wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2026 – 10:32 PM EDT

PDB ID	:	3B9J / pdb_00003b9j
Title	:	Structure of Xanthine Oxidase with 2-hydroxy-6-methylpurine
Authors	:	Pauff, J.M.; Zhang, J.; Bell, C.E.; Hille, R.
Deposited on	:	2007-11-05
Resolution	:	2.30 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:

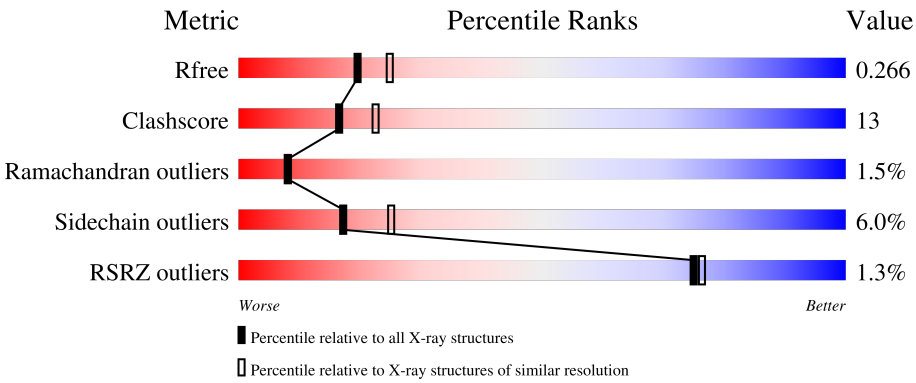
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 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	219	% 60% 12% • 26%
1	I	219	% 60% 11% • 26%
2	B	350	% 70% 15% • 13%
2	J	350	% 71% 14% • 13%
3	C	763	2% 75% 19% • ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	K	763	% 73% 21%

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	290	C	1335	-	-	X	-
7	290	K	1335	-	-	X	-
9	ZXF	K	1336	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19847 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 oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	162	1239	778	222	227	12	0	0	0
1	I	162	1215	764	214	225	12	0	0	0

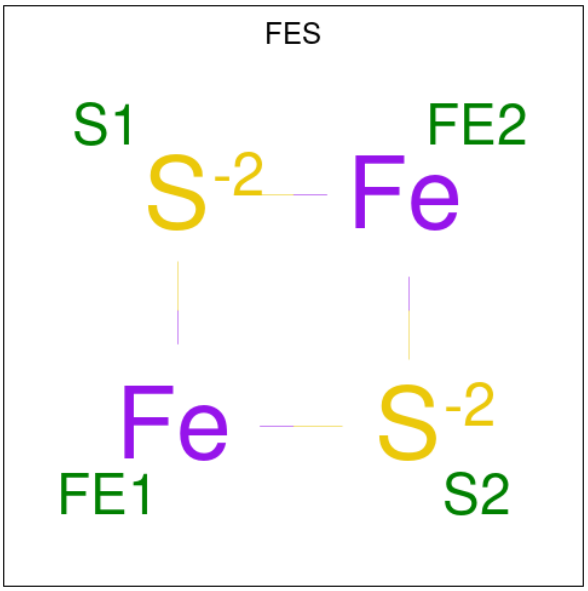
- Molecule 2 is a protein called xanthine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	305	2381	1533	400	435	13	0	0	0
2	J	305	2356	1516	393	434	13	0	0	0

- Molecule 3 is a protein called xanthine oxidase.

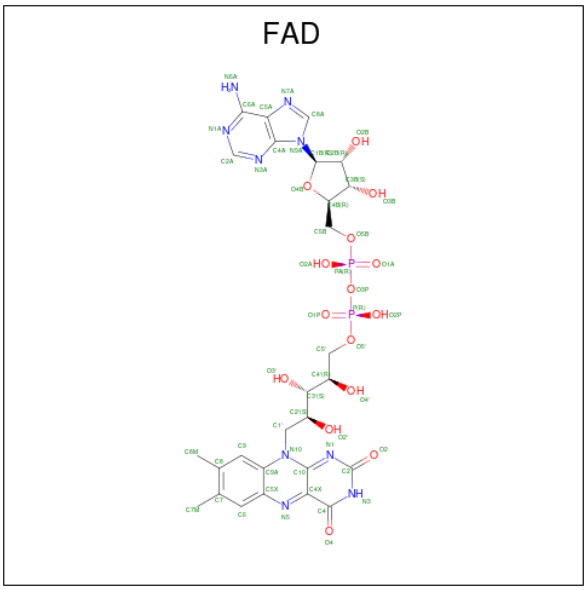
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	758	5835	3688	1005	1107	35	0	0	0
3	K	747	5759	3645	987	1093	34	0	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	I	1	4	2	2	0	0
			Total	Fe	S		
4	I	1	4	2	2	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

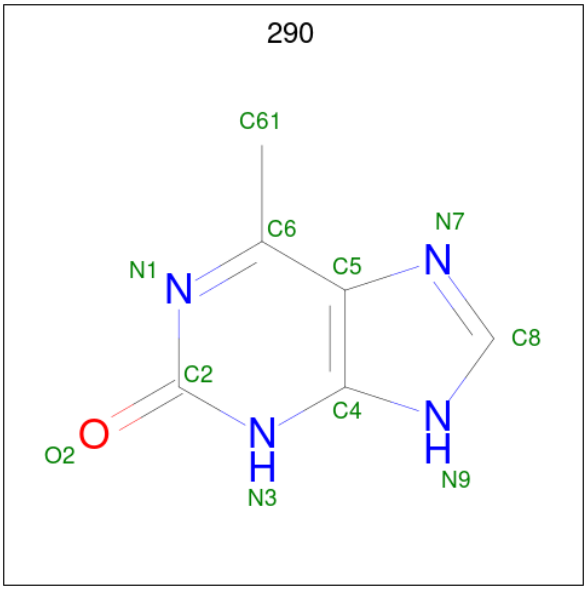


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
5	J	1	53	27	9	15	2	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

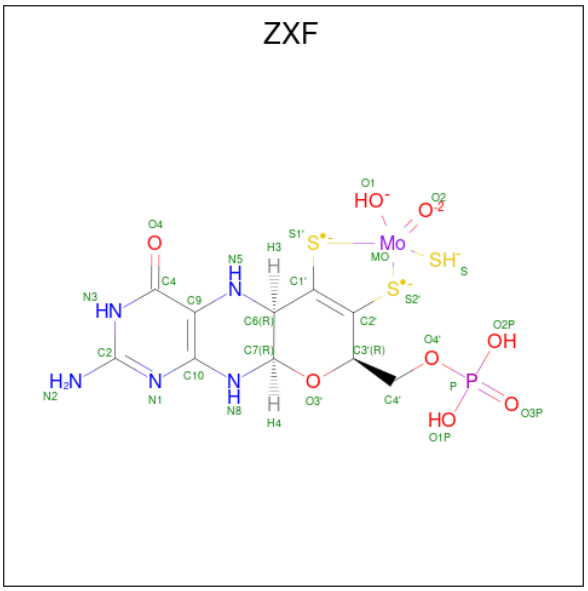
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	C	1	1	1	0	0

- Molecule 7 is 6-methyl-3,9-dihydro-2H-purin-2-one (CCD ID: 290) (formula: $C_6H_6N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	C	1	11	6	4	1	0	0
			Total	C	N	O		
7	K	1	11	6	4	1	0	0

- Molecule 8 is Molybdopterin hydoxy-oxo-thiol-molybdenum (CCD ID: ZXF) (formula: $C_{10}H_{14}MoN_5O_8PS_3$).



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

- Molecule 9 is water.

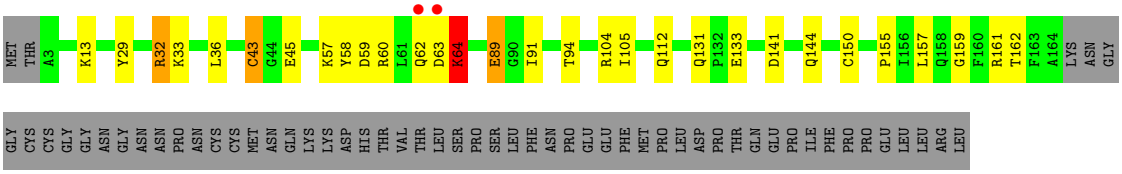
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	68	68	68	0	0
9	B	87	87	87	0	0
9	C	247	247	247	0	0
9	I	73	73	73	0	0
9	J	90	90	90	0	0
9	K	296	296	296	0	0

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.

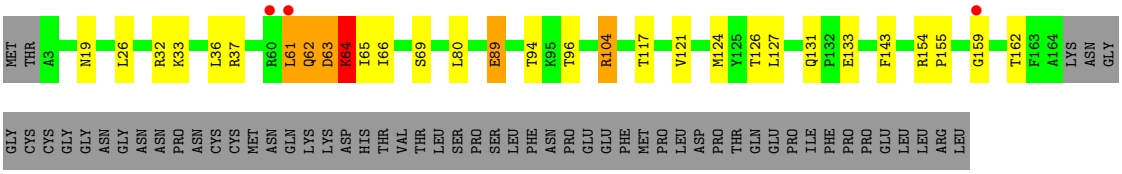
- Molecule 1: xanthine oxidase

Chain A:



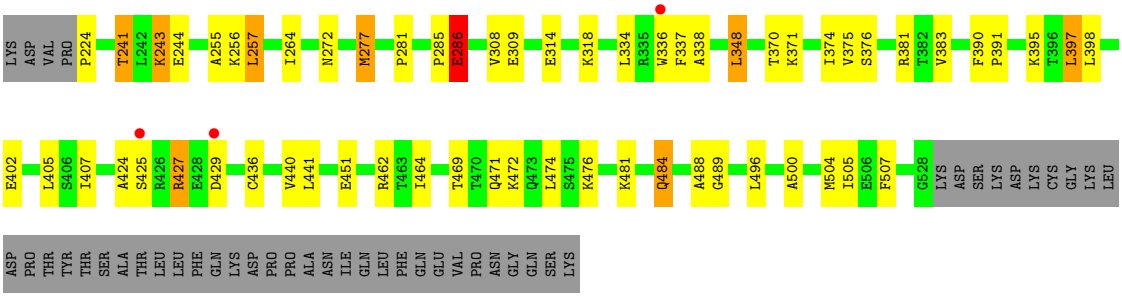
- Molecule 1: xanthine oxidase

Chain I:



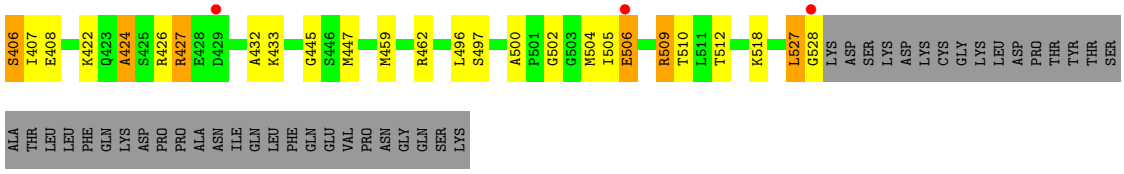
- Molecule 2: xanthine oxidase

Chain B:



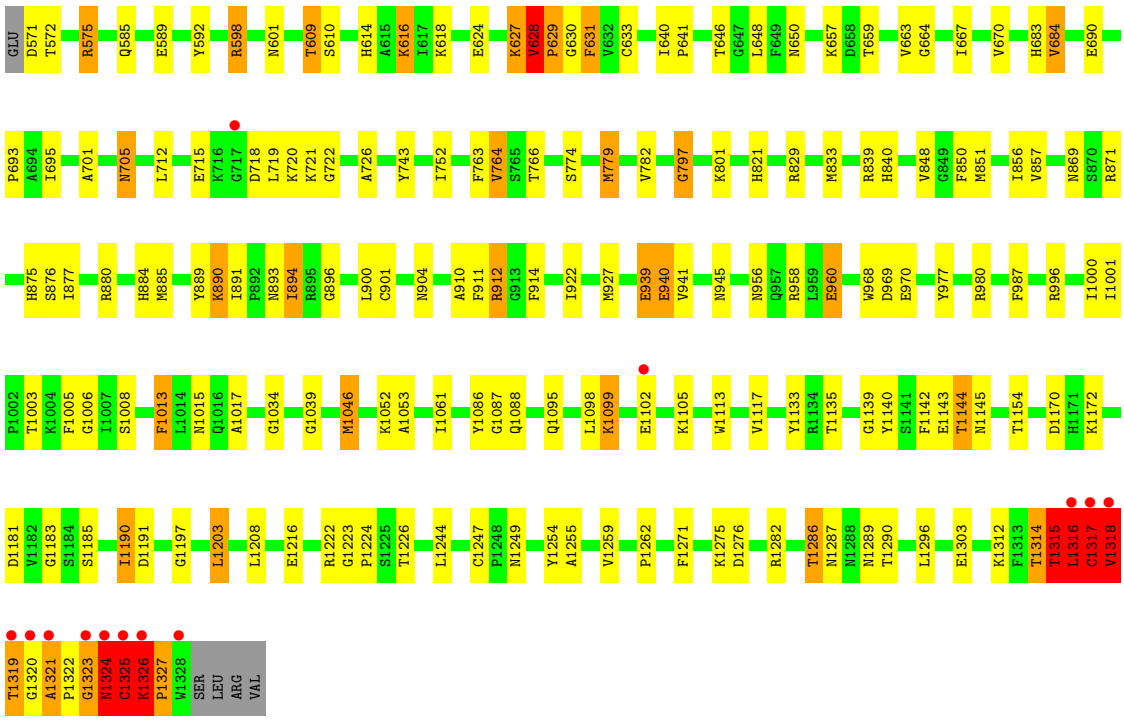
- Molecule 2: xanthine oxidase

Chain J:



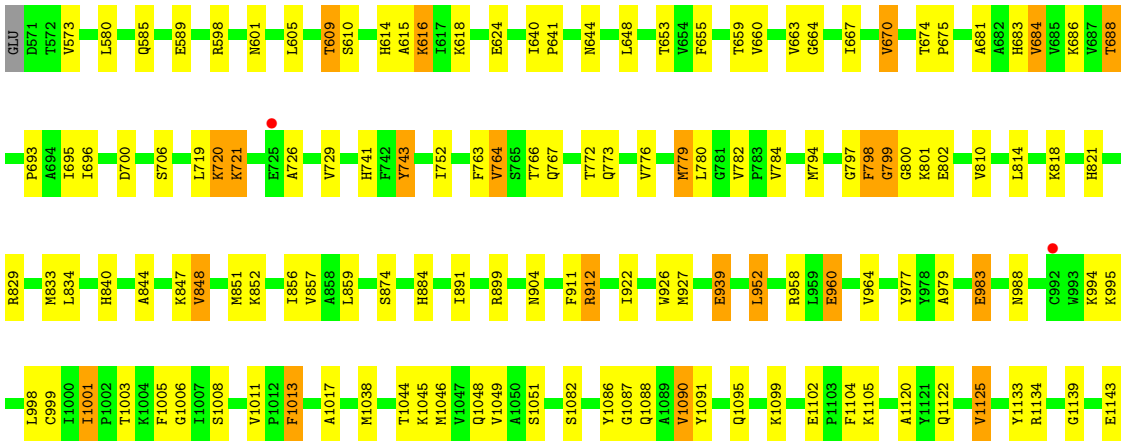
• Molecule 3: xanthine oxidase

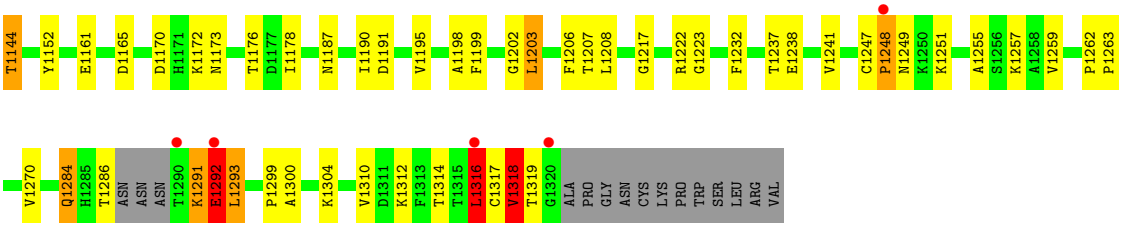
Chain C:



• Molecule 3: xanthine oxidase

Chain K:




T1144
Y1152
E1161
D1165
D1170
H1171
K1172
N1173
T1176
D1177
I1178
N1187
I1190
D1191
V1195
A1198
F1199
G1202
L1203
F1206
T1207
L1208
G1217
R1222
G1223
F1232
T1237
E1238
V1241
C1247
P1248
N1249
K1250
K1251
A1255
S1256
K1257
A1258
V1259
P1262
P1263
V1270
Q1284
H1285
T1286
ASN
ASN
ASN
T1290
K1291
E1292
L1293
P1299
A1300
K1304
V1310
D1311
K1312
F1313
T1314
T1315
L1316
C1317
V1318
T1319
G1320
ALA
PRO
GLY
ASN
CYS
LYS
PRO
TRP
SER
LEU
ARG
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.19Å 73.79Å 146.50Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	144.34 – 2.30 144.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (144.34-2.30) 96.2 (144.34-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.263 0.197 , 0.266	Depositor DCC
R_{free} test set	6568 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19847	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 290, CA, FAD, FES, ZXF

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	1.10	2/1261 (0.2%)	1.07	1/1702 (0.1%)
1	I	1.00	1/1237 (0.1%)	1.01	1/1672 (0.1%)
2	B	0.96	0/2430	1.04	2/3282 (0.1%)
2	J	0.91	0/2403	1.01	1/3248 (0.0%)
3	C	1.08	7/5963 (0.1%)	1.19	23/8078 (0.3%)
3	K	1.00	4/5885 (0.1%)	1.09	6/7971 (0.1%)
All	All	1.02	14/19179 (0.1%)	1.10	34/25953 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	I	0	1
3	C	3	10
3	K	0	5
All	All	3	17

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1315	THR	CA-C	-6.54	1.44	1.52
1	I	96	THR	CA-C	6.15	1.55	1.52
1	A	91	ILE	CA-CB	5.67	1.61	1.54
1	A	105	ILE	CA-CB	5.63	1.62	1.54
3	C	1315	THR	CA-CB	-5.61	1.44	1.53

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1318	VAL	N-CA-C	18.24	130.71	113.20
3	C	628	VAL	N-CA-C	11.74	134.23	108.88
3	C	1318	VAL	CB-CA-C	-11.66	99.16	110.70
3	C	1314	THR	N-CA-C	9.25	121.13	111.14
3	C	1326	LYS	N-CA-C	8.96	136.07	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1315	THR	CA
3	C	1319	THR	CA
3	C	1326	LYS	CA

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	LYS	Peptide
3	C	1314	THR	Peptide
3	C	627	LYS	Peptide
3	C	628	VAL	Peptide
3	C	630	GLY	Peptide

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	1239	0	1245	26	0
1	I	1215	0	1201	20	0
2	B	2381	0	2437	58	0
2	J	2356	0	2394	50	0
3	C	5835	0	5747	173	0
3	K	5759	0	5679	167	0
4	A	8	0	0	0	0
4	I	8	0	0	0	0
5	B	53	0	31	2	0
5	J	53	0	31	3	0
6	C	1	0	0	0	0
7	C	11	0	6	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	11	0	6	7	0
8	C	28	0	0	0	0
8	K	28	0	0	0	0
9	A	68	0	0	7	0
9	B	87	0	0	6	0
9	C	247	0	0	29	0
9	I	73	0	0	2	0
9	J	90	0	0	5	0
9	K	296	0	0	26	0
All	All	19847	0	18777	487	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 13.

The worst 5 of 487 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)
7:K:1335:290:C8	9:K:1336:ZXF:O1	1.75	1.32
3:K:1046:MET:HE1	3:K:1086:TYR:C	1.55	1.30
3:C:640:ILE:HG23	3:C:779:MET:HE3	1.21	1.20
7:K:1335:290:H8	9:K:1336:ZXF:O1	1.30	1.15
3:C:683:HIS:HB2	9:C:1420:HOH:O	1.46	1.12

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	160/219 (73%)	151 (94%)	7 (4%)	2 (1%)	9 10
1	I	160/219 (73%)	150 (94%)	7 (4%)	3 (2%)	6 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	303/350 (87%)	286 (94%)	16 (5%)	1 (0%)	36	46
2	J	303/350 (87%)	286 (94%)	12 (4%)	5 (2%)	7	7
3	C	756/763 (99%)	710 (94%)	30 (4%)	16 (2%)	5	4
3	K	743/763 (97%)	704 (95%)	29 (4%)	10 (1%)	9	10
All	All	2425/2664 (91%)	2287 (94%)	101 (4%)	37 (2%)	8	8

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
2	B	286	GLU
3	C	1316	LEU
3	C	1317	CYS
3	C	1323	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	135/187 (72%)	130 (96%)	5 (4%)	30	45
1	I	130/187 (70%)	124 (95%)	6 (5%)	24	36
2	B	259/302 (86%)	245 (95%)	14 (5%)	20	29
2	J	254/302 (84%)	237 (93%)	17 (7%)	15	21
3	C	630/639 (99%)	588 (93%)	42 (7%)	15	21
3	K	623/639 (98%)	586 (94%)	37 (6%)	18	26
All	All	2031/2256 (90%)	1910 (94%)	121 (6%)	17	25

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1290	THR
3	K	1122	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	295	GLU
3	K	1099	LYS
3	K	1284	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	146	ASN
3	K	626	GLN
3	K	1307	ASN
2	J	226	GLN
2	J	333	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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FES	A	602	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FES	I	602	1	0,4,4	-	-	-		
7	290	C	1335	-	11,12,12	1.21	1 (9%)	10,17,17	2.29	3 (30%)
4	FES	A	601	1	0,4,4	-	-	-		
9	ZXF	K	1336	-	24,31,31	2.88	4 (16%)	22,52,52	3.36	11 (50%)
4	FES	I	601	1	0,4,4	-	-	-		
7	290	K	1335	-	11,12,12	1.25	1 (9%)	10,17,17	2.15	2 (20%)
5	FAD	B	606	-	58,58,58	1.14	3 (5%)	85,89,89	1.83	23 (27%)
5	FAD	J	606	-	58,58,58	1.18	4 (6%)	85,89,89	1.75	17 (20%)
9	ZXF	C	1336	-	24,31,31	3.96	6 (25%)	22,52,52	3.05	11 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	A	602	1	-	-	0/1/1/1
4	FES	I	602	1	-	-	0/1/1/1
7	290	C	1335	-	-	-	0/2/2/2
4	FES	A	601	1	-	-	0/1/1/1
9	ZXF	K	1336	-	-	3/6/46/46	0/4/4/4
4	FES	I	601	1	-	-	0/1/1/1
7	290	K	1335	-	-	-	0/2/2/2
5	FAD	B	606	-	-	0/34/50/50	0/6/6/6
5	FAD	J	606	-	-	5/34/50/50	0/6/6/6
9	ZXF	C	1336	-	-	1/6/46/46	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1336	ZXF	MO-S2'	14.37	2.59	2.39
9	K	1336	ZXF	MO-S2'	11.68	2.56	2.39
9	C	1336	ZXF	MO-S1'	9.90	2.53	2.39
9	C	1336	ZXF	C9-C10	5.21	1.47	1.38
9	K	1336	ZXF	C9-C10	4.95	1.47	1.38

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	1336	ZXF	C1'-C2'-S2'	10.52	126.12	120.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1336	ZXF	C1'-C2'-S2'	7.89	124.63	120.15
5	B	606	FAD	N3A-C2A-N1A	-7.58	117.10	128.58
5	J	606	FAD	N3A-C2A-N1A	-6.78	118.32	128.58
9	C	1336	ZXF	C2'-C1'-S1'	6.10	123.61	120.15

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1336	ZXF	C3'-C4'-O4'-P
9	K	1336	ZXF	C4'-O4'-P-O2P
5	J	606	FAD	C2'-C3'-C4'-C5'
9	K	1336	ZXF	C4'-O4'-P-O1P
5	J	606	FAD	C2'-C3'-C4'-O4'

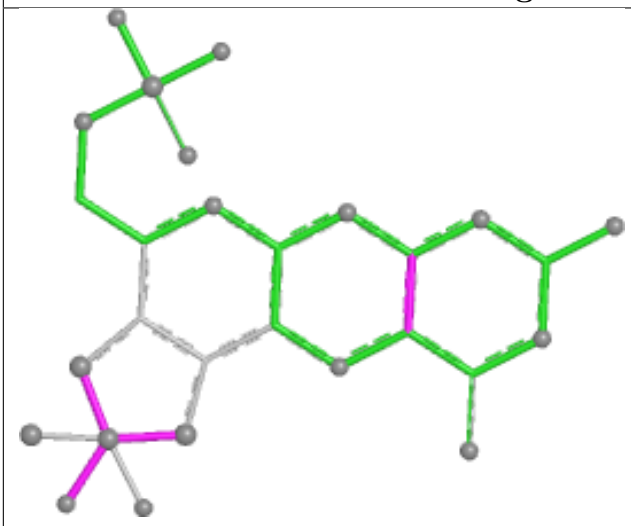
There are no ring outliers.

6 monomers are involved in 24 short contacts:

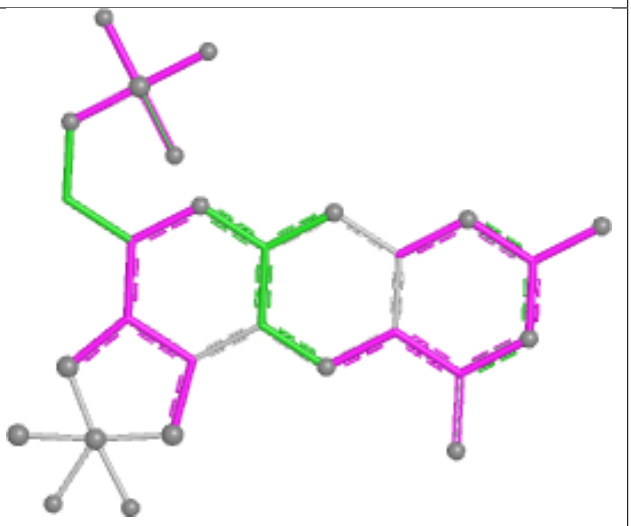
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1335	290	4	0
9	K	1336	ZXF	9	0
7	K	1335	290	7	0
5	B	606	FAD	2	0
5	J	606	FAD	3	0
9	C	1336	ZXF	7	0

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.

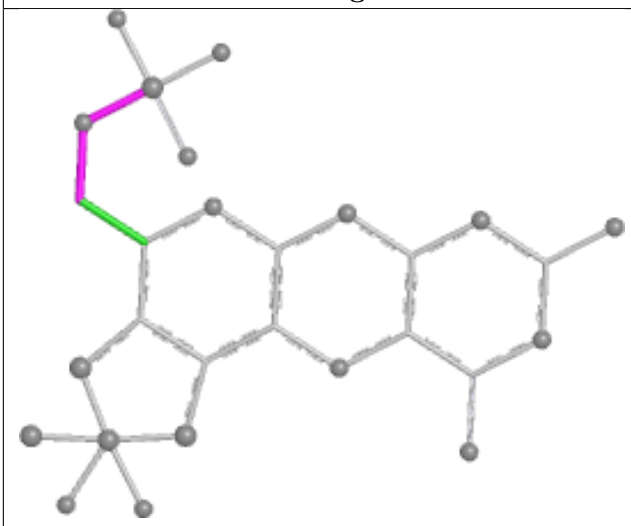
Ligand ZXF K 1336



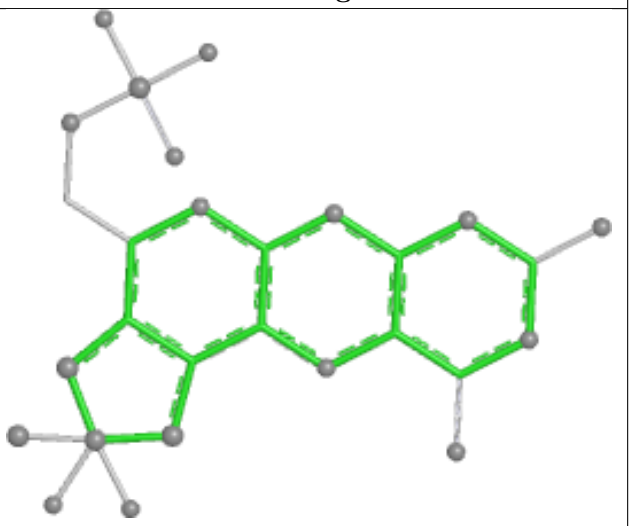
Bond lengths



Bond angles

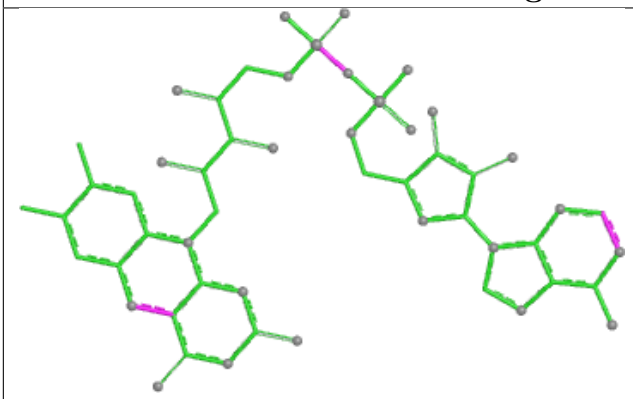


Torsions

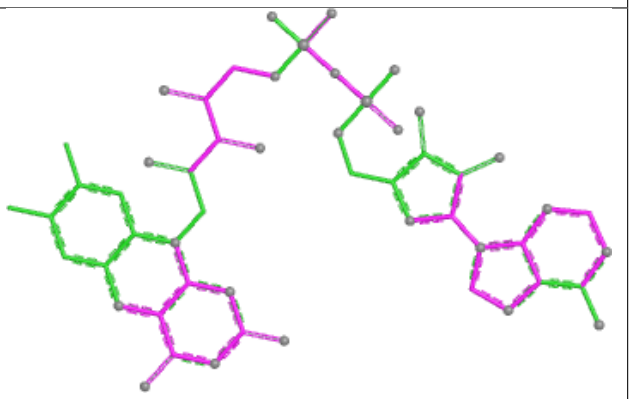


Rings

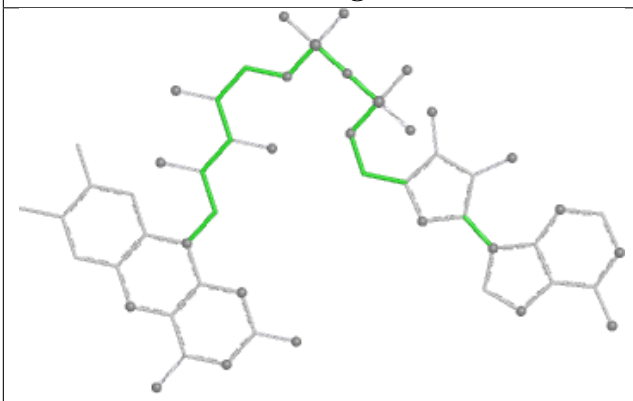
Ligand FAD B 606



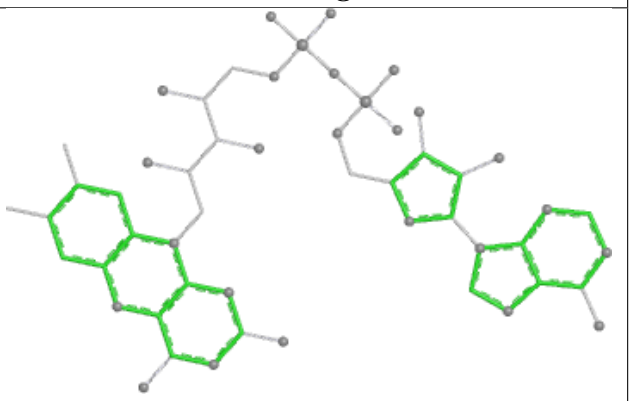
Bond lengths



Bond angles

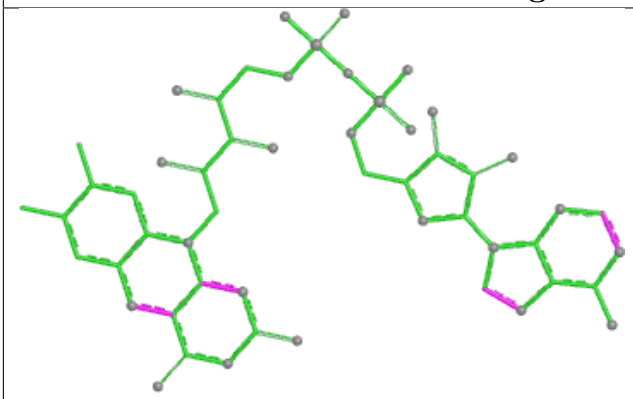


Torsions

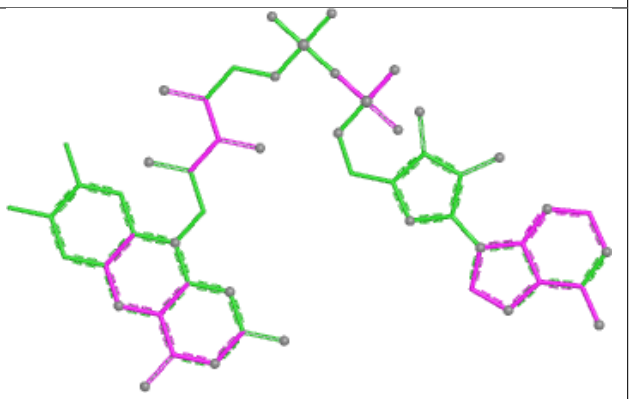


Rings

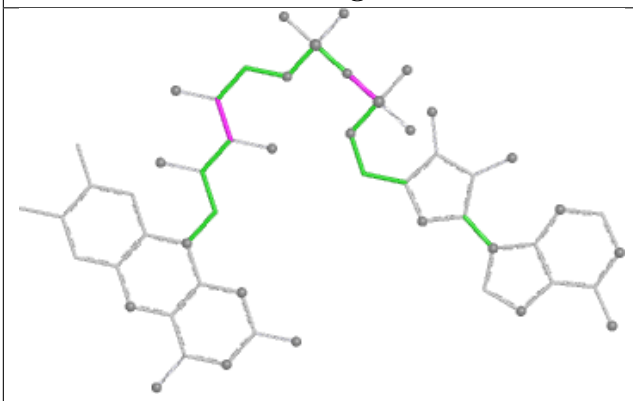
Ligand FAD J 606



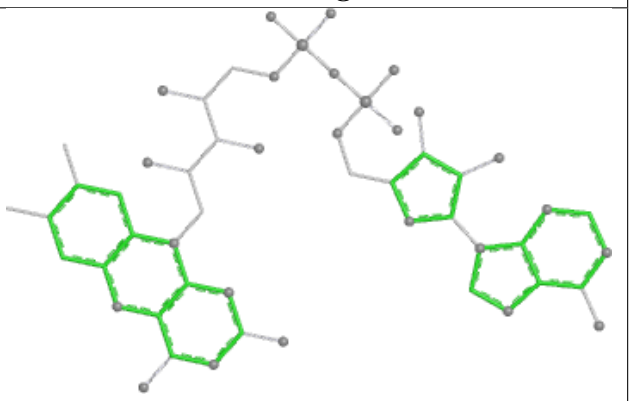
Bond lengths



Bond angles

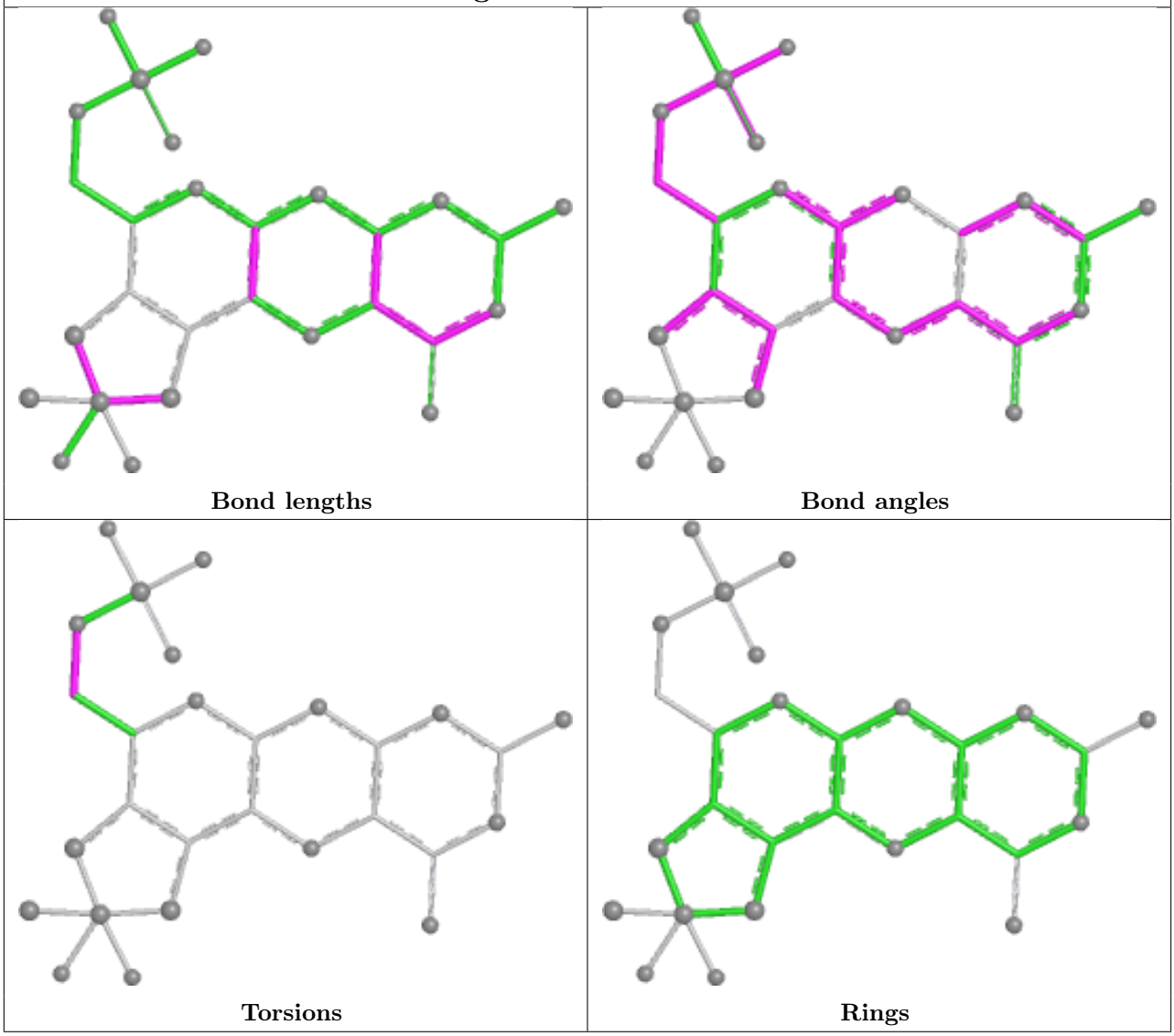


Torsions



Rings

Ligand ZXF C 1336



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	162/219 (73%)	-0.26	2 (1%)	76	77	13, 21, 37, 50	0
1	I	162/219 (73%)	-0.10	3 (1%)	66	68	17, 27, 44, 54	0
2	B	305/350 (87%)	-0.03	3 (0%)	79	80	15, 28, 39, 43	0
2	J	305/350 (87%)	0.14	3 (0%)	79	80	22, 34, 44, 47	0
3	C	758/763 (99%)	-0.09	13 (1%)	69	70	13, 25, 39, 51	0
3	K	747/763 (97%)	-0.15	7 (0%)	81	82	12, 25, 40, 55	0
All	All	2439/2664 (91%)	-0.08	31 (1%)	75	76	12, 26, 41, 55	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1325	CYS	6.9
3	C	1323	GLY	4.3
3	K	1316	LEU	4.2
3	C	1328	TRP	3.9
3	C	1321	ALA	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)

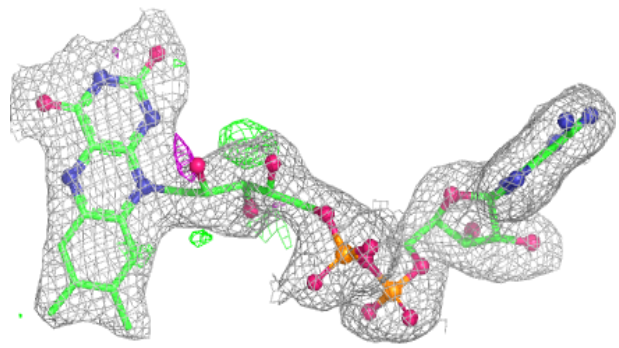
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

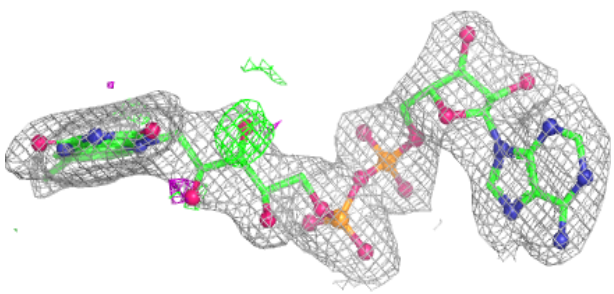
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	C	1	1/1	0.84	0.15	49,49,49,49	0
7	290	C	1335	11/11	0.84	0.14	30,31,32,32	0
7	290	K	1335	11/11	0.93	0.09	19,21,22,23	0
5	FAD	J	606	53/53	0.95	0.07	19,25,30,37	0
9	ZXF	K	1336	28/28	0.95	0.09	27,29,44,46	0
5	FAD	B	606	53/53	0.96	0.06	13,22,25,27	0
9	ZXF	C	1336	28/28	0.97	0.07	20,25,45,49	0
4	FES	A	602	4/4	0.99	0.03	13,14,16,18	0
4	FES	I	601	4/4	0.99	0.03	19,19,20,21	0
4	FES	A	601	4/4	0.99	0.03	13,16,18,18	0
4	FES	I	602	4/4	1.00	0.03	19,19,19,20	0

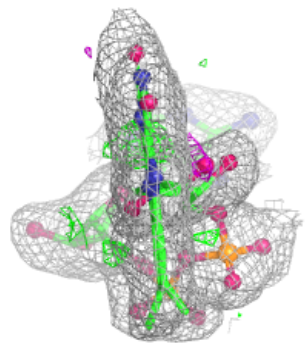
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD J 606:

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

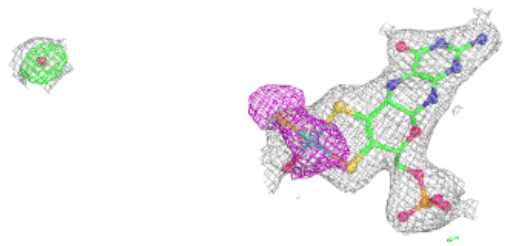


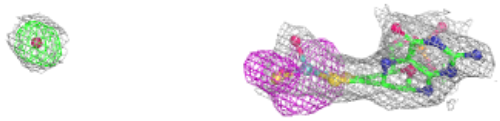




Electron density around ZXF K 1336:

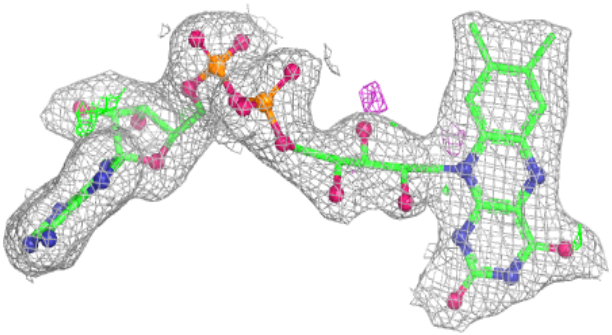
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

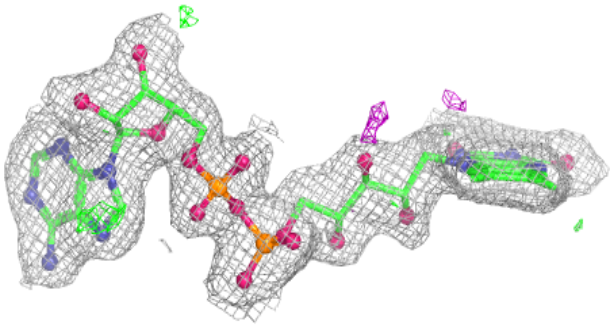


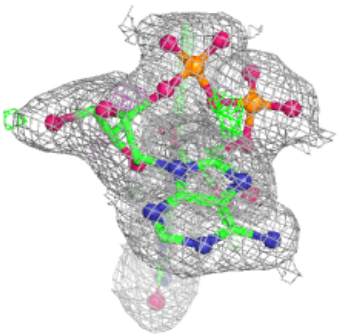


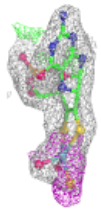
Electron density around FAD B 606:

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







Electron density around ZXF C 1336: $2mF_o$-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.