wwPDB X-ray Structure Validation Summary Report (i)

Jan 29, 2024 – 10:06 PM EST

PDB ID	:	1FIQ
Title	:	CRYSTAL STRUCTURE OF XANTHINE OXIDASE FROM BOVINE MILK
Authors	:	Enroth, C.; Eger, B.T.; Okamoto, K.; Nishino, T.; Nishino, T.; Pai, E.F.
Deposited on	:	2000-08-04
Resolution	:	2.50 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 (1)) were used in the production of this report:

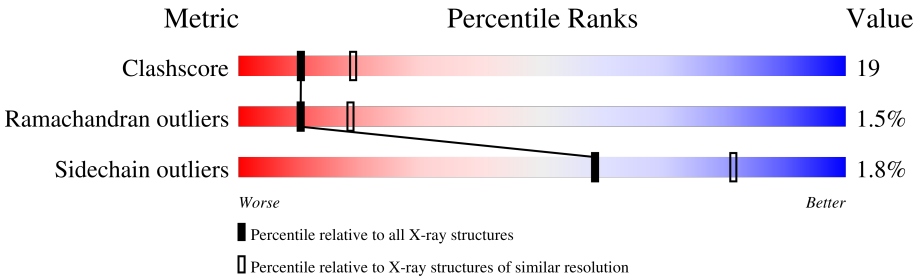
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	219	54% 19% • 25%
2	B	350	54% 32% • 13%
3	C	763	63% 33% ••

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	MOS	C	1334	-	-	X	-
9	GOL	C	1336	-	X	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10106 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	164	1255	788	225	230	12	0	0	0

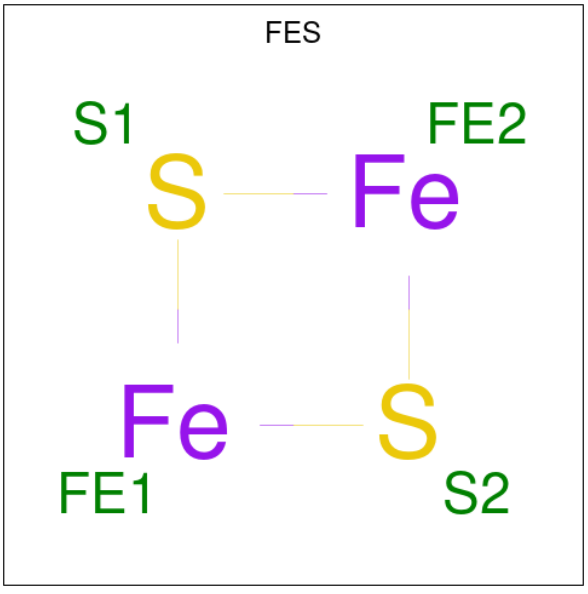
- Molecule 2 is a protein called XANTHINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	305	2389	1539	402	435	13	0	0	0

- Molecule 3 is a protein called XANTHINE OXIDASE.

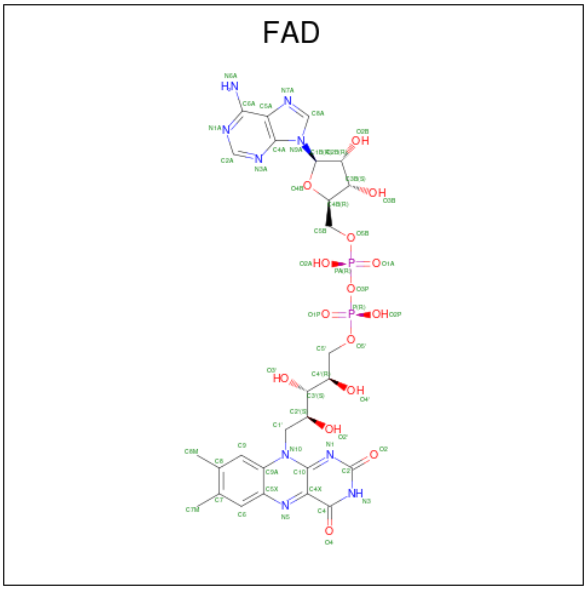
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	745	5761	3643	992	1093	33	0	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



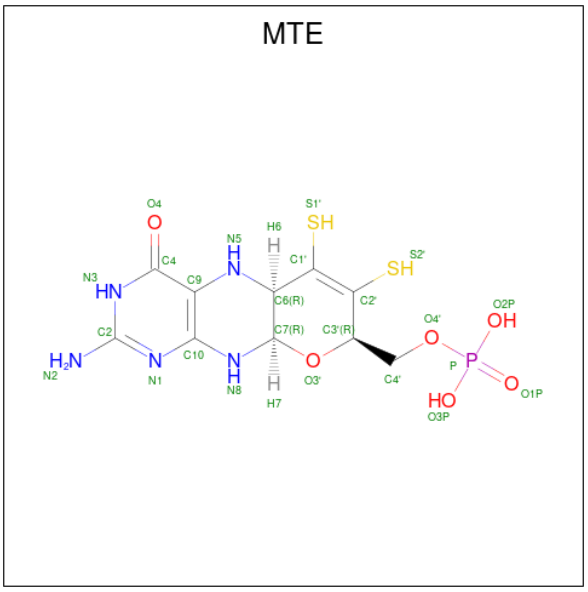
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		

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



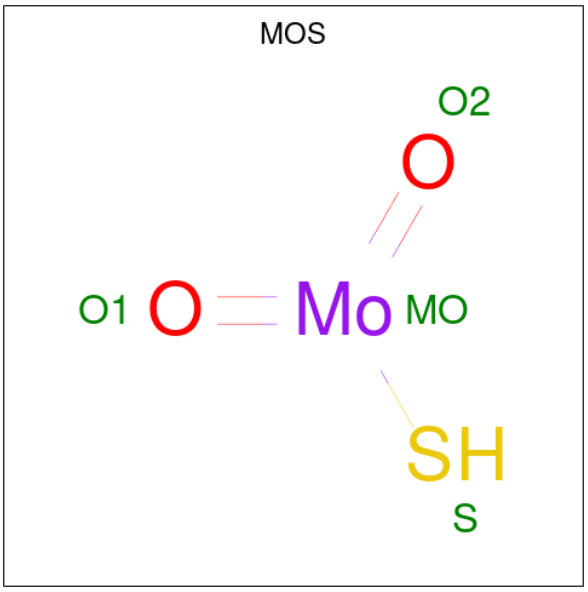
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



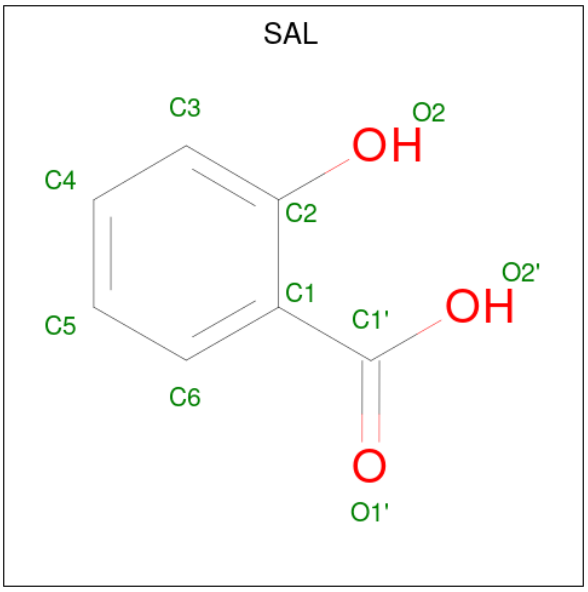
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



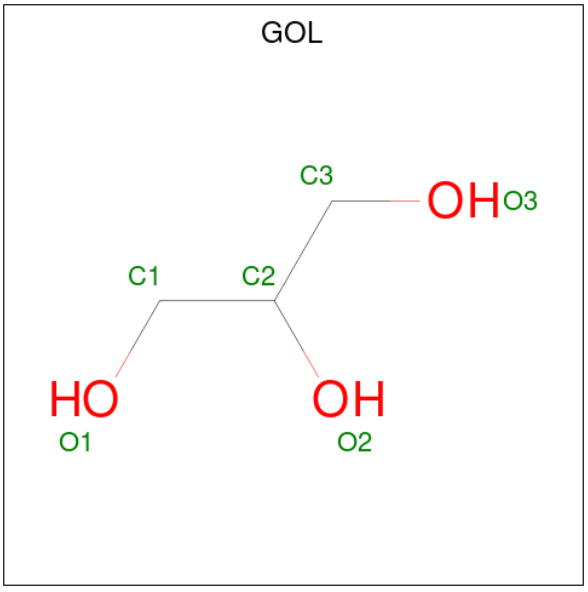
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 8 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 10 7 3	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	94	Total O 94 94	0	0
10	B	119	Total O 119 119	0	0
10	C	383	Total O 383 383	0	0

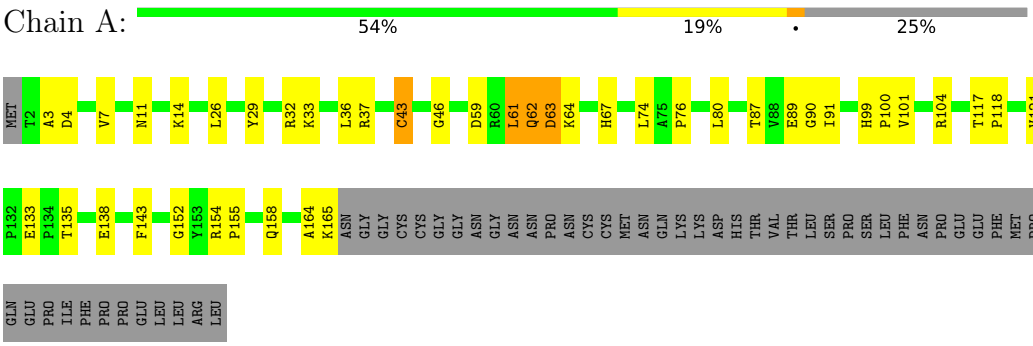
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

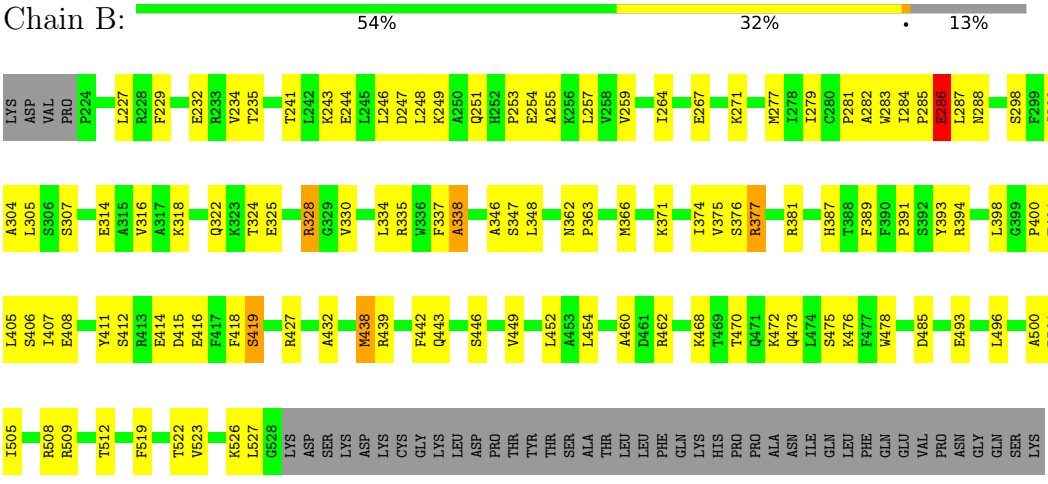
• Molecule 1: XANTHINE OXIDASE

Chain A:



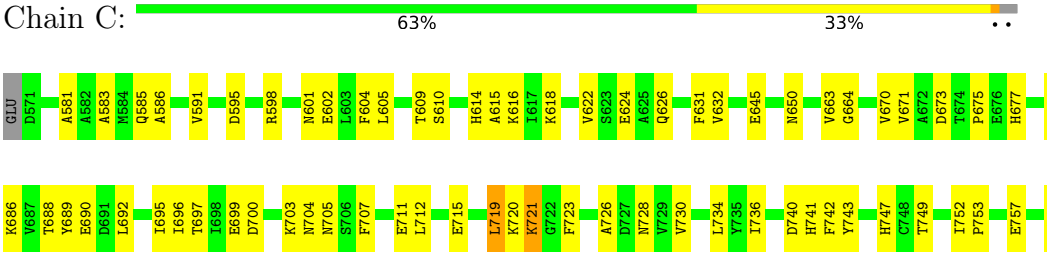
• Molecule 2: XANTHINE OXIDASE

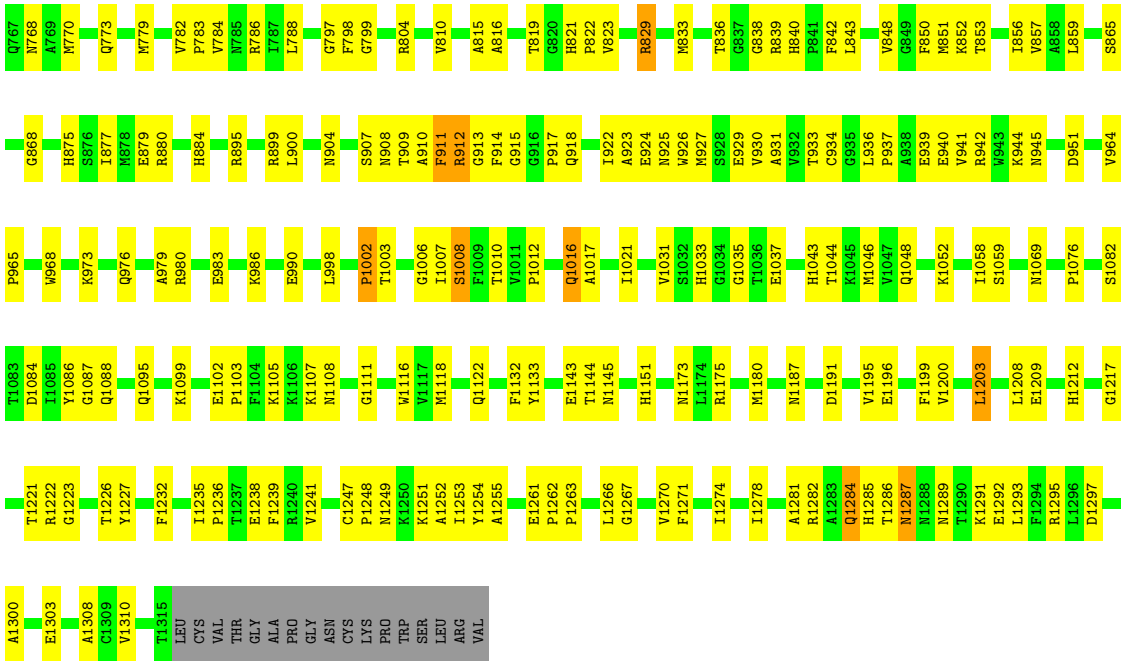
Chain B:



• Molecule 3: XANTHINE OXIDASE

Chain C:




Q767 N768 A769 M770 Q773 M779 V782 P783 V784 N785 R786 I787 L788 G797 F798 G799 R804 V810 A815 A816 T819 G820 H821 P822 V823 R829 M833 T836 G837 G838 R839 H840 P841 F842 L843 V848 G849 F850 M851 K852 T853 I856 V857 A858 L859 S865
G868 H875 S876 I877 M878 E879 R880 H884 R895 R899 L900 N904 S907 N908 T909 A910 F911 R912 G913 F914 G915 G916 P917 Q918 I922 A923 E924 N925 W926 M927 S928 E929 V930 A931 V932 T933 C934 G935 L936 P937 A938 E939 E940 V941 R942 W943 K944 N945 D951 V964
P965 W968 K973 Q976 A979 R980 E983 K986 E990 L998 P1002 T1003 G1006 I1007 S1008 F1009 T1010 V1011 P1012 Q1016 A1017 I1021 V1031 S1032 H1033 G1034 G1035 T1036 E1037 H1043 T1044 K1045 M1046 V1047 Q1048 K1052 I1058 S1059 N1069 P1076 S1082
T1083 D1084 I1085 Y1086 G1087 Q1088 Q1095 K1099 E1102 P1103 F1104 K1105 K1106 K1107 N1108 G1111 W1116 V1117 M1118 Q1122 F1132 Y1133 E1143 T1144 N1145 H1151 N1173 L1174 R1175 M1180 N1187 D1191 V1195 E1196 F1199 V1200 L1203 L1208 E1209 H1212 G1217
T1221 R1222 G1223 T1226 Y1227 F1232 I1235 P1236 T1237 E1238 F1239 R1240 V1241 C1247 P1248 N1249 K1250 K1251 A1252 I1253 Y1254 A1255 E1261 P1262 P1263 L1266 G1267 V1270 F1271 I1274 I1278 A1281 R1282 A1283 Q1284 H1285 T1286 N1287 N1288 N1289 T1290 K1291 E1292 L1293 F1294 R1295 L1296 D1297
A1300 E1303 A1308 C1309 V1310 T1315 LEU CYS VAL THR GLY ALA PRO GLY ASN CYS LYS PRO TRP SER LEU ARG VAL

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	117.83Å 165.40Å 154.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.9 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.212 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10106	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MOS, SAL, FES, FAD, MTE

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	0.37	0/1277	0.66	0/1723
2	B	0.33	0/2438	0.59	1/3290 (0.0%)
3	C	0.35	0/5888	0.62	0/7974
All	All	0.35	0/9603	0.62	1/12987 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	286	GLU	N-CA-C	-5.80	95.34	111.00

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	1255	0	1265	42	0
2	B	2389	0	2459	103	0
3	C	5761	0	5685	223	1
4	A	8	0	0	1	0
5	B	53	0	31	1	0
6	C	24	0	10	1	0
7	C	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	10	0	4	0	0
9	C	6	0	3	5	0
10	A	94	0	0	3	0
10	B	119	0	0	1	0
10	C	383	0	0	6	2
All	All	10106	0	9457	357	3

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 19.

The worst 5 of 357 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)
2:B:374:ILE:HD12	2:B:381:ARG:HH12	1.27	0.97
3:C:1046:MET:HE1	3:C:1087:GLY:HA2	1.47	0.97
3:C:1289:ASN:HB3	3:C:1292:GLU:HB2	1.55	0.89
3:C:618:LYS:HD3	3:C:688:THR:HG21	1.58	0.84
3:C:833:MET:HE3	3:C:1222:ARG:C	1.99	0.83

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1509:HOH:O	10:C:1509:HOH:O[3_556]	1.82	0.38
3:C:973:LYS:NZ	3:C:973:LYS:NZ[4_556]	1.86	0.34
10:C:1598:HOH:O	10:C:1598:HOH:O[3_556]	1.99	0.21

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	162/219 (74%)	152 (94%)	5 (3%)	5 (3%)	4 5
2	B	303/350 (87%)	274 (90%)	25 (8%)	4 (1%)	12 21
3	C	743/763 (97%)	687 (92%)	47 (6%)	9 (1%)	13 24
All	All	1208/1332 (91%)	1113 (92%)	77 (6%)	18 (2%)	10 18

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	64	LYS
3	C	1008	SER
3	C	1287	ASN
2	B	282	ALA

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	137/187 (73%)	137 (100%)	0	100 100
2	B	261/302 (86%)	254 (97%)	7 (3%)	44 71
3	C	624/639 (98%)	613 (98%)	11 (2%)	59 81
All	All	1022/1128 (91%)	1004 (98%)	18 (2%)	59 81

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1016	GLN
3	C	1239	PHE
3	C	1208	LEU
3	C	743	TYR
3	C	1002	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	704	ASN
3	C	1287	ASN
3	C	840	HIS
3	C	1048	GLN
3	C	821	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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	601	1	0,4,4	-	-	-		
8	SAL	C	1335	-	10,10,10	1.83	4 (40%)	13,13,13	2.08	4 (30%)
7	MOS	C	1334	6	0,3,3	-	-	-		
9	GOL	C	1336	-	5,5,5	6.33	5 (100%)	5,5,5	5.69	3 (60%)
6	MTE	C	1333	7	21,26,26	6.98	14 (66%)	21,40,40	4.94	11 (52%)
4	FES	A	602	1	0,4,4	-	-	-		
5	FAD	B	606	-	53,58,58	4.72	38 (71%)	68,89,89	2.19	22 (32%)

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	601	1	-	-	0/1/1/1
8	SAL	C	1335	-	-	0/4/4/4	0/1/1/1
9	GOL	C	1336	-	-	2/4/4/4	-
6	MTE	C	1333	7	-	6/6/34/34	0/3/3/3
4	FES	A	602	1	-	-	0/1/1/1
5	FAD	B	606	-	-	2/30/50/50	0/6/6/6

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1333	MTE	C7-C6	21.01	1.70	1.53
6	C	1333	MTE	C9-C10	13.44	1.66	1.41
5	B	606	FAD	C4A-N3A	12.51	1.52	1.35
5	B	606	FAD	C9A-N10	11.65	1.61	1.41
9	C	1336	GOL	C3-C2	-10.94	1.06	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1333	MTE	C4-C9-N5	12.00	129.19	119.12
6	C	1333	MTE	P-O4'-C4'	11.80	150.81	118.30
9	C	1336	GOL	O3-C3-C2	9.99	158.08	110.20
9	C	1336	GOL	O2-C2-C3	6.84	139.23	109.12
6	C	1333	MTE	O2P-P-O4'	6.30	123.50	106.73

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1333	MTE	C3'-C4'-O4'-P
6	C	1333	MTE	C4'-O4'-P-O1P
6	C	1333	MTE	C4'-O4'-P-O2P
6	C	1333	MTE	C4'-O4'-P-O3P
9	C	1336	GOL	O1-C1-C2-O2

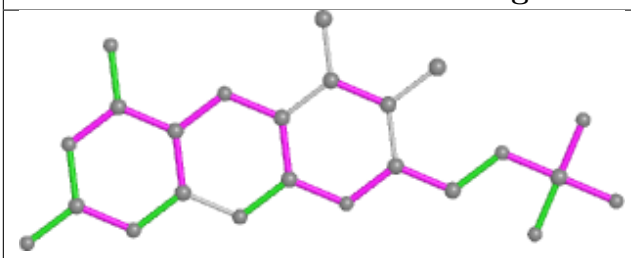
There are no ring outliers.

5 monomers are involved in 11 short contacts:

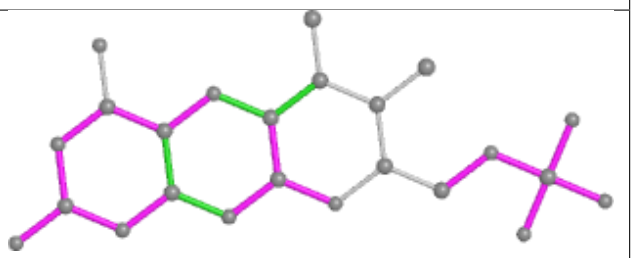
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1334	MOS	3	0
9	C	1336	GOL	5	0
6	C	1333	MTE	1	0
4	A	602	FES	1	0
5	B	606	FAD	1	0

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.

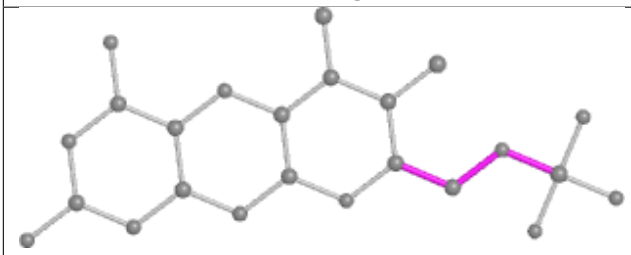
Ligand MTE C 1333



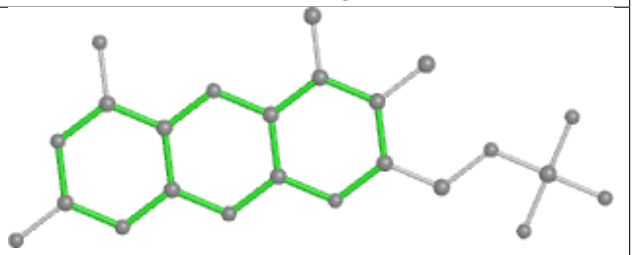
Bond lengths



Bond angles

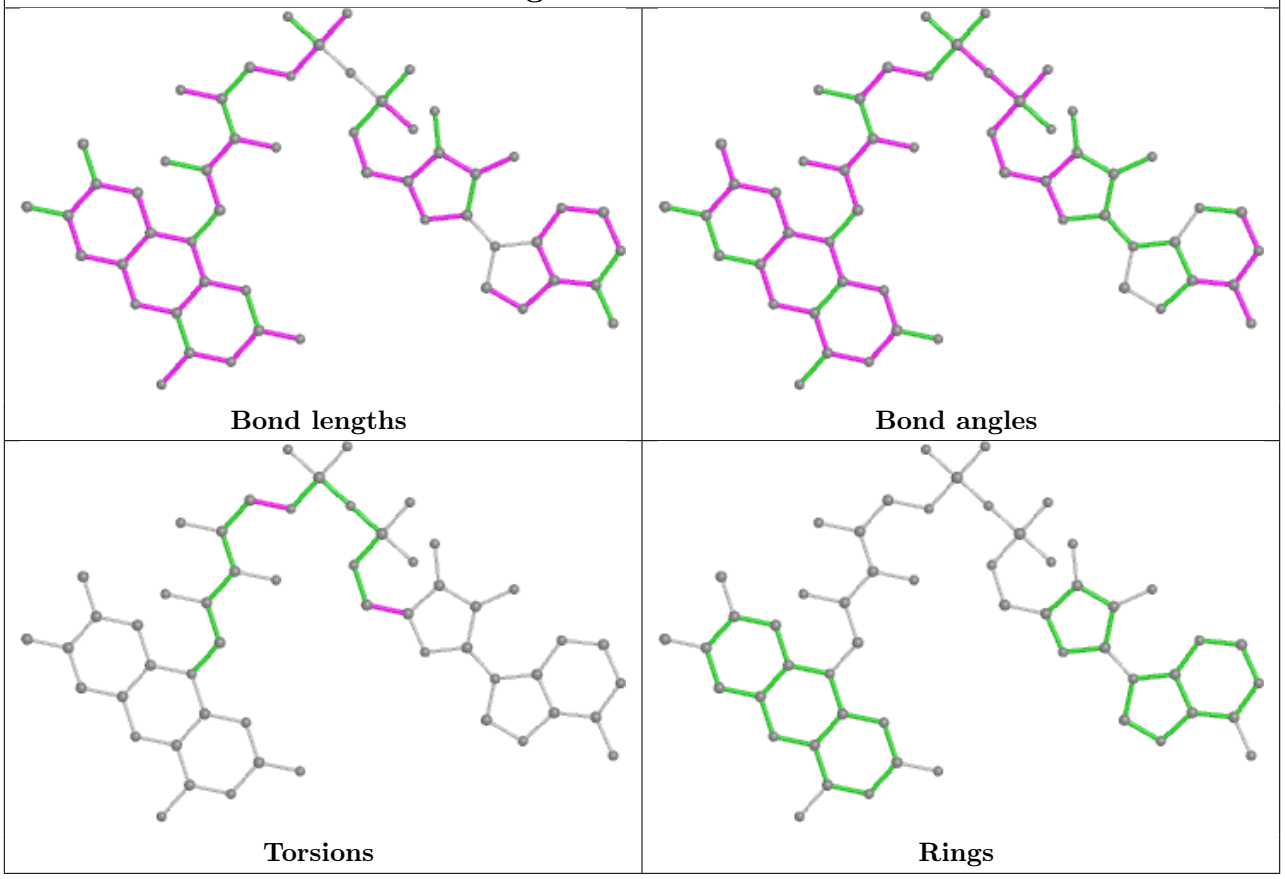


Torsions



Rings

Ligand FAD B 606



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.