



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:12 pm BST

PDB ID : 2W55  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

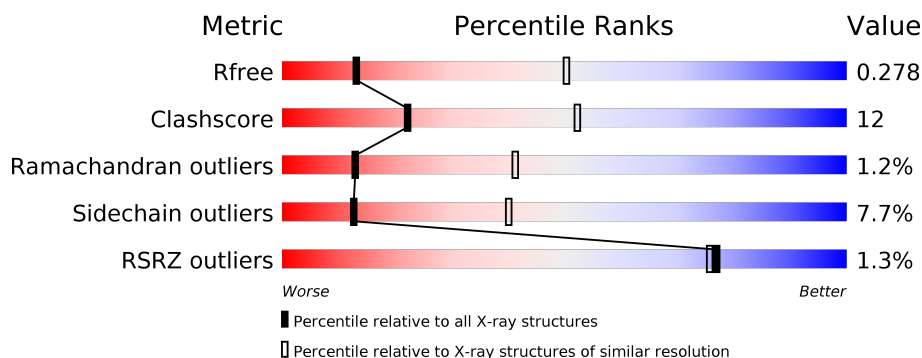
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	462	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>• •</div> </div> </div>
1	C	462	<div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	E	462	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	G	462	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>• •</div> </div> </div>
2	B	777	<div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
2	D	777	<div> <div>68%</div> <div>27%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	777	
2	H	777	

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
1	A	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	C	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	E	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	G	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	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

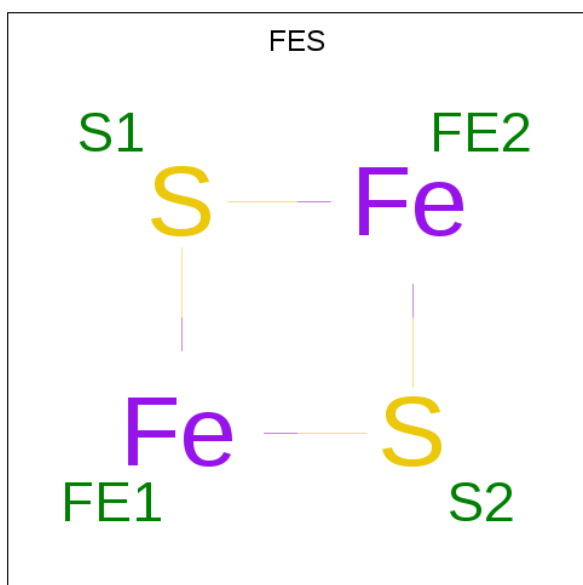
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

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

There are 8 discrepancies between the modelled and reference sequences:

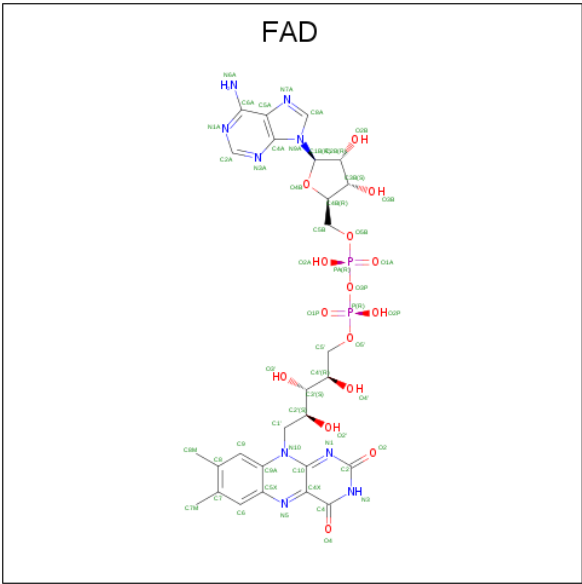
Chain	Residue	Modelled	Actual	Comment	Reference
B	232	GLN	GLU	engineered mutation	UNP O54051
B	772	ARG	GLY	conflict	UNP O54051
D	232	GLN	GLU	engineered mutation	UNP O54051
D	772	ARG	GLY	conflict	UNP O54051
F	232	GLN	GLU	engineered mutation	UNP O54051
F	772	ARG	GLY	conflict	UNP O54051
H	232	GLN	GLU	engineered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

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



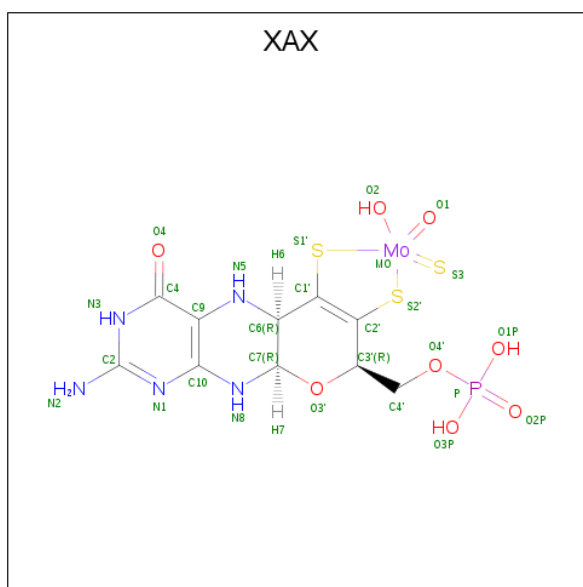
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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 {[ (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 (three-letter code: XAX) (formula: C<sub>10</sub>H<sub>13</sub>MoN<sub>5</sub>O<sub>8</sub>PS<sub>3</sub>).

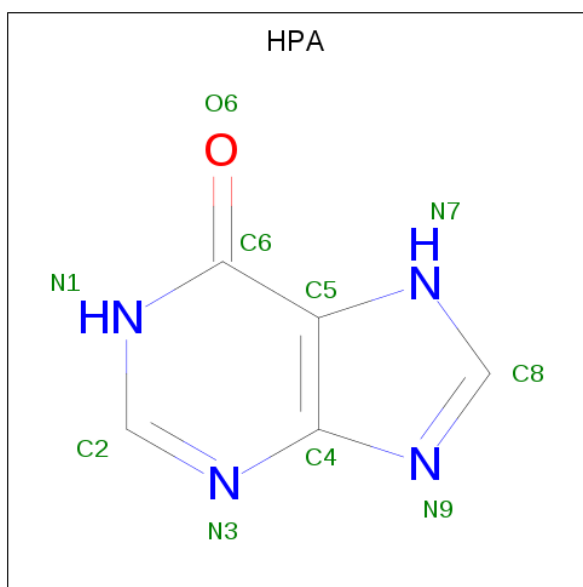


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	D	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	F	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	H	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

- Molecule 6 is BARIUM ION (three-letter code: BA) (formula: Ba).

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

- Molecule 7 is HYPOXANTHINE (three-letter code: HPA) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O).



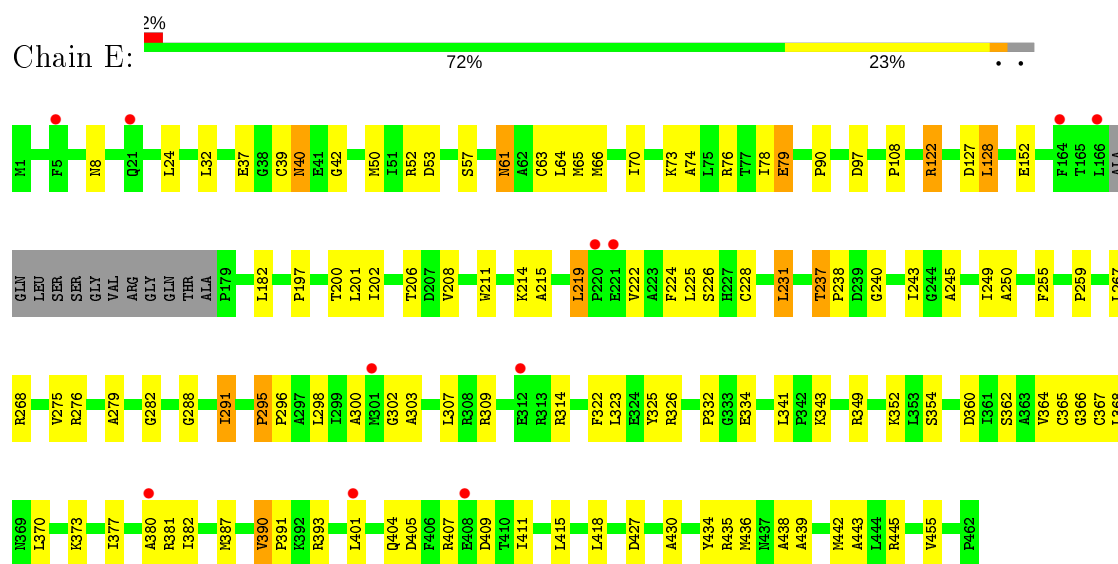
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			10	5	4	1		
7	D	1	Total	C	N	O	0	0
			10	5	4	1		
7	F	1	Total	C	N	O	0	0
			10	5	4	1		
7	H	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 8 is water.

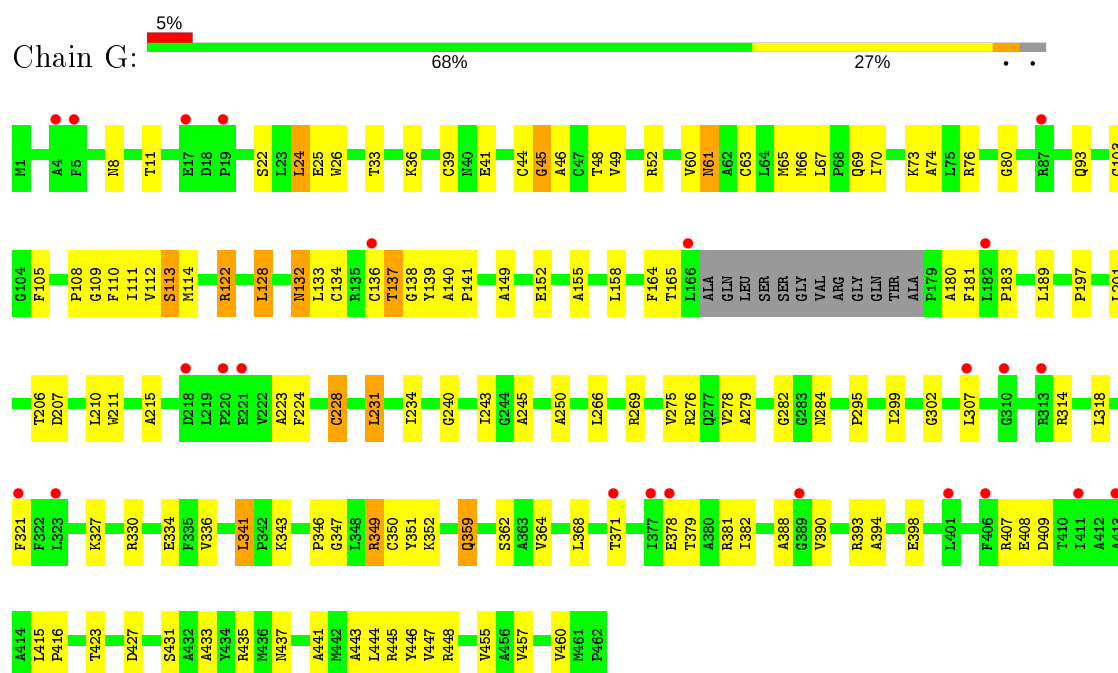
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	O	0	0
			4	4		
8	B	8	Total	O	0	0
			8	8		
8	C	3	Total	O	0	0
			3	3		
8	D	11	Total	O	0	0
			11	11		
8	E	1	Total	O	0	0
			1	1		
8	F	12	Total	O	0	0
			12	12		
8	G	1	Total	O	0	0
			1	1		
8	H	3	Total	O	0	0
			3	3		



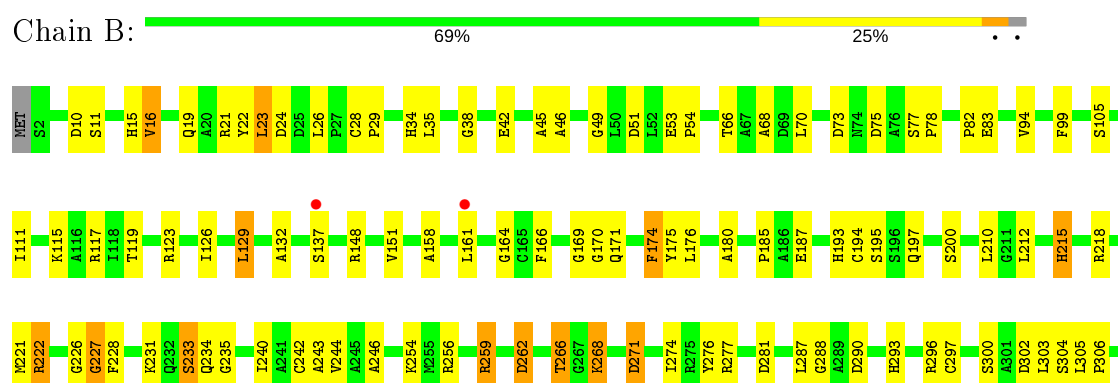


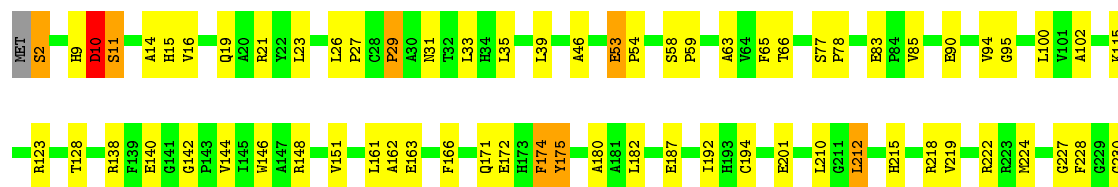


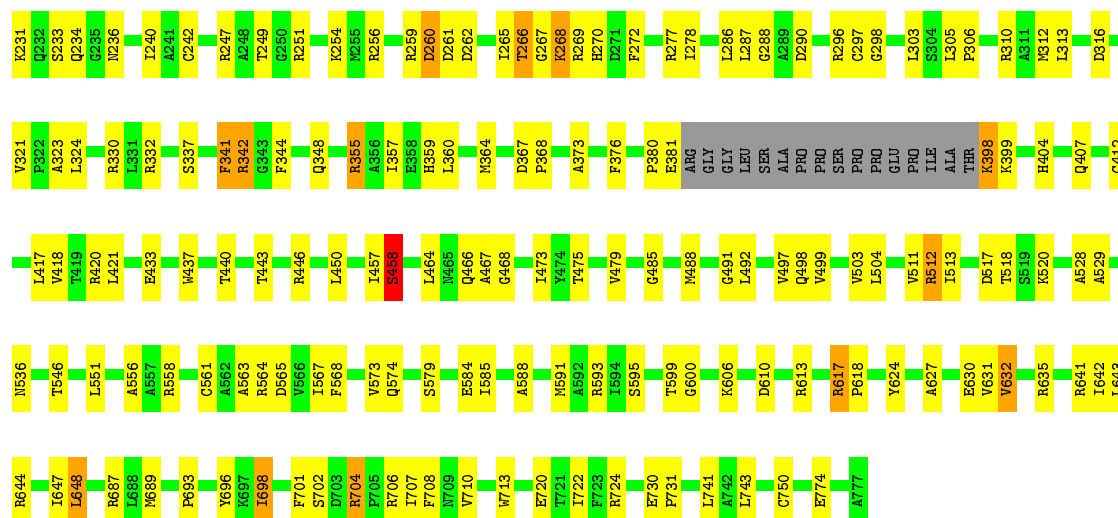
• Molecule 1: XANTHINE DEHYDROGENASE



• Molecule 2: XANTHINE DEHYDROGENASE

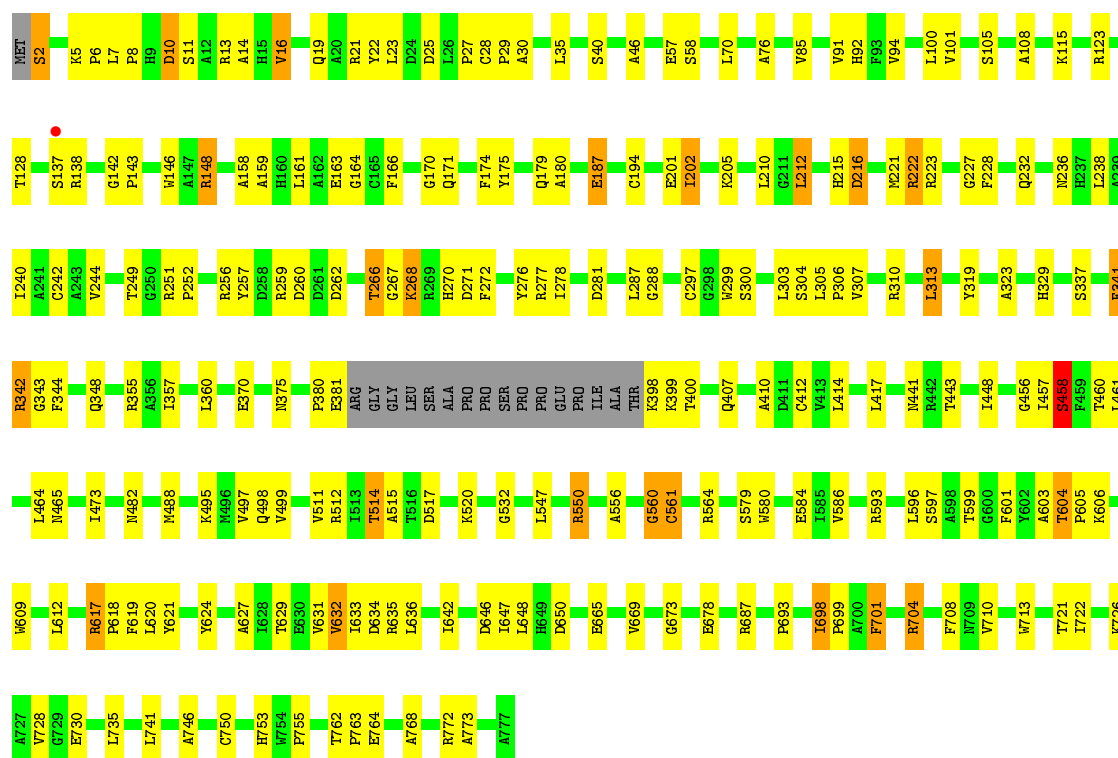






• Molecule 2: XANTHINE DEHYDROGENASE

Chain H: 69% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.74Å 140.57Å 157.61Å 109.45° 106.10° 101.09°	Depositor
Resolution (Å)	50.00 – 3.40 49.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-3.40) 77.9 (49.83-3.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality [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, FAD, 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	0.36	0/3438	0.54	0/4658
1	C	0.35	0/3438	0.54	0/4658
1	E	0.35	0/3438	0.53	0/4658
1	G	0.36	0/3438	0.55	0/4658
2	B	0.35	0/5844	0.53	0/7941
2	D	0.36	0/5844	0.55	0/7941
2	F	0.37	0/5844	0.56	0/7941
2	H	0.36	0/5844	0.53	0/7941
All	All	0.36	0/37128	0.54	0/50396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	69	0
1	C	3375	0	3368	64	0
1	E	3375	0	3369	72	0
1	G	3375	0	3371	87	0
2	B	5716	0	5633	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5716	0	5633	155	0
2	F	5716	0	5633	145	0
2	H	5716	0	5633	142	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	3	0
4	G	53	0	31	8	0
5	B	28	0	8	4	0
5	D	28	0	8	7	0
5	F	28	0	8	8	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	851	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 851 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	14	44
1	C	446/462 (96%)	405 (91%)	37 (8%)	4 (1%)	17	49
1	E	446/462 (96%)	406 (91%)	34 (8%)	6 (1%)	12	39
1	G	446/462 (96%)	393 (88%)	47 (10%)	6 (1%)	12	39
2	B	756/777 (97%)	707 (94%)	39 (5%)	10 (1%)	12	39
2	D	756/777 (97%)	685 (91%)	65 (9%)	6 (1%)	19	51
2	F	756/777 (97%)	690 (91%)	58 (8%)	8 (1%)	14	44
2	H	756/777 (97%)	699 (92%)	46 (6%)	11 (2%)	10	36
All	All	4808/4956 (97%)	4379 (91%)	373 (8%)	56 (1%)	13	41

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 ⓘ

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%)	310 (91%)	29 (9%)	10	35
1	C	339/347 (98%)	316 (93%)	23 (7%)	16	45
1	E	339/347 (98%)	321 (95%)	18 (5%)	22	52
1	G	339/347 (98%)	318 (94%)	21 (6%)	18	48
2	B	571/584 (98%)	526 (92%)	45 (8%)	12	39
2	D	571/584 (98%)	523 (92%)	48 (8%)	11	36
2	F	571/584 (98%)	521 (91%)	50 (9%)	10	33
2	H	571/584 (98%)	524 (92%)	47 (8%)	11	37
All	All	3640/3724 (98%)	3359 (92%)	281 (8%)	13	40

5 of 281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	464	LEU
1	E	349	ARG
2	H	441	ASN
2	D	514	THR
2	D	720	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	422	GLN
2	D	753	HIS
2	H	293	HIS
2	D	426	ASN
2	D	466	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates 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$
7	HPA	H	1780	-	8,11,11	2.24	3 (37%)	5,15,15	3.03	3 (60%)
4	FAD	C	1465	-	51,58,58	1.72	6 (11%)	60,89,89	1.55	9 (15%)
7	HPA	B	1780	-	8,11,11	2.39	3 (37%)	5,15,15	2.95	3 (60%)
4	FAD	E	1465	-	51,58,58	1.75	6 (11%)	60,89,89	1.51	8 (13%)
7	HPA	D	1780	-	8,11,11	2.18	3 (37%)	5,15,15	3.02	3 (60%)
4	FAD	G	1465	-	51,58,58	1.79	6 (11%)	60,89,89	1.57	11 (18%)
3	FES	E	1464	1	0,4,4	0.00	-	-	-	-
5	XAX	H	1778	-	20,31,31	3.92	5 (25%)	22,52,52	2.36	7 (31%)
5	XAX	F	1778	-	20,31,31	3.80	5 (25%)	22,52,52	2.22	6 (27%)
3	FES	G	1464	1	0,4,4	0.00	-	-	-	-
3	FES	E	1463	1	0,4,4	0.00	-	-	-	-
5	XAX	B	1778	-	20,31,31	3.80	5 (25%)	22,52,52	2.44	6 (27%)
3	FES	G	1463	1	0,4,4	0.00	-	-	-	-
3	FES	A	1463	1	0,4,4	0.00	-	-	-	-
3	FES	A	1464	1	0,4,4	0.00	-	-	-	-
3	FES	C	1463	1	0,4,4	0.00	-	-	-	-
5	XAX	D	1778	-	20,31,31	3.89	6 (30%)	22,52,52	2.08	4 (18%)
3	FES	C	1464	1	0,4,4	0.00	-	-	-	-
7	HPA	F	1780	-	8,11,11	2.30	3 (37%)	5,15,15	2.77	3 (60%)
4	FAD	A	1465	-	51,58,58	1.80	7 (13%)	60,89,89	1.51	9 (15%)

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
7	HPA	H	1780	-	-	-	0/2/2/2
4	FAD	C	1465	-	-	11/30/50/50	0/6/6/6
7	HPA	B	1780	-	-	-	0/2/2/2
4	FAD	E	1465	-	-	10/30/50/50	0/6/6/6
7	HPA	D	1780	-	-	-	0/2/2/2
4	FAD	G	1465	-	-	12/30/50/50	0/6/6/6
3	FES	E	1464	1	-	-	0/1/1/1
5	XAX	H	1778	-	1/1/7/9	2/6/46/46	0/4/4/4
3	FES	C	1464	1	-	-	0/1/1/1
3	FES	G	1464	1	-	-	0/1/1/1
3	FES	E	1463	1	-	-	0/1/1/1
5	XAX	B	1778	-	1/1/7/9	3/6/46/46	0/4/4/4
3	FES	G	1463	1	-	-	0/1/1/1
3	FES	A	1463	1	-	-	0/1/1/1
5	XAX	F	1778	-	1/1/7/9	2/6/46/46	0/4/4/4
3	FES	C	1463	1	-	-	0/1/1/1
5	XAX	D	1778	-	1/1/7/9	2/6/46/46	0/4/4/4
3	FES	A	1464	1	-	-	0/1/1/1
7	HPA	F	1780	-	-	-	0/2/2/2
4	FAD	A	1465	-	-	18/30/50/50	0/6/6/6

The worst 5 of 58 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	-8.29	1.33	1.45

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1778	XAX	C4-C9-N5	6.53	124.60	119.12
5	F	1778	XAX	C4-C9-N5	5.95	124.11	119.12
4	G	1465	FAD	C4-N3-C2	5.95	120.16	115.14
5	D	1778	XAX	C4-C9-N5	5.88	124.05	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	H	1778	XAX	C4-C9-N5	5.76	123.96	119.12

All (4) chirality outliers are listed below:

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

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1778	XAX	O3'-C3'-C4'-O4'
4	E	1465	FAD	C2'-C1'-N10-C9A
4	E	1465	FAD	N10-C1'-C2'-O2'
4	E	1465	FAD	N10-C1'-C2'-C3'
4	E	1465	FAD	C2'-C3'-C4'-O4'

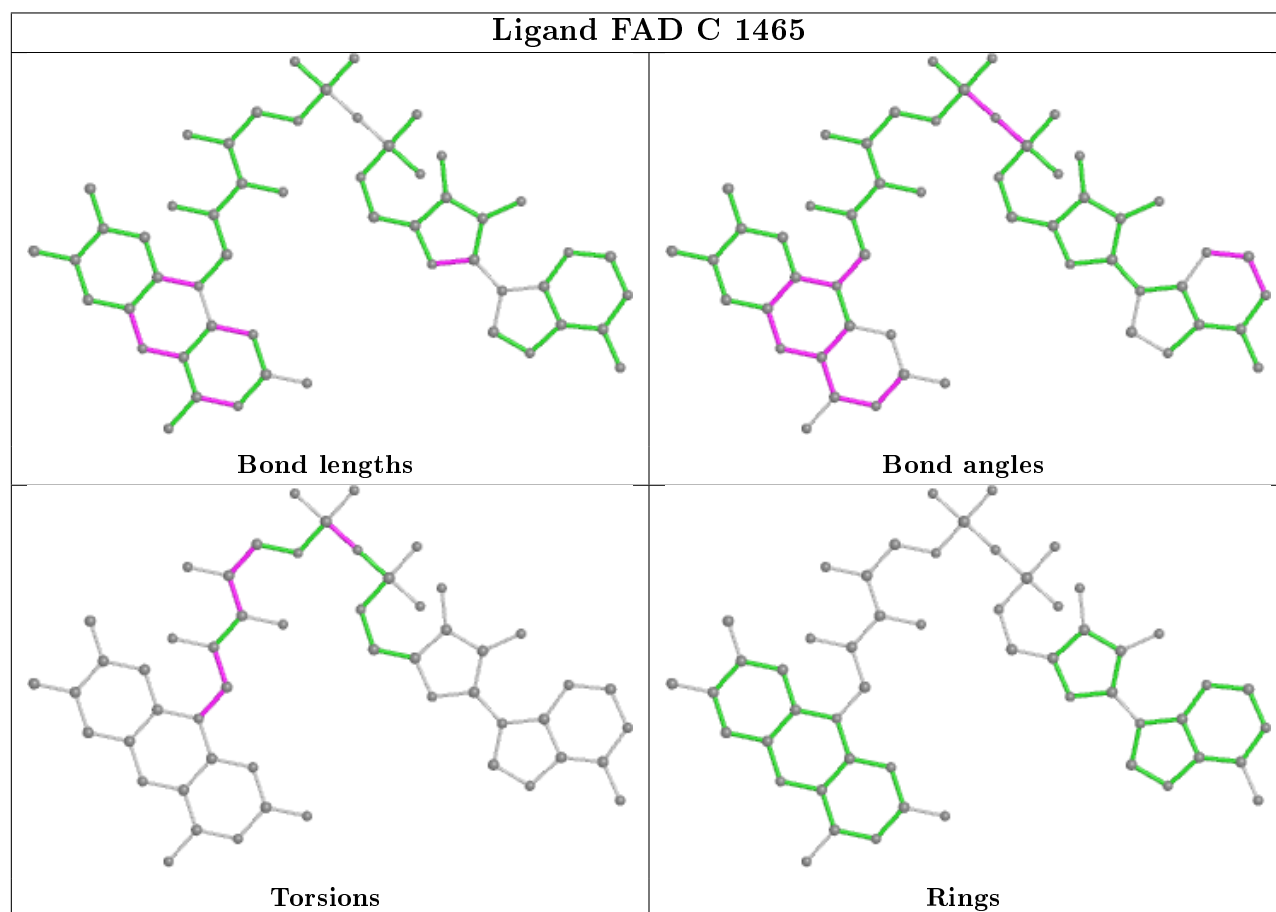
There are no ring outliers.

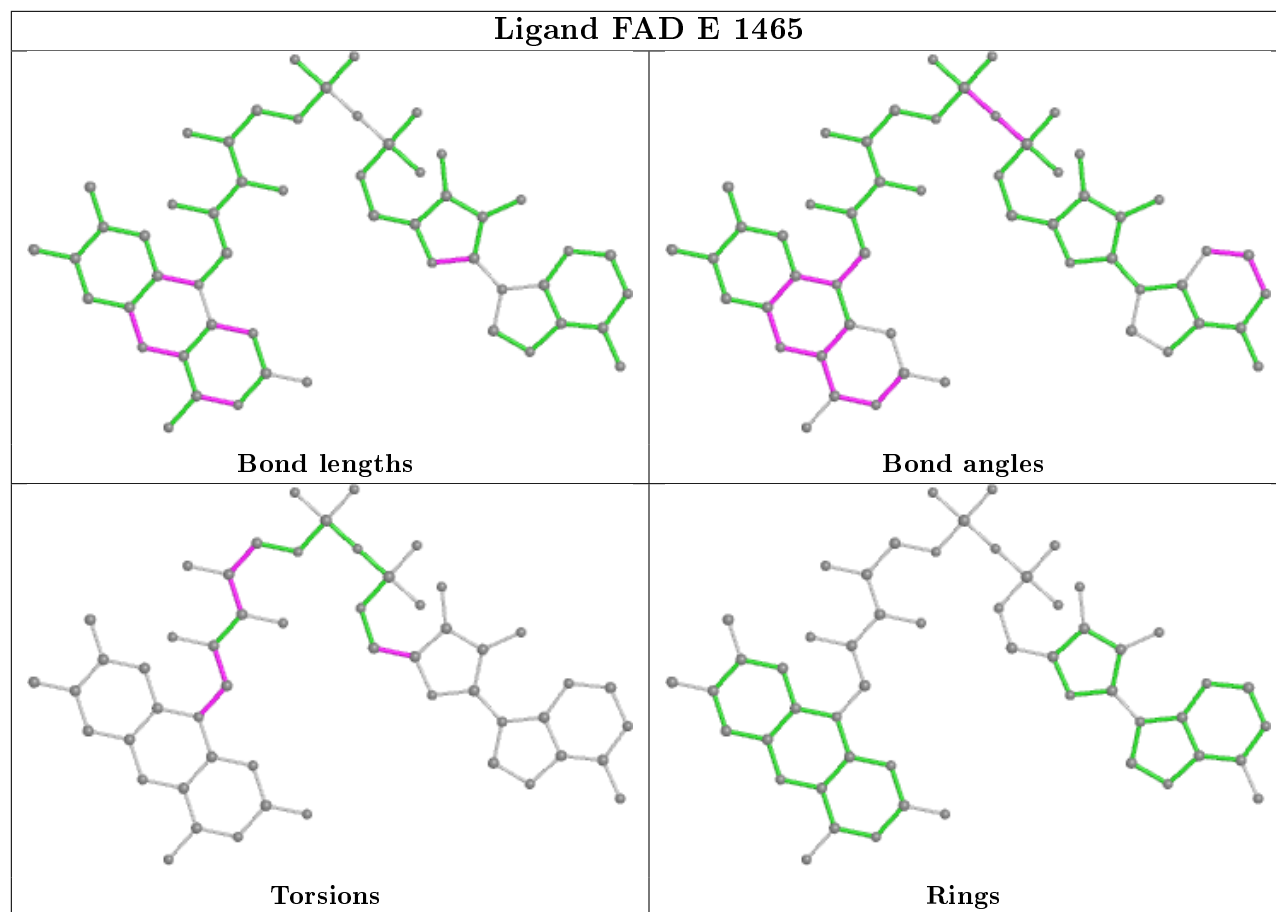
12 monomers are involved in 55 short contacts:

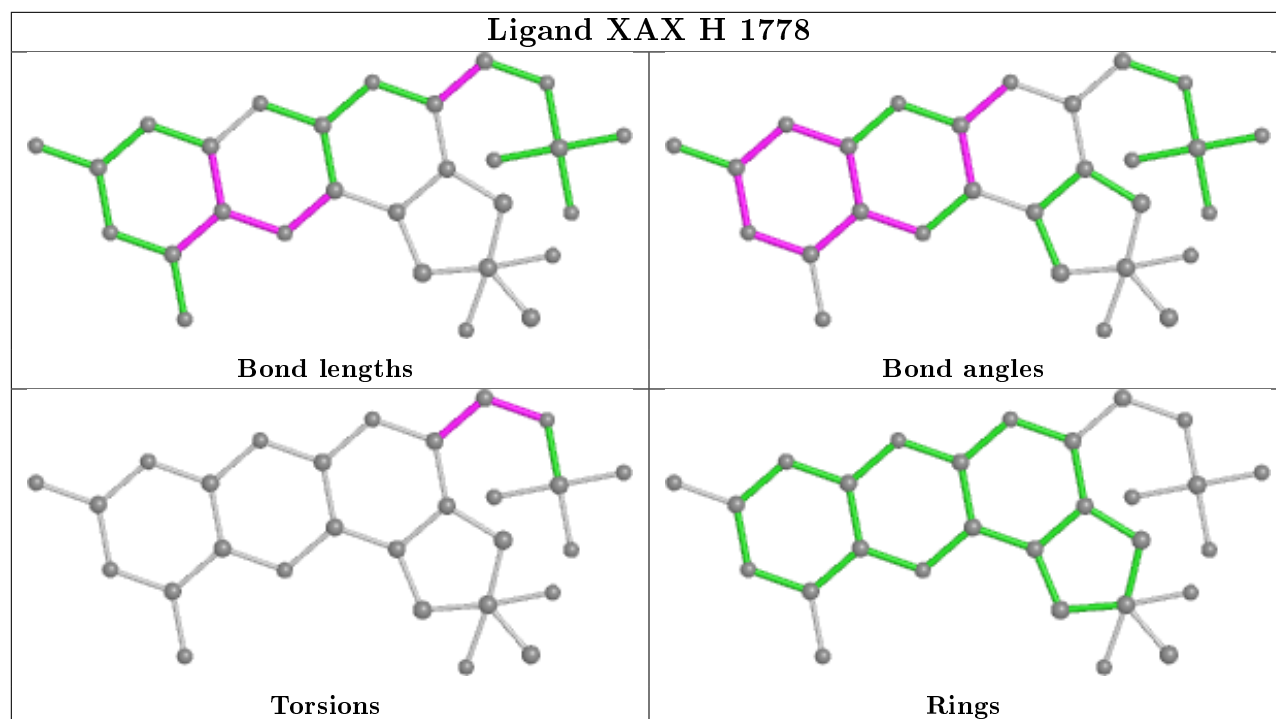
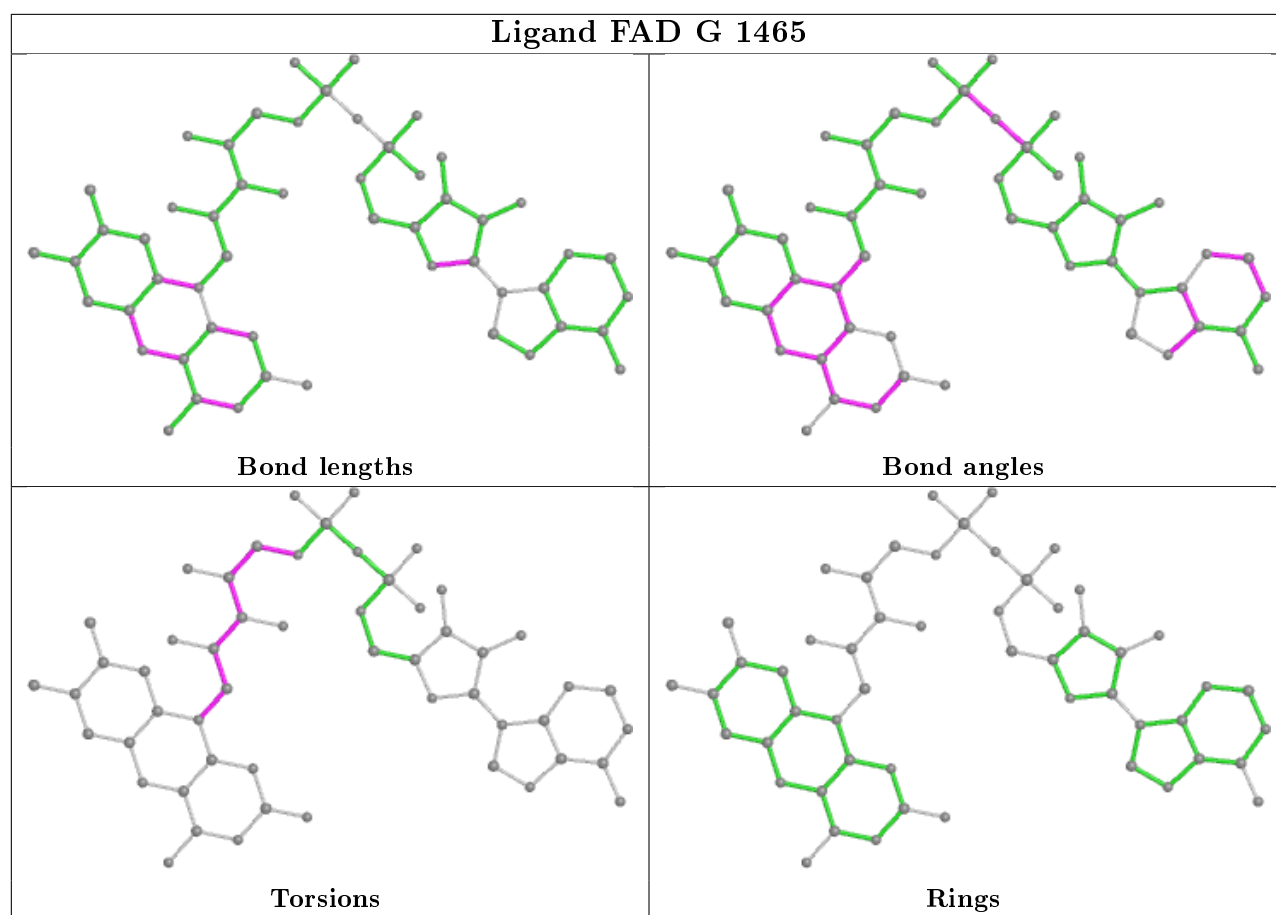
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	1780	HPA	7	0
4	C	1465	FAD	5	0
4	E	1465	FAD	3	0
7	D	1780	HPA	3	0
4	G	1465	FAD	8	0
5	H	1778	XAX	4	0
5	F	1778	XAX	8	0
3	G	1464	FES	1	0
5	B	1778	XAX	4	0
5	D	1778	XAX	7	0
7	F	1780	HPA	1	0
4	A	1465	FAD	6	0

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

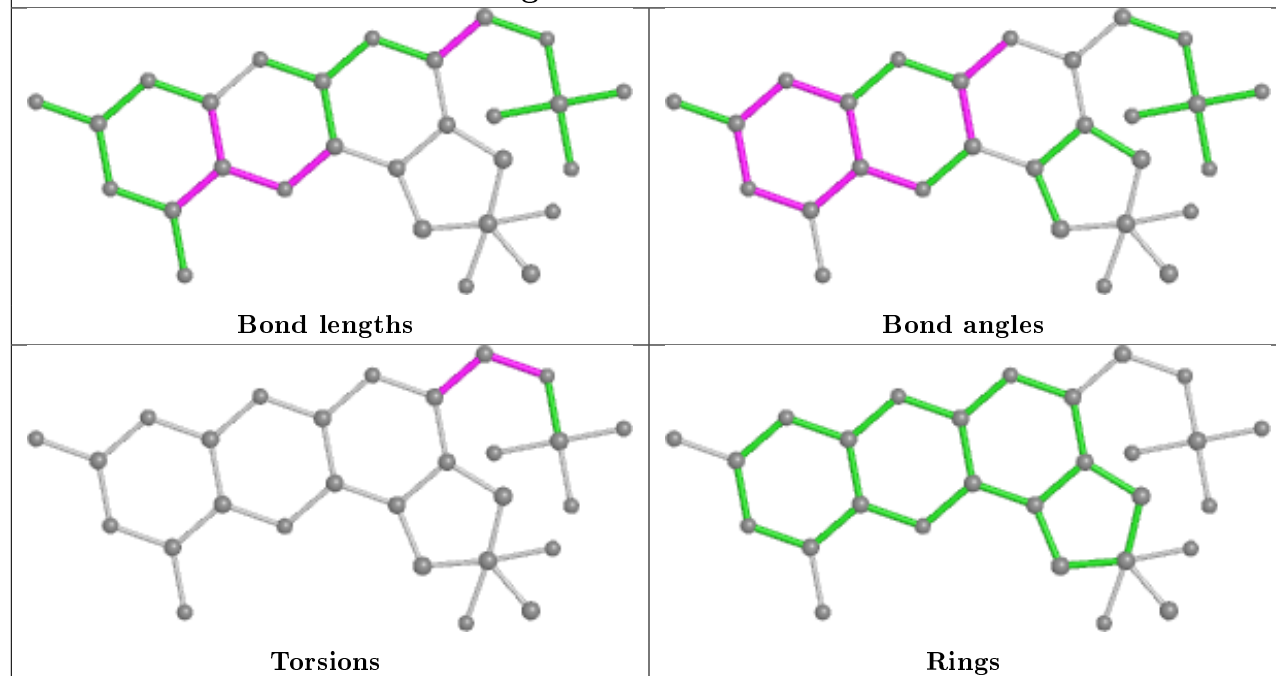
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



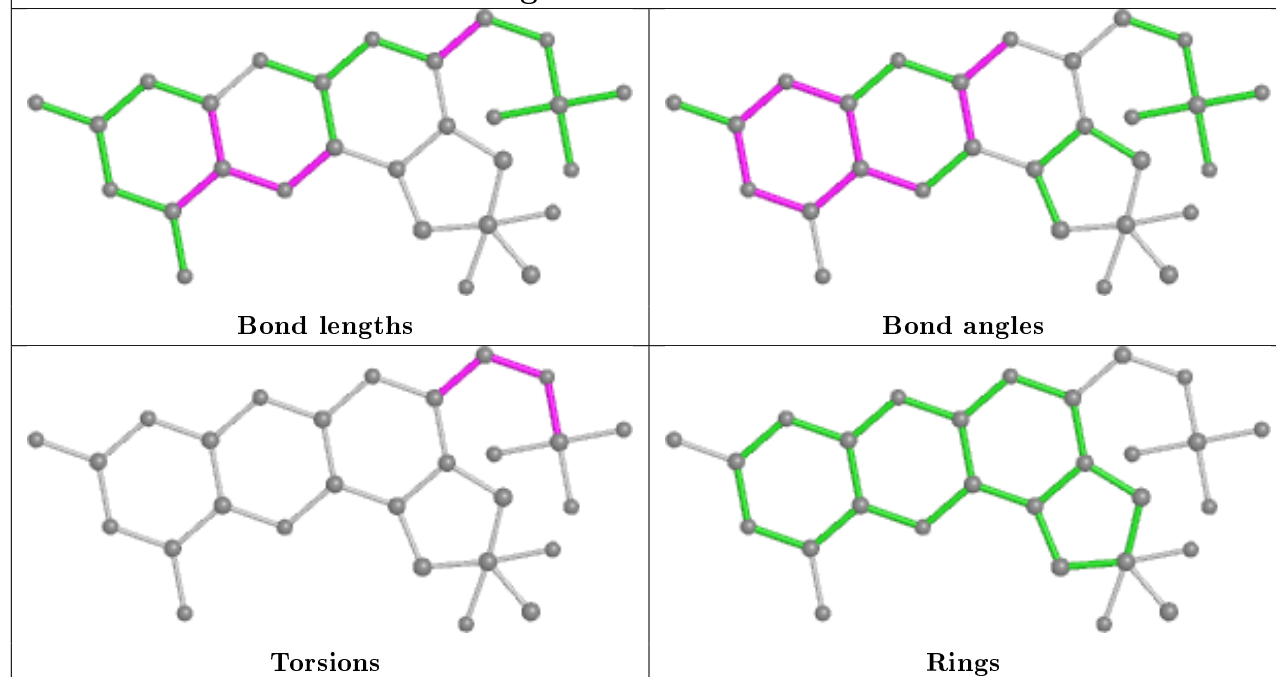




## Ligand XAX F 1778

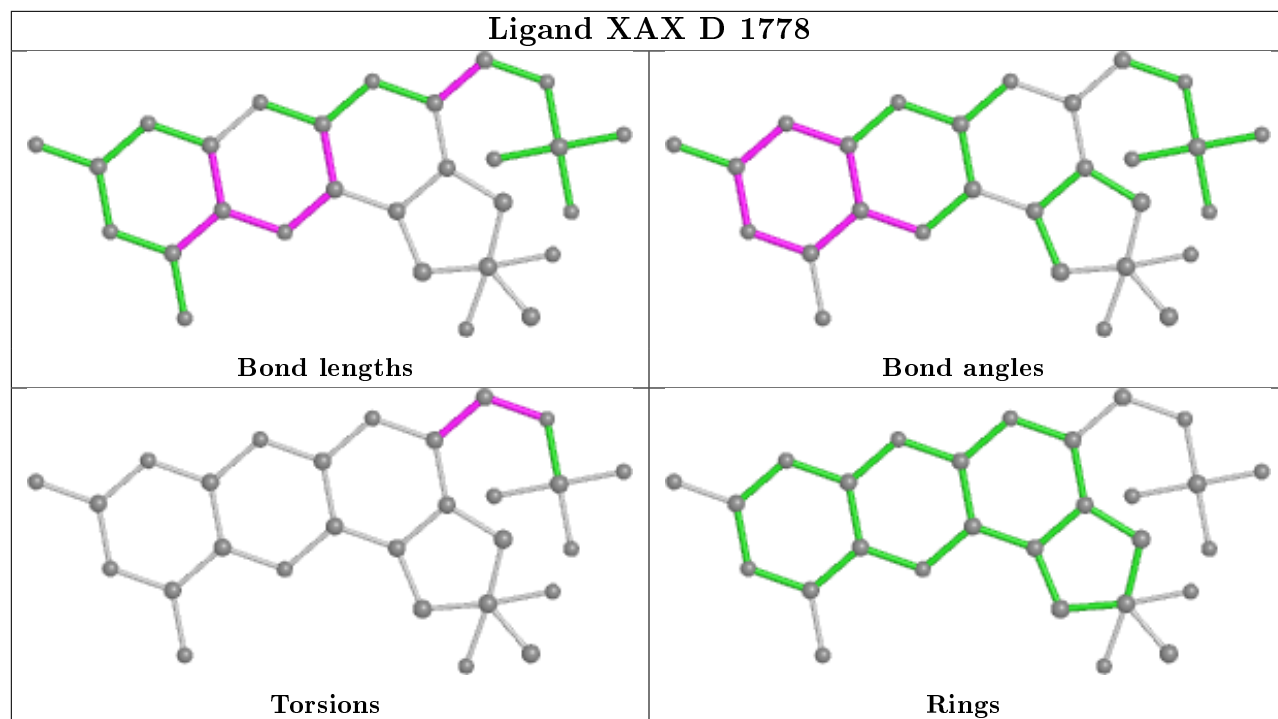


## Ligand XAX B 1778

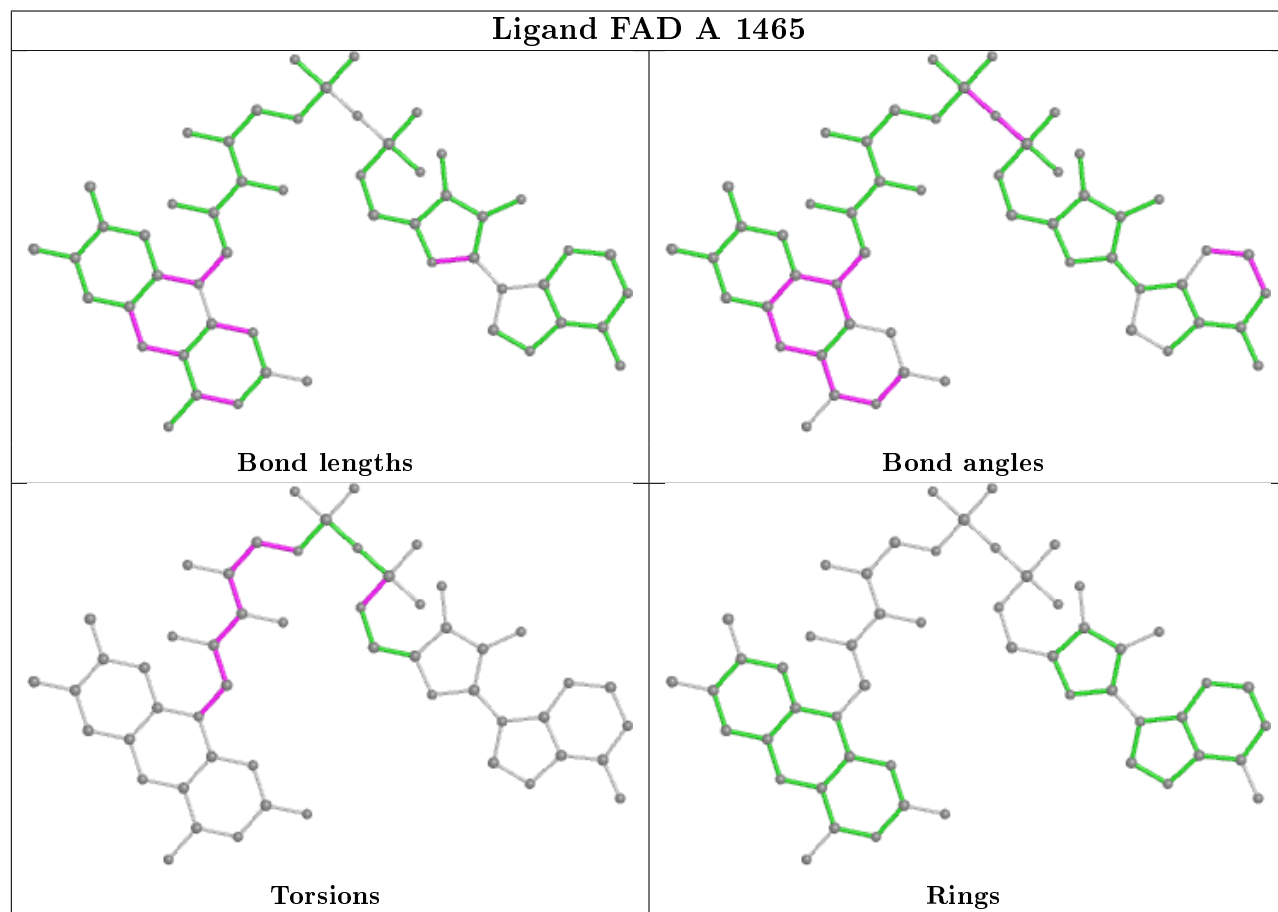




## Ligand XAX D 1778



## 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	450/462 (97%)	0.31	20 (4%) 34 34	41, 43, 44, 45	0
1	C	450/462 (97%)	-0.10	2 (0%) 92 92	41, 43, 44, 45	0
1	E	450/462 (97%)	0.16	11 (2%) 59 57	41, 43, 44, 45	0
1	G	450/462 (97%)	0.25	24 (5%) 26 27	42, 43, 44, 45	0
2	B	760/777 (97%)	-0.13	3 (0%) 92 92	40, 43, 44, 46	0
2	D	760/777 (97%)	-0.29	2 (0%) 94 93	41, 43, 44, 46	0
2	F	760/777 (97%)	-0.29	0 100 100	41, 43, 44, 46	0
2	H	760/777 (97%)	-0.23	1 (0%) 95 96	41, 43, 44, 46	0
All	All	4840/4956 (97%)	-0.09	63 (1%) 77 76	40, 43, 44, 46	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	17	GLU	4.0
1	G	411	ILE	3.8
1	A	413	ALA	3.5
1	G	378	GLU	3.5
1	A	240	GLY	3.5

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

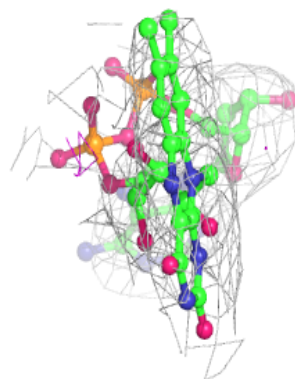
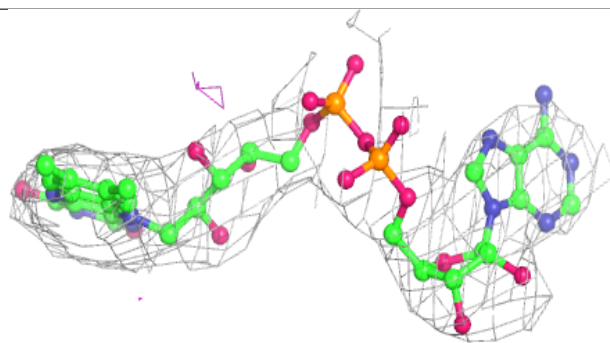
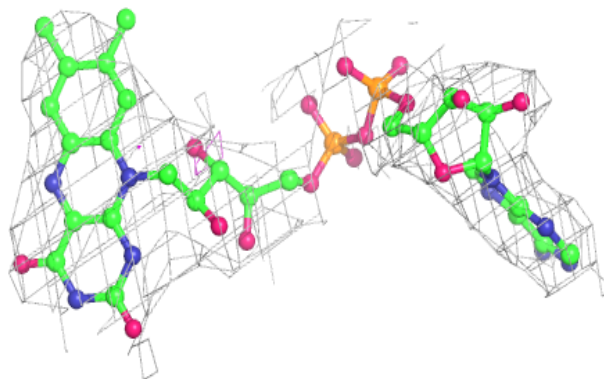
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	HPA	D	1780	10/10	0.88	0.26	43,43,43,43	0
4	FAD	E	1465	53/53	0.93	0.18	62,66,78,78	0
4	FAD	G	1465	53/53	0.93	0.17	74,76,79,80	0
7	HPA	H	1780	10/10	0.93	0.14	43,43,43,43	0
7	HPA	F	1780	10/10	0.94	0.15	43,43,43,43	0
4	FAD	A	1465	53/53	0.94	0.17	72,74,76,76	0
4	FAD	C	1465	53/53	0.95	0.17	46,51,55,55	0
7	HPA	B	1780	10/10	0.95	0.13	43,43,43,43	0
3	FES	E	1464	4/4	0.95	0.28	97,98,98,99	4
5	XAX	B	1778	28/28	0.96	0.37	52,55,60,61	28
5	XAX	H	1778	28/28	0.97	0.25	52,55,62,63	28
6	BA	H	1779	1/1	0.97	0.08	115,115,115,115	0
3	FES	C	1464	4/4	0.97	0.26	107,108,108,108	4
3	FES	G	1464	4/4	0.97	0.29	66,66,66,66	4
5	XAX	D	1778	28/28	0.98	0.28	37,42,47,49	28
5	XAX	F	1778	28/28	0.98	0.28	39,41,47,49	28
3	FES	A	1464	4/4	0.98	0.41	84,84,84,85	4
6	BA	D	1779	1/1	0.99	0.04	105,105,105,105	0
6	BA	F	1779	1/1	0.99	0.07	98,98,98,98	0
3	FES	A	1463	4/4	0.99	0.33	29,30,30,30	4
6	BA	B	1779	1/1	0.99	0.06	108,108,108,108	0
3	FES	G	1463	4/4	0.99	0.27	44,45,45,46	4
3	FES	E	1463	4/4	0.99	0.26	32,32,32,33	4
3	FES	C	1463	4/4	0.99	0.29	24,25,25,25	4

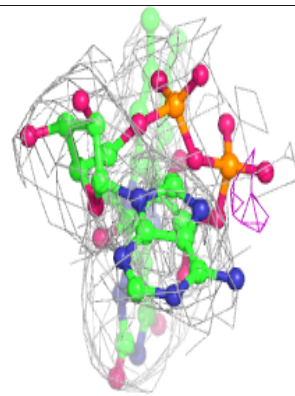
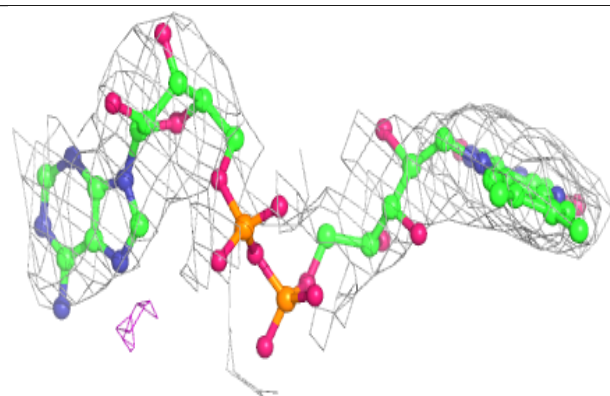
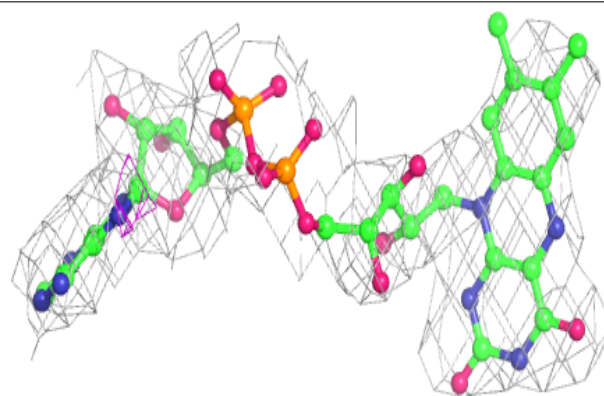
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD 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)

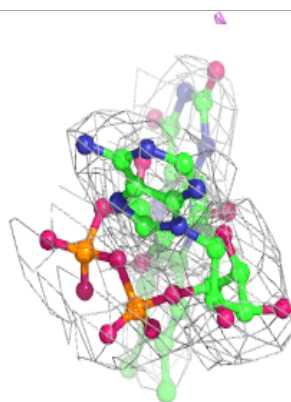
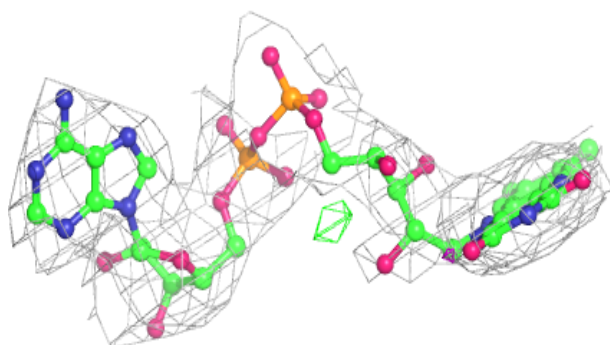
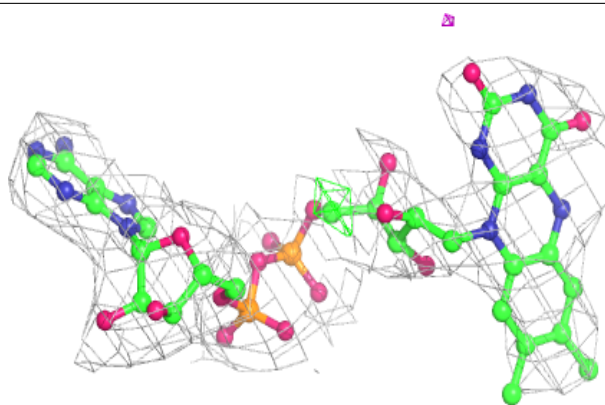
**Electron density around FAD G 1465:**

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

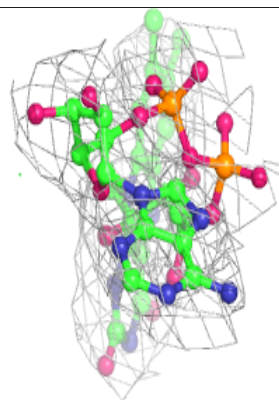
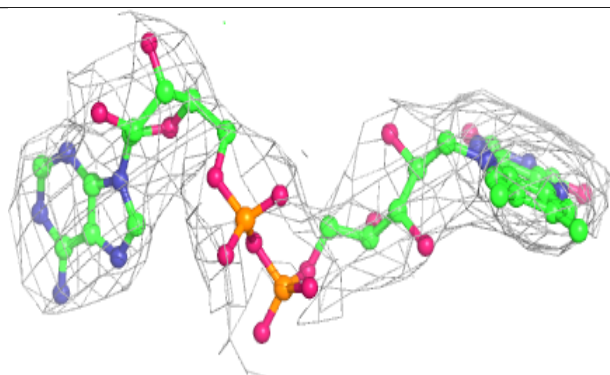
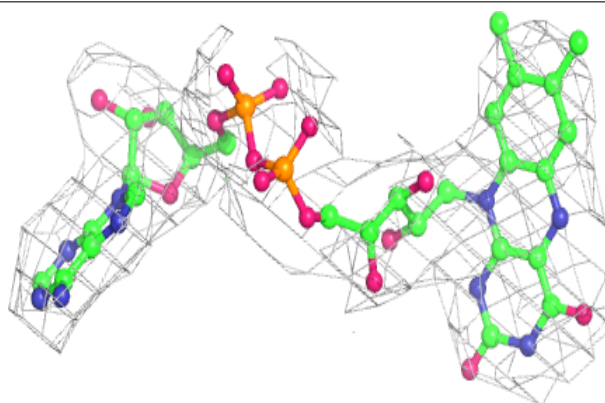


**Electron density around FAD A 1465:**

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

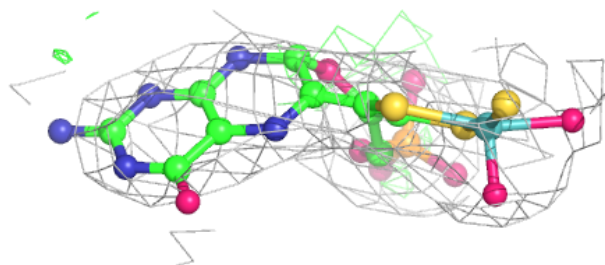
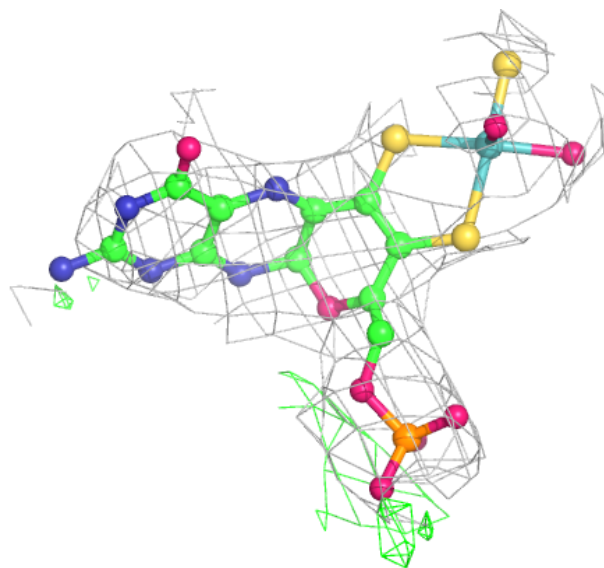
**Electron density around FAD C 1465:**

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



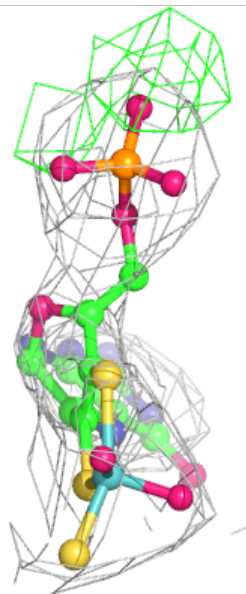
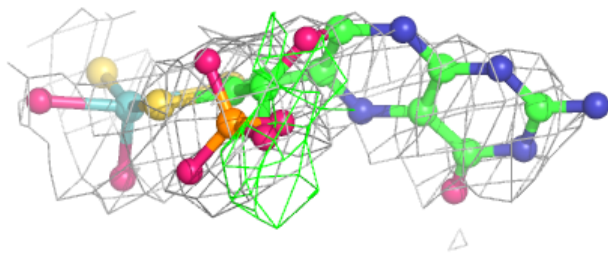
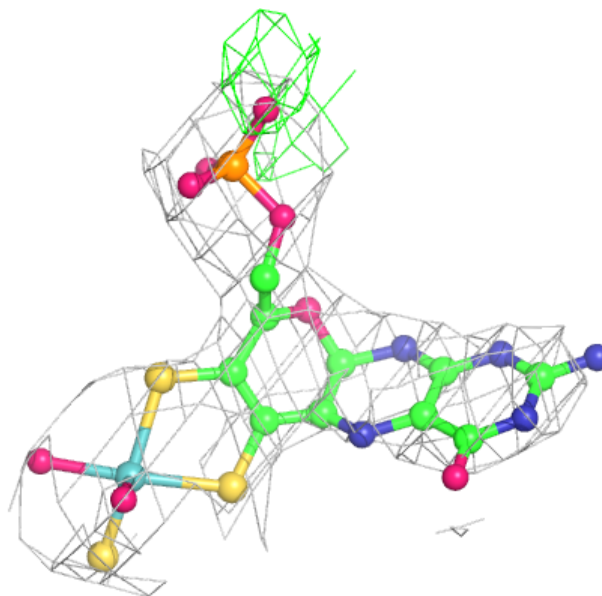
**Electron density around XAX B 1778:**

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



**Electron density around XAX H 1778:**

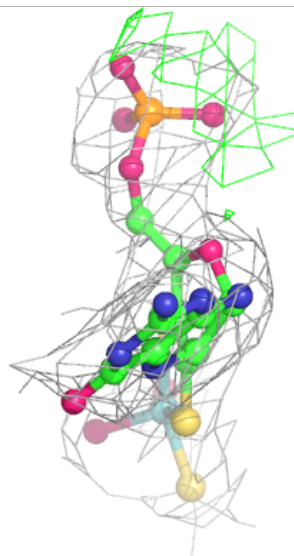
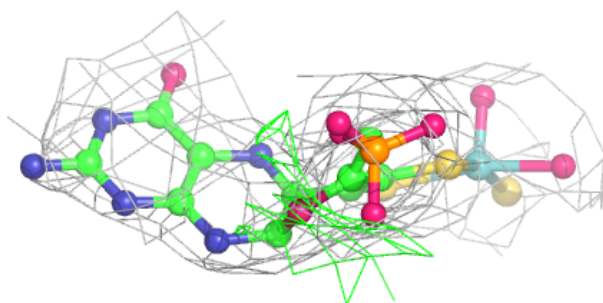
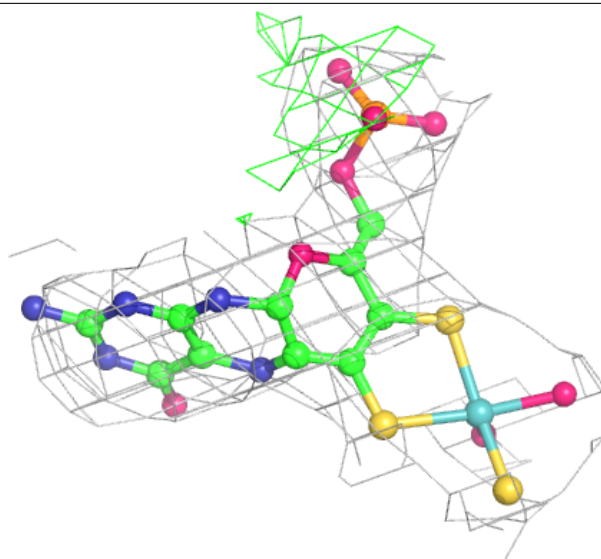
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





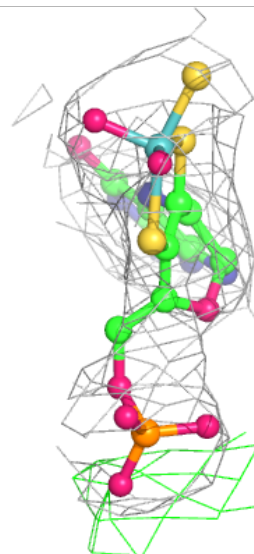
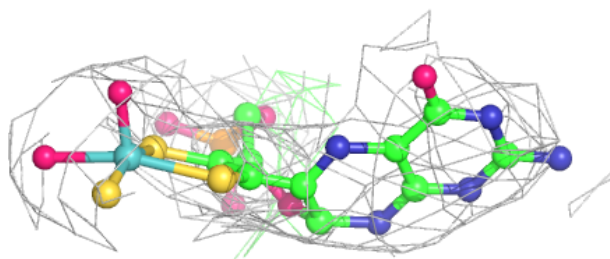
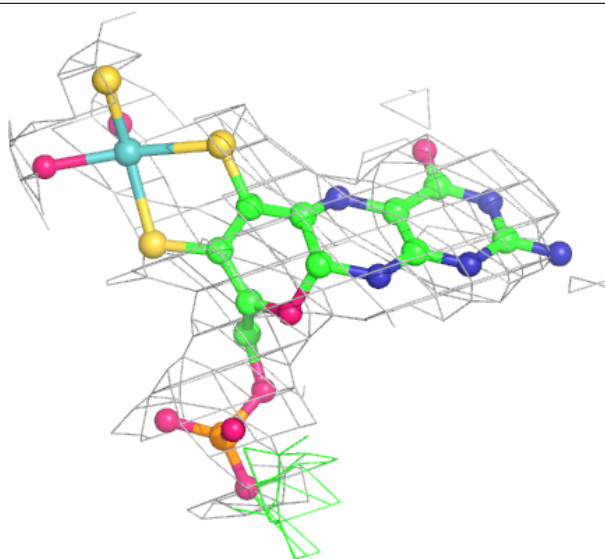
**Electron density around XAX D 1778:**

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



**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.