wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 04:57 am GMT

PDB ID	:	2CKJ
Title	:	Human milk xanthine oxidoreductase
Authors	:	Pearson, A.R.; Godber, B.L.J.; Eisenthal, R.; Taylor, G.L.; Harrison, R.
Deposited on	:	2006-04-19
Resolution	:	3.59 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:

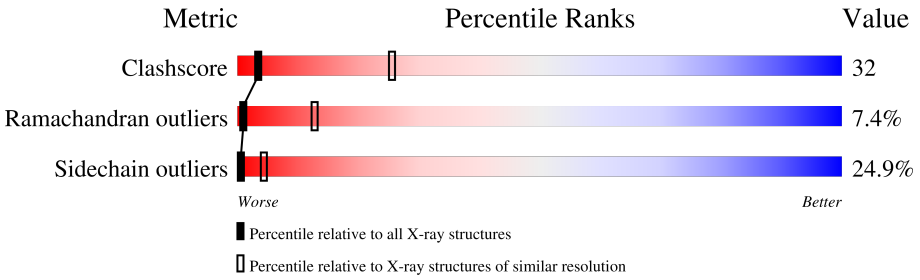
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.59 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	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

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	1333	34% 34% 20% 6% 5%
1	B	1333	35% 35% 20% 7% .
1	C	1333	35% 36% 18% 8% .
1	D	1333	36% 34% 20% 7% .

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
2	FES	A	3002	-	-	X	-
2	FES	B	3002	-	-	X	-
4	GOL	A	3007	-	-	X	-
4	GOL	B	3007	-	-	X	-
4	GOL	C	3007	-	-	X	-
4	GOL	D	3007	-	-	X	-

2 Entry composition (i)

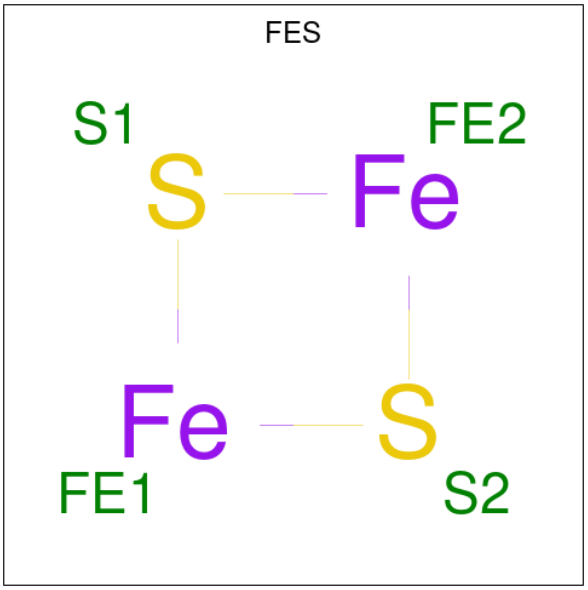
There are 6 unique types of molecules in this entry. The entry contains 39807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1264	Total	C	N	O	S	0	0	0
			9764	6195	1679	1826	64			
1	B	1289	Total	C	N	O	S	0	0	0
			9951	6307	1713	1865	66			
1	C	1283	Total	C	N	O	S	0	0	0
			9905	6280	1706	1854	65			
1	D	1283	Total	C	N	O	S	0	0	0
			9910	6281	1707	1856	66			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

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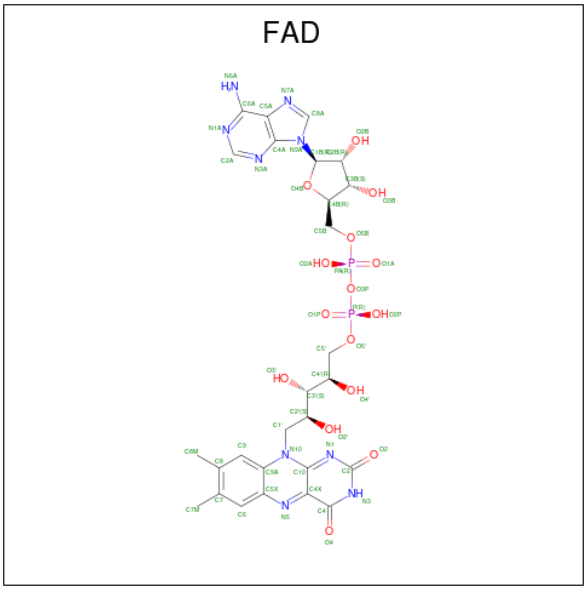
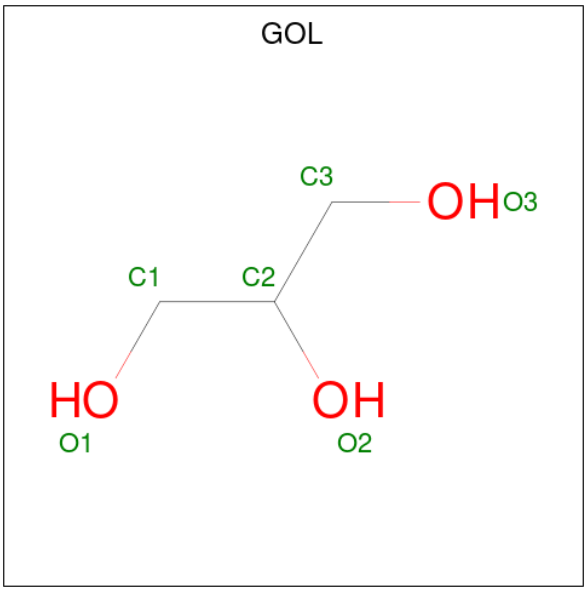
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



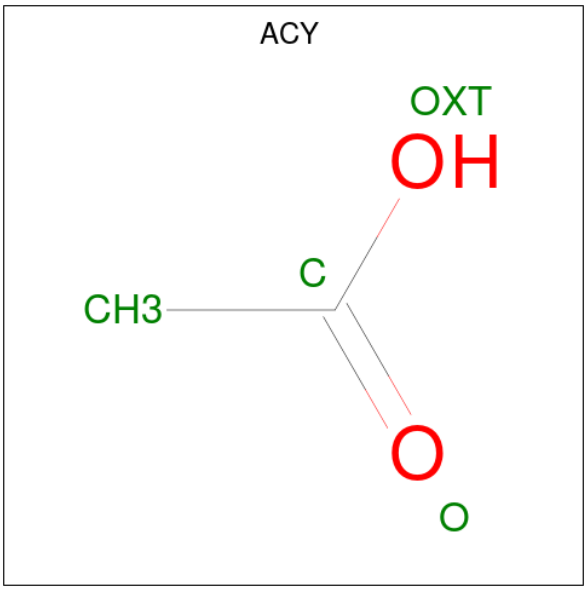
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



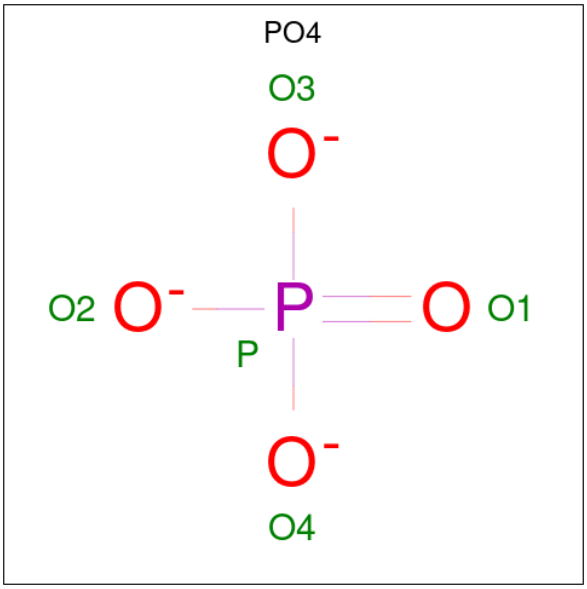
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O P 5 4 1	0	0

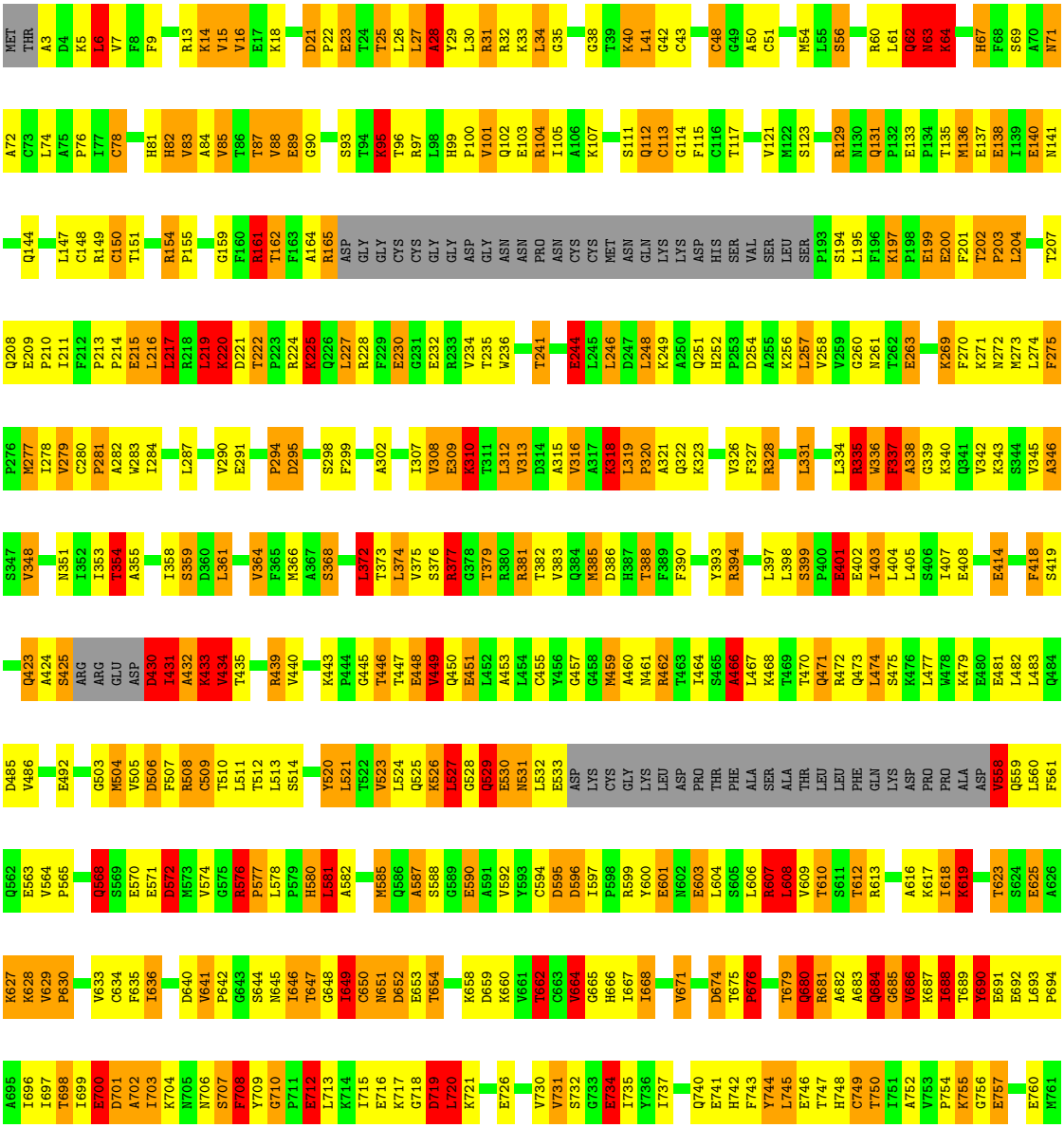
3 Residue-property plots (i)

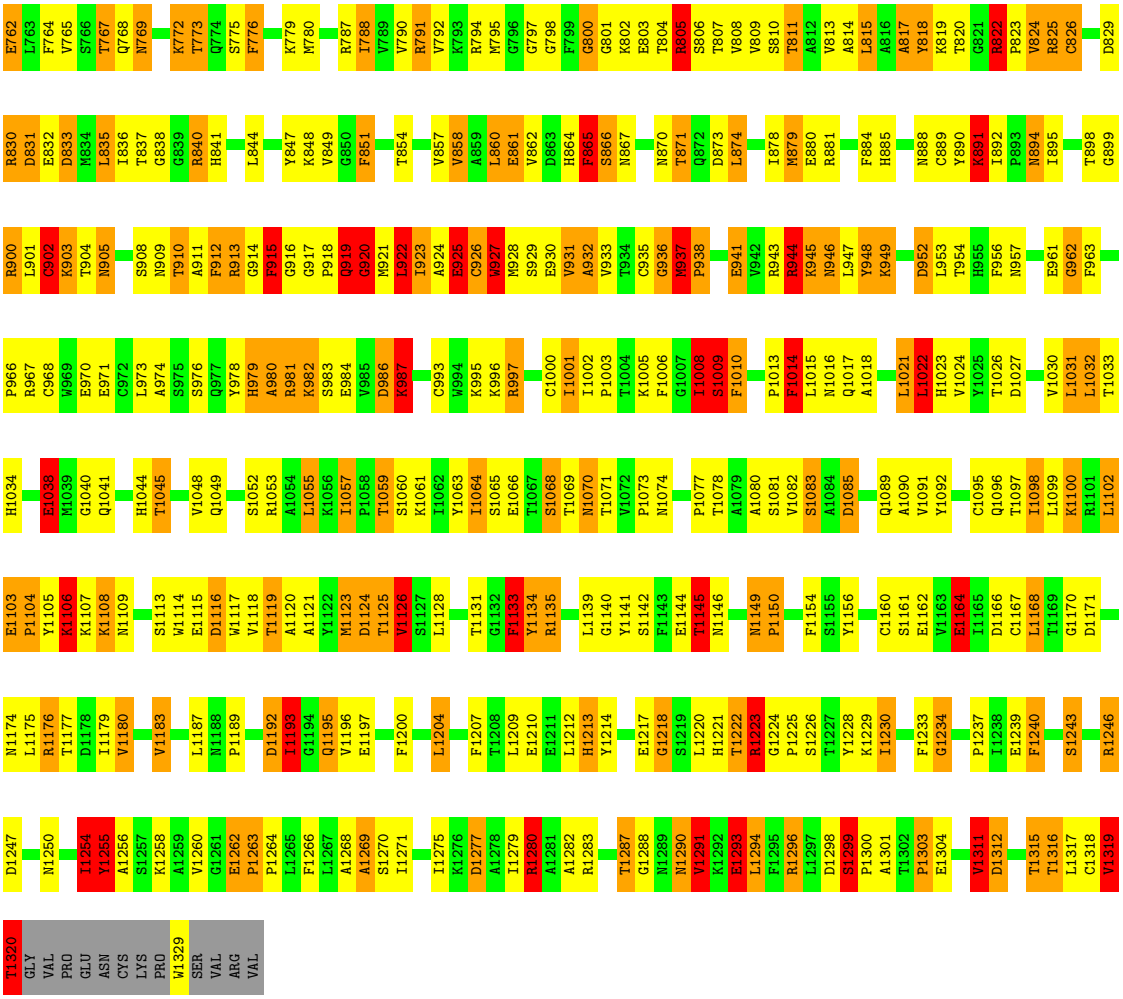
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 OXIDOREDUCTASE

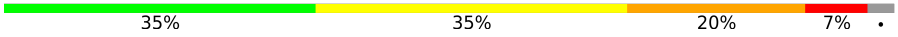
Chain A:

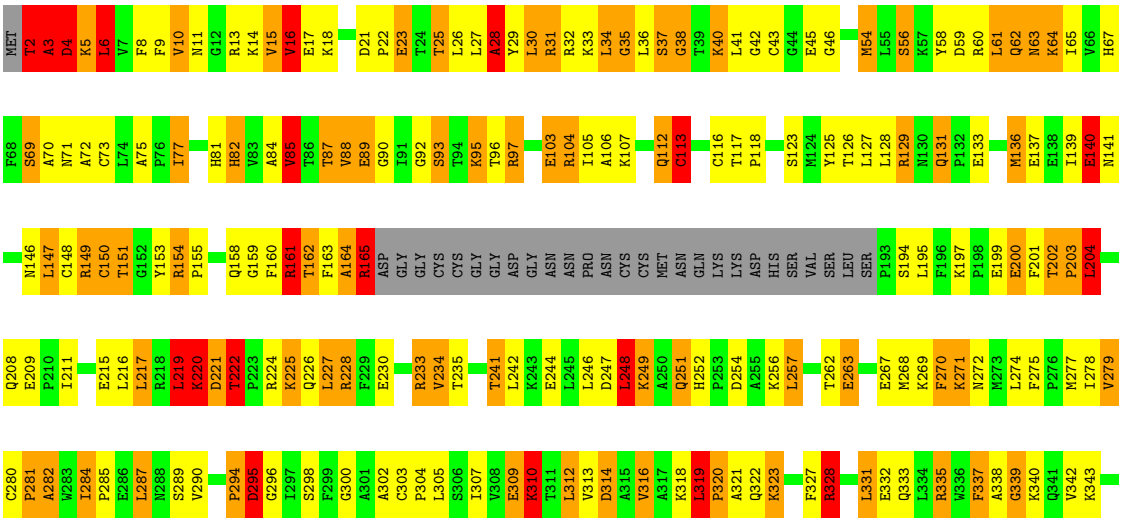


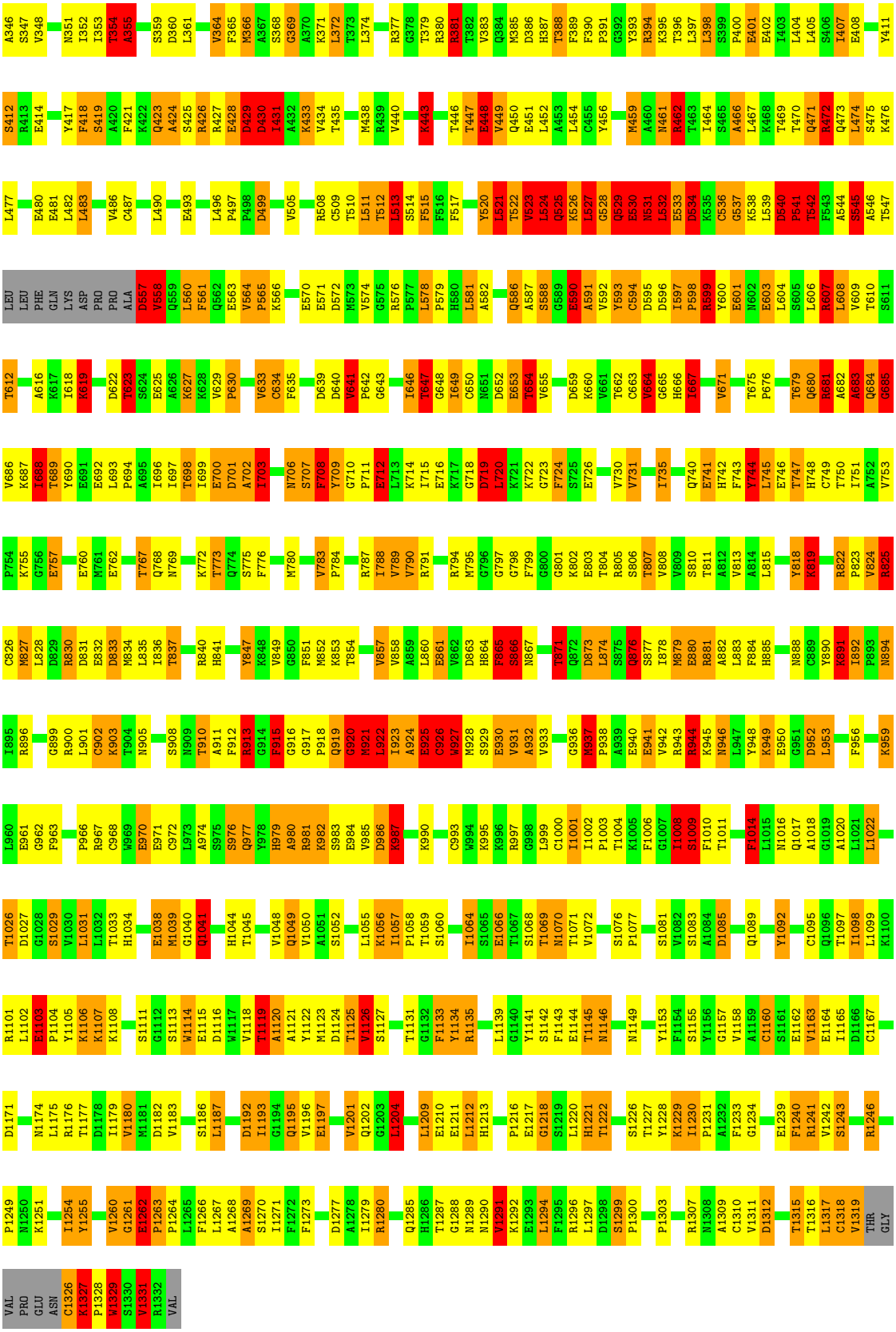


• Molecule 1: XANTHINE OXIDOREDUCTASE

Chain B:

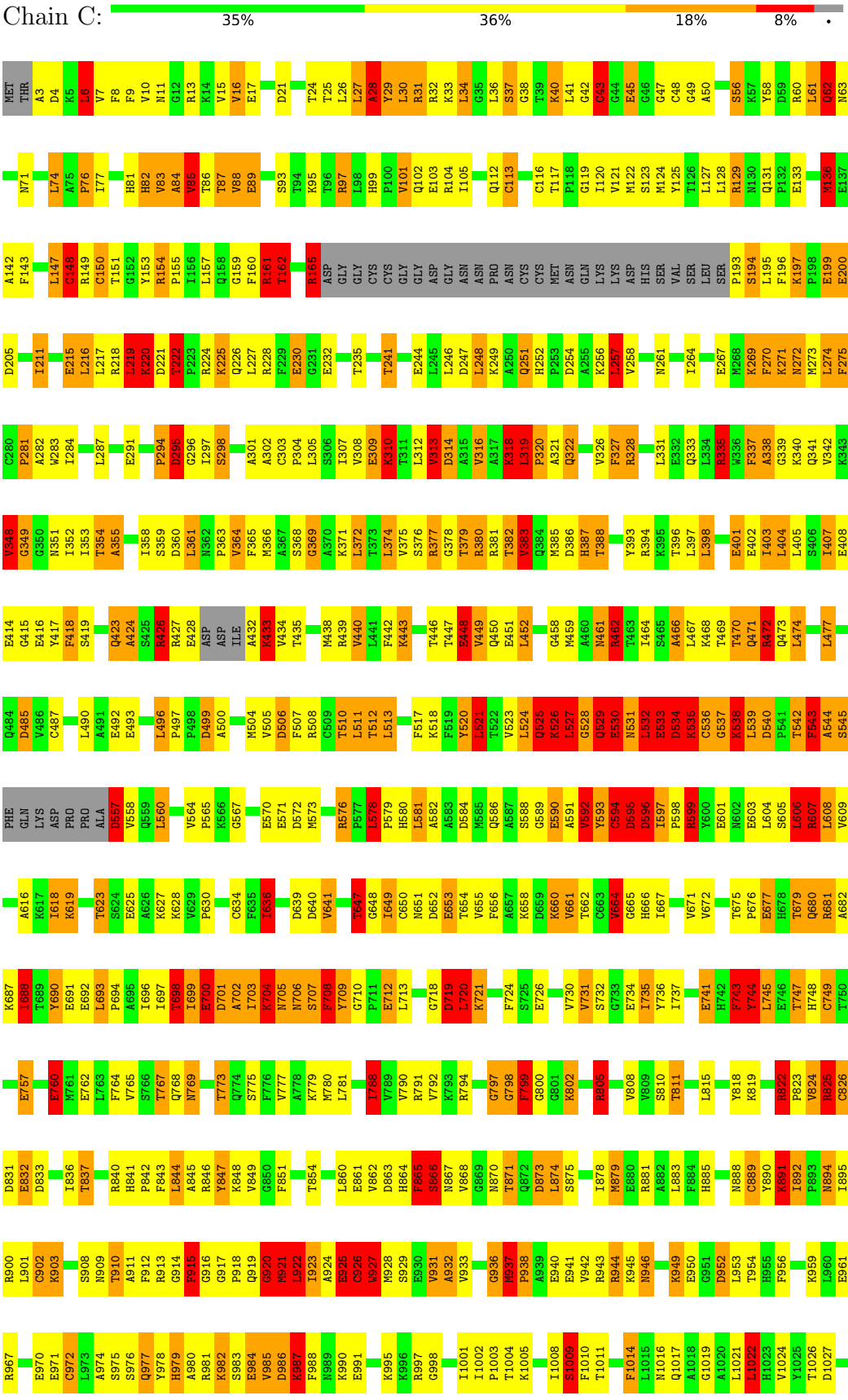


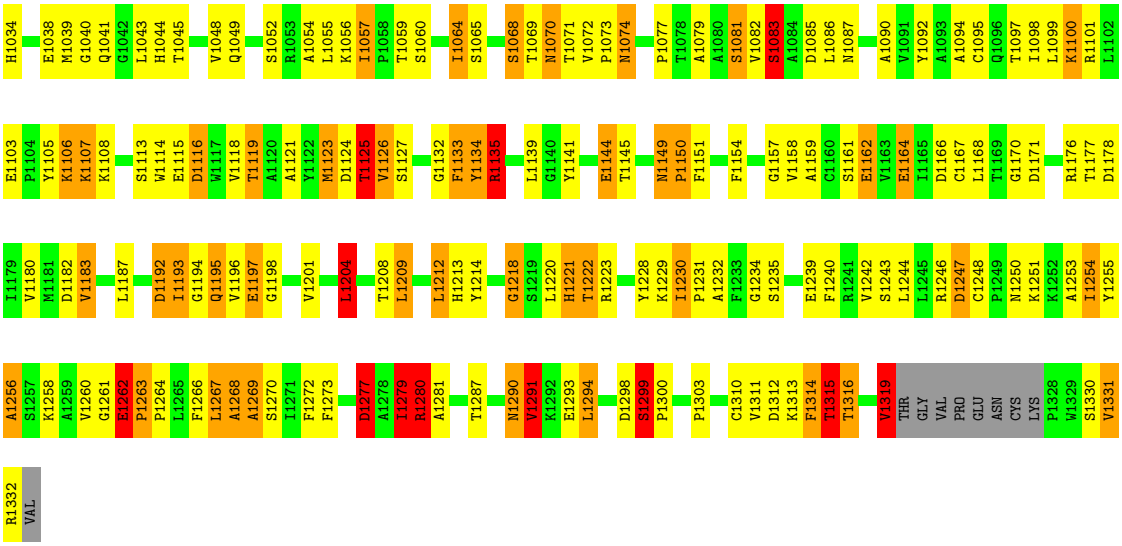




• Molecule 1: XANTHINE OXIDOREDUCTASE

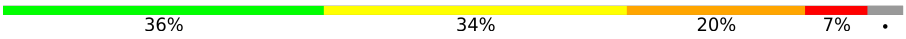
Chain C:

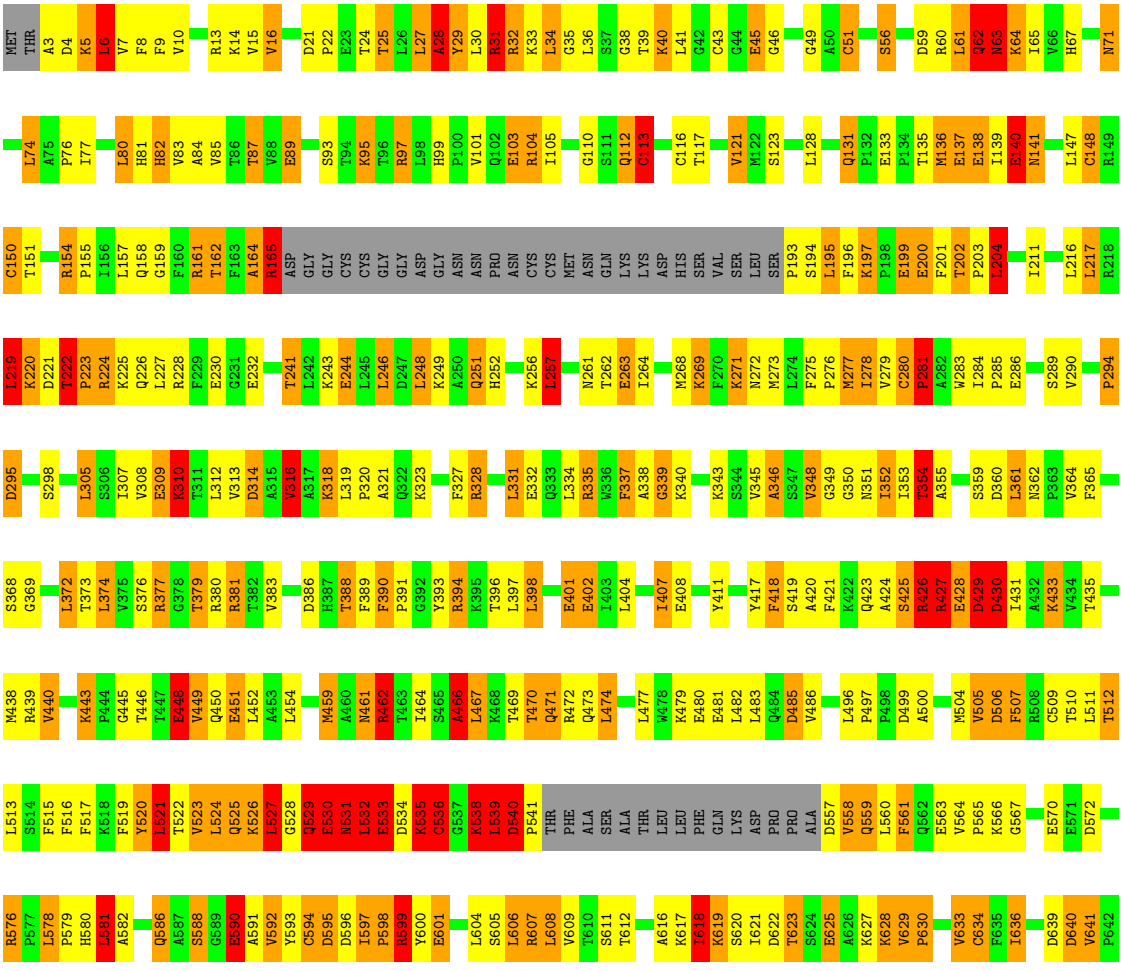


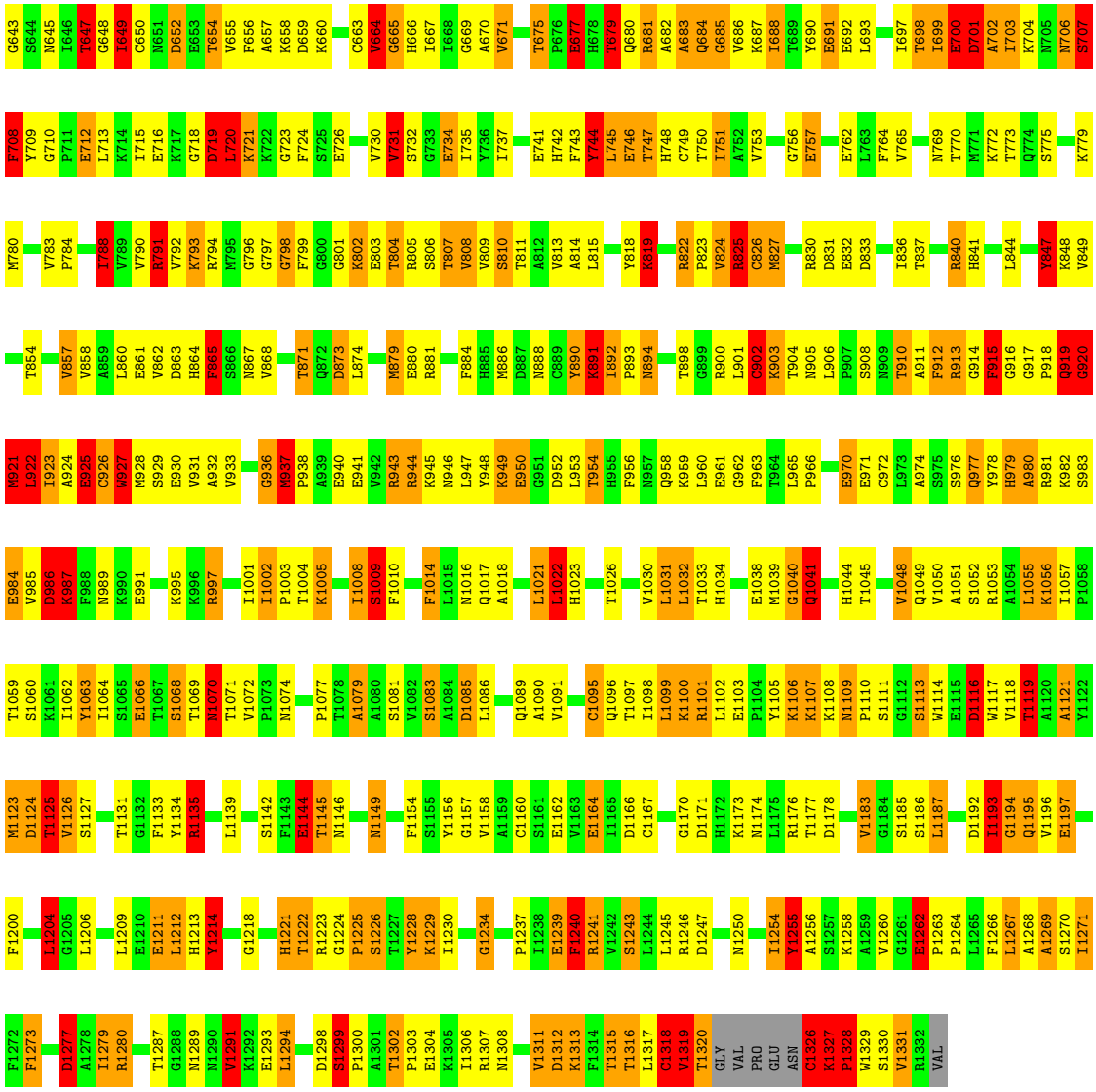


• Molecule 1: XANTHINE OXIDOREDUCTASE

Chain D:






G643 S644 N645 I646 T647 G648 I649 C650 N651 D652 E653 T654 V655 F656 A657 K658 D659 K660 C663 V664 G665 H666 I667 I668 G669 A670 V671 T675 P676 E677 H678 I679 Q680 R681 A682 A683 Q684 G685 V686 K687 I688 T689 Y690 E691 E692 L693 I697 T698 I699 E700 D701 A702 I703 K704 N705 N706 S707
F708 Y709 G710 P711 E712 L713 K714 I715 E716 K717 G718 D719 L720 K721 K722 G723 F724 S725 E726 V730 V731 S732 G733 E734 I735 Y736 I737 E741 H742 F743 Y744 L745 E746 T747 H748 C749 T750 I751 A752 V753 G756 E757 E762 L763 F764 V765 N769 T770 M771 K772 T773 Q774 S775 K779
M780 V783 P784 I788 V789 V790 R791 V792 K793 R794 M795 G796 G797 G798 F799 G800 G801 K802 E803 T804 R805 S806 T807 V808 V809 S810 T811 A812 V813 A814 L815 Y818 K819 R822 P823 V824 R825 C826 M827 R830 D831 E832 D833 I836 T837 R840 H841 L844 Y847 K848 V849
T854 V857 V858 A859 L860 E861 V862 D863 H864 F865 S866 N867 V868 T871 Q872 D873 L874 M879 E880 R881 F884 H885 M886 D887 N888 C889 Y890 K891 I892 P893 N894 T898 G899 R900 L901 C902 K903 T904 N905 L906 P907 S908 N909 T910 A911 F912 R913 G914 F915 G916 G917 P918 Q919 G920
M921 L922 I923 A924 E925 C926 W927 M928 S929 E930 V931 A932 V933 G936 M937 P938 A939 E940 E941 V942 R943 R944 K945 N946 L947 Y948 K949 E950 G951 D952 L953 T954 H955 F956 N957 Q958 K959 L960 E961 G962 F963 T964 L965 P966 E970 E971 C972 L973 A974 S975 S976 Q977 Y978 H979 A980 R981 K982 S983
E984 V985 D986 K987 F988 N989 K990 E991 K995 K996 R997 I1001 I1002 P1003 T1004 K1005 I1008 S1009 F1010 F1014 L1015 N1016 Q1017 A1018 L1021 L1022 H1023 T1026 V1030 L1031 L1032 T1033 H1034 E1038 M1039 G1040 Q1041 H1044 T1045 V1048 Q1049 V1050 A1051 S1052 R1053 A1054 L1055 K1056 I1057 P1058
T1059 S1060 K1061 I1062 Y1063 I1064 S1065 E1066 T1067 S1068 T1069 N1070 T1071 V1072 P1073 N1074 P1077 T1078 A1079 A1080 S1081 V1082 S1083 A1084 D1085 L1086 Q1089 A1090 V1091 C1095 Q1096 T1097 I1098 L1099 K1100 R1101 L1102 E1103 P1104 Y1105 K1106 K1107 K1108 N1109 P1110 S1111 G1112 S1113 W1114 E1115 D1116 W1117 V1118 T1119 A1120 A1121 Y1122
M1123 D1124 T1125 V1126 S1127 T1131 G1132 F1133 Y1134 R1135 L1139 S1142 F1143 E1144 T1145 N1146 N1149 F1154 S1155 Y1156 G1157 V1158 A1159 C1160 S1161 E1162 V1163 E1164 I1165 D1166 C1167 G1170 D1171 H1172 K1173 N1174 L1175 R1176 T1177 D1178 V1183 G1184 S1185 S1186 L1187 D1192 I1193 G1194 Q1195 V1196 E1197
F1200 L1204 G1205 L1206 L1209 E1210 E1211 L1212 H1213 Y1214 G1218 H1221 T1222 R1223 G1224 P1225 S1226 T1227 Y1228 K1229 I1230 G1234 P1237 I1238 E1239 F1240 R1241 V1242 S1243 L1244 L1245 R1246 D1247 N1250 I1254 Y1255 A1256 S1257 K1258 A1259 V1260 G1261 E1262 P1263 P1264 L1265 F1266 L1267 A1268 A1269 S1270 I1271
F1272 F1273 D1277 A1278 I1279 R1280 T1287 G1288 N1289 N1290 V1291 K1292 E1293 L1294 D1298 S1299 P1300 A1301 T1302 P1303 E1304 K1305 I1306 R1307 N1308 V1311 D1312 K1313 F1314 T1315 T1316 L1317 C1318 V1319 T1320 GLY VAL PRO GLU ASN C1326 K1327 P1328 W1329 S1330 V1331 R1332 VAL

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	197.73Å 197.73Å 285.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.76 – 3.59	Depositor
% Data completeness (in resolution range)	98.2 (30.76-3.59)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	39807	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: ACY, GOL, FAD, FES, PO4

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	2.11	336/9969 (3.4%)	1.70	184/13492 (1.4%)
1	B	2.14	334/10160 (3.3%)	1.73	211/13751 (1.5%)
1	C	2.10	326/10113 (3.2%)	1.72	202/13685 (1.5%)
1	D	2.06	304/10118 (3.0%)	1.70	175/13693 (1.3%)
All	All	2.10	1300/40360 (3.2%)	1.71	772/54621 (1.4%)

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	40
1	B	1	54
1	C	1	49
1	D	0	55
All	All	2	198

The worst 5 of 1300 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1318	CYS	CB-SG	17.07	2.11	1.82
1	A	762	GLU	CG-CD	16.49	1.76	1.51
1	A	78	CYS	CB-SG	16.00	2.09	1.82
1	B	3	ALA	N-CA	15.65	1.77	1.46
1	B	762	GLU	CD-OE1	15.23	1.42	1.25

The worst 5 of 772 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	794	ARG	NE-CZ-NH2	-14.57	113.02	120.30
1	A	830	ARG	NE-CZ-NH1	13.47	127.04	120.30
1	C	825	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	B	599	ARG	CG-CD-NE	13.40	139.94	111.80
1	C	599	ARG	NE-CZ-NH1	13.04	126.82	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	165	ARG	CA
1	C	165	ARG	CA

5 of 198 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	GLU	Peptide
1	A	164	ALA	Peptide
1	A	202	THR	Peptide
1	A	222	THR	Peptide
1	A	294	PRO	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	9764	0	9788	628	0
1	B	9951	0	9967	711	0
1	C	9905	0	9922	648	0
1	D	9910	0	9929	634	0
2	A	8	0	0	2	0
2	B	8	0	0	2	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	53	0	30	12	0
3	B	53	0	29	6	0
3	C	53	0	29	10	0
3	D	53	0	29	14	0
4	A	6	0	8	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	14	0
4	C	6	0	8	4	0
4	D	6	0	8	10	0
5	D	4	0	3	0	0
6	D	5	0	0	1	0
All	All	39807	0	39758	2568	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 32.

The worst 5 of 2568 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:D:793:LYS:CG	1:D:793:LYS:CD	1.74	1.62
1:C:1319:VAL:CA	1:C:1319:VAL:CB	1.77	1.61
1:D:903:LYS:CD	1:D:903:LYS:CE	1.75	1.61
1:B:1319:VAL:CA	1:B:1319:VAL:CB	1.78	1.61
1:A:318:LYS:CE	1:A:318:LYS:CD	1.76	1.61

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	1255/1333 (94%)	1002 (80%)	168 (13%)	85 (7%)	1 15
1	B	1281/1333 (96%)	1021 (80%)	158 (12%)	102 (8%)	1 11
1	C	1273/1333 (96%)	1011 (79%)	168 (13%)	94 (7%)	1 13
1	D	1275/1333 (96%)	1006 (79%)	174 (14%)	95 (8%)	1 12
All	All	5084/5332 (95%)	4040 (80%)	668 (13%)	376 (7%)	1 13

5 of 376 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	219	LEU
1	A	220	LYS
1	A	272	ASN
1	A	449	VAL

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	1067/1126 (95%)	807 (76%)	260 (24%)	0	4
1	B	1088/1126 (97%)	812 (75%)	276 (25%)	0	4
1	C	1082/1126 (96%)	814 (75%)	268 (25%)	0	4
1	D	1084/1126 (96%)	813 (75%)	271 (25%)	0	4
All	All	4321/4504 (96%)	3246 (75%)	1075 (25%)	0	4

5 of 1075 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	630	PRO
1	D	720	LEU
1	D	623	THR
1	D	1131	THR
1	B	619	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	768	GLN
1	D	158	GLN
1	C	909	ASN
1	C	1070	ASN
1	D	651	ASN

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)

18 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	$\#\|Z\| > 2$
2	FES	C	3002	1	0,4,4	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
2	FES	D	3002	1	0,4,4	-	-	-		
4	GOL	B	3007	-	5,5,5	0.61	0	5,5,5	0.75	0
4	GOL	D	3007	-	5,5,5	0.85	0	5,5,5	1.30	1 (20%)
3	FAD	B	3006	-	53,58,58	2.07	14 (26%)	68,89,89	2.32	25 (36%)
4	GOL	A	3007	-	5,5,5	0.59	0	5,5,5	0.95	0
3	FAD	D	3006	-	53,58,58	2.28	11 (20%)	68,89,89	2.46	28 (41%)
4	GOL	C	3007	-	5,5,5	0.52	0	5,5,5	0.53	0
6	PO4	D	3009	-	4,4,4	1.07	0	6,6,6	1.86	1 (16%)
2	FES	D	3001	1	0,4,4	-	-	-		
2	FES	B	3001	1	0,4,4	-	-	-		
3	FAD	C	3006	-	53,58,58	2.02	14 (26%)	68,89,89	2.48	29 (42%)
3	FAD	A	3006	-	53,58,58	1.84	12 (22%)	68,89,89	1.99	25 (36%)
2	FES	A	3001	1	0,4,4	-	-	-		
2	FES	B	3002	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FES	C	3001	1	0,4,4	-	-	-		
5	ACY	D	3008	-	3,3,3	1.13	0	3,3,3	1.52	0

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
2	FES	C	3002	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	D	3002	1	-	-	0/1/1/1
4	GOL	B	3007	-	-	2/4/4/4	-
4	GOL	D	3007	-	-	0/4/4/4	-
2	FES	C	3001	1	-	-	0/1/1/1
3	FAD	B	3006	-	-	8/30/50/50	0/6/6/6
4	GOL	A	3007	-	-	2/4/4/4	-
3	FAD	D	3006	-	-	9/30/50/50	0/6/6/6
4	GOL	C	3007	-	-	2/4/4/4	-
2	FES	D	3001	1	-	-	0/1/1/1
2	FES	B	3001	1	-	-	0/1/1/1
3	FAD	A	3006	-	-	6/30/50/50	0/6/6/6
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	B	3002	1	-	-	0/1/1/1
3	FAD	C	3006	-	-	8/30/50/50	0/6/6/6

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3006	FAD	C2A-N3A	10.49	1.49	1.32
3	D	3006	FAD	C2A-N1A	7.07	1.47	1.33
3	B	3006	FAD	C2A-N3A	7.04	1.43	1.32
3	C	3006	FAD	C2A-N3A	6.02	1.41	1.32
3	A	3006	FAD	C2A-N1A	5.43	1.44	1.33

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3006	FAD	C1B-N9A-C4A	6.77	138.54	126.64
3	C	3006	FAD	C1B-N9A-C4A	6.74	138.48	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3006	FAD	C1B-N9A-C4A	6.65	138.32	126.64
3	C	3006	FAD	O2'-C2'-C1'	-5.79	95.79	109.80
3	D	3006	FAD	C4-C4X-C10	5.74	126.43	116.79

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3006	FAD	C5B-O5B-PA-O3P
3	B	3006	FAD	C5B-O5B-PA-O1A
3	B	3006	FAD	C5B-O5B-PA-O2A
3	B	3006	FAD	C5B-O5B-PA-O3P
3	B	3006	FAD	C2'-C3'-C4'-O4'

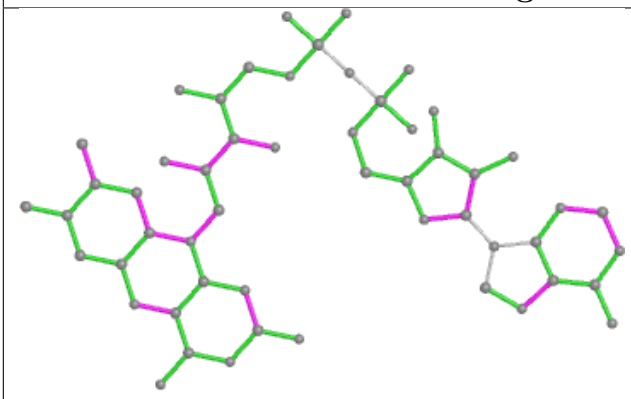
There are no ring outliers.

11 monomers are involved in 81 short contacts:

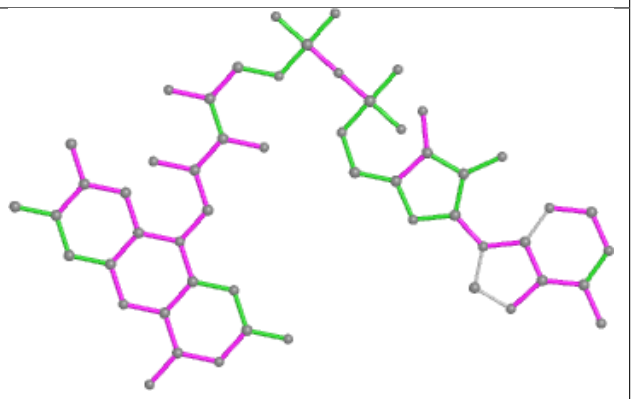
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	FES	2	0
4	B	3007	GOL	14	0
4	D	3007	GOL	10	0
3	B	3006	FAD	6	0
4	A	3007	GOL	6	0
3	D	3006	FAD	14	0
4	C	3007	GOL	4	0
6	D	3009	PO4	1	0
3	C	3006	FAD	10	0
3	A	3006	FAD	12	0
2	B	3002	FES	2	0

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.

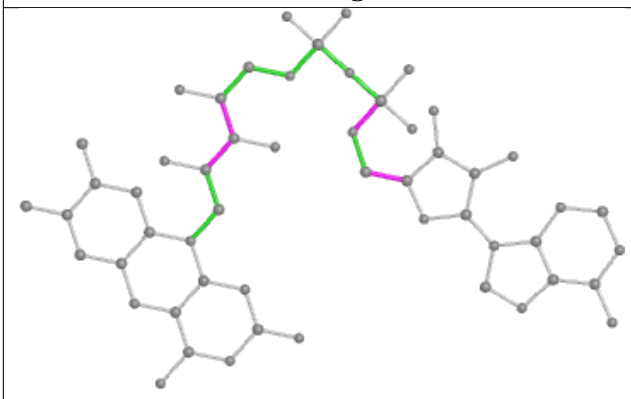
Ligand FAD B 3006



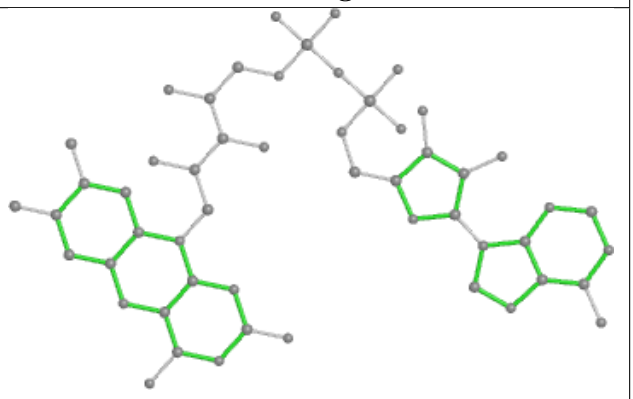
Bond lengths



Bond angles

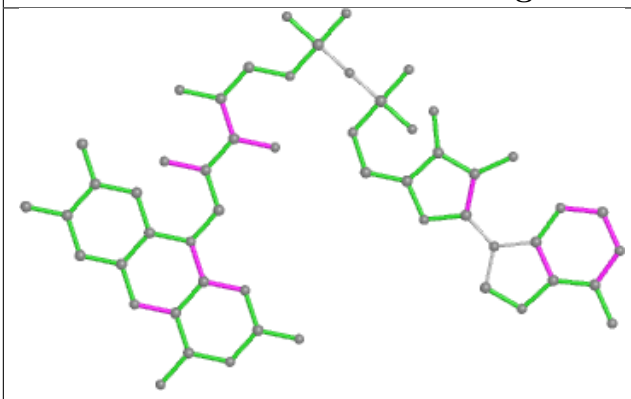


Torsions

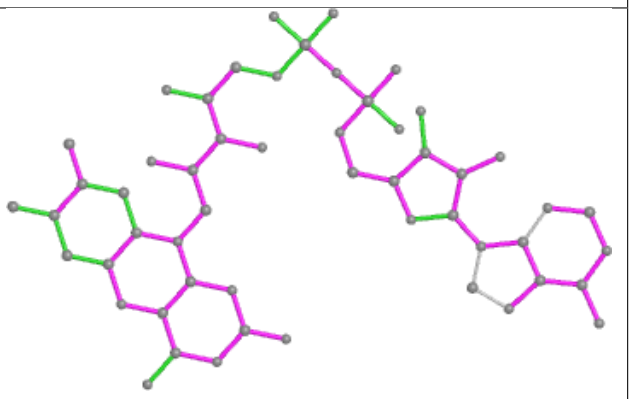


Rings

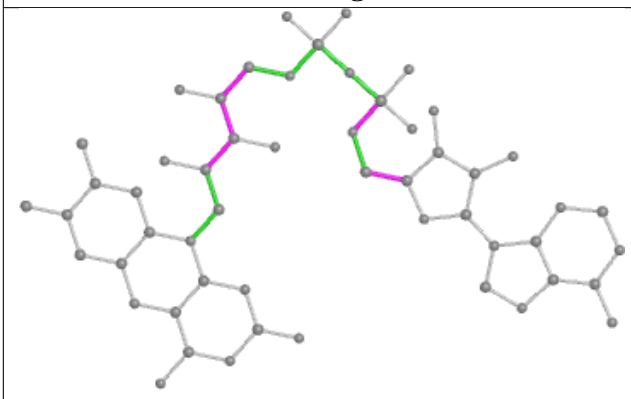
Ligand FAD D 3006



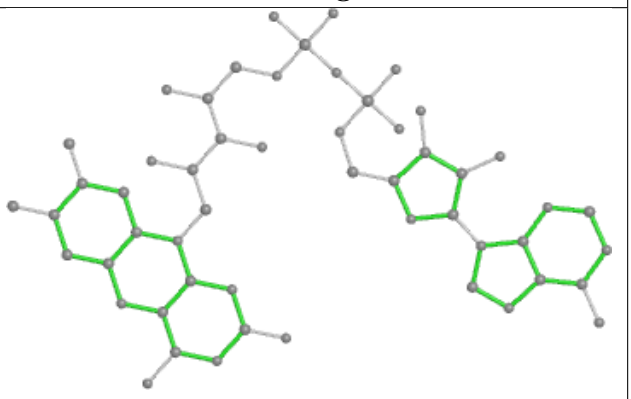
Bond lengths



Bond angles

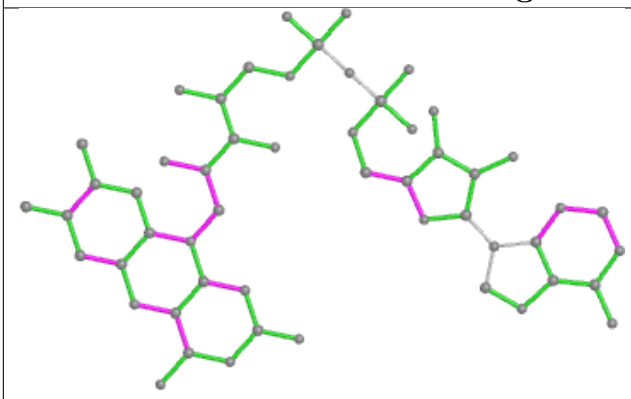


Torsions

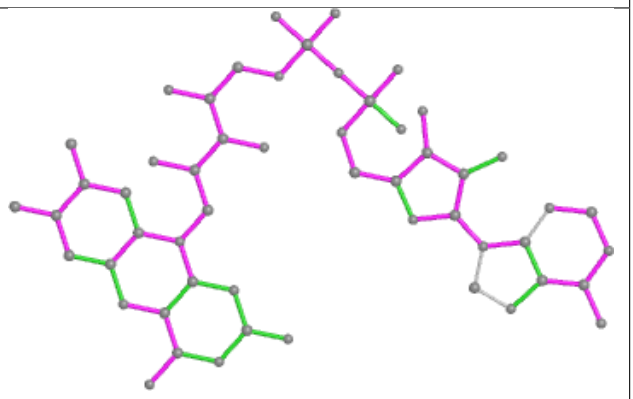


Rings

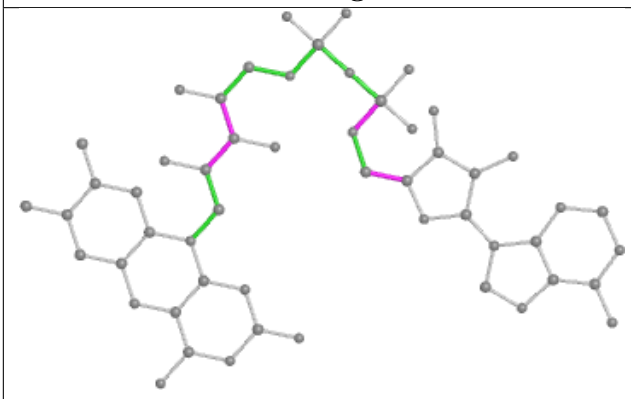
Ligand FAD C 3006



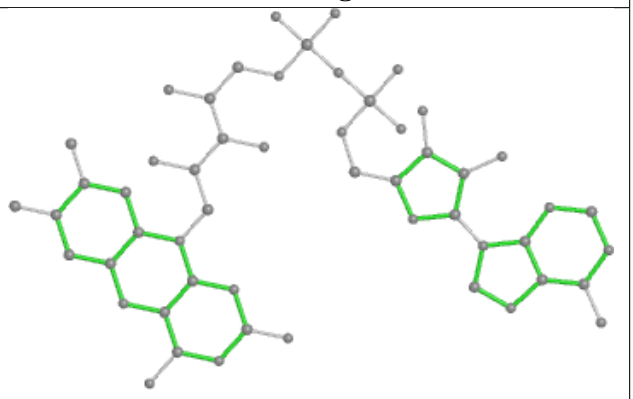
Bond lengths



Bond angles

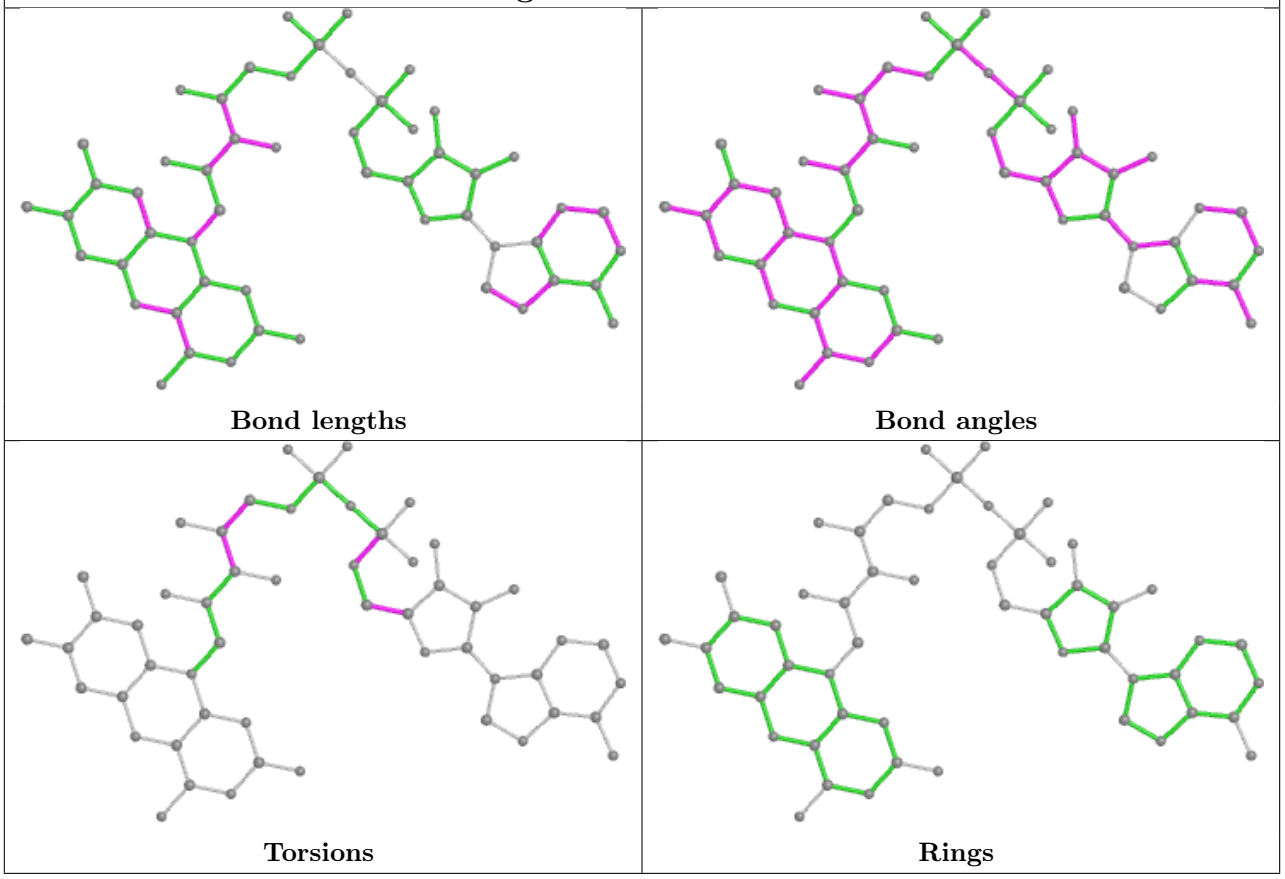


Torsions



Rings

Ligand FAD A 3006



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.