wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 09:12 pm BST

PDB ID	:	2W3R / pdb_00002w3r
Title	:	Crystal Structure of Xanthine Dehydrogenase (desulfo form) from Rhodobacter capsulatus in complex with hypoxanthine
Authors	:	Dietzel, U.; Kuper, J.; Leimkuhler, S.; Kisker, C.
Deposited on	:	2008-11-14
Resolution	:	2.90 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:

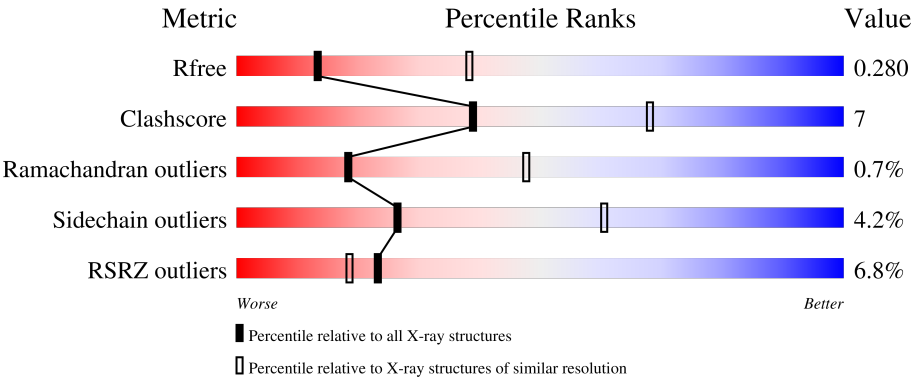
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	13% 79% 18% ·
1	C	462	20% 84% 13% · ·
1	E	462	12% 78% 18% · ·
1	G	462	13% 75% 21% · ·
2	B	777	2% 82% 14% · ·

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Mol	Chain	Length	Quality of chain
2	D	777	3% 78% 19%
2	F	777	2% 81% 15%
2	H	777	% 80% 16%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	DYI	B	1781	X	-	-	-
7	DYI	D	1781	X	-	-	-
7	DYI	F	1781	X	-	-	-
7	DYI	H	1781	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 36853 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
1	A	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			

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

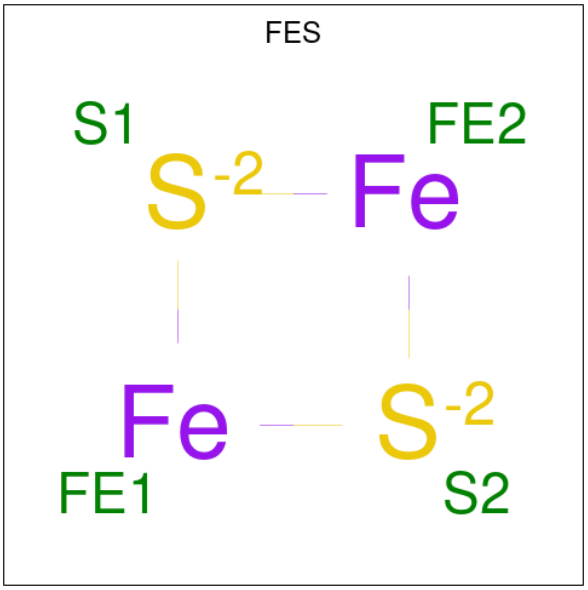
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

There are 4 discrepancies between the modelled and reference sequences:

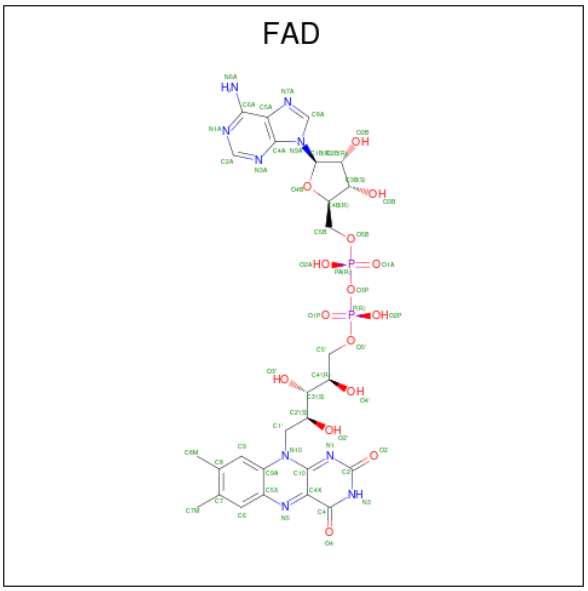
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	UNP O54051
D	772	ARG	GLY	conflict	UNP O54051
F	772	ARG	GLY	conflict	UNP O54051
H	772	ARG	GLY	conflict	UNP O54051

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



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

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

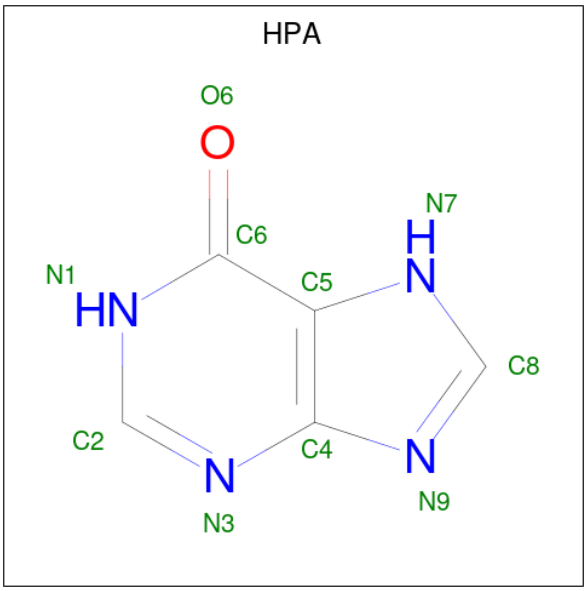


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

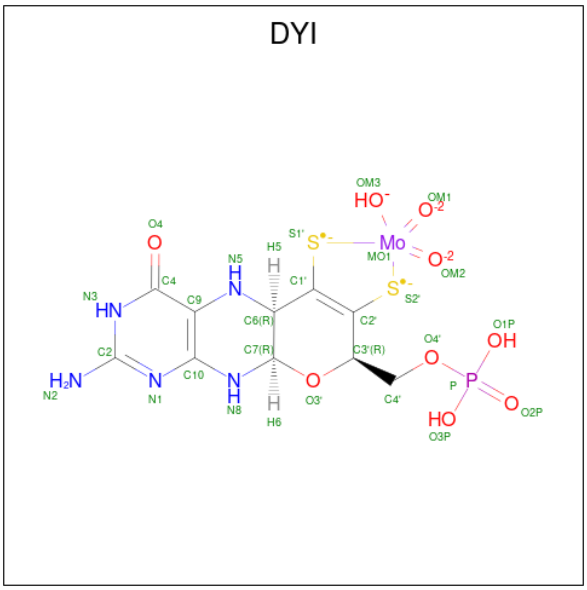
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 is HYPOXANTHINE (CCD ID: HPA) (formula: $C_5H_4N_4O$).



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

- Molecule 7 is Molybdopterin hydrox dioxo molybdenum (CCD ID: DYI) (formula: $C_{10}H_{13}MoN_5O_9PS_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
7	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	9	1	2		
7	D	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	9	1	2		
7	F	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	9	1	2		
7	H	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	9	1	2		

- Molecule 8 is water.

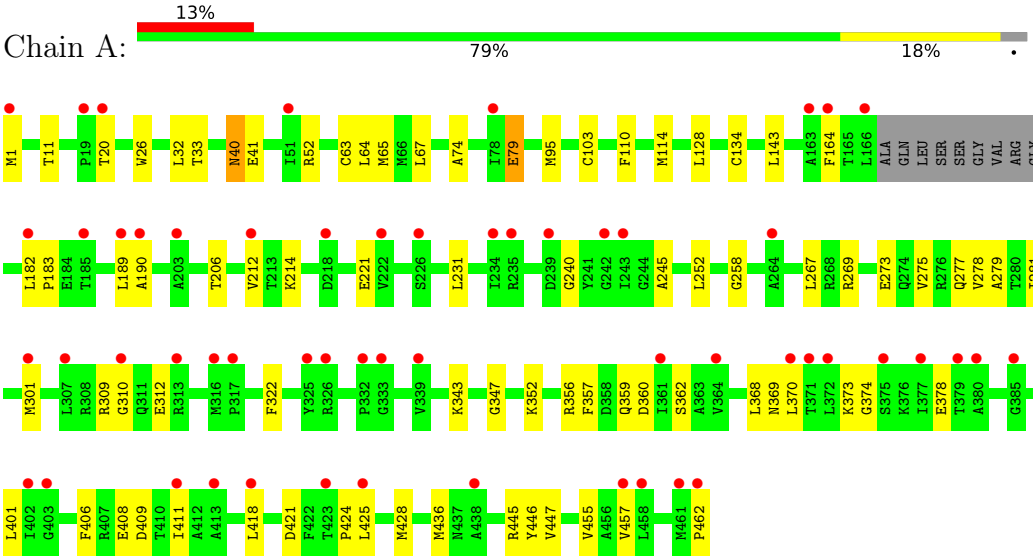
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		
8	B	15	Total	O	0	0
			15	15		
8	C	10	Total	O	0	0
			10	10		
8	D	16	Total	O	0	0
			16	16		
8	E	2	Total	O	0	0
			2	2		
8	F	11	Total	O	0	0
			11	11		
8	G	5	Total	O	0	0
			5	5		
8	H	16	Total	O	0	0
			16	16		

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.

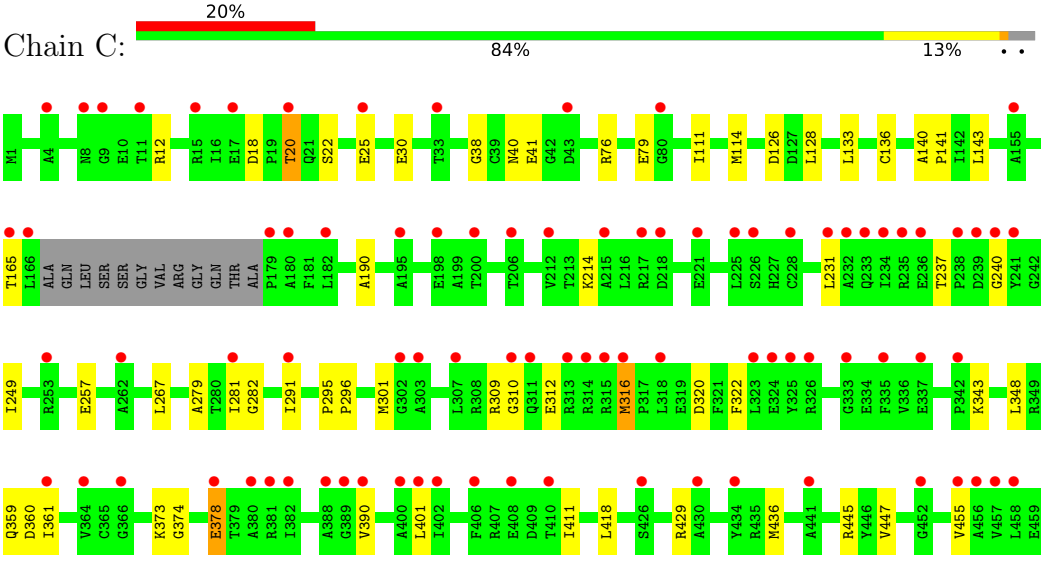
• Molecule 1: XANTHINE DEHYDROGENASE

Chain A:



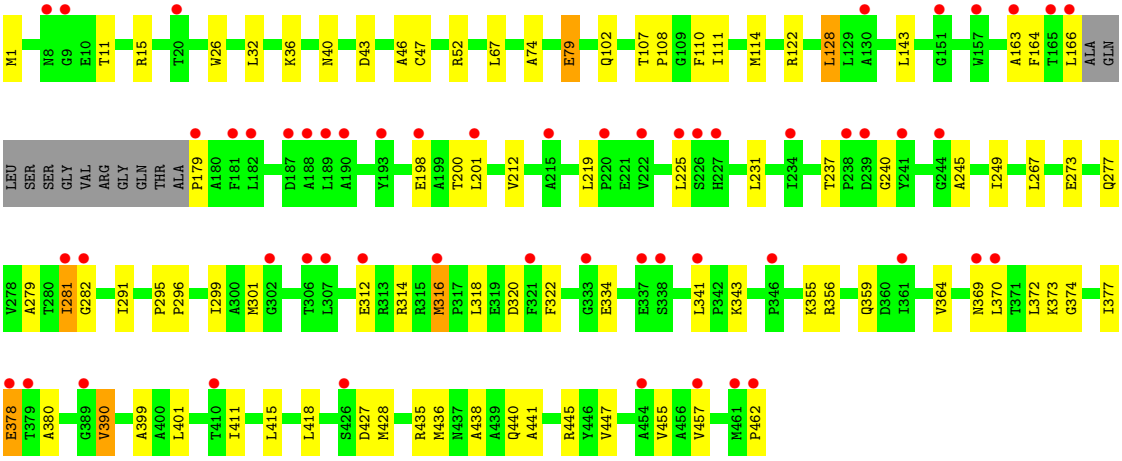
• Molecule 1: XANTHINE DEHYDROGENASE

Chain C:



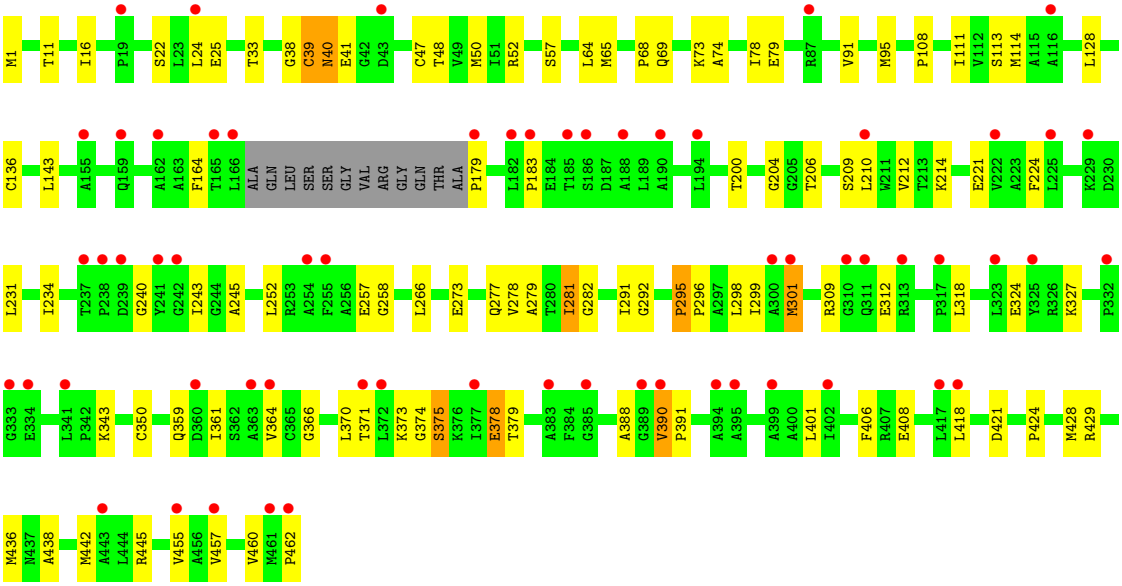
• Molecule 1: XANTHINE DEHYDROGENASE

Chain E:



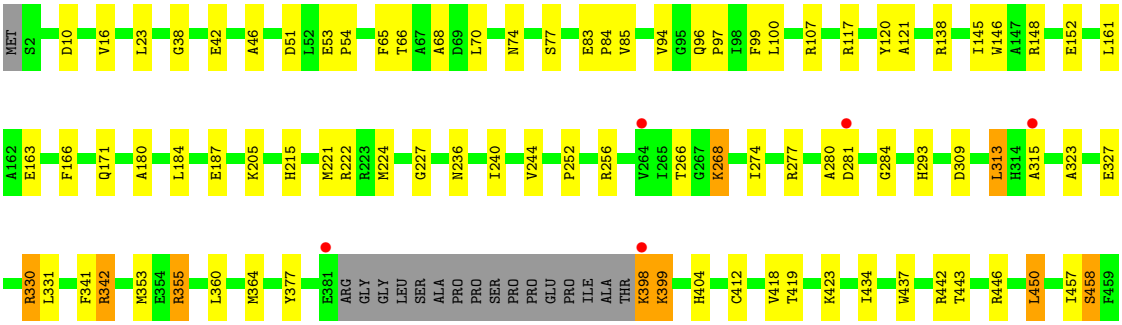
• Molecule 1: XANTHINE DEHYDROGENASE

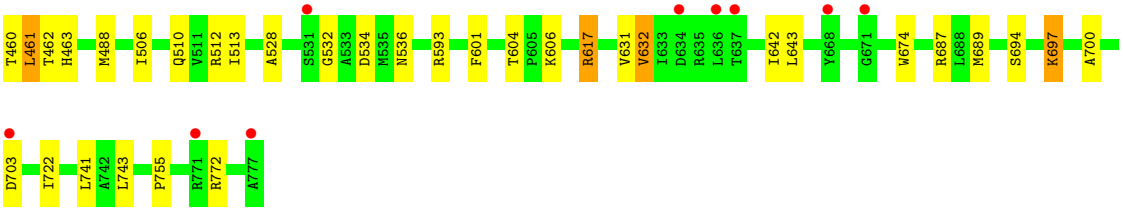
Chain G:



• Molecule 2: XANTHINE DEHYDROGENASE

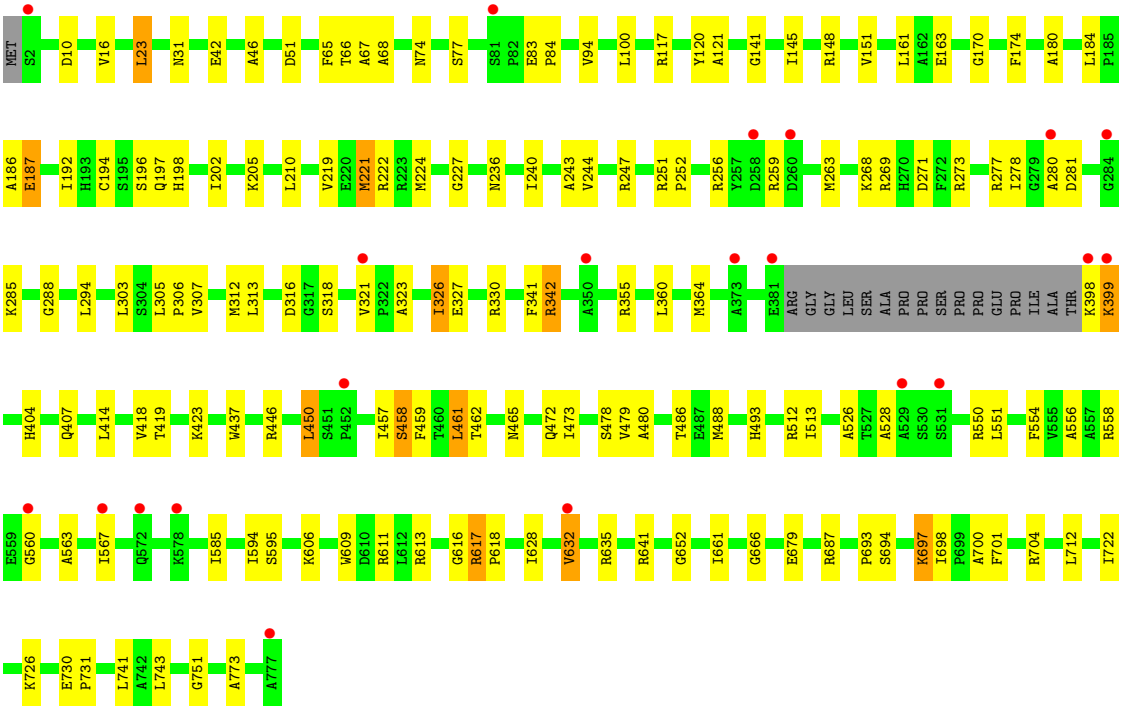
Chain B:





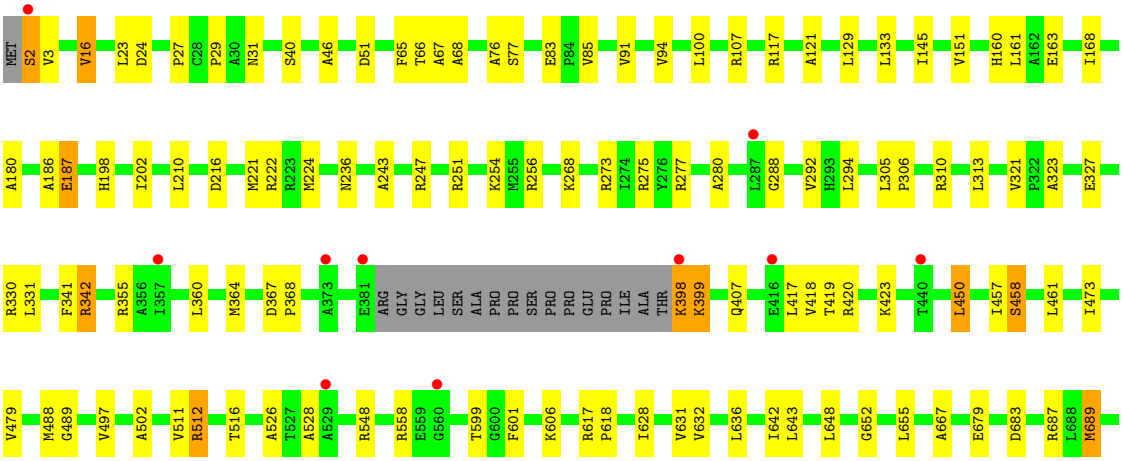
• Molecule 2: XANTHINE DEHYDROGENASE

Chain D:



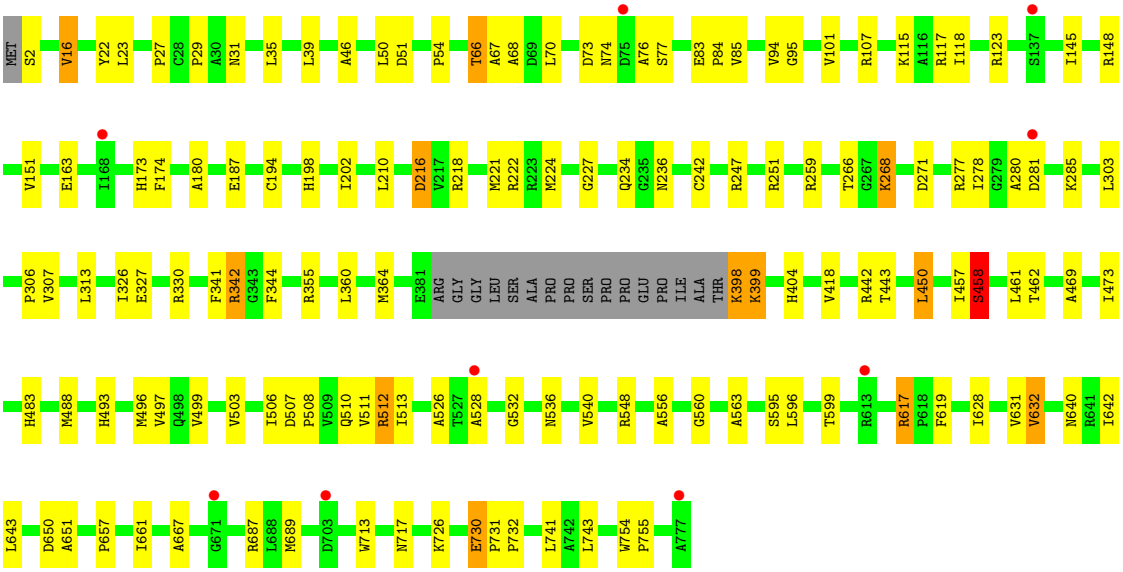
• Molecule 2: XANTHINE DEHYDROGENASE

Chain F:



• Molecule 2: XANTHINE DEHYDROGENASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.77Å 139.94Å 158.04Å 109.33° 106.15° 101.05°	Depositor
Resolution (Å)	51.23 – 2.90 51.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (51.23-2.90) 98.2 (51.23-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.240 , 0.281 0.240 , 0.280	Depositor DCC
R_{free} test set	7476 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	36853	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DYI, HPA, FAD, CA, FES

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	0.44	0/3439	0.81	2/4659 (0.0%)
1	C	0.43	0/3439	0.79	0/4659
1	E	0.45	0/3439	0.81	0/4659
1	G	0.46	0/3439	0.81	3/4659 (0.1%)
2	B	0.44	0/5845	0.81	1/7942 (0.0%)
2	D	0.42	0/5845	0.81	1/7942 (0.0%)
2	F	0.43	0/5845	0.80	0/7942
2	H	0.45	0/5845	0.81	1/7942 (0.0%)
All	All	0.44	0/37136	0.81	8/50404 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	462	THR	N-CA-C	6.22	119.04	111.82
2	H	462	THR	N-CA-C	5.85	118.41	111.33
2	B	462	THR	N-CA-C	5.69	117.48	111.28
1	G	258	GLY	CA-C-N	5.56	125.03	119.24
1	G	258	GLY	C-N-CA	5.56	125.03	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3367	47	0
1	C	3376	0	3367	36	0
1	E	3376	0	3367	50	0
1	G	3376	0	3367	60	0
2	B	5717	0	5631	67	0
2	D	5717	0	5630	92	0
2	F	5717	0	5631	77	0
2	H	5717	0	5631	84	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	5	0
4	C	53	0	31	3	0
4	E	53	0	31	3	0
4	G	53	0	31	4	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	B	10	0	4	2	0
6	D	10	0	4	1	0
6	F	10	0	4	1	0
6	H	10	0	4	0	0
7	B	28	0	0	3	0
7	D	28	0	0	3	0
7	F	28	0	0	3	0
7	H	28	0	0	3	0
8	A	6	0	0	0	0
8	B	15	0	0	1	0
8	C	10	0	0	1	0
8	D	16	0	0	0	0
8	E	2	0	0	0	0
8	F	11	0	0	0	0
8	G	5	0	0	0	0
8	H	16	0	0	1	0
All	All	36853	0	36131	493	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 7.

The worst 5 of 493 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:HB1	1:A:310:GLY:HA2	1.53	0.91
1:A:445:ARG:HG3	1:A:455:VAL:HG11	1.56	0.86
2:F:31:ASN:HB2	2:F:251:ARG:HD3	1.62	0.82
1:G:136:CYS:HB2	3:G:1463:FES:S2	2.21	0.81
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.61	0.80

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%)	415 (93%)	29 (6%)	2 (0%)	30	59
1	C	446/462 (96%)	425 (95%)	19 (4%)	2 (0%)	30	59
1	E	446/462 (96%)	416 (93%)	29 (6%)	1 (0%)	43	72
1	G	446/462 (96%)	415 (93%)	27 (6%)	4 (1%)	14	41
2	B	756/777 (97%)	722 (96%)	28 (4%)	6 (1%)	16	44
2	D	756/777 (97%)	725 (96%)	24 (3%)	7 (1%)	14	41
2	F	756/777 (97%)	721 (95%)	32 (4%)	3 (0%)	30	59
2	H	756/777 (97%)	711 (94%)	38 (5%)	7 (1%)	14	41
All	All	4808/4956 (97%)	4550 (95%)	226 (5%)	32 (1%)	18	48

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	458	SER
2	D	187	GLU
2	D	458	SER
2	F	187	GLU
2	F	458	SER

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%)	325 (96%)	14 (4%)	27	61
1	C	339/347 (98%)	325 (96%)	14 (4%)	27	61
1	E	339/347 (98%)	324 (96%)	15 (4%)	25	59
1	G	339/347 (98%)	324 (96%)	15 (4%)	25	59
2	B	571/584 (98%)	548 (96%)	23 (4%)	28	62
2	D	571/584 (98%)	543 (95%)	28 (5%)	22	54
2	F	571/584 (98%)	550 (96%)	21 (4%)	30	64
2	H	571/584 (98%)	548 (96%)	23 (4%)	28	62
All	All	3640/3724 (98%)	3487 (96%)	153 (4%)	26	60

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	33	THR
2	H	398	LYS
1	G	128	LEU
2	H	2	SER
2	H	617	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	426	ASN
2	H	72	HIS
2	F	441	ASN
1	G	40	ASN
2	H	234	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
6	HPA	B	1780	-	10,11,11	1.76	1 (10%)	11,15,15	3.44	8 (72%)
3	FES	A	1464	1	0,4,4	-	-	-		
3	FES	E	1464	1	0,4,4	-	-	-		
7	DYI	D	1781	-	20,31,31	4.14	4 (20%)	20,52,52	2.01	5 (25%)
4	FAD	E	1465	-	56,58,58	1.26	4 (7%)	81,89,89	1.62	16 (19%)
4	FAD	C	1465	-	56,58,58	1.25	4 (7%)	81,89,89	1.67	16 (19%)
3	FES	C	1463	1	0,4,4	-	-	-		
4	FAD	A	1465	-	56,58,58	1.27	5 (8%)	81,89,89	1.63	16 (19%)
3	FES	C	1464	1	0,4,4	-	-	-		
3	FES	E	1463	1	0,4,4	-	-	-		
4	FAD	G	1465	-	56,58,58	1.27	5 (8%)	81,89,89	1.60	16 (19%)
6	HPA	D	1780	-	10,11,11	1.76	1 (10%)	11,15,15	3.50	8 (72%)
7	DYI	B	1781	-	20,31,31	4.03	4 (20%)	20,52,52	2.02	5 (25%)
7	DYI	F	1781	-	20,31,31	4.11	4 (20%)	20,52,52	1.79	5 (25%)
6	HPA	F	1780	-	10,11,11	1.77	1 (10%)	11,15,15	3.50	8 (72%)
7	DYI	H	1781	-	20,31,31	4.06	5 (25%)	20,52,52	1.82	6 (30%)
3	FES	G	1464	1	0,4,4	-	-	-		
3	FES	A	1463	1	0,4,4	-	-	-		
6	HPA	H	1780	-	10,11,11	1.77	1 (10%)	11,15,15	3.55	8 (72%)
3	FES	G	1463	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HPA	B	1780	-	-	-	0/2/2/2
3	FES	A	1464	1	-	-	0/1/1/1
3	FES	E	1464	1	-	-	0/1/1/1
7	DYI	D	1781	-	1/1/7/9	5/6/46/46	0/4/4/4
4	FAD	E	1465	-	-	9/34/50/50	0/6/6/6
4	FAD	C	1465	-	-	10/34/50/50	0/6/6/6
3	FES	C	1463	1	-	-	0/1/1/1
4	FAD	A	1465	-	-	10/34/50/50	0/6/6/6
3	FES	C	1464	1	-	-	0/1/1/1
3	FES	E	1463	1	-	-	0/1/1/1
4	FAD	G	1465	-	-	11/34/50/50	0/6/6/6
6	HPA	D	1780	-	-	-	0/2/2/2
7	DYI	B	1781	-	1/1/7/9	3/6/46/46	0/4/4/4
7	DYI	F	1781	-	1/1/7/9	5/6/46/46	0/4/4/4
6	HPA	F	1780	-	-	-	0/2/2/2
7	DYI	H	1781	-	1/1/7/9	1/6/46/46	0/4/4/4
3	FES	G	1464	1	-	-	0/1/1/1
3	FES	A	1463	1	-	-	0/1/1/1
6	HPA	H	1780	-	-	-	0/2/2/2
3	FES	G	1463	1	-	-	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1781	DYI	C4'-C3'	-13.60	1.33	1.52
7	H	1781	DYI	C4'-C3'	-13.25	1.34	1.52
7	B	1781	DYI	C4'-C3'	-13.03	1.34	1.52
7	F	1781	DYI	C4'-C3'	-12.88	1.34	1.52
7	F	1781	DYI	C6-N5	-11.06	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})
6	H	1780	HPA	C5-C6-N1	5.83	120.02	110.57
4	A	1465	FAD	C5A-C4A-N3A	-5.74	119.27	126.75
4	E	1465	FAD	C5A-C4A-N3A	-5.66	119.37	126.75
4	C	1465	FAD	C5A-C4A-N3A	-5.66	119.37	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1780	HPA	C5-C6-N1	5.63	119.70	110.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1781	DYI	C3'
7	D	1781	DYI	C3'
7	F	1781	DYI	C3'
7	H	1781	DYI	C3'

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1465	FAD	N10-C1'-C2'-O2'
4	A	1465	FAD	N10-C1'-C2'-C3'
4	A	1465	FAD	C2'-C3'-C4'-O4'
4	A	1465	FAD	C2'-C3'-C4'-C5'
4	A	1465	FAD	O3'-C3'-C4'-O4'

There are no ring outliers.

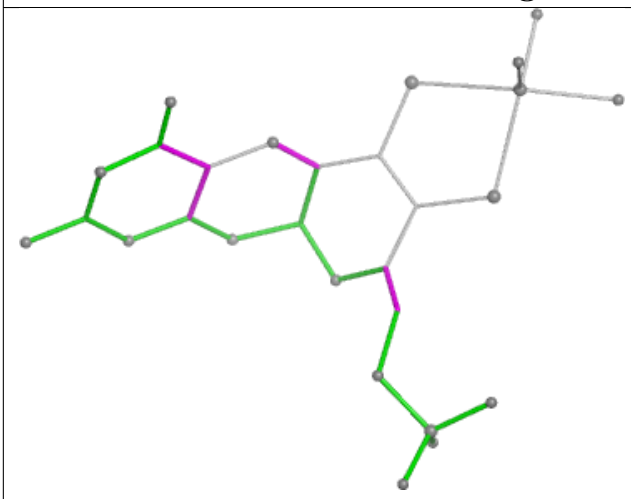
12 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1780	HPA	2	0
7	D	1781	DYI	3	0
4	E	1465	FAD	3	0
4	C	1465	FAD	3	0
4	A	1465	FAD	5	0
4	G	1465	FAD	4	0
6	D	1780	HPA	1	0
7	B	1781	DYI	3	0
7	F	1781	DYI	3	0
6	F	1780	HPA	1	0
7	H	1781	DYI	3	0
3	G	1463	FES	1	0

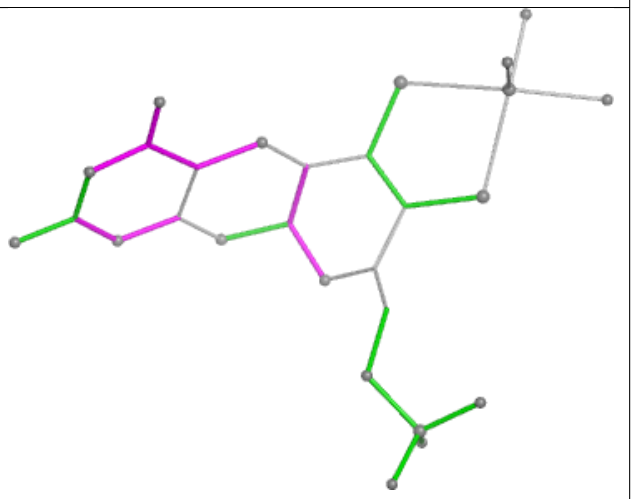
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

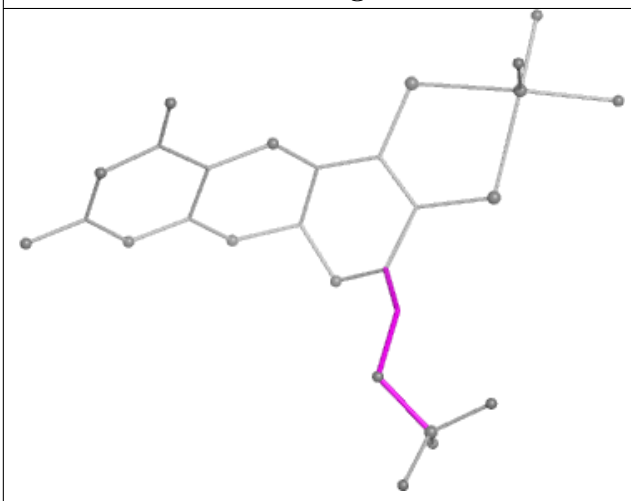
Ligand DYI D 1781



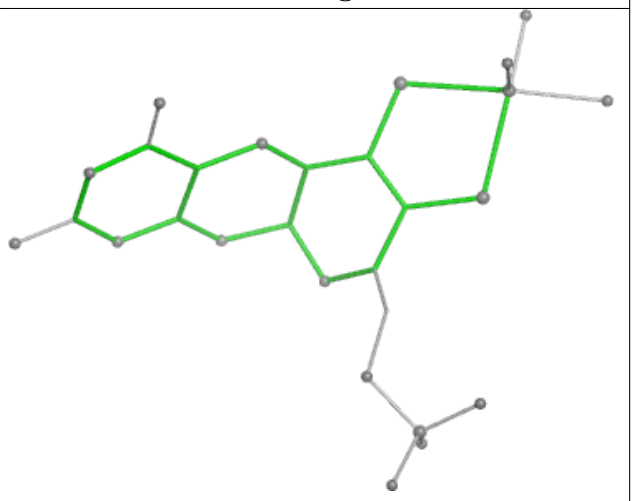
Bond lengths



Bond angles

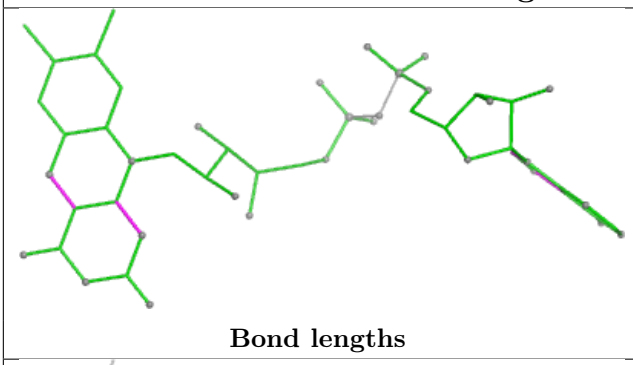


Torsions

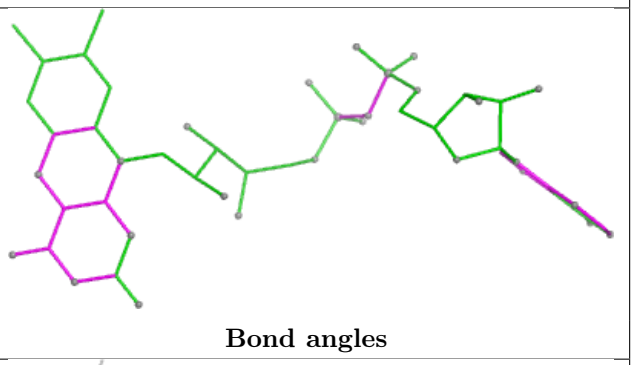


Rings

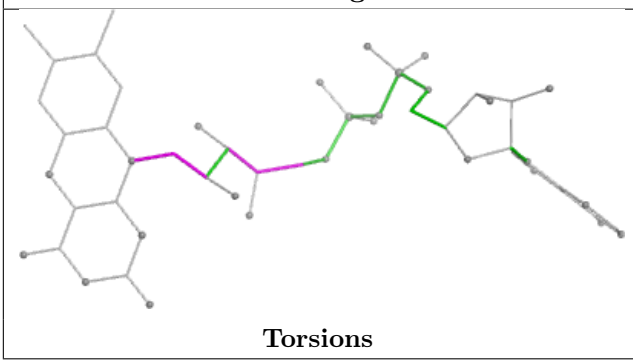
Ligand FAD E 1465



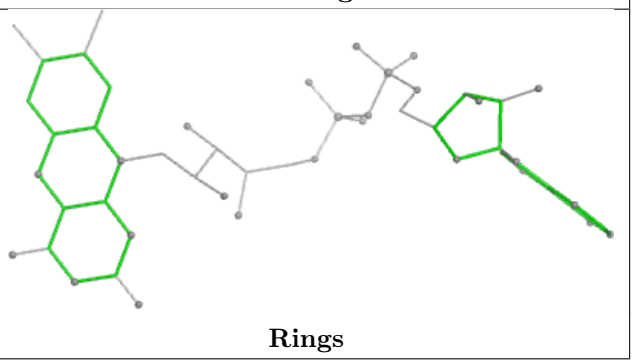
Bond lengths



Bond angles

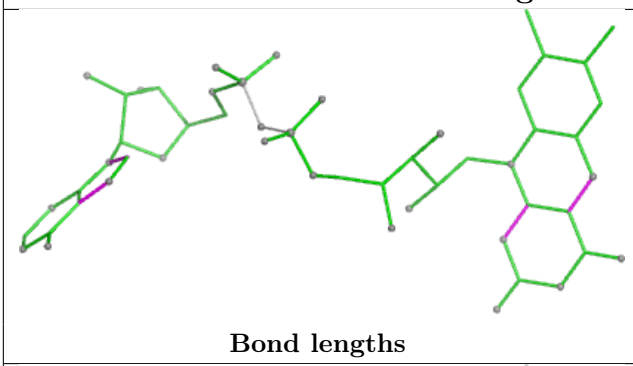


Torsions

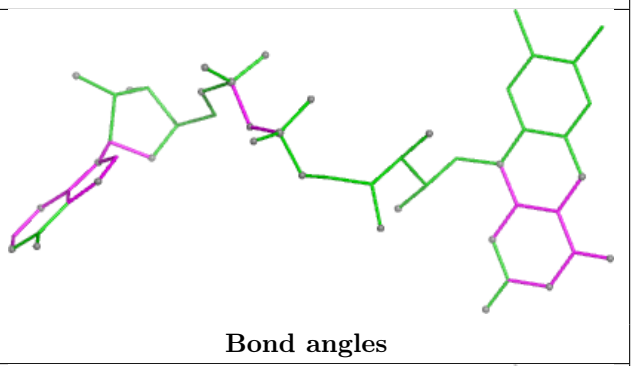


Rings

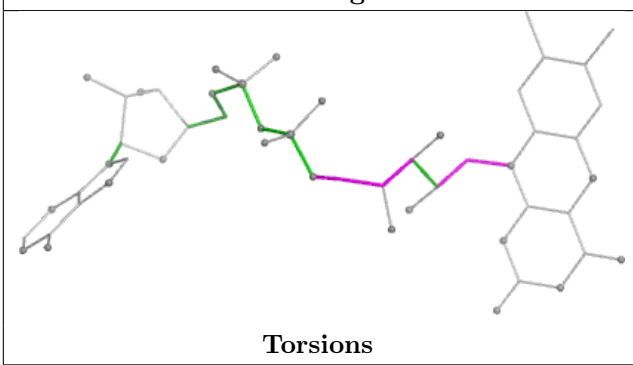
Ligand FAD C 1465



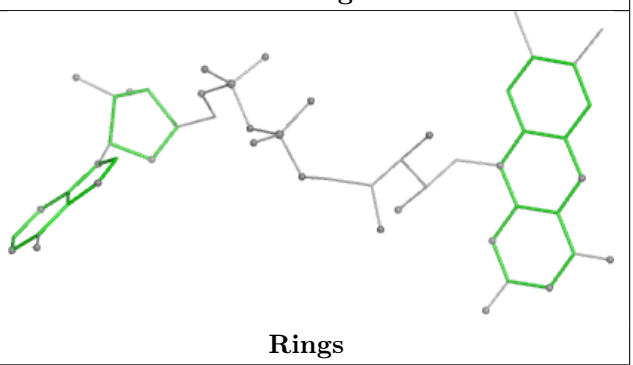
Bond lengths



Bond angles

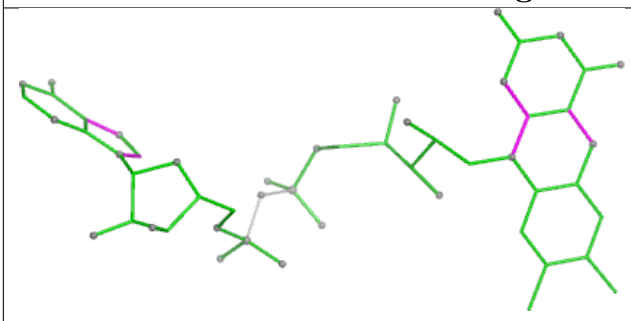


Torsions

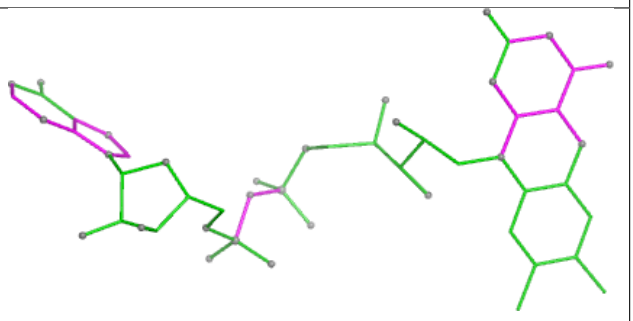


Rings

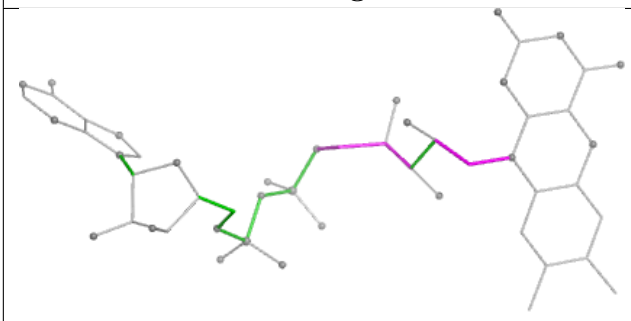
Ligand FAD A 1465



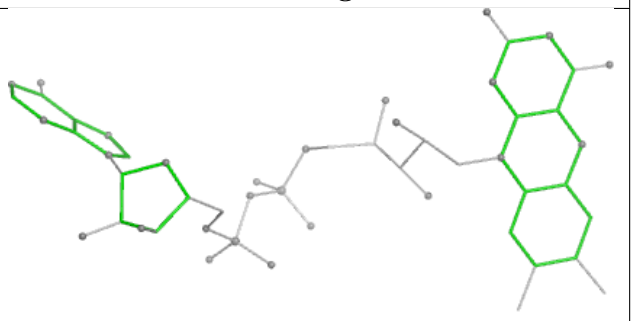
Bond lengths



Bond angles

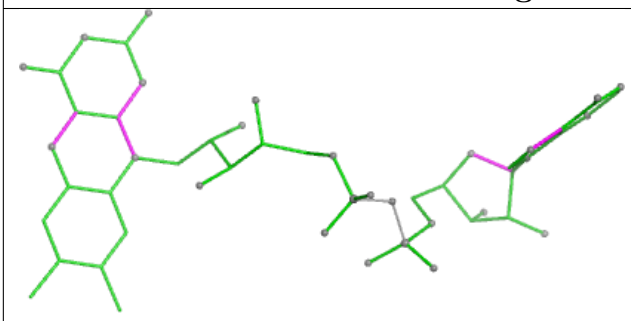


Torsions

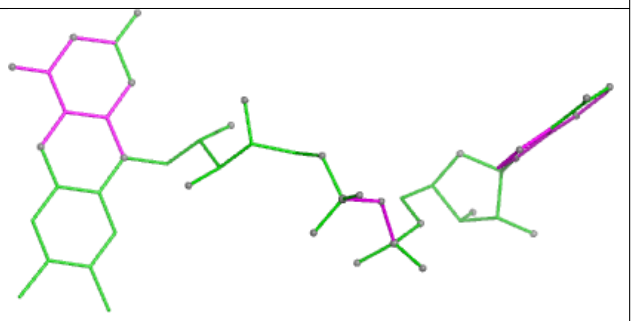


Rings

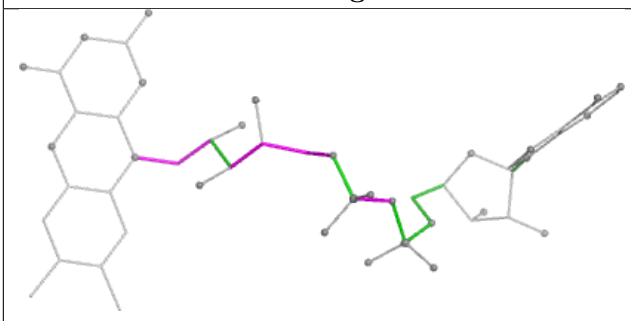
Ligand FAD G 1465



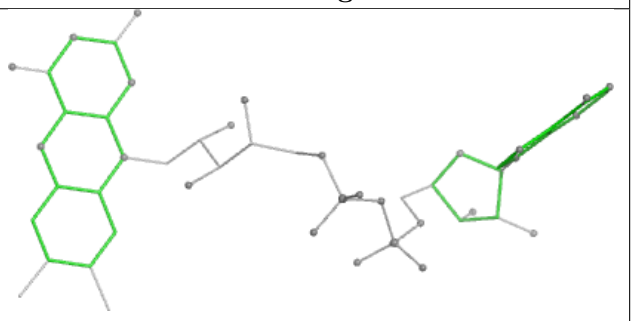
Bond lengths



Bond angles

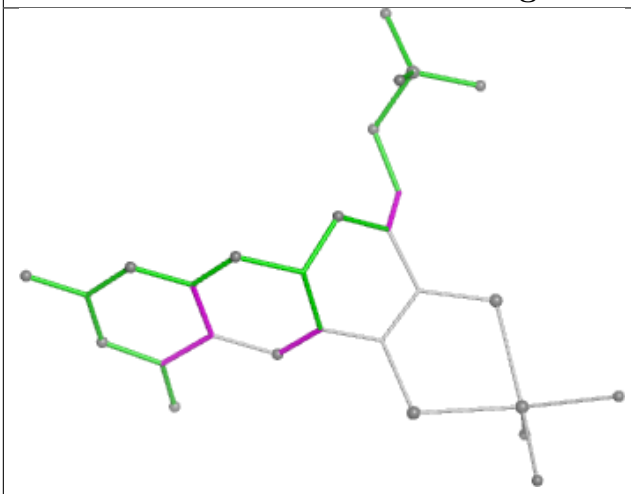


Torsions

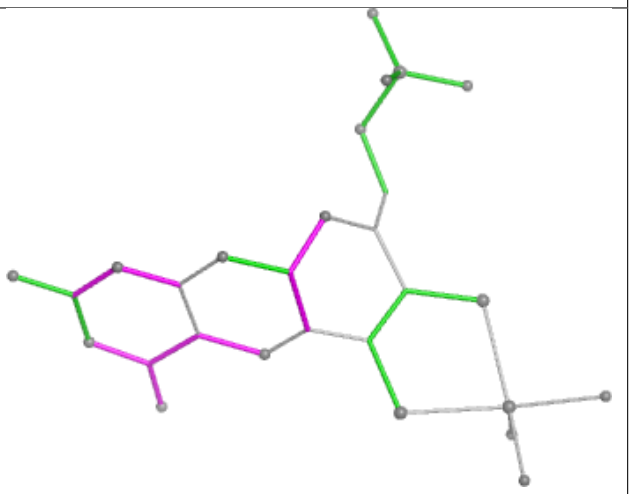


Rings

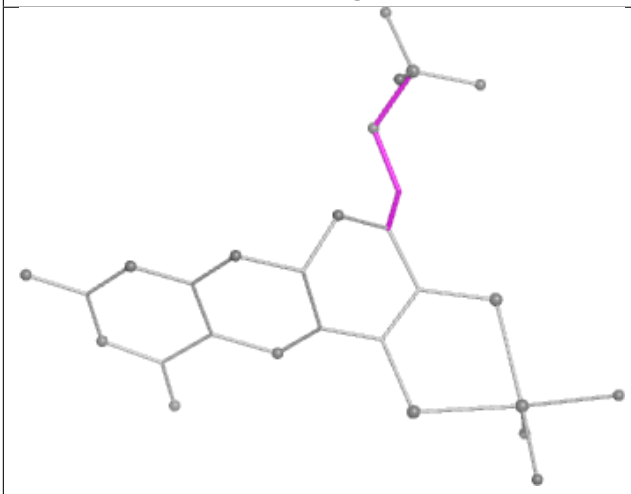
Ligand DYI B 1781



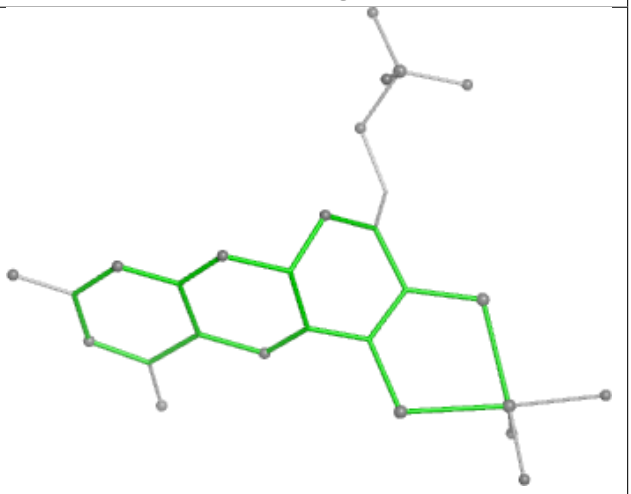
Bond lengths



Bond angles

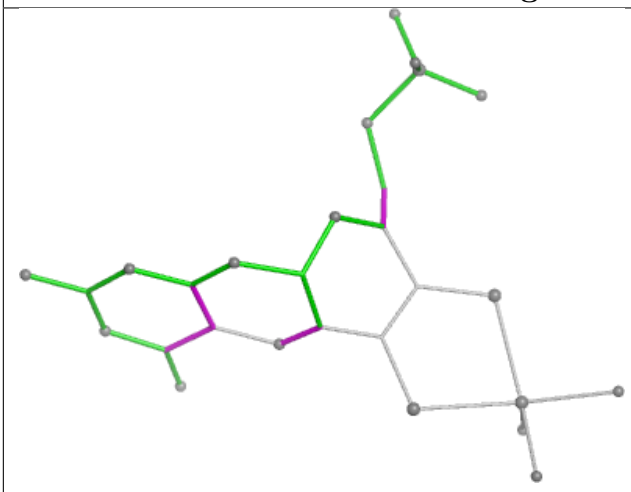


Torsions

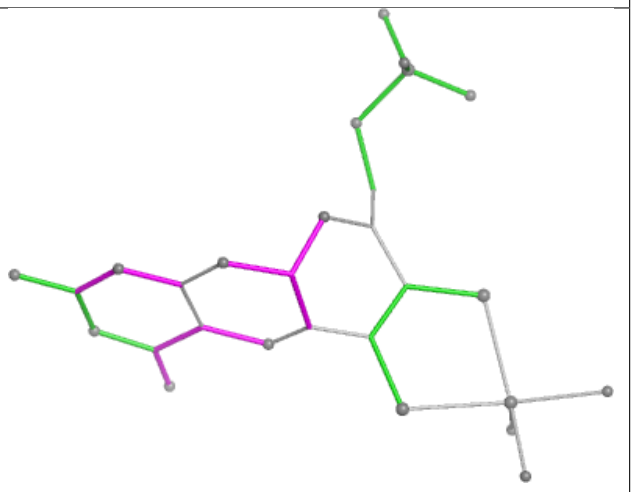


Rings

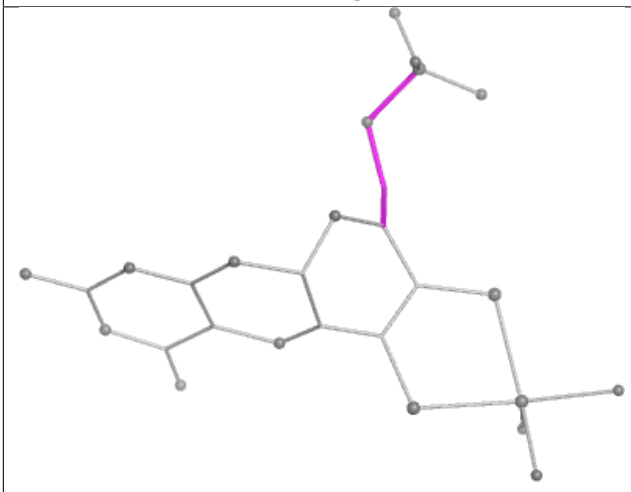
Ligand DYI F 1781



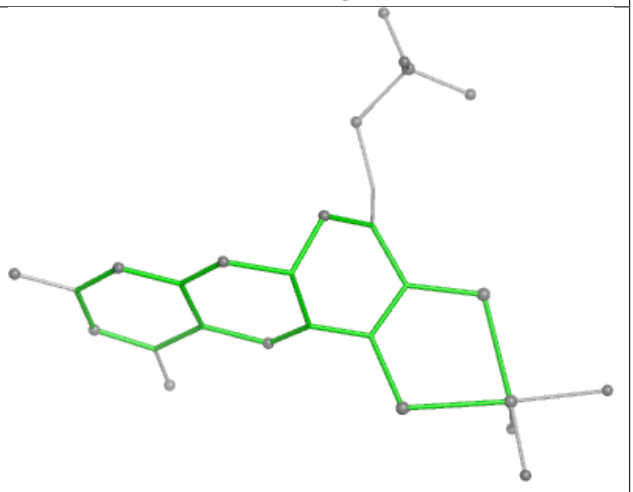
Bond lengths



Bond angles

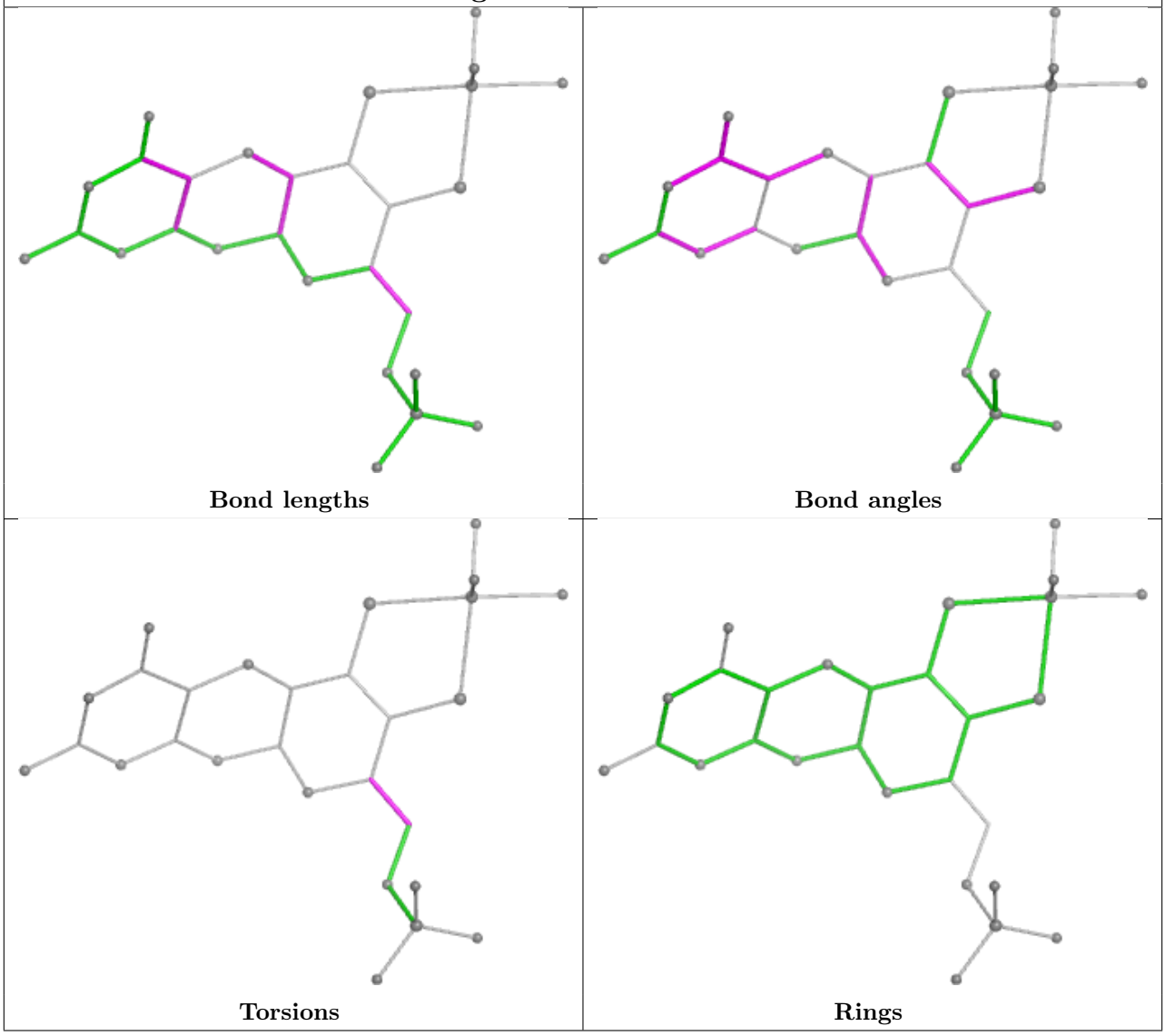


Torsions



Rings

Ligand DYI H 1781



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	450/462 (97%)	1.10	58 (12%) 7 6	40, 63, 78, 79	0
1	C	450/462 (97%)	1.37	94 (20%) 2 2	40, 63, 77, 79	0
1	E	450/462 (97%)	1.16	55 (12%) 8 7	40, 63, 78, 79	0
1	G	450/462 (97%)	1.27	62 (13%) 6 5	40, 63, 78, 79	0
2	B	760/777 (97%)	0.46	14 (1%) 67 59	34, 47, 60, 65	0
2	D	760/777 (97%)	0.61	21 (2%) 55 46	34, 46, 60, 65	0
2	F	760/777 (97%)	0.57	14 (1%) 67 59	35, 46, 60, 65	0
2	H	760/777 (97%)	0.56	9 (1%) 76 69	35, 47, 60, 66	0
All	All	4840/4956 (97%)	0.80	327 (6%) 23 18	34, 51, 75, 79	0

The worst 5 of 327 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	166	LEU	7.9
1	C	166	LEU	5.8
1	G	166	LEU	5.5
1	A	166	LEU	5.2
2	D	560	GLY	5.0

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 oligosaccharides in this entry.

6.4 Ligands (i)

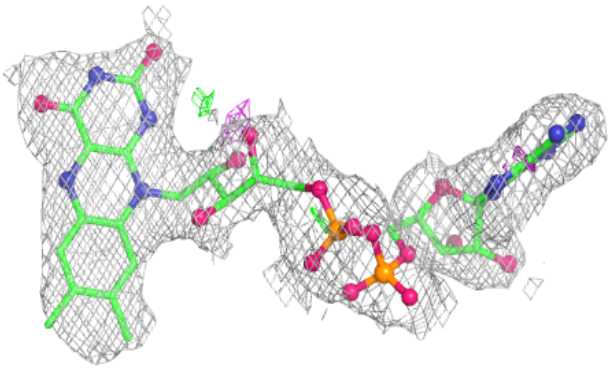
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

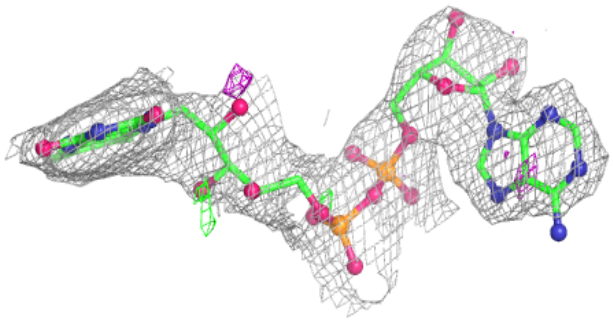
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	HPA	F	1780	10/10	0.80	0.19	55,56,57,57	0
6	HPA	B	1780	10/10	0.81	0.19	57,58,58,58	0
6	HPA	D	1780	10/10	0.82	0.19	52,53,54,54	0
6	HPA	H	1780	10/10	0.83	0.15	59,59,60,60	0
4	FAD	G	1465	53/53	0.88	0.15	68,70,76,76	0
4	FAD	A	1465	53/53	0.90	0.12	58,61,68,68	0
4	FAD	E	1465	53/53	0.92	0.12	51,58,73,73	0
7	DYI	H	1781	28/28	0.92	0.18	60,61,65,66	27
7	DYI	B	1781	28/28	0.93	0.18	50,52,55,58	27
4	FAD	C	1465	53/53	0.94	0.10	32,35,44,44	0
7	DYI	D	1781	28/28	0.96	0.13	30,37,39,40	27
7	DYI	F	1781	28/28	0.96	0.14	39,41,42,42	27
5	CA	H	1779	1/1	0.96	0.07	65,65,65,65	0
5	CA	B	1779	1/1	0.97	0.05	55,55,55,55	0
5	CA	D	1779	1/1	0.97	0.04	48,48,48,48	0
5	CA	F	1779	1/1	0.97	0.07	54,54,54,54	0
3	FES	C	1464	4/4	0.98	0.07	42,42,44,46	0
3	FES	E	1463	4/4	0.98	0.05	43,43,45,45	0
3	FES	E	1464	4/4	0.98	0.07	55,56,56,58	0
3	FES	G	1463	4/4	0.98	0.04	47,49,50,50	0
3	FES	A	1464	4/4	0.98	0.06	52,52,53,53	0
3	FES	C	1463	4/4	0.99	0.06	38,40,40,41	0
3	FES	G	1464	4/4	0.99	0.06	53,55,55,56	0
3	FES	A	1463	4/4	0.99	0.04	41,42,42,43	0

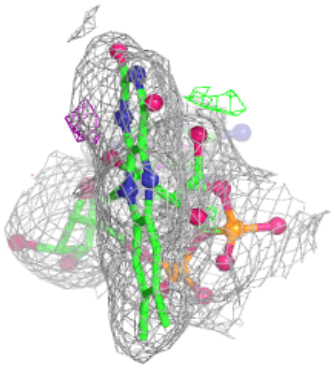
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

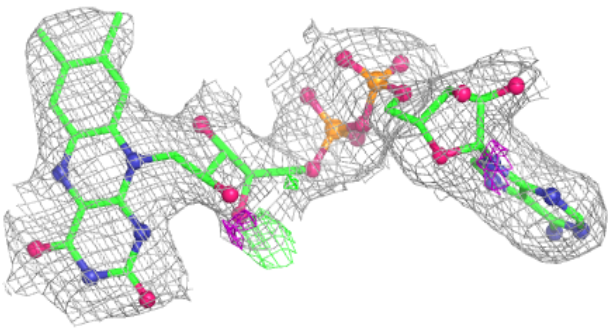


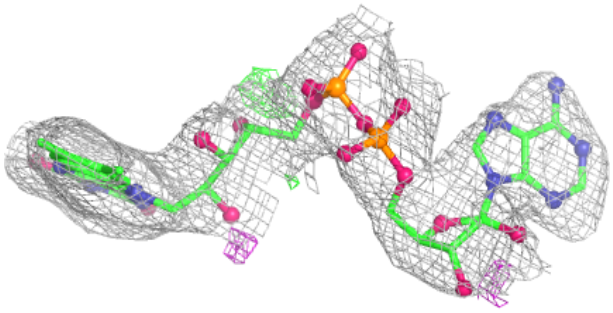


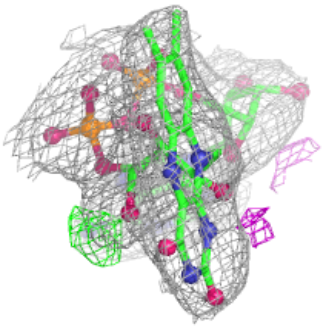


Electron density around FAD A 1465:

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

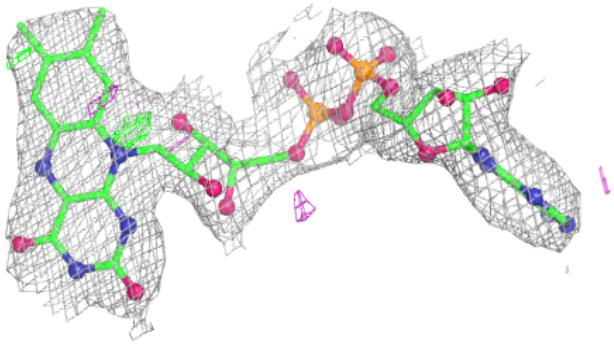


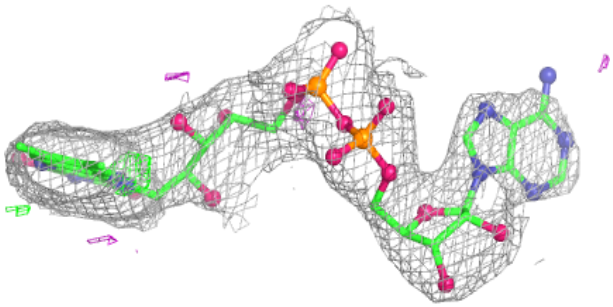


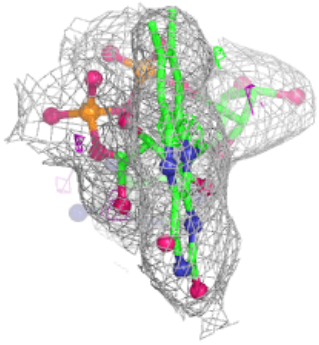


Electron density around FAD E 1465:

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

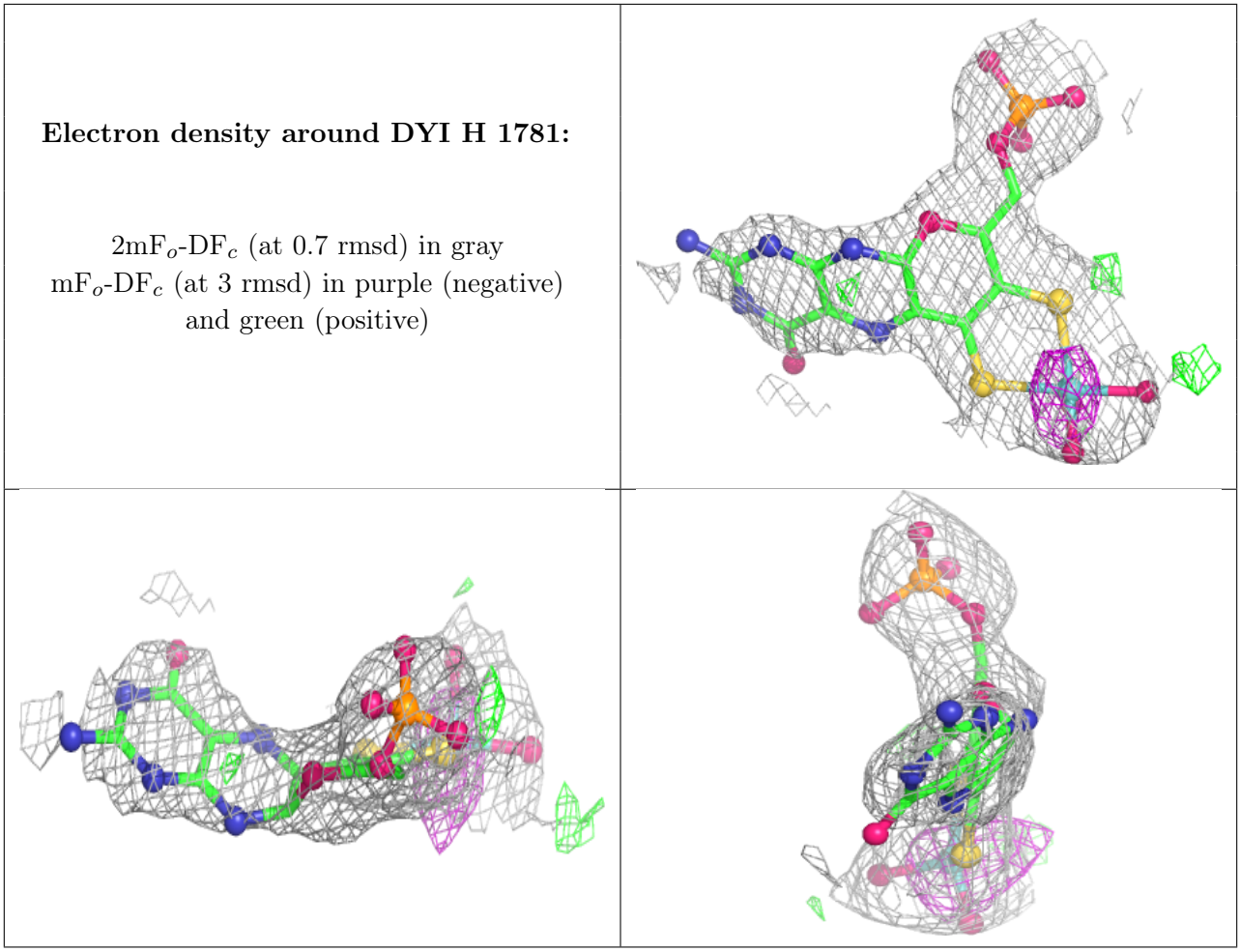






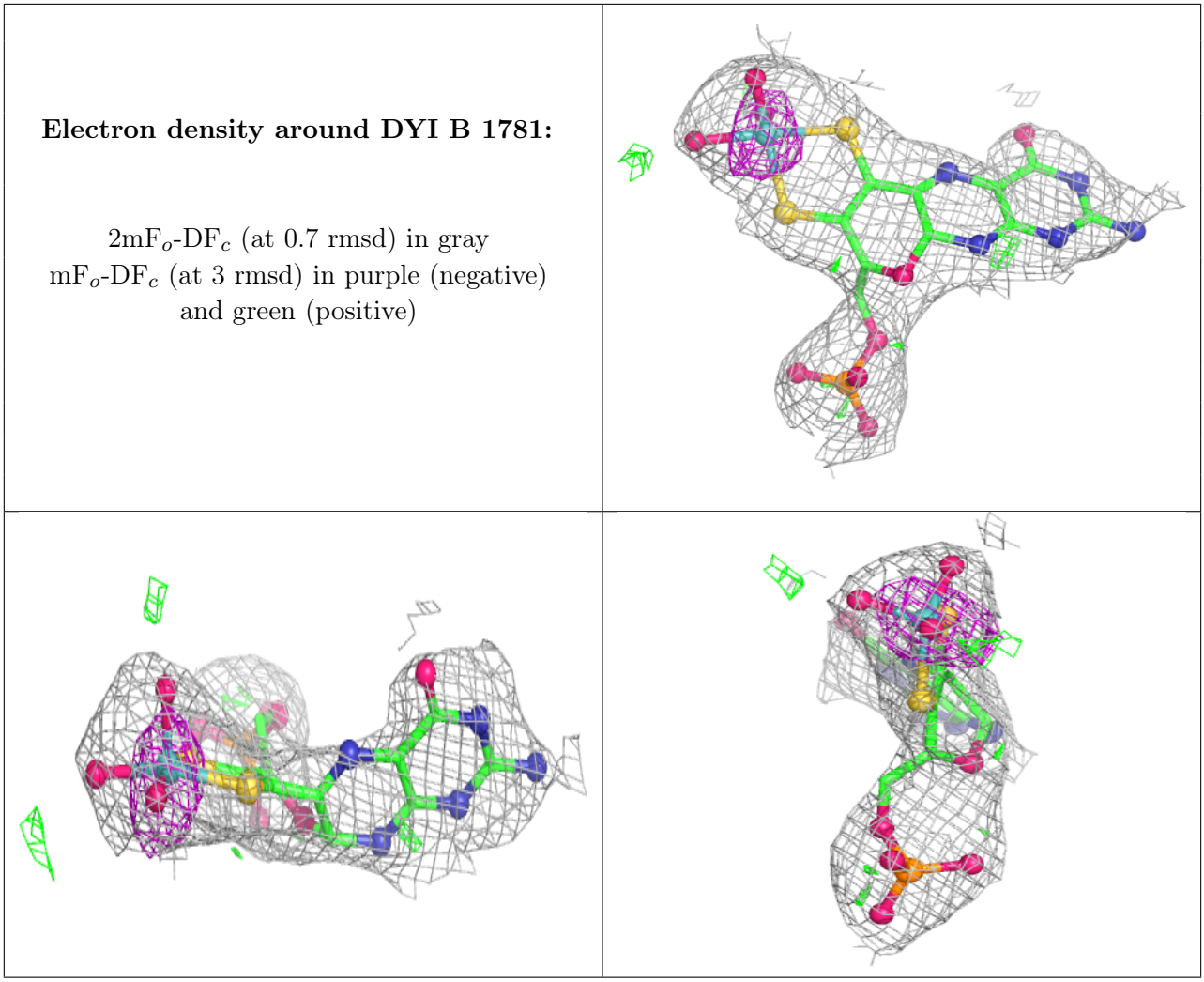
Electron density around DYI H 1781:

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



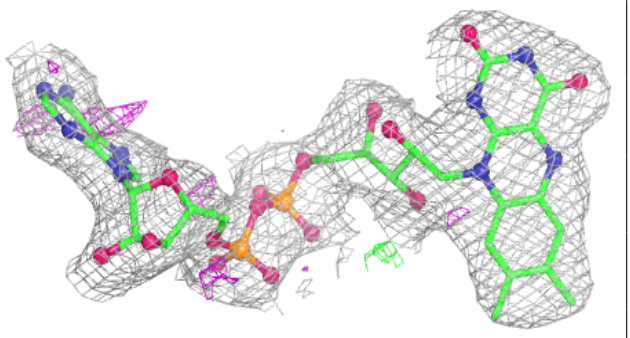
Electron density around DYI B 1781:

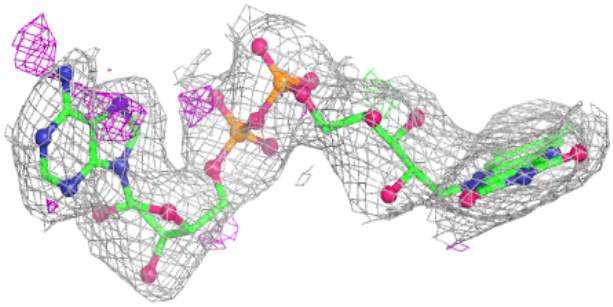
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

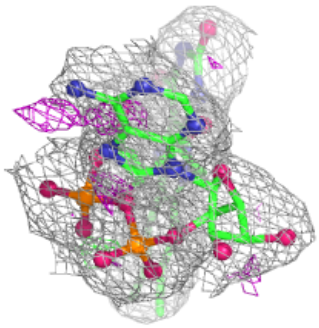


Electron density around FAD C 1465:

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

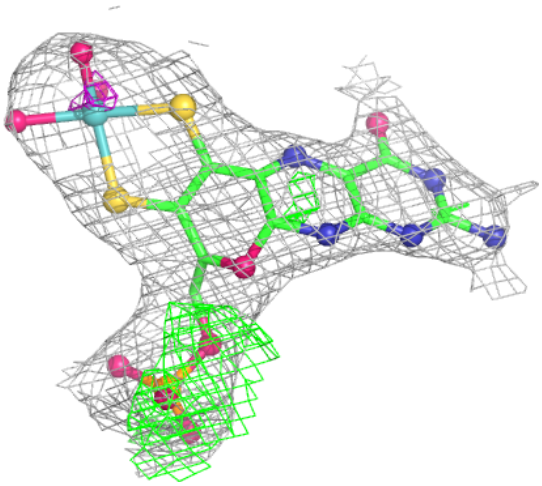


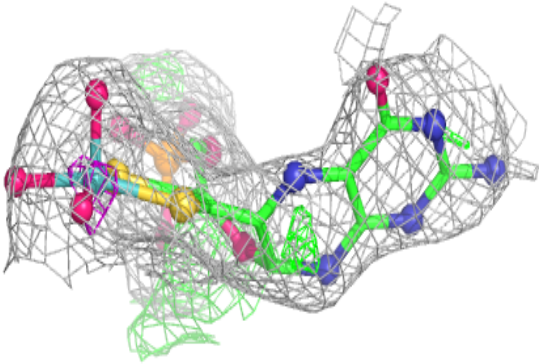


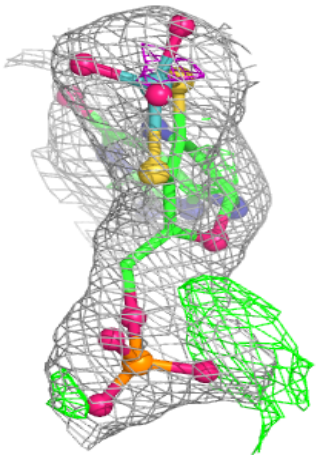


Electron density around DYI D 1781:

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

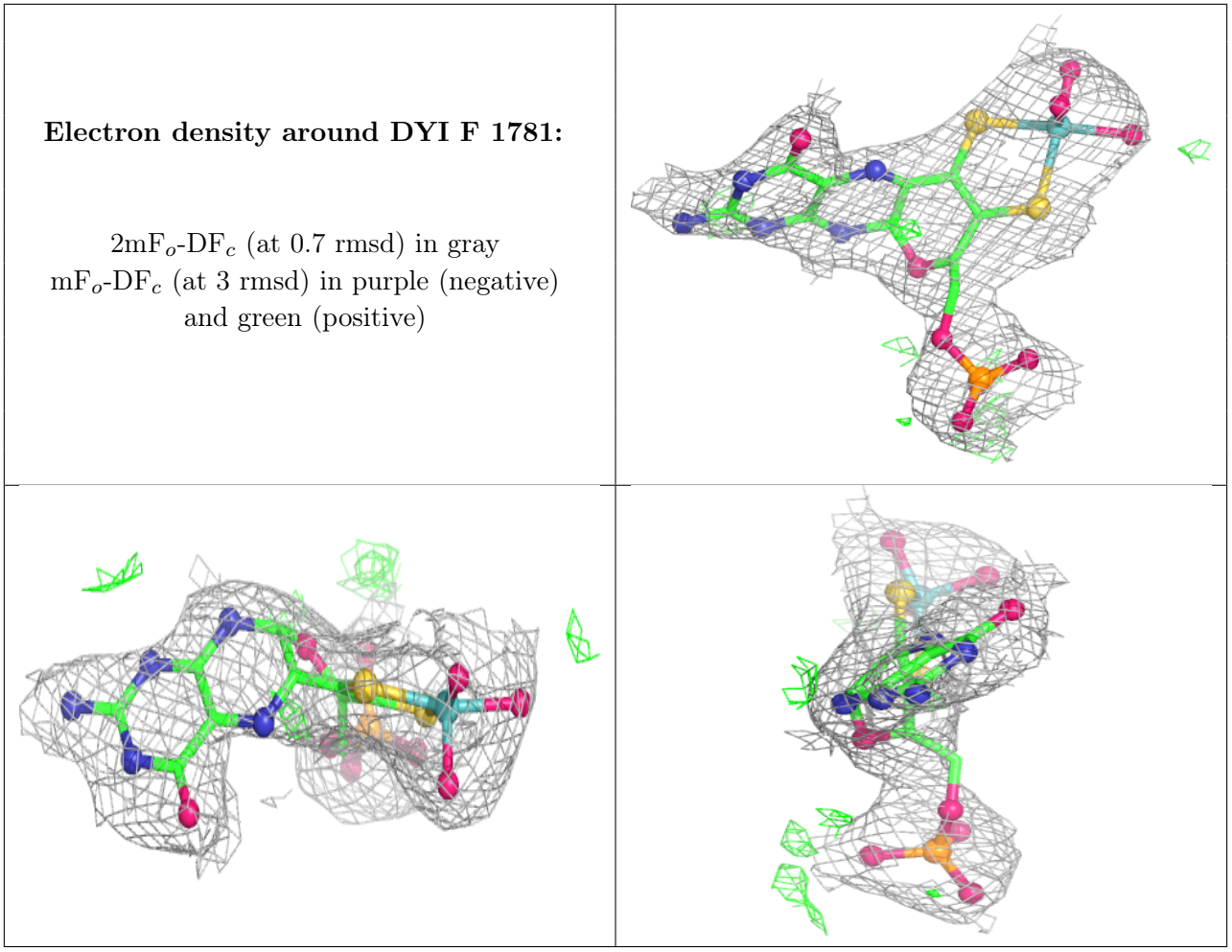






Electron density around DYI F 1781:

$2mF_o$-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.