



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:57 PM GMT

PDB ID : 2GAG  
Title : Heterotetrameric sarcosine: structure of a diflavin metaloenzyme at 1.85 Å resolution  
Authors : Chen, Z.W.; Hassan-Abdulah, A.; Zhao, G.; Jorns, M.S.; Mathews, F.S.  
Deposited on : 2006-03-08  
Resolution : 1.85 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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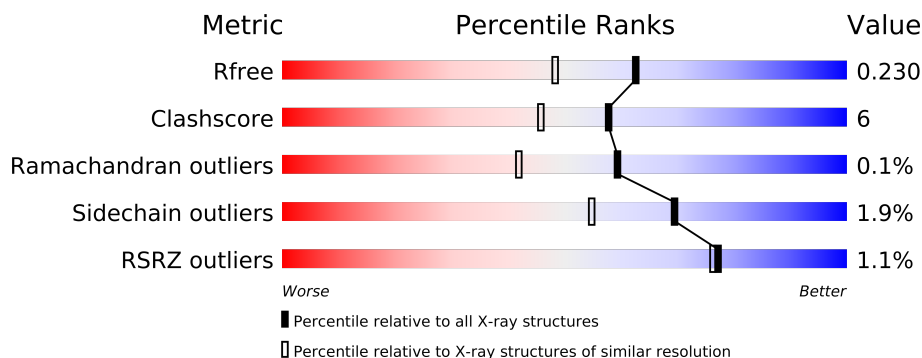
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.85 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))
$R_{free}$	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	965	
2	B	405	
3	C	210	
4	D	99	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	GOL	A	998	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14136 atoms, of which 0 are hydrogen and 0 are deuterium.

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 heterotetrameric sarcosine oxidase alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	965	Total	C	N	O	S	0	0	0
			7261	4520	1294	1428	19			

- Molecule 2 is a protein called heterotetrameric sarcosine oxidase beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3098	1969	542	576	11			

- Molecule 3 is a protein called heterotetrameric sarcosine oxidase gamma-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	S	0	0	0
			1396	877	248	266	5			

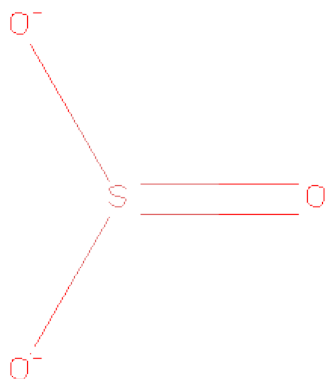
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	203	LEU	-	CLONING ARTIFACT	GB 63146667
C	204	GLU	-	CLONING ARTIFACT	GB 63146667
C	205	HIS	-	EXPRESSION TAG	GB 63146667
C	206	HIS	-	EXPRESSION TAG	GB 63146667
C	207	HIS	-	EXPRESSION TAG	GB 63146667
C	208	HIS	-	EXPRESSION TAG	GB 63146667
C	209	HIS	-	EXPRESSION TAG	GB 63146667
C	210	HIS	-	EXPRESSION TAG	GB 63146667

- Molecule 4 is a protein called heterotetrameric sarcosine oxidase delta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	0	0	0
			747	480	134	128	5			

- Molecule 5 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).

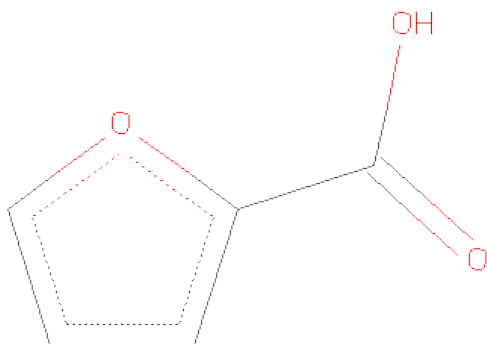


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

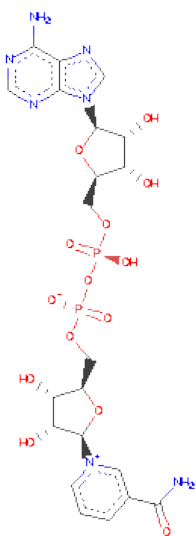
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is 2-FUROIC ACID (three-letter code: FOA) (formula: C<sub>5</sub>H<sub>4</sub>O<sub>3</sub>).



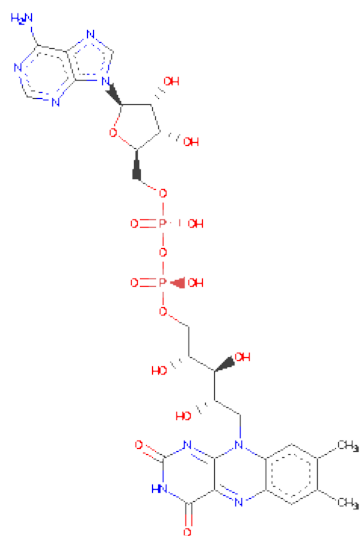
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	5	3		
7	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 8 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



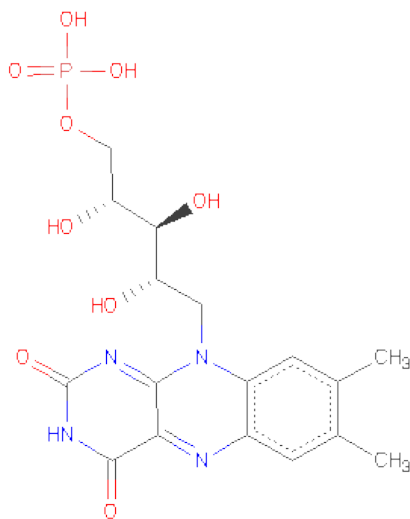
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 10 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 12 is water.

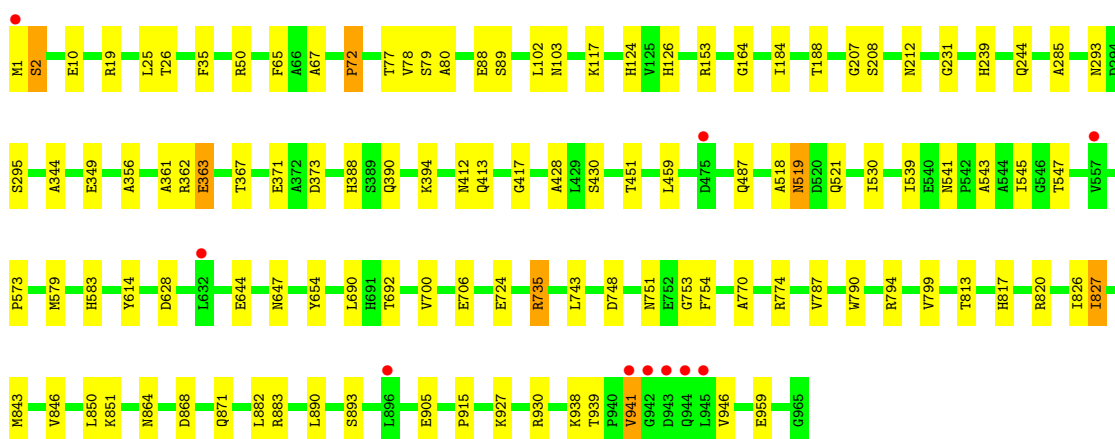
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	876	Total	O	0	0
			876	876		
12	B	313	Total	O	0	0
			313	313		
12	C	175	Total	O	0	0
			175	175		
12	D	115	Total	O	0	0
			115	115		

### 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 errors 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.

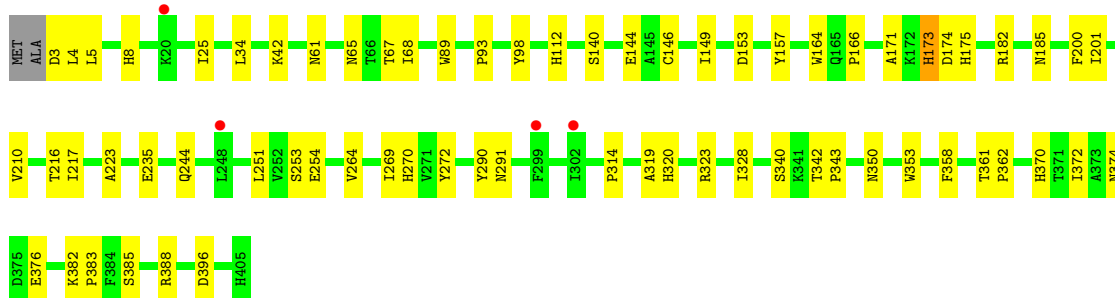
- Molecule 1: heterotetrameric sarcosine oxidase alpha-subunit

Chain A: 



- Molecule 2: heterotetrameric sarcosine oxidase beta-subunit

Chain B: 



- Molecule 3: heterotetrameric sarcosine oxidase gamma-subunit

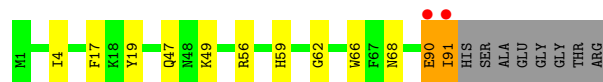
Chain C: 





- Molecule 4: heterotetrameric sarcosine oxidase delta-subunit

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.19Å 132.41Å 197.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 48.93 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.8 (40.00-1.85) 91.7 (48.93-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.82 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.189 , 0.230 0.189 , 0.230	Depositor DCC
$R_{free}$ test set	7613 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 157520 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NAD, FMN, SO3, FOA, 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	0.47	0/7389	0.71	1/10052 (0.0%)
2	B	0.47	0/3179	0.73	3/4323 (0.1%)
3	C	0.48	0/1426	0.70	1/1954 (0.1%)
4	D	0.56	0/773	0.73	0/1047
All	All	0.48	0/12767	0.71	5/17376 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	319	ALA	N-CA-C	-6.72	92.87	111.00
1	A	2	SER	N-CA-C	6.29	127.98	111.00
2	B	269	ILE	N-CA-C	-5.83	95.27	111.00
3	C	164	LEU	N-CA-C	-5.20	96.95	111.00
2	B	270	HIS	N-CA-C	5.16	124.93	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7261	0	7143	91	0
2	B	3098	0	3013	48	0
3	C	1396	0	1385	17	0
4	D	747	0	710	10	0
5	B	4	0	0	1	0
6	D	1	0	0	0	0
7	A	8	0	3	0	0
7	B	8	0	3	4	0
8	A	44	0	26	0	0
9	B	53	0	31	2	0
10	B	31	0	15	1	0
11	A	6	0	8	1	0
12	A	876	0	0	12	0
12	B	313	0	0	5	0
12	C	175	0	0	1	0
12	D	115	0	0	0	0
All	All	14136	0	12337	157	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 157 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:MET:HB3	1:A:285:ALA:HB3	1.47	0.94
1:A:647:ASN:HD21	1:A:654:TYR:H	1.16	0.94
2:B:173:HIS:HD1	2:B:174:ASP:H	1.21	0.88
2:B:350:ASN:HD21	2:B:353:TRP:HE1	1.26	0.82
2:B:61:ASN:HD21	2:B:328:ILE:H	1.30	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	963/965 (100%)	934 (97%)	28 (3%)	1 (0%)	59 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	401/405 (99%)	385 (96%)	16 (4%)	0	100	100
3	C	188/210 (90%)	181 (96%)	7 (4%)	0	100	100
4	D	89/99 (90%)	86 (97%)	3 (3%)	0	100	100
All	All	1641/1679 (98%)	1586 (97%)	54 (3%)	1 (0%)	59	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	PRO

### 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	749/749 (100%)	734 (98%)	15 (2%)	68	52
2	B	319/320 (100%)	314 (98%)	5 (2%)	75	62
3	C	143/161 (89%)	140 (98%)	3 (2%)	66	50
4	D	74/79 (94%)	72 (97%)	2 (3%)	57	39
All	All	1285/1309 (98%)	1260 (98%)	25 (2%)	69	55

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

Mol	Chain	Res	Type
1	A	851	LYS
1	A	941	VAL
4	D	90	GLU
1	A	883	ARG
1	A	959	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	817	HIS

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Mol	Chain	Res	Type
2	B	15	ASN
3	C	77	GLN
1	A	830	GLN
1	A	871	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\# Z  > 2$
7	FOA	A	997	-	8,8,8	1.17	1 (12%)	9,10,10	1.54	1 (11%)
11	GOL	A	998	-	5,5,5	0.26	0	5,5,5	0.61	0
8	NAD	A	999	-	48,48,48	2.72	20 (41%)	73,73,73	2.64	21 (28%)
9	FAD	B	501	-	58,58,58	2.70	26 (44%)	85,89,89	2.02	15 (17%)
10	FMN	B	502	2	33,33,33	4.62	14 (42%)	46,50,50	4.68	22 (47%)
7	FOA	B	503	-	8,8,8	1.54	2 (25%)	9,10,10	2.61	1 (11%)
5	SO3	B	504	-	3,3,3	0.88	0	2,3,3	0.48	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
7	FOA	A	997	-	-	0/0/4/4	0/1/1/1
11	GOL	A	998	-	-	0/4/4/4	0/0/0/0
8	NAD	A	999	-	-	0/30/62/62	0/3/5/5
9	FAD	B	501	-	-	0/34/50/50	0/1/6/6
10	FMN	B	502	2	1/1/4/4	0/18/18/18	0/0/3/3
7	FOA	B	503	-	-	0/0/4/4	0/1/1/1
5	SO3	B	504	-	-	0/0/0/0	0/0/0/0

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	502	FMN	C1'-C2'	-20.87	1.31	1.51
10	B	502	FMN	C9A-C5A	7.17	1.57	1.42
8	A	999	NAD	C4A-N3A	6.72	1.45	1.35
8	A	999	NAD	C8A-N9A	6.64	1.46	1.36
9	B	501	FAD	C5X-N5	6.33	1.45	1.35

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	502	FMN	C2'-C1'-N10	17.69	135.91	112.45
10	B	502	FMN	C4A-C10-N10	-16.37	112.34	120.51
8	A	999	NAD	N3A-C2A-N1A	-13.10	117.75	128.71
9	B	501	FAD	N3A-C2A-N1A	-10.16	120.21	128.71
10	B	502	FMN	C2-N1-C10	8.61	123.66	114.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	502	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	965/965 (100%)	-0.06	10 (1%) 79 78	17, 27, 44, 75	0
2	B	403/405 (99%)	-0.04	4 (0%) 79 78	17, 28, 43, 58	0
3	C	190/210 (90%)	-0.13	3 (1%) 68 68	19, 27, 41, 64	0
4	D	91/99 (91%)	-0.14	2 (2%) 59 57	17, 25, 39, 77	0
All	All	1649/1679 (98%)	-0.07	19 (1%) 77 73	17, 27, 43, 77	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	91	ILE	7.8
1	A	942	GLY	7.7
1	A	1	MET	7.2
1	A	896	LEU	4.9
1	A	943	ASP	4.8

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
11	GOL	A	998	6/6	0.26	4.69	50,53,56,57	0
7	FOA	B	503	8/8	0.13	1.56	21,30,33,33	0
6	ZN	D	101	1/1	0.08	1.02	21,21,21,21	0
7	FOA	A	997	8/8	0.11	0.58	28,32,38,39	0
5	SO3	B	504	4/4	0.11	-0.07	45,49,53,54	0
8	NAD	A	999	44/44	0.10	-0.17	17,21,27,29	0
10	FMN	B	502	31/31	0.12	-0.35	16,21,25,26	0
9	FAD	B	501	53/53	0.08	-0.61	16,24,29,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.