



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:35 am GMT

PDB ID : 2GAH  
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 : 2.00 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](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

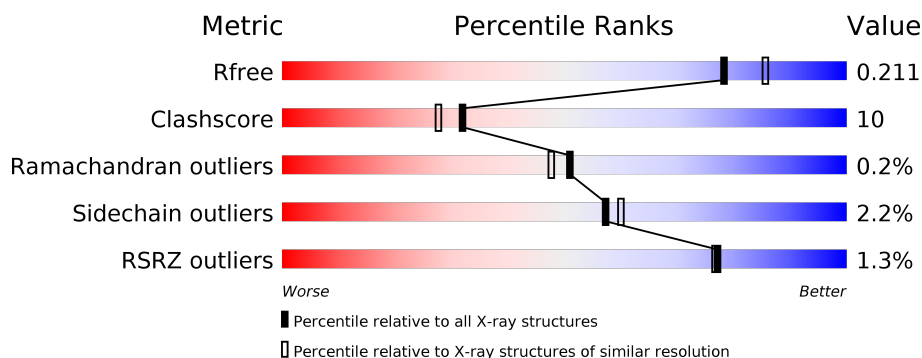
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	965	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 82%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>10%</span> <span>82%</span> <span>18%</span> </div> </div>
2	B	405	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 20%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>20%</span> <span>78%</span> </div> </div>
3	C	210	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 19%, green 70%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>70%</span> <span>19%</span> <span>10%</span> </div> </div>
4	D	99	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 10%, green 78%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>78%</span> <span>10%</span> <span>8%</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	FMN	B	502	X	-	-	-
9	FOA	B	503	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14343 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 heterotetrameric sarcosine oxidase alpha-subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	965	7261	4520	1294	1428	2	17	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	90	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	155	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	267	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	419	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	503	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	579	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	609	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	626	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	661	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	667	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	673	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	757	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	816	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	843	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	904	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	403	3098	1969	542	576	3	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	62	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	160	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	187	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	236	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	265	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	283	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	306	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	333	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0

- 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	Se	0	0	0
			1396	877	248	266	2	3			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	23	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ7
C	176	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ7
C	193	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ7
C	203	LEU	-	CLONING ARTIFACT	UNP Q3ZDQ7
C	204	GLU	-	CLONING ARTIFACT	UNP Q3ZDQ7
C	205	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	206	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	207	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	208	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	209	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	210	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7

- 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	Se	0	0	0
			747	480	134	128	3	2			

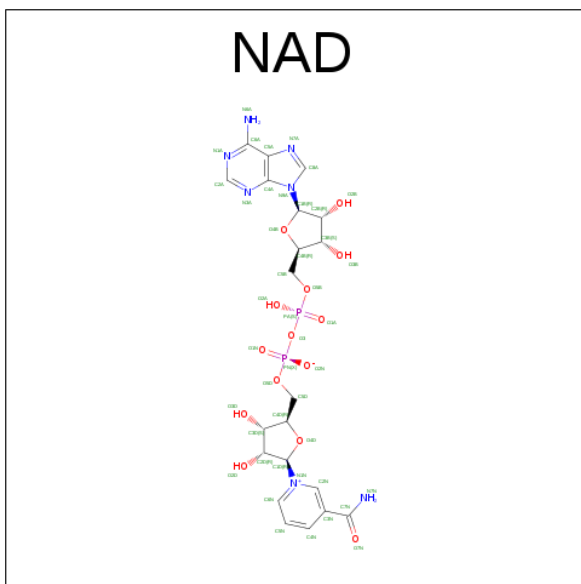
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ9
D	2	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ9

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

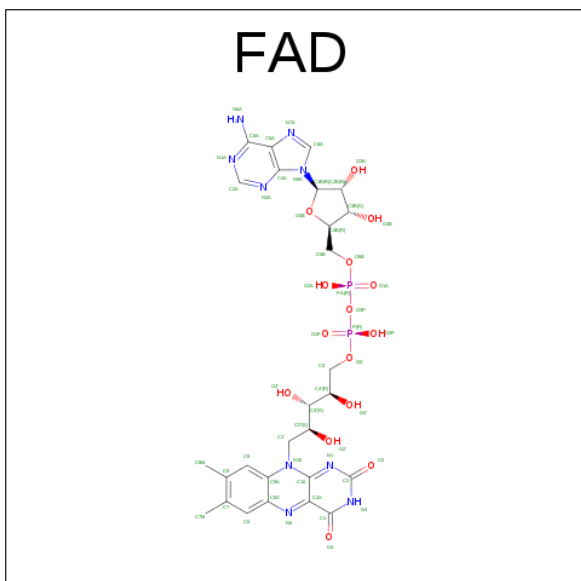
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Zn	0	0
			1	1		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



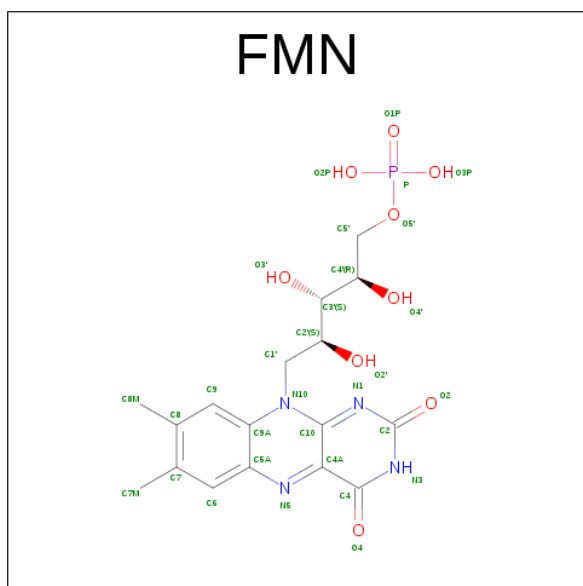
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



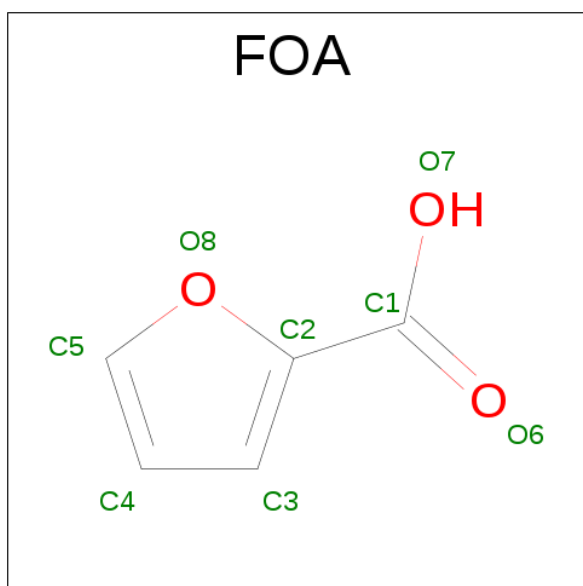
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 9 is 2-FUROIC ACID (three-letter code: FOA) (formula:  $C_5H_4O_3$ ).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	986	Total	O	0	0
			986	986		
10	B	421	Total	O	0	0
			421	421		
10	C	189	Total	O	0	0
			189	189		
10	D	108	Total	O	0	0
			108	108		



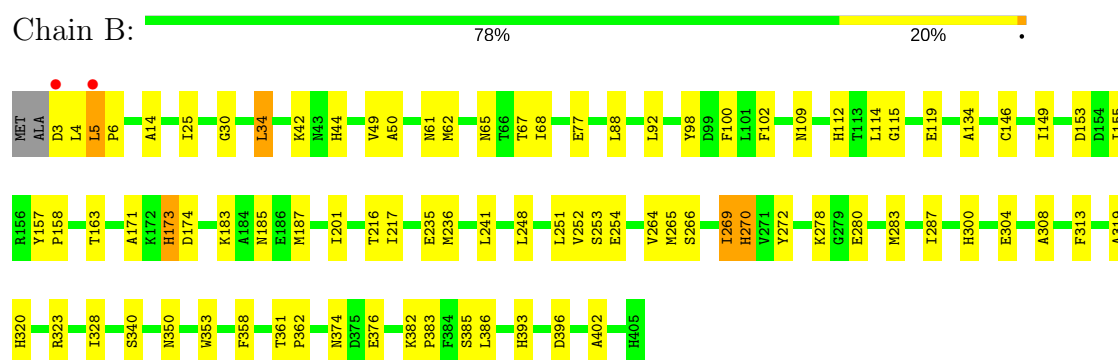
### 3 Residue-property plots

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.

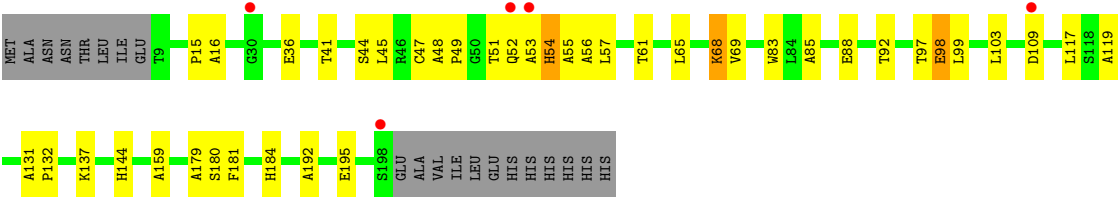
- Molecule 1: heterotetrameric sarcosine oxidase alpha-subunit



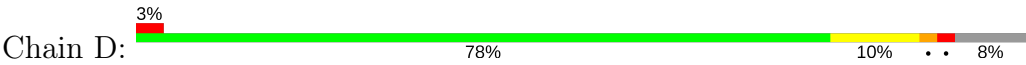
- Molecule 2: heterotetrameric sarcosine oxidase beta-subunit



- Molecule 3: heterotetrameric sarcosine oxidase gamma-subunit



● Molecule 4: heterotetrameric sarcosine oxidase delta-subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.26Å 132.77Å 198.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.57 – 2.00 20.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.4 (20.57-2.00) 86.5 (20.57-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.174 , 0.211 0.174 , 0.211	Depositor DCC
$R_{free}$ test set	5028 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ZN, FOA, NAD, 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	0.37	0/7373	0.60	0/10004
2	B	0.38	0/3171	0.64	3/4299 (0.1%)
3	C	0.35	0/1423	0.64	1/1945 (0.1%)
4	D	0.66	3/772 (0.4%)	0.95	7/1044 (0.7%)
All	All	0.39	3/12739 (0.0%)	0.64	11/17292 (0.1%)

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
4	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	90	GLU	CG-CD	8.63	1.64	1.51
4	D	90	GLU	CB-CG	6.37	1.64	1.52
4	D	90	GLU	N-CA	-5.80	1.34	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	90	GLU	N-CA-CB	-11.43	90.03	110.60
4	D	91	ILE	N-CA-C	8.73	134.58	111.00
4	D	88	ARG	C-N-CD	8.65	146.56	128.40
4	D	90	GLU	CB-CG-CD	7.40	134.17	114.20
2	B	319	ALA	N-CA-C	-5.94	94.95	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	89	PRO	Peptide

## 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	7261	0	7143	151	0
2	B	3098	0	3013	63	0
3	C	1396	0	1385	38	0
4	D	747	0	710	13	0
5	D	1	0	0	0	0
6	A	44	0	26	0	0
7	B	53	0	31	4	0
8	B	31	0	17	2	0
9	B	8	0	3	4	0
10	A	986	0	0	20	0
10	B	421	0	0	5	0
10	C	189	0	0	6	0
10	D	108	0	0	1	0
All	All	14343	0	12328	253	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 10.

The worst 5 of 253 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:656:LYS:H	1:A:656:LYS:HD2	1.26	0.98
1:A:647:ASN:HD21	1:A:654:TYR:H	1.21	0.86
2:B:173:HIS:HD1	2:B:174:ASP:H	1.28	0.82
4:D:70:LEU:HD13	4:D:91:ILE:HD13	1.61	0.82
1:A:541:ASN:HD21	1:A:543:ALA:HB3	1.43	0.81

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%)	931 (97%)	29 (3%)	3 (0%)	44	40
2	B	401/405 (99%)	388 (97%)	13 (3%)	0	100	100
3	C	188/210 (90%)	179 (95%)	9 (5%)	0	100	100
4	D	89/99 (90%)	85 (96%)	3 (3%)	1 (1%)	17	9
All	All	1641/1679 (98%)	1583 (96%)	54 (3%)	4 (0%)	51	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	72	PRO
1	A	943	ASP
4	D	89	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	749/732 (102%)	735 (98%)	14 (2%)	62	66
2	B	319/312 (102%)	310 (97%)	9 (3%)	49	49
3	C	143/158 (90%)	140 (98%)	3 (2%)	59	62
4	D	74/77 (96%)	72 (97%)	2 (3%)	50	51
All	All	1285/1279 (100%)	1257 (98%)	28 (2%)	57	60

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	943	ASP
2	B	5	LEU
3	C	109	ASP
1	A	944	GLN
2	B	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	647	ASN
1	A	916	ASN
3	C	77	GLN
1	A	751	ASN
1	A	830	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
6	NAD	A	999	-	41,48,48	2.54	13 (31%)	43,73,73	2.66	12 (27%)
7	FAD	B	501	-	51,58,58	3.13	22 (43%)	54,89,89	2.41	12 (22%)
8	FMN	B	502	2	31,33,33	3.66	18 (58%)	38,50,50	4.54	21 (55%)
9	FOA	B	503	-	2,8,8	1.95	1 (50%)	1,10,10	1.54	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
6	NAD	A	999	-	-	0/22/62/62	0/5/5/5
7	FAD	B	501	-	-	0/28/50/50	0/6/6/6
8	FMN	B	502	2	1/1/4/4	0/16/18/18	0/3/3/3
9	FOA	B	503	-	-	0/0/4/4	0/0/1/1

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	FAD	P-O5'	-6.13	1.33	1.59
7	B	501	FAD	O5B-C5B	-4.40	1.27	1.44
8	B	502	FMN	C1'-N10	-4.24	1.44	1.48
6	A	999	NAD	C2B-C1B	-3.12	1.48	1.53
8	B	502	FMN	O5'-C5'	-2.95	1.33	1.44

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	999	NAD	N3A-C2A-N1A	-13.63	116.99	128.86
7	B	501	FAD	N3A-C2A-N1A	-10.68	119.56	128.86
8	B	502	FMN	C4A-C10-N10	-9.88	113.66	120.52
8	B	502	FMN	C4-C4A-C10	-6.64	114.59	119.96
8	B	502	FMN	C8M-C8-C9	-4.94	107.97	120.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	502	FMN	C2'

There are no torsion outliers.



There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	FAD	4	0
8	B	502	FMN	2	0
9	B	503	FOA	4	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 [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, 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	948/965 (98%)	-0.38	11 (1%) 79 78	13, 21, 36, 65	0
2	B	395/405 (97%)	-0.49	2 (0%) 90 90	12, 18, 32, 70	0
3	C	187/210 (89%)	-0.13	5 (2%) 55 54	16, 24, 41, 59	0
4	D	89/99 (89%)	-0.24	3 (3%) 46 46	16, 21, 34, 73	0
All	All	1619/1679 (96%)	-0.37	21 (1%) 77 77	12, 21, 36, 73	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	91	ILE	4.7
4	D	90	GLU	4.4
1	A	459	LEU	4.0
1	A	943	ASP	3.9
1	A	746	THR	3.7

### 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	FOA	B	503	8/8	0.94	0.12	1.75	17,22,24,26	0
7	FAD	B	501	53/53	0.97	0.09	-0.15	13,17,20,22	0
6	NAD	A	999	44/44	0.98	0.08	-0.44	11,17,22,25	0
8	FMN	B	502	31/31	0.98	0.07	-0.99	10,15,18,20	0
5	ZN	D	101	1/1	1.00	0.03	-3.53	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.