Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 09:52 PM EDT

PDB ID	:	6KSB
Title	:	Crystal Structure of E447A M130G Acyl-CoA Dehydrogenase FadE5 mutant from Mycobacteria smegmatis in complex with C16CoA
Authors	:	Liu, X.; Chen, X.B.
Deposited on	:	2019-08-23
Resolution	:	1.97 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:

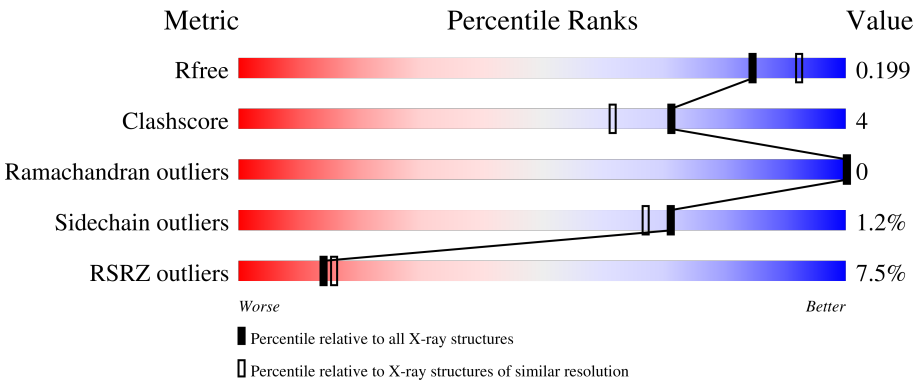
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.97 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	611	7% 92% 7%
1	B	611	8% 90% 9%

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
2	GOL	A	701	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19584 atoms, of which 9352 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.

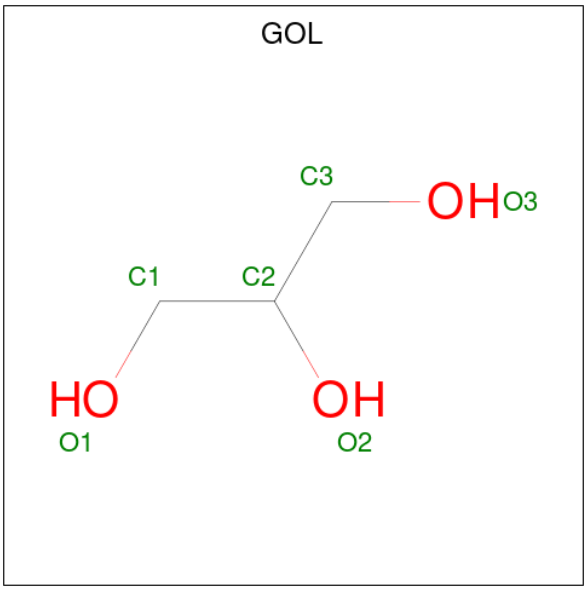
- Molecule 1 is a protein called Acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	608	9224	2951	4569	791	892	21	0	0	0
1	B	609	9252	2955	4589	793	894	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

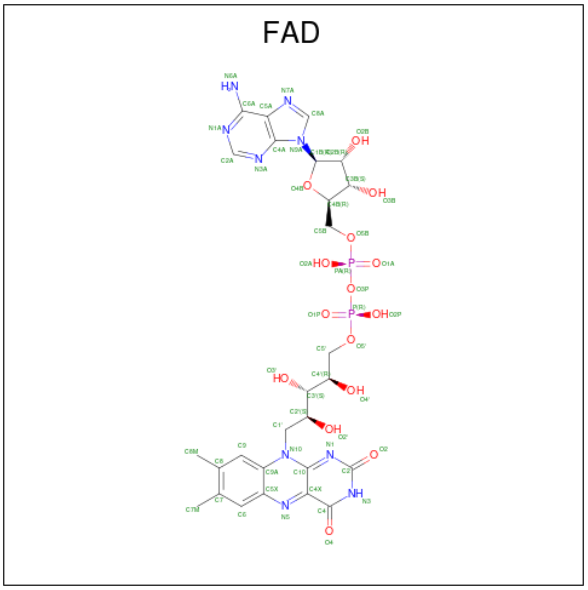
Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	MET	engineered mutation	UNP A0A0D6G5A8
A	447	ALA	GLU	engineered mutation	UNP A0A0D6G5A8
B	130	GLY	MET	engineered mutation	UNP A0A0D6G5A8
B	447	ALA	GLU	engineered mutation	UNP A0A0D6G5A8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



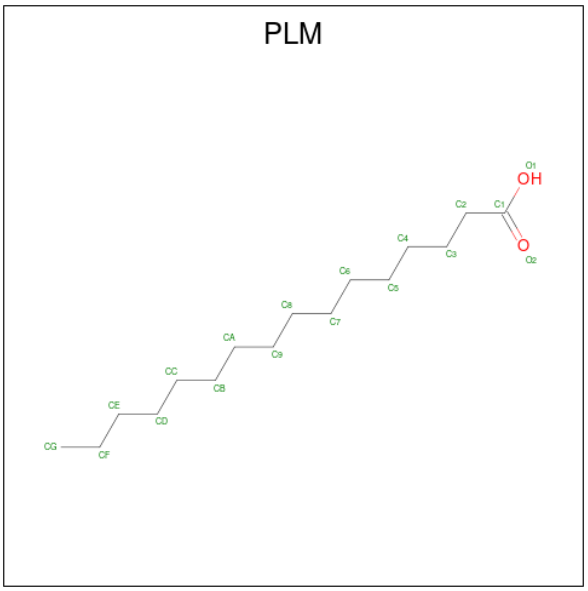
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	11	3	5	3	0	0
			Total	C	H	O		
2	B	1	12	3	6	3	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



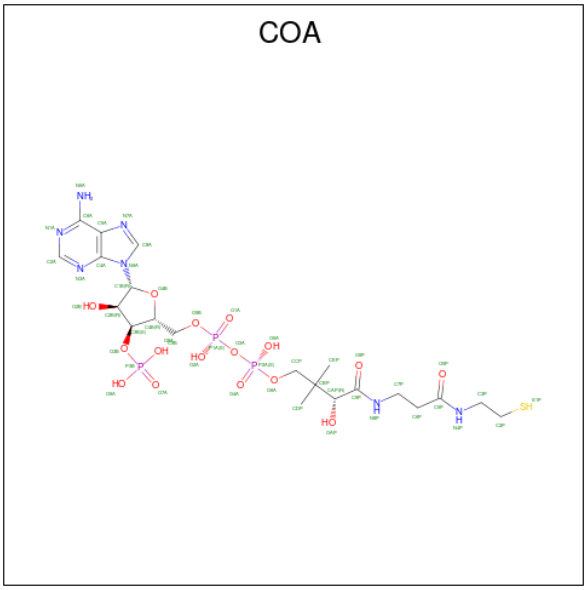
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	84	27	31	9	15	2	0	0
			Total	C	H	N	O	P		
3	B	1	83	27	30	9	15	2	0	0

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	47	16	30	1	0	0
4	B	1	47	16	30	1	0	0

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
5	A	1	79	21	31	7	16	3	1	0	0
5	B	1	79	21	31	7	16	3	1	0	0

- Molecule 6 is water.

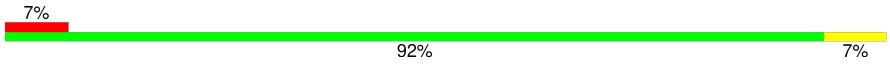
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	333	333	333	0	0
			Total	O		
6	B	333	333	333	0	0

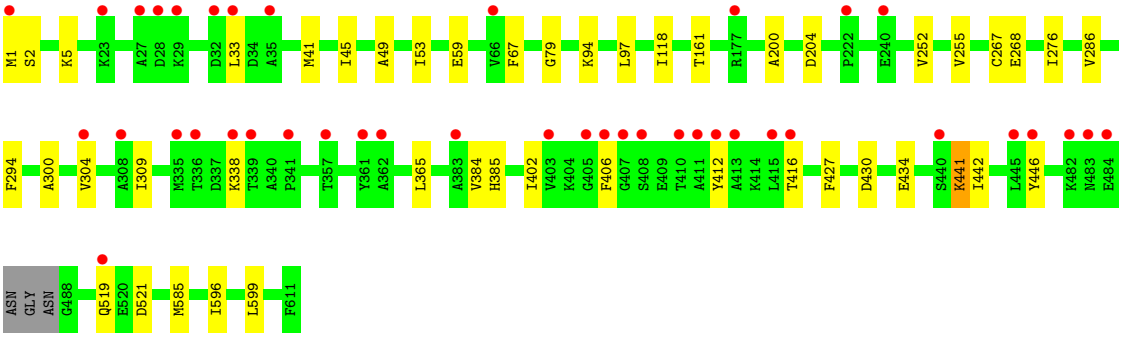
3 Residue-property plots (i)

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: Acyl-CoA dehydrogenase

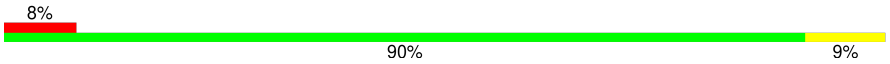
Chain A:

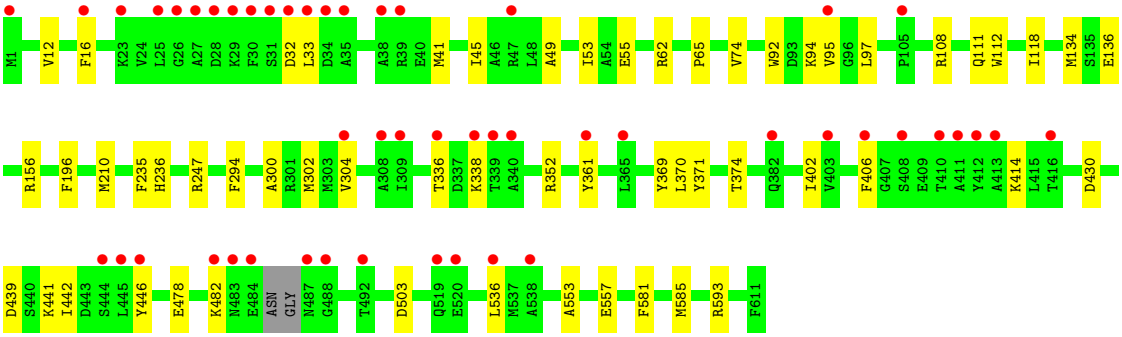




- Molecule 1: Acyl-CoA dehydrogenase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.62Å 199.10Å 73.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.97 49.34 – 1.97	Depositor EDS
% Data completeness (in resolution range)	85.2 (49.34-1.97) 85.2 (49.34-1.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.164 , 0.199 0.166 , 0.199	Depositor DCC
R_{free} test set	4418 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19584	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: PLM, COA, FAD, GOL

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	0.67	2/4747 (0.0%)	0.70	1/6422 (0.0%)
1	B	0.64	0/4755	0.68	3/6433 (0.0%)
All	All	0.65	2/9502 (0.0%)	0.69	4/12855 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	ILE	C-N	8.32	1.50	1.34
1	A	434	GLU	CD-OE1	-5.78	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	439	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	62	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	352	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	204	ASP	CB-CG-OD1	5.24	123.01	118.30

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	4655	4569	4583	29	0
1	B	4663	4589	4589	37	0
2	A	6	5	8	0	0
2	B	6	6	8	0	0
3	A	53	31	31	3	0
3	B	53	30	31	6	0
4	A	17	30	31	0	0
4	B	17	30	31	1	0
5	A	48	31	30	1	0
5	B	48	31	30	2	0
6	A	333	0	0	6	1
6	B	333	0	0	7	1
All	All	10232	9352	9372	67	2

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 4.

All (67) 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)
5:B:704:COA:C1B	5:B:704:COA:O4B	1.63	1.23
1:B:442:ILE:HD11	3:B:702:FAD:HM83	1.36	1.04
1:B:442:ILE:CD1	3:B:702:FAD:HM83	1.89	1.01
1:A:521:ASP:OD1	6:A:801:HOH:O	2.08	0.72
1:B:55:GLU:OE2	6:B:801:HOH:O	2.10	0.69
1:A:338:LYS:HD2	6:B:810:HOH:O	1.92	0.68
1:A:519:GLN:HB3	6:A:803:HOH:O	1.93	0.67
1:B:210:MET:SD	6:B:1077:HOH:O	2.53	0.67
1:B:442:ILE:HD13	3:B:702:FAD:HM83	1.78	0.63
1:A:309:ILE:HG12	1:A:365:LEU:HB3	1.81	0.63
1:B:442:ILE:HD11	3:B:702:FAD:C8M	2.23	0.62
1:B:581:PHE:HA	1:B:585:MET:HE2	1.83	0.61
1:B:94:LYS:HG3	1:B:97:LEU:HD22	1.82	0.61
1:A:33:LEU:HD11	1:A:41:MET:CE	2.32	0.59
1:A:442:ILE:HD11	3:A:702:FAD:HM83	1.86	0.56
1:A:286:VAL:HG11	6:A:1098:HOH:O	2.05	0.55
1:B:134:MET:HE2	4:B:703:PLM:HC2	1.89	0.55
1:A:1:MET:HG2	1:A:2:SER:H	1.74	0.53
1:A:33:LEU:HD11	1:A:41:MET:HE1	1.91	0.53
1:A:385:HIS:O	6:A:802:HOH:O	2.19	0.53
3:B:702:FAD:C2	5:B:704:COA:S1P	2.96	0.52
1:B:196:PHE:O	3:B:702:FAD:C4X	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLU:OE2	6:B:803:HOH:O	2.20	0.51
1:A:252:VAL:HG13	1:A:267:CYS:HB3	1.93	0.50
1:B:336:THR:OG1	6:B:802:HOH:O	2.19	0.50
1:B:370:LEU:O	1:B:374:THR:HG23	2.10	0.50
1:B:33:LEU:HD11	1:B:41:MET:HE1	1.93	0.50
1:B:45:ILE:HD12	1:B:92:TRP:CE3	2.46	0.50
1:A:67:PHE:HB2	1:A:255:VAL:HG23	1.94	0.49
1:A:94:LYS:HG2	1:A:97:LEU:HD22	1.94	0.49
1:A:442:ILE:CD1	3:A:702:FAD:HM83	2.42	0.49
1:B:45:ILE:HD11	1:B:118:ILE:HD11	1.95	0.48
1:A:338:LYS:HG3	6:B:1032:HOH:O	2.12	0.48
1:A:33:LEU:HD11	1:A:41:MET:HE3	1.95	0.48
1:B:402:ILE:HD13	1:B:536:LEU:HD12	1.96	0.48
1:B:478:GLU:CG	1:B:482:LYS:HE3	2.44	0.47
1:A:300:ALA:O	1:A:304:VAL:HG23	2.14	0.47
3:A:702:FAD:C2	5:A:704:COA:S1P	3.03	0.47
1:B:32:ASP:OD1	1:B:32:ASP:N	2.43	0.47
1:B:300:ALA:O	1:B:304:VAL:HG23	2.15	0.47
1:A:268:GLU:HB2	6:A:853:HOH:O	2.15	0.47
1:B:402:ILE:O	1:B:406:PHE:HB3	2.16	0.46
1:B:108:ARG:NH2	1:B:111:GLN:OE1	2.49	0.45
1:A:596:ILE:HA	1:A:599:LEU:HG	1.97	0.45
1:A:45:ILE:HD11	1:A:118:ILE:HD11	1.97	0.45
1:B:12:VAL:HG13	1:B:16:PHE:CD2	2.53	0.44
1:B:361:TYR:CE2	1:B:414:LYS:HE3	2.52	0.44
1:B:503:ASP:HA	1:B:593:ARG:HD3	2.01	0.43
1:B:95:VAL:HG12	1:B:111:GLN:HG3	2.01	0.42
1:A:59:GLU:OE1	1:A:79:GLY:HA3	2.20	0.42
1:B:65:PRO:HB3	1:B:74:VAL:CG1	2.50	0.42
1:B:12:VAL:HG13	1:B:16:PHE:HD2	1.85	0.42
1:A:94:LYS:HG2	1:A:97:LEU:CD2	2.50	0.42
1:A:384:VAL:HG23	1:A:385:HIS:CD2	2.55	0.42
1:A:416:THR:HG23	1:B:441:LYS:HE2	2.02	0.41
6:A:1079:HOH:O	1:B:338:LYS:HE2	2.20	0.41
1:A:412:TYR:CE1	1:A:441:LYS:HD2	2.55	0.41
1:A:402:ILE:O	1:A:406:PHE:HB3	2.21	0.41
1:B:112:TRP:CE2	1:B:302:MET:HG2	2.56	0.41
1:A:161:THR:HG21	1:A:200:ALA:HA	2.02	0.41
1:B:236:HIS:HE1	6:B:1007:HOH:O	2.03	0.41
1:A:427:PHE:CZ	1:B:442:ILE:HB	2.55	0.41
1:B:553:ALA:O	1:B:557:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HA	1:A:53:ILE:HB	2.03	0.40
1:B:235:PHE:CE1	1:B:247:ARG:HD3	2.56	0.40
1:B:371:TYR:O	1:B:374:THR:OG1	2.26	0.40
1:B:49:ALA:HA	1:B:53:ILE:HB	2.03	0.40

All (2) 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)
6:A:811:HOH:O	6:A:985:HOH:O[4_555]	1.99	0.21
6:B:1010:HOH:O	6:B:1111:HOH:O[2_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	604/611 (99%)	590 (98%)	14 (2%)	0	100	100
1	B	605/611 (99%)	593 (98%)	12 (2%)	0	100	100
All	All	1209/1222 (99%)	1183 (98%)	26 (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	475/477 (100%)	469 (99%)	6 (1%)	69	64
1	B	476/477 (100%)	471 (99%)	5 (1%)	73	70
All	All	951/954 (100%)	940 (99%)	11 (1%)	71	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	294	PHE
1	A	430	ASP
1	A	441	LYS
1	A	446	TYR
1	A	585	MET
1	B	156	ARG
1	B	294	PHE
1	B	369	TYR
1	B	430	ASP
1	B	446	TYR

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	236	HIS

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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PLM	B	703	5	15,16,17	0.78	0	14,15,17	0.84	0
5	COA	A	704	4	43,50,50	3.35	12 (27%)	56,75,75	1.98	12 (21%)
3	FAD	B	702	-	54,58,58	0.73	0	71,89,89	0.73	2 (2%)
5	COA	B	704	4	43,50,50	3.45	13 (30%)	56,75,75	1.82	12 (21%)
2	GOL	A	701	-	5,5,5	1.09	0	5,5,5	2.10	2 (40%)
4	PLM	A	703	5	15,16,17	0.77	0	14,15,17	0.76	0
2	GOL	B	701	-	5,5,5	0.73	0	5,5,5	1.19	0
3	FAD	A	702	-	54,58,58	1.31	9 (16%)	71,89,89	0.74	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLM	B	703	5	-	9/14/14/15	-
5	COA	A	704	4	-	4/44/64/64	0/3/3/3
3	FAD	B	702	-	-	2/30/50/50	0/6/6/6
5	COA	B	704	4	-	2/44/64/64	0/3/3/3
2	GOL	A	701	-	-	4/4/4/4	-
4	PLM	A	703	5	-	8/14/14/15	-
2	GOL	B	701	-	-	2/4/4/4	-
3	FAD	A	702	-	-	1/30/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	COA	O4B-C1B	17.23	1.63	1.40
5	A	704	COA	O4B-C1B	16.80	1.62	1.40
5	B	704	COA	O4B-C4B	-6.35	1.30	1.45
5	A	704	COA	O4B-C4B	-6.21	1.31	1.45
5	B	704	COA	C5P-N4P	5.50	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	COA	C9P-N8P	5.09	1.45	1.33
5	A	704	COA	C5P-N4P	4.97	1.45	1.33
5	B	704	COA	C9P-N8P	4.89	1.45	1.33
5	B	704	COA	P1A-O3A	4.23	1.64	1.59
5	A	704	COA	P2A-O3A	4.03	1.63	1.59
5	B	704	COA	P3B-O3B	3.87	1.66	1.59
5	B	704	COA	O2B-C2B	3.81	1.52	1.43
3	A	702	FAD	P-O3P	-3.74	1.55	1.59
5	A	704	COA	O5P-C5P	-3.65	1.16	1.23
5	B	704	COA	P2A-O3A	3.55	1.63	1.59
5	A	704	COA	P1A-O3A	3.25	1.63	1.59
5	A	704	COA	O2B-C2B	3.21	1.50	1.43
5	A	704	COA	P3B-O3B	3.11	1.65	1.59
5	B	704	COA	C6A-N6A	3.09	1.45	1.34
5	A	704	COA	C6A-N6A	3.05	1.45	1.34
3	A	702	FAD	C2-N1	-2.61	1.30	1.36
3	A	702	FAD	C2-N3	-2.55	1.33	1.39
5	A	704	COA	O3B-C3B	-2.49	1.35	1.44
5	B	704	COA	O9P-C9P	-2.41	1.18	1.23
5	B	704	COA	C2A-N3A	2.38	1.35	1.32
5	A	704	COA	OAP-CAP	-2.17	1.38	1.42
3	A	702	FAD	P-O2P	-2.15	1.45	1.55
5	B	704	COA	O5P-C5P	-2.13	1.19	1.23
3	A	702	FAD	O3'-C3'	-2.11	1.37	1.43
3	A	702	FAD	C9-C8	-2.11	1.36	1.39
3	A	702	FAD	C8A-N7A	-2.11	1.30	1.34
5	B	704	COA	P2A-O6A	2.07	1.67	1.59
3	A	702	FAD	PA-O2A	-2.00	1.46	1.55
3	A	702	FAD	C1B-N9A	-2.00	1.45	1.49

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704	COA	N3A-C2A-N1A	-6.74	119.53	128.67
5	B	704	COA	N3A-C2A-N1A	-6.29	120.14	128.67
5	A	704	COA	C5A-C6A-N6A	6.17	129.72	120.31
5	B	704	COA	C5A-C6A-N6A	5.20	128.24	120.31
5	B	704	COA	C3B-C2B-C1B	4.58	109.96	99.89
5	A	704	COA	O4B-C1B-N9A	-4.47	102.82	108.75
5	A	704	COA	C3B-C2B-C1B	4.03	108.75	99.89
5	A	704	COA	N6A-C6A-N1A	-4.00	109.78	118.33
2	A	701	GOL	O2-C2-C3	3.69	124.48	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	704	COA	N6A-C6A-N1A	-3.56	110.73	118.33
5	B	704	COA	C6P-C7P-N8P	-3.36	104.85	112.00
3	A	702	FAD	C5A-C6A-N6A	3.01	124.89	120.31
5	A	704	COA	C7P-N8P-C9P	-2.84	117.44	122.55
2	A	701	GOL	C3-C2-C1	-2.84	101.39	111.80
5	B	704	COA	O4B-C1B-N9A	-2.73	105.13	108.75
5	A	704	COA	C3P-N4P-C5P	-2.68	117.83	122.82
5	B	704	COA	C3P-N4P-C5P	-2.55	118.08	122.82
3	B	702	FAD	C5A-C6A-N6A	2.53	124.16	120.31
5	A	704	COA	P3B-O3B-C3B	-2.46	116.85	123.43
5	A	704	COA	O5P-C5P-N4P	-2.37	118.38	123.03
5	B	704	COA	CDP-CBP-CCP	2.32	112.05	108.22
5	A	704	COA	C2P-C3P-N4P	-2.25	107.20	112.31
3	B	702	FAD	O4'-C4'-C5'	-2.24	105.04	109.99
5	B	704	COA	P3B-O3B-C3B	-2.22	117.51	123.43
5	A	704	COA	C6P-C7P-N8P	-2.21	107.30	112.00
5	B	704	COA	C2P-C3P-N4P	-2.20	107.31	112.31
5	B	704	COA	O5P-C5P-N4P	-2.16	118.79	123.03
5	A	704	COA	O5A-P2A-O3A	2.15	113.07	107.27
5	B	704	COA	C2B-C3B-C4B	-2.01	99.72	103.24

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-C3
2	B	701	GOL	C1-C2-C3-O3
3	B	702	FAD	C2'-C1'-N10-C10
4	A	703	PLM	O2-C1-C2-C3
4	A	703	PLM	C1-C2-C3-C4
4	B	703	PLM	C1-C2-C3-C4
4	A	703	PLM	C3-C4-C5-C6
2	A	701	GOL	C1-C2-C3-O3
2	A	701	GOL	O1-C1-C2-O2
2	B	701	GOL	O2-C2-C3-O3
4	B	703	PLM	C9-CA-CB-CC
4	A	703	PLM	CB-CC-CD-CE
4	A	703	PLM	C6-C7-C8-C9
4	B	703	PLM	C6-C7-C8-C9
4	B	703	PLM	C7-C8-C9-CA
4	B	703	PLM	CC-CD-CE-CF
2	A	701	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	702	FAD	O2'-C2'-C3'-C4'
3	B	702	FAD	C1'-C2'-C3'-O3'
4	B	703	PLM	CA-CB-CC-CD
4	B	703	PLM	C2-C3-C4-C5
4	B	703	PLM	C5-C6-C7-C8
5	B	704	COA	S1P-C2P-C3P-N4P
4	B	703	PLM	CD-CE-CF-CG
4	A	703	PLM	C8-C9-CA-CB
4	A	703	PLM	CC-CD-CE-CF
5	A	704	COA	P2A-O3A-P1A-O1A
5	A	704	COA	O9P-C9P-CAP-OAP
4	A	703	PLM	CA-CB-CC-CD
5	A	704	COA	N8P-C9P-CAP-OAP
5	B	704	COA	N8P-C9P-CAP-OAP
5	A	704	COA	P2A-O3A-P1A-O2A

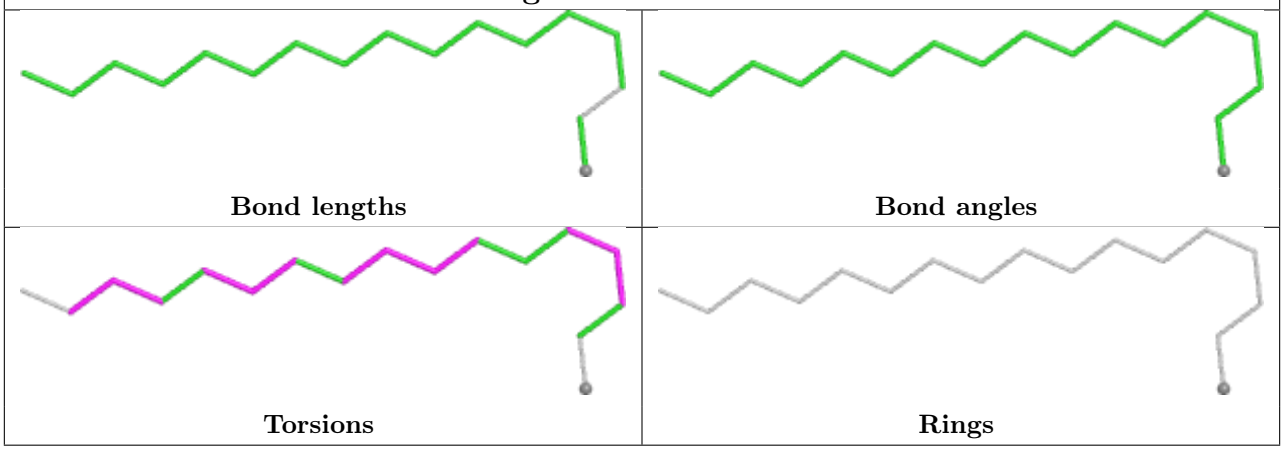
There are no ring outliers.

5 monomers are involved in 11 short contacts:

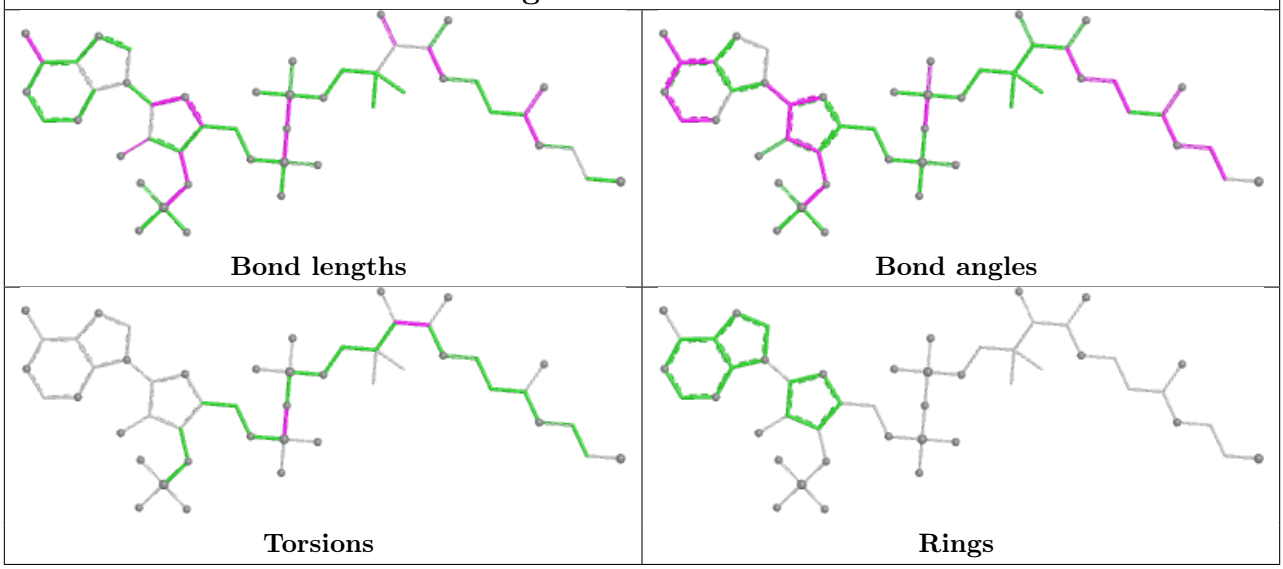
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	PLM	1	0
5	A	704	COA	1	0
3	B	702	FAD	6	0
5	B	704	COA	2	0
3	A	702	FAD	3	0

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

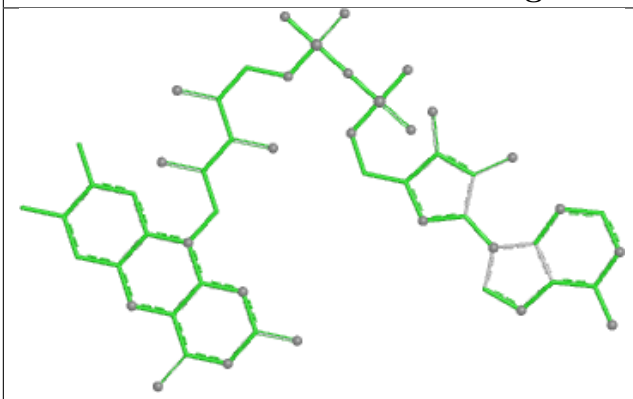
Ligand PLM B 703



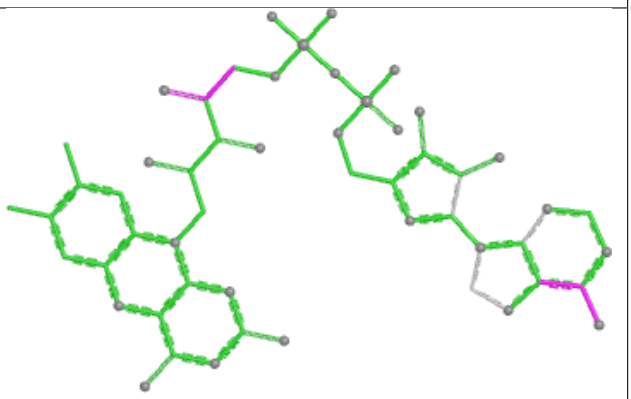
Ligand COA A 704



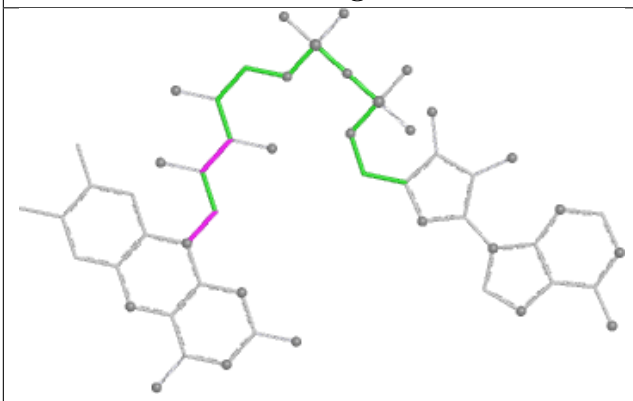
Ligand FAD B 702



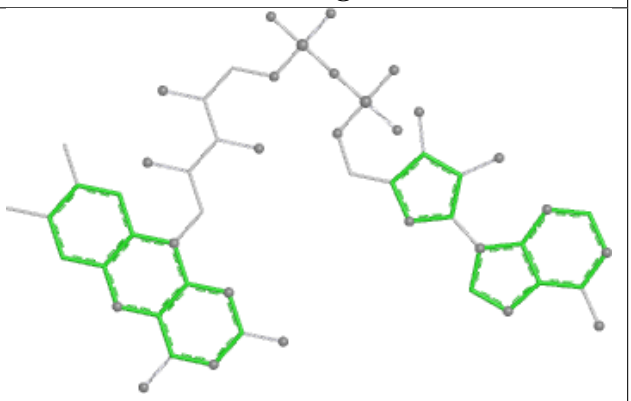
Bond lengths



Bond angles

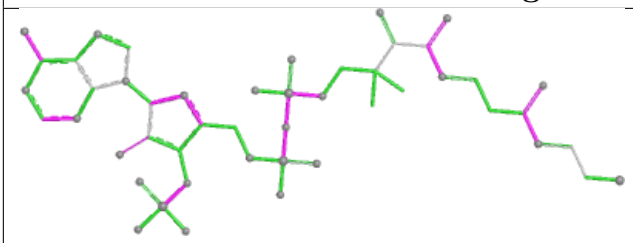


Torsions

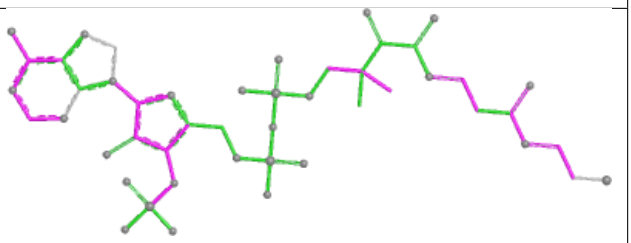


Rings

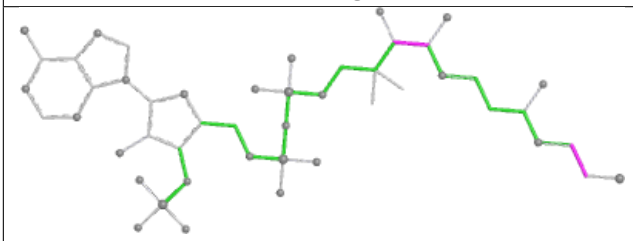
Ligand COA B 704



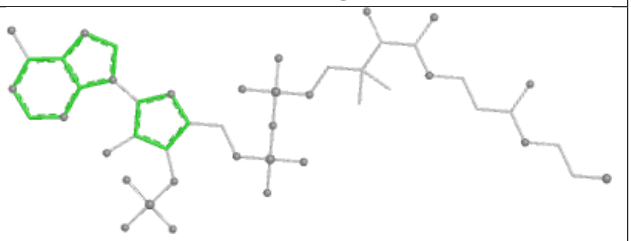
Bond lengths



Bond angles

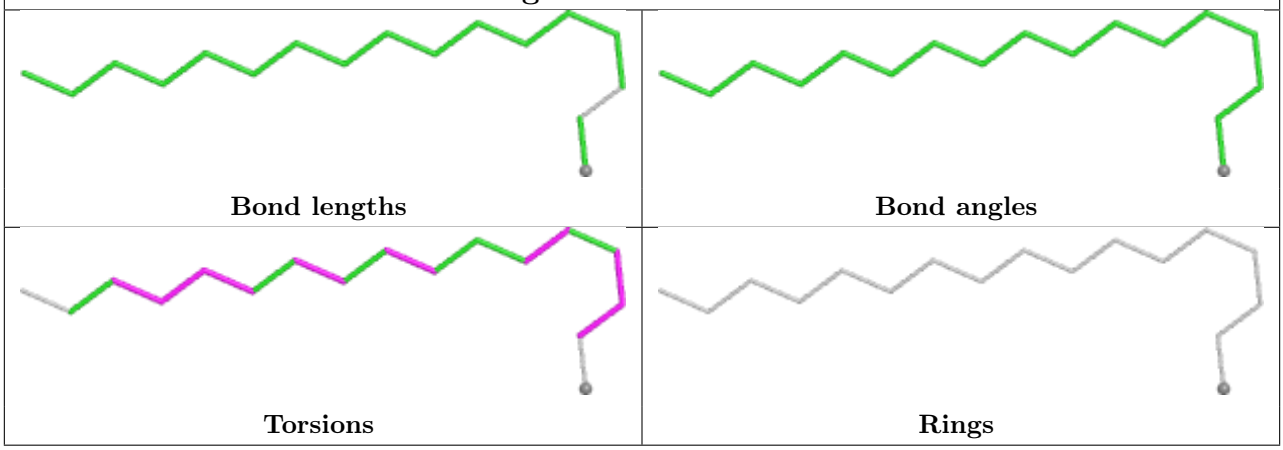


Torsions

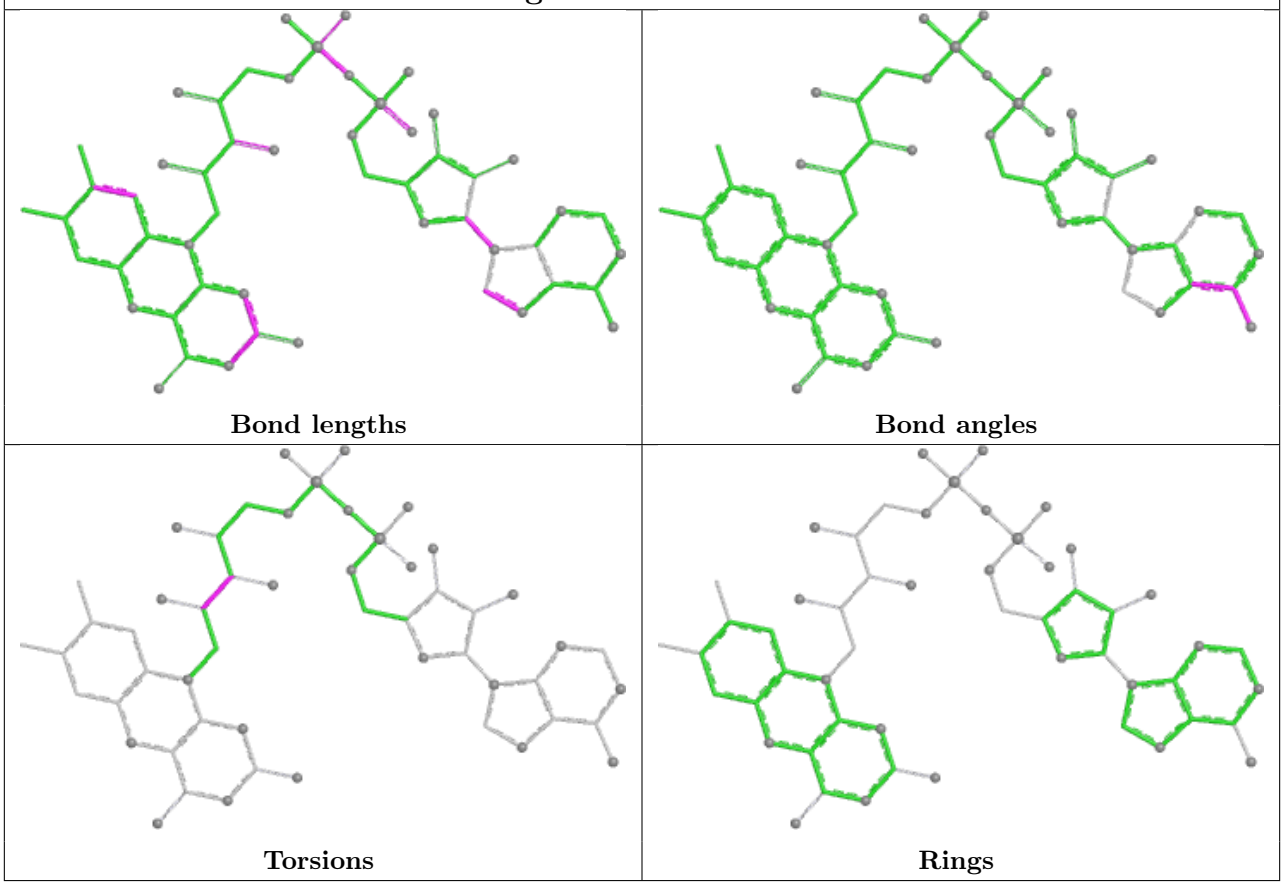


Rings

Ligand PLM A 703



Ligand FAD A 702



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	608/611 (99%)	0.44	41 (6%)	17	19	16, 25, 45, 77	0
1	B	609/611 (99%)	0.51	50 (8%)	11	13	18, 26, 44, 78	0
All	All	1217/1222 (99%)	0.47	91 (7%)	14	16	16, 26, 45, 78	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	ALA	8.4
1	B	28	ASP	5.6
1	B	31	SER	5.3
1	A	1	MET	4.9
1	A	484	GLU	4.8
1	B	1	MET	4.4
1	B	33	LEU	4.2
1	A	304	VAL	3.8
1	B	410	THR	3.8
1	B	25	LEU	3.7
1	A	412	TYR	3.7
1	A	413	ALA	3.7
1	B	487	ASN	3.7
1	B	412	TYR	3.6
1	B	339	THR	3.6
1	B	23	LYS	3.6
1	A	339	THR	3.6
1	B	32	ASP	3.5
1	A	482	LYS	3.5
1	B	411	ALA	3.4
1	B	406	PHE	3.3
1	B	26	GLY	3.3
1	A	446	TYR	3.3
1	B	336	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	338	LYS	3.2
1	B	413	ALA	3.2
1	A	483	ASN	3.2
1	B	95	VAL	3.2
1	A	361	TYR	3.1
1	A	308	ALA	3.1
1	A	32	ASP	3.1
1	B	16	PHE	3.0
1	A	416	THR	2.8
1	B	519	GLN	2.8
1	B	340	ALA	2.8
1	A	411	ALA	2.8
1	B	29	LYS	2.8
1	B	484	GLU	2.8
1	B	492	THR	2.7
1	B	105	PRO	2.7
1	A	519	GLN	2.7
1	B	408	SER	2.7
1	A	341	PRO	2.7
1	B	361	TYR	2.7
1	A	28	ASP	2.6
1	B	482	LYS	2.6
1	B	416	THR	2.6
1	A	35	ALA	2.5
1	B	338	LYS	2.5
1	A	66	VAL	2.5
1	B	34	ASP	2.5
1	B	365	LEU	2.5
1	B	536	LEU	2.4
1	B	382	GLN	2.4
1	B	520	GLU	2.4
1	B	30	PHE	2.4
1	A	408	SER	2.4
1	B	39	ARG	2.4
1	A	357	THR	2.4
1	A	222	PRO	2.4
1	A	403	VAL	2.4
1	A	415	LEU	2.3
1	A	27	ALA	2.3
1	A	410	THR	2.3
1	A	407	GLY	2.3
1	B	446	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	29	LYS	2.3
1	B	444	SER	2.3
1	A	336	THR	2.3
1	B	308	ALA	2.2
1	B	488	GLY	2.2
1	B	445	LEU	2.2
1	A	383	ALA	2.2
1	A	405	GLY	2.2
1	B	304	VAL	2.2
1	A	445	LEU	2.1
1	A	406	PHE	2.1
1	A	440	SER	2.1
1	B	403	VAL	2.1
1	B	309	ILE	2.1
1	B	483	ASN	2.1
1	B	538	ALA	2.1
1	B	47	ARG	2.1
1	A	23	LYS	2.1
1	A	33	LEU	2.1
1	A	362	ALA	2.1
1	A	177	ARG	2.0
1	B	35	ALA	2.0
1	B	38	ALA	2.0
1	A	240	GLU	2.0
1	A	335	MET	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)

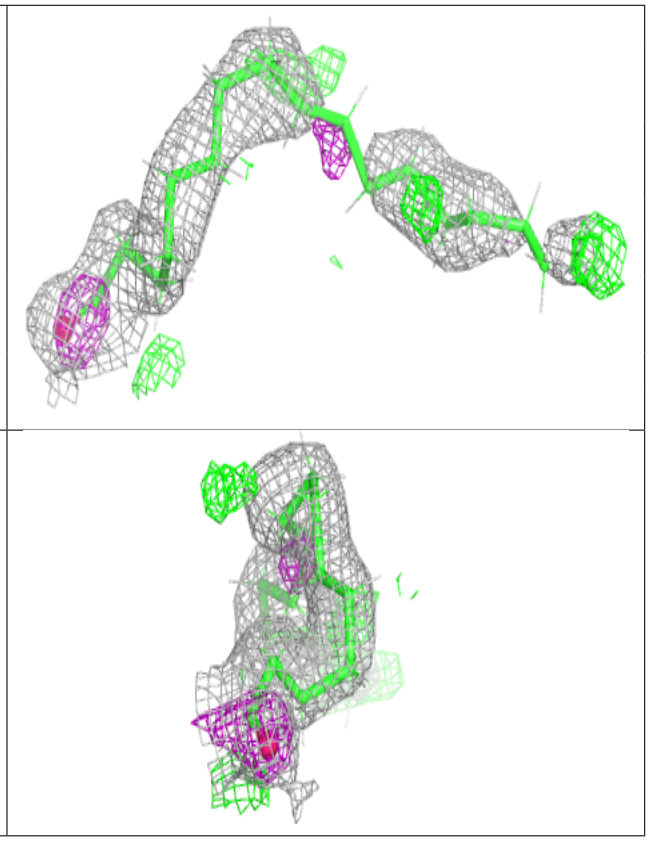
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PLM	B	703	17/18	0.85	0.24	24,52,69,70	0
4	PLM	A	703	17/18	0.86	0.25	25,53,79,86	0
2	GOL	A	701	6/6	0.94	0.17	24,30,41,41	0
5	COA	A	704	48/48	0.94	0.12	23,31,37,38	0
3	FAD	A	702	53/53	0.95	0.14	17,25,35,39	0
2	GOL	B	701	6/6	0.95	0.09	23,33,41,43	0
5	COA	B	704	48/48	0.95	0.12	24,31,36,41	0
3	FAD	B	702	53/53	0.96	0.13	18,23,35,38	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.

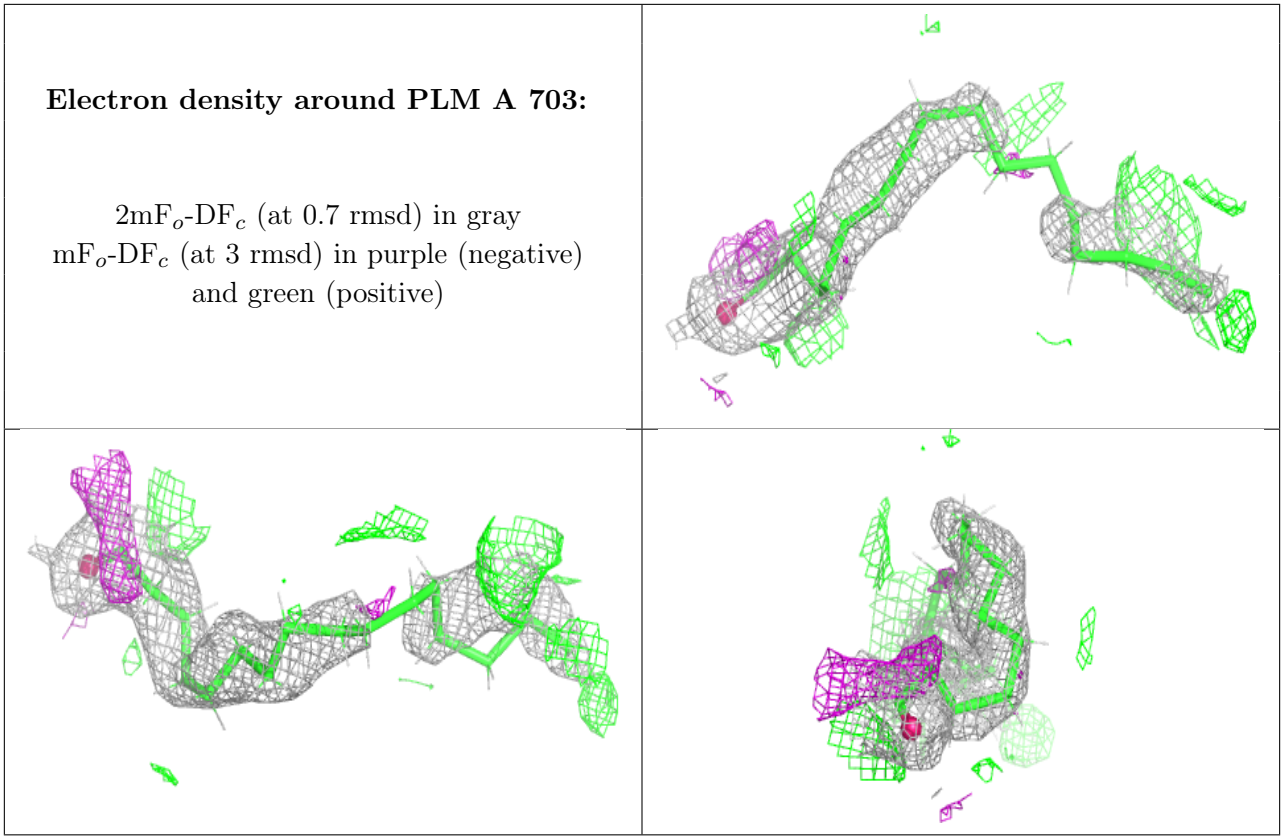
Electron density around PLM B 703:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



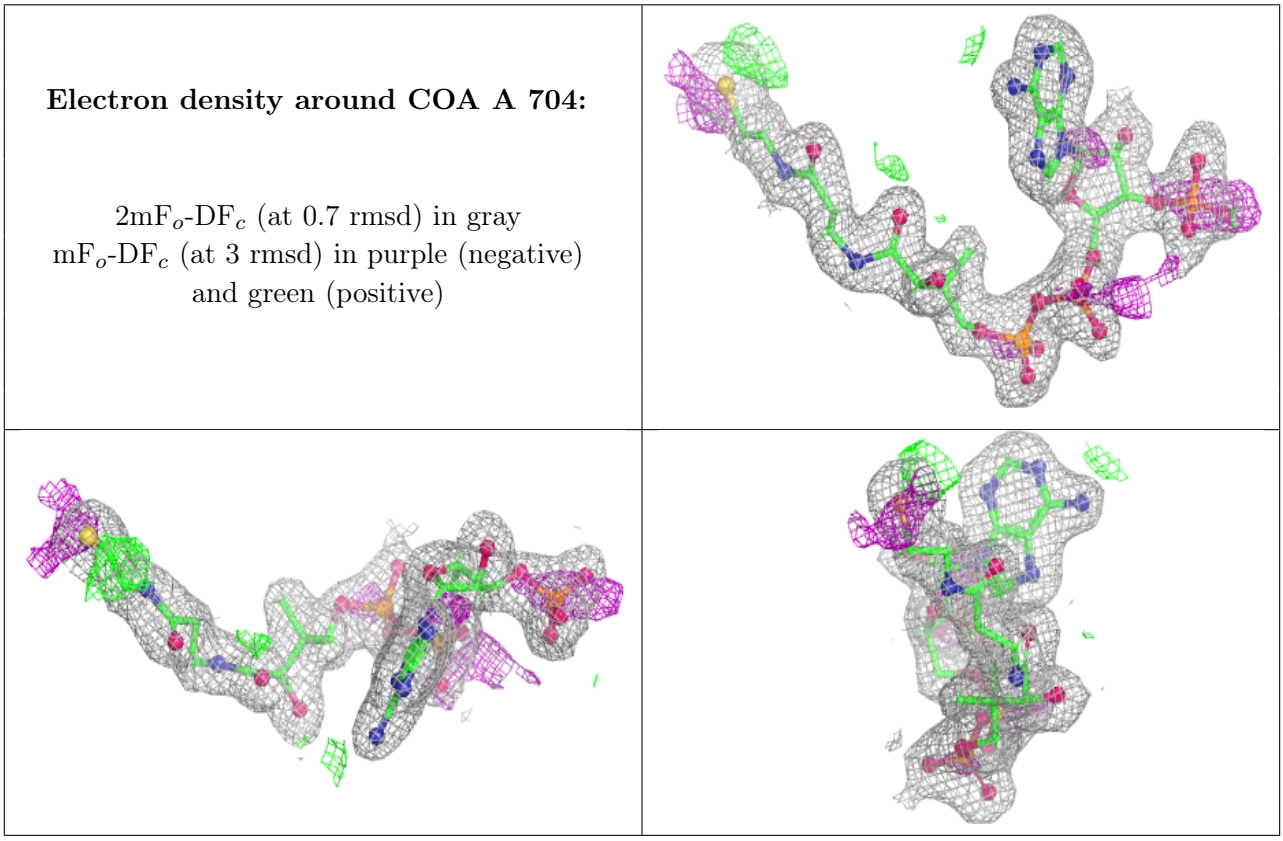
Electron density around PLM A 703:

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



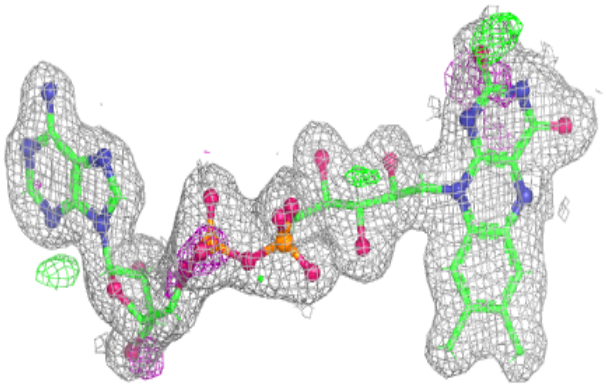
Electron density around COA A 704:

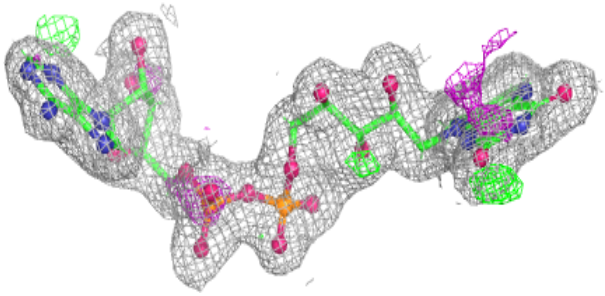
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

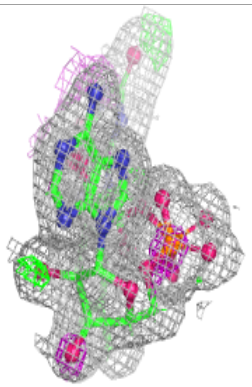


Electron density around FAD A 702:

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

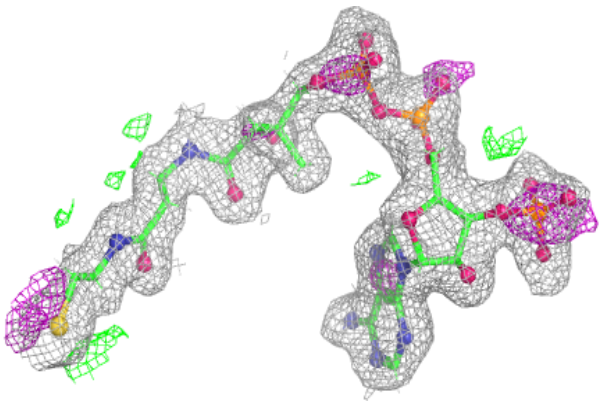


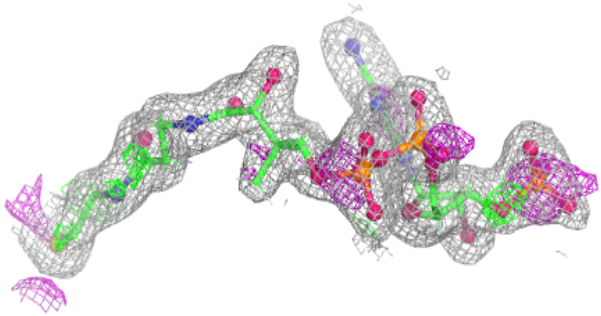


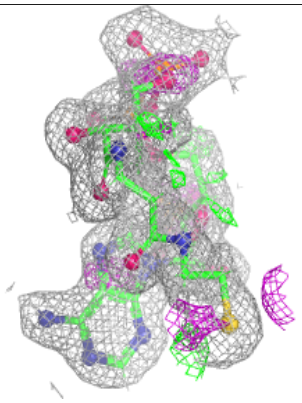


Electron density around COA B 704:

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

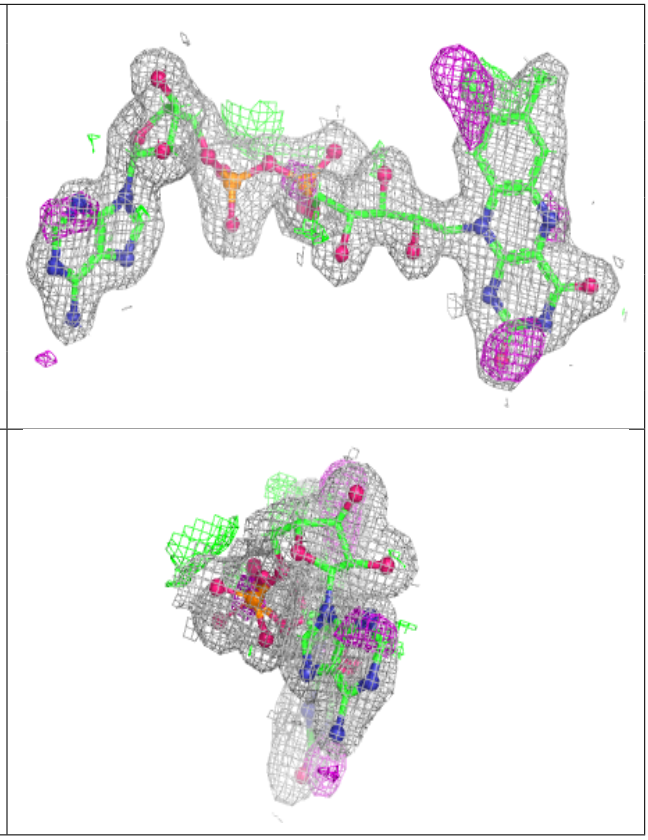






Electron density around FAD B 702:

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



6.5 Other polymers (i)

There are no such residues in this entry.