Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 12:40 AM EDT

PDB ID	:	5IMS
Title	:	Saccharomyces cerevisiae acetohydroxyacid synthase
Authors	:	Guddat, L.W.; Lonhienne, T.
Deposited on	:	2016-03-06
Resolution	:	1.98 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:

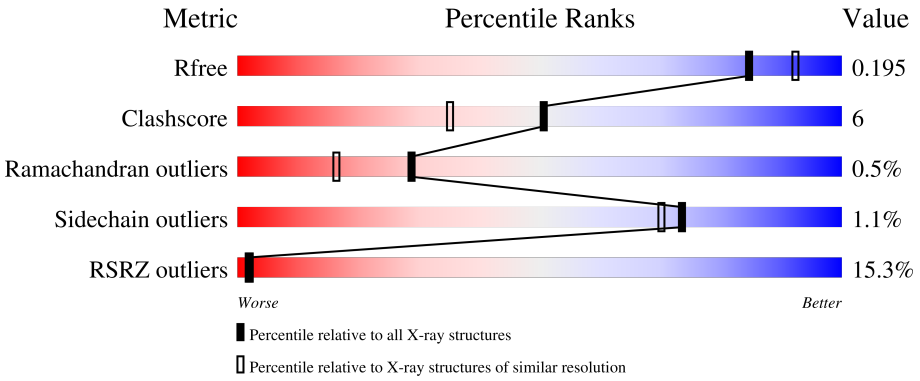
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	5% 75% 5% 20%
1	B	677	20% 71% 12% • 16%

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
7	ACT	A	708	-	-	X	-
7	ACT	B	712	-	-	X	-
7	ACT	B	713	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9452 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
1	A	541	Total	C	N	O	S	0	3	0
			4111	2604	709	779	19			
1	B	567	Total	C	N	O	S	0	1	0
			4325	2740	747	818	20			

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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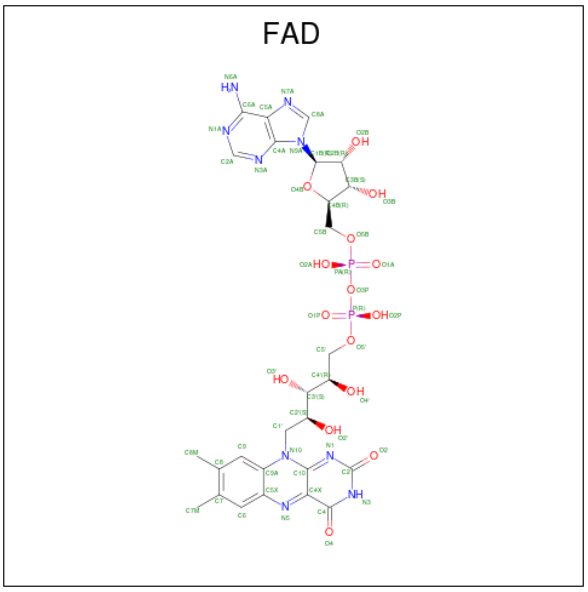
Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	expression tag	UNP P07342
B	32	ALA	-	expression tag	UNP P07342
B	33	ALA	-	expression tag	UNP P07342
B	34	ALA	-	expression tag	UNP P07342
B	35	LYS	-	expression tag	UNP P07342
B	36	PHE	-	expression tag	UNP P07342
B	37	GLU	-	expression tag	UNP P07342
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 FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

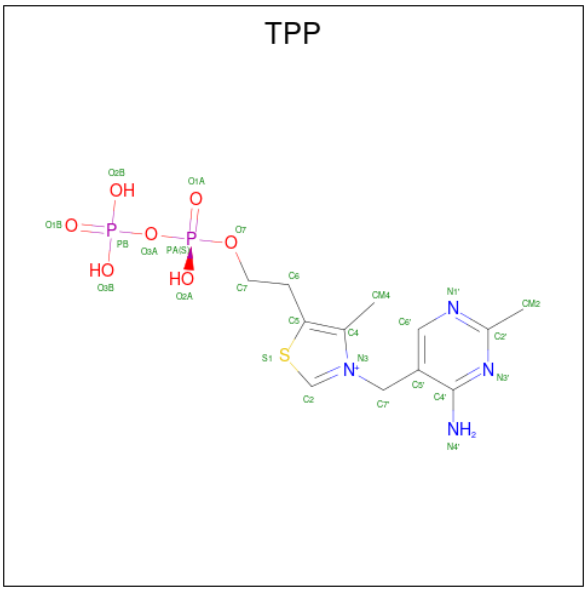


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

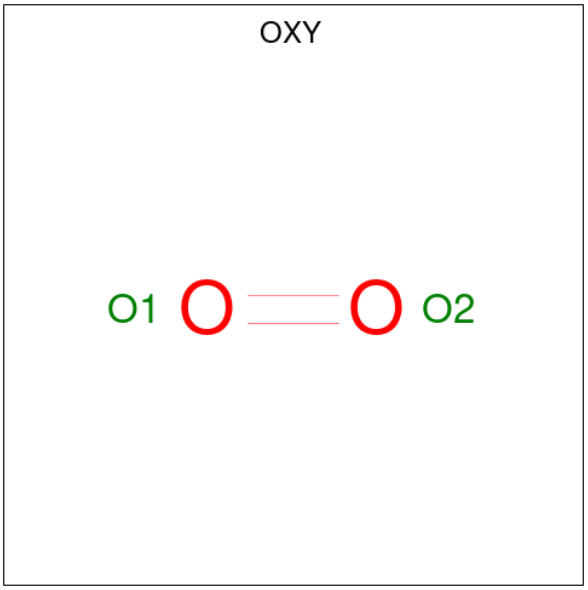
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



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

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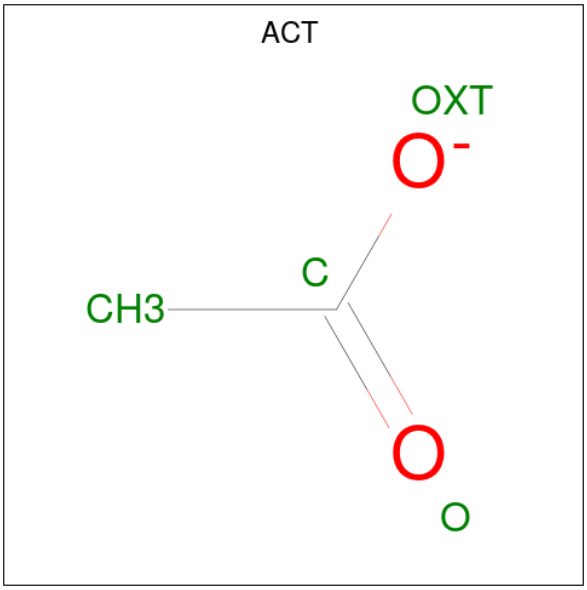
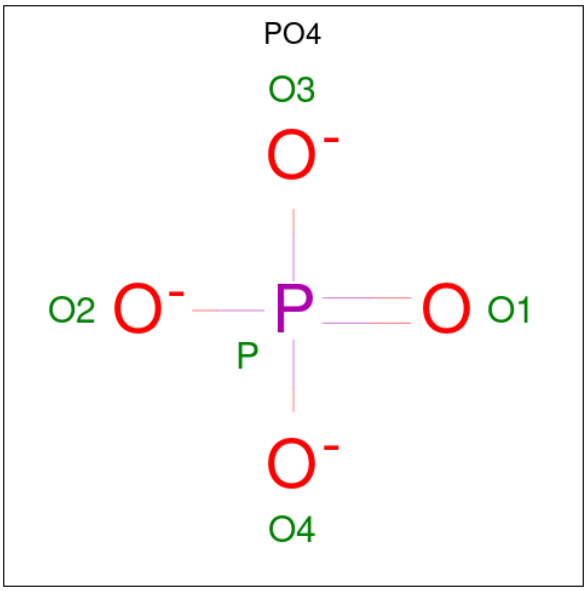
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 9 is water.

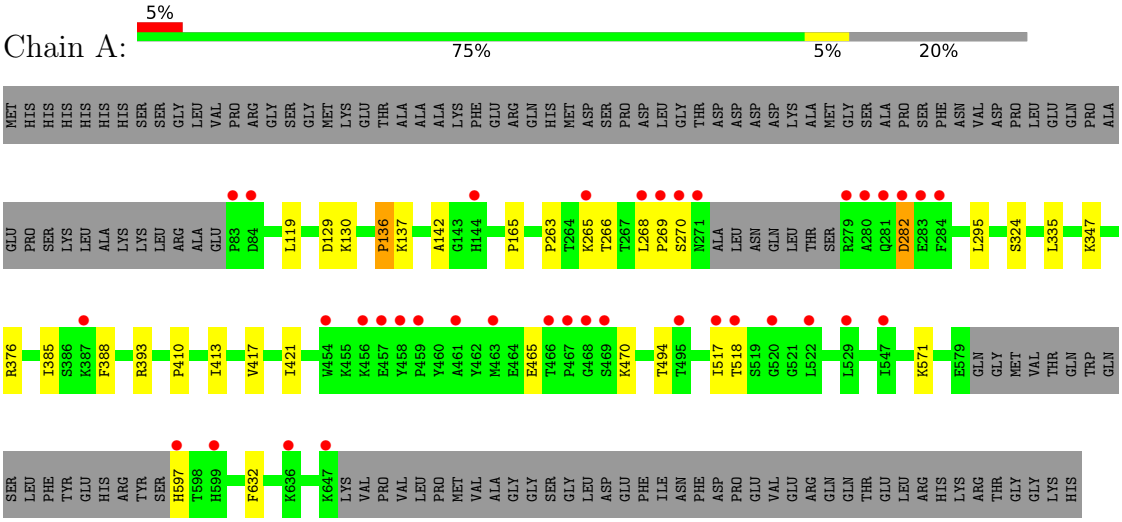
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	492	Total O 492 492	0	0
9	B	327	Total O 327 327	0	0

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.

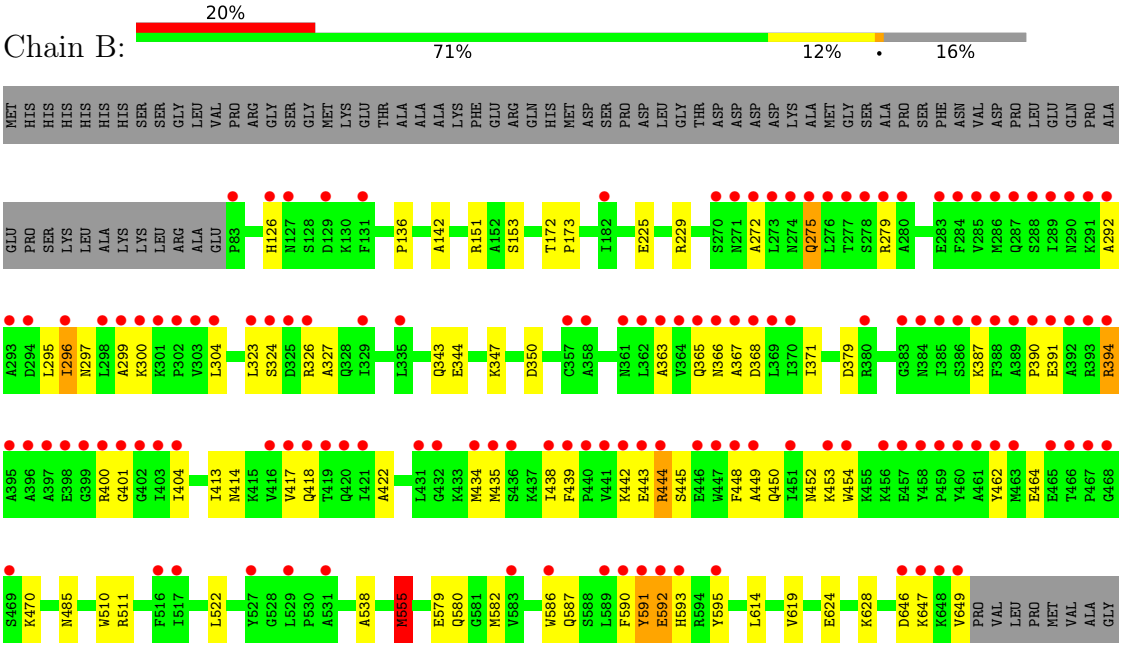
• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain A:



• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain B:



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	95.68Å 110.18Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.18 – 1.98 42.18 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.18-1.98) 99.0 (42.18-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.193 0.168 , 0.195	Depositor DCC
R_{free} test set	2000 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.3	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	9452	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: OXY, MG, K, PO4, ACT, TPP, 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	0.73	0/4195	0.69	1/5689 (0.0%)
1	B	0.68	0/4414	0.70	1/5989 (0.0%)
All	All	0.70	0/8609	0.70	2/11678 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	555	MET	CA-CB-CG	-9.17	97.72	113.30
1	A	129	ASP	CB-CG-OD1	5.83	123.54	118.30

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	4111	0	4143	23	0
1	B	4325	0	4349	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	26	0	16	1	0
5	B	26	0	16	1	0
6	A	6	0	0	1	0
6	B	12	0	0	1	0
7	A	4	0	3	2	0
7	B	8	0	6	2	0
8	B	5	0	0	0	0
9	A	492	0	0	5	1
9	B	327	0	0	11	1
All	All	9452	0	8595	99	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 6.

All (99) 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:368:ASP:OD2	1:B:400:ARG:NH2	2.01	0.92
1:B:296:ILE:HD11	1:B:438:ILE:HD12	1.51	0.92
1:B:327:ALA:O	1:B:444:ARG:NH1	2.04	0.89
1:A:388:PHE:O	1:A:393:ARG:NH1	2.09	0.86
1:B:326:ARG:NH2	1:B:438:ILE:O	2.14	0.81
1:B:579:GLU:HB2	1:B:647:LYS:HE2	1.62	0.81
1:B:580:GLN:HB3	1:B:647:LYS:HB3	1.62	0.81
1:B:434:MET:HG2	1:B:438:ILE:HD11	1.64	0.79
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.64	0.78
6:B:708:OXY:O1	9:B:801:HOH:O	2.03	0.76
1:A:376:ARG:NH2	9:A:801:HOH:O	2.22	0.72
1:B:590:PHE:O	1:B:592:GLU:N	2.20	0.71
1:B:297:ASN:HD21	1:B:439:PHE:H	1.36	0.71
1:B:297:ASN:O	1:B:300:LYS:NZ	2.24	0.70
1:B:450:GLN:O	1:B:452:ASN:N	2.23	0.70
7:B:712:ACT:H2	7:B:713:ACT:H1	1.73	0.69
1:B:279:ARG:HG2	1:B:279:ARG:HH11	1.60	0.66
1:B:297:ASN:ND2	1:B:439:PHE:H	1.96	0.63
1:B:587:GLN:NE2	1:B:592:GLU:OE2	2.31	0.63
1:B:272:ALA:HA	1:B:275:GLN:HE21	1.64	0.62
1:B:272:ALA:HA	1:B:275:GLN:NE2	2.15	0.62
1:B:126:HIS:ND1	9:B:804:HOH:O	2.31	0.61
7:A:708:ACT:H3	9:B:875:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:MET:HG2	9:B:801:HOH:O	2.01	0.60
1:B:442:LYS:HD2	1:B:442:LYS:H	1.66	0.60
1:A:295:LEU:HD12	1:A:421:ILE:HD12	1.84	0.59
1:B:485:ASN:ND2	9:B:806:HOH:O	2.35	0.58
5:B:704:TPP:H2	9:B:875:HOH:O	2.03	0.58
1:B:297:ASN:HD21	1:B:439:PHE:N	2.01	0.58
1:B:151:ARG:NH2	9:B:802:HOH:O	2.09	0.57
1:B:579:GLU:CB	1:B:647:LYS:HE2	2.33	0.57
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.36	0.56
1:B:391:GLU:OE2	1:B:394:ARG:NH2	2.39	0.56
1:A:130:LYS:HD2	9:A:978:HOH:O	2.07	0.54
1:B:470:LYS:HE3	1:B:646:ASP:HA	1.91	0.53
1:B:324:SER:OG	1:B:347:LYS:HE2	2.08	0.53
1:A:263:PRO:HB3	1:A:265:LYS:HE2	1.92	0.52
1:B:450:GLN:NE2	1:B:454:TRP:HE1	2.08	0.52
1:A:335:LEU:HD22	9:A:1110:HOH:O	2.10	0.52
1:B:296:ILE:CD1	1:B:438:ILE:HD12	2.32	0.51
1:B:300:LYS:HA	1:B:444:ARG:NH2	2.26	0.51
1:B:443:GLU:CD	1:B:444:ARG:H	2.13	0.51
1:B:387:LYS:O	1:B:390:PRO:HD3	2.10	0.51
1:B:619:VAL:HG13	1:B:624:GLU:HG3	1.93	0.51
1:B:365:GLN:O	1:B:390:PRO:HD2	2.12	0.50
1:B:323:LEU:HA	1:B:435:MET:HE1	1.93	0.49
1:B:442:LYS:HD2	1:B:442:LYS:N	2.27	0.49
1:B:343:GLN:NE2	1:B:510:TRP:H	2.11	0.49
1:B:591:TYR:O	1:B:593:HIS:N	2.46	0.49
1:B:153:SER:HB3	1:B:538:ALA:HB1	1.95	0.48
1:B:413:ILE:HD13	1:B:422:ALA:HB1	1.96	0.48
1:B:344:GLU:HG3	1:B:511:ARG:NE	2.29	0.47
1:B:449:ALA:O	1:B:453:LYS:HE2	2.14	0.47
1:A:282:ASP:N	1:A:282:ASP:OD1	2.47	0.47
1:B:434:MET:CG	1:B:438:ILE:HD11	2.38	0.47
6:A:706:OXY:O1	7:A:708:ACT:O	2.31	0.47
1:A:324:SER:OG	1:A:347:LYS:HE2	2.14	0.47
1:A:597:HIS:HB2	9:A:1116:HOH:O	2.14	0.47
1:B:350:ASP:HB3	9:B:828:HOH:O	2.14	0.47
1:B:586:TRP:CZ3	1:B:595:TYR:CE1	3.03	0.47
1:A:268:LEU:HA	1:A:269:PRO:HD2	1.80	0.46
1:B:225:GLU:HG2	1:B:229:ARG:HG2	1.96	0.46
1:B:462:TYR:CE1	1:B:464:GLU:HG2	2.51	0.46
1:B:300:LYS:HA	1:B:444:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LYS:NZ	9:A:812:HOH:O	2.49	0.45
1:B:363:ALA:N	1:B:454:TRP:HZ3	2.15	0.45
1:B:413:ILE:HG22	1:B:414:ASN:ND2	2.32	0.45
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.99	0.45
1:A:136:PRO:HG3	1:A:142:ALA:HB2	2.00	0.44
7:B:712:ACT:CH3	7:B:713:ACT:H1	2.43	0.44
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.52	0.44
1:B:297:ASN:HD22	1:B:297:ASN:HA	1.60	0.44
1:B:299:ALA:O	1:B:300:LYS:HD2	2.18	0.44
1:A:137:LYS:O	1:B:555:MET:HG2	2.17	0.43
1:A:263:PRO:HB2	1:A:266:THR:HG23	2.00	0.43
1:A:335:LEU:HD21	1:A:518:THR:HG21	2.01	0.43
1:B:292:ALA:HB1	1:B:404:ILE:HD13	2.01	0.43
1:B:414:ASN:HA	1:B:417:VAL:O	2.19	0.43
1:B:579:GLU:H	1:B:647:LYS:HE2	1.84	0.42
1:A:410:PRO:HA	1:A:413:ILE:HD12	2.01	0.42
1:B:445:SER:O	1:B:449:ALA:HB3	2.18	0.42
1:B:279:ARG:HH11	1:B:279:ARG:CG	2.30	0.42
1:B:442:LYS:H	1:B:442:LYS:CD	2.32	0.41
1:B:443:GLU:OE2	1:B:448:PHE:HB3	2.18	0.41
1:B:470:LYS:NZ	9:B:805:HOH:O	2.34	0.41
1:A:465:GLU:OE2	1:A:465:GLU:N	2.52	0.41
5:A:704:TPP:H2	9:B:833:HOH:O	2.20	0.41
1:B:379:ASP:HB3	9:B:1065:HOH:O	2.18	0.41
1:B:136:PRO:HG3	1:B:142:ALA:HB2	2.02	0.41
1:B:296:ILE:CD1	1:B:438:ILE:HG23	2.51	0.41
1:B:579:GLU:H	1:B:647:LYS:CE	2.33	0.41
1:A:165:PRO:HD3	1:B:522:LEU:HG	2.03	0.41
1:A:494:THR:HG22	1:A:517:ILE:HB	2.03	0.41
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.03	0.41
1:B:418:GLN:OE1	1:B:418:GLN:N	2.54	0.41
1:B:295:LEU:HD21	1:B:401:GLY:HA2	2.02	0.41
1:B:442:LYS:N	1:B:442:LYS:CD	2.84	0.41
1:A:385:ILE:HD12	1:A:385:ILE:HA	1.90	0.40
1:B:172:THR:HB	1:B:173:PRO:HD3	2.04	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)
9:A:1212:HOH:O	9:B:824:HOH:O[3_544]	2.16	0.04

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	538/677 (80%)	534 (99%)	3 (1%)	1 (0%)	47	38
1	B	566/677 (84%)	544 (96%)	18 (3%)	4 (1%)	22	11
All	All	1104/1354 (82%)	1078 (98%)	21 (2%)	5 (0%)	29	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	591	TYR
1	B	592	GLU
1	A	270	SER
1	B	367	ALA
1	B	366	ASN

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	442/556 (80%)	439 (99%)	3 (1%)	84	83
1	B	465/556 (84%)	458 (98%)	7 (2%)	65	59
All	All	907/1112 (82%)	897 (99%)	10 (1%)	73	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	136	PRO
1	A	282	ASP
1	B	275	GLN
1	B	296	ILE
1	B	394	ARG
1	B	444	ARG
1	B	555	MET
1	B	614	LEU
1	B	649	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	275	GLN
1	B	297	ASN
1	B	587	GLN

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 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\#\|Z\|>2$
6	OXY	B	710	-	1,1,1	0.04	0	-		
7	ACT	B	713	-	3,3,3	0.74	0	3,3,3	0.92	0
6	OXY	A	705	-	1,1,1	0.14	0	-		
6	OXY	A	706	-	1,1,1	0.15	0	-		
6	OXY	B	705	-	1,1,1	0.16	0	-		
3	FAD	A	702	-	53,58,58	1.59	9 (16%)	68,89,89	1.45	12 (17%)
6	OXY	B	709	-	1,1,1	0.00	0	-		
6	OXY	A	707	-	1,1,1	0.14	0	-		
6	OXY	B	707	-	1,1,1	0.18	0	-		
7	ACT	B	712	-	3,3,3	0.82	0	3,3,3	0.64	0
3	FAD	B	702	-	53,58,58	1.70	12 (22%)	68,89,89	1.48	15 (22%)
6	OXY	B	706	-	1,1,1	0.16	0	-		
5	TPP	B	704	4	22,27,27	2.13	5 (22%)	29,40,40	2.26	9 (31%)
6	OXY	B	708	-	1,1,1	0.05	0	-		
7	ACT	A	708	-	3,3,3	0.72	0	3,3,3	1.09	0
5	TPP	A	704	4	22,27,27	1.81	6 (27%)	29,40,40	2.43	10 (34%)
8	PO4	B	711	-	4,4,4	0.87	0	6,6,6	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TPP	A	704	4	-	3/16/17/17	0/2/2/2
3	FAD	B	702	-	-	2/30/50/50	0/6/6/6
3	FAD	A	702	-	-	3/30/50/50	0/6/6/6
5	TPP	B	704	4	-	3/16/17/17	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	TPP	C6-C5	6.94	1.54	1.50
5	A	704	TPP	C6-C5	4.94	1.53	1.50
5	B	704	TPP	C4-N3	-4.76	1.35	1.39
3	B	702	FAD	C4X-N5	4.76	1.40	1.30
3	A	702	FAD	C4X-N5	4.65	1.39	1.30
3	A	702	FAD	C10-N1	4.55	1.42	1.33
3	B	702	FAD	C2B-C1B	-4.50	1.46	1.53
3	B	702	FAD	C10-N1	4.19	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C2B-C1B	-3.76	1.48	1.53
3	B	702	FAD	O4B-C1B	3.20	1.45	1.41
5	A	704	TPP	C4'-N4'	3.06	1.41	1.34
3	B	702	FAD	C9-C9A	2.84	1.44	1.39
5	A	704	TPP	C4-N3	-2.80	1.37	1.39
3	A	702	FAD	C2'-C3'	2.62	1.58	1.53
5	A	704	TPP	C6'-N1'	2.49	1.39	1.34
3	B	702	FAD	C2'-C3'	2.46	1.58	1.53
3	B	702	FAD	C7M-C7	2.46	1.55	1.51
5	A	704	TPP	C4'-N3'	2.45	1.38	1.35
5	B	704	TPP	C2'-N1'	2.42	1.38	1.34
3	B	702	FAD	O3'-C3'	-2.40	1.37	1.43
3	A	702	FAD	O4B-C1B	2.34	1.44	1.41
3	B	702	FAD	C1'-N10	-2.33	1.42	1.48
3	B	702	FAD	C2-N1	2.32	1.42	1.36
5	A	704	TPP	C7'-C5'	2.27	1.56	1.51
3	B	702	FAD	C8M-C8	2.24	1.55	1.51
3	A	702	FAD	C1'-N10	-2.24	1.42	1.48
3	B	702	FAD	C4X-C10	-2.23	1.37	1.44
5	B	704	TPP	C4'-N4'	2.19	1.39	1.34
3	A	702	FAD	C7M-C7	2.18	1.55	1.51
5	B	704	TPP	C7'-C5'	2.08	1.55	1.51
3	A	702	FAD	C4X-C4	2.02	1.51	1.44
3	A	702	FAD	O3'-C3'	-2.00	1.38	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704	TPP	C6-C5-C4	6.23	132.43	127.43
5	B	704	TPP	CM2-C2'-N1'	5.97	123.71	117.14
5	A	704	TPP	CM2-C2'-N1'	4.96	122.60	117.14
5	B	704	TPP	N1'-C2'-N3'	-4.30	118.13	125.54
5	A	704	TPP	N1'-C2'-N3'	-4.28	118.17	125.54
3	A	702	FAD	N3A-C2A-N1A	-4.19	122.12	128.68
5	B	704	TPP	C7'-N3-C2	-4.12	117.91	125.35
3	B	702	FAD	N3A-C2A-N1A	-3.74	122.84	128.68
3	B	702	FAD	O4-C4-C4X	-3.70	116.77	126.60
5	A	704	TPP	C7'-N3-C2	-3.70	118.67	125.35
5	B	704	TPP	C5-C4-N3	3.69	114.96	107.57
5	A	704	TPP	C6'-N1'-C2'	3.68	122.22	115.96
5	B	704	TPP	CM4-C4-C5	-3.49	119.98	127.60
3	B	702	FAD	C4-N3-C2	-3.47	119.23	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	FAD	C4X-C4-N3	3.46	121.98	113.19
5	B	704	TPP	C6'-N1'-C2'	3.33	121.63	115.96
5	A	704	TPP	O2B-PB-O3A	3.27	115.59	104.64
5	A	704	TPP	C5-C4-N3	3.19	113.95	107.57
5	A	704	TPP	CM4-C4-C5	-3.18	120.64	127.60
3	A	702	FAD	C4X-C10-N10	3.06	120.96	116.48
3	B	702	FAD	C10-N1-C2	3.05	123.01	116.90
5	A	704	TPP	PA-O3A-PB	-2.98	122.59	132.83
3	A	702	FAD	O2-C2-N1	-2.94	116.96	121.83
3	B	702	FAD	C4-C4X-N5	2.88	122.33	118.23
3	B	702	FAD	C4A-C5A-N7A	-2.85	106.43	109.40
3	A	702	FAD	C5'-C4'-C3'	-2.85	106.70	112.20
3	A	702	FAD	O4-C4-C4X	-2.75	119.31	126.60
5	B	704	TPP	C6-C5-C4	2.73	129.62	127.43
3	B	702	FAD	O4'-C4'-C3'	2.73	115.73	109.10
3	A	702	FAD	C4A-C5A-N7A	-2.70	106.58	109.40
3	B	702	FAD	C9A-N10-C10	-2.56	116.77	120.77
3	A	702	FAD	C4-N3-C2	-2.52	120.98	125.64
3	B	702	FAD	C5'-C4'-C3'	-2.38	107.60	112.20
3	B	702	FAD	C4X-C10-N10	2.36	119.93	116.48
5	B	704	TPP	PA-O3A-PB	-2.34	124.80	132.83
3	B	702	FAD	C4X-C10-N1	-2.27	119.47	124.73
3	A	702	FAD	C4X-C4-N3	2.26	118.93	113.19
5	A	704	TPP	CM4-C4-N3	2.26	125.41	122.53
3	A	702	FAD	C4X-C10-N1	-2.25	119.51	124.73
3	A	702	FAD	C10-N1-C2	2.19	121.28	116.90
5	B	704	TPP	O3B-PB-O2B	2.18	115.98	107.64
3	A	702	FAD	C10-C4X-N5	-2.16	120.28	124.86
3	B	702	FAD	C1B-N9A-C4A	-2.15	122.87	126.64
3	B	702	FAD	C9A-C5X-N5	-2.10	120.15	122.43
3	A	702	FAD	C5X-C9A-N10	2.07	120.09	117.95
3	B	702	FAD	C10-C4X-N5	-2.06	120.49	124.86

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	FAD	P-O3P-PA-O5B
3	B	702	FAD	P-O3P-PA-O5B
5	A	704	TPP	C4-C5-C6-C7
5	A	704	TPP	PA-O3A-PB-O3B
5	B	704	TPP	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	B	704	TPP	PA-O3A-PB-O2B
3	B	702	FAD	O4B-C4B-C5B-O5B
5	B	704	TPP	PA-O3A-PB-O3B
5	A	704	TPP	C7-O7-PA-O1A
3	A	702	FAD	O4B-C4B-C5B-O5B
3	A	702	FAD	O3'-C3'-C4'-C5'

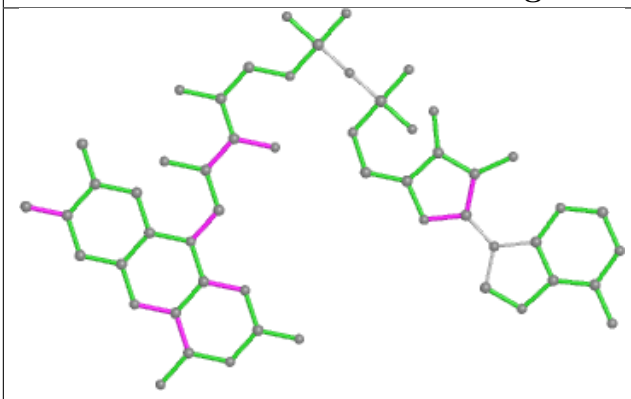
There are no ring outliers.

7 monomers are involved in 7 short contacts:

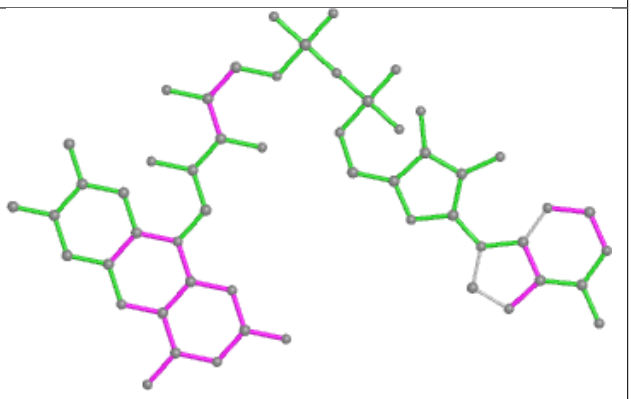
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	713	ACT	2	0
6	A	706	OXY	1	0
7	B	712	ACT	2	0
5	B	704	TPP	1	0
6	B	708	OXY	1	0
7	A	708	ACT	2	0
5	A	704	TPP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

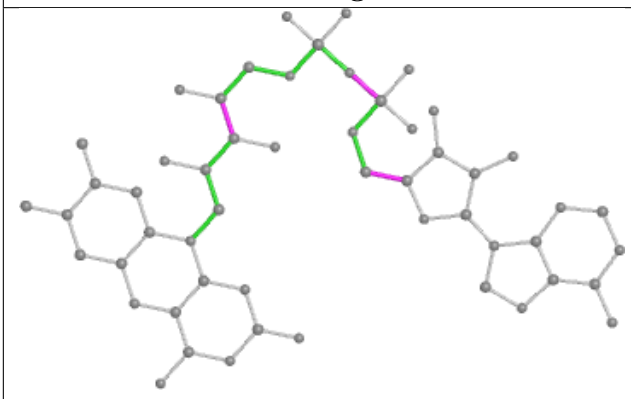
Ligand FAD A 702



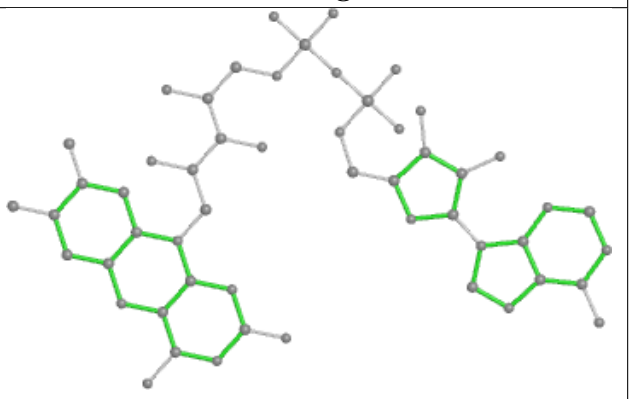
Bond lengths



Bond angles

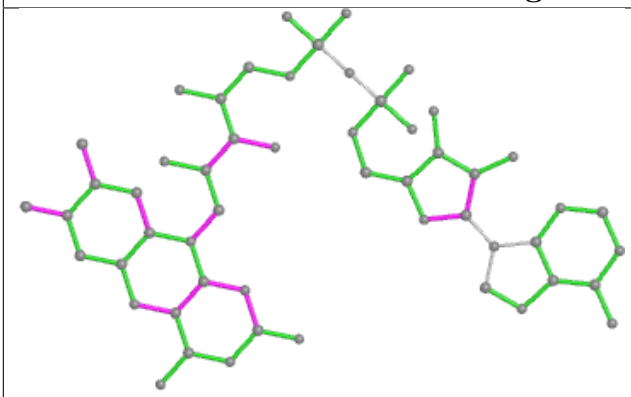


Torsions

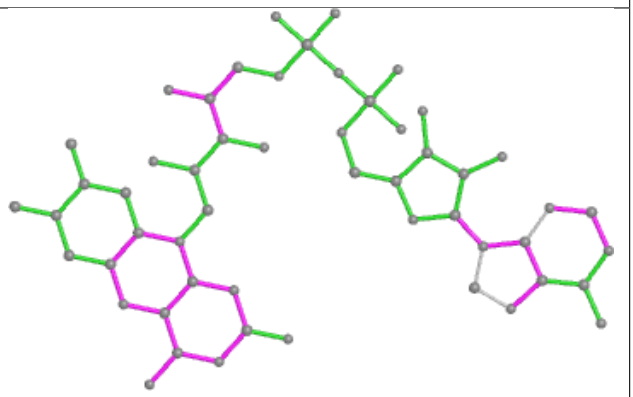


Rings

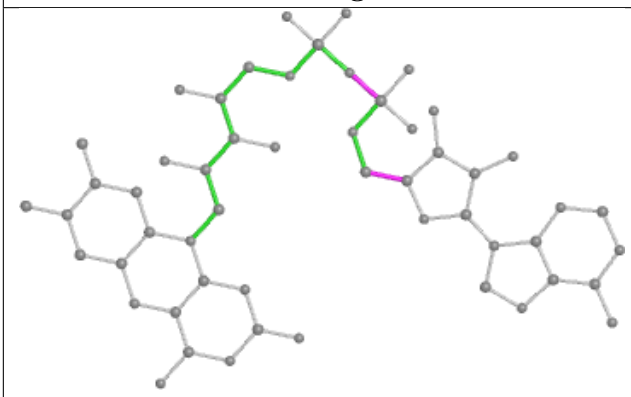
Ligand FAD B 702



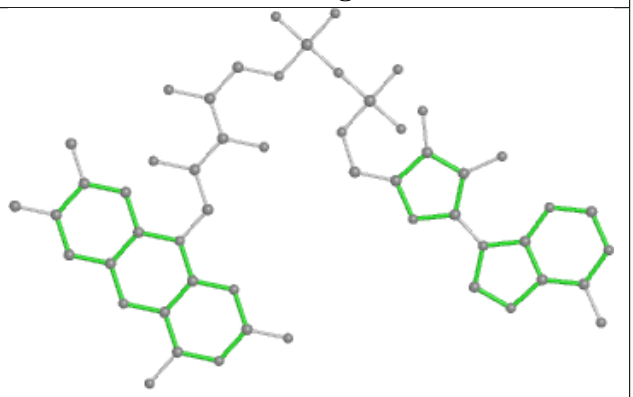
Bond lengths



Bond angles

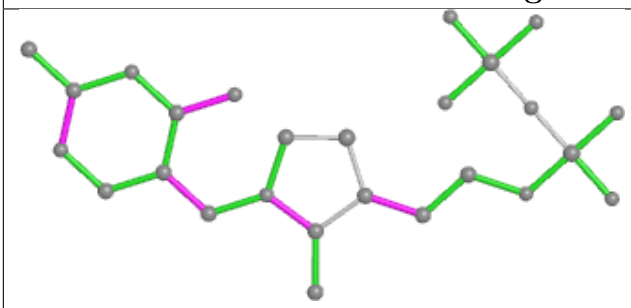


Torsions

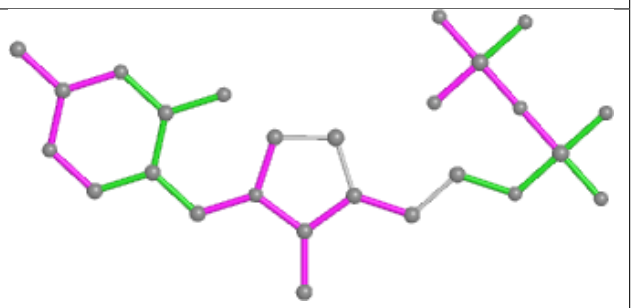


Rings

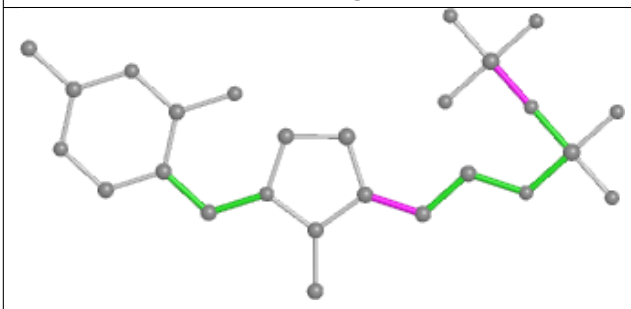
Ligand TPP B 704



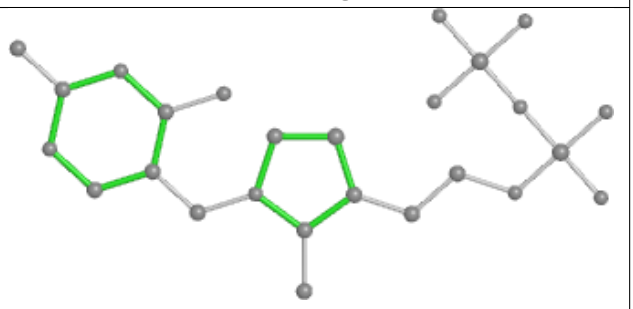
Bond lengths



Bond angles

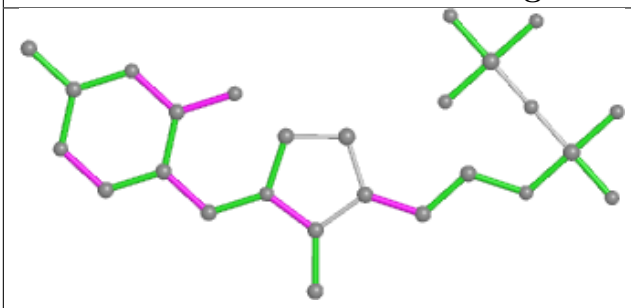


Torsions

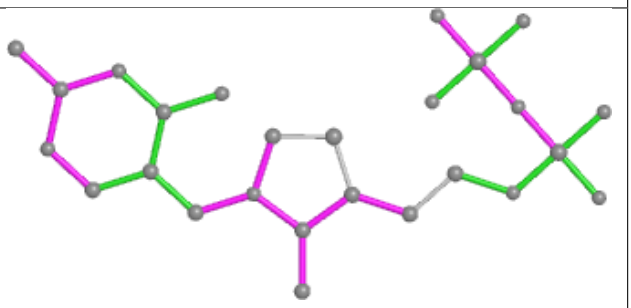


Rings

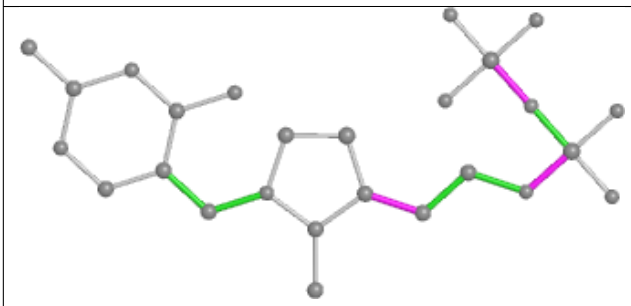
Ligand TPP A 704



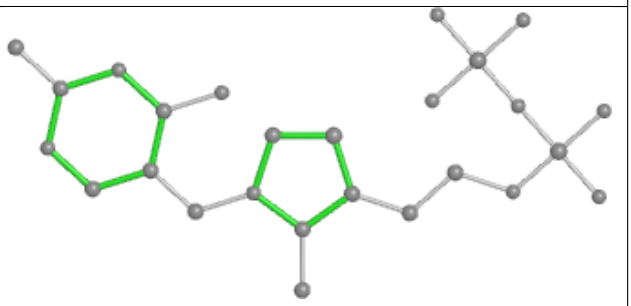
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	541/677 (79%)	0.28	37 (6%) 17 19	19, 29, 62, 112	0
1	B	567/677 (83%)	1.28	133 (23%) 0 0	19, 37, 117, 144	0
All	All	1108/1354 (81%)	0.79	170 (15%) 2 2	19, 32, 105, 144	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	591	TYR	10.6
1	B	448	PHE	9.2
1	B	451	ILE	8.9
1	B	387	LYS	8.2
1	B	396	ALA	8.1
1	B	454	TRP	8.1
1	B	273	LEU	7.9
1	B	458	TYR	7.9
1	B	390	PRO	7.8
1	B	362	LEU	7.7
1	B	649	VAL	7.6
1	B	296	ILE	7.3
1	B	449	ALA	7.2
1	B	392	ALA	7.0
1	B	385	ILE	6.9
1	B	463	MET	6.7
1	B	394	ARG	6.6
1	B	274	ASN	6.6
1	B	365	GLN	6.6
1	B	402	GLY	6.6
1	B	364	VAL	6.3
1	B	397	ALA	6.1
1	B	590	PHE	6.0
1	A	458	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	401	GLY	5.8
1	B	388	PHE	5.8
1	A	280	ALA	5.6
1	B	447	TRP	5.2
1	A	281	GLN	5.2
1	B	293	ALA	5.2
1	B	369	LEU	5.2
1	B	326	ARG	5.1
1	B	595	TYR	5.1
1	B	467	PRO	5.1
1	A	268	LEU	5.0
1	A	467	PRO	5.0
1	B	461	ALA	5.0
1	A	271	ASN	4.9
1	B	462	TYR	4.9
1	B	438	ILE	4.9
1	A	463	MET	4.9
1	B	416	VAL	4.8
1	B	285	VAL	4.8
1	B	439	PHE	4.8
1	B	386	SER	4.7
1	B	417	VAL	4.7
1	B	441	VAL	4.7
1	B	292	ALA	4.6
1	B	436	SER	4.6
1	B	393	ARG	4.5
1	B	298	LEU	4.5
1	B	279	ARG	4.5
1	B	400	ARG	4.5
1	B	127	ASN	4.5
1	B	419	THR	4.5
1	B	395	ALA	4.5
1	B	466	THR	4.5
1	B	299	ALA	4.4
1	B	383	GLY	4.4
1	A	270	SER	4.4
1	B	435	MET	4.2
1	B	647	LYS	4.2
1	A	597	HIS	4.2
1	B	272	ALA	4.2
1	B	384	ASN	4.2
1	A	83	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	367	ALA	4.1
1	A	466	THR	4.1
1	B	468	GLY	4.1
1	A	599	HIS	4.0
1	B	324	SER	4.0
1	B	358	ALA	4.0
1	B	276	LEU	3.9
1	B	368	ASP	3.9
1	B	646	ASP	3.8
1	B	456	LYS	3.8
1	B	442	LYS	3.8
1	B	294	ASP	3.8
1	B	403	ILE	3.8
1	B	366	ASN	3.8
1	B	459	PRO	3.8
1	B	329	ILE	3.7
1	B	370	ILE	3.7
1	B	287	GLN	3.7
1	B	303	VAL	3.7
1	B	453	LYS	3.7
1	A	269	PRO	3.6
1	B	648	LYS	3.6
1	B	592	GLU	3.6
1	B	284	PHE	3.6
1	B	443	GLU	3.6
1	A	279	ARG	3.6
1	B	593	HIS	3.5
1	B	277	THR	3.5
1	B	460	TYR	3.5
1	B	418	GLN	3.4
1	B	302	PRO	3.4
1	B	275	GLN	3.4
1	B	398	GLU	3.4
1	B	361	ASN	3.3
1	B	271	ASN	3.3
1	B	420	GLN	3.2
1	A	265	LYS	3.2
1	B	586	TRP	3.2
1	B	389	ALA	3.2
1	B	589	LEU	3.0
1	B	301	LYS	3.0
1	B	286	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	468	GLY	2.9
1	B	280	ALA	2.9
1	B	399	GLY	2.8
1	A	469	SER	2.8
1	B	469	SER	2.8
1	B	83	PRO	2.8
1	B	289	ILE	2.8
1	B	527	TYR	2.8
1	B	283	GLU	2.8
1	B	431	LEU	2.7
1	B	444	ARG	2.7
1	A	283	GLU	2.7
1	A	456	LYS	2.7
1	B	335	LEU	2.7
1	B	129	ASP	2.6
1	B	531	ALA	2.6
1	B	126	HIS	2.6
1	A	457	GLU	2.6
1	A	517	ILE	2.6
1	B	270	SER	2.5
1	A	454	TRP	2.5
1	B	517	ILE	2.5
1	B	391	GLU	2.5
1	B	457	GLU	2.5
1	A	461	ALA	2.5
1	A	282	ASP	2.5
1	B	380	ARG	2.5
1	B	434	MET	2.5
1	B	325	ASP	2.4
1	A	647	LYS	2.4
1	B	446	GLU	2.4
1	A	529	LEU	2.3
1	B	182	ILE	2.3
1	B	290	ASN	2.3
1	A	459	PRO	2.3
1	B	291	LYS	2.3
1	B	516	PHE	2.3
1	B	288	SER	2.3
1	B	300	LYS	2.3
1	B	363	ALA	2.3
1	A	522	LEU	2.3
1	B	357	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	284	PHE	2.2
1	B	304	LEU	2.2
1	B	131	PHE	2.2
1	B	583	VAL	2.2
1	A	495	THR	2.1
1	A	518	THR	2.1
1	B	465	GLU	2.1
1	B	278	SER	2.1
1	B	440	PRO	2.1
1	B	323	LEU	2.1
1	A	547	ILE	2.1
1	B	421	ILE	2.1
1	B	529	LEU	2.1
1	A	520	GLY	2.1
1	A	387	LYS	2.1
1	A	84	ASP	2.1
1	A	144	HIS	2.0
1	A	636	LYS	2.0
1	B	404	ILE	2.0
1	B	432	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OXY	A	705	2/2	0.74	0.22	55,55,55,60	0
6	OXY	B	706	2/2	0.80	0.38	84,84,84,85	0
6	OXY	A	706	2/2	0.83	0.26	69,69,69,71	0

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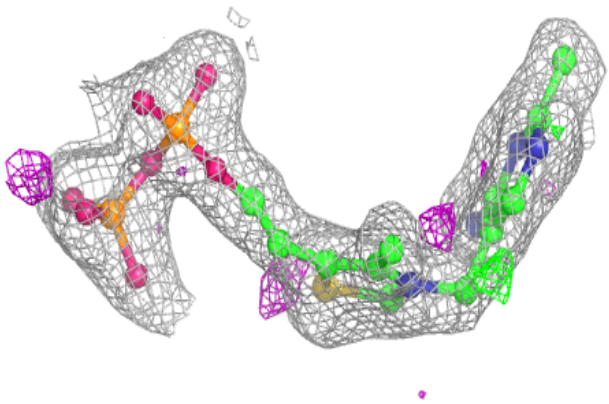
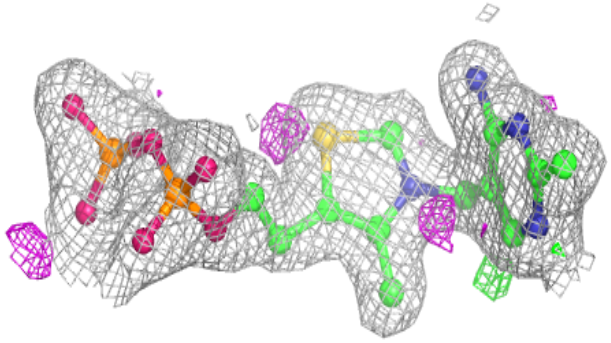
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OXY	B	709	2/2	0.83	0.36	64,64,64,69	0
7	ACT	B	712	4/4	0.84	0.18	56,57,63,65	0
6	OXY	B	705	2/2	0.89	0.14	68,68,68,69	0
7	ACT	A	708	4/4	0.90	0.15	41,57,57,61	0
6	OXY	B	708	2/2	0.90	0.25	59,59,59,61	0
7	ACT	B	713	4/4	0.90	0.14	57,58,71,73	0
4	MG	B	703	1/1	0.95	0.05	25,25,25,25	0
4	MG	A	703	1/1	0.95	0.05	35,35,35,35	0
8	PO4	B	711	5/5	0.95	0.12	57,66,70,71	0
6	OXY	B	707	2/2	0.96	0.16	61,61,61,62	0
6	OXY	B	710	2/2	0.96	0.39	40,40,40,48	0
5	TPP	A	704	26/26	0.96	0.10	21,30,37,56	0
5	TPP	B	704	26/26	0.97	0.10	19,22,26,28	0
6	OXY	A	707	2/2	0.97	0.17	48,48,48,53	0
3	FAD	B	702	53/53	0.97	0.13	33,41,66,74	0
2	K	A	701	1/1	0.98	0.07	34,34,34,34	0
2	K	B	701	1/1	0.98	0.09	41,41,41,41	0
3	FAD	A	702	53/53	0.98	0.12	25,31,64,70	0

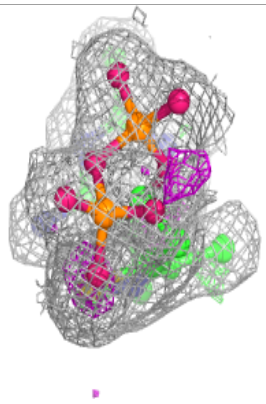
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 704:

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

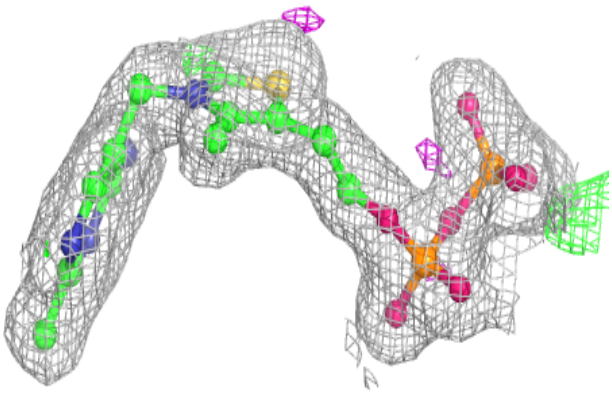


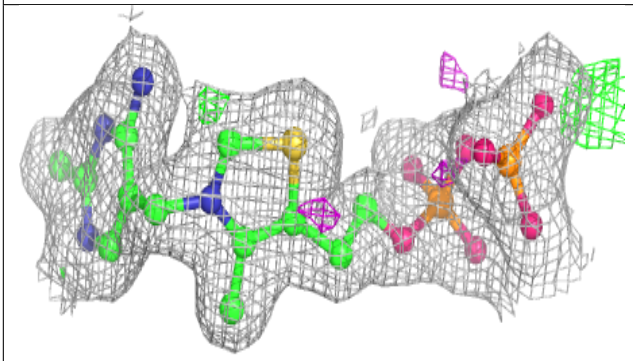


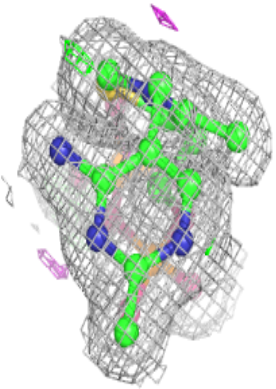


Electron density around TPP B 704:

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

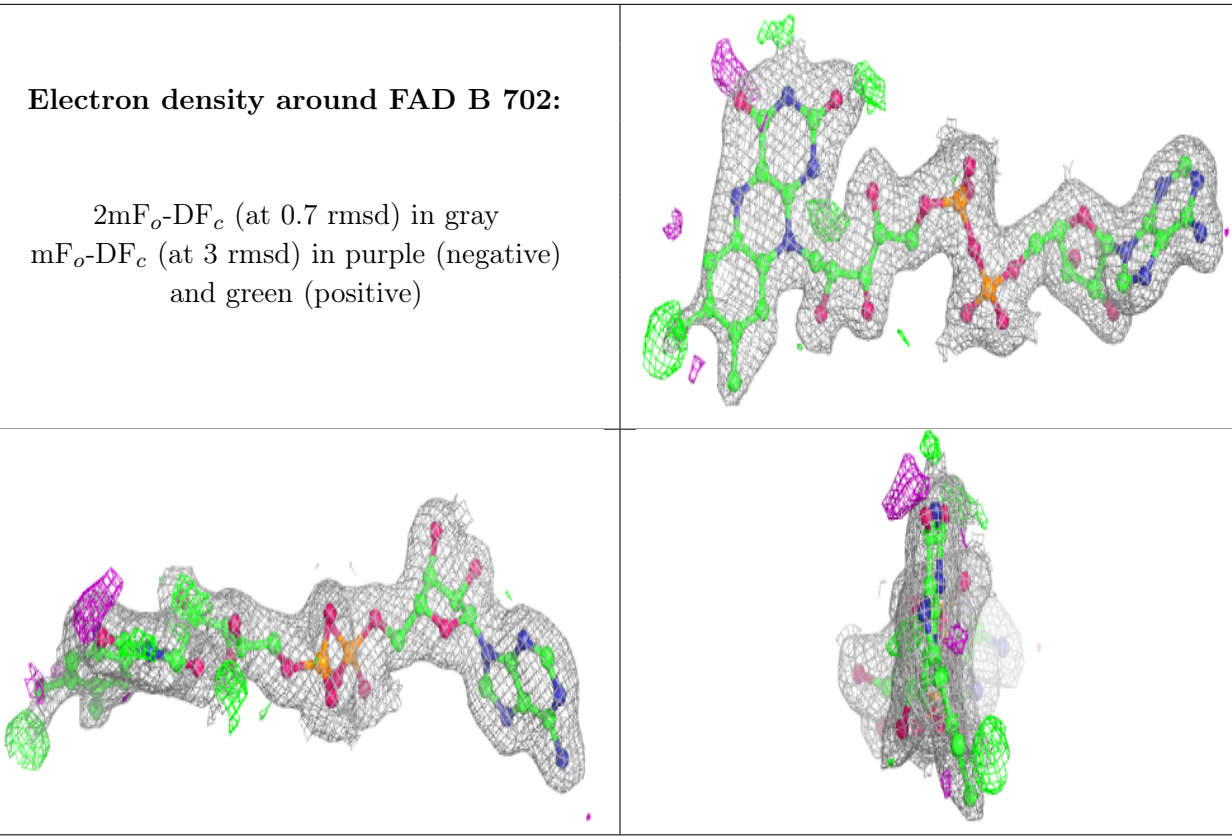






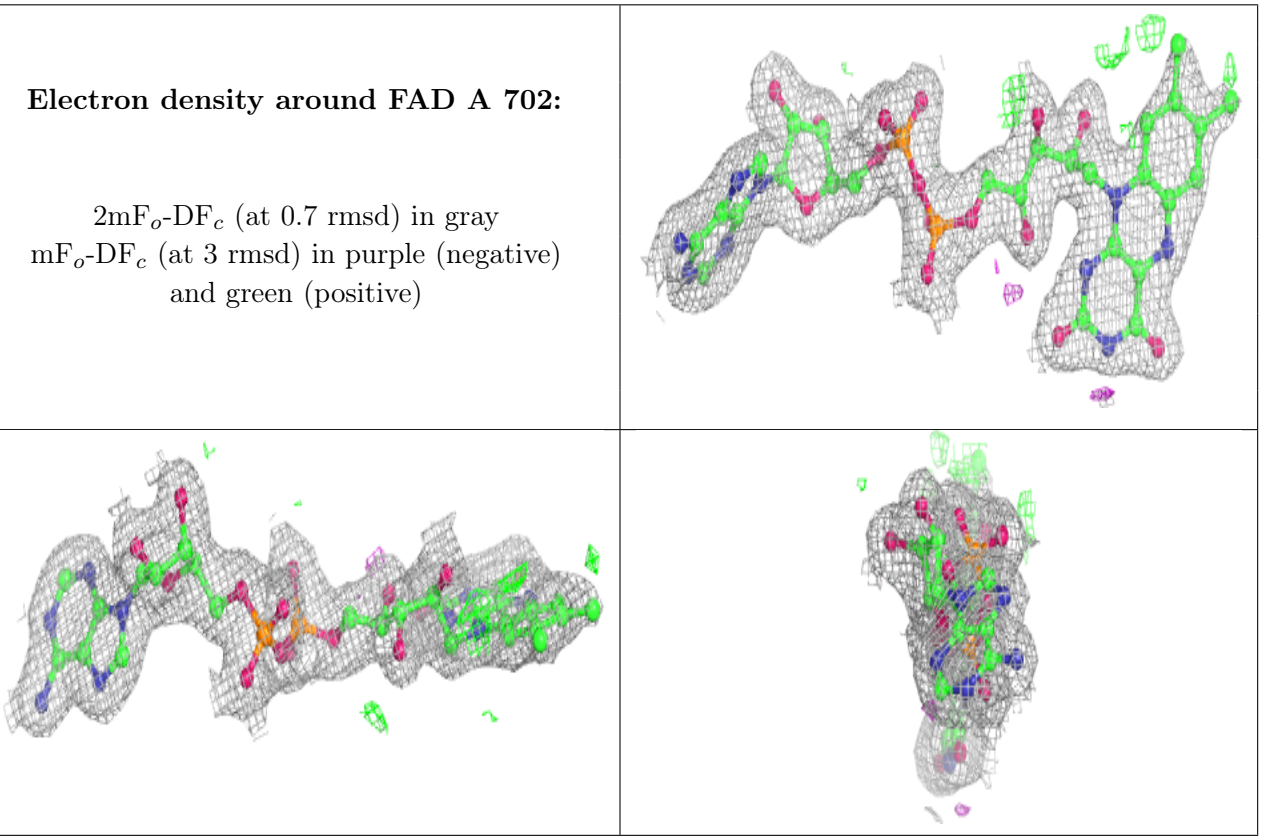
Electron density around FAD B 702:

$2mF_o$-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 702:

$2mF_o$-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.