Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 01:39 AM EST

PDB ID	:	6BD3
Title	:	Saccharomyces cerevisiae acetohydroxyacid synthase
Authors	:	Guddat, L.W.; Lonhienne, T.
Deposited on	:	2017-10-21
Resolution	:	2.28 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:

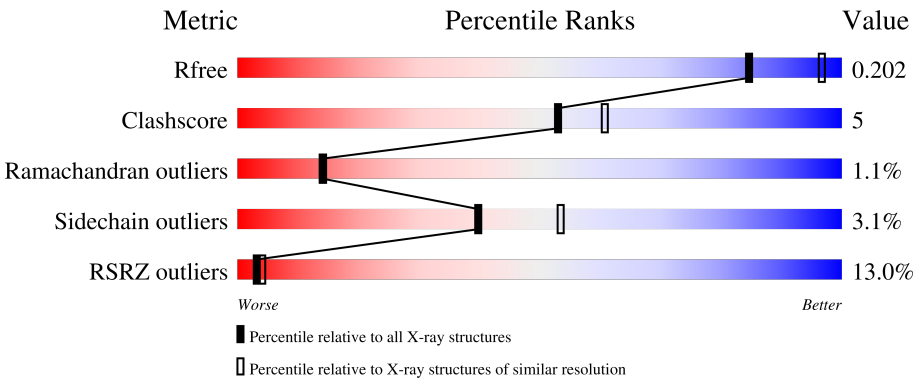
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	3% 73% 6% 21%
1	B	677	18% 69% 11% • 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OXY	B	704	-	-	-	X
5	OXY	B	709	-	-	X	-
6	CO2	A	706	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 8823 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 catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	538	4073	2581	701	772	19	0	0	0
1	B	558	4237	2684	729	804	20	0	0	0

There are 94 discrepancies between the modelled and reference sequences:

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	expression tag	UNP P07342
B	32	ALA	-	expression tag	UNP P07342
B	33	ALA	-	expression tag	UNP P07342
B	34	ALA	-	expression tag	UNP P07342
B	35	LYS	-	expression tag	UNP P07342
B	36	PHE	-	expression tag	UNP P07342
B	37	GLU	-	expression tag	UNP P07342
B	38	ARG	-	expression tag	UNP P07342
B	39	GLN	-	expression tag	UNP P07342
B	40	HIS	-	expression tag	UNP P07342
B	41	MET	-	expression tag	UNP P07342
B	42	ASP	-	expression tag	UNP P07342
B	43	SER	-	expression tag	UNP P07342
B	44	PRO	-	expression tag	UNP P07342
B	45	ASP	-	expression tag	UNP P07342
B	46	LEU	-	expression tag	UNP P07342
B	47	GLY	-	expression tag	UNP P07342
B	48	THR	-	expression tag	UNP P07342
B	49	ASP	-	expression tag	UNP P07342
B	50	ASP	-	expression tag	UNP P07342
B	51	ASP	-	expression tag	UNP P07342
B	52	ASP	-	expression tag	UNP P07342
B	53	LYS	-	expression tag	UNP P07342
B	54	ALA	-	expression tag	UNP P07342
B	55	MET	-	expression tag	UNP P07342
B	56	GLY	-	expression tag	UNP P07342
B	57	SER	-	expression tag	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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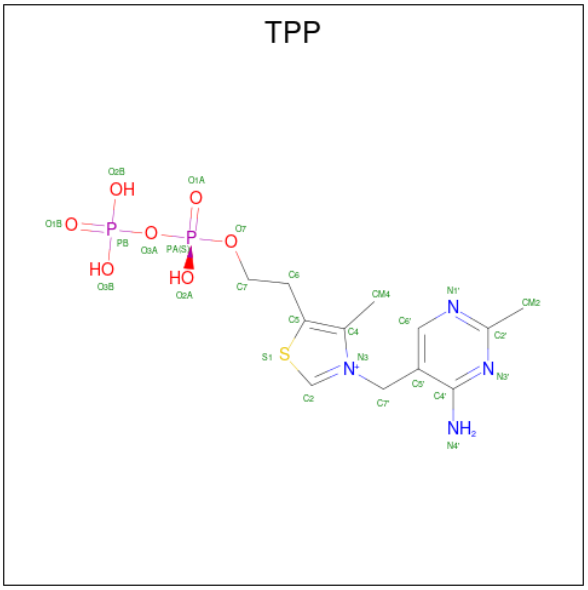
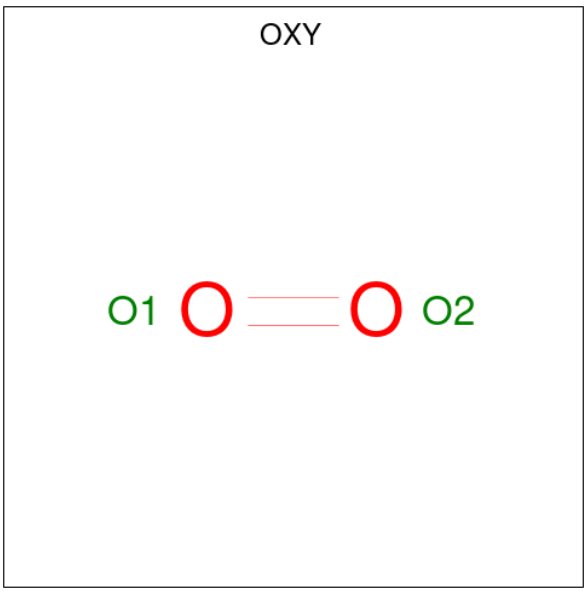
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



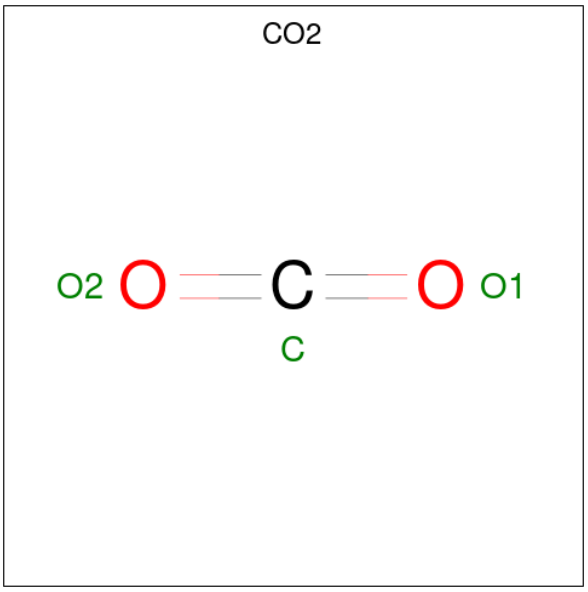
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	26	12	4	7	2	1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



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

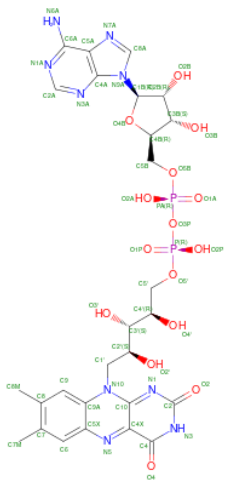
- Molecule 6 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

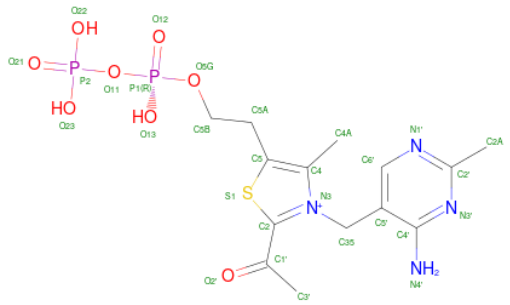
FAD



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

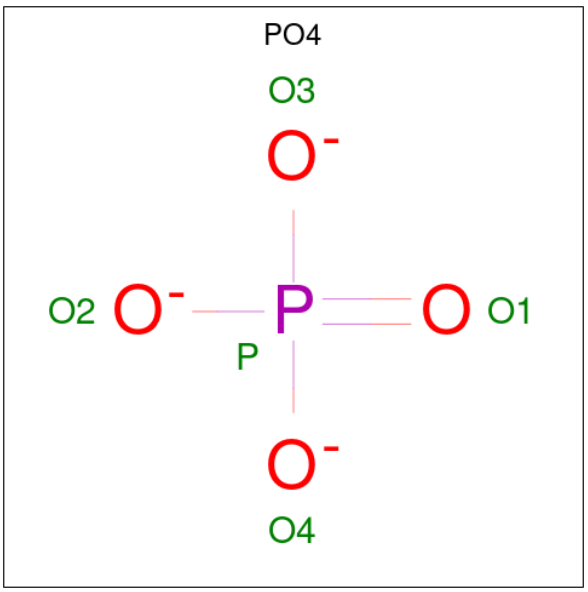
- Molecule 8 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$).

HTL



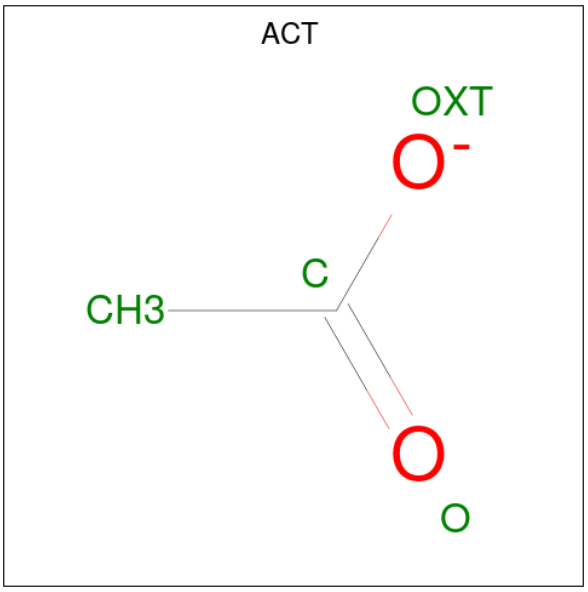
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
8	B	1	29	14	4	8	2	1	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
9	B	1	5	4	1	0	0

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	B	1	4	2	2	0	0

- Molecule 11 is water.

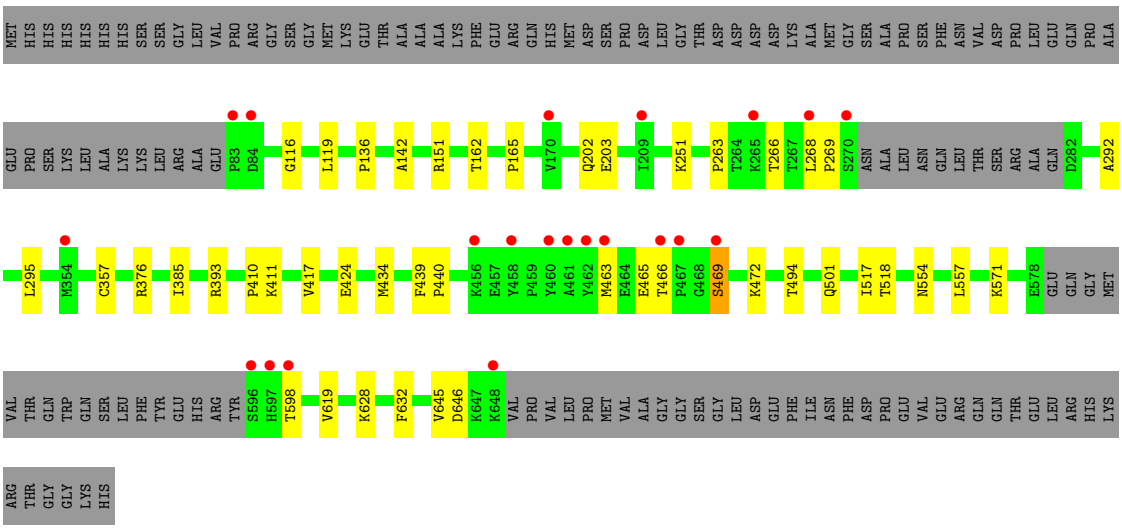
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	210	210	210	0	0
			Total	O		
11	B	110	110	110	0	0

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.

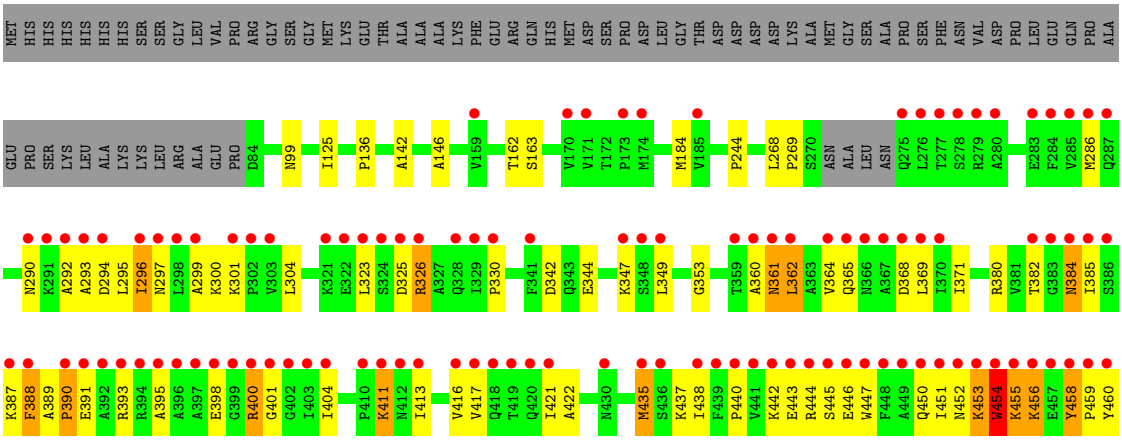
• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

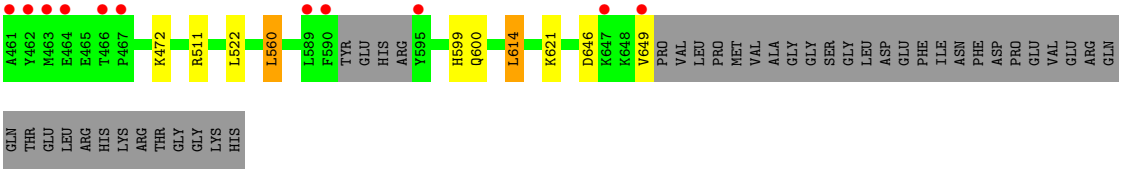
Chain A:



• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain B:




A461 Y462 M463 E464 E465 T466 P467 K472 R511 L522 L560 L589 F590 TYR GLU HIS ARG Y595 H599 Q600 L614 K621 D646 K647 K648 V649 PRO VAL LEU PRO MET VAL ALA GLY GLY SER GLY LEU ASP GLU PHE ILE ASN PHE ASP PRO GLU VAL GLU ARG GLN
GLN THR GLU LEU ARG HIS LYS ARG THR GLY GLY LYS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.90Å 108.77Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 2.28 47.95 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.31-2.28) 99.6 (47.95-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.171 , 0.201 0.174 , 0.202	Depositor DCC
R_{free} test set	2000 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.4	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	0.96	EDS
Total number of atoms	8823	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, PO4, CO2, K, MG, HTL, OXY, ACT, TPP

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	0.26	0/4154	0.43	0/5634
1	B	0.25	0/4321	0.46	0/5862
All	All	0.25	0/8475	0.45	0/11496

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	4073	0	4109	24	0
1	B	4237	0	4258	63	0
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	26	0	16	3	0
5	A	4	0	0	1	0
5	B	12	0	0	3	0
6	A	3	0	0	3	0
7	A	53	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	53	0	30	2	0
8	B	29	0	18	1	0
9	B	5	0	0	1	0
10	B	4	0	3	1	0
11	A	210	0	0	1	0
11	B	110	0	0	0	0
All	All	8823	0	8464	92	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 5.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LYS:O	1:B:455:LYS:N	2.12	0.82
1:B:455:LYS:H	1:B:456:LYS:HB2	1.48	0.76
1:B:295:LEU:HD11	1:B:401:GLY:HA2	1.69	0.74
1:A:385:ILE:O	1:A:393:ARG:NH2	2.20	0.74
1:A:151:ARG:NH1	1:A:518:THR:O	2.24	0.71
1:B:330:PRO:HB2	1:B:349:LEU:HD11	1.74	0.70
1:B:326:ARG:NH2	1:B:438:ILE:O	2.24	0.69
1:B:353:GLY:O	1:B:361:ASN:ND2	2.27	0.67
1:B:325:ASP:OD1	1:B:347:LYS:NZ	2.30	0.65
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.80	0.64
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.78	0.64
1:B:292:ALA:HB2	1:B:421:ILE:HG21	1.80	0.63
1:A:162:THR:OG1	5:A:705:OXY:O1	2.17	0.62
1:B:296:ILE:HG22	1:B:369:LEU:HD21	1.85	0.58
1:A:292:ALA:HB3	1:A:434:MET:HE1	1.85	0.57
1:B:162:THR:OG1	5:B:709:OXY:O1	2.22	0.57
4:A:703:TPP:H7'2	10:B:712:ACT:OXT	2.06	0.56
1:B:296:ILE:HD11	1:B:438:ILE:HG23	1.86	0.56
1:B:395:ALA:HA	1:B:400:ARG:HB3	1.87	0.55
1:B:296:ILE:O	1:B:299:ALA:HB2	2.06	0.55
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.88	0.55
1:B:382:THR:HG22	1:B:388:PHE:HE1	1.72	0.54
1:B:416:VAL:HG12	1:B:417:VAL:HG23	1.89	0.54
1:B:472:LYS:NZ	1:B:646:ASP:OD2	2.36	0.54
1:B:286:MET:O	1:B:290:ASN:ND2	2.42	0.53
1:A:466:THR:OG1	1:A:469:SER:OG	2.26	0.53
1:B:292:ALA:HB1	1:B:404:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ALA:HB1	1:B:401:GLY:N	2.23	0.52
1:A:494:THR:HG22	1:A:517:ILE:HB	1.91	0.52
1:B:301:LYS:HD2	1:B:447:TRP:CE3	2.44	0.52
1:A:501:GLN:NE2	1:A:518:THR:OG1	2.41	0.52
1:B:368:ASP:OD1	1:B:369:LEU:N	2.44	0.51
1:A:116:GLY:H	6:A:706:CO2:C	2.24	0.51
1:B:300:LYS:HB3	1:B:368:ASP:OD2	2.10	0.50
4:A:703:TPP:HN42	4:A:703:TPP:H2	1.76	0.50
1:B:384:ASN:OD1	1:B:384:ASN:N	2.41	0.50
6:A:706:CO2:O2	5:B:704:OXY:O1	2.30	0.50
1:B:362:LEU:HB3	1:B:454:TRP:CH2	2.46	0.50
1:B:146:ALA:HB3	1:B:184:MET:HE2	1.94	0.49
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.42	0.49
1:B:560:LEU:HG	1:B:614:LEU:HD21	1.94	0.49
6:A:706:CO2:C	8:B:703:HTL:C1'	2.90	0.49
1:B:385:ILE:HD12	1:B:385:ILE:H	1.78	0.49
1:B:294:ASP:HA	1:B:297:ASN:HB2	1.94	0.49
1:A:619:VAL:HG22	1:A:628:LYS:HG3	1.95	0.48
1:B:599:HIS:ND1	9:B:710:PO4:O1	2.44	0.48
1:B:342:ASP:OD2	1:B:511:ARG:NH2	2.38	0.47
1:B:361:ASN:OD1	1:B:361:ASN:N	2.33	0.47
1:A:465:GLU:HG2	1:A:472:LYS:HG2	1.95	0.47
1:B:413:ILE:HD13	1:B:422:ALA:HB1	1.96	0.46
1:B:451:ILE:HA	1:B:454:TRP:HE3	1.81	0.46
1:B:296:ILE:HD11	1:B:438:ILE:HD12	1.98	0.46
4:A:703:TPP:HN42	4:A:703:TPP:C2	2.29	0.46
1:B:365:GLN:O	1:B:391:GLU:HB3	2.16	0.45
1:B:163:SER:OG	5:B:709:OXY:O2	2.29	0.45
1:B:450:GLN:O	1:B:450:GLN:NE2	2.47	0.45
1:A:251:LYS:NZ	11:A:807:HOH:O	2.45	0.45
1:B:99:ASN:HD22	1:B:125:ILE:HD13	1.82	0.45
1:B:360:ALA:O	1:B:364:VAL:HG23	2.17	0.45
1:B:380:ARG:HD3	7:B:711:FAD:C5X	2.47	0.44
1:B:411:LYS:HD2	1:B:411:LYS:H	1.80	0.44
1:A:554:ASN:HA	1:A:557:LEU:HD23	1.99	0.44
1:A:465:GLU:OE2	1:A:472:LYS:N	2.37	0.44
1:A:410:PRO:HG3	1:A:424:GLU:OE2	2.17	0.44
1:B:388:PHE:CD2	1:B:389:ALA:HB2	2.53	0.44
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.99	0.44
1:B:388:PHE:HA	1:B:390:PRO:HD3	2.00	0.43
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LYS:N	1:B:456:LYS:HB2	2.24	0.43
1:B:444:ARG:O	1:B:446:GLU:N	2.52	0.43
1:A:268:LEU:HA	1:A:269:PRO:HD3	1.92	0.42
1:B:300:LYS:O	1:B:301:LYS:HD3	2.19	0.42
1:B:388:PHE:HA	1:B:389:ALA:HA	1.60	0.42
1:B:447:TRP:CE3	1:B:447:TRP:HA	2.53	0.42
1:B:290:ASN:HD22	1:B:437:LYS:NZ	2.17	0.42
1:A:472:LYS:NZ	1:A:646:ASP:OD2	2.44	0.42
1:B:323:LEU:HA	1:B:435:MET:HE1	2.01	0.42
1:A:263:PRO:HB2	1:A:266:THR:HG23	2.01	0.42
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.90	0.42
1:B:99:ASN:HA	1:B:125:ILE:HD11	2.01	0.42
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.02	0.42
1:B:621:LYS:HB2	1:B:621:LYS:HE3	1.83	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.88	0.41
1:B:447:TRP:O	1:B:451:ILE:HG12	2.21	0.41
1:B:184:MET:O	1:B:244:PRO:HA	2.21	0.41
7:B:711:FAD:H9	7:B:711:FAD:H1'1	1.73	0.40
1:A:439:PHE:HA	1:A:440:PRO:HD3	1.96	0.40
1:B:268:LEU:HA	1:B:269:PRO:HD3	1.89	0.40
1:B:290:ASN:HA	1:B:293:ALA:HB3	2.03	0.40
1:B:290:ASN:HD22	1:B:437:LYS:HZ3	1.70	0.40
1:B:362:LEU:HB3	1:B:454:TRP:CZ2	2.56	0.40
1:B:453:LYS:O	1:B:456:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	532/677 (79%)	521 (98%)	9 (2%)	2 (0%)	34 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	552/677 (82%)	516 (94%)	26 (5%)	10 (2%)	8	7
All	All	1084/1354 (80%)	1037 (96%)	35 (3%)	12 (1%)	14	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	GLU
1	B	387	LYS
1	B	454	TRP
1	B	459	PRO
1	A	463	MET
1	B	445	SER
1	B	455	LYS
1	B	453	LYS
1	B	458	TYR
1	B	398	GLU
1	B	440	PRO
1	B	390	PRO

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	439/556 (79%)	432 (98%)	7 (2%)	62	76
1	B	456/556 (82%)	435 (95%)	21 (5%)	27	35
All	All	895/1112 (80%)	867 (97%)	28 (3%)	40	53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	357	CYS
1	A	376	ARG
1	A	411	LYS

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Mol	Chain	Res	Type
1	A	469	SER
1	A	598	THR
1	A	645	VAL
1	B	296	ILE
1	B	326	ARG
1	B	361	ASN
1	B	362	LEU
1	B	384	ASN
1	B	388	PHE
1	B	393	ARG
1	B	400	ARG
1	B	411	LYS
1	B	435	MET
1	B	442	LYS
1	B	443	GLU
1	B	452	ASN
1	B	454	TRP
1	B	456	LYS
1	B	458	TYR
1	B	460	TYR
1	B	560	LEU
1	B	600	GLN
1	B	614	LEU
1	B	649	VAL

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

Mol	Chain	Res	Type
1	B	290	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
7	FAD	A	707	-	53,58,58	1.68	10 (18%)	68,89,89	1.36	11 (16%)
5	OXY	B	706	-	1,1,1	0.15	0	-		
5	OXY	B	707	-	1,1,1	0.16	0	-		
5	OXY	B	705	-	1,1,1	0.15	0	-		
10	ACT	B	712	-	3,3,3	0.74	0	3,3,3	0.79	0
5	OXY	A	705	-	1,1,1	0.14	0	-		
5	OXY	B	708	-	1,1,1	0.15	0	-		
9	PO4	B	710	-	4,4,4	0.92	0	6,6,6	0.45	0
5	OXY	B	704	-	1,1,1	0.08	0	-		
5	OXY	A	704	-	1,1,1	0.15	0	-		
5	OXY	B	709	-	1,1,1	0.15	0	-		
8	HTL	B	703	3	23,30,30	4.18	11 (47%)	31,45,45	2.74	9 (29%)
6	CO2	A	706	-	2,2,2	1.04	0	1,1,1	0.50	0
4	TPP	A	703	3	22,27,27	1.81	3 (13%)	29,40,40	2.07	10 (34%)
7	FAD	B	711	-	53,58,58	1.71	11 (20%)	68,89,89	1.40	11 (16%)

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
8	HTL	B	703	3	-	4/16/21/21	0/2/2/2
7	FAD	A	707	-	-	6/30/50/50	0/6/6/6
4	TPP	A	703	3	-	6/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FAD	B	711	-	-	2/30/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	703	HTL	C5-S1	-14.47	1.47	1.74
8	B	703	HTL	C4-N3	7.80	1.56	1.39
4	A	703	TPP	C4-N3	-6.13	1.34	1.39
7	B	711	FAD	C10-N1	5.25	1.44	1.33
8	B	703	HTL	O2'-C1'	5.22	1.39	1.22
8	B	703	HTL	C5A-C5	5.12	1.53	1.50
7	A	707	FAD	C10-N1	5.00	1.43	1.33
7	B	711	FAD	C4X-N5	4.73	1.39	1.30
7	A	707	FAD	C4X-N5	4.58	1.39	1.30
7	B	711	FAD	C2B-C1B	-4.47	1.47	1.53
7	A	707	FAD	C2B-C1B	-4.44	1.47	1.53
8	B	703	HTL	C5'-C4'	-3.67	1.36	1.42
8	B	703	HTL	P2-O22	-3.49	1.41	1.54
4	A	703	TPP	C4'-N4'	3.42	1.42	1.34
8	B	703	HTL	C4'-N4'	3.38	1.42	1.34
8	B	703	HTL	P1-O13	-3.38	1.39	1.55
4	A	703	TPP	C6-C5	3.12	1.52	1.50
7	B	711	FAD	O4B-C1B	3.11	1.45	1.41
7	A	707	FAD	O4B-C1B	2.97	1.45	1.41
7	B	711	FAD	C2-N1	2.75	1.43	1.36
7	B	711	FAD	O3'-C3'	-2.69	1.36	1.43
7	A	707	FAD	O3'-C3'	-2.63	1.36	1.43
7	A	707	FAD	C2'-C3'	2.56	1.58	1.53
7	A	707	FAD	C2-N1	2.53	1.42	1.36
7	B	711	FAD	C1'-N10	-2.52	1.41	1.48
8	B	703	HTL	P2-O23	-2.41	1.45	1.54
7	A	707	FAD	C1'-N10	-2.41	1.42	1.48
7	B	711	FAD	C2'-C3'	2.31	1.57	1.53
8	B	703	HTL	P2-O21	-2.28	1.43	1.50
7	A	707	FAD	C1'-C2'	2.18	1.55	1.52
8	B	703	HTL	P1-O12	-2.18	1.43	1.50
7	A	707	FAD	C4X-C4	2.15	1.52	1.44
7	B	711	FAD	C4X-C4	2.14	1.52	1.44
7	B	711	FAD	C1'-C2'	2.10	1.55	1.52
7	B	711	FAD	C2B-C3B	-2.06	1.47	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	703	HTL	C4-N3-C2	-11.27	102.36	108.64
8	B	703	HTL	C5A-C5-C4	-5.67	122.88	127.43
4	A	703	TPP	PA-O3A-PB	-4.88	116.07	132.83
7	A	707	FAD	N3A-C2A-N1A	-4.14	122.22	128.68
7	B	711	FAD	N3A-C2A-N1A	-4.13	122.22	128.68
4	A	703	TPP	C7'-N3-C2	-3.77	118.54	125.35
4	A	703	TPP	N1'-C2'-N3'	-3.73	119.12	125.54
4	A	703	TPP	C6'-N1'-C2'	3.47	121.87	115.96
8	B	703	HTL	C6'-C5'-C4'	3.37	120.31	115.72
8	B	703	HTL	C2A-C2'-N1'	3.36	120.84	117.14
4	A	703	TPP	CM2-C2'-N1'	3.36	120.83	117.14
8	B	703	HTL	P1-O11-P2	-3.30	121.49	132.83
7	A	707	FAD	C4A-C5A-N7A	-3.28	105.98	109.40
7	B	711	FAD	C9A-C5X-N5	-3.15	119.01	122.43
7	B	711	FAD	C4-N3-C2	-3.15	119.83	125.64
7	A	707	FAD	C4-N3-C2	-3.08	119.95	125.64
7	B	711	FAD	C4A-C5A-N7A	-3.04	106.23	109.40
4	A	703	TPP	C5-C4-N3	3.00	113.57	107.57
7	B	711	FAD	C4-C4X-N5	2.99	122.49	118.23
7	B	711	FAD	C4X-C4-N3	2.99	120.78	113.19
7	A	707	FAD	C4X-C10-N10	2.93	120.77	116.48
7	A	707	FAD	C4X-C4-N3	2.81	120.34	113.19
7	B	711	FAD	C10-C4X-N5	-2.74	119.05	124.86
7	A	707	FAD	C4X-C10-N1	-2.73	118.38	124.73
8	B	703	HTL	N1'-C2'-N3'	-2.65	120.98	125.54
7	B	711	FAD	O4-C4-C4X	-2.64	119.59	126.60
7	B	711	FAD	C4X-C10-N1	-2.61	118.68	124.73
7	B	711	FAD	C9A-N10-C10	-2.53	116.83	120.77
4	A	703	TPP	C5'-C6'-N1'	-2.50	119.65	123.82
4	A	703	TPP	CM4-C4-C5	-2.44	122.26	127.60
7	A	707	FAD	C10-N1-C2	2.40	121.71	116.90
7	B	711	FAD	C10-N1-C2	2.40	121.70	116.90
7	A	707	FAD	C10-C4X-N5	-2.35	119.88	124.86
7	A	707	FAD	O4-C4-C4X	-2.34	120.38	126.60
8	B	703	HTL	C5'-C6'-N1'	-2.31	119.98	123.82
8	B	703	HTL	C6'-N1'-C2'	2.22	119.73	115.96
7	A	707	FAD	C4-C4X-N5	2.19	121.35	118.23
4	A	703	TPP	C5'-C7'-N3	-2.18	109.64	113.28
8	B	703	HTL	O23-P2-O11	2.14	111.81	104.64
7	A	707	FAD	C3B-C2B-C1B	2.09	104.12	100.98
4	A	703	TPP	C6'-C5'-C4'	2.01	118.45	115.72

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	TPP	C5-C6-C7-O7
4	A	703	TPP	C7-O7-PA-O2A
8	B	703	HTL	C4-C5-C5A-C5B
8	B	703	HTL	P1-O11-P2-O23
4	A	703	TPP	PB-O3A-PA-O7
7	A	707	FAD	P-O3P-PA-O5B
7	B	711	FAD	P-O3P-PA-O5B
4	A	703	TPP	C7-O7-PA-O3A
4	A	703	TPP	C7-O7-PA-O1A
4	A	703	TPP	C4-C5-C6-C7
7	A	707	FAD	C2'-C3'-C4'-O4'
7	A	707	FAD	C2'-C3'-C4'-C5'
8	B	703	HTL	P1-O11-P2-O22
7	A	707	FAD	O4B-C4B-C5B-O5B
7	A	707	FAD	PA-O3P-P-O2P
7	B	711	FAD	O4B-C4B-C5B-O5B
7	A	707	FAD	O3'-C3'-C4'-C5'
8	B	703	HTL	P1-O11-P2-O21

There are no ring outliers.

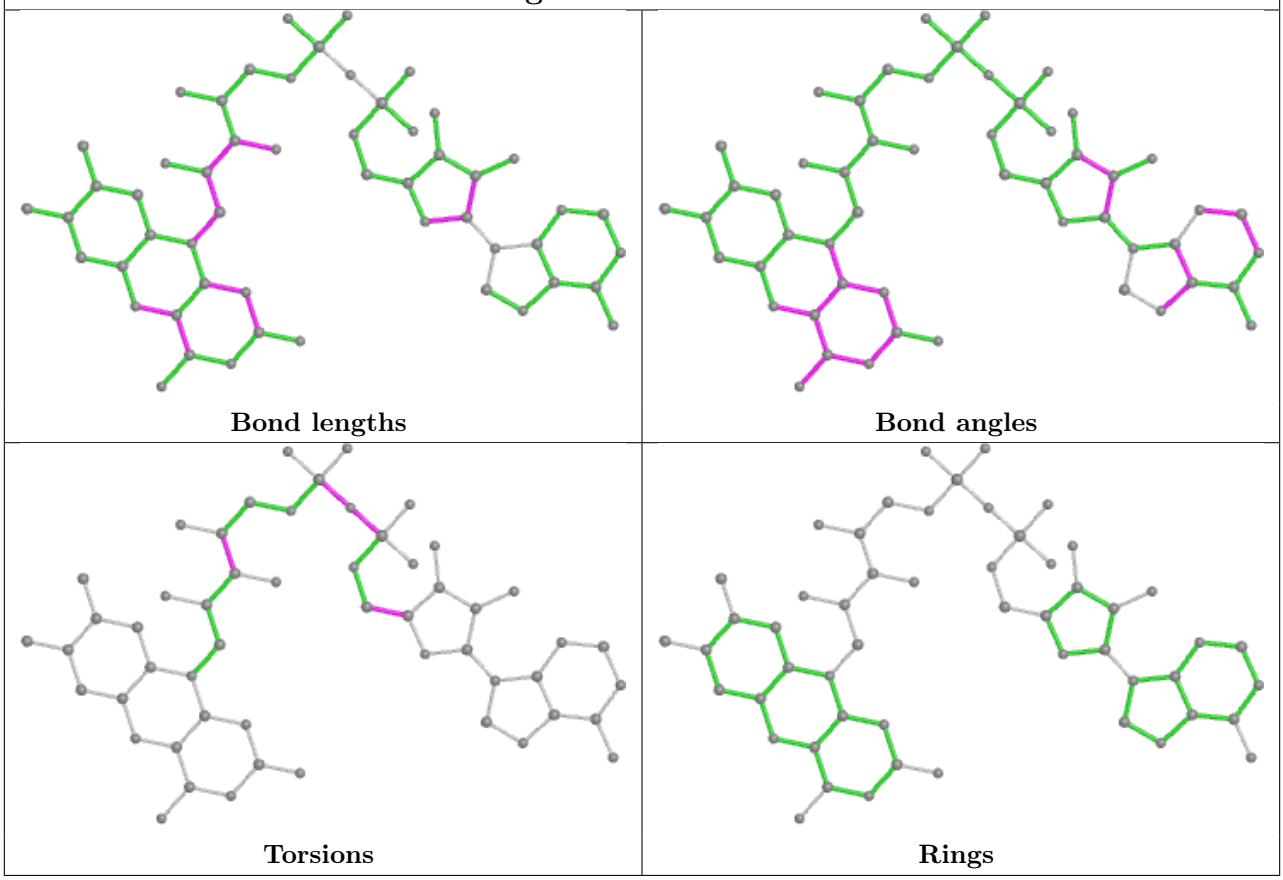
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	712	ACT	1	0
5	A	705	OXY	1	0
9	B	710	PO4	1	0
5	B	704	OXY	1	0
5	B	709	OXY	2	0
8	B	703	HTL	1	0
6	A	706	CO2	3	0
4	A	703	TPP	3	0
7	B	711	FAD	2	0

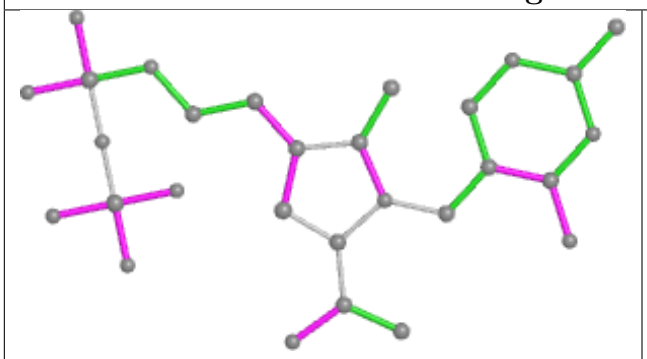
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

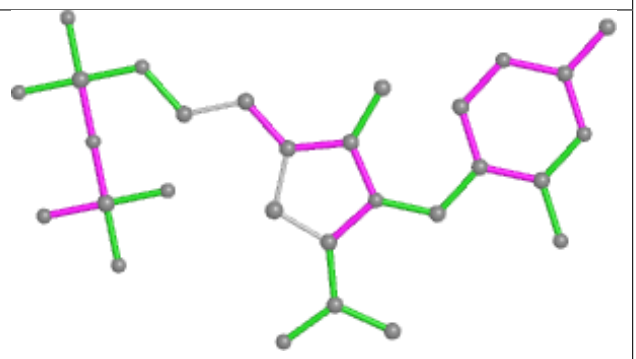
Ligand FAD A 707



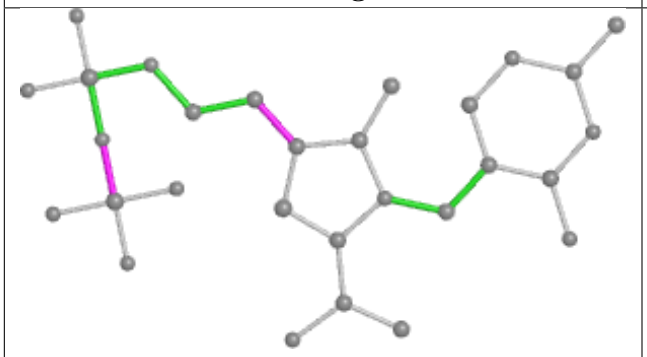
Ligand HTL B 703



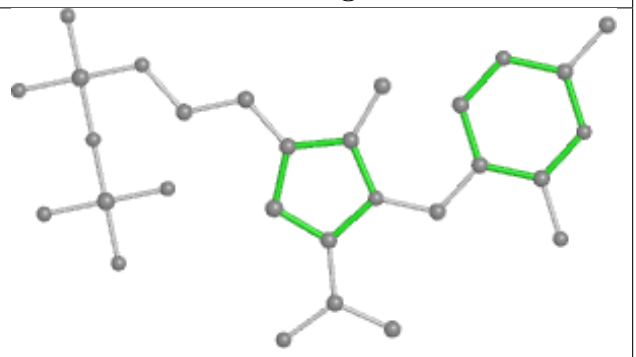
Bond lengths



Bond angles

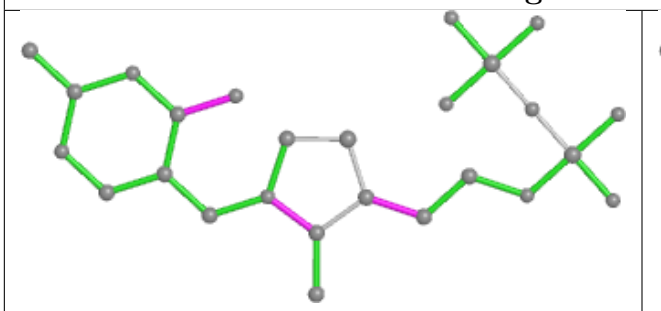


Torsions

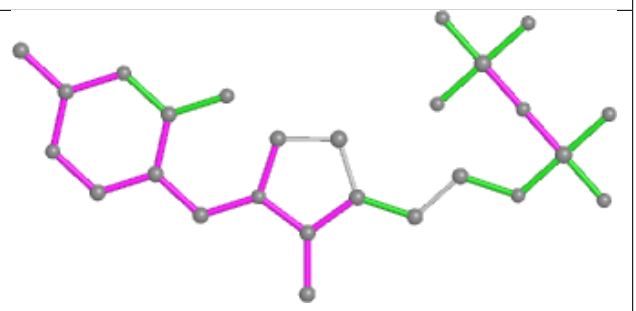


Rings

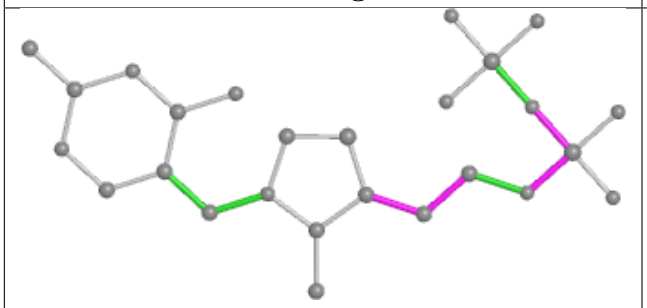
Ligand TPP A 703



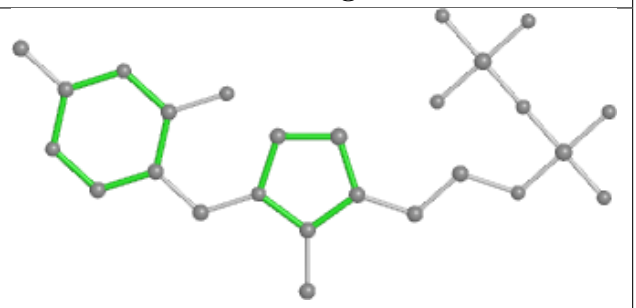
Bond lengths



Bond angles

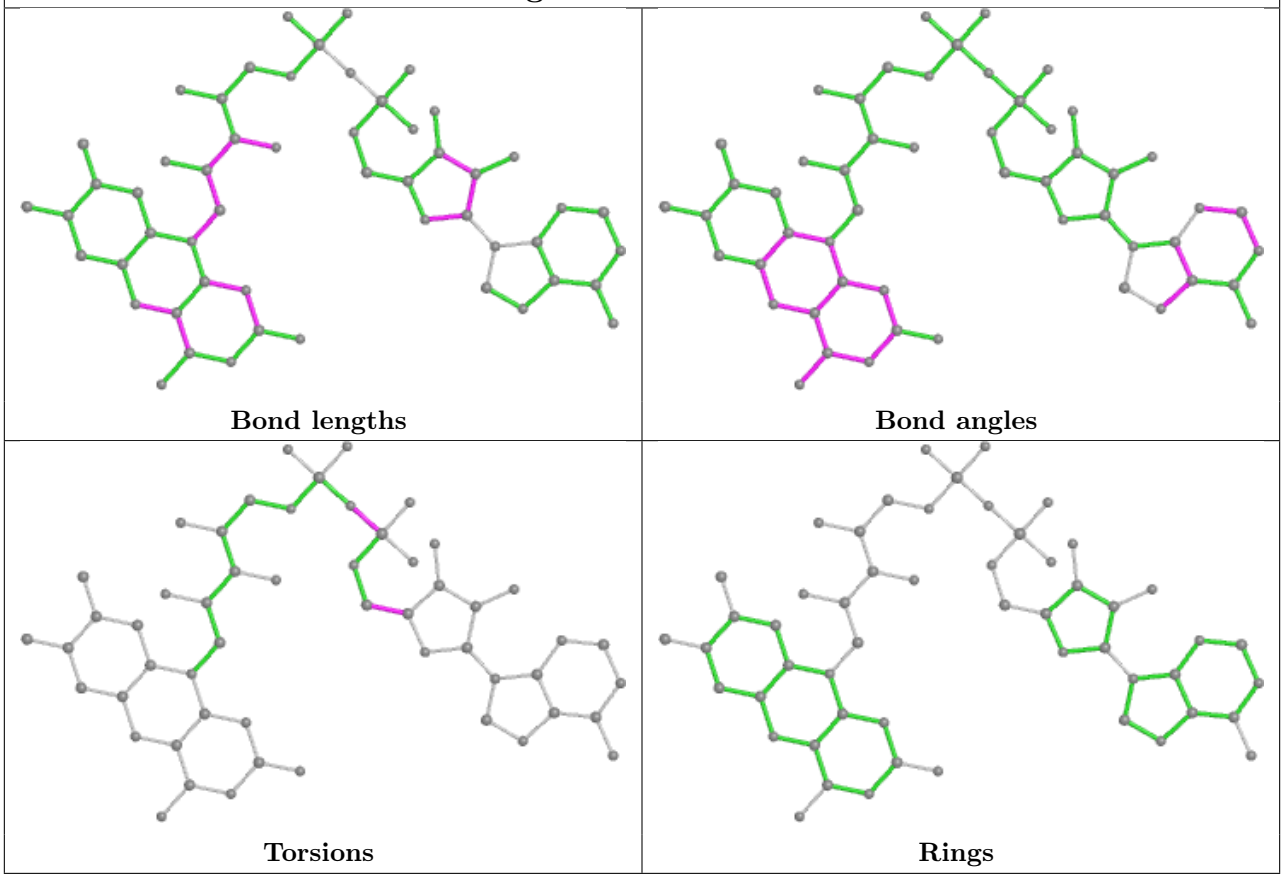


Torsions



Rings

Ligand FAD B 711



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	538/677 (79%)	0.11	21 (3%)	39	44	28, 43, 89, 168	0
1	B	558/677 (82%)	1.14	122 (21%)	0	1	28, 56, 144, 172	0
All	All	1096/1354 (80%)	0.63	143 (13%)	3	4	28, 47, 134, 172	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	451	ILE	10.0
1	B	590	PHE	9.5
1	B	402	GLY	9.2
1	A	463	MET	8.7
1	B	394	ARG	8.5
1	B	296	ILE	8.2
1	B	460	TYR	7.6
1	B	390	PRO	7.0
1	B	396	ALA	6.9
1	B	367	ALA	6.7
1	B	293	ALA	6.4
1	B	447	TRP	6.3
1	B	366	ASN	6.2
1	B	441	VAL	6.1
1	B	444	ARG	6.1
1	B	448	PHE	6.0
1	B	454	TRP	6.0
1	B	303	VAL	5.8
1	B	458	TYR	5.7
1	B	368	ASP	5.6
1	B	439	PHE	5.6
1	B	649	VAL	5.5
1	B	392	ALA	5.5
1	B	595	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	461	ALA	5.3
1	B	370	ILE	5.2
1	B	285	VAL	5.1
1	B	329	ILE	5.1
1	B	299	ALA	5.0
1	B	362	LEU	5.0
1	B	416	VAL	5.0
1	B	438	ILE	5.0
1	B	397	ALA	4.9
1	B	459	PRO	4.9
1	B	324	SER	4.9
1	B	450	GLN	4.8
1	B	446	GLU	4.8
1	B	453	LYS	4.7
1	B	403	ILE	4.6
1	A	458	TYR	4.6
1	B	364	VAL	4.6
1	B	466	THR	4.6
1	B	330	PRO	4.4
1	B	294	ASP	4.4
1	B	326	ARG	4.3
1	B	419	THR	4.3
1	B	391	GLU	4.3
1	B	463	MET	4.3
1	B	325	ASP	4.2
1	A	456	LYS	4.2
1	B	287	GLN	4.2
1	B	452	ASN	4.1
1	A	467	PRO	4.0
1	A	462	TYR	4.0
1	B	589	LEU	4.0
1	B	462	TYR	4.0
1	B	302	PRO	4.0
1	B	401	GLY	4.0
1	B	398	GLU	4.0
1	B	298	LEU	3.9
1	B	418	GLN	3.9
1	B	443	GLU	3.9
1	B	276	LEU	3.9
1	A	83	PRO	3.8
1	B	369	LEU	3.8
1	B	400	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	466	THR	3.8
1	B	286	MET	3.8
1	B	279	ARG	3.8
1	B	283	GLU	3.7
1	B	456	LYS	3.7
1	B	383	GLY	3.7
1	B	284	PHE	3.7
1	B	395	ALA	3.7
1	B	445	SER	3.7
1	B	384	ASN	3.7
1	B	387	LYS	3.6
1	B	297	ASN	3.6
1	B	436	SER	3.6
1	B	449	ALA	3.5
1	A	596	SER	3.5
1	B	290	ASN	3.5
1	A	268	LEU	3.5
1	B	417	VAL	3.4
1	B	328	GLN	3.4
1	B	393	ARG	3.4
1	B	442	LYS	3.4
1	B	301	LYS	3.3
1	B	388	PHE	3.3
1	B	277	THR	3.3
1	A	265	LYS	3.3
1	B	385	ILE	3.3
1	B	347	LYS	3.3
1	B	435	MET	3.2
1	B	420	GLN	3.2
1	B	455	LYS	3.2
1	B	321	LYS	3.1
1	B	278	SER	3.1
1	A	597	HIS	3.0
1	B	467	PRO	3.0
1	B	360	ALA	2.9
1	B	647	LYS	2.9
1	B	410	PRO	2.9
1	B	365	GLN	2.9
1	B	292	ALA	2.8
1	A	84	ASP	2.7
1	B	341	PHE	2.7
1	B	359	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	421	ILE	2.6
1	B	280	ALA	2.6
1	B	386	SER	2.6
1	B	170	VAL	2.6
1	B	349	LEU	2.5
1	B	413	ILE	2.5
1	B	348	SER	2.5
1	A	460	TYR	2.4
1	B	361	ASN	2.4
1	B	404	ILE	2.4
1	B	457	GLU	2.4
1	B	399	GLY	2.3
1	B	323	LEU	2.3
1	B	322	GLU	2.3
1	B	440	PRO	2.3
1	B	159	VAL	2.3
1	A	270	SER	2.3
1	B	185	VAL	2.2
1	B	173	PRO	2.2
1	A	469	SER	2.2
1	B	461	ALA	2.2
1	A	648	LYS	2.2
1	B	411	LYS	2.2
1	A	170	VAL	2.2
1	A	354	MET	2.2
1	B	291	LYS	2.2
1	B	412	ASN	2.1
1	B	174	MET	2.1
1	B	275	GLN	2.1
1	B	464	GLU	2.1
1	A	209	ILE	2.1
1	A	598	THR	2.1
1	B	430	ASN	2.1
1	B	382	THR	2.1
1	B	171	VAL	2.1

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)

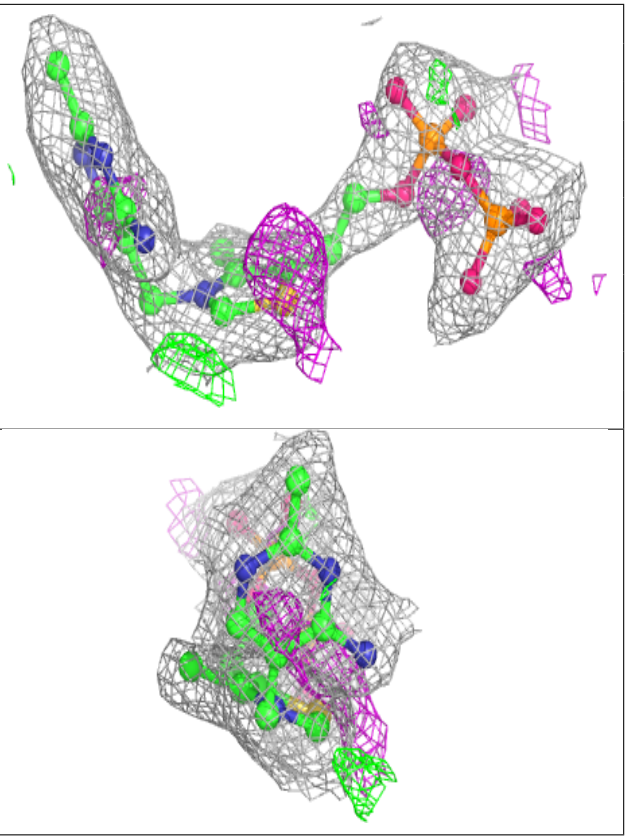
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OXY	B	704	2/2	0.53	0.43	79,79,79,87	0
5	OXY	B	707	2/2	0.65	0.34	69,69,69,76	0
5	OXY	B	708	2/2	0.72	0.33	99,99,99,101	0
5	OXY	B	705	2/2	0.74	0.31	111,111,111,111	0
6	CO2	A	706	3/3	0.77	0.35	85,85,88,88	0
10	ACT	B	712	4/4	0.83	0.22	95,96,97,99	0
5	OXY	B	706	2/2	0.85	0.38	83,83,83,84	0
4	TPP	A	703	26/26	0.90	0.16	27,58,71,550	0
3	MG	B	702	1/1	0.90	0.05	40,40,40,40	0
3	MG	A	702	1/1	0.91	0.14	64,64,64,64	0
8	HTL	B	703	29/29	0.92	0.15	29,38,50,52	2
9	PO4	B	710	5/5	0.92	0.16	111,116,121,122	0
5	OXY	A	704	2/2	0.92	0.26	83,83,83,86	0
5	OXY	A	705	2/2	0.93	0.24	76,76,76,77	0
5	OXY	B	709	2/2	0.95	0.23	73,73,73,76	0
7	FAD	B	711	53/53	0.96	0.14	48,60,80,82	0
2	K	A	701	1/1	0.96	0.10	49,49,49,49	0
7	FAD	A	707	53/53	0.97	0.12	32,46,78,83	0
2	K	B	701	1/1	0.98	0.08	63,63,63,63	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.

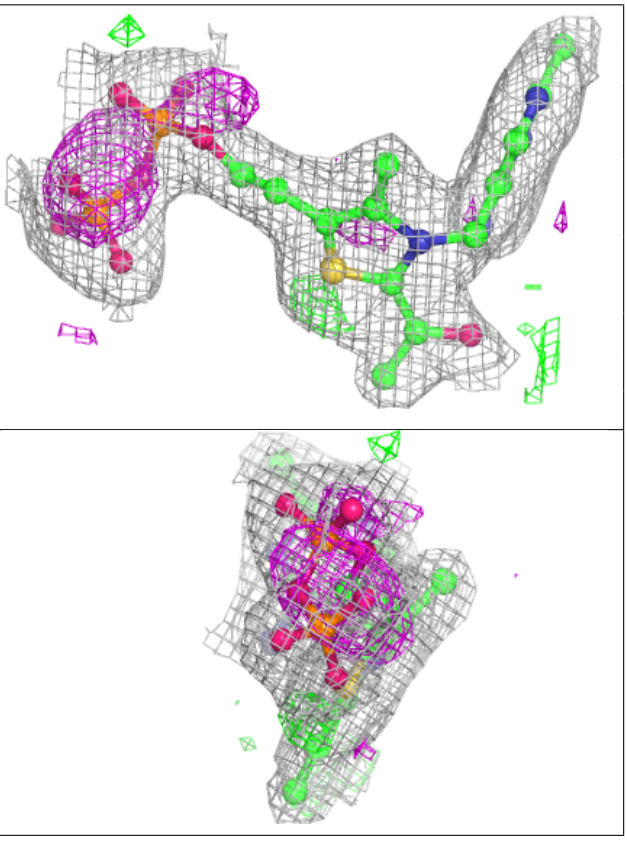
Electron density around TPP A 703:

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



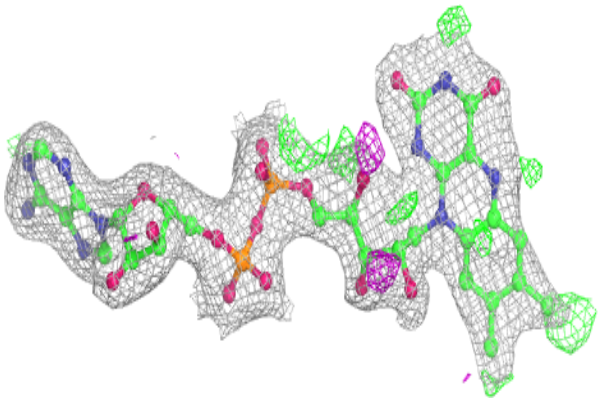
Electron density around HTL B 703:

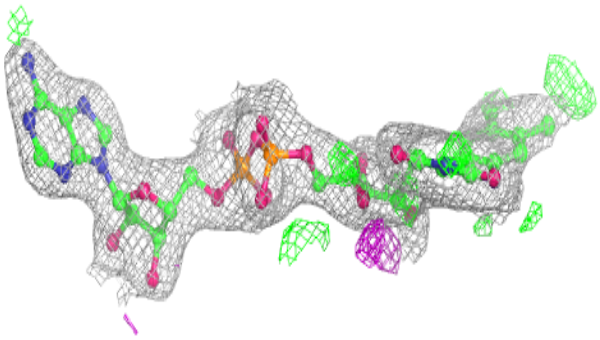
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

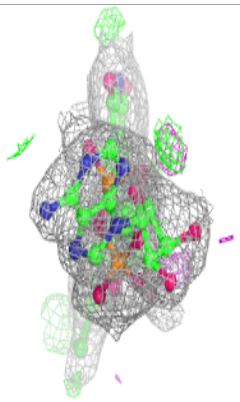


Electron density around FAD B 711:

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

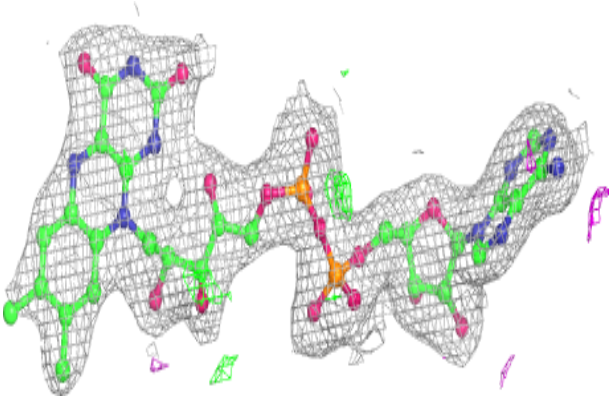


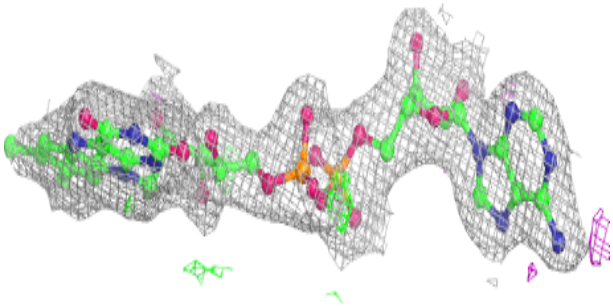


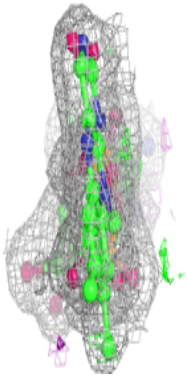


Electron density around FAD A 707:

$2mF_o$-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.