



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 08:44 PM EDT

PDB ID : 3UNC / pdb_00003unc
Title : Crystal Structure of Bovine Milk Xanthine Dehydrogenase to 1.65Å Resolution
Authors : Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.
Deposited on : 2011-11-15
Resolution : 1.65 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 ⓘ 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 ⓘ](#)) 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

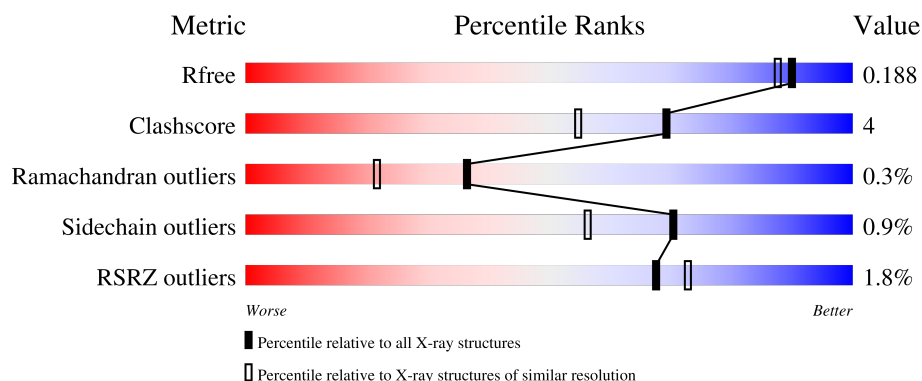
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1332	
1	B	1332	

2 Entry composition [i](#)

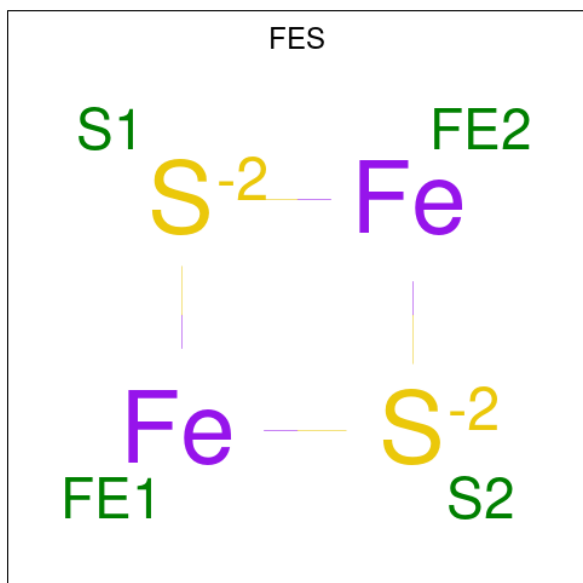
There are 9 unique types of molecules in this entry. The entry contains 22475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1286	Total 10084	C 6408	N 1726	O 1884	S 66	0	13	0
1	B	1289	Total 10073	C 6400	N 1723	O 1883	S 67	0	9	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- # FAD
-
- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD), a crucial coenzyme. The molecule is composed of three main parts: a riboflavin (isoalloxazine) ring system, a ribitol linker, and an adenosine moiety.
- Riboflavin (Isoalloxazine) Ring System:** This is the top part of the structure, featuring a fused bicyclic system with nitrogen atoms (N1, N3, N7, N9) and carbonyl groups (C2=O, C4=O, C6=O). It is attached to a ribitol chain via a glycosidic bond at the N1 position.
 - Ribitol Linker:** A five-carbon chain (C1-C5) that connects the riboflavin to the adenosine moiety. It has hydroxyl groups at C2, C3, and C4, and is linked to the riboflavin at C1 and the adenosine at C5.
 - Adenosine Moiety:** This part consists of an adenine base (a fused bicyclic system with N1, N3, N7, N9 and C2, C4, C6, C8) attached to a ribose sugar (C1'-C5'). The ribose has hydroxyl groups at C2', C3', and C4', and is linked to the ribitol linker at C5'.
- The structure is color-coded: the riboflavin ring is blue, the ribitol linker is red, and the adenosine moiety is green. The overall structure is shown in a perspective view, highlighting the spatial arrangement of the atoms and bonds.

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

- SAL
-
- The chemical structure of Salicylic acid (SAL) is shown. It consists of a benzene ring with a carboxylic acid group attached. The atoms are labeled as follows: C1, C2, C3, C4, C5, and C6 for the benzene ring carbons; C1' for the carbonyl carbon; O1' for the carbonyl oxygen; O2 for the phenolic hydroxyl oxygen; and O2' for the carboxylic acid hydroxyl oxygen. The labels are in green, and the oxygen atoms and their associated hydroxyl groups are in red.

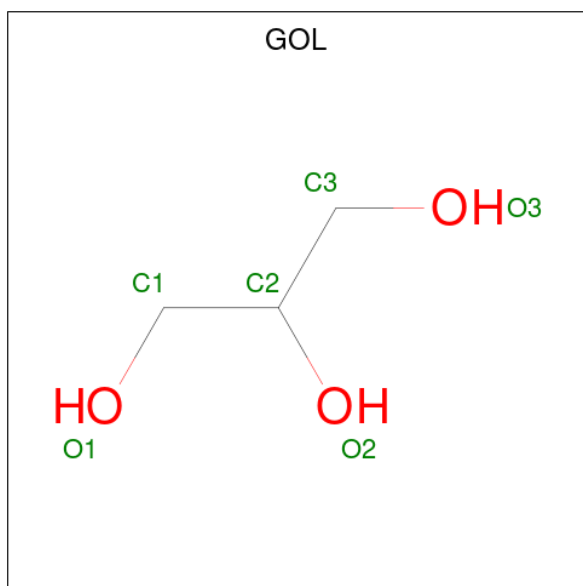
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	7	3		

WORLDWIDE
PDB
PROTEIN DATA BANK

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



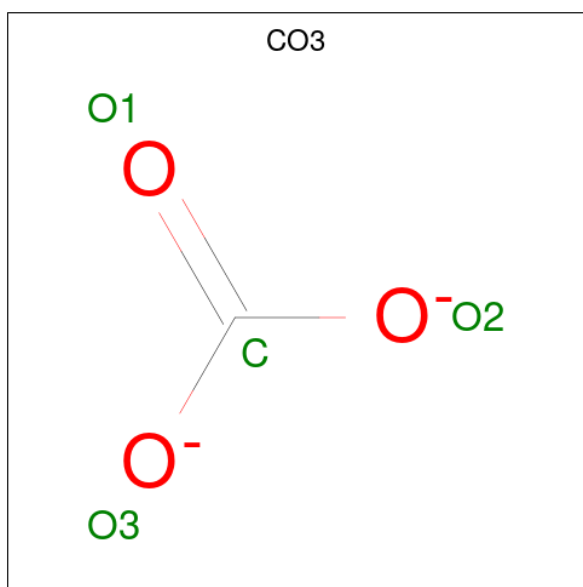
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

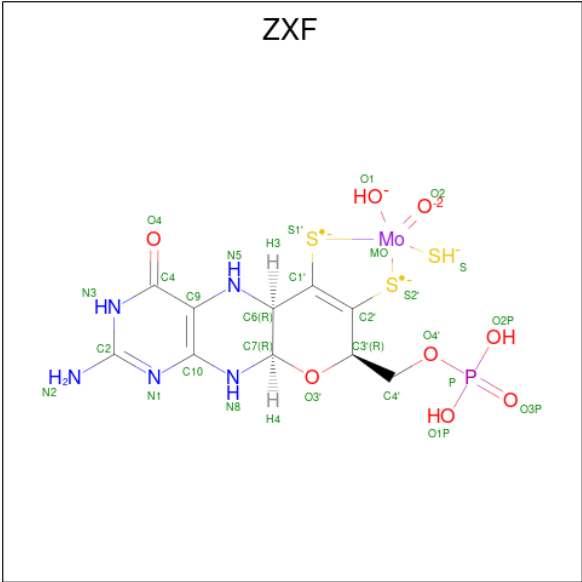


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		

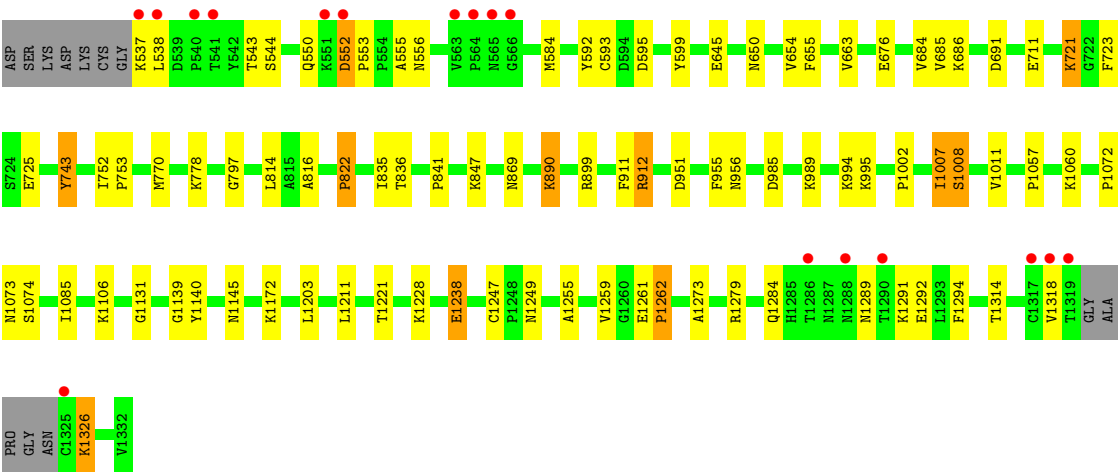
- Molecule 8 is Molybdopterin hydroxy-oxo-thiol-molybdenum (CCD ID: ZXF) (formula: C₁₀H₁₄MoN₅O₈PS₃).



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	990	Total	O	0	0
			990	990		
9	B	976	Total	O	0	0
			976	976		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.57Å 124.37Å 148.18Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.65) 93.1 (20.00-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 1.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.196 0.166 , 0.188	Depositor DCC
R_{free} test set	4755 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22475	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SAL, FES, GOL, CO3, ZXF, CA

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	0.56	0/10302	0.98	38/13941 (0.3%)
1	B	0.57	0/10291	0.98	41/13927 (0.3%)
All	All	0.56	0/20593	0.98	79/27868 (0.3%)

There are no bond length outliers.

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	ILE	N-CA-C	9.00	121.12	111.58
1	A	835	ILE	N-CA-C	8.93	121.04	111.58
1	A	1011	VAL	N-CA-C	-8.81	98.83	107.55
1	B	836	THR	N-CA-C	8.51	123.49	113.20
1	B	869	ASN	N-CA-C	8.47	123.23	113.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10084	0	10078	73	0
1	B	10073	0	10064	67	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	1	0
3	B	53	0	31	1	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
5	A	66	0	88	3	0
5	B	78	0	104	2	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	28	0	0	0	0
8	B	28	0	0	0	0
9	A	990	0	0	9	0
9	B	976	0	0	9	0
All	All	22475	0	20404	144	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 4.

The worst 5 of 144 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:A:1211:LEU:HA	1:A:1221[B]:THR:HG21	1.47	0.95
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.33	0.93
1:B:1211:LEU:HA	1:B:1221[B]:THR:HG21	1.54	0.89
1:A:131:GLN:HE21	1:A:133:GLU:H	1.26	0.82
1:B:131:GLN:HE21	1:B:133:GLU:H	1.28	0.81

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	1291/1332 (97%)	1254 (97%)	34 (3%)	3 (0%)	43	27
1	B	1290/1332 (97%)	1259 (98%)	27 (2%)	4 (0%)	36	21
All	All	2581/2664 (97%)	2513 (97%)	61 (2%)	7 (0%)	36	21

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	912	ARG
1	A	797	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1104/1128 (98%)	1096 (99%)	8 (1%)	76	64
1	B	1103/1128 (98%)	1090 (99%)	13 (1%)	63	45
All	All	2207/2256 (98%)	2186 (99%)	21 (1%)	70	52

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1002	PRO
1	B	1247[A]	CYS
1	B	1326	LYS
1	B	1247[B]	CYS
1	B	1106	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	251	GLN

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Mol	Chain	Res	Type
1	B	565	ASN
1	B	1284	GLN
1	B	556	ASN
1	B	626	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 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\# Z > 2$
5	GOL	B	1339	-	5,5,5	0.31	0	5,5,5	0.18	0
5	GOL	B	1344	-	5,5,5	0.48	0	5,5,5	0.39	0
5	GOL	A	1349	-	5,5,5	0.46	0	5,5,5	0.32	0
5	GOL	A	1339	-	5,5,5	0.34	0	5,5,5	0.22	0
5	GOL	B	1342	-	5,5,5	0.46	0	5,5,5	0.31	0
3	FAD	A	1337	-	58,58,58	2.00	17 (29%)	85,89,89	1.94	20 (23%)
5	GOL	A	1345	-	5,5,5	0.50	0	5,5,5	0.43	0
2	FES	A	1334	1	0,4,4	-	-	-	-	-
5	GOL	B	1346	-	5,5,5	0.40	0	5,5,5	0.30	0
5	GOL	B	1347	-	5,5,5	0.45	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SAL	A	1338	-	10,10,10	2.05	5 (50%)	13,13,13	2.02	4 (30%)
5	GOL	B	1341	-	5,5,5	0.42	0	5,5,5	0.35	0
6	CO3	B	1352	-	3,3,3	0.42	0	2,3,3	0.11	0
2	FES	B	1334	1	0,4,4	-	-	-	-	-
6	CO3	A	1350	-	3,3,3	0.32	0	2,3,3	0.26	0
9	ZXF	B	1354	-	24,31,31	2.72	7 (29%)	22,52,52	2.88	9 (40%)
5	GOL	A	1340	-	5,5,5	0.30	0	5,5,5	0.19	0
5	GOL	B	1343	-	5,5,5	0.28	0	5,5,5	0.21	0
5	GOL	A	1348	-	5,5,5	0.53	0	5,5,5	0.24	0
2	FES	A	1333	1	0,4,4	-	-	-	-	-
5	GOL	B	1351	-	5,5,5	0.52	0	5,5,5	0.21	0
5	GOL	B	1350	-	5,5,5	0.56	0	5,5,5	0.53	0
4	SAL	B	1338	-	10,10,10	2.15	5 (50%)	13,13,13	2.00	3 (23%)
9	ZXF	A	1352	-	24,31,31	2.69	7 (29%)	22,52,52	2.99	10 (45%)
5	GOL	B	1345	-	5,5,5	0.39	0	5,5,5	0.29	0
5	GOL	B	1348	-	5,5,5	0.59	0	5,5,5	0.33	0
2	FES	B	1333	1	0,4,4	-	-	-	-	-
5	GOL	A	1346	-	5,5,5	0.46	0	5,5,5	0.28	0
5	GOL	A	1341	-	5,5,5	0.41	0	5,5,5	0.37	0
5	GOL	A	1342	-	5,5,5	0.46	0	5,5,5	0.30	0
5	GOL	A	1343	-	5,5,5	0.30	0	5,5,5	0.15	0
5	GOL	B	1349	-	5,5,5	0.24	0	5,5,5	0.27	0
5	GOL	A	1347	-	5,5,5	0.47	0	5,5,5	0.27	0
5	GOL	A	1344	-	5,5,5	0.44	0	5,5,5	0.44	0
5	GOL	B	1340	-	5,5,5	0.37	0	5,5,5	0.24	0
3	FAD	B	1337	-	58,58,58	1.97	16 (27%)	85,89,89	1.95	18 (21%)

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	GOL	B	1339	-	-	0/4/4/4	-
5	GOL	B	1344	-	-	2/4/4/4	-
5	GOL	A	1349	-	-	4/4/4/4	-
5	GOL	A	1339	-	-	0/4/4/4	-
5	GOL	B	1342	-	-	0/4/4/4	-
3	FAD	A	1337	-	-	6/34/50/50	0/6/6/6
5	GOL	A	1345	-	-	1/4/4/4	-
2	FES	A	1334	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1346	-	-	0/4/4/4	-
5	GOL	B	1347	-	-	0/4/4/4	-
4	SAL	A	1338	-	-	0/4/4/4	0/1/1/1
5	GOL	B	1341	-	-	0/4/4/4	-
2	FES	B	1334	1	-	-	0/1/1/1
9	ZXF	B	1354	-	-	1/6/46/46	0/4/4/4
5	GOL	A	1340	-	-	0/4/4/4	-
5	GOL	B	1343	-	-	0/4/4/4	-
5	GOL	A	1348	-	-	0/4/4/4	-
2	FES	A	1333	1	-	-	0/1/1/1
5	GOL	B	1351	-	-	0/4/4/4	-
5	GOL	B	1350	-	-	3/4/4/4	-
4	SAL	B	1338	-	-	0/4/4/4	0/1/1/1
9	ZXF	A	1352	-	-	1/6/46/46	0/4/4/4
5	GOL	B	1345	-	-	4/4/4/4	-
5	GOL	B	1348	-	-	0/4/4/4	-
2	FES	B	1333	1	-	-	0/1/1/1
5	GOL	A	1346	-	-	0/4/4/4	-
5	GOL	A	1341	-	-	0/4/4/4	-
5	GOL	A	1342	-	-	1/4/4/4	-
5	GOL	A	1343	-	-	0/4/4/4	-
5	GOL	B	1349	-	-	2/4/4/4	-
5	GOL	A	1347	-	-	0/4/4/4	-
5	GOL	A	1344	-	-	3/4/4/4	-
5	GOL	B	1340	-	-	0/4/4/4	-
3	FAD	B	1337	-	-	6/34/50/50	0/6/6/6

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1354	ZXF	C10-N8	8.71	1.44	1.35
9	A	1352	ZXF	C10-N8	8.59	1.44	1.35
3	B	1337	FAD	C9A-C5X	5.39	1.49	1.41
9	B	1354	ZXF	C9-C10	5.12	1.47	1.38
9	A	1352	ZXF	O4-C4	5.08	1.33	1.23

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1337	FAD	C5X-C9A-N10	-6.66	111.95	117.97
9	A	1352	ZXF	C2-N1-C10	6.39	124.63	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1354	ZXF	C2-N1-C10	6.36	124.58	113.36
3	B	1337	FAD	C9-C9A-N10	6.31	130.34	121.85
9	A	1352	ZXF	C7-C6-N5	6.23	113.98	107.87

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

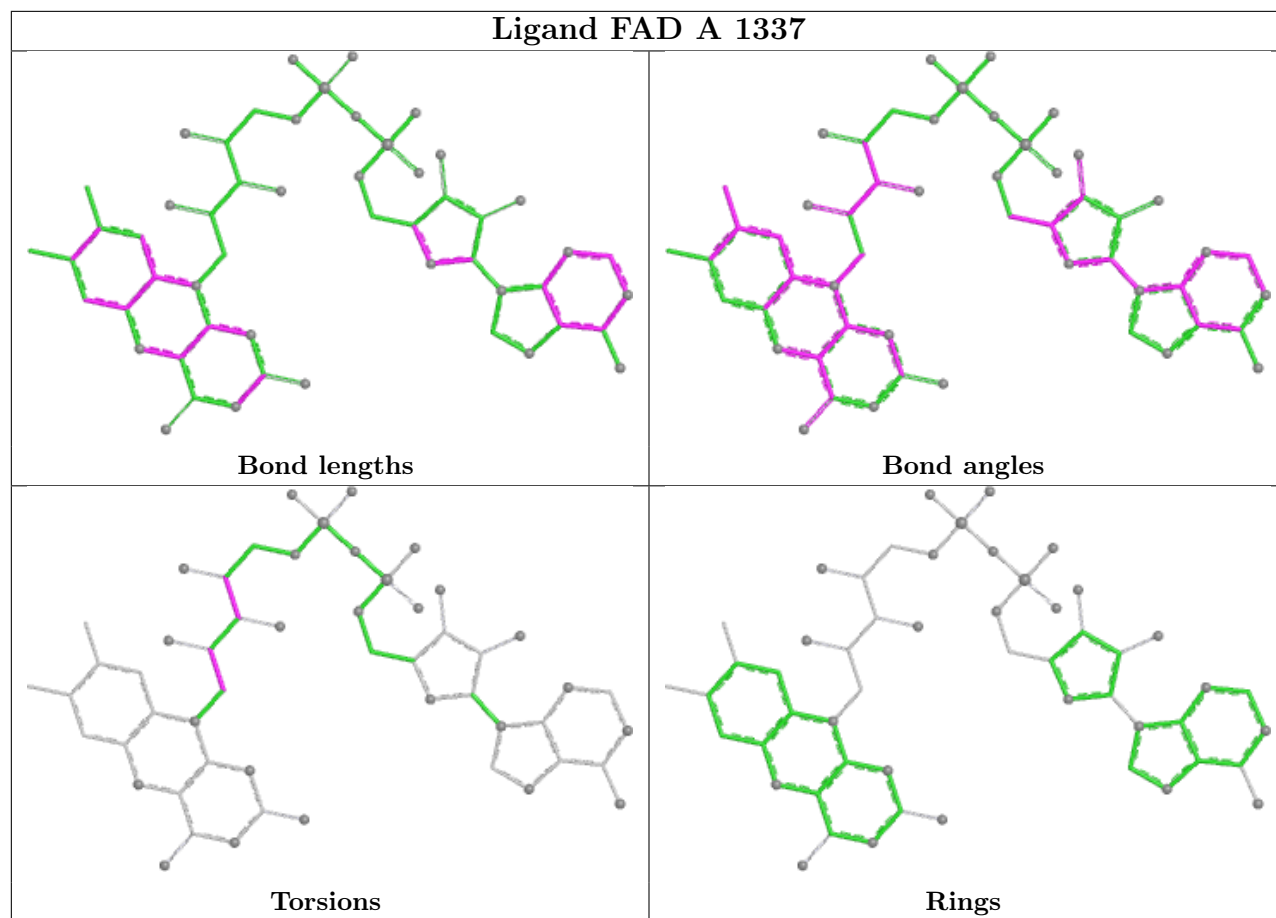
Mol	Chain	Res	Type	Atoms
3	A	1337	FAD	N10-C1'-C2'-O2'
3	A	1337	FAD	N10-C1'-C2'-C3'
3	B	1337	FAD	N10-C1'-C2'-O2'
3	B	1337	FAD	N10-C1'-C2'-C3'
5	A	1349	GOL	O1-C1-C2-C3

There are no ring outliers.

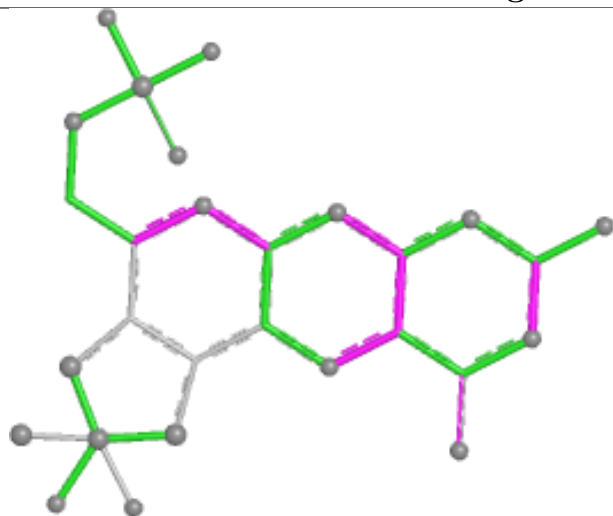
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1337	FAD	1	0
5	A	1345	GOL	3	0
9	B	1354	ZXF	4	0
9	A	1352	ZXF	1	0
5	B	1345	GOL	1	0
5	B	1349	GOL	1	0
3	B	1337	FAD	1	0

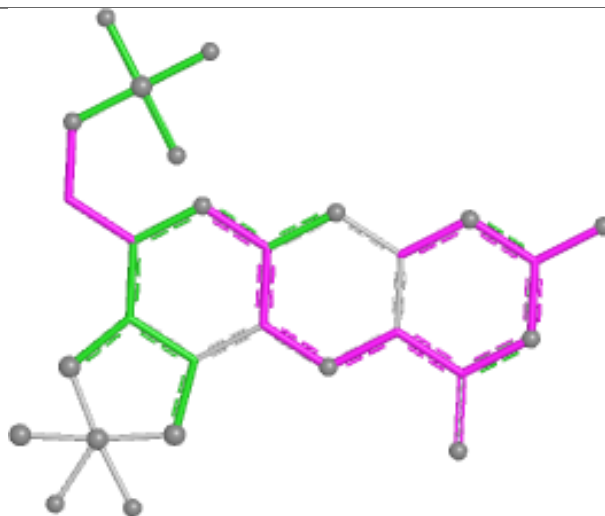
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



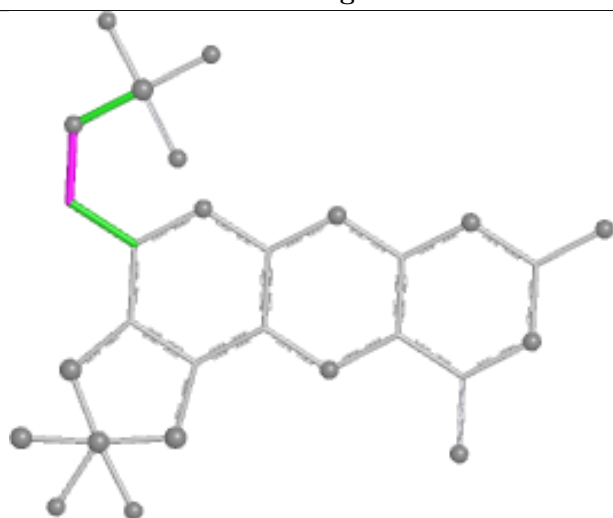
Ligand ZXF B 1354



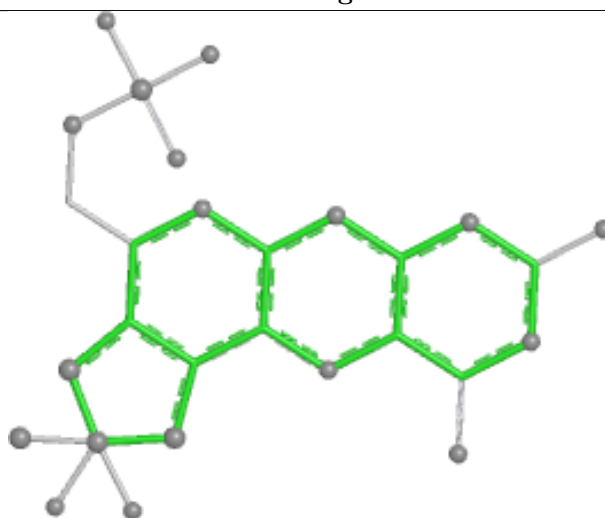
Bond lengths



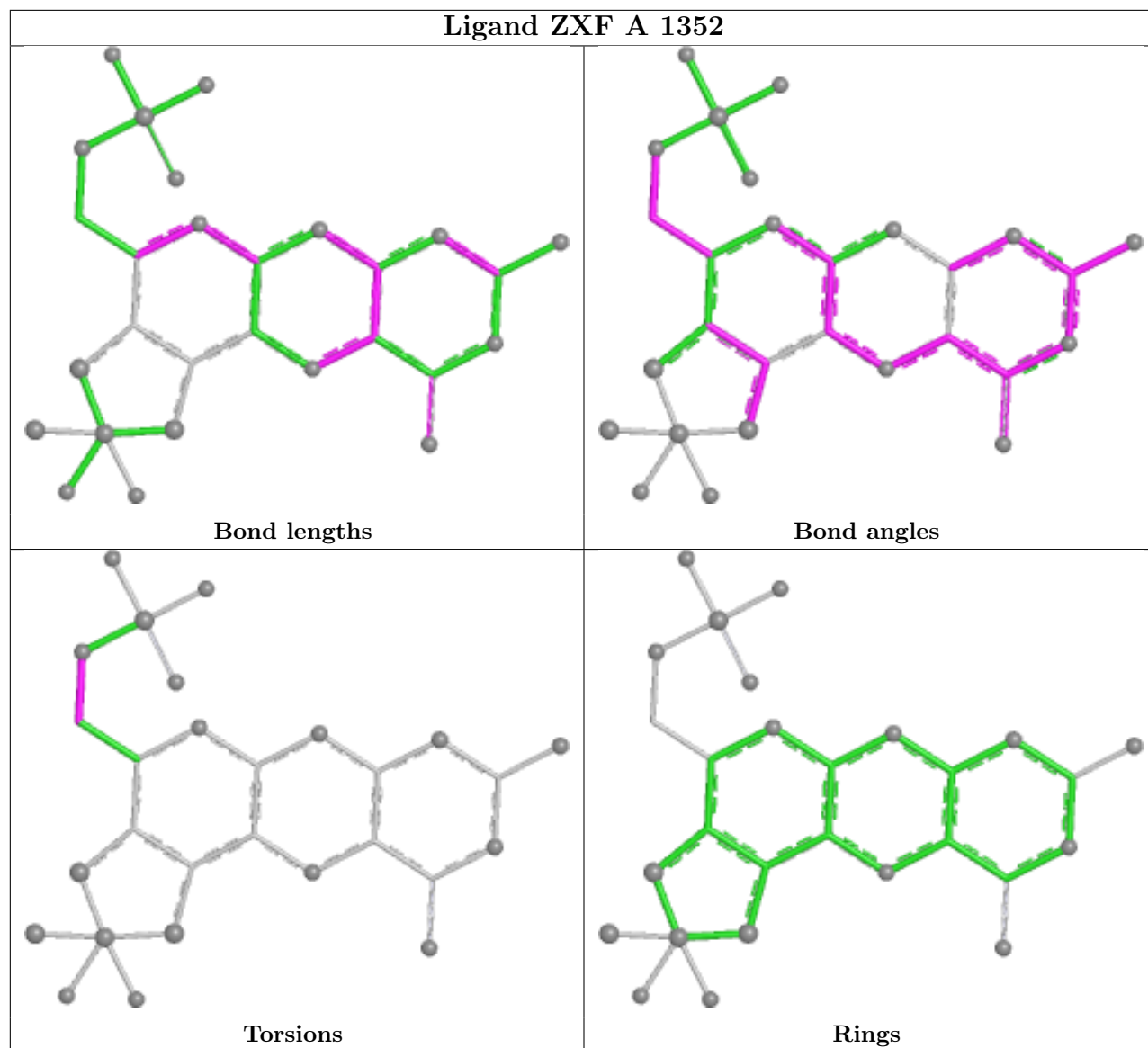
Bond angles

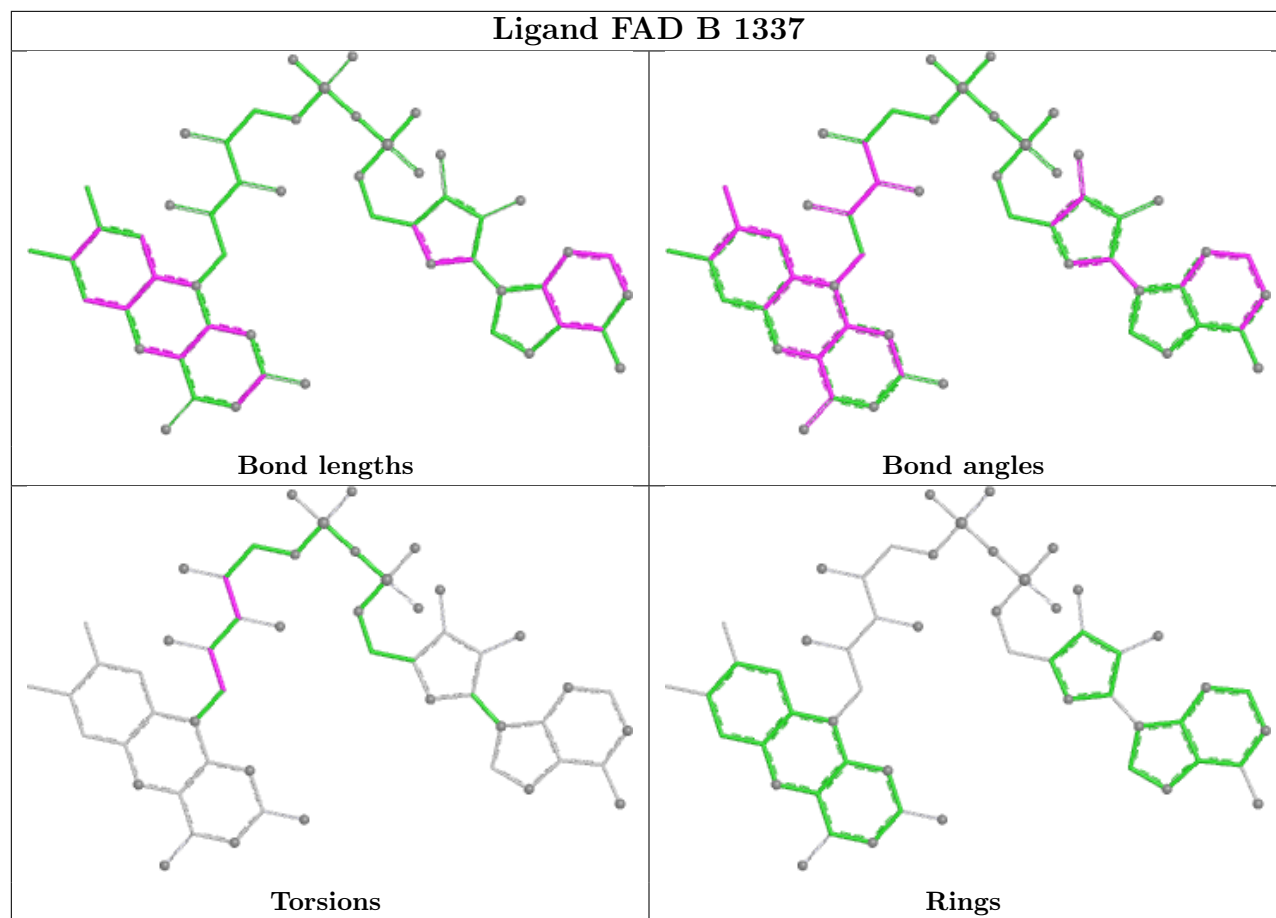


Torsions



Rings





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	1286/1332 (96%)	-0.14	24 (1%) 66 71	9, 21, 36, 61	13 (1%)
1	B	1289/1332 (96%)	-0.07	23 (1%) 67 73	9, 21, 36, 57	9 (0%)
All	All	2575/2664 (96%)	-0.11	47 (1%) 67 73	9, 21, 36, 61	22 (0%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1317	CYS	5.1
1	B	528	GLY	4.2
1	A	61	LEU	3.9
1	B	61	LEU	3.7
1	A	222	VAL	3.6

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](#)

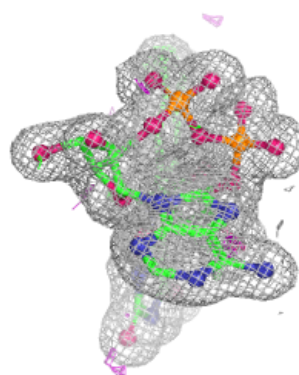
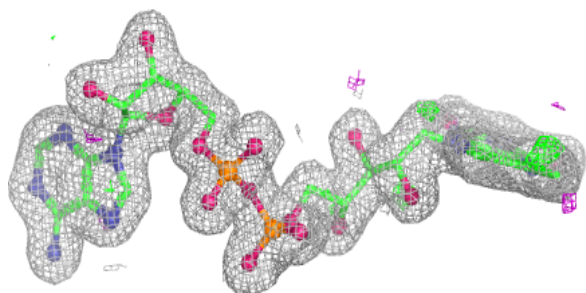
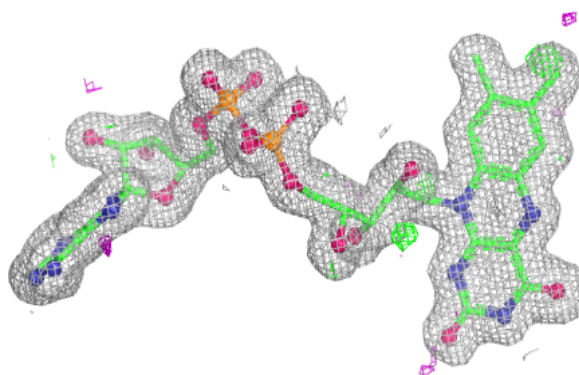
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	1345	6/6	0.73	0.20	41,49,50,52	0
5	GOL	B	1351	6/6	0.75	0.14	41,45,45,46	0
5	GOL	B	1349	6/6	0.76	0.18	48,51,52,52	0
5	GOL	B	1342	6/6	0.77	0.14	54,54,54,54	0
5	GOL	B	1344	6/6	0.77	0.17	40,41,42,43	0
5	GOL	A	1344	6/6	0.79	0.15	39,40,40,42	0
5	GOL	A	1349	6/6	0.80	0.15	31,41,43,43	0
5	GOL	A	1340	6/6	0.83	0.13	31,32,33,34	0
5	GOL	B	1340	6/6	0.84	0.13	31,34,36,38	0
5	GOL	B	1350	6/6	0.85	0.15	43,44,45,46	0
5	GOL	B	1345	6/6	0.85	0.13	36,40,43,45	0
5	GOL	A	1347	6/6	0.86	0.12	36,38,40,42	0
5	GOL	A	1342	6/6	0.88	0.10	45,45,46,47	0
5	GOL	A	1348	6/6	0.89	0.10	31,34,35,38	0
5	GOL	A	1341	6/6	0.90	0.10	24,29,30,31	0
5	GOL	A	1343	6/6	0.90	0.13	20,27,29,32	0
5	GOL	B	1343	6/6	0.91	0.13	22,28,29,32	0
5	GOL	B	1348	6/6	0.92	0.09	32,35,35,36	0
5	GOL	B	1347	6/6	0.92	0.09	32,34,35,36	0
5	GOL	B	1346	6/6	0.93	0.14	23,26,26,28	0
4	SAL	B	1338	10/10	0.93	0.08	23,24,25,26	0
5	GOL	A	1346	6/6	0.94	0.11	23,25,26,29	0
5	GOL	B	1341	6/6	0.94	0.09	23,29,31,34	0
4	SAL	A	1338	10/10	0.95	0.07	22,23,24,24	0
5	GOL	A	1339	6/6	0.95	0.07	19,20,20,22	0
5	GOL	B	1339	6/6	0.97	0.05	20,21,22,22	0
6	CO3	A	1350	4/4	0.97	0.04	14,15,16,16	0
3	FAD	B	1337	53/53	0.98	0.05	15,17,21,23	0
3	FAD	A	1337	53/53	0.98	0.04	15,18,22,24	0
6	CO3	B	1352	4/4	0.98	0.04	16,17,17,17	0
7	CA	A	1351	1/1	0.99	0.02	17,17,17,17	0
7	CA	B	1353	1/1	0.99	0.04	18,18,18,18	0
9	ZXF	A	1352	28/28	0.99	0.06	16,18,21,29	0
9	ZXF	B	1354	28/28	0.99	0.06	15,18,20,28	0
2	FES	B	1333	4/4	1.00	0.03	13,14,14,14	0
2	FES	B	1334	4/4	1.00	0.03	13,14,14,15	0
2	FES	A	1333	4/4	1.00	0.02	14,14,15,15	0
2	FES	A	1334	4/4	1.00	0.02	14,14,14,15	0

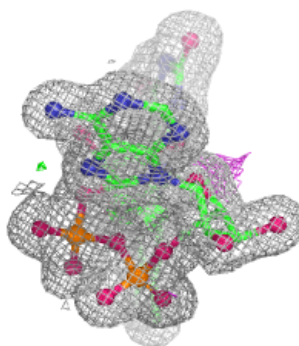
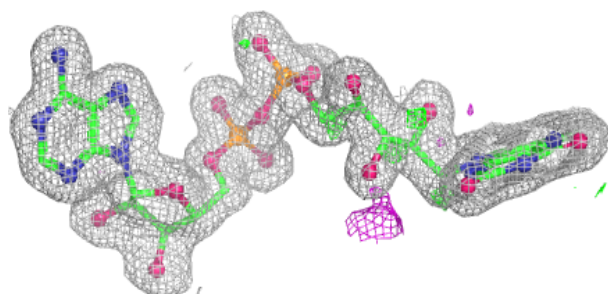
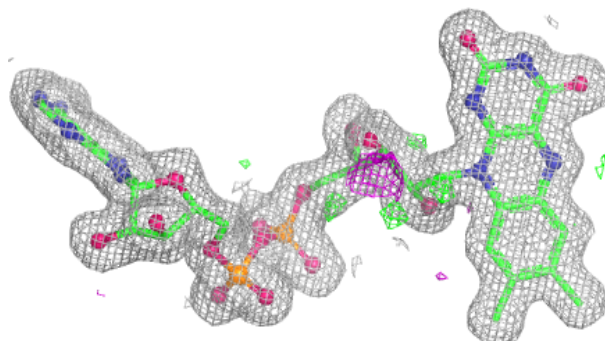
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1337:

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

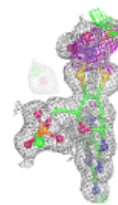
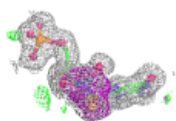
**Electron density around FAD A 1337:**

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



Electron density around ZXF A 1352:

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

**Electron density around ZXF B 1354:**

$2mF_o-DF_c$ (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.