W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 11:23 am BST

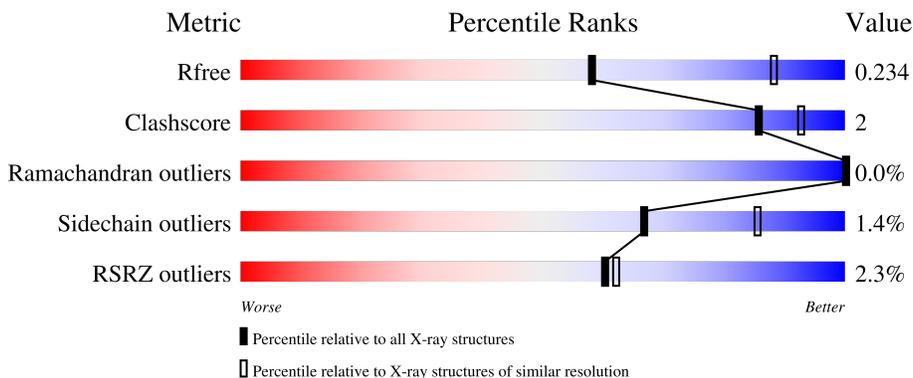|		
PDB ID	:	8RPI
Title	:	JanthE from Janthinobacterium sp. HH01, lactyl-ThDP
Authors	:	Lanza, L.; Leogrande, C.; Rabe von Pappenheim, F.; Tittmann, K.; Mueller, M.
Deposited on	:	2024-01-16
Resolution	:	2.71 Å(reported)

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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 2.71 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		2
Ramachandran outliers		0.0%
Sidechain outliers		1.4%
RSRZ outliers		2.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	619	% 93% 5% ·
1	B	619	2% 92% 6% ··
1	C	619	3% 93% 5% ·
1	D	619	2% 92% 7% ·
1	E	619	% 93% 5% ·

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Mol	Chain	Length	Quality of chain
1	F	619	
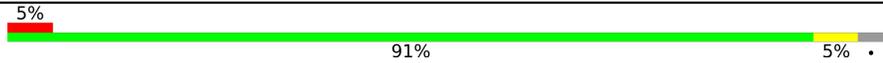
5%

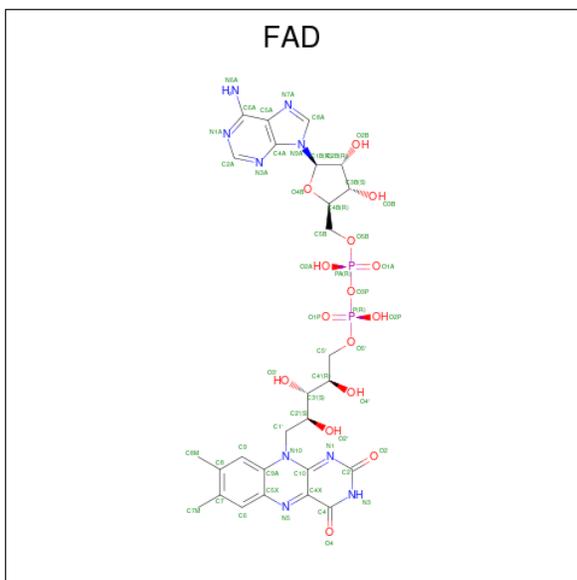91%

5%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 56761 atoms, of which 27989 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 Thiamine pyrophosphate-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	B	608	Total	C	H	N	O	S	0	6	0
			9349	2974	4653	822	869	31			
1	C	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	D	608	Total	C	H	N	O	S	0	6	0
			9351	2974	4655	822	869	31			
1	E	605	Total	C	H	N	O	S	0	6	0
			9321	2965	4643	818	863	32			
1	F	598	Total	C	H	N	O	S	0	4	0
			9177	2924	4563	805	854	31			

- 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 84	C 27	H 31	N 9	O 15	P 2	0	0
2	B	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0
2	C	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0
2	D	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0
2	E	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0
2	F	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

- Molecule 4 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-CARBOXY-1-HYDROXYETHYL)-5-(2-{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDL) (formula: $C_{15}H_{23}N_4O_{10}P_2S$) (labeled as "Ligand of Interest" by depositor).
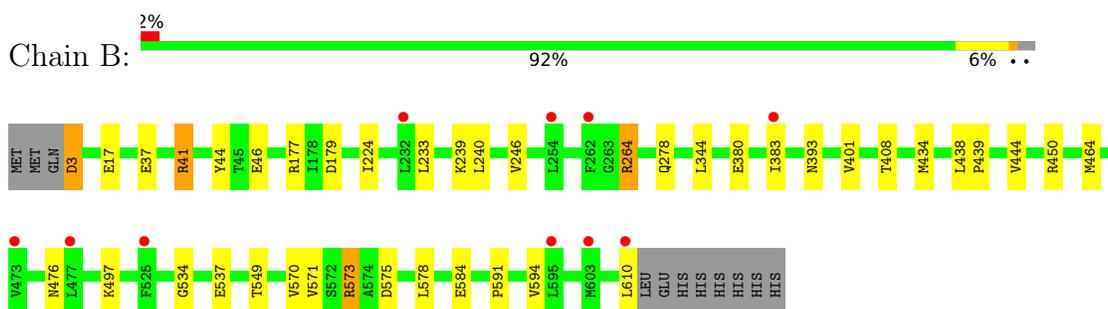
TDL

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			32	15	4	10	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			32	15	4	10	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			32	15	4	10	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			32	15	4	10	2	1		
4	E	1	Total	C	N	O	P	S	0	0
			32	15	4	10	2	1		
4	F	1	Total	C	N	O	P	S	0	0
			32	15	4	10	2	1		

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).

2PE

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	B	1	59	18	31	10	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total 48	O 48	0	0
6	B	36	Total 36	O 36	0	0
6	C	32	Total 32	O 32	0	0
6	D	43	Total 43	O 43	0	0
6	E	37	Total 37	O 37	0	0
6	F	14	Total 14	O 14	0	0

3   Residue-property plots ⓘ

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: Thiamine pyrophosphate-binding protein
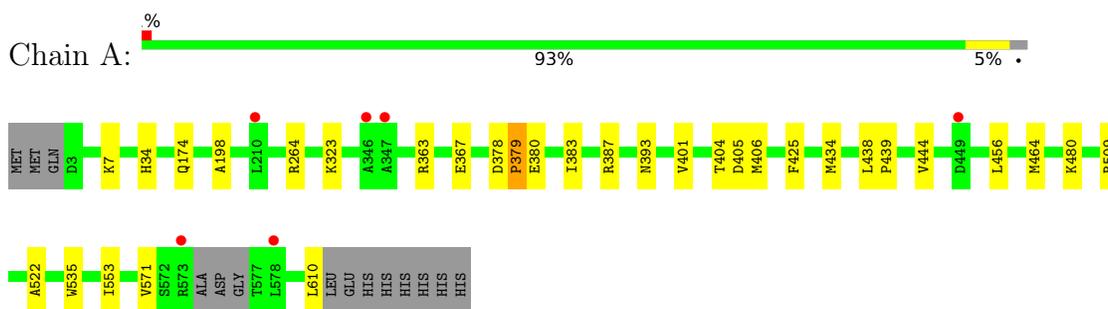
Chain A:

• Molecule 1: Thiamine pyrophosphate-binding protein

Chain B:

• Molecule 1: Thiamine pyrophosphate-binding protein

Chain C:

• Molecule 1: Thiamine pyrophosphate-binding protein

Chain D:

• Molecule 1: Thiamine pyrophosphate-binding protein

Chain E:

• Molecule 1: Thiamine pyrophosphate-binding protein

Chain F:
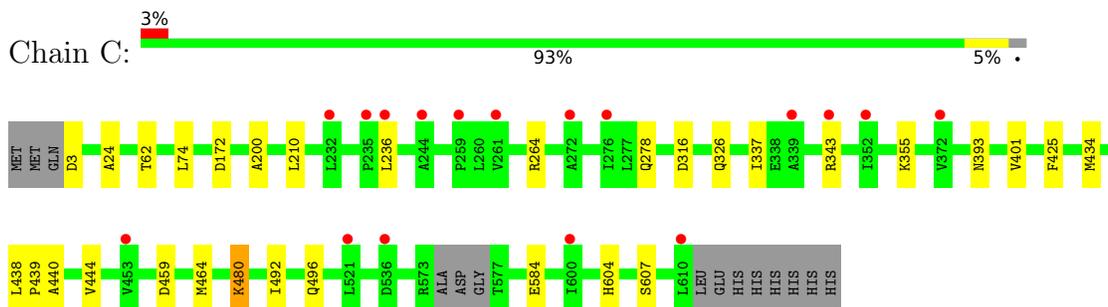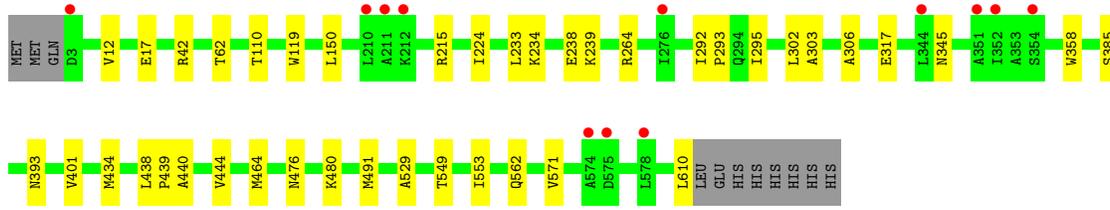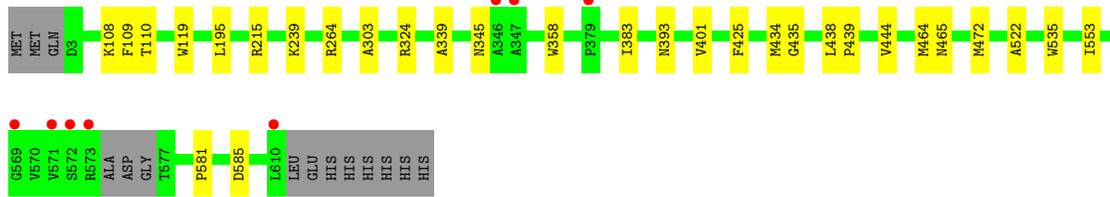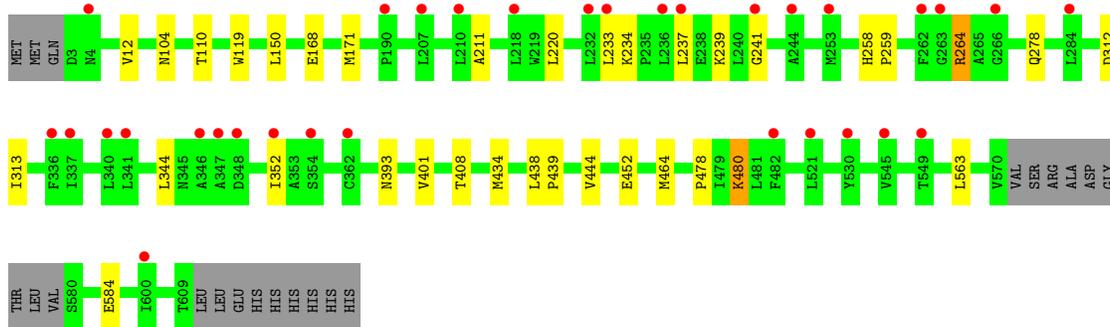
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.15Å 118.54Å 202.05Å 90.00° 96.72° 90.00°	Depositor
Resolution (Å)	85.69 – 2.71 85.69 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.5 (85.69-2.71) 95.5 (85.69-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.234 0.195 , 0.234	Depositor DCC
R_{free} test set	5315 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 27.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	56761	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: TDL, MG, FAD, 2PE

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	0.32	0/4779	0.51	0/6483
1	B	0.36	0/4814	0.53	1/6531 (0.0%)
1	C	0.28	0/4779	0.50	0/6483
1	D	0.27	0/4814	0.50	0/6531
1	E	0.28	0/4797	0.50	0/6507
1	F	0.28	0/4727	0.50	0/6412
All	All	0.30	0/28710	0.51	1/38947 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	179	ASP	CB-CG-OD1	5.19	122.97	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	4667	4629	4629	15	0
1	B	4696	4653	4649	21	0
1	C	4667	4629	4629	16	0
1	D	4696	4655	4649	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4678	4643	4633	15	0
1	F	4614	4563	4561	21	0
2	A	53	31	31	0	0
2	B	53	31	31	1	0
2	C	53	31	31	0	0
2	D	53	31	31	0	0
2	E	53	31	31	0	0
2	F	53	31	31	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	32	0	19	3	0
4	B	32	0	19	4	0
4	C	32	0	19	4	0
4	D	32	0	19	4	0
4	E	32	0	19	4	0
4	F	32	0	19	4	0
5	B	28	31	38	2	0
6	A	48	0	0	1	0
6	B	36	0	0	3	0
6	C	32	0	0	0	0
6	D	43	0	0	1	0
6	E	37	0	0	0	0
6	F	14	0	0	1	0
All	All	28772	27989	28088	122	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.

The worst 5 of 122 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:37:GLU:OE2	1:B:41:ARG:NH1	2.07	0.87
1:B:537:GLU:N	1:B:537:GLU:OE1	2.18	0.77
1:A:174:GLN:OE1	6:A:802:HOH:O	2.10	0.69
1:C:434:MET:SD	4:C:703:TDL:HM43	2.34	0.68
1:D:434:MET:SD	4:D:703:TDL:HM43	2.34	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	605/619 (98%)	592 (98%)	12 (2%)	1 (0%)	47	72
1	B	612/619 (99%)	595 (97%)	17 (3%)	0	100	100
1	C	605/619 (98%)	587 (97%)	18 (3%)	0	100	100
1	D	612/619 (99%)	593 (97%)	19 (3%)	0	100	100
1	E	607/619 (98%)	587 (97%)	20 (3%)	0	100	100
1	F	598/619 (97%)	575 (96%)	23 (4%)	0	100	100
All	All	3639/3714 (98%)	3529 (97%)	109 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	PRO

5.3.2 Protein sidechains ⓘ

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	492/500 (98%)	485 (99%)	7 (1%)	67	85
1	B	494/500 (99%)	483 (98%)	11 (2%)	52	78
1	C	492/500 (98%)	486 (99%)	6 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	494/500 (99%)	487 (99%)	7 (1%)	67	85
1	E	494/500 (99%)	490 (99%)	4 (1%)	81	92
1	F	485/500 (97%)	480 (99%)	5 (1%)	76	90
All	All	2951/3000 (98%)	2911 (99%)	40 (1%)	67	85

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	480	LYS
1	F	264	ARG
1	D	491	MET
1	E	393	ASN
1	F	464	MET

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

Mol	Chain	Res	Type
1	A	34	HIS
1	C	326	GLN
1	C	475	HIS

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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	TDL	A	703	3	26,33,33	0.77	0	30,51,51	0.86	1 (3%)
2	FAD	F	701	-	53,58,58	0.48	0	68,89,89	0.51	1 (1%)
5	2PE	B	703	-	27,27,27	0.15	0	26,26,26	1.03	1 (3%)
2	FAD	E	701	-	53,58,58	0.50	0	68,89,89	0.57	2 (2%)
4	TDL	B	704	3	26,33,33	0.77	0	30,51,51	0.92	1 (3%)
2	FAD	C	701	-	53,58,58	0.50	0	68,89,89	0.53	1 (1%)
4	TDL	C	703	3	26,33,33	0.78	0	30,51,51	0.87	1 (3%)
2	FAD	D	701	-	53,58,58	0.48	0	68,89,89	0.48	1 (1%)
4	TDL	F	703	3	26,33,33	0.79	0	30,51,51	0.88	1 (3%)
4	TDL	E	703	3	26,33,33	0.79	0	30,51,51	0.90	1 (3%)
2	FAD	A	701	-	53,58,58	0.54	0	68,89,89	0.49	1 (1%)
2	FAD	B	701	-	53,58,58	0.50	0	68,89,89	0.49	1 (1%)
4	TDL	D	703	3	26,33,33	0.76	0	30,51,51	0.84	1 (3%)

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	TDL	A	703	3	-	2/22/29/29	0/2/2/2
2	FAD	F	701	-	-	9/30/50/50	0/6/6/6
5	2PE	B	703	-	-	7/25/25/25	-
2	FAD	E	701	-	-	7/30/50/50	0/6/6/6
4	TDL	B	704	3	-	3/22/29/29	0/2/2/2
2	FAD	C	701	-	-	7/30/50/50	0/6/6/6
4	TDL	C	703	3	-	4/22/29/29	0/2/2/2
2	FAD	D	701	-	-	9/30/50/50	0/6/6/6
4	TDL	F	703	3	-	5/22/29/29	0/2/2/2
4	TDL	E	703	3	-	6/22/29/29	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	701	-	-	8/30/50/50	0/6/6/6
2	FAD	B	701	-	-	7/30/50/50	0/6/6/6
4	TDL	D	703	3	-	4/22/29/29	0/2/2/2

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	704	TDL	C5-C4-N3	2.76	113.42	107.66
4	F	703	TDL	C5-C4-N3	2.73	113.38	107.66
4	A	703	TDL	C5-C4-N3	2.69	113.29	107.66
4	C	703	TDL	C5-C4-N3	2.67	113.24	107.66
4	D	703	TDL	C5-C4-N3	2.67	113.24	107.66

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5B-O5B-PA-O1A
2	A	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	TDL	3	0
2	F	701	FAD	3	0
5	B	703	2PE	2	0
4	B	704	TDL	4	0
4	C	703	TDL	4	0
4	F	703	TDL	4	0
4	E	703	TDL	4	0
2	B	701	FAD	1	0
4	D	703	TDL	4	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 TDL A 703

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD F 701

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE B 703

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD E 701

Bond lengths

Bond angles

Torsions

Rings

Ligand TDL B 704

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 701

Bond lengths

Bond angles

Torsions

Rings

Ligand TDL C 703

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 701

Bond lengths

Bond angles

Torsions

Rings

Ligand TDL F 703

Bond lengths

Bond angles

Torsions

Rings

Ligand TDL E 703

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand TDL D 703

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, 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(Å²)	Q<0.9
1	A	605/619 (97%)	0.13	6 (0%)	82	83	40, 55, 75, 107	0
1	B	608/619 (98%)	0.18	10 (1%)	72	74	39, 56, 73, 99	0
1	C	605/619 (97%)	0.20	17 (2%)	53	54	44, 58, 81, 100	0
1	D	608/619 (98%)	0.21	12 (1%)	65	67	39, 53, 77, 117	0
1	E	605/619 (97%)	0.16	8 (1%)	77	78	42, 54, 74, 102	0
1	F	598/619 (96%)	0.44	32 (5%)	25	25	41, 71, 98, 126	0
All	All	3629/3714 (97%)	0.22	85 (2%)	60	62	39, 57, 86, 126	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	572	SER	5.0
1	A	347	ALA	5.0
1	F	233	LEU	4.7
1	E	347	ALA	4.2
1	F	348	ASP	4.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	2PE	B	703	28/28	0.79	0.27	75,100,122,123	0
3	MG	C	702	1/1	0.87	0.20	52,52,52,52	0
3	MG	F	702	1/1	0.89	0.20	60,60,60,60	0
3	MG	A	702	1/1	0.90	0.16	55,55,55,55	0
3	MG	E	702	1/1	0.93	0.15	58,58,58,58	0
2	FAD	F	701	53/53	0.95	0.17	65,74,87,92	0
4	TDL	B	704	32/32	0.96	0.17	45,50,56,60	0
2	FAD	B	701	53/53	0.97	0.16	46,52,63,65	0
2	FAD	C	701	53/53	0.97	0.20	50,56,68,71	0
4	TDL	A	703	32/32	0.97	0.17	46,54,58,60	0
3	MG	B	702	1/1	0.97	0.16	49,49,49,49	0
4	TDL	C	703	32/32	0.97	0.18	44,53,58,61	0
4	TDL	D	703	32/32	0.97	0.18	46,49,55,56	0
4	TDL	E	703	32/32	0.97	0.20	48,55,59,62	0
4	TDL	F	703	32/32	0.97	0.20	54,60,67,68	0
2	FAD	D	701	53/53	0.97	0.18	44,49,59,64	0
2	FAD	A	701	53/53	0.98	0.17	39,49,59,60	0
2	FAD	E	701	53/53	0.98	0.18	40,46,55,57	0
3	MG	D	702	1/1	0.98	0.18	49,49,49,49	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 2PE B 703:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
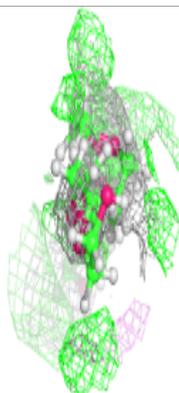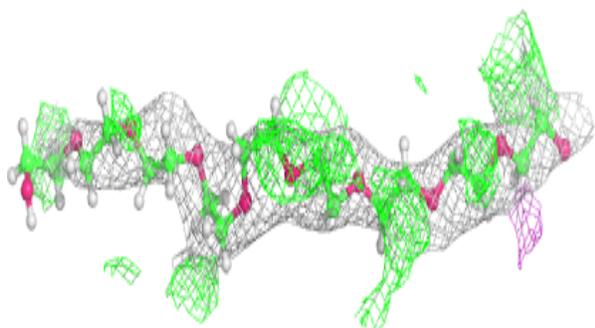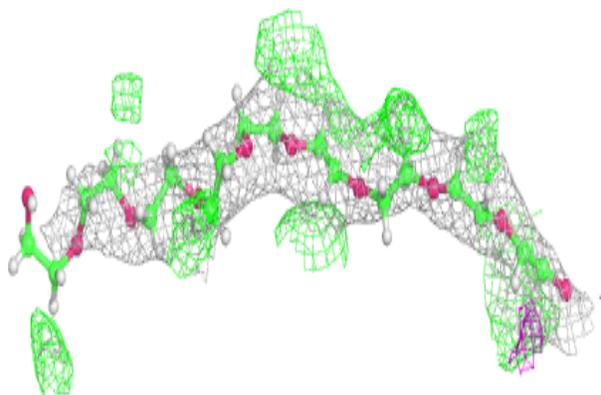
Electron density around FAD F 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
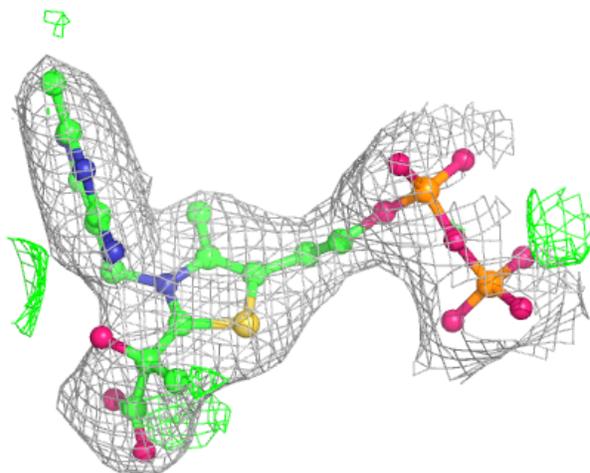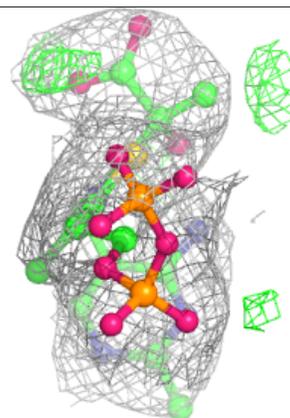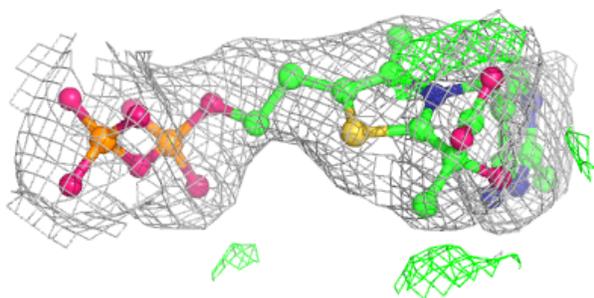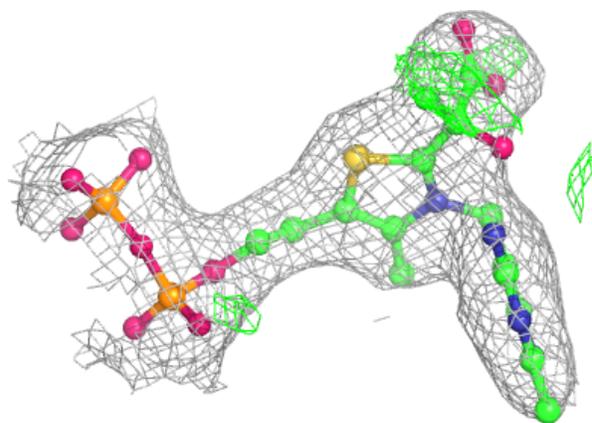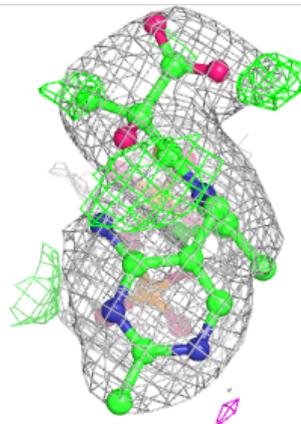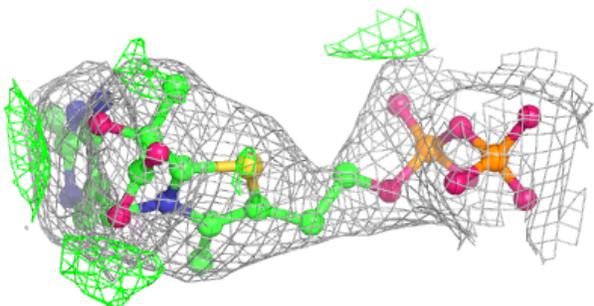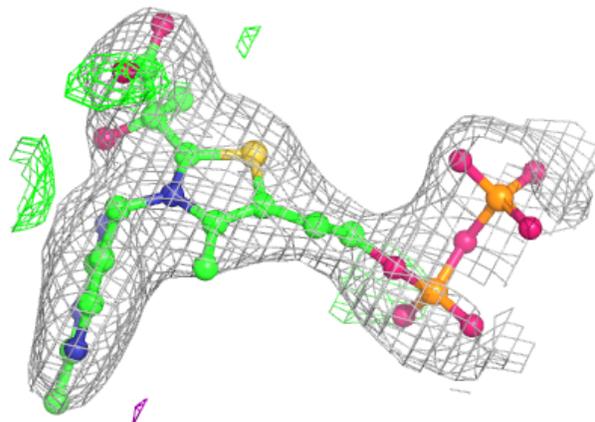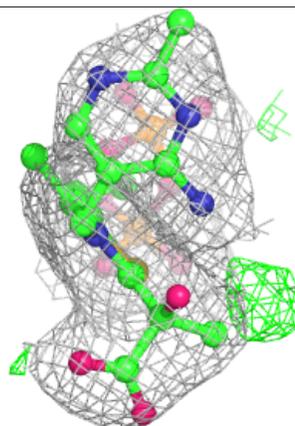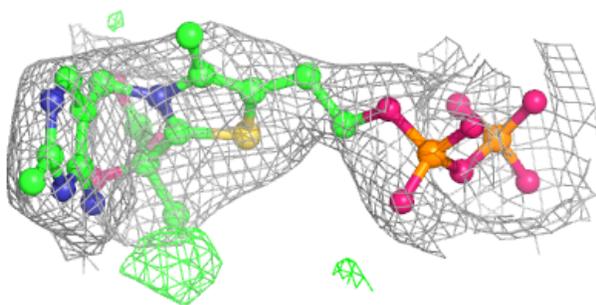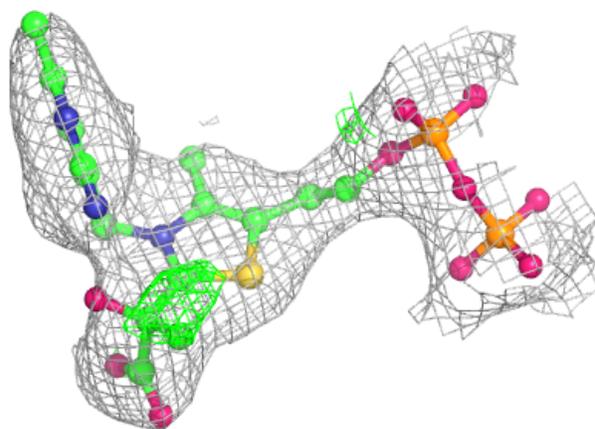and green (positive)
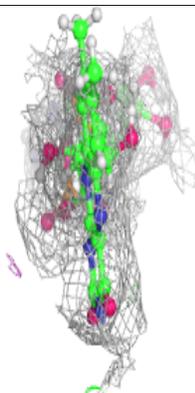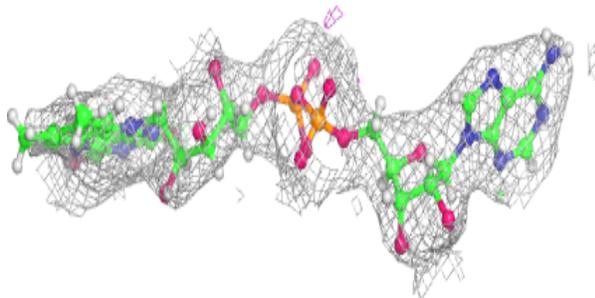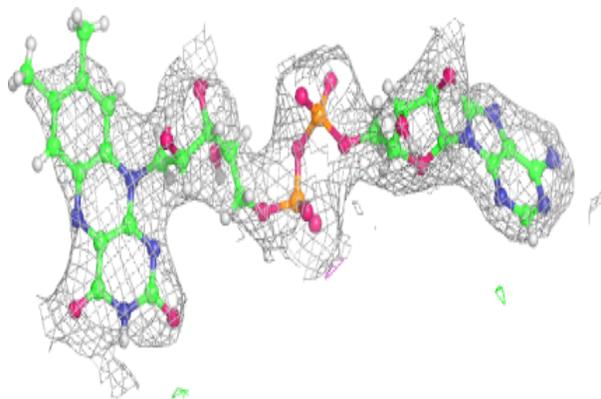
Electron density around TDL B 704:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
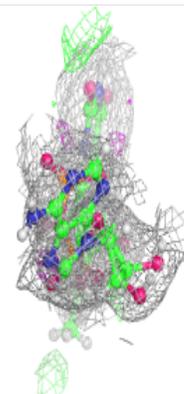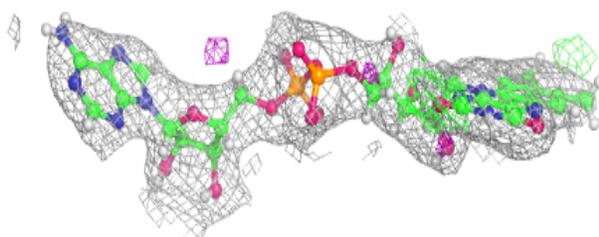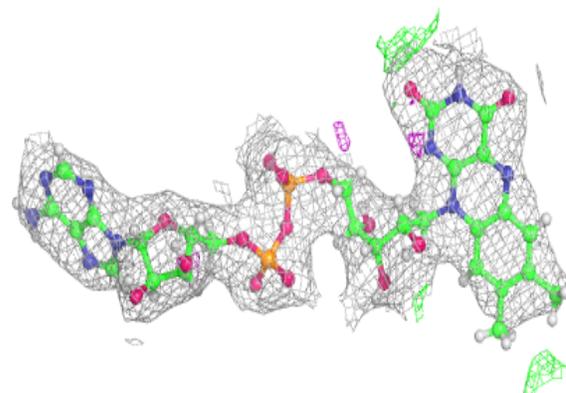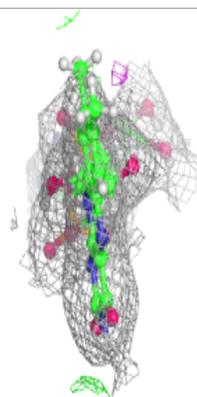and green (positive)
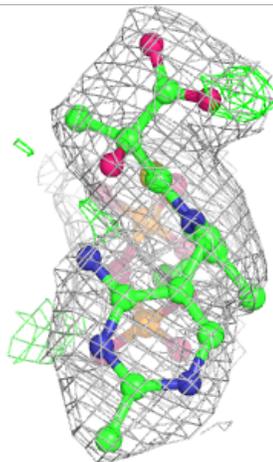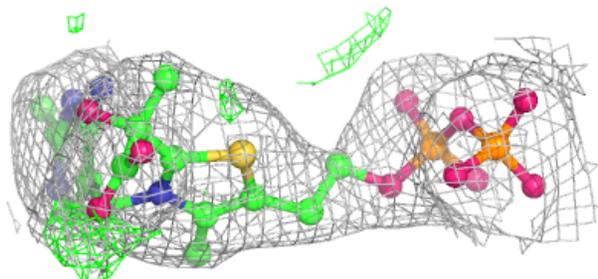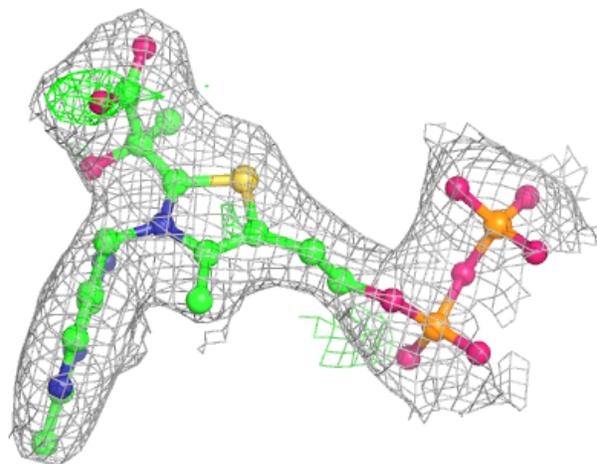
Electron density around FAD B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
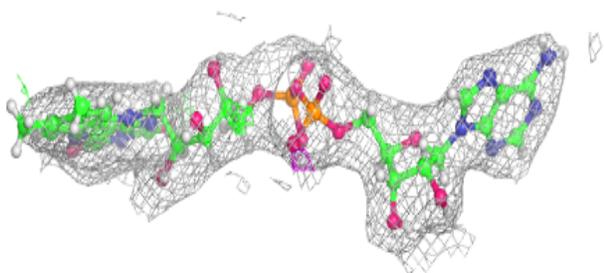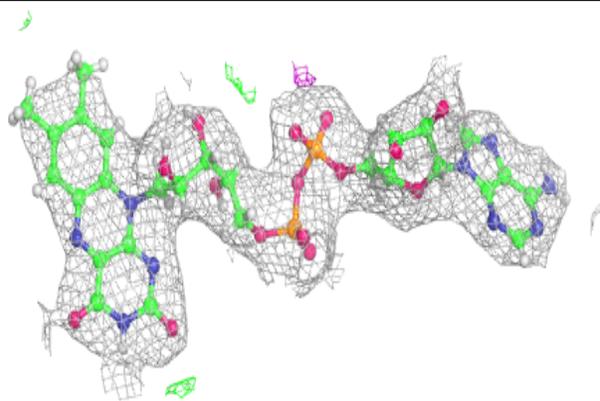and green (positive)
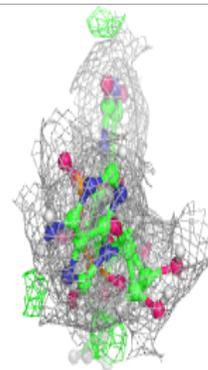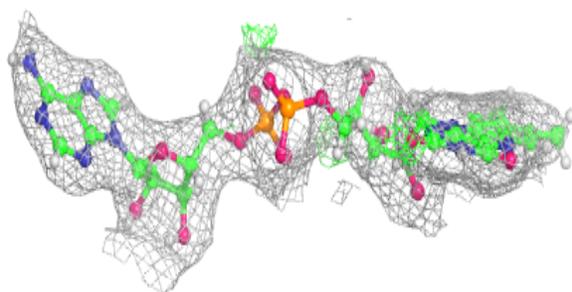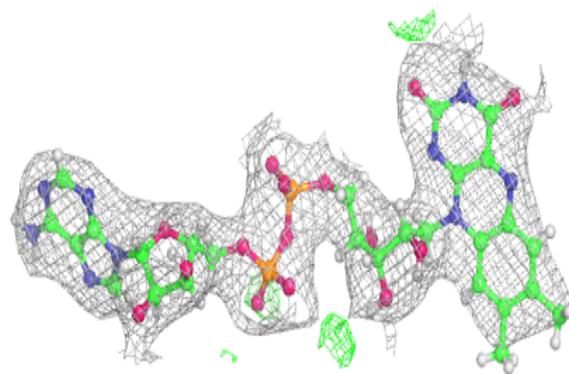
Electron density around FAD C 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
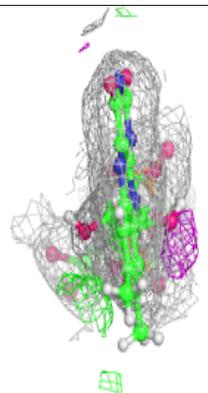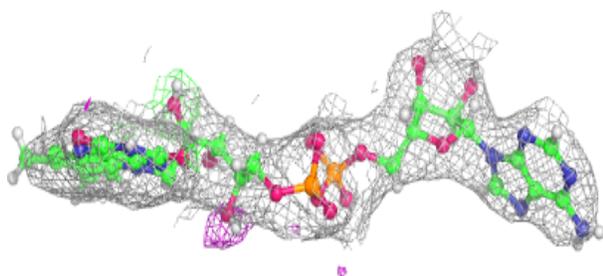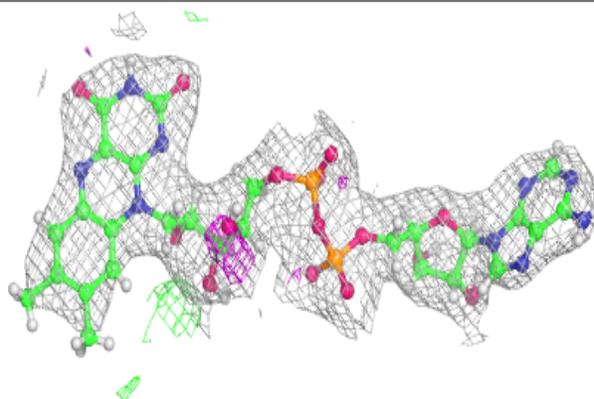
Electron density around TDL A 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
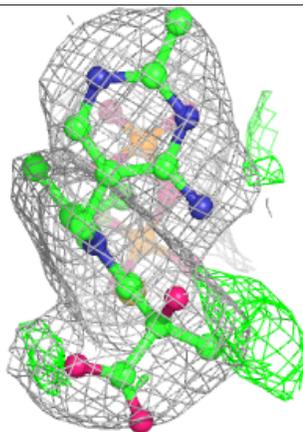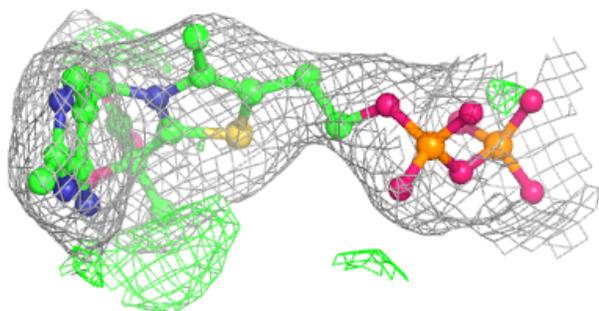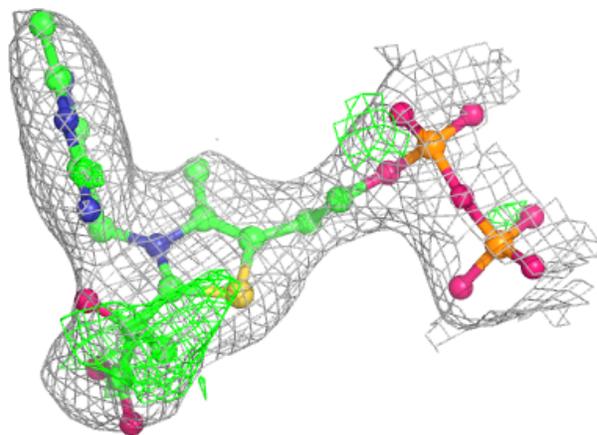
Electron density around TDL C 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
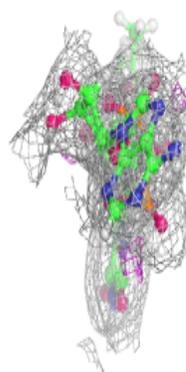and green (positive)
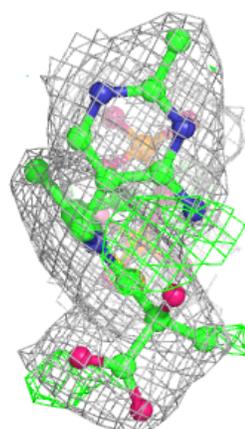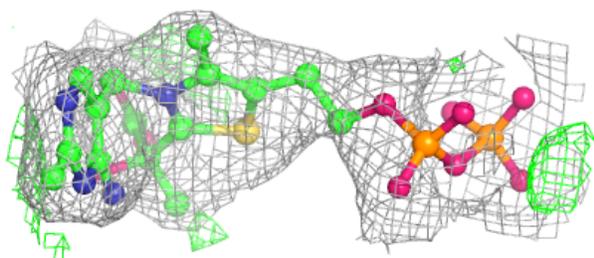
Electron density around TDL D 703:

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

Electron density around TDL E 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 TDL F 703:

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

Electron density around FAD D 701:

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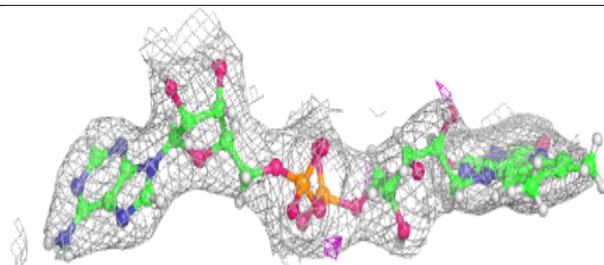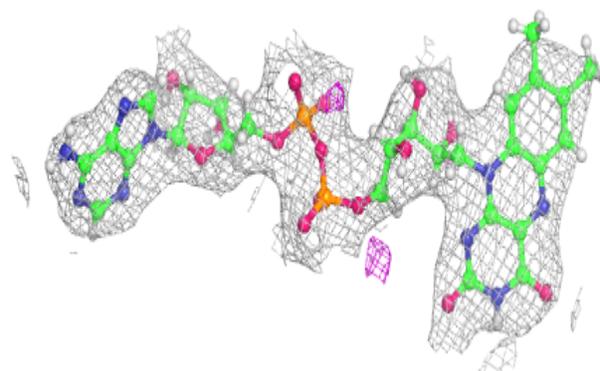$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

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 FAD E 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.