



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:16 pm GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

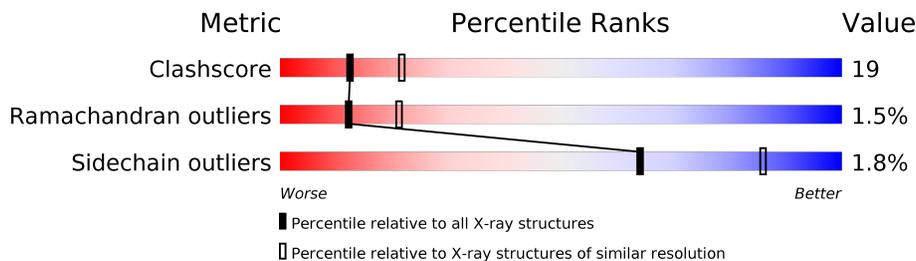
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	219	
2	B	350	
3	C	763	

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
6	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

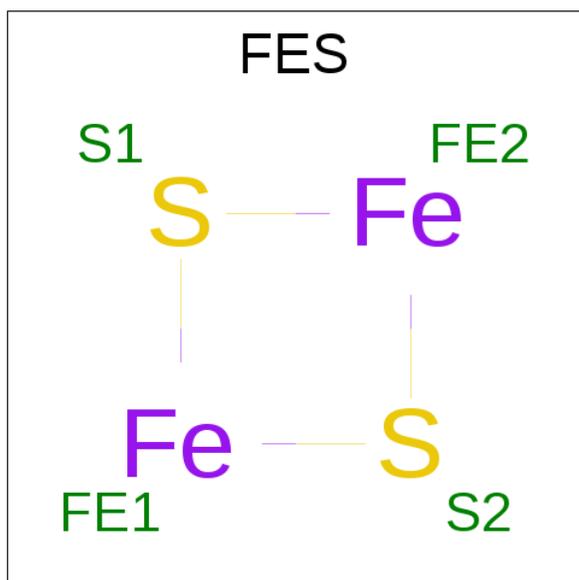
- Molecule 2 is a protein called XANTHINE OXIDASE.

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.

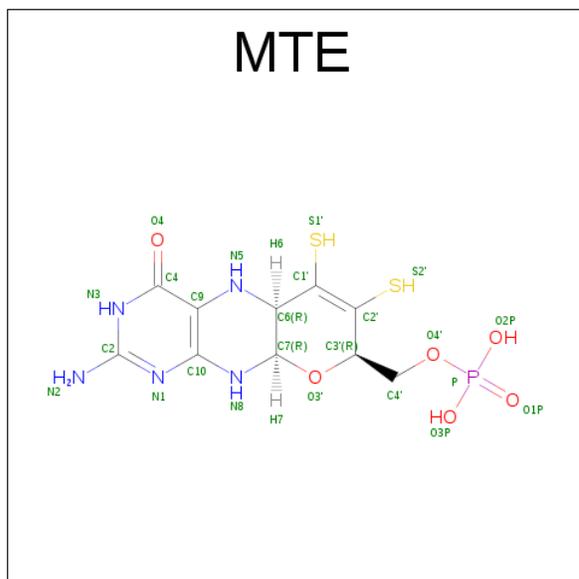
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	745	5761	3643	992	1093	33	0	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



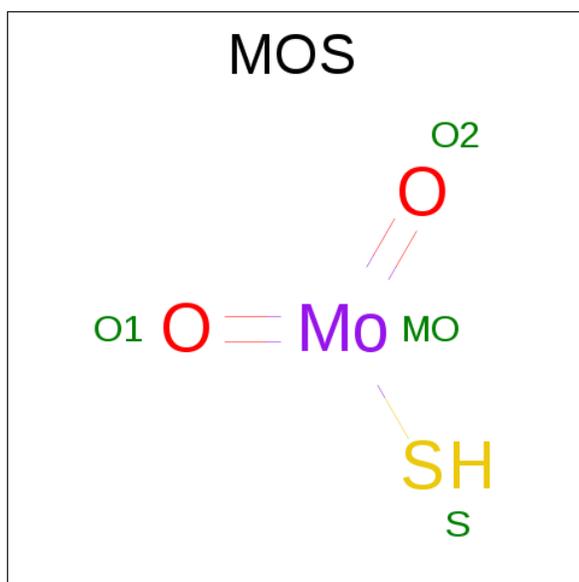
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is 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: C₁₀H₁₄N₅O₆PS₂).



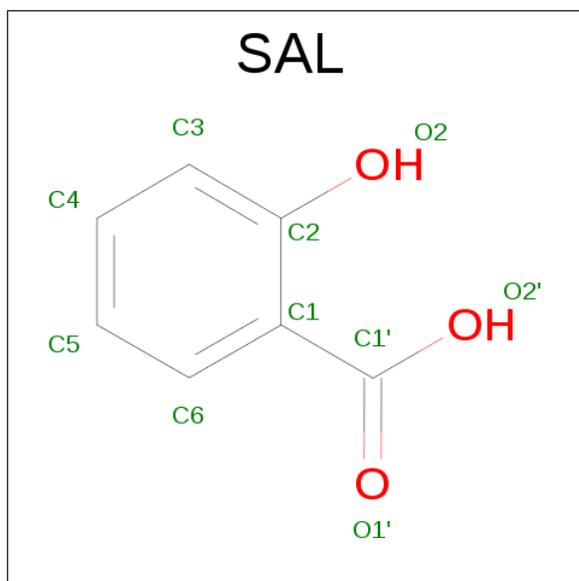
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 6 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO₂S).



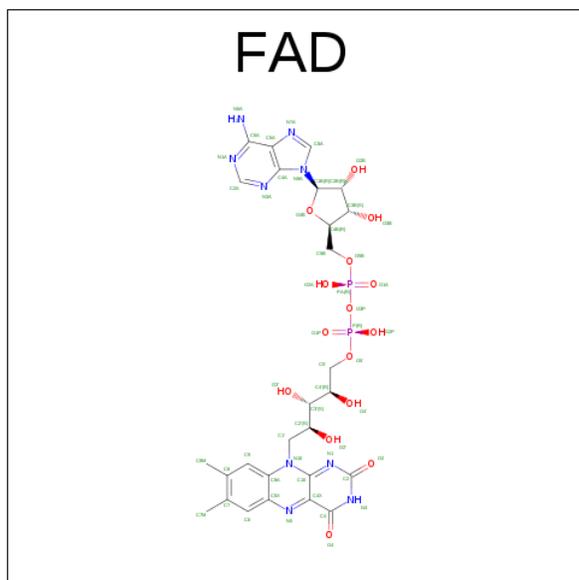
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Mo	O	S		
6	C	1	4	1	2	1	0	0

- Molecule 7 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: C₇H₆O₃).



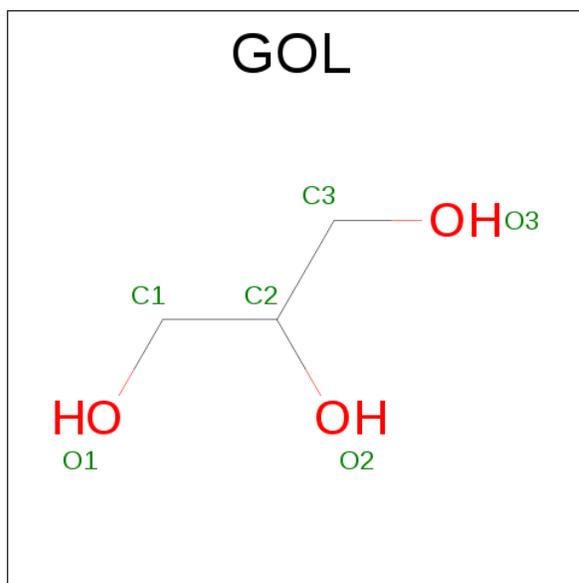
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	10	7	3	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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



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

- Molecule 10 is water.

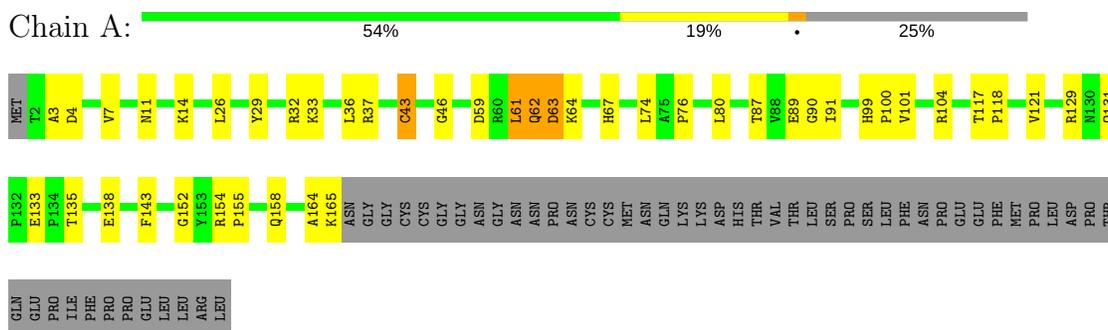
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	94	Total 94	O 94	0	0
10	B	119	Total 119	O 119	0	0
10	C	383	Total 383	O 383	0	0

3 Residue-property plots

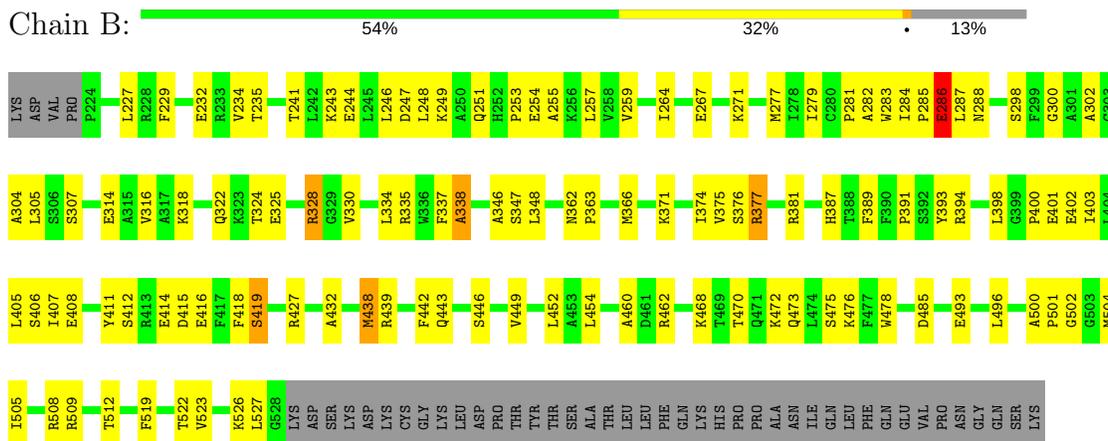
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: XANTHINE OXIDASE



- Molecule 2: XANTHINE OXIDASE



- Molecule 3: XANTHINE OXIDASE



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	10106	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

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: GOL, SAL, MOS, 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(°)	Ideal(°)
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 [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	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	C	24	0	10	1	0
6	C	4	0	0	3	0
7	C	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	53	0	31	1	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%)	5	6
2	B	303/350 (87%)	274 (90%)	25 (8%)	4 (1%)	14	25
3	C	743/763 (97%)	687 (92%)	47 (6%)	9 (1%)	15	27
All	All	1208/1332 (91%)	1113 (92%)	77 (6%)	18 (2%)	12	21

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%)	50	77
3	C	624/639 (98%)	613 (98%)	11 (2%)	64	86
All	All	1022/1128 (91%)	1004 (98%)	18 (2%)	64	86

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

Mol	Chain	Res	Type
3	C	743	TYR
3	C	829	ARG
3	C	1016	GLN
2	B	485	ASP
3	C	723	PHE

Some 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	677	HIS
3	C	728	ASN
3	C	1108	ASN
3	C	683	HIS
3	C	704	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 carbohydrates 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	0.00	-	0,4,4	0.00	-
4	FES	A	602	1	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	B	606	-	51,58,58	5.13	37 (72%)	54,89,89	2.76	19 (35%)
5	MTE	C	1333	6	21,26,26	7.22	14 (66%)	19,40,40	4.51	10 (52%)
6	MOS	C	1334	5	0,3,3	0.00	-	0,3,3	0.00	-
7	SAL	C	1335	-	7,10,10	1.63	2 (28%)	9,13,13	1.24	0
9	GOL	C	1336	-	5,5,5	6.90	5 (100%)	5,5,5	5.41	3 (60%)

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	-	0/0/4/4	0/1/1/1
4	FES	A	602	1	-	0/0/4/4	0/1/1/1
8	FAD	B	606	-	-	0/28/50/50	0/6/6/6
5	MTE	C	1333	6	-	1/6/34/34	0/3/3/3
6	MOS	C	1334	5	-	0/0/0/0	0/0/0/0
7	SAL	C	1335	-	-	0/0/4/4	0/1/1/1
9	GOL	C	1336	-	-	0/4/4/4	0/0/0/0

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1336	GOL	C3-C2	-12.30	1.06	1.52
5	C	1333	MTE	P-O4'	-7.00	1.37	1.60
5	C	1333	MTE	C4'-C3'	-6.70	1.42	1.52
9	C	1336	GOL	O2-C2	-5.94	1.25	1.43
5	C	1333	MTE	P-O3P	-5.87	1.30	1.54

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	606	FAD	C5X-C9A-N10	-6.89	112.54	117.66
8	B	606	FAD	C4-C4X-C10	-6.30	114.87	119.96
5	C	1333	MTE	O4'-P-O1P	-5.93	89.85	106.47
8	B	606	FAD	O5B-PA-O1A	-5.64	86.47	109.25
8	B	606	FAD	C4X-C10-N10	-5.41	116.76	120.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1333	MTE	P-O4'-C4'-C3'

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	FES	1	0
8	B	606	FAD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1333	MTE	1	0
6	C	1334	MOS	3	0
9	C	1336	GOL	5	0

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.