wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 07:14 AM EDT

PDB ID	:	1VDV / pdb_00001vdv
Title	:	Bovine Milk Xanthine Dehydrogenase Y-700 Bound Form
Authors	:	Fukunari, A.; Okamoto, K.; Nishino, T.; Eger, B.T.; Pai, E.F.; Kamezawa, M.; Yamada, I.; Kato, N.
Deposited on	:	2004-03-25
Resolution	:	1.98 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:

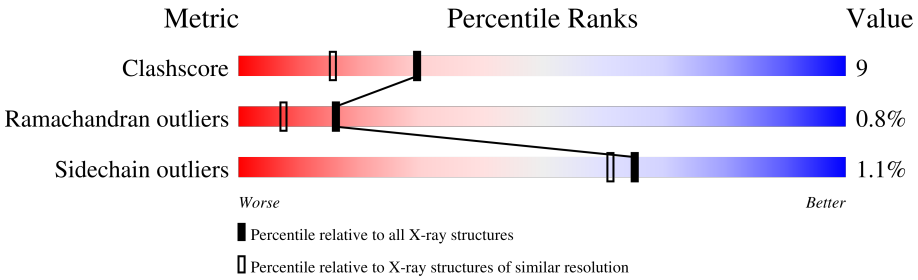
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & 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 1.98 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	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

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	1332	79% 17%
1	B	1332	80% 15%

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	ACY	A	5201	-	-	X	-
7	ACY	B	5202	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 22610 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/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1299	Total	C	N	O	S	0	0	0
			10077	6404	1728	1884	61			
1	B	1296	Total	C	N	O	S	0	0	0
			10054	6391	1724	1878	61			

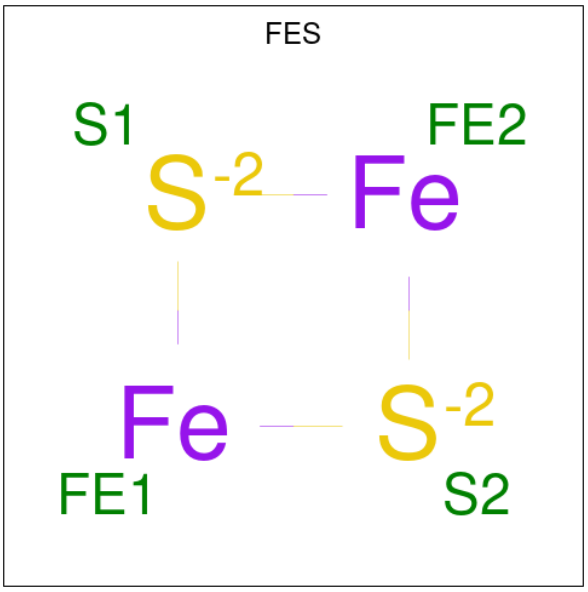
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P80457
B	1	MET	-	initiating methionine	UNP P80457

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

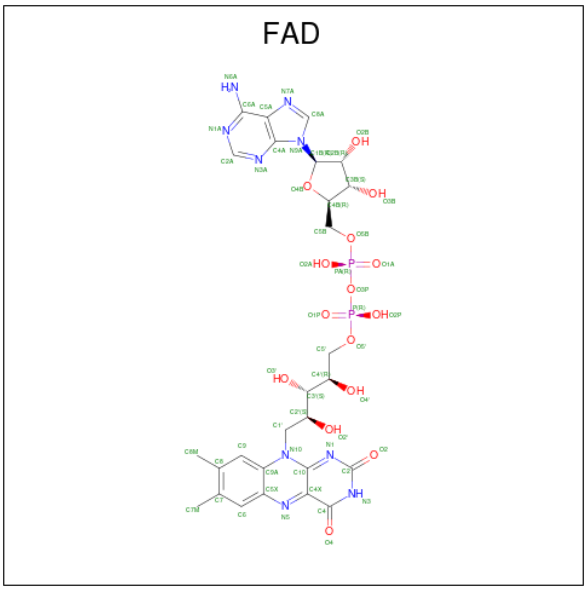
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

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



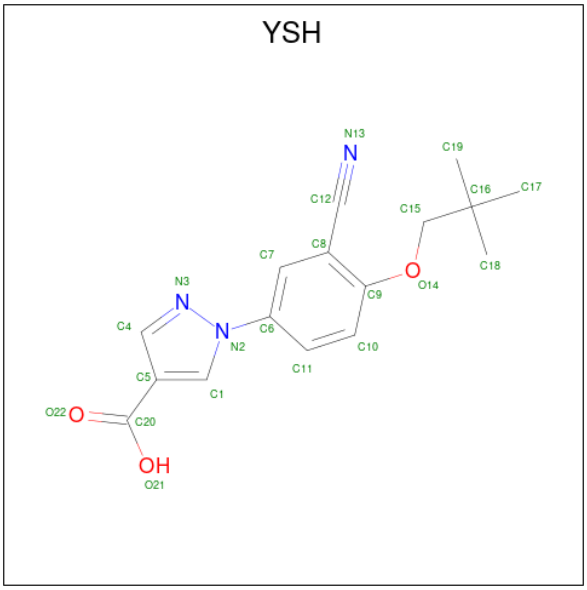
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0

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



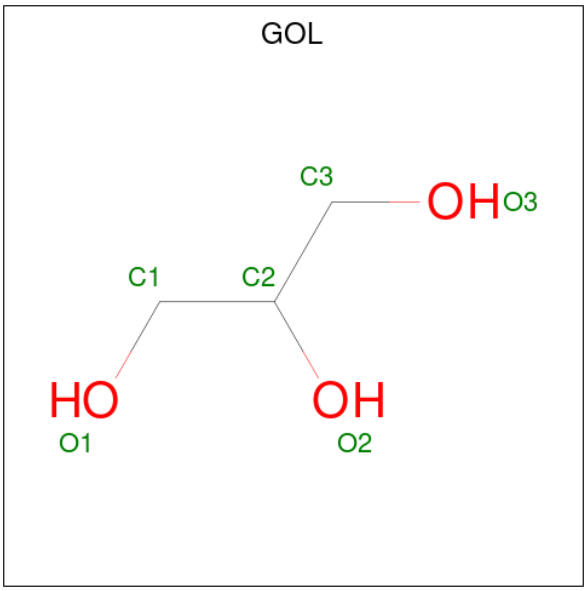
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is 1-[3-CYANO-4-(NEOPENTYLOXY)PHENYL]-1H-PYRAZOLE-4-CARBOXYLIC ACID (CCD ID: YSH) (formula: $C_{16}H_{17}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	16	3	3		
5	B	1	Total	C	N	O	0	0
			22	16	3	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



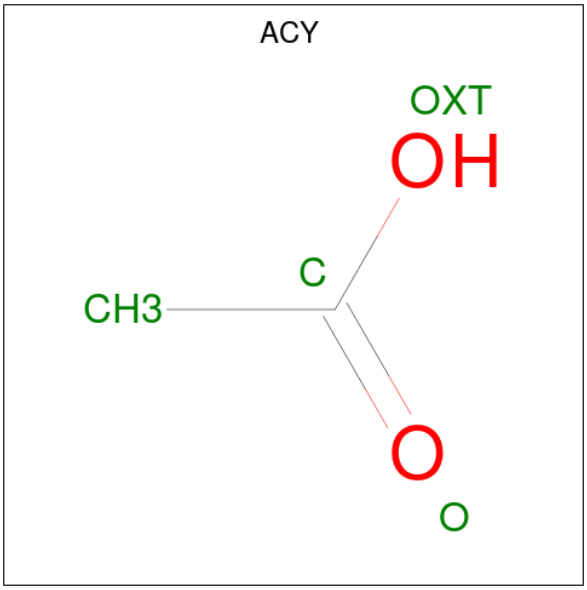
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0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

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

- Molecule 7 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is Molybdopterin hydoxy-oxo-thiol-molybdenum (CCD ID: HOH) (formula: H_2O).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1086	Total	O	0	0
			1086	1086		
9	B	1033	Total	O	0	0
			1033	1033		

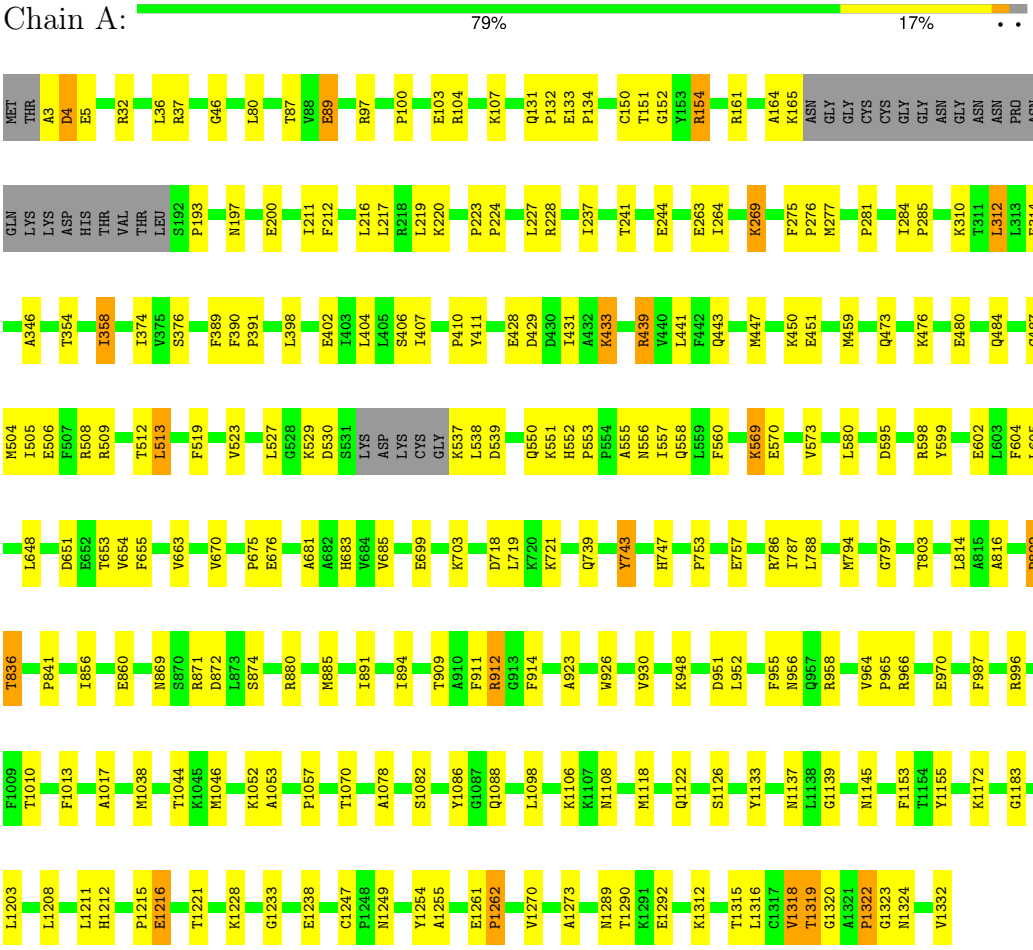
3 Residue-property plots (i)

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.

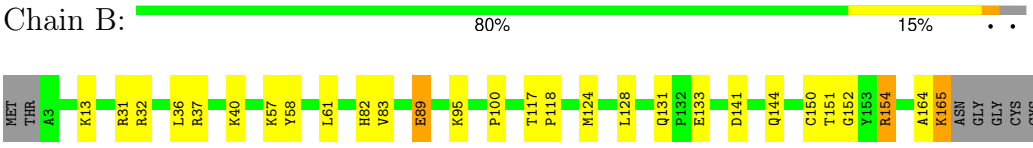
• Molecule 1: Xanthine dehydrogenase/oxidase

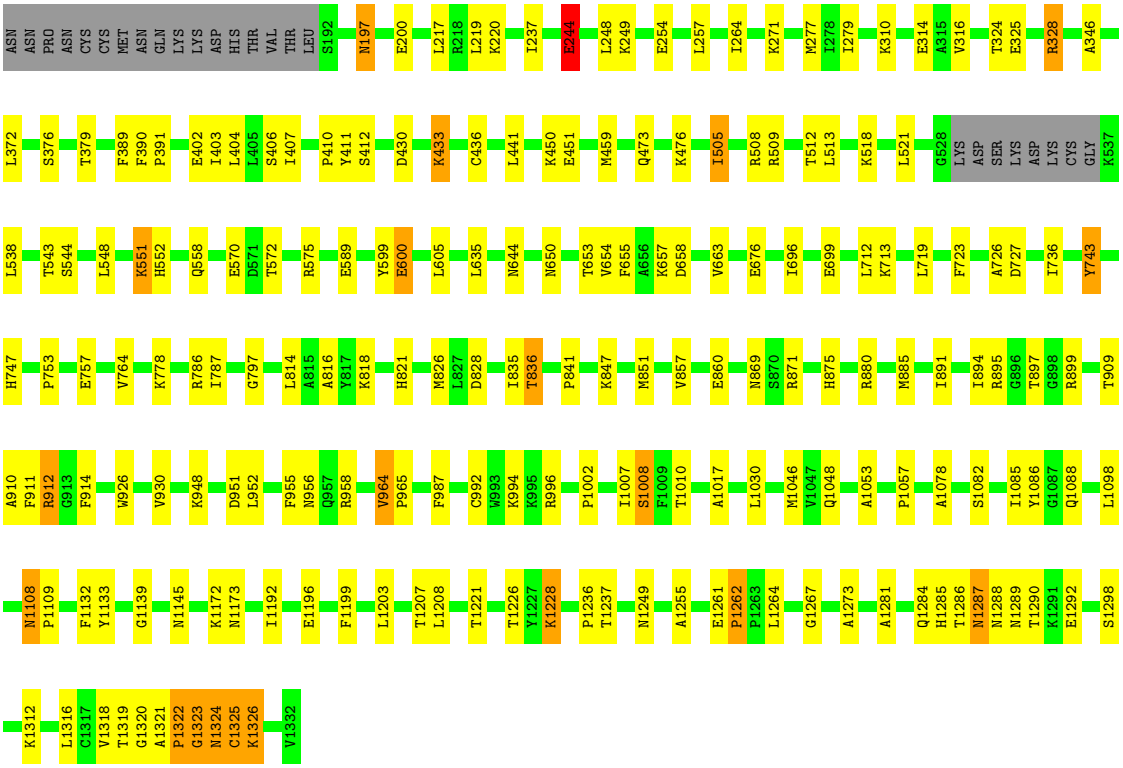
Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:




ASN ASN PRO ASN CYS CYS MET ASN GLN LYS LYS ASP HIS THR VAL THR LEU S192 N197 E200 L217 R218 L219 K220 I237 E244 L248 K249 E254 L257 I264 K271 M277 I278 I279 K310 E314 A315 V316 T324 E325 R328 A346
L372 S376 T379 F389 F390 P391 E402 I403 L404 L405 S406 I407 P410 Y411 S412 D430 K433 C436 L441 K450 E451 M459 Q473 K476 I505 R508 R509 T512 L513 K518 L521 G528 LYS ASP SER LYS ASP LYS CYS GLY K537
L538 T543 S544 L548 K551 H552 Q558 E570 D571 T572 R575 E589 Y599 E600 L605 L635 N644 N650 T653 V654 F655 A656 K657 D658 V663 E676 I696 E699 L712 K713 L719 F723 A726 D727 I736 Y743
H747 P753 E757 V764 K778 R786 I787 G797 L814 A815 A816 Y817 K818 H821 M826 L827 D828 I835 T836 P841 K847 M851 V857 E860 N869 S870 R871 H875 R880 M885 I891 I894 R895 G896 T897 G898 R899 T909
A910 F911 R912 G913 F914 W926 V930 K948 D951 L952 F955 N956 Q957 R958 V964 P965 F987 C992 W993 K994 K995 R996 P1002 I1007 S1008 F1009 T1010 A1017 L1030 M1046 V1047 Q1048 A1053 P1057 A1078 S1082 I1085 Y1086 G1087 Q1088 L1098
N1108 P1109 F1132 Y1133 G1139 N1145 K1172 N1173 I1192 E1196 F1199 L1203 T1207 L1208 T1221 T1226 Y1227 K1228 P1236 T1237 N1249 A1255 E1261 P1262 P1263 L1264 G1267 A1273 A1281 Q1284 H1285 T1286 N1287 N1288 N1289 T1290 K1291 E1292 S1298
K1312 L1316 C1317 V1318 T1319 G1320 A1321 P1322 G1323 N1324 C1325 K1326 V1332

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.82Å 123.94Å 148.89Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	20.00 – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.178 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22610	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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, ZXF, FES, CA, ACY, YSH, FAD

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	0/10298	0.91	41/13939 (0.3%)
1	B	0.36	0/10275	0.91	40/13909 (0.3%)
All	All	0.36	0/20573	0.91	81/27848 (0.3%)

There are no bond length outliers.

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	835	ILE	N-CA-C	10.79	123.01	111.58
1	A	835	ILE	N-CA-C	10.43	122.64	111.58
1	B	151	THR	N-CA-C	10.30	123.77	111.82
1	A	151	THR	N-CA-C	10.11	123.55	111.82
1	B	836	THR	N-CA-C	8.76	123.80	113.20

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	10077	0	10076	182	0
1	B	10054	0	10053	167	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	0	1	0
3	B	8	0	0	0	0
4	A	53	0	31	3	0
4	B	53	0	31	2	0
5	A	22	0	16	3	0
5	B	22	0	16	3	0
6	A	66	0	88	8	0
6	B	60	0	80	8	0
7	A	4	0	3	4	0
7	B	4	0	3	4	0
8	A	28	0	0	0	0
8	B	28	0	0	0	0
9	A	1086	0	0	10	0
9	B	1033	0	0	9	0
All	All	22610	0	20397	351	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 9.

The worst 5 of 351 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:B:5102:YSH:N2	5:B:5102:YSH:C1	1.70	1.52
5:A:5101:YSH:N2	5:A:5101:YSH:C1	1.68	1.51
1:A:3:ALA:HB1	1:A:228:ARG:H	1.20	1.06
1:A:537:LYS:HG2	1:A:538:LEU:H	1.28	0.98
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.30	0.97

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	1293/1332 (97%)	1244 (96%)	41 (3%)	8 (1%)	21 12
1	B	1290/1332 (97%)	1234 (96%)	44 (3%)	12 (1%)	14 6
All	All	2583/2664 (97%)	2478 (96%)	85 (3%)	20 (1%)	16 7

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	B	1008	SER
1	B	1287	ASN
1	B	1324	ASN

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	1101/1128 (98%)	1086 (99%)	15 (1%)	59 54
1	B	1098/1128 (97%)	1088 (99%)	10 (1%)	70 67
All	All	2199/2256 (98%)	2174 (99%)	25 (1%)	65 61

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1332	VAL
1	B	154	ARG
1	B	1002	PRO
1	B	100	PRO
1	B	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	626	GLN

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Mol	Chain	Res	Type
1	B	1145	ASN
1	B	650	ASN
1	B	869	ASN
1	B	1220	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 4 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
3	FES	B	4002	1	0,4,4	-	-	-		
5	YSH	A	5101	-	23,23,23	7.30	13 (56%)	33,33,33	4.20	12 (36%)
6	GOL	A	5019	-	5,5,5	0.33	0	5,5,5	0.32	0
5	YSH	B	5102	-	23,23,23	7.44	15 (65%)	33,33,33	4.14	11 (33%)
6	GOL	B	5012	-	5,5,5	0.23	0	5,5,5	0.45	0
6	GOL	A	5005	-	5,5,5	0.31	0	5,5,5	0.36	0
6	GOL	A	5016	-	5,5,5	0.28	0	5,5,5	0.51	0
6	GOL	B	5022	-	5,5,5	0.23	0	5,5,5	0.39	0
7	ACY	B	5202	-	3,3,3	1.19	0	3,3,3	1.70	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	5002	-	5,5,5	0.23	0	5,5,5	0.39	0
3	FES	B	4001	1	0,4,4	-	-	-		
4	FAD	B	4005	-	58,58,58	2.37	24 (41%)	85,89,89	2.07	31 (36%)
7	ACY	A	5201	-	3,3,3	1.09	0	3,3,3	1.76	1 (33%)
3	FES	A	3002	1	0,4,4	-	-	-		
6	GOL	B	5015	-	5,5,5	0.26	0	5,5,5	0.33	0
6	GOL	B	5009	-	5,5,5	0.32	0	5,5,5	0.32	0
4	FAD	A	3005	-	58,58,58	2.27	19 (32%)	85,89,89	2.09	29 (34%)
9	ZXF	B	5304	-	24,31,31	5.87	12 (50%)	22,52,52	4.58	13 (59%)
6	GOL	B	5013	-	5,5,5	0.23	0	5,5,5	0.32	0
6	GOL	B	5007	-	5,5,5	0.29	0	5,5,5	0.34	0
6	GOL	A	5003	-	5,5,5	0.32	0	5,5,5	0.35	0
6	GOL	B	5014	-	5,5,5	0.22	0	5,5,5	0.40	0
9	ZXF	A	5305	-	24,31,31	6.18	13 (54%)	22,52,52	4.53	13 (59%)
6	GOL	A	5017	-	5,5,5	0.28	0	5,5,5	0.34	0
6	GOL	A	5018	-	5,5,5	0.35	0	5,5,5	0.29	0
6	GOL	B	5021	-	5,5,5	0.28	0	5,5,5	0.42	0
6	GOL	A	5004	-	5,5,5	0.29	0	5,5,5	0.35	0
6	GOL	A	5006	-	5,5,5	0.25	0	5,5,5	0.44	0
6	GOL	A	5001	-	5,5,5	0.32	0	5,5,5	0.42	0
6	GOL	B	5008	-	5,5,5	0.27	0	5,5,5	0.42	0
6	GOL	B	5020	-	5,5,5	0.26	0	5,5,5	0.36	0
6	GOL	A	5011	-	5,5,5	0.21	0	5,5,5	0.40	0
3	FES	A	3001	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	YSH	A	5101	-	-	0/16/16/16	0/2/2/2
6	GOL	A	5019	-	-	0/4/4/4	-
3	FES	B	4002	1	-	-	0/1/1/1
5	YSH	B	5102	-	-	2/16/16/16	0/2/2/2
6	GOL	B	5012	-	-	0/4/4/4	-
6	GOL	A	5005	-	-	0/4/4/4	-
6	GOL	A	5016	-	-	0/4/4/4	-
6	GOL	B	5022	-	-	0/4/4/4	-
6	GOL	A	5002	-	-	0/4/4/4	-
3	FES	B	4001	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	B	4005	-	-	2/34/50/50	0/6/6/6
3	FES	A	3002	1	-	-	0/1/1/1
6	GOL	B	5015	-	-	0/4/4/4	-
6	GOL	B	5009	-	-	0/4/4/4	-
4	FAD	A	3005	-	-	4/34/50/50	0/6/6/6
9	ZXF	B	5304	-	-	6/6/46/46	0/4/4/4
6	GOL	B	5013	-	-	0/4/4/4	-
6	GOL	B	5007	-	-	0/4/4/4	-
6	GOL	A	5003	-	-	0/4/4/4	-
6	GOL	B	5014	-	-	0/4/4/4	-
9	ZXF	A	5305	-	-	4/6/46/46	0/4/4/4
6	GOL	A	5017	-	-	0/4/4/4	-
6	GOL	A	5018	-	-	0/4/4/4	-
6	GOL	B	5021	-	-	0/4/4/4	-
6	GOL	A	5004	-	-	0/4/4/4	-
6	GOL	A	5006	-	-	0/4/4/4	-
6	GOL	A	5001	-	-	0/4/4/4	-
6	GOL	B	5008	-	-	0/4/4/4	-
6	GOL	B	5020	-	-	0/4/4/4	-
6	GOL	A	5011	-	-	0/4/4/4	-
3	FES	A	3001	1	-	-	0/1/1/1

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5102	YSH	C1-C5	21.19	1.71	1.38
5	A	5101	YSH	C1-C5	20.87	1.71	1.38
5	B	5102	YSH	C1-N2	19.56	1.70	1.35
9	A	5305	ZXF	C7-C6	19.00	1.68	1.53
5	A	5101	YSH	C1-N2	18.95	1.68	1.35

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	5101	YSH	C5-C1-N2	-14.03	90.97	107.09
5	B	5102	YSH	C5-C1-N2	-13.97	91.05	107.09
9	B	5304	ZXF	C2'-C1'-S1'	13.58	127.86	120.15
9	A	5305	ZXF	C2'-C1'-S1'	13.21	127.65	120.15
5	B	5102	YSH	C4-N3-N2	12.88	114.44	104.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
4	B	4005	FAD	N10-C1'-C2'-O2'
4	B	4005	FAD	N10-C1'-C2'-C3'
5	B	5102	YSH	N13-C12-C8-C9

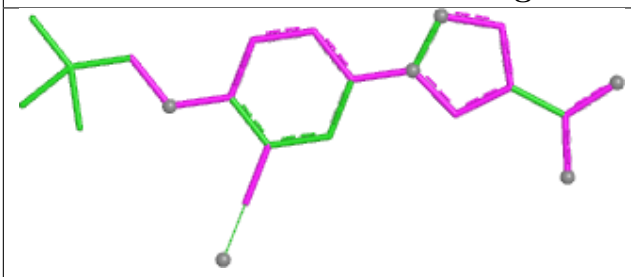
There are no ring outliers.

19 monomers are involved in 41 short contacts:

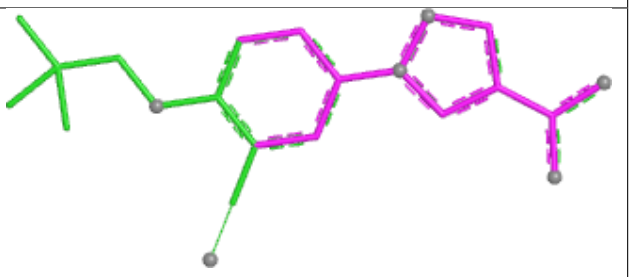
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5101	YSH	3	0
6	A	5019	GOL	1	0
5	B	5102	YSH	3	0
6	B	5022	GOL	2	0
7	B	5202	ACY	4	0
6	A	5002	GOL	2	0
4	B	4005	FAD	2	0
7	A	5201	ACY	4	0
3	A	3002	FES	1	0
4	A	3005	FAD	3	0
9	B	5304	ZXF	3	0
6	B	5013	GOL	1	0
6	B	5014	GOL	2	0
9	A	5305	ZXF	2	0
6	A	5006	GOL	2	0
6	A	5001	GOL	1	0
6	B	5008	GOL	2	0
6	B	5020	GOL	1	0
6	A	5011	GOL	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.

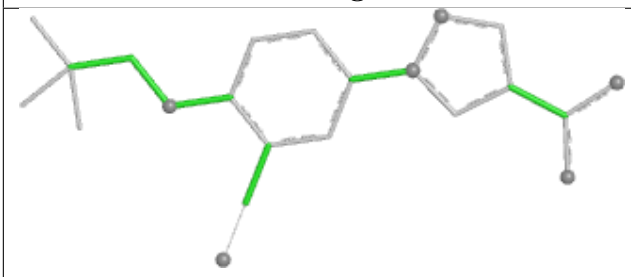
Ligand YSH A 5101



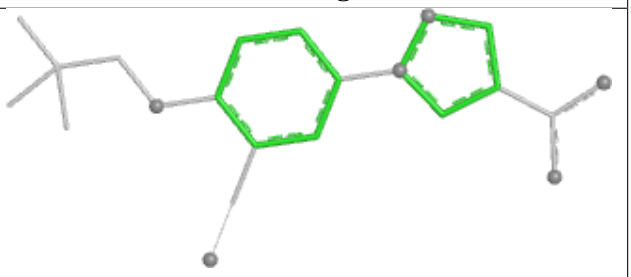
Bond lengths



Bond angles

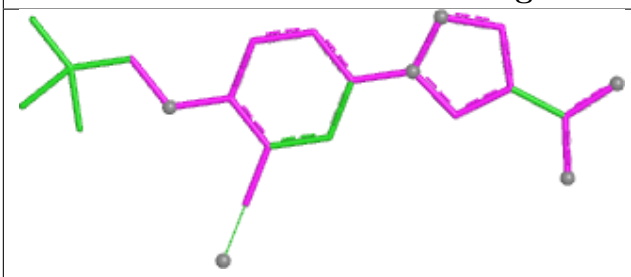


Torsions

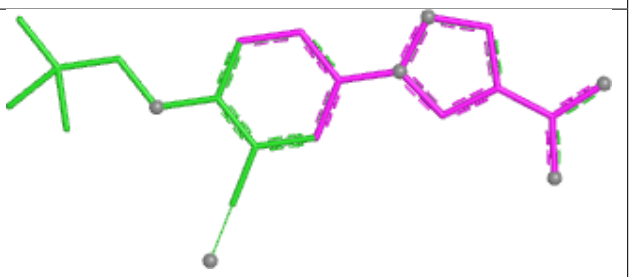


Rings

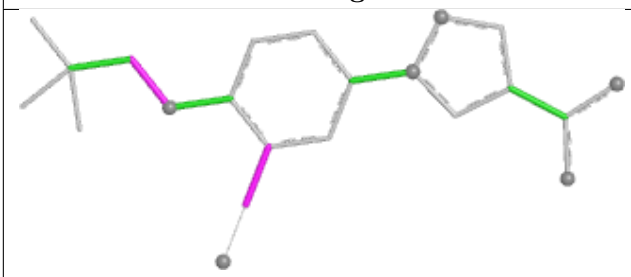
Ligand YSH B 5102



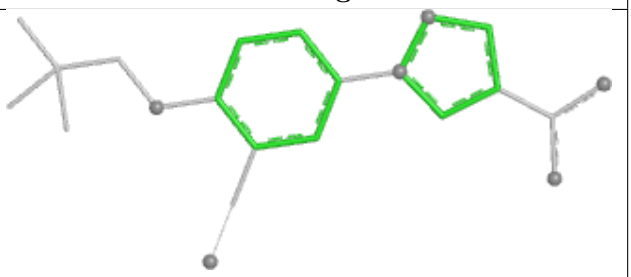
Bond lengths



Bond angles

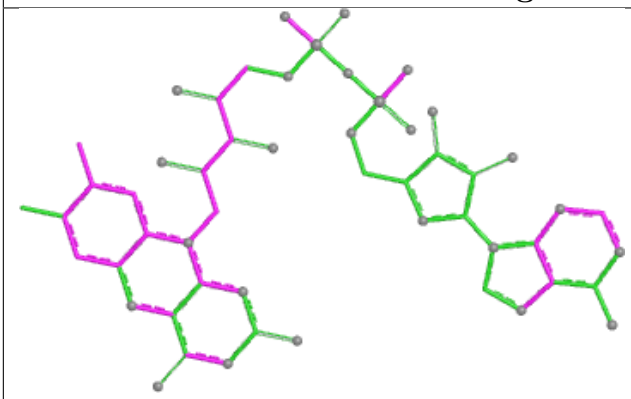


Torsions

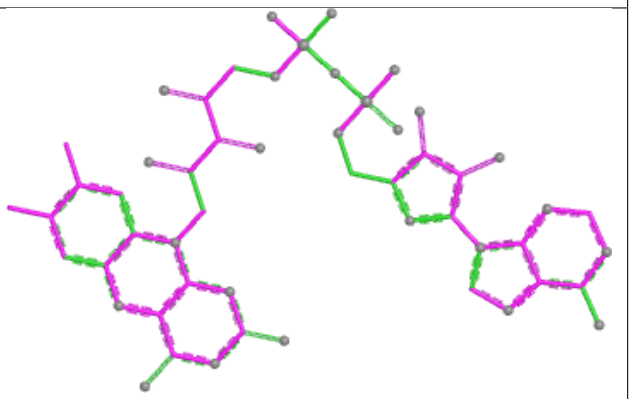


Rings

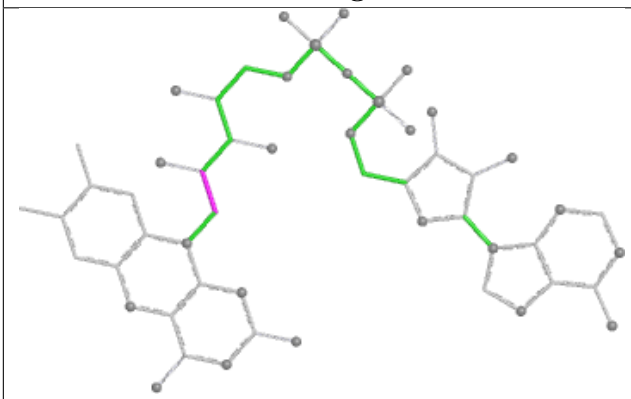
Ligand FAD B 4005



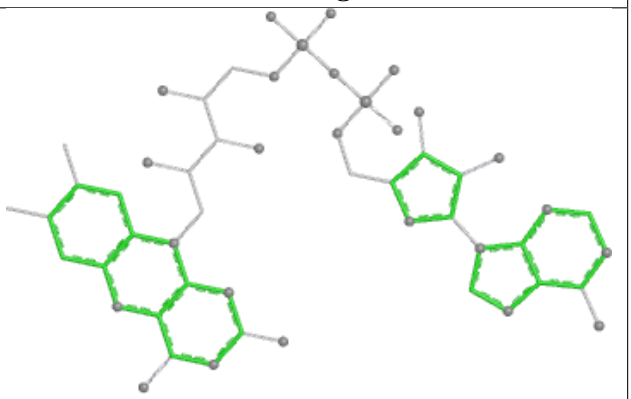
Bond lengths



Bond angles

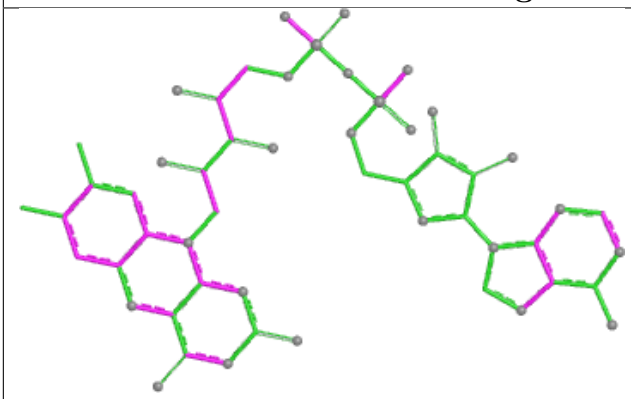


Torsions

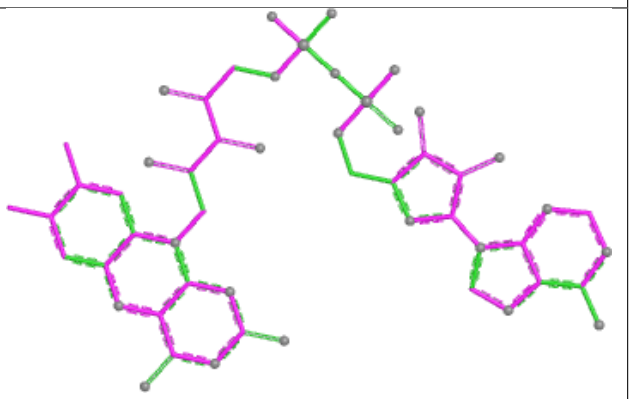


Rings

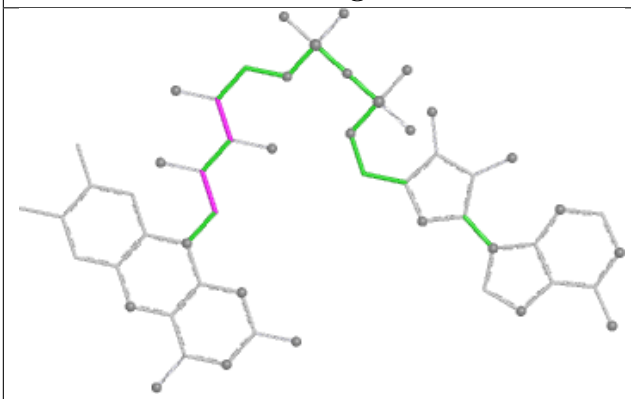
Ligand FAD A 3005



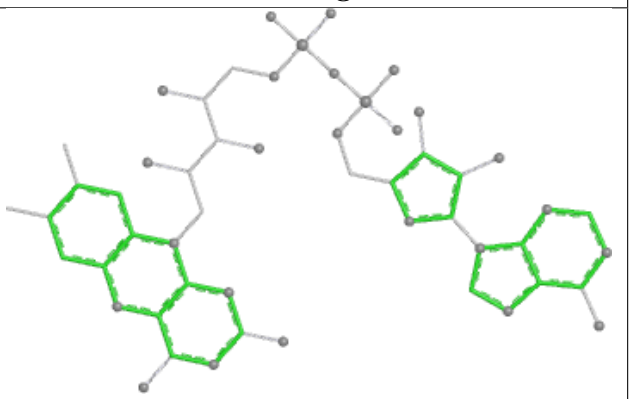
Bond lengths



Bond angles

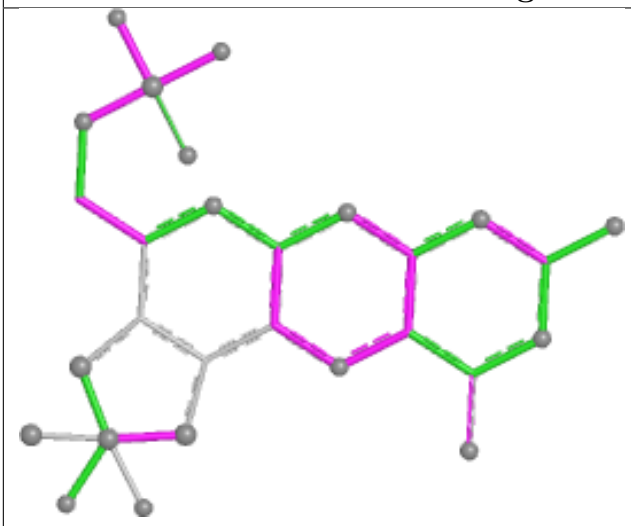


Torsions

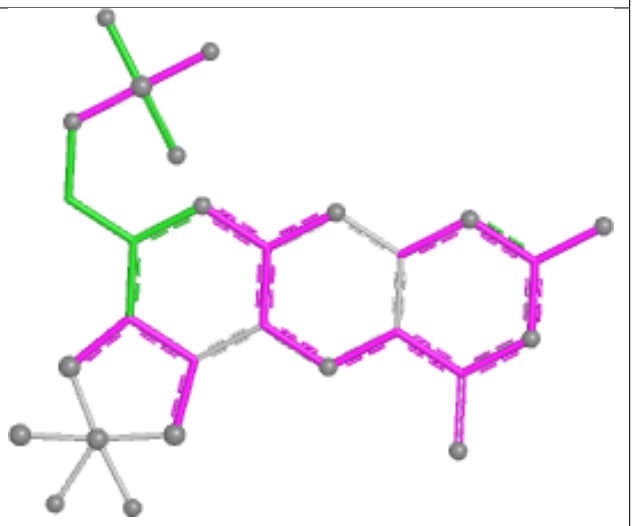


Rings

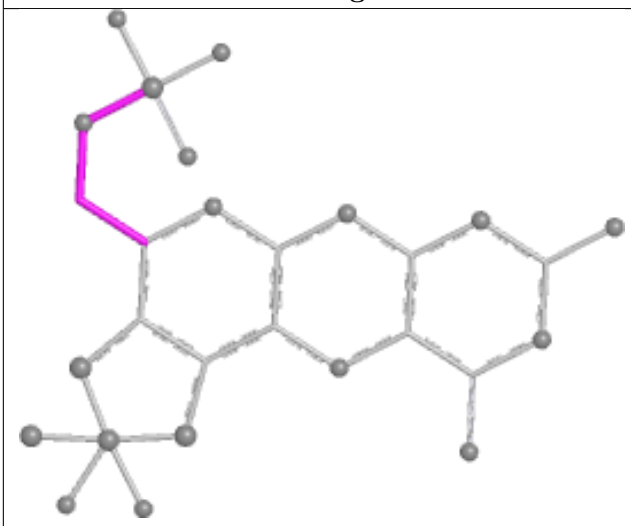
Ligand ZXF B 5304



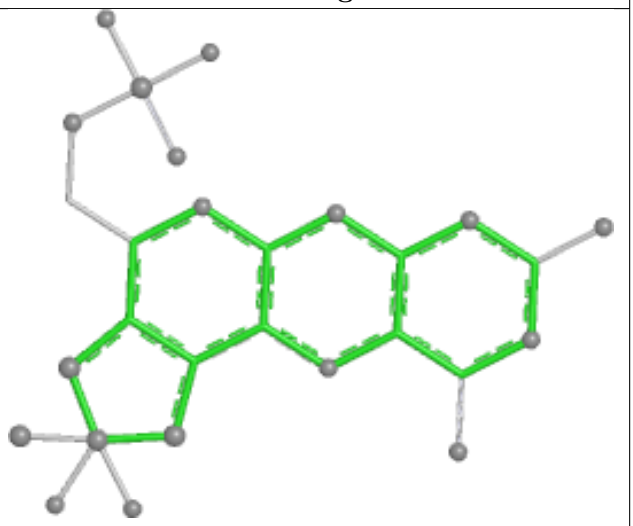
Bond lengths



Bond angles

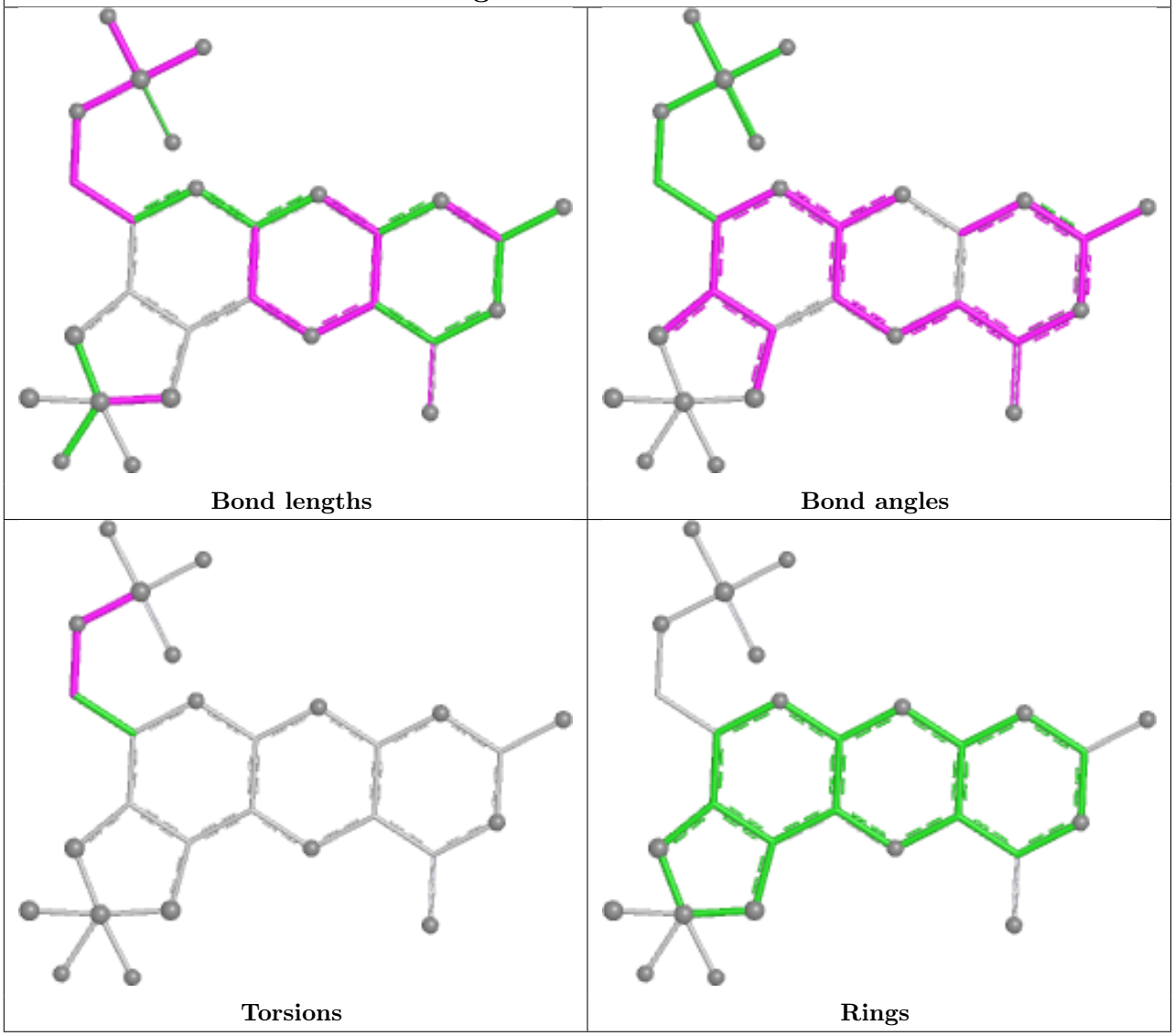


Torsions



Rings

Ligand ZXF A 5305



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.