wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 09:11 pm BST

PDB ID	:	2W55 / pdb_00002w55
Title	:	Crystal Structure of Xanthine Dehydrogenase (E232Q variant) from Rhodobacter capsulatus in Complex with Hypoxanthine
Authors	:	Doebbler, J.A.; Truglio, J.J.; Leimkuhler, S.; Kisker, C.
Deposited on	:	2008-12-04
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

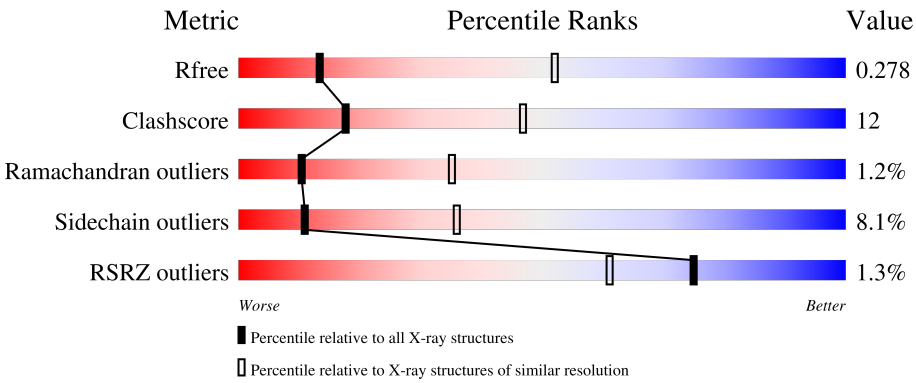
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	462	2% 68% 27%
1	C	462	% 70% 24%
1	E	462	2% 68% 26%
1	G	462	3% 65% 29%
2	B	777	% 69% 26%

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Mol	Chain	Length	Quality of chain
2	D	777	% 66% 28%
2	F	777	% 66% 29%
2	H	777	% 68% 27%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	XAX	B	1778	X	-	-	-
5	XAX	D	1778	X	-	-	-
5	XAX	F	1778	X	-	-	-
5	XAX	H	1778	X	-	-	-
7	HPA	H	1780	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 36807 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 XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3375	2115	608	627	25	0	0	0
1	C	450	3375	2115	608	627	25	0	0	0
1	E	450	3375	2115	608	627	25	0	0	0
1	G	450	3375	2115	608	627	25	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	TRP	LEU	conflict	UNP O54050
C	26	TRP	LEU	conflict	UNP O54050
E	26	TRP	LEU	conflict	UNP O54050
G	26	TRP	LEU	conflict	UNP O54050

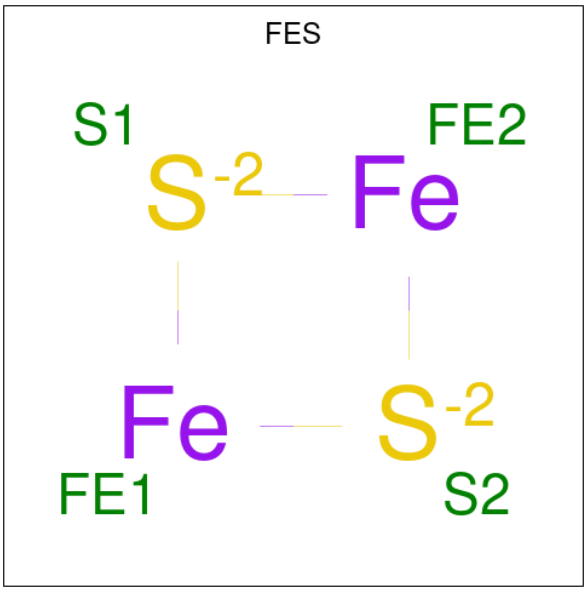
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	760	5716	3581	1057	1052	26	0	0	0
2	D	760	5716	3581	1057	1052	26	0	0	0
2	F	760	5716	3581	1057	1052	26	0	0	0
2	H	760	5716	3581	1057	1052	26	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

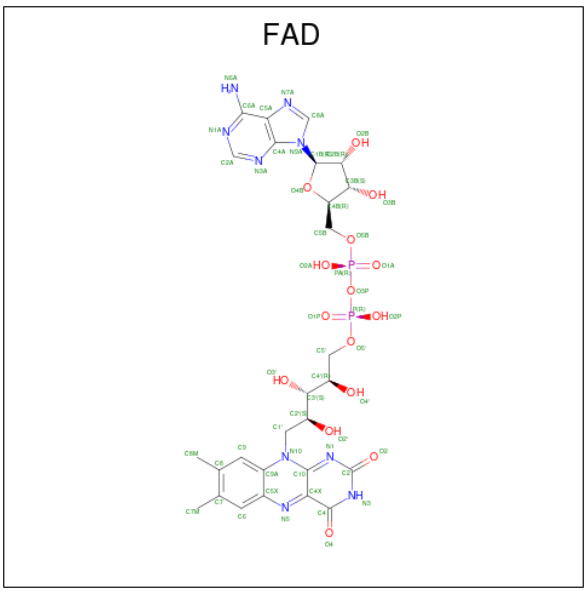
Chain	Residue	Modelled	Actual	Comment	Reference
B	232	GLN	GLU	engineered mutation	UNP O54051
B	772	ARG	GLY	conflict	UNP O54051
D	232	GLN	GLU	engineered mutation	UNP O54051
D	772	ARG	GLY	conflict	UNP O54051
F	232	GLN	GLU	engineered mutation	UNP O54051
F	772	ARG	GLY	conflict	UNP O54051
H	232	GLN	GLU	engineered mutation	UNP O54051
H	772	ARG	GLY	conflict	UNP O54051

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



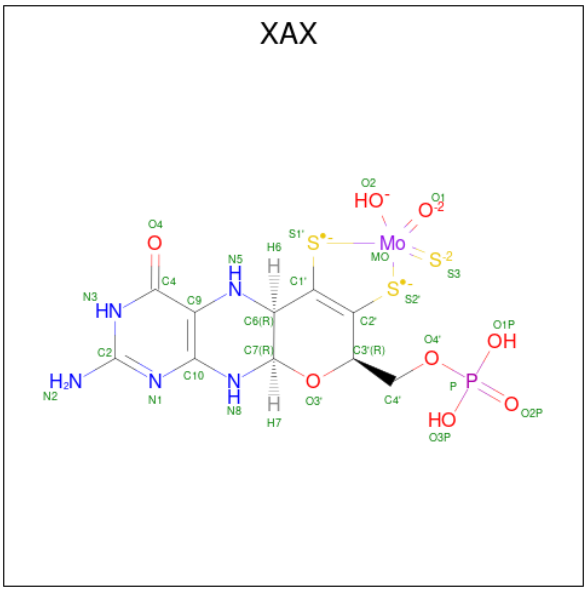
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0
			Total	Fe	S		
3	A	1	4	2	2	0	0
			Total	Fe	S		
3	C	1	4	2	2	0	0
			Total	Fe	S		
3	C	1	4	2	2	0	0
			Total	Fe	S		
3	E	1	4	2	2	0	0
			Total	Fe	S		
3	E	1	4	2	2	0	0
			Total	Fe	S		
3	G	1	4	2	2	0	0
			Total	Fe	S		
3	G	1	4	2	2	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is {[(5aR,8R,9aR)-2-amino-4-oxo-6,7-di(sulfanyl-kappaS)-3,5,5a,8,9a,10-hexahydro-4H-pyrano[3,2-g]pteridin-8-yl]methyl dihydrogenato(2-) phosphate}(hydroxy)oxo(thioxo) molybdenum (CCD ID: XAX) (formula: $C_{10}H_{13}MoN_5O_8PS_3$).

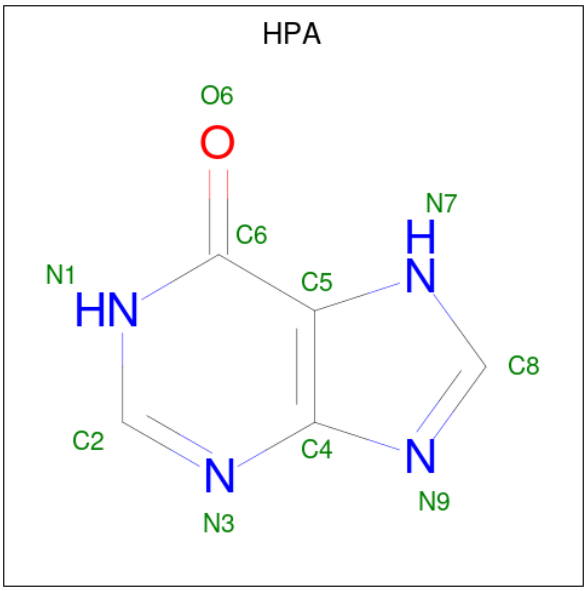


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Mo	N	O	P	S		
5	B	1	28	10	1	5	8	1	3	0	0
5	D	1	28	10	1	5	8	1	3	0	0
5	F	1	28	10	1	5	8	1	3	0	0
5	H	1	28	10	1	5	8	1	3	0	0

- Molecule 6 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ba		
6	B	1	1	1	0	0
6	D	1	1	1	0	0
6	F	1	1	1	0	0
6	H	1	1	1	0	0

- Molecule 7 is HYPOXANTHINE (CCD ID: HPA) (formula: $C_5H_4N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	10	5	4	1	0	0
7	D	1	10	5	4	1	0	0
7	F	1	10	5	4	1	0	0
7	H	1	10	5	4	1	0	0

- Molecule 8 is water.

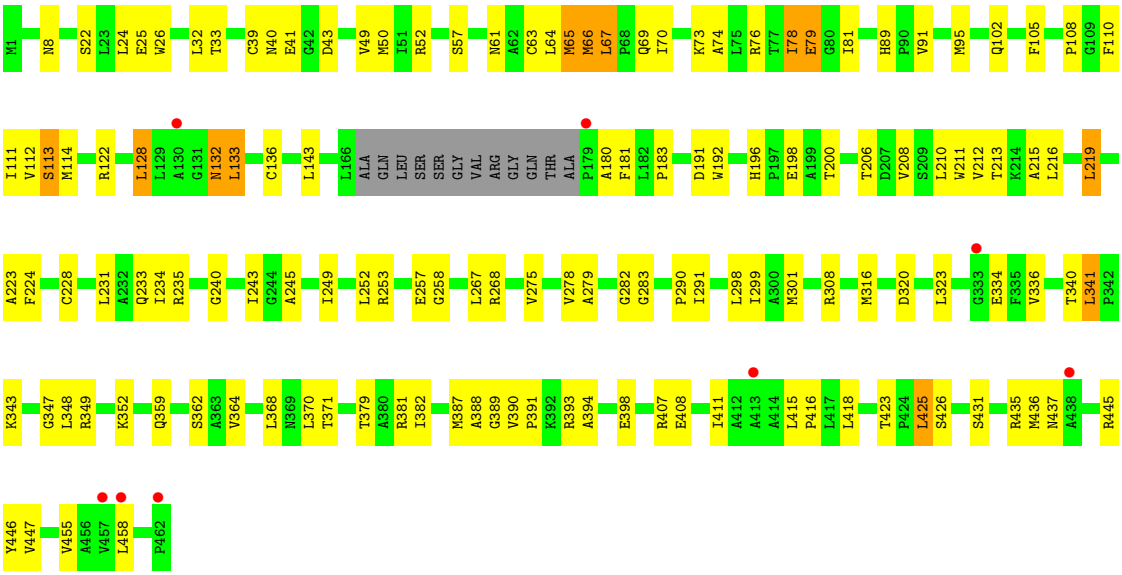
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	4	4	4	0	0
8	B	8	8	8	0	0
8	C	3	3	3	0	0
8	D	11	11	11	0	0
8	E	1	1	1	0	0
8	F	12	12	12	0	0
8	G	1	1	1	0	0
8	H	3	3	3	0	0

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.

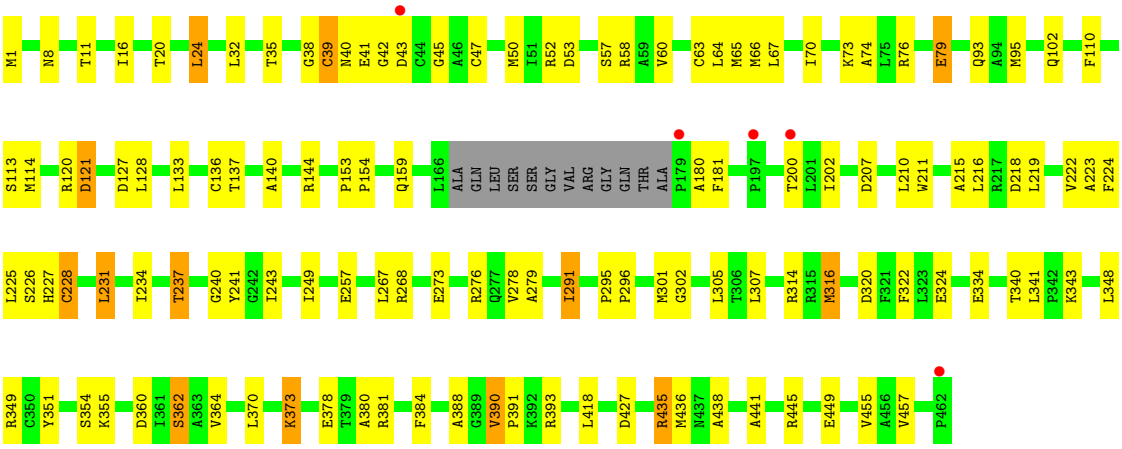
• Molecule 1: XANTHINE DEHYDROGENASE

Chain A: 2% 68% 27%



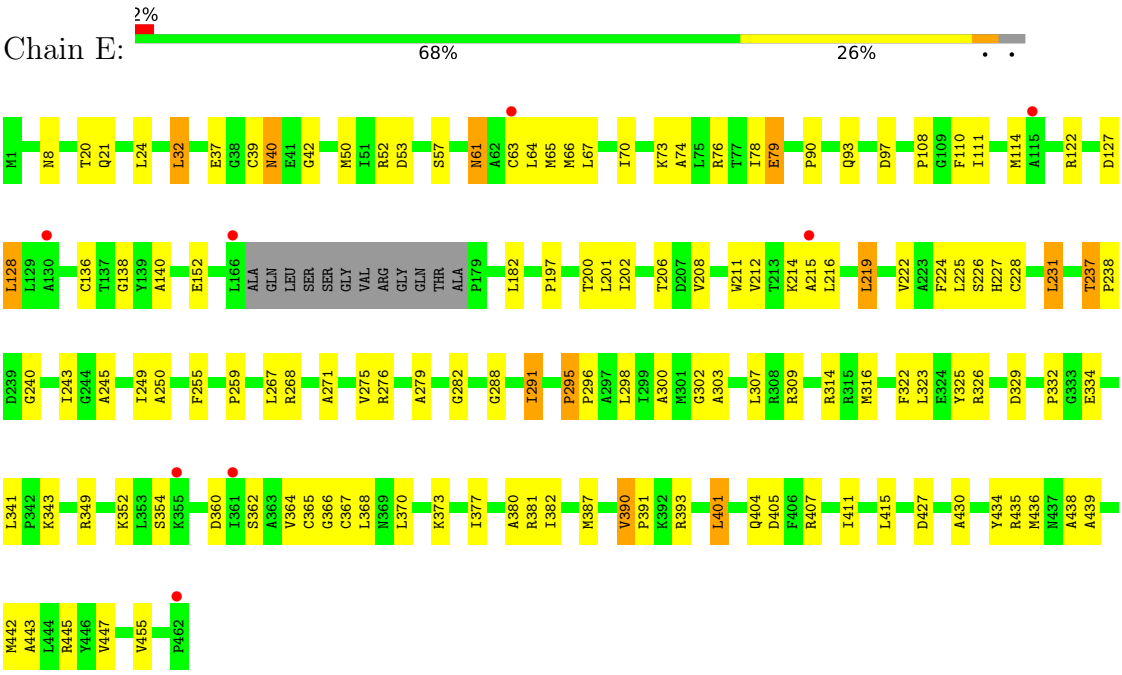
• Molecule 1: XANTHINE DEHYDROGENASE

Chain C: % 70% 24%



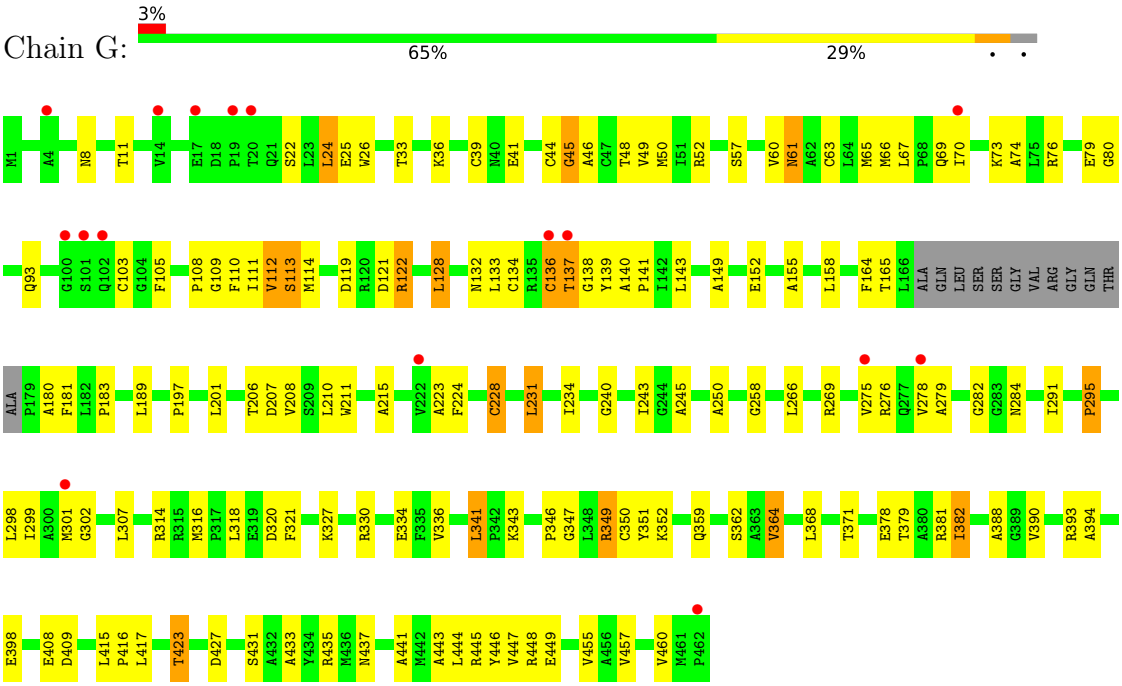
• Molecule 1: XANTHINE DEHYDROGENASE

Chain E:



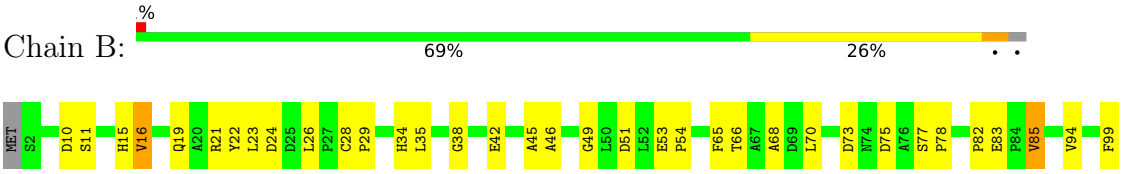
• Molecule 1: XANTHINE DEHYDROGENASE

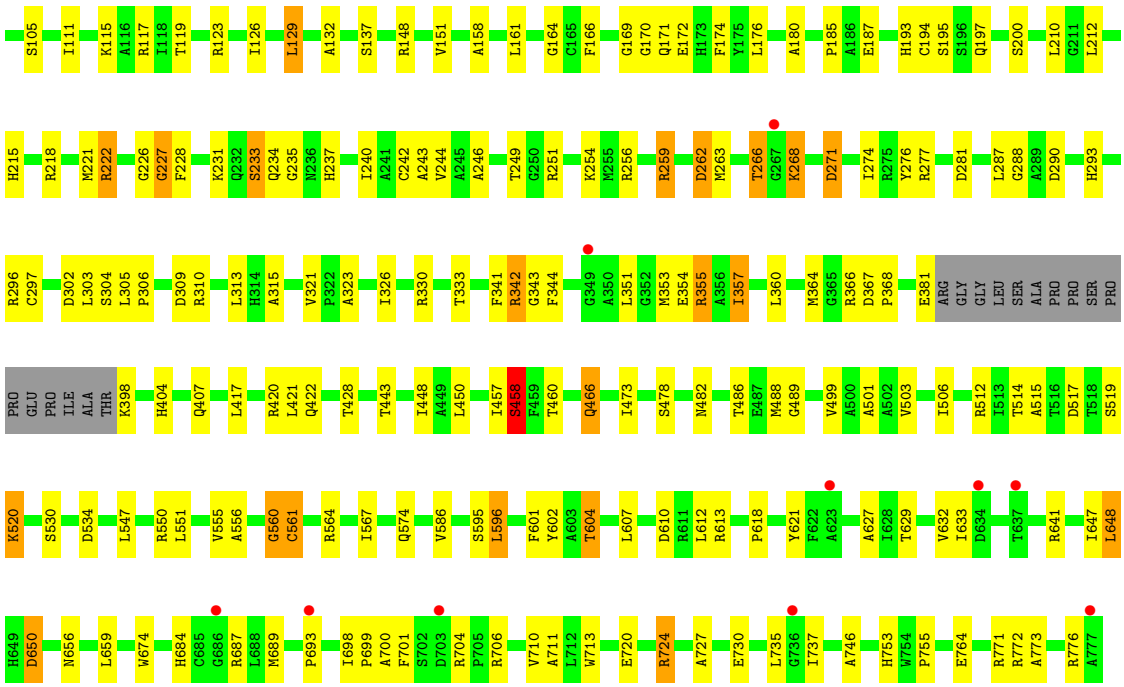
Chain G:



• Molecule 2: XANTHINE DEHYDROGENASE

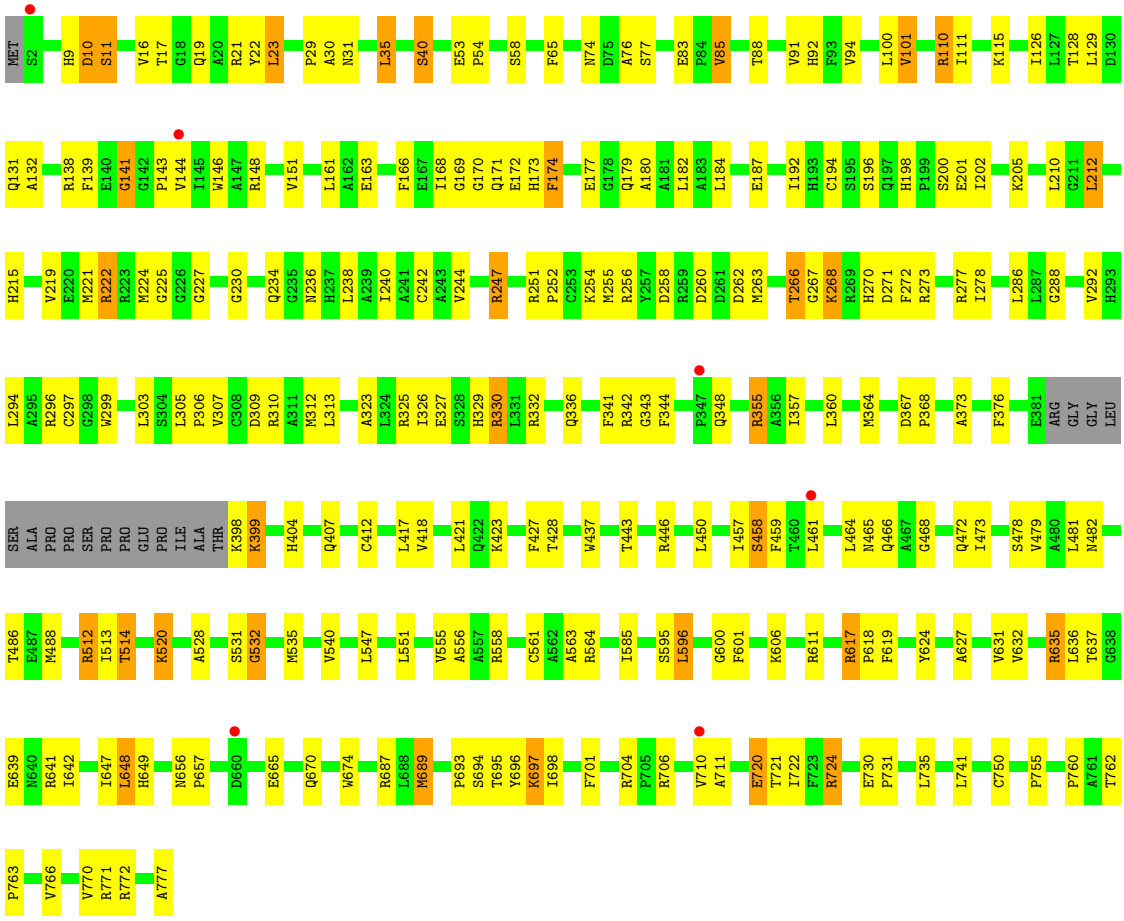
Chain B:





- Molecule 2: XANTHINE DEHYDROGENASE

Chain D:



• Molecule 2: XANTHINE DEHYDROGENASE

Chain F: % 66% 29% • •

MET S2 H9 D10 S11 A14 H15 V16 Q19 A20 R21 Y22 L23 L26 P27 C28 P29 A30 N31 T32 L33 H34 L35 L39 A46 E53 P54 S58 A63 V64 F65 T66 S77 P78 S81 P82 E83 P84 V85 E90 V94 G95 L100 V101 A102

K115 R123 T128 R138 F139 E140 G141 G142 P143 V144 I145 W146 A147 R148 V151 H160 L161 A162 E163 F166 Q171 E172 H173 F174 Y175 A180 A181 L182 E187 I192 H193 C194 E201 I202 V206 L210 G211 L212 R218 V219 E220 M221 R222 R223 M224

G227 F228 G229 G230 K231 Q232 S233 Q234 G235 N236 I240 A241 C242 R247 A248 T249 G250 R251 K254 M255 R256 R259 D260 D261 D262 I265 T266 G267 K268 R269 H270 D271 F272 R277 I278 L286 L287 G288 A289 D290 R296 C297 G298 L303 S304 L305 P306 R310 A311 M312

L313 D316 V321 P322 A323 L324 S328 H329 R330 L331 R332 S337 F341 R342 G343 F344 Q348 R355 A356 I357 E358 H359 L360 M364 D367 P368 A373 F376 P380 E381 ARG GLY GLY LEU SER ALA PRO PRO SER PRO PRO PRO GLU PRO ILE ALA THR K398 K399

H404 Q407 C412 L417 V418 T419 R420 L421 Q422 K423 T429 E433 W437 T440 T443 R446 L450 I457 S458 L461 L464 N465 Q466 A467 G468 I473 Y474 T475 V479 G485 T486 E487 M488 G491 L492 V497 Q498 V499 V503 L504

V511 R512 I513 D517 T518 S519 K520 A526 T527 A528 A529 N536 G537 M538 K541 T546 L547 R548 L551 A556 A557 R558 C561 A562 A563 R564 D565 V566 I567 F568 V573 Q574 S579 E584 I585 A588 M591 A592 R593 I594 S595 T599 G600 F601 Y602

K606 L607 D610 R613 R617 P618 Y624 A627 E630 V631 V632 R635 R641 I642 I643 R644 I647 L648 S654 G686 R687 L688 M689 P693 Y696 K697 I698 F701 S702 D703 R704 P705 R706 I707 V710 W713 D714 Q715 E720 T721 I722 F723

R724 E730 P731 L741 A742 L743 C750 T762 P763 E774 A777

• Molecule 2: XANTHINE DEHYDROGENASE

Chain H: % 68% 27% • •

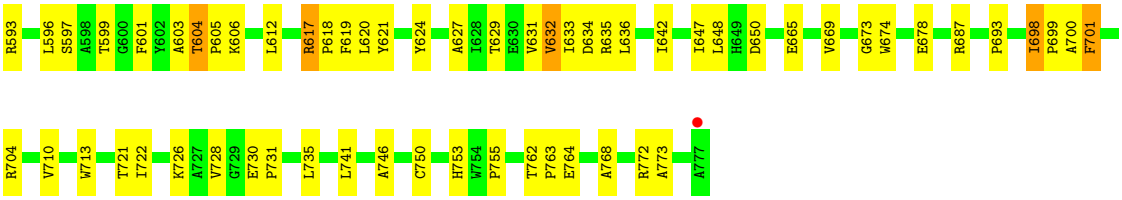
MET S2 K5 P6 L7 P8 H9 D10 S11 A12 R13 A14 H15 V16 Q19 Y22 L23 D24 D25 L26 P27 C28 P29 A30 N31 L35 S40 A46 E57 S58 L70 A76 V85 V91 H92 F93 V94 L100 V101 S105 A108 K115 R123

T128 S137 R138 G142 P143 W146 A147 R148 A158 A159 H160 L161 A162 E163 G164 C165 F166 G170 Q171 E172 H173 F174 Q179 A180 E187 C194 E201 I202 Q203 H204 K205 L210 G211 L212 D216 E220 M221 R222 R223 M224 G227 F228 Q232 N236 H237

L238 A239 I240 A241 C242 A243 V244 T249 G250 R251 P252 R256 Y257 D258 R259 D260 D261 D262 M263 T266 G267 K268 R269 H270 D271 F272 Y276 R277 I278 D281 L287 G288 C297 G298 W299 S300 L303 S304 L305 P306 V307 R310 L313 Y319 A323 I326

H329 T335 Q336 S337 F341 R342 G343 F344 Q348 R355 A356 I357 L360 E370 N375 P380 E381 ARG GLY GLY LEU SER ALA PRO PRO PRO PRO GLU PRO ILE ALA THR K398 K399 T400 Q407 A410 D411 C412 V413 L414 L417 N441 R442 T443 I448

A449 L450 G456 I457 S458 F459 T460 L461 L464 N465 I473 N482 T486 E487 M488 K495 M496 V497 Q498 V499 V509 Q510 V511 R512 I513 T514 A515 T516 D517 K520 G532 L547 R548 G549 R550 A556 G560 C561 R564 S579 W580 E584 I585 V586


R593
L596 S597 A598 T599 G600 F601 Y602 A603 T604 P605 K606
L612
R617 P618 F619 L620 Y621
Y624
A627 I628 T629 E630 V631 V632 I633 D634 R635 L636
I642
I647 L648 H649 D650
E665
V669
G673 W674
E678
R687
P693
I698 P699 A700 F701
R704
V710
W713
T721 I722
K726 A727 V728 G729 E730 P731
L735
L741
A746
C750
H753 W754 P755
T762 P763 E764
A768
R772 A773
A777

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.74Å 140.57Å 157.61Å 109.45° 106.10° 101.09°	Depositor
Resolution (Å)	50.00 – 3.40 50.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-3.40) 77.8 (50.00-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.221 , 0.270 0.225 , 0.278	Depositor DCC
R_{free} test set	3708 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	36807	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7034e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: XAX, HPA, BA, FES, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.48	0/3438	0.85	3/4658 (0.1%)
1	C	0.48	0/3438	0.84	3/4658 (0.1%)
1	E	0.48	0/3438	0.84	2/4658 (0.0%)
1	G	0.50	0/3438	0.85	6/4658 (0.1%)
2	B	0.47	0/5844	0.85	3/7941 (0.0%)
2	D	0.48	0/5844	0.87	1/7941 (0.0%)
2	F	0.48	0/5844	0.88	8/7941 (0.1%)
2	H	0.48	0/5844	0.85	1/7941 (0.0%)
All	All	0.48	0/37128	0.86	27/50396 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	CYS	N-CA-C	6.58	119.43	111.40
1	E	136	CYS	N-CA-C	5.77	118.68	111.24
2	F	81	SER	CA-C-N	5.77	125.77	119.89
2	F	81	SER	C-N-CA	5.77	125.77	119.89
2	B	85	VAL	N-CA-C	-5.53	106.42	111.67

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	3375	0	3368	77	0
1	C	3375	0	3368	72	0
1	E	3375	0	3369	75	0
1	G	3375	0	3371	94	0
2	B	5716	0	5633	137	0
2	D	5716	0	5633	166	0
2	F	5716	0	5633	150	0
2	H	5716	0	5633	151	0
3	A	8	0	0	0	0
3	C	8	0	0	0	0
3	E	8	0	0	0	0
3	G	8	0	0	1	0
4	A	53	0	31	6	0
4	C	53	0	31	5	0
4	E	53	0	31	2	0
4	G	53	0	31	7	0
5	B	28	0	8	4	0
5	D	28	0	8	7	0
5	F	28	0	8	7	0
5	H	28	0	8	4	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	10	0	4	0	0
7	D	10	0	4	3	0
7	F	10	0	4	1	0
7	H	10	0	4	7	0
8	A	4	0	0	0	0
8	B	8	0	0	1	0
8	C	3	0	0	1	0
8	D	11	0	0	0	0
8	E	1	0	0	0	0
8	F	12	0	0	0	0
8	G	1	0	0	0	0
8	H	3	0	0	0	0
All	All	36807	0	36180	906	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 12.

The worst 5 of 906 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:F:1778:XAX:O1	7:F:1780:HPA:H2	1.49	1.12
2:D:179:GLN:HB3	2:D:238:LEU:HD11	1.45	0.99
1:C:445:ARG:HG3	1:C:455:VAL:HG11	1.50	0.94
2:H:457:ILE:O	2:H:458:SER:HB2	1.62	0.93
2:F:138:ARG:HD3	2:F:142:GLY:H	1.34	0.92

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	446/462 (96%)	394 (88%)	47 (10%)	5 (1%)	11	38
1	C	446/462 (96%)	405 (91%)	37 (8%)	4 (1%)	14	42
1	E	446/462 (96%)	406 (91%)	34 (8%)	6 (1%)	9	33
1	G	446/462 (96%)	393 (88%)	47 (10%)	6 (1%)	9	33
2	B	756/777 (97%)	707 (94%)	39 (5%)	10 (1%)	9	33
2	D	756/777 (97%)	685 (91%)	65 (9%)	6 (1%)	16	44
2	F	756/777 (97%)	690 (91%)	58 (8%)	8 (1%)	11	38
2	H	756/777 (97%)	699 (92%)	46 (6%)	11 (2%)	8	30
All	All	4808/4956 (97%)	4379 (91%)	373 (8%)	56 (1%)	10	35

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	458	SER
1	C	39	CYS
2	D	187	GLU
2	D	458	SER
2	D	532	GLY

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	339/347 (98%)	308 (91%)	31 (9%)	9	30
1	C	339/347 (98%)	313 (92%)	26 (8%)	12	37
1	E	339/347 (98%)	314 (93%)	25 (7%)	13	38
1	G	339/347 (98%)	311 (92%)	28 (8%)	10	35
2	B	571/584 (98%)	532 (93%)	39 (7%)	14	40
2	D	571/584 (98%)	520 (91%)	51 (9%)	9	31
2	F	571/584 (98%)	518 (91%)	53 (9%)	8	29
2	H	571/584 (98%)	530 (93%)	41 (7%)	13	39
All	All	3640/3724 (98%)	3346 (92%)	294 (8%)	11	36

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	112	VAL
2	H	617	ARG
1	G	228	CYS
2	H	202	ILE
2	D	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	15	HIS
1	G	93	GLN
2	F	236	ASN
2	F	466	GLN
1	G	260	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
3	FES	A	1463	1	0,4,4	-	-	-		
3	FES	A	1464	1	0,4,4	-	-	-		
5	XAX	B	1778	-	20,31,31	4.02	4 (20%)	20,52,52	2.18	5 (25%)
3	FES	E	1464	1	0,4,4	-	-	-		
7	HPA	D	1780	-	10,11,11	1.75	1 (10%)	11,15,15	3.34	8 (72%)
3	FES	C	1464	1	0,4,4	-	-	-		
4	FAD	G	1465	-	56,58,58	1.33	6 (10%)	81,89,89	1.67	16 (19%)
5	XAX	F	1778	-	20,31,31	4.09	4 (20%)	20,52,52	1.85	6 (30%)
7	HPA	F	1780	-	10,11,11	1.86	2 (20%)	11,15,15	3.26	8 (72%)
3	FES	G	1463	1	0,4,4	-	-	-		
4	FAD	C	1465	-	56,58,58	1.27	4 (7%)	81,89,89	1.65	16 (19%)
5	XAX	H	1778	-	20,31,31	4.15	4 (20%)	20,52,52	2.06	4 (20%)
4	FAD	E	1465	-	56,58,58	1.29	4 (7%)	81,89,89	1.64	17 (20%)
3	FES	G	1464	1	0,4,4	-	-	-		
4	FAD	A	1465	-	56,58,58	1.36	6 (10%)	81,89,89	1.62	16 (19%)
7	HPA	B	1780	-	10,11,11	1.84	2 (20%)	11,15,15	3.56	9 (81%)
7	HPA	H	1780	-	10,11,11	1.76	1 (10%)	11,15,15	3.53	8 (72%)
3	FES	E	1463	1	0,4,4	-	-	-		
3	FES	C	1463	1	0,4,4	-	-	-		
5	XAX	D	1778	-	20,31,31	4.17	5 (25%)	20,52,52	1.74	4 (20%)

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
3	FES	A	1463	1	-	-	0/1/1/1
3	FES	C	1463	1	-	-	0/1/1/1
5	XAX	B	1778	-	1/1/7/9	3/6/46/46	0/4/4/4
3	FES	E	1464	1	-	-	0/1/1/1
7	HPA	D	1780	-	-	-	0/2/2/2
3	FES	C	1464	1	-	-	0/1/1/1
4	FAD	G	1465	-	-	11/34/50/50	0/6/6/6
5	XAX	F	1778	-	1/1/7/9	2/6/46/46	0/4/4/4
7	HPA	F	1780	-	-	-	0/2/2/2
3	FES	G	1463	1	-	-	0/1/1/1
4	FAD	C	1465	-	-	10/34/50/50	0/6/6/6
5	XAX	H	1778	-	1/1/7/9	2/6/46/46	0/4/4/4
4	FAD	E	1465	-	-	10/34/50/50	0/6/6/6
3	FES	G	1464	1	-	-	0/1/1/1
4	FAD	A	1465	-	-	17/34/50/50	0/6/6/6
7	HPA	B	1780	-	-	-	0/2/2/2
7	HPA	H	1780	-	-	-	0/2/2/2
3	FES	E	1463	1	-	-	0/1/1/1
3	FES	A	1464	1	-	-	0/1/1/1
5	XAX	D	1778	-	1/1/7/9	2/6/46/46	0/4/4/4

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1778	XAX	C4'-C3'	-13.94	1.33	1.52
5	D	1778	XAX	C4'-C3'	-13.34	1.34	1.52
5	B	1778	XAX	C4'-C3'	-13.23	1.34	1.52
5	F	1778	XAX	C4'-C3'	-12.83	1.34	1.52
5	F	1778	XAX	C6-N5	-11.17	1.33	1.46

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1465	FAD	C5A-C4A-N3A	-6.02	118.89	126.75
7	H	1780	HPA	C5-C6-N1	6.00	120.29	110.57
4	A	1465	FAD	C5A-C4A-N3A	-5.70	119.31	126.75
4	E	1465	FAD	C5A-C4A-N3A	-5.66	119.36	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1778	XAX	O3'-C7-C6	5.59	112.69	108.96

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1778	XAX	C3'
5	D	1778	XAX	C3'
5	F	1778	XAX	C3'
5	H	1778	XAX	C3'

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1465	FAD	N10-C1'-C2'-C3'
4	A	1465	FAD	C1'-C2'-C3'-O3'
4	A	1465	FAD	C1'-C2'-C3'-C4'
4	A	1465	FAD	C2'-C3'-C4'-O4'
4	A	1465	FAD	C2'-C3'-C4'-C5'

There are no ring outliers.

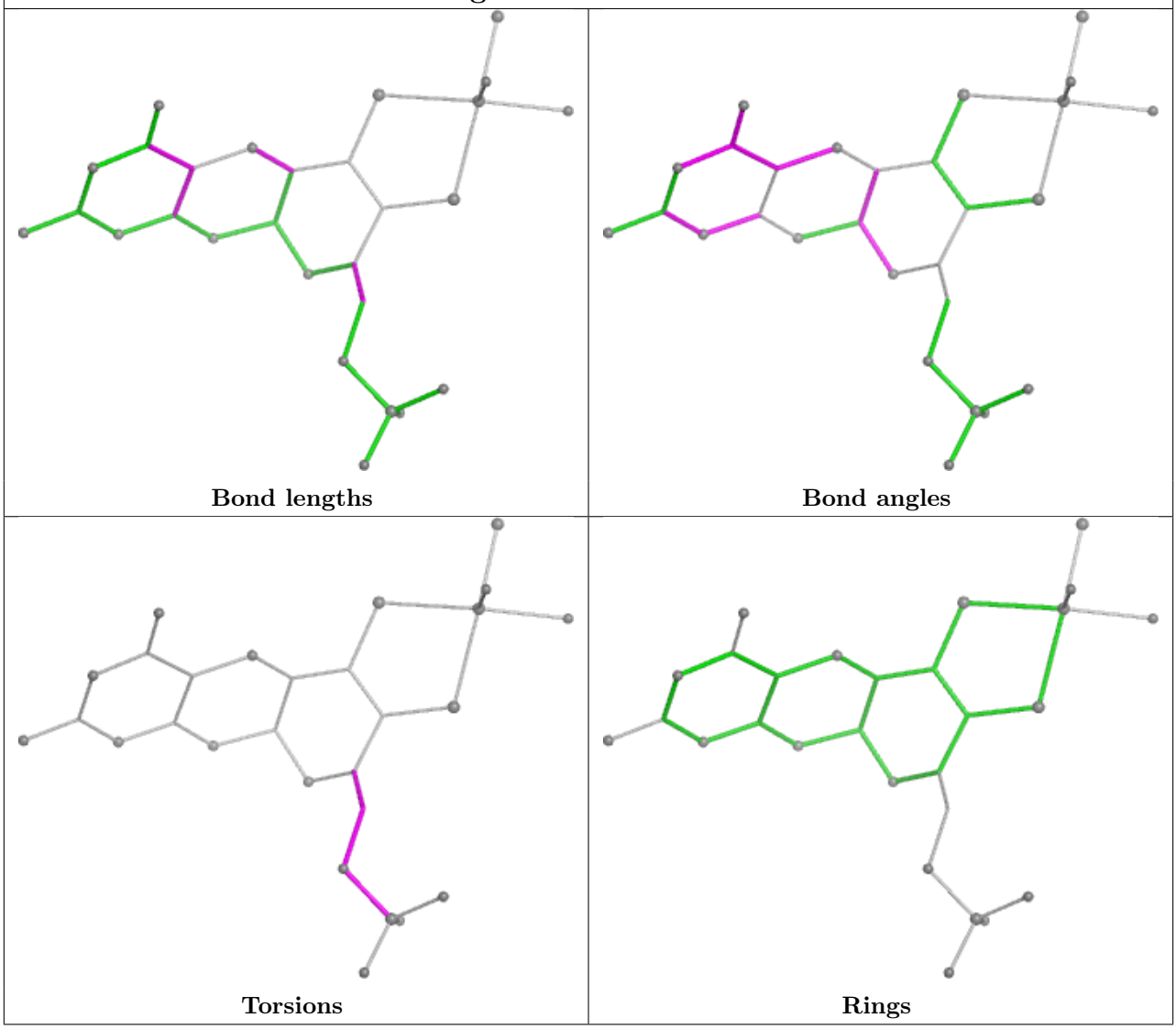
12 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1778	XAX	4	0
7	D	1780	HPA	3	0
4	G	1465	FAD	7	0
5	F	1778	XAX	7	0
7	F	1780	HPA	1	0
4	C	1465	FAD	5	0
5	H	1778	XAX	4	0
4	E	1465	FAD	2	0
3	G	1464	FES	1	0
4	A	1465	FAD	6	0
7	H	1780	HPA	7	0
5	D	1778	XAX	7	0

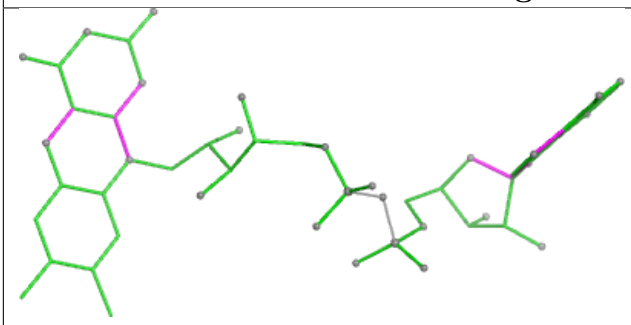
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

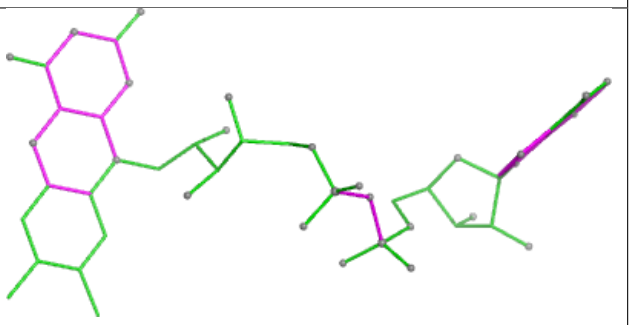
Ligand XAX B 1778



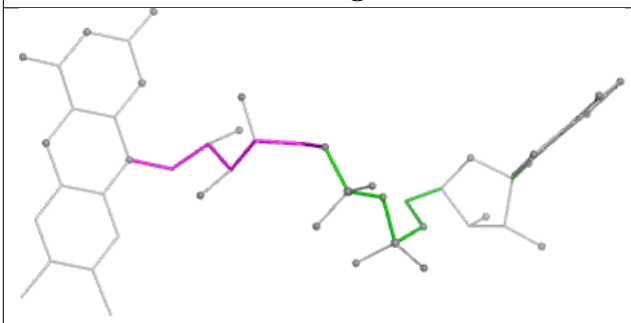
Ligand FAD G 1465



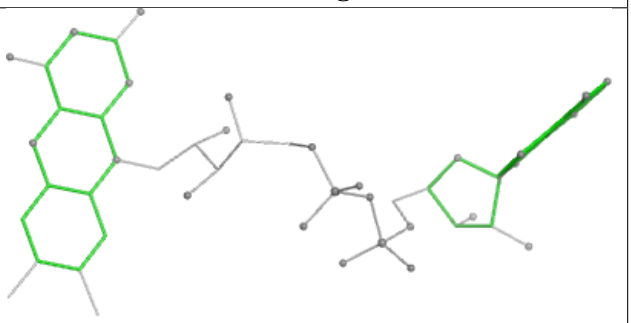
Bond lengths



Bond angles

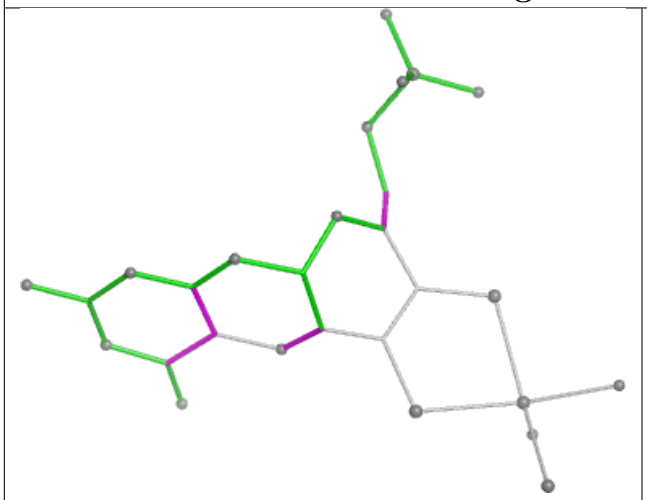


Torsions



Rings

Ligand XAX F 1778



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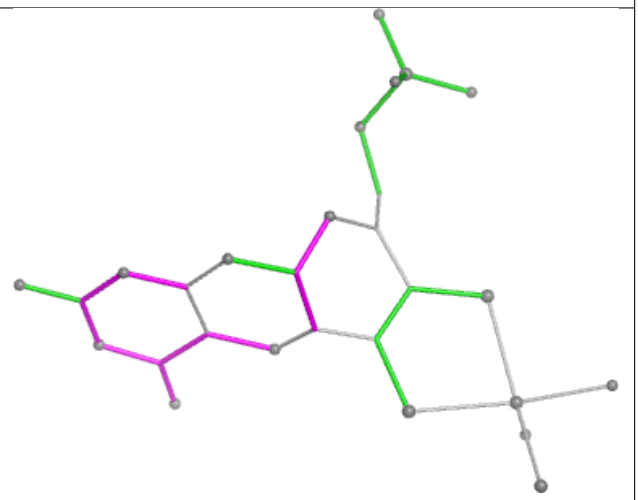
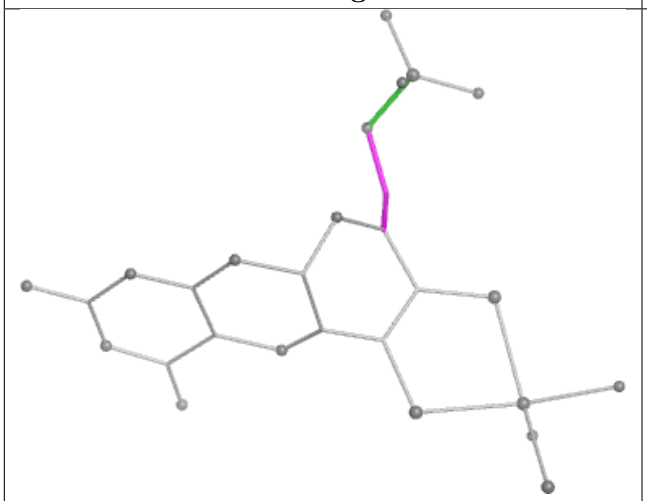
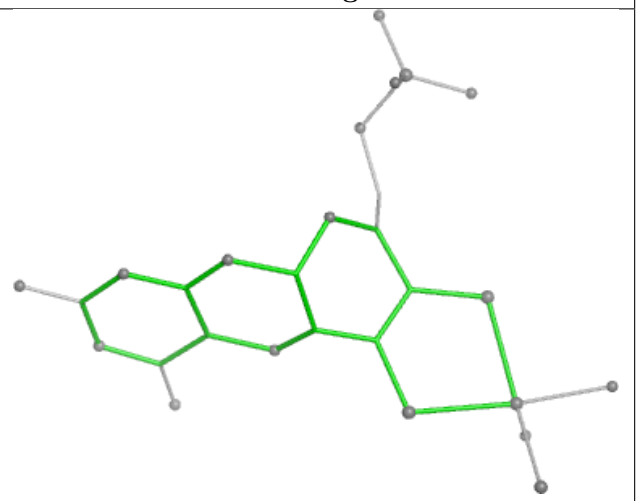


Bond angles

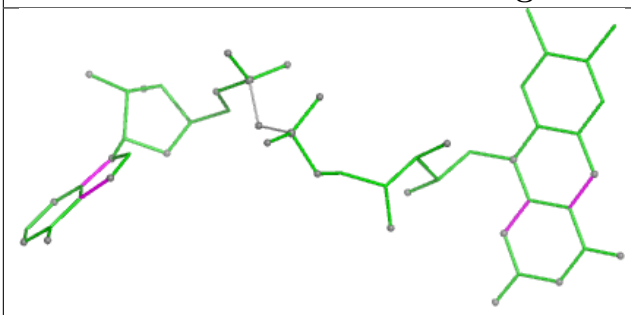


Torsions

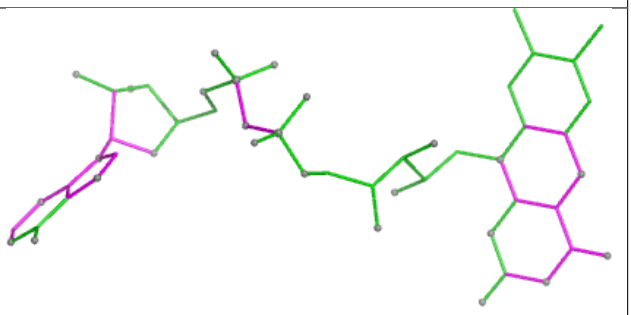


Rings

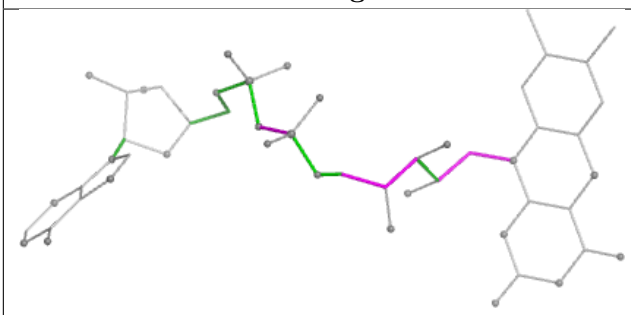
Ligand FAD C 1465



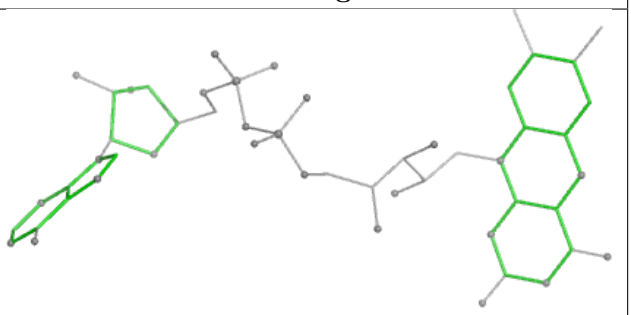
Bond lengths



Bond angles

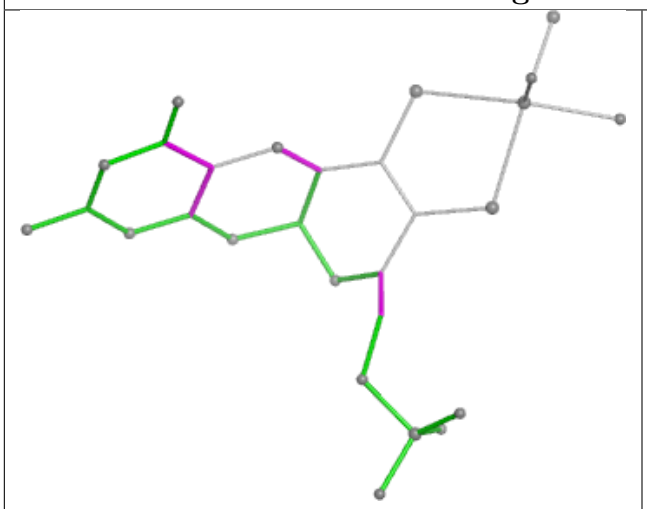


Torsions

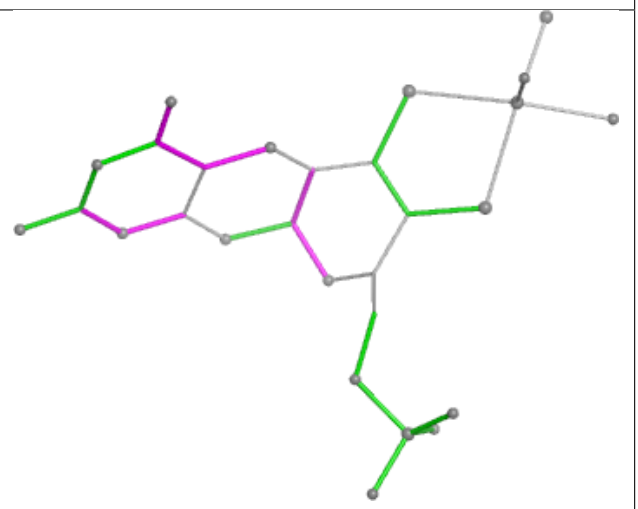


Rings

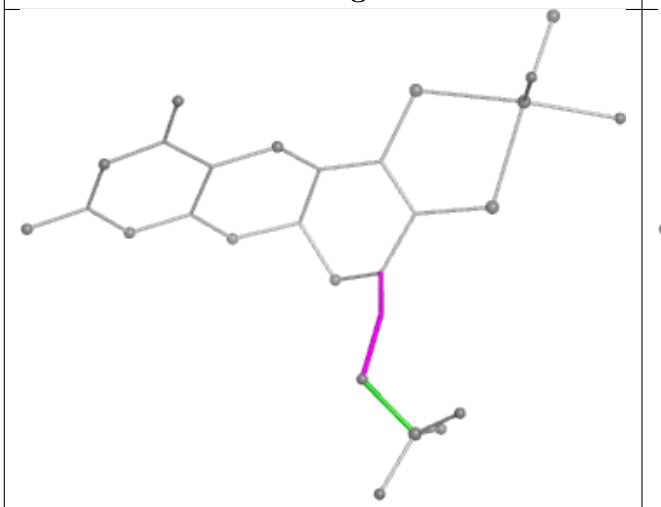
Ligand XAX H 1778



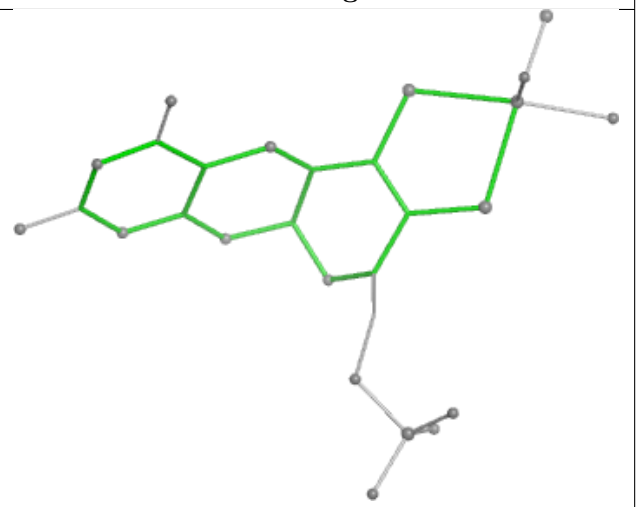
Bond lengths



Bond angles

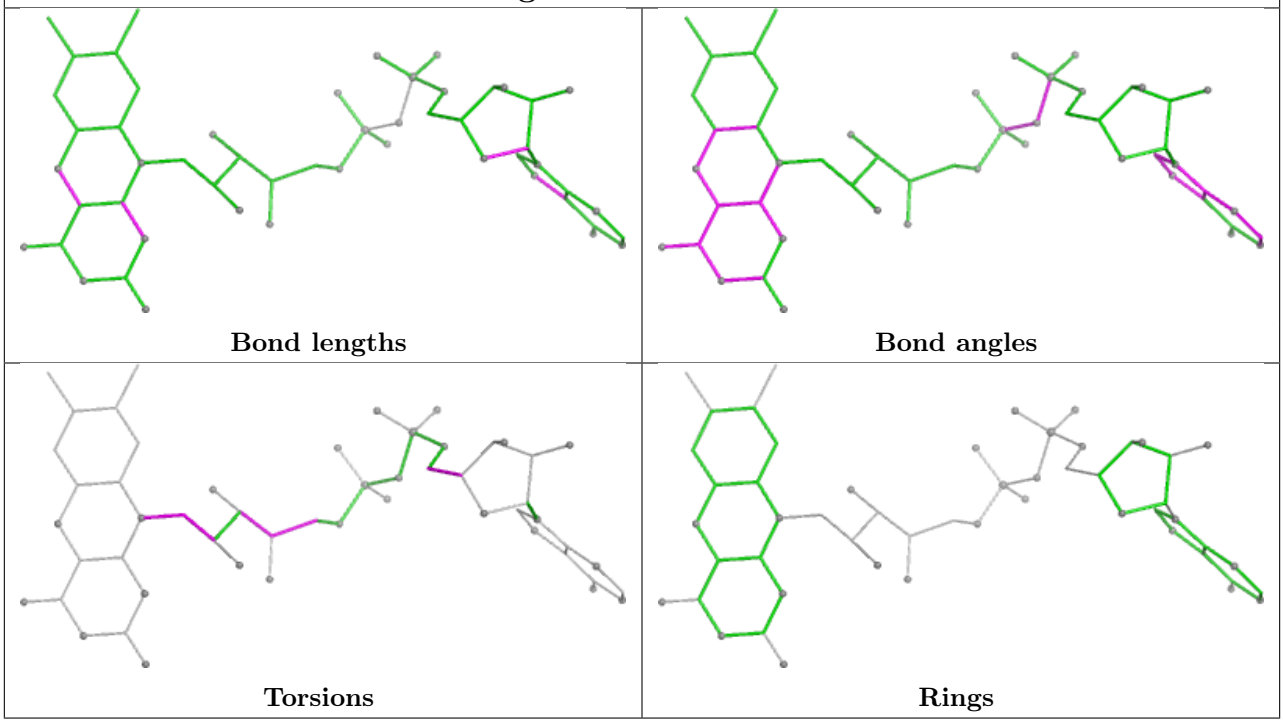


Torsions

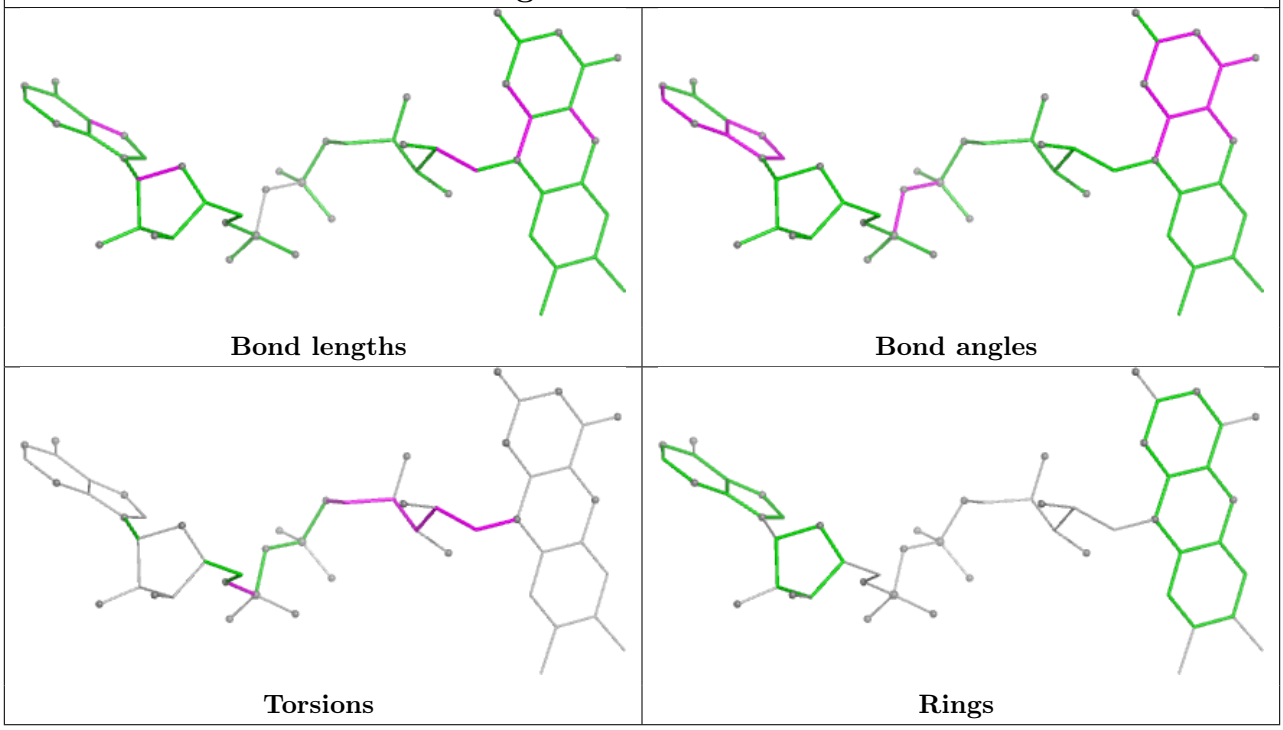


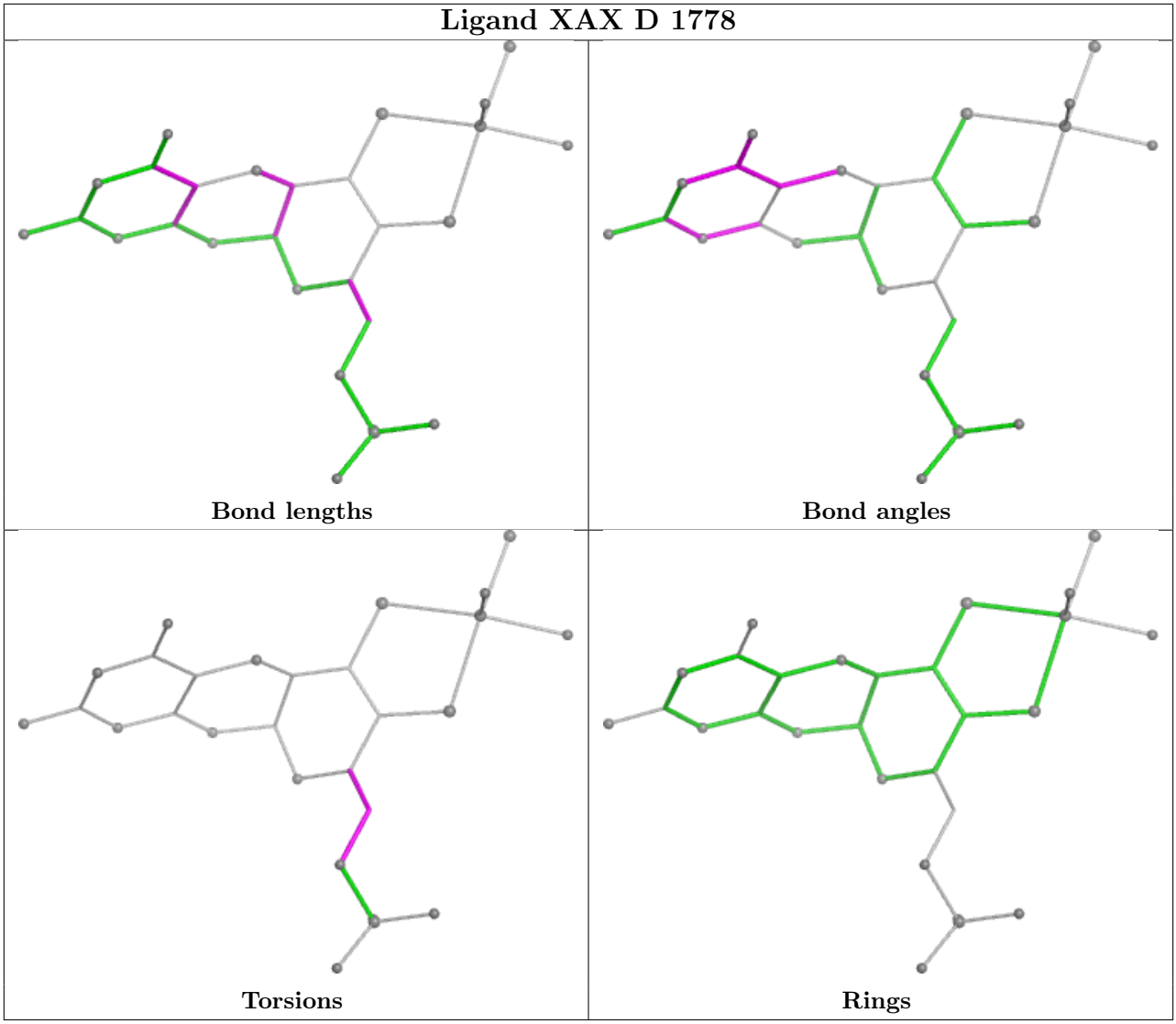
Rings

Ligand FAD E 1465



Ligand FAD A 1465





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	450/462 (97%)	0.16	8 (1%)	67	53	41, 43, 44, 45	0
1	C	450/462 (97%)	0.01	5 (1%)	78	65	41, 43, 44, 45	0
1	E	450/462 (97%)	0.22	8 (1%)	67	53	41, 43, 44, 45	0
1	G	450/462 (97%)	0.26	16 (3%)	46	33	42, 43, 44, 45	0
2	B	760/777 (97%)	0.14	10 (1%)	75	61	40, 43, 44, 46	0
2	D	760/777 (97%)	-0.01	6 (0%)	82	71	41, 43, 44, 46	0
2	F	760/777 (97%)	-0.03	6 (0%)	82	71	41, 43, 44, 46	0
2	H	760/777 (97%)	-0.10	4 (0%)	87	78	41, 43, 44, 46	0
All	All	4840/4956 (97%)	0.06	63 (1%)	75	61	40, 43, 44, 46	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	462	PRO	6.4
1	E	462	PRO	6.4
2	H	137	SER	4.9
1	C	179	PRO	3.9
1	E	355	LYS	3.5

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 oligosaccharides in this entry.

6.4 Ligands (i)

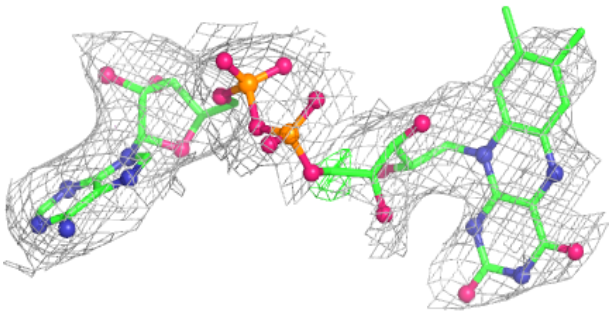
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

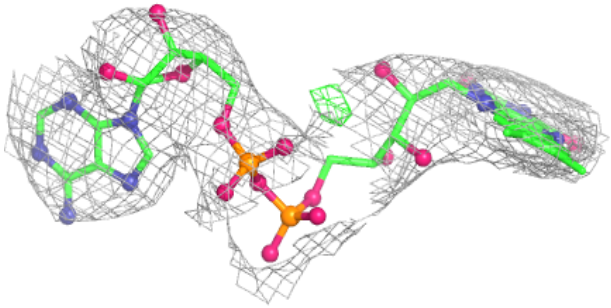
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	HPA	D	1780	10/10	0.83	0.14	43,43,43,43	0
7	HPA	B	1780	10/10	0.85	0.11	43,43,43,43	0
7	HPA	H	1780	10/10	0.89	0.12	43,43,43,43	0
4	FAD	A	1465	53/53	0.90	0.09	72,74,76,76	0
4	FAD	G	1465	53/53	0.91	0.09	74,76,79,80	0
7	HPA	F	1780	10/10	0.91	0.18	43,43,43,43	0
3	FES	E	1464	4/4	0.91	0.12	97,98,98,99	4
3	FES	G	1464	4/4	0.92	0.12	66,66,66,66	4
5	XAX	H	1778	28/28	0.93	0.15	52,55,62,63	28
5	XAX	B	1778	28/28	0.94	0.13	52,55,60,61	28
4	FAD	E	1465	53/53	0.94	0.09	62,66,78,78	0
3	FES	C	1464	4/4	0.94	0.08	107,108,108,108	4
5	XAX	F	1778	28/28	0.95	0.11	39,41,47,49	28
3	FES	A	1464	4/4	0.96	0.13	84,84,84,85	4
6	BA	H	1779	1/1	0.96	0.13	115,115,115,115	0
4	FAD	C	1465	53/53	0.96	0.07	46,51,55,55	0
6	BA	F	1779	1/1	0.97	0.14	98,98,98,98	0
5	XAX	D	1778	28/28	0.97	0.09	37,42,47,49	28
6	BA	B	1779	1/1	0.97	0.15	108,108,108,108	0
3	FES	G	1463	4/4	0.98	0.10	44,45,45,46	4
6	BA	D	1779	1/1	0.98	0.13	105,105,105,105	0
3	FES	A	1463	4/4	0.99	0.09	29,30,30,30	4
3	FES	E	1463	4/4	0.99	0.10	32,32,32,33	4
3	FES	C	1463	4/4	0.99	0.10	24,25,25,25	4

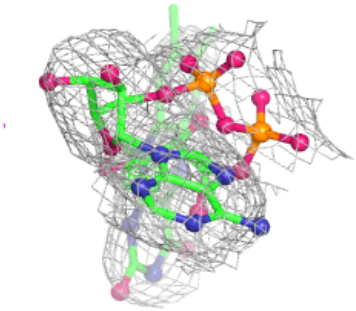
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1465:

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

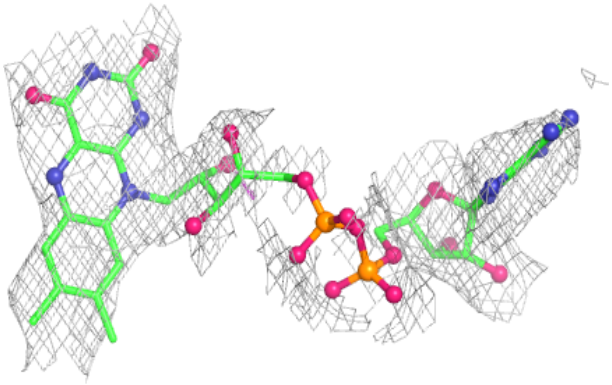


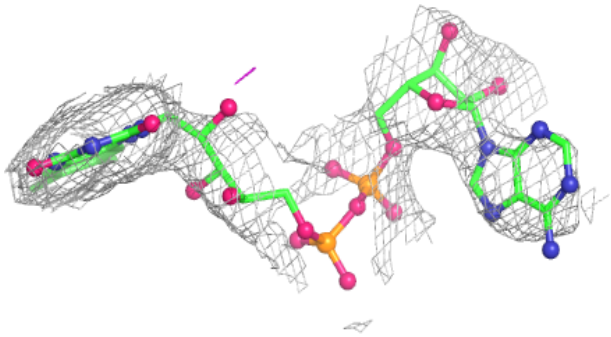


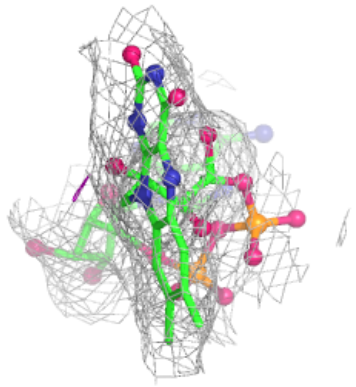


Electron density around FAD G 1465:

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

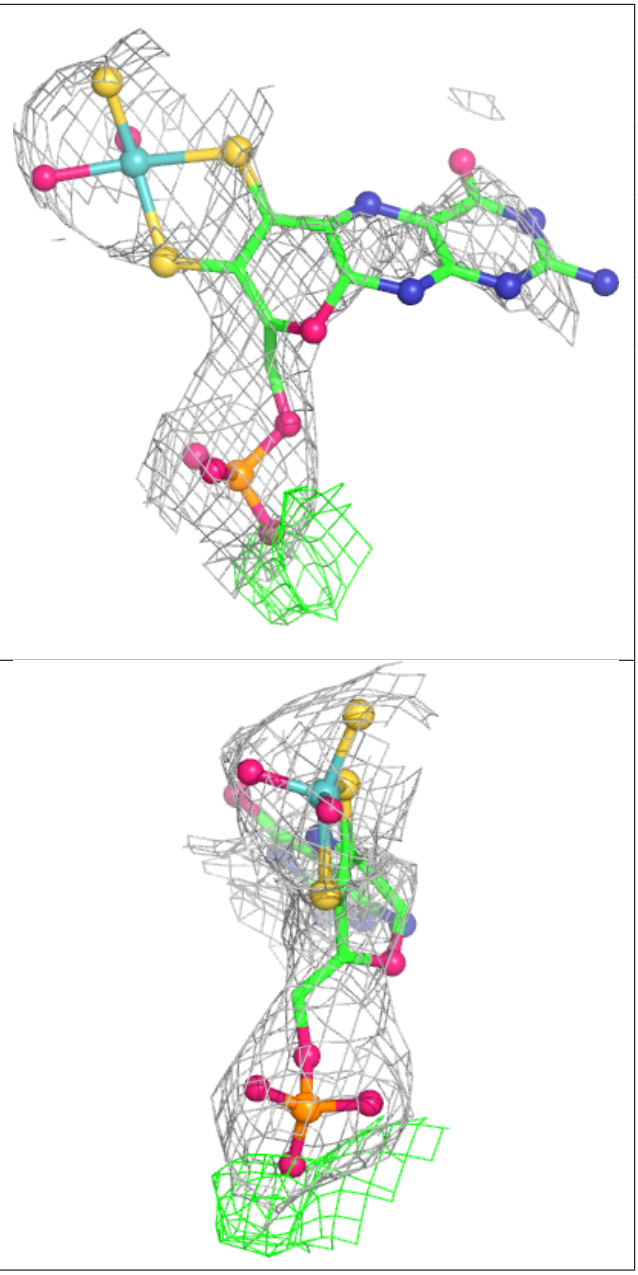






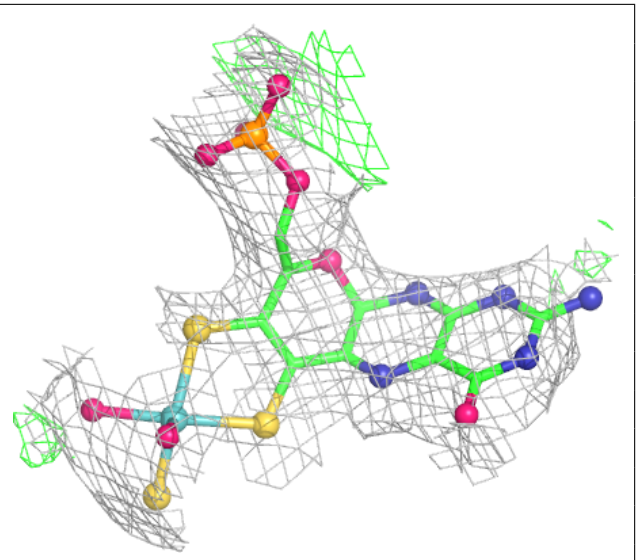
Electron density around XAX H 1778:

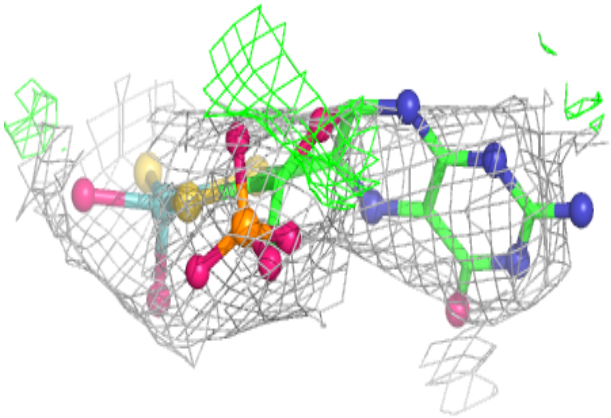
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

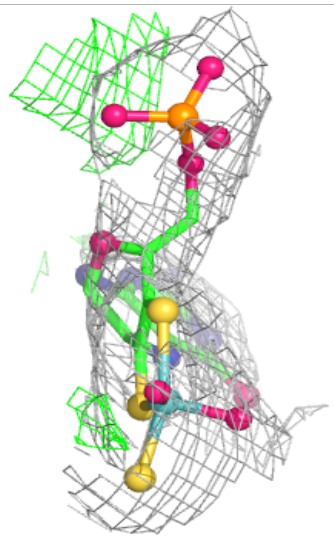


Electron density around XAX B 1778:

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

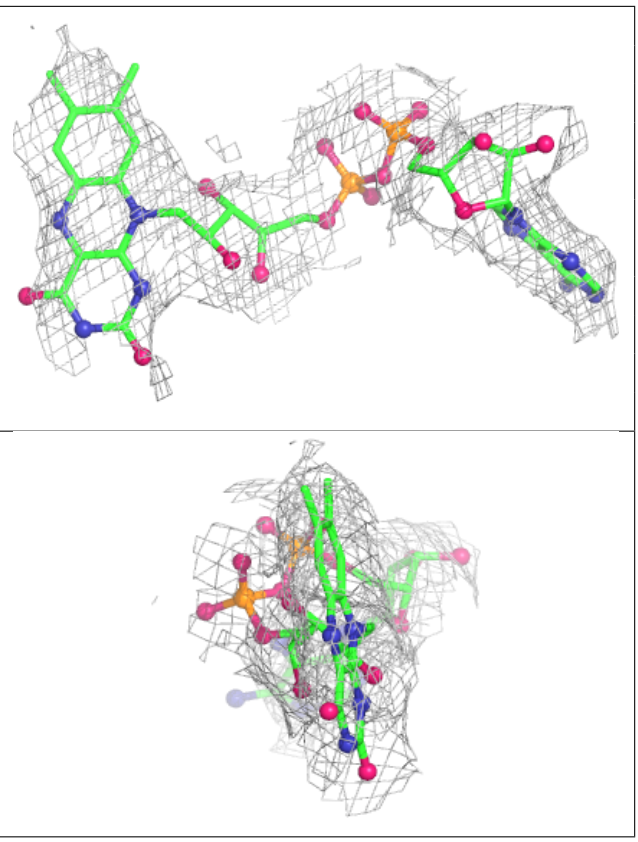






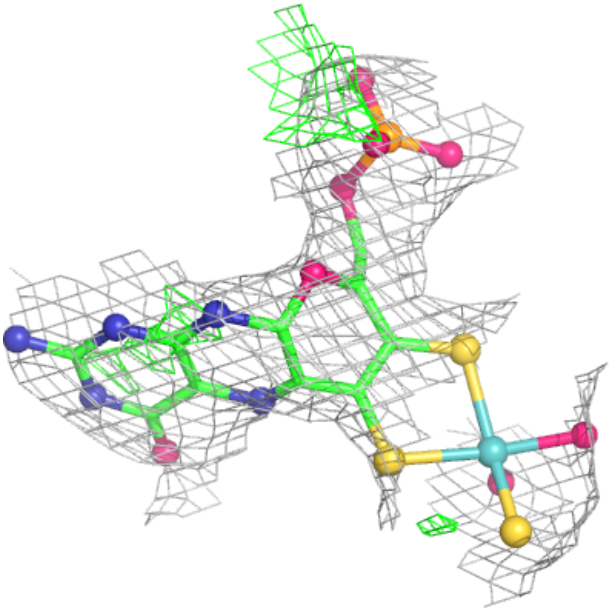
Electron density around FAD E 1465:

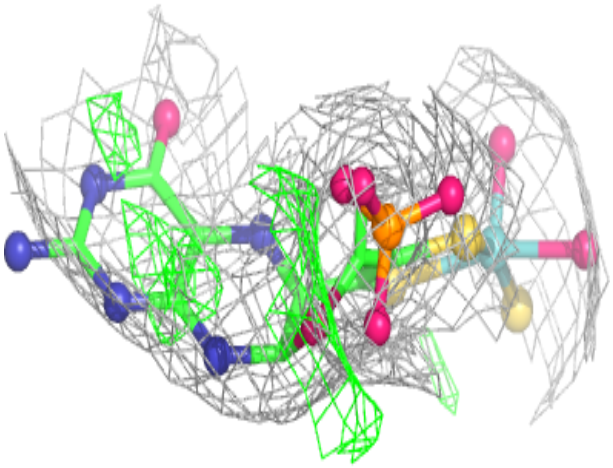
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

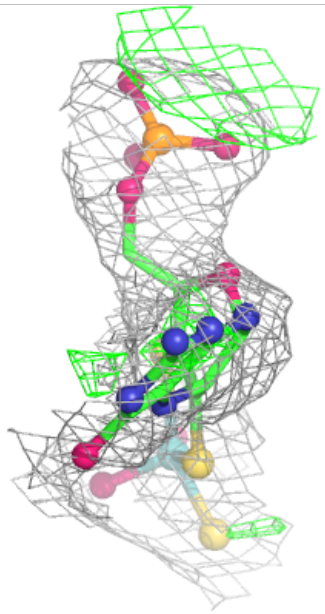


Electron density around XAX F 1778:

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

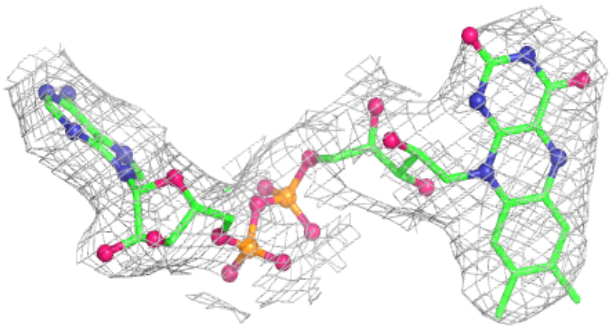


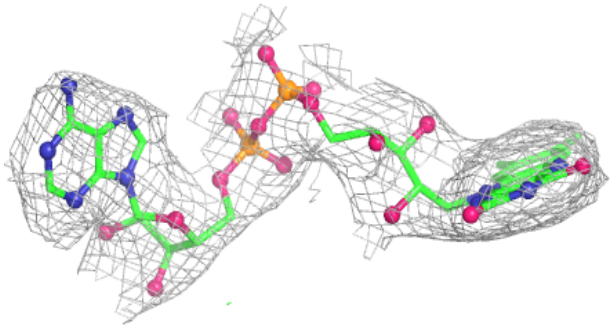


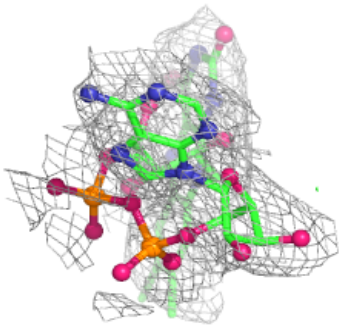


Electron density around FAD C 1465:

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

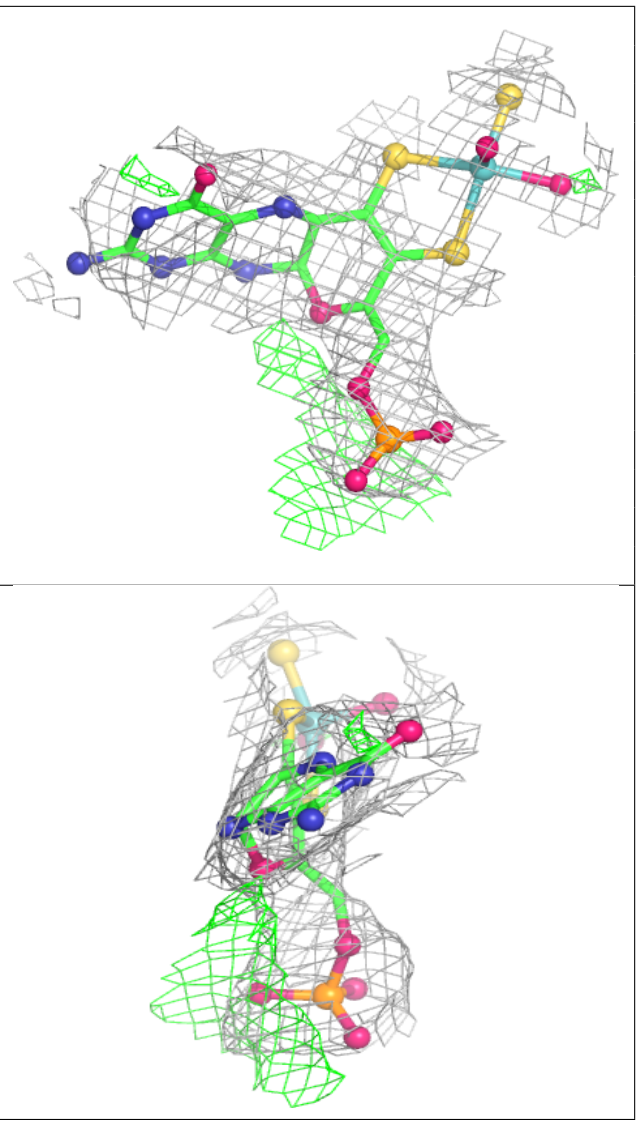






Electron density around XAX D 1778:

$2mF_o$-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.