



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:09 PM BST

PDB ID : 6DEP
Title : Crystal structure of Candida albicans acetohydroxyacid synthase in complex with the herbicide sulfometuron methyl
Authors : Garcia, M.D.; Guddat, L.W.
Deposited on : 2018-05-12
Resolution : 2.15 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 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	:	2.13.1
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)	:	2.13.1

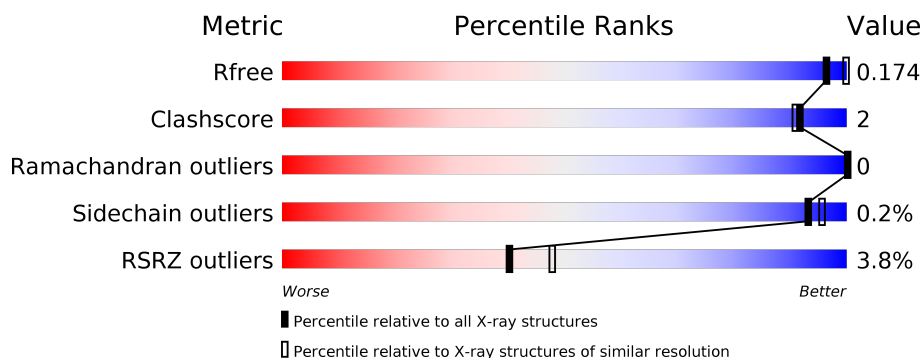
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	682	<div> <div>3%</div> <div>85%</div> <div>12%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5387 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	16	0
			4623	2942	782	877	22			

There are 45 discrepancies between the modelled and reference sequences:

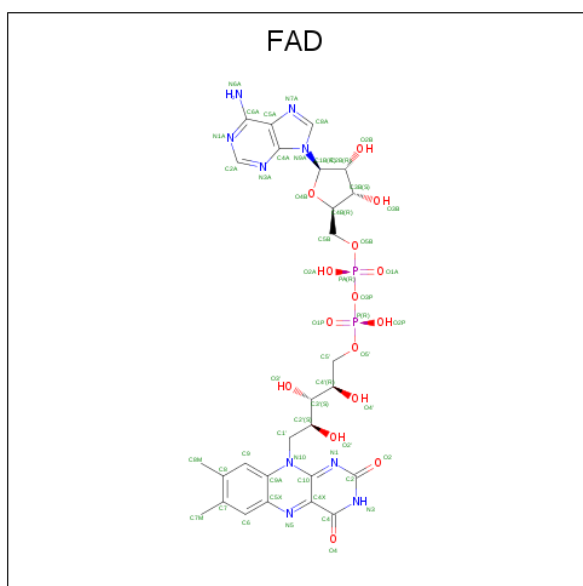
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP A0A1D8PJF9
A	3	HIS	-	expression tag	UNP A0A1D8PJF9
A	4	HIS	-	expression tag	UNP A0A1D8PJF9
A	5	HIS	-	expression tag	UNP A0A1D8PJF9
A	6	HIS	-	expression tag	UNP A0A1D8PJF9
A	7	HIS	-	expression tag	UNP A0A1D8PJF9
A	8	HIS	-	expression tag	UNP A0A1D8PJF9
A	9	SER	-	expression tag	UNP A0A1D8PJF9
A	10	SER	-	expression tag	UNP A0A1D8PJF9
A	11	GLY	-	expression tag	UNP A0A1D8PJF9
A	12	LEU	-	expression tag	UNP A0A1D8PJF9
A	13	VAL	-	expression tag	UNP A0A1D8PJF9
A	14	PRO	-	expression tag	UNP A0A1D8PJF9
A	15	ARG	-	expression tag	UNP A0A1D8PJF9
A	16	GLY	-	expression tag	UNP A0A1D8PJF9
A	17	SER	-	expression tag	UNP A0A1D8PJF9
A	18	GLY	-	expression tag	UNP A0A1D8PJF9
A	19	MET	-	expression tag	UNP A0A1D8PJF9
A	20	LYS	-	expression tag	UNP A0A1D8PJF9
A	21	GLU	-	expression tag	UNP A0A1D8PJF9
A	22	THR	-	expression tag	UNP A0A1D8PJF9
A	23	ALA	-	expression tag	UNP A0A1D8PJF9
A	24	ALA	-	expression tag	UNP A0A1D8PJF9
A	25	ALA	-	expression tag	UNP A0A1D8PJF9
A	26	LYS	-	expression tag	UNP A0A1D8PJF9
A	27	PHE	-	expression tag	UNP A0A1D8PJF9
A	28	GLU	-	expression tag	UNP A0A1D8PJF9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ARG	-	expression tag	UNP A0A1D8PJF9
A	30	GLN	-	expression tag	UNP A0A1D8PJF9
A	31	HIS	-	expression tag	UNP A0A1D8PJF9
A	32	MET	-	expression tag	UNP A0A1D8PJF9
A	33	ASP	-	expression tag	UNP A0A1D8PJF9
A	34	SER	-	expression tag	UNP A0A1D8PJF9
A	35	PRO	-	expression tag	UNP A0A1D8PJF9
A	36	ASP	-	expression tag	UNP A0A1D8PJF9
A	37	LEU	-	expression tag	UNP A0A1D8PJF9
A	38	GLY	-	expression tag	UNP A0A1D8PJF9
A	39	THR	-	expression tag	UNP A0A1D8PJF9
A	40	ASP	-	expression tag	UNP A0A1D8PJF9
A	41	ASP	-	expression tag	UNP A0A1D8PJF9
A	42	ASP	-	expression tag	UNP A0A1D8PJF9
A	43	ASP	-	expression tag	UNP A0A1D8PJF9
A	44	LYS	-	expression tag	UNP A0A1D8PJF9
A	45	ALA	-	expression tag	UNP A0A1D8PJF9
A	46	MET	-	expression tag	UNP A0A1D8PJF9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

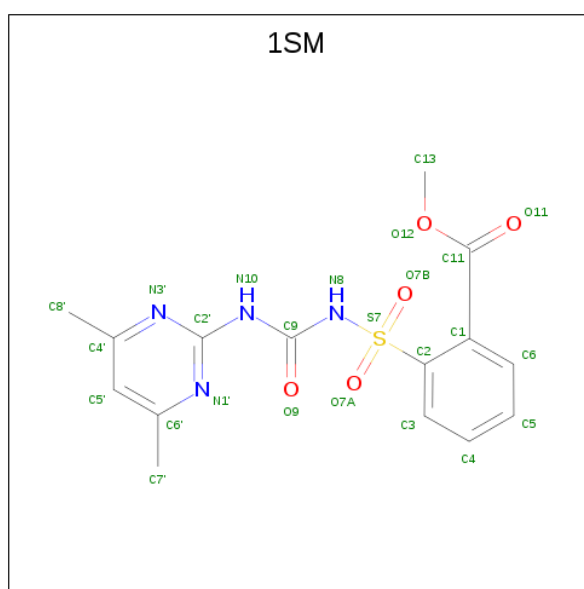
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

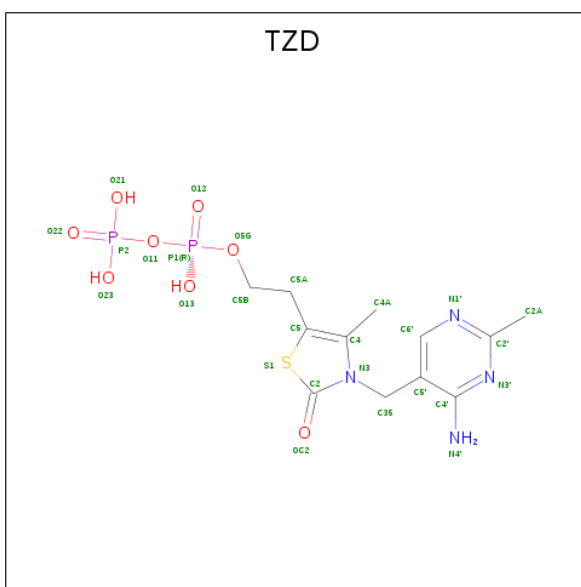
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is METHYL 2-[(4,6-DIMETHYLPYRIMIDIN-2-YL)AMINO]CARBONYL}AMINO)SULFONYL]BENZOATE (three-letter code: 1SM) (formula: C₁₅H₁₆N₄O₅S).



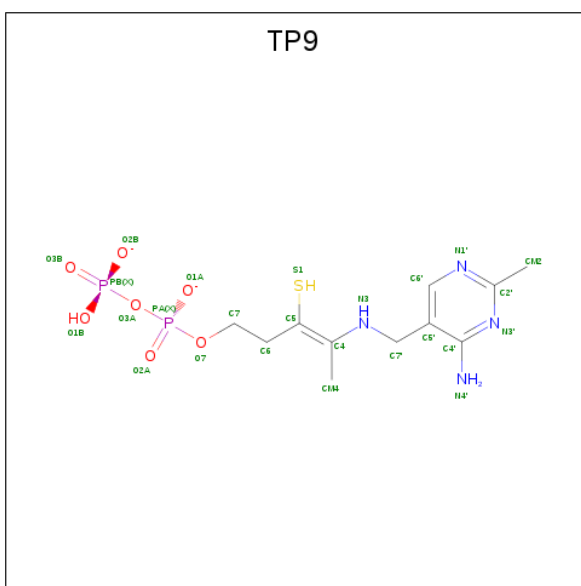
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			25	15	4	5	1		

- Molecule 6 is 2-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-2-OXO-2,3-DIHYDRO-1,3-THIAZOL-5-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TZD) (formula: C₁₂H₁₈N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	1
			27	12	4	8	2	1		

- Molecule 7 is (3Z)-4-[[[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]AMINO}-3-MERCAPTOPYRUVATE-3-EN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: TP9) (formula: $C_{11}H_{18}N_4O_7P_2S$).

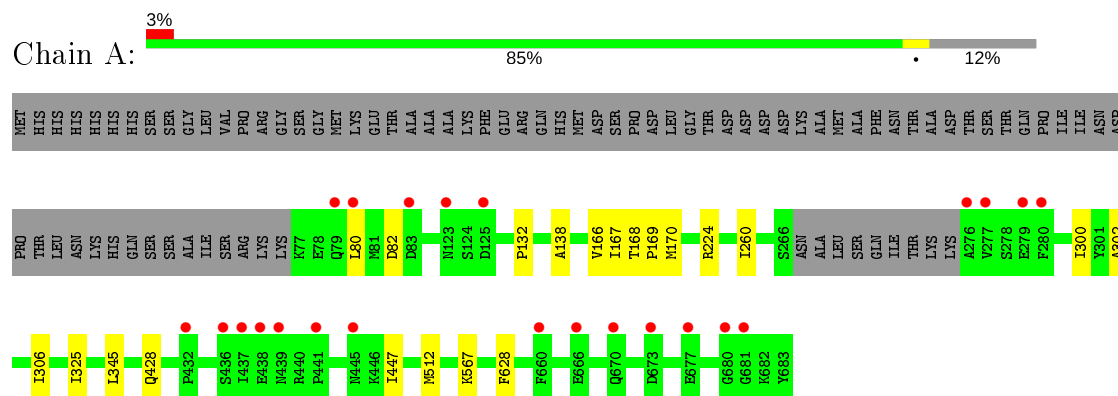


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	S	0	1
			25	11	4	7	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	632	Total 632	O 632	0	0

- Molecule 1: Acetolactate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	175.89Å 175.89Å 177.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.65 – 2.15 46.65 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.65-2.15) 99.6 (46.65-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.144 , 0.172 0.151 , 0.174	Depositor DCC
R_{free} test set	2000 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5387	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, 1SM, TZD, FAD, TP9

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	0.23	0/4752	0.43	0/6449

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	4623	0	4666	13	0
2	A	53	0	31	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	25	0	16	0	0
6	A	27	0	15	1	0
7	A	25	0	17	0	0
8	A	632	0	0	4	0
All	All	5387	0	4745	15	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (15) 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:132:PRO:HG3	1:A:138:ALA:HB2	1.81	0.61
1:A:428:GLN:NE2	8:A:809:HOH:O	2.34	0.61
1:A:260:ILE:N	8:A:801:HOH:O	2.43	0.51
1:A:567:LYS:HB3	1:A:628:PHE:CZ	2.49	0.48
1:A:166[B]:VAL:HG23	1:A:170:MET:HE1	1.96	0.47
1:A:167:ILE:HD13	1:A:170:MET:HE3	1.97	0.46
6:A:705[A]:TZD:H4'2	6:A:705[A]:TZD:C2	2.30	0.45
1:A:224:ARG:NH1	8:A:808:HOH:O	2.50	0.44
1:A:82:ASP:HB2	1:A:260:ILE:HG13	1.99	0.44
1:A:302:ALA:HB1	1:A:306[B]:ILE:HD12	2.00	0.43
1:A:168:THR:HB	1:A:169:PRO:HD3	2.01	0.43
1:A:345:LEU:HD21	1:A:447:ILE:HG23	2.01	0.41
1:A:80:LEU:O	8:A:801:HOH:O	2.21	0.41
1:A:300:ILE:HG13	1:A:325:ILE:HG21	2.03	0.40
2:A:701:FAD:H1'1	2:A:701:FAD:H9	1.75	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	610/682 (89%)	600 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	499/563 (89%)	498 (100%)	1 (0%)	93	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	512	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	TZD	A	705[A]	4	23,28,28	3.49	6 (26%)	28,42,42	1.61	7 (25%)
5	1SM	A	704	-	26,26,26	1.35	3 (11%)	36,37,37	3.16	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	701	-	51,58,58	2.21	11 (21%)	60,89,89	1.56	11 (18%)
7	TP9	A	706[B]	4	21,25,25	2.04	2 (9%)	28,36,36	1.80	6 (21%)

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
6	TZD	A	705[A]	4	-	4/16/17/17	0/2/2/2
5	ISM	A	704	-	-	9/21/21/21	0/2/2/2
2	FAD	A	701	-	-	3/30/50/50	0/6/6/6
7	TP9	A	706[B]	4	-	0/17/22/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705[A]	TZD	C5-S1	-11.75	1.52	1.74
2	A	701	FAD	C10-N1	7.95	1.43	1.33
7	A	706[B]	TP9	C4-N3	7.91	1.42	1.32
6	A	705[A]	TZD	C4-N3	7.79	1.56	1.39
6	A	705[A]	TZD	C5A-C5	6.25	1.53	1.50
2	A	701	FAD	C4-C4X	6.22	1.52	1.41
2	A	701	FAD	C1'-N10	-5.84	1.42	1.48
2	A	701	FAD	C4X-N5	4.62	1.39	1.33
2	A	701	FAD	C2B-C1B	-4.57	1.46	1.53
5	A	704	ISM	C2'-N10	3.69	1.43	1.38
5	A	704	ISM	O12-C11	3.48	1.41	1.33
6	A	705[A]	TZD	C4'-N4'	3.26	1.42	1.34
2	A	701	FAD	C4-N3	3.18	1.38	1.33
7	A	706[B]	TP9	C4'-N4'	3.17	1.42	1.34
2	A	701	FAD	O4B-C1B	2.94	1.45	1.41
6	A	705[A]	TZD	C5'-C4'	-2.60	1.38	1.42
2	A	701	FAD	O3'-C3'	-2.58	1.36	1.43
5	A	704	ISM	C9-N10	2.57	1.42	1.37
2	A	701	FAD	C2'-C3'	2.36	1.57	1.53
6	A	705[A]	TZD	C35-N3	-2.27	1.44	1.48
2	A	701	FAD	C2-N1	2.26	1.42	1.38
2	A	701	FAD	C2B-C3B	-2.17	1.47	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	ISM	O7B-S7-O7A	-15.44	100.57	119.55
2	A	701	FAD	C4-N3-C2	6.32	120.48	115.14
5	A	704	ISM	C2-S7-N8	6.07	113.21	106.06
7	A	706[B]	TP9	CM4-C4-N3	-5.90	111.42	118.00
5	A	704	ISM	O12-C11-C1	4.46	119.71	112.30
2	A	701	FAD	N3A-C2A-N1A	-4.17	122.16	128.68
2	A	701	FAD	C1'-N10-C9A	3.36	120.94	118.29
6	A	705[A]	TZD	N1'-C2'-N3'	-3.28	119.90	125.54
2	A	701	FAD	C4-C4X-N5	3.06	122.09	118.60
7	A	706[B]	TP9	C6'-N1'-C2'	3.04	121.13	115.96
7	A	706[B]	TP9	C5'-C6'-N1'	-3.04	118.76	123.82
6	A	705[A]	TZD	C6'-C5'-C4'	2.95	119.73	115.72
2	A	701	FAD	C9A-N10-C10	-2.94	118.06	121.91
2	A	701	FAD	C4A-C5A-N7A	-2.85	106.43	109.40
5	A	704	ISM	C7'-C6'-N1'	2.84	121.09	116.56
6	A	705[A]	TZD	C6'-N1'-C2'	2.82	120.77	115.96
6	A	705[A]	TZD	C4A-C4-N3	2.72	126.12	122.69
5	A	704	ISM	C2'-N10-C9	-2.70	127.52	130.40
7	A	706[B]	TP9	C7'-N3-C4	-2.66	122.31	125.97
6	A	705[A]	TZD	C5'-C6'-N1'	-2.63	119.44	123.82
6	A	705[A]	TZD	C2A-C2'-N1'	2.61	120.01	117.14
2	A	701	FAD	C4-C4X-C10	-2.53	118.28	119.95
7	A	706[B]	TP9	PA-O3A-PB	-2.38	124.65	132.83
2	A	701	FAD	C4X-C4-N3	-2.38	120.18	123.43
2	A	701	FAD	C10-C4X-N5	-2.35	119.63	121.26
5	A	704	ISM	C2'-N3'-C4'	2.22	120.81	115.99
2	A	701	FAD	C5X-C9A-N10	2.21	119.32	117.72
6	A	705[A]	TZD	P1-O11-P2	-2.15	125.45	132.83
5	A	704	ISM	N10-C2'-N1'	2.12	122.67	116.46
5	A	704	ISM	N3'-C2'-N1'	-2.03	123.02	126.23
2	A	701	FAD	C5'-C4'-C3'	-2.02	108.30	112.20
7	A	706[B]	TP9	N4'-C4'-N3'	2.01	119.87	117.03

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C2'-C1'-N10-C9A
5	A	704	ISM	C1-C2-S7-O7A
5	A	704	ISM	N8-C9-N10-C2'
5	A	704	ISM	C3-C2-S7-O7A
5	A	704	ISM	C3-C2-S7-N8
5	A	704	ISM	C1-C2-S7-N8

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Mol	Chain	Res	Type	Atoms
2	A	701	FAD	P-O3P-PA-O5B
6	A	705[A]	TZD	C5-C5A-C5B-O5G
6	A	705[A]	TZD	C4-C5-C5A-C5B
5	A	704	ISM	C6-C1-C11-O12
5	A	704	ISM	O9-C9-N10-C2'
5	A	704	ISM	C2-C1-C11-O12
6	A	705[A]	TZD	P1-O11-P2-O23
2	A	701	FAD	O4B-C4B-C5B-O5B
6	A	705[A]	TZD	C5B-O5G-P1-O12
5	A	704	ISM	C6-C1-C11-O11

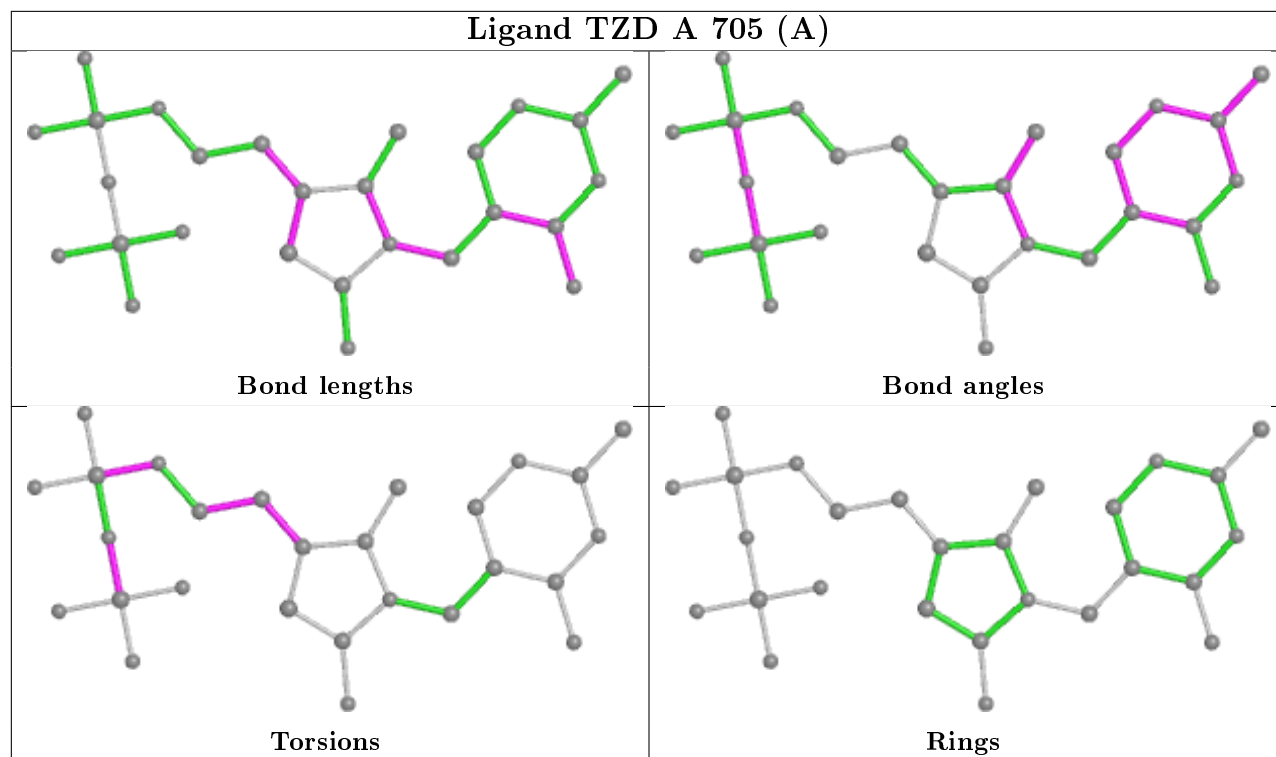
There are no ring outliers.

2 monomers are involved in 2 short contacts:

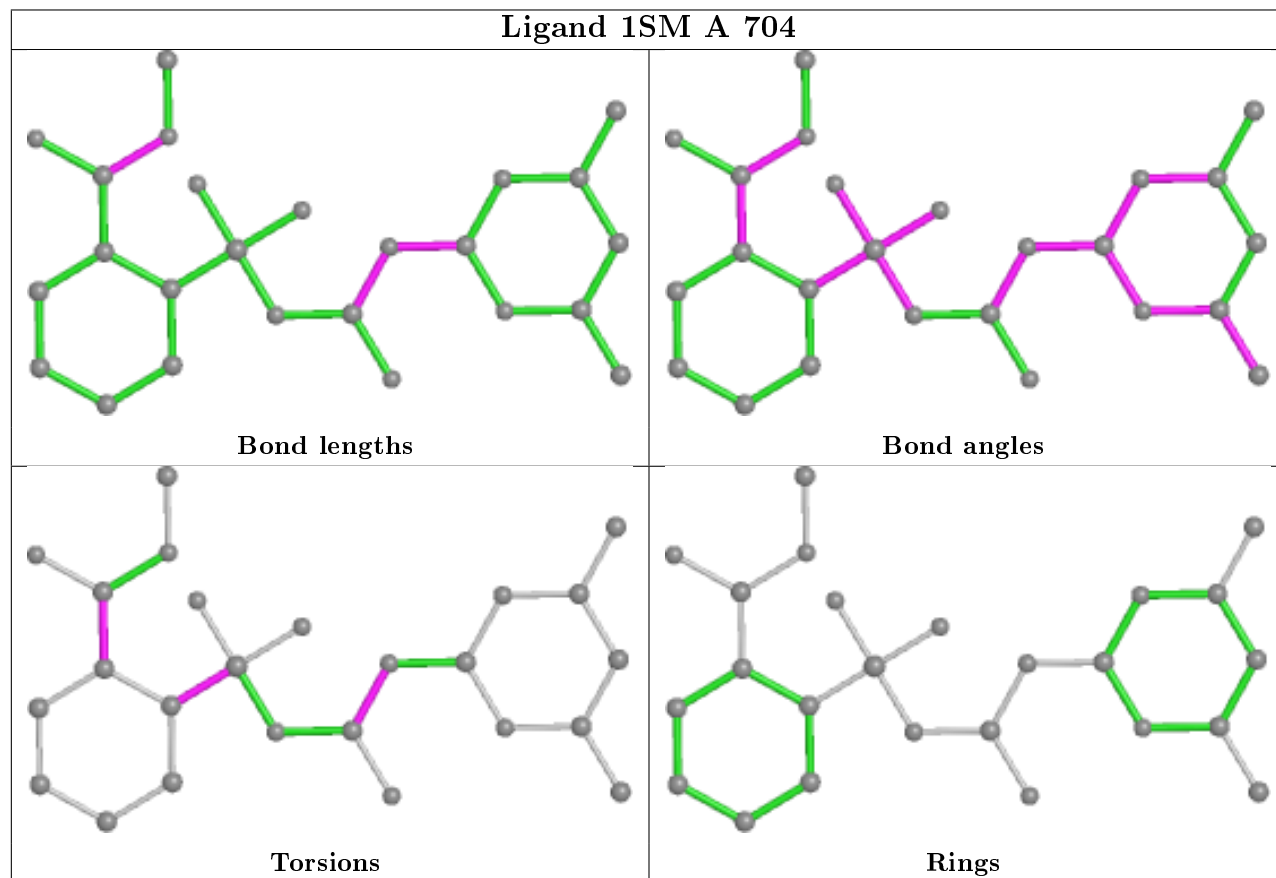
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	705[A]	TZD	1	0
2	A	701	FAD	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

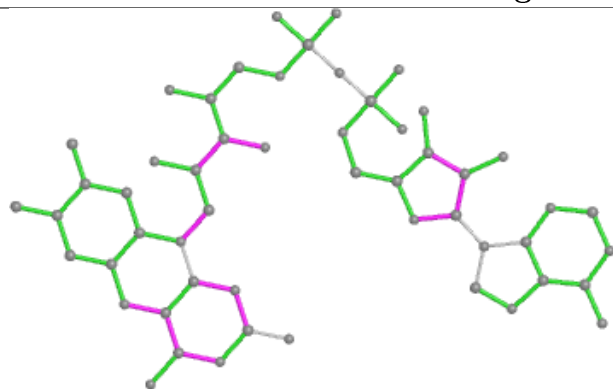
Ligand TZD A 705 (A)



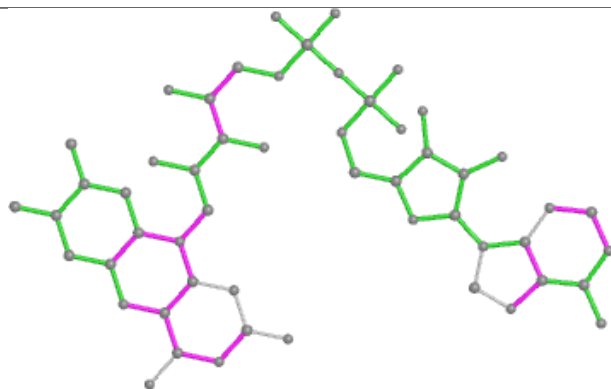
Ligand 1SM A 704



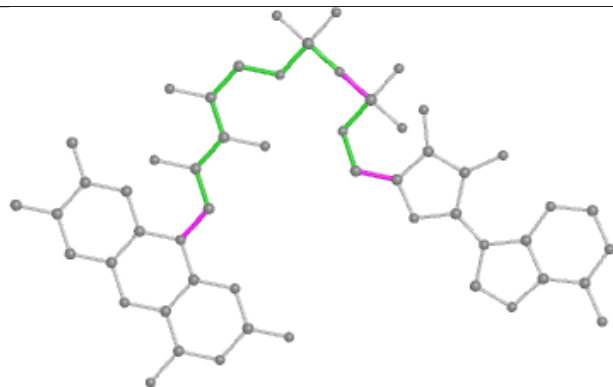
Ligand FAD A 701



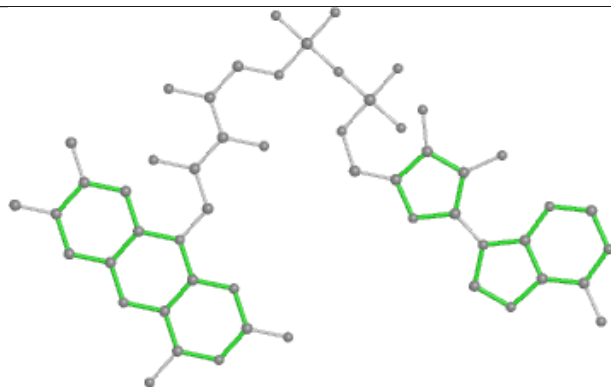
Bond lengths



Bond angles

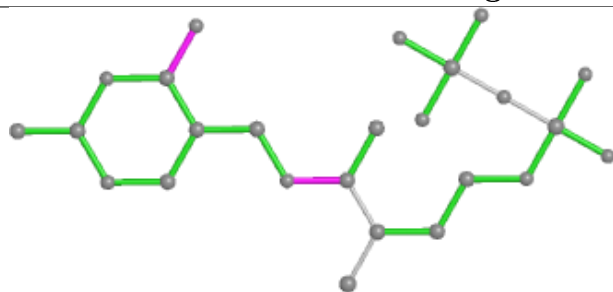


Torsions

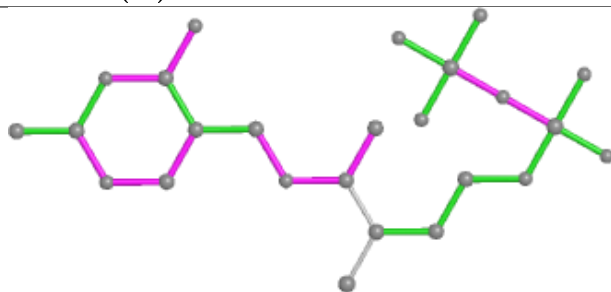


Rings

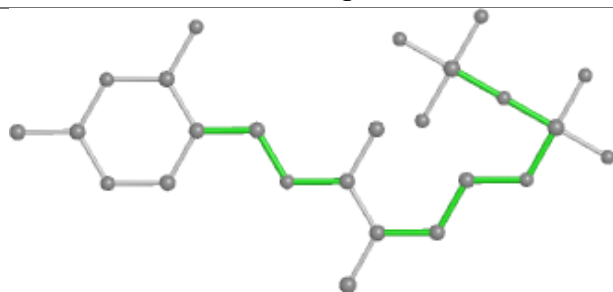
Ligand TP9 A 706 (B)



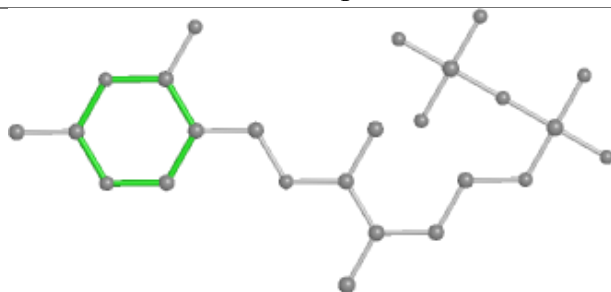
Bond lengths



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, 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	598/682 (87%)	-0.21	23 (3%)	40 48	18, 29, 52, 99	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	VAL	7.1
1	A	276	ALA	4.0
1	A	280	PHE	3.9
1	A	681	GLY	3.5
1	A	439	ASN	3.3
1	A	436[A]	SER	3.3
1	A	279	GLU	3.3
1	A	437	ILE	3.2
1	A	441	PRO	3.1
1	A	677	GLU	3.0
1	A	80	LEU	2.8
1	A	438	GLU	2.8
1	A	680	GLY	2.7
1	A	666	GLU	2.7
1	A	670	GLN	2.6
1	A	125	ASP	2.6
1	A	79	GLN	2.5
1	A	445	ASN	2.4
1	A	660	PHE	2.4
1	A	673	ASP	2.4
1	A	123	ASN	2.3
1	A	432	PRO	2.1
1	A	83	ASP	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](#)

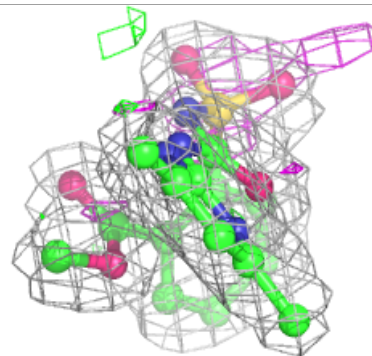
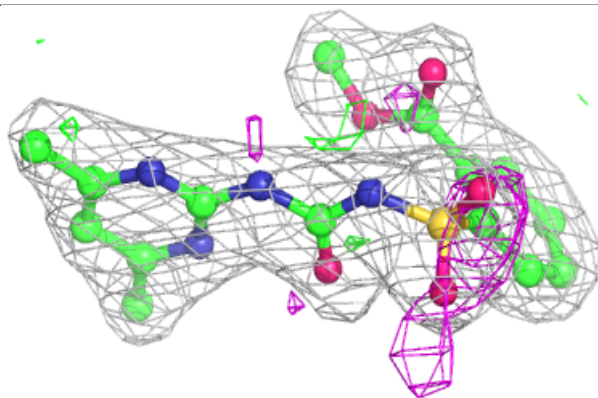
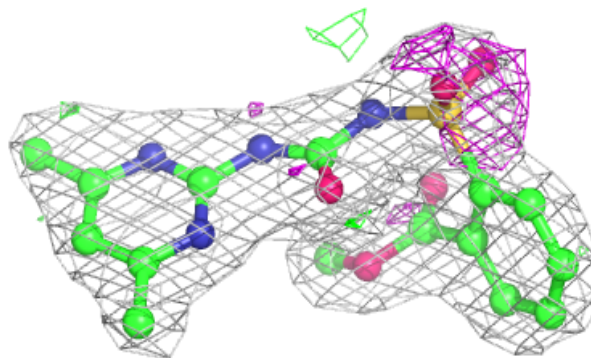
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ISM	A	704	25/25	0.95	0.10	26,35,40,42	0
4	MG	A	703	1/1	0.97	0.07	17,17,17,17	0
6	TZD	A	705[A]	27/27	0.98	0.12	17,22,27,30	27
2	FAD	A	701	53/53	0.98	0.09	17,23,26,30	0
3	K	A	702	1/1	0.98	0.09	29,29,29,29	0
7	TP9	A	706[B]	25/25	0.98	0.12	17,22,23,35	25

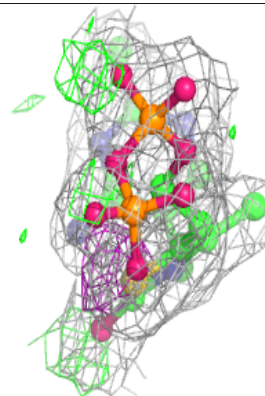
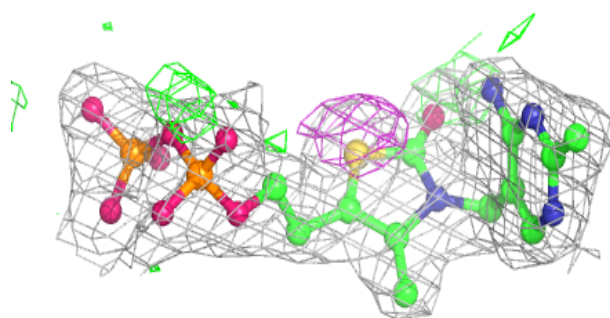
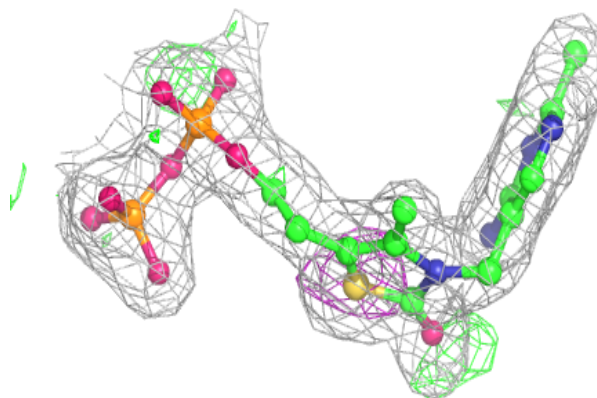
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1SM 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)

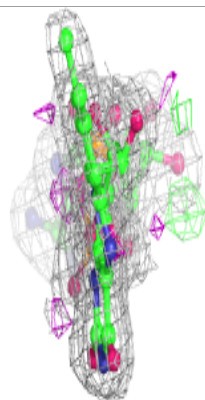
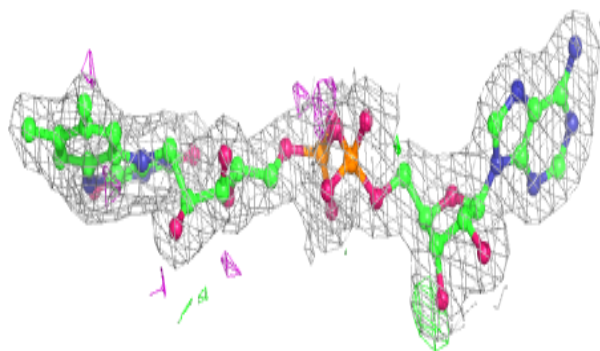
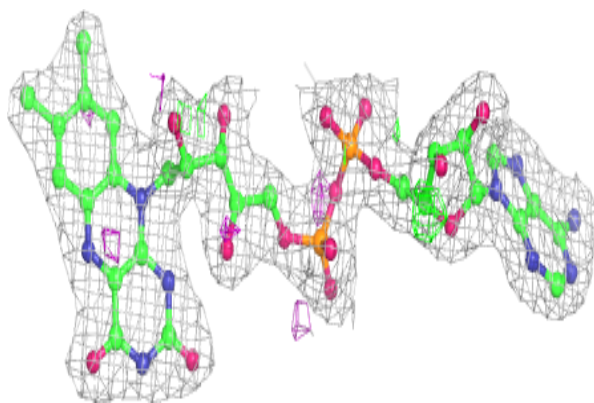
**Electron density around TZD A 705 (A):**

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

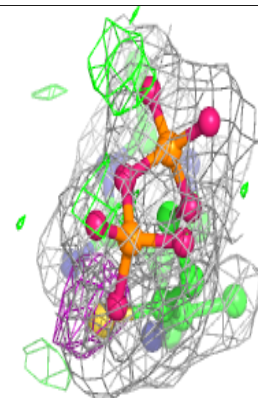
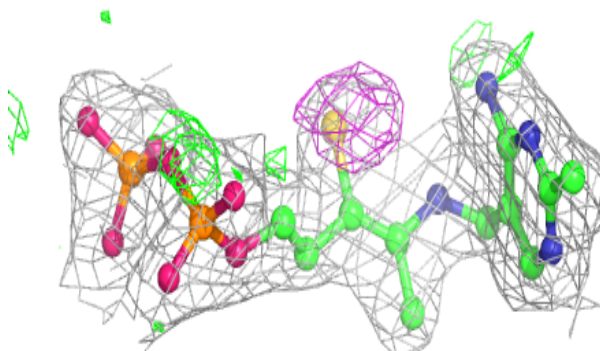
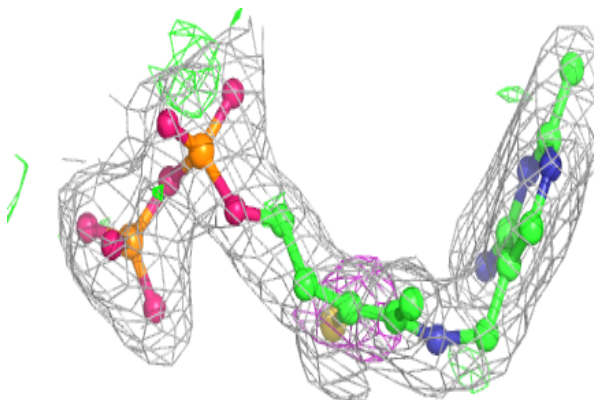


Electron density around FAD A 701:

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

**Electron density around TP9 A 706 (B):**

$2mF_o-DF_c$ (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.