



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:31 PM BST

PDB ID : 1YKG  
Title : Solution structure of the flavodoxin-like domain from the Escherichia coli sulfite reductase  
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Deposited on : 2005-01-18

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>  
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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

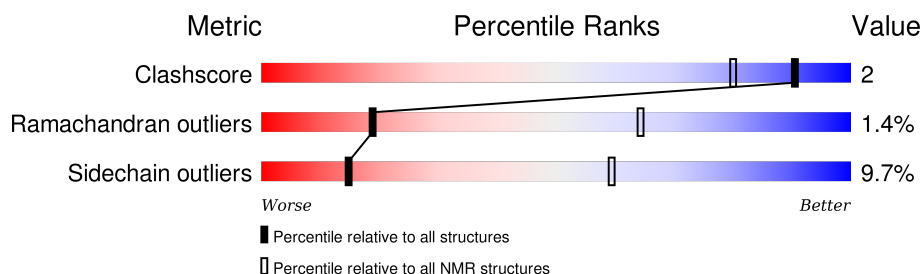
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	167	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	FMN	300	15	-

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:63-A:133, A:145-A:204 (131)	0.27	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13, 14, 15
2	1, 11

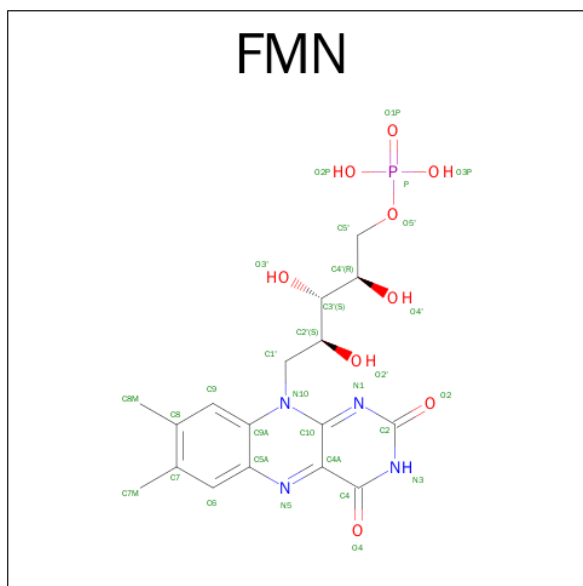
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2311 atoms, of which 1154 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sulfite reductase [NADPH] flavoprotein alpha-component.

Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	
			2261	712	1135	194	219	1	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



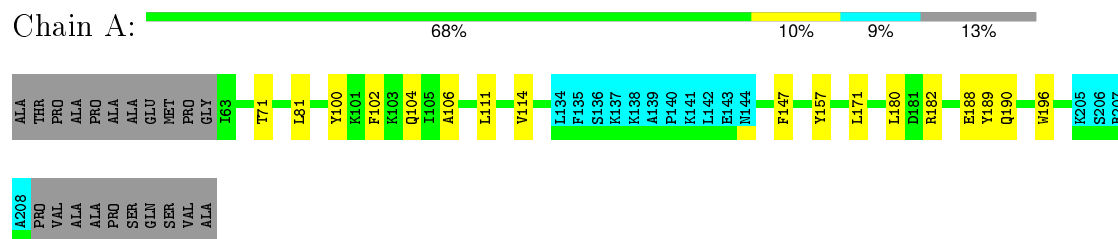
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			50	17	19	4	9	1

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

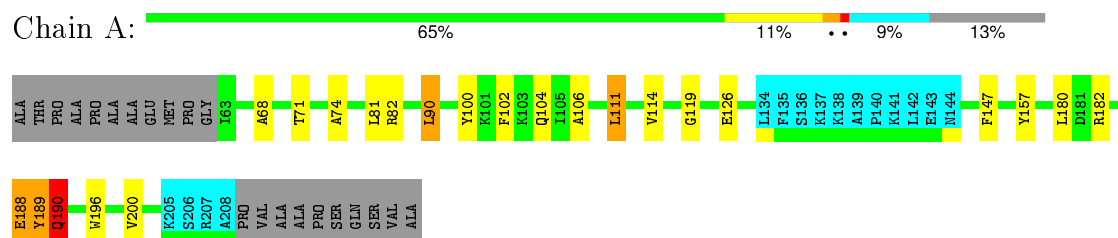


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

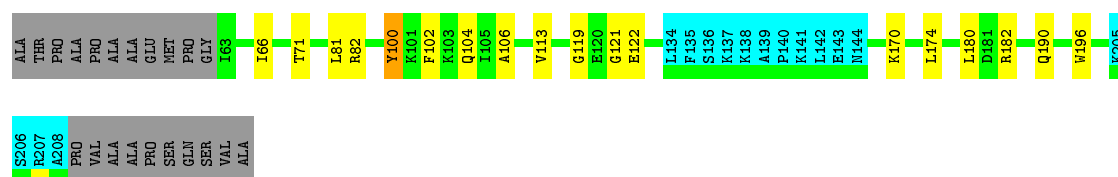
- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



#### 4.2.2 Score per residue for model 2

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

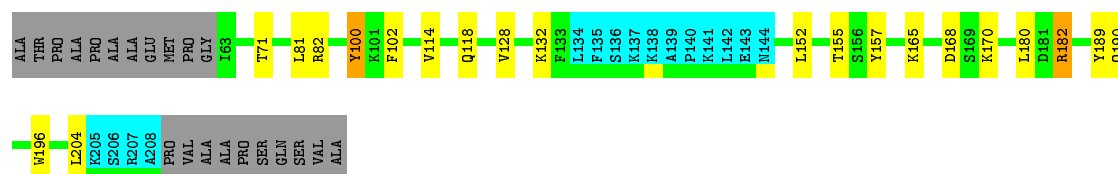




#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

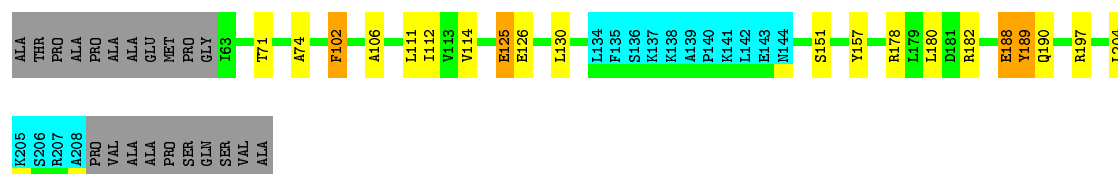
Chain A: 66% 11% 9% 13%



#### 4.2.4 Score per residue for model 4

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

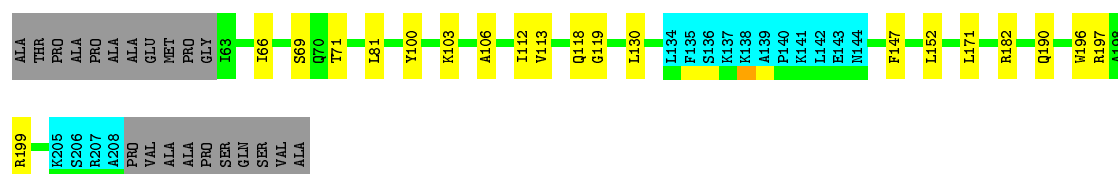
Chain A: 66% 10% 9% 13%



#### 4.2.5 Score per residue for model 5

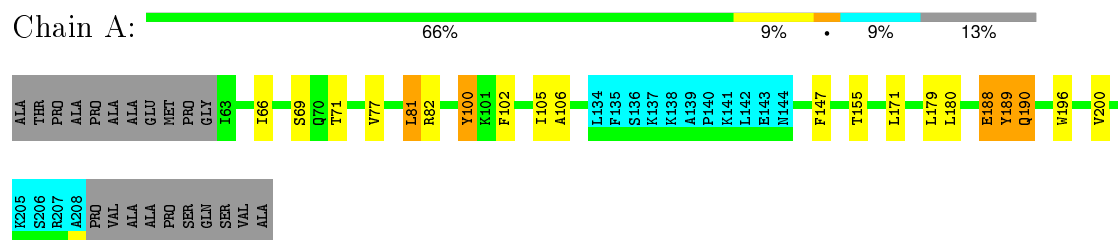
- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

Chain A: 66% 12% 9% 13%



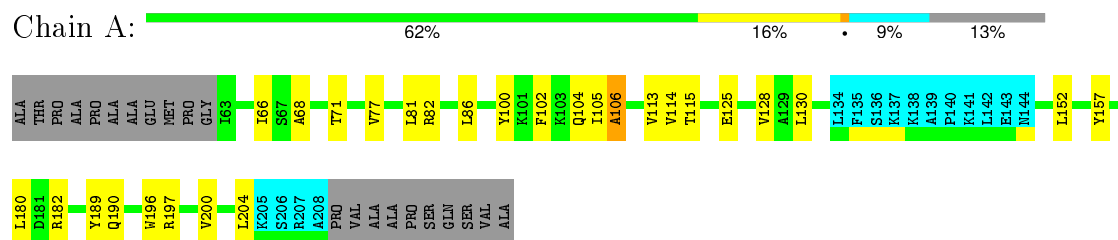
#### 4.2.6 Score per residue for model 6

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



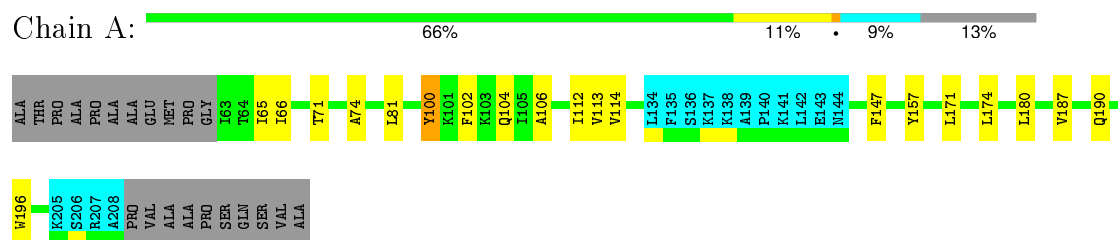
#### 4.2.7 Score per residue for model 7

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



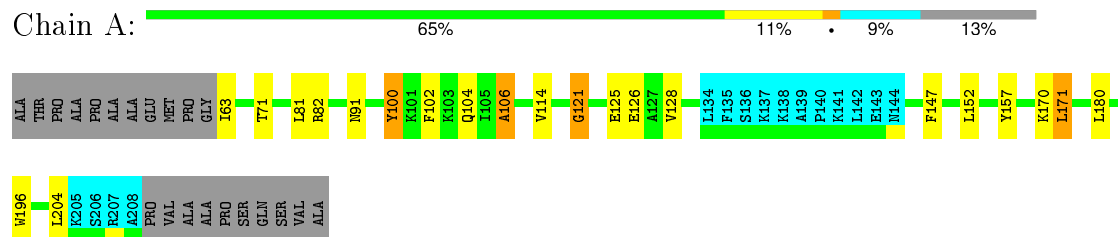
#### 4.2.8 Score per residue for model 8

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



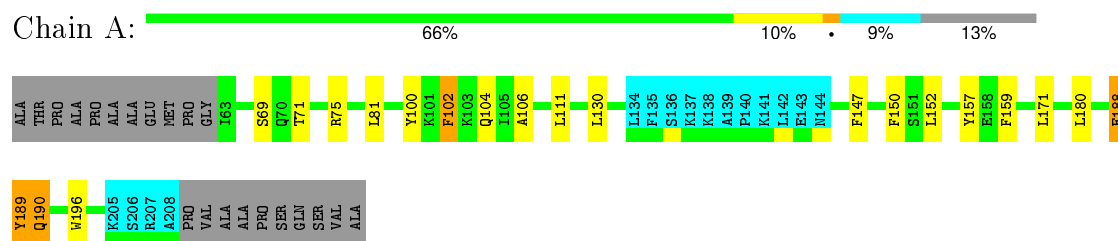
#### 4.2.9 Score per residue for model 9

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



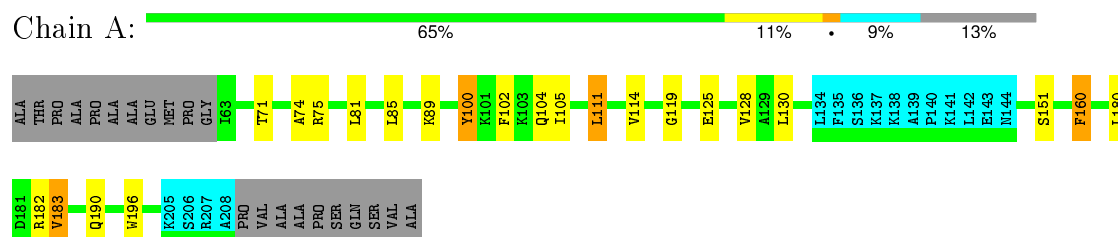
### 4.2.10 Score per residue for model 10

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



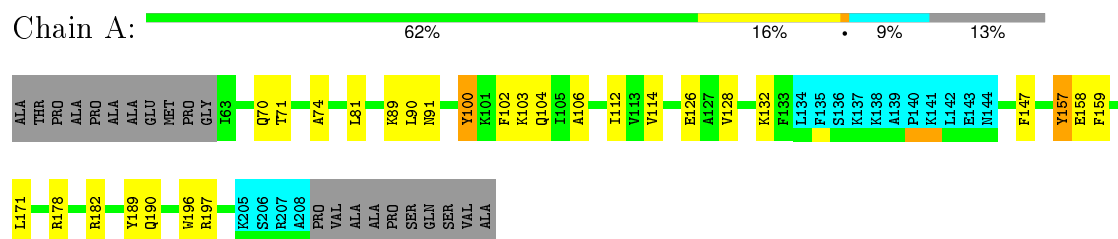
### 4.2.11 Score per residue for model 11

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



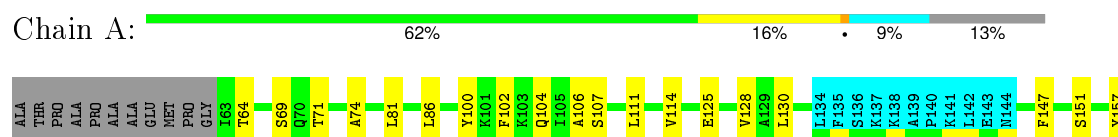
### 4.2.12 Score per residue for model 12

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

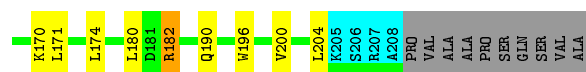


### 4.2.13 Score per residue for model 13

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component



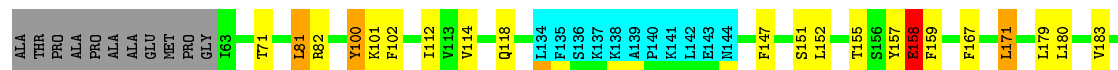




#### 4.2.14 Score per residue for model 14

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

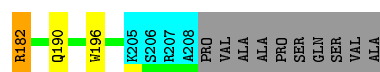
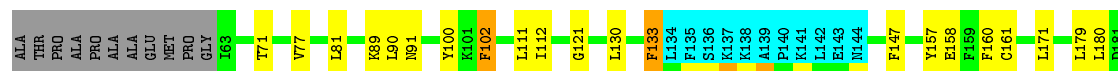
Chain A: 65% 11% 9% 13%



#### 4.2.15 Score per residue for model 15

- Molecule 1: Sulfite reductase [NADPH] flavoprotein alpha-component

Chain A: 64% 13% 9% 13%



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 15 calculated structures, 15 were deposited, based on the following criterion: *initial selection based on experimental energy target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DISCOVER	structure solution	2.98
Sculptor	refinement	1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

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 (average) 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	0.58±0.00	0±0/1021 (0.0±0.0%)	1.05±0.02	3±1/1381 (0.2±0.1%)
All	All	0.58	0/15315 (0.0%)	1.05	45/20715 (0.2%)

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	Planarity
1	A	0.0±0.0	3.7±1.1
All	All	0	55

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	182	ARG	NE-CZ-NH2	-7.07	116.76	120.30	13	1
1	A	125	GLU	C-N-CA	7.05	139.34	121.70	4	1
1	A	100	TYR	CB-CG-CD2	-6.84	116.90	121.00	11	9
1	A	106	ALA	N-CA-CB	-5.66	102.18	110.10	7	11
1	A	183	VAL	CA-CB-CG2	5.54	119.20	110.90	11	1
1	A	190	GLN	CA-C-N	5.43	129.14	117.20	1	14
1	A	90	LEU	N-CA-C	5.39	125.56	111.00	12	2
1	A	100	TYR	CB-CG-CD1	5.33	124.20	121.00	9	2
1	A	150	PHE	CB-CG-CD1	-5.30	117.09	120.80	10	1
1	A	152	LEU	CB-CA-C	5.18	120.03	110.20	10	1
1	A	68	ALA	CB-CA-C	5.14	117.81	110.10	1	1
1	A	158	GLU	CA-C-O	-5.13	109.32	120.10	14	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	71	THR	Mainchain	15
1	A	102	PHE	Sidechain	12
1	A	157	TYR	Sidechain	11
1	A	188	GLU	Mainchain	4
1	A	189	TYR	Sidechain	3
1	A	121	GLY	Mainchain	2
1	A	197	ARG	Sidechain	1
1	A	125	GLU	Mainchain	1
1	A	182	ARG	Sidechain	1
1	A	178	ARG	Sidechain	1
1	A	75	ARG	Sidechain	1
1	A	100	TYR	Sidechain	1
1	A	158	GLU	Mainchain	1
1	A	147	PHE	Sidechain	1

## 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1006	1000	998	4±2
All	All	15555	15285	15255	66

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 2.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:HD23	1:A:196:TRP:CZ3	0.79	2.11	6	2
1:A:81:LEU:HD22	1:A:196:TRP:CZ3	0.73	2.19	5	3
1:A:81:LEU:HD13	1:A:196:TRP:CZ3	0.71	2.20	7	6
1:A:81:LEU:HD22	1:A:196:TRP:CH2	0.67	2.24	10	6
1:A:125:GLU:O	1:A:128:VAL:HG12	0.66	1.90	7	3
1:A:157:TYR:O	1:A:159:PHE:N	0.63	2.31	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:PHE:CD2	1:A:171:LEU:HD23	0.59	2.33	14	2
1:A:147:PHE:CD2	1:A:171:LEU:HD13	0.58	2.33	12	7
1:A:81:LEU:HD11	1:A:200:VAL:CG2	0.57	2.29	13	3
1:A:160:PHE:O	1:A:161:CYS:HB3	0.54	2.02	15	1
1:A:167:PHE:O	1:A:171:LEU:HD22	0.53	2.04	14	1
1:A:128:VAL:O	1:A:132:LYS:HB2	0.53	2.04	3	1
1:A:119:GLY:O	1:A:122:GLU:OE1	0.52	2.28	2	1
1:A:68:ALA:HB3	1:A:115:THR:HA	0.51	1.82	7	1
1:A:81:LEU:HD21	1:A:200:VAL:CG2	0.48	2.38	6	1
1:A:74:ALA:HB1	1:A:114:VAL:HG23	0.48	1.85	12	5
1:A:147:PHE:CZ	1:A:171:LEU:HB3	0.48	2.43	14	1
1:A:81:LEU:HD21	1:A:200:VAL:HG21	0.48	1.86	6	1
1:A:81:LEU:HD12	1:A:197:ARG:HG3	0.48	1.86	7	1
1:A:188:GLU:O	1:A:190:GLN:N	0.46	2.45	6	3
1:A:160:PHE:O	1:A:161:CYS:CB	0.46	2.63	15	1
1:A:128:VAL:O	1:A:132:LYS:CB	0.45	2.64	12	1
1:A:111:LEU:O	1:A:111:LEU:HD23	0.45	2.11	11	1
1:A:68:ALA:N	1:A:114:VAL:O	0.43	2.50	7	1
1:A:63:ILE:N	1:A:91:ASN:O	0.43	2.51	9	1
1:A:125:GLU:O	1:A:128:VAL:HG22	0.43	2.14	13	1
1:A:74:ALA:HB1	1:A:114:VAL:CG1	0.43	2.44	1	1
1:A:168:ASP:OD2	1:A:182:ARG:NH1	0.42	2.53	3	1
1:A:111:LEU:HD23	1:A:111:LEU:O	0.42	2.14	1	1
1:A:65:ILE:HG23	1:A:112:ILE:HG22	0.41	1.91	8	1
1:A:85:LEU:O	1:A:89:LYS:N	0.41	2.53	11	1
1:A:69:SER:OG	1:A:74:ALA:HB3	0.41	2.16	13	1
1:A:111:LEU:C	1:A:111:LEU:HD23	0.41	2.36	11	1
1:A:74:ALA:HB1	1:A:114:VAL:CG2	0.40	2.46	11	1
1:A:104:GLN:O	1:A:107:SER:N	0.40	2.53	13	1
1:A:81:LEU:CD2	1:A:196:TRP:CZ3	0.40	3.04	12	1

## 6.3 Torsion angles ⓘ

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	130/167 (78%)	123±1 (95±1%)	5±1 (4±1%)	2±1 (1±1%)	19	64
All	All	1950/2505 (78%)	1852 (95%)	71 (4%)	27 (1%)	19	64

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	189	TYR	4
1	A	119	GLY	3
1	A	102	PHE	2
1	A	89	LYS	2
1	A	105	ILE	2
1	A	158	GLU	2
1	A	90	LEU	2
1	A	91	ASN	2
1	A	121	GLY	2
1	A	106	ALA	2
1	A	126	GLU	1
1	A	160	PHE	1
1	A	159	PHE	1
1	A	187	VAL	1

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	104/130 (80%)	94±2 (90±2%)	10±2 (10±2%)	15	59
All	All	1560/1950 (80%)	1408 (90%)	152 (10%)	15	59

All 44 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	180	LEU	13
1	A	100	TYR	12
1	A	182	ARG	10
1	A	104	GLN	8

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Mol	Chain	Res	Type	Models (Total)
1	A	130	LEU	7
1	A	82	ARG	7
1	A	111	LEU	6
1	A	66	ILE	5
1	A	112	ILE	5
1	A	204	LEU	5
1	A	152	LEU	5
1	A	113	VAL	4
1	A	151	SER	4
1	A	189	TYR	4
1	A	170	LYS	4
1	A	69	SER	3
1	A	126	GLU	3
1	A	114	VAL	3
1	A	179	LEU	3
1	A	118	GLN	3
1	A	77	VAL	3
1	A	102	PHE	3
1	A	155	THR	3
1	A	86	LEU	2
1	A	81	LEU	2
1	A	103	LYS	2
1	A	197	ARG	2
1	A	174	LEU	2
1	A	190	GLN	2
1	A	171	LEU	2
1	A	183	VAL	2
1	A	101	LYS	1
1	A	70	GLN	1
1	A	64	THR	1
1	A	75	ARG	1
1	A	133	PHE	1
1	A	105	ILE	1
1	A	188	GLU	1
1	A	159	PHE	1
1	A	165	LYS	1
1	A	160	PHE	1
1	A	158	GLU	1
1	A	199	ARG	1
1	A	178	ARG	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	FMN	A	300	-	31,33,33	1.69±0.05	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	FMN	A	300	-	32,50,50	2.17±0.09	1±0 (4±1%)

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
2	FMN	A	300	-	3±0,3,4,4	0±0,18,18,18	0±0,3,3,3

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	300	FMN	C2-N1-C10	9.28	121.30	113.39	11	15
2	A	300	FMN	C5A-C9A-N10	5.74	121.88	117.58	14	4
2	A	300	FMN	C1'-N10-C9A	5.48	125.18	118.83	6	3

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	300	FMN	C4'	15
2	A	300	FMN	C2'	15
2	A	300	FMN	C3'	15

There are no torsion outliers.

There are no ring outliers.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided