



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:26 pm GMT

PDB ID : 1RVV  
Title : SYNTHASE/RIBOFLAVIN SYNTHASE COMPLEX OF BACILLUS SUB-  
TILIS  
Authors : Ritsert, K.; Huber, R.; Turk, D.; Ladenstein, R.; Schmidt-Baese, K.; Bacher,  
A.  
Deposited on : 1995-10-25  
Resolution : 2.40 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) : **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) : trunk28620

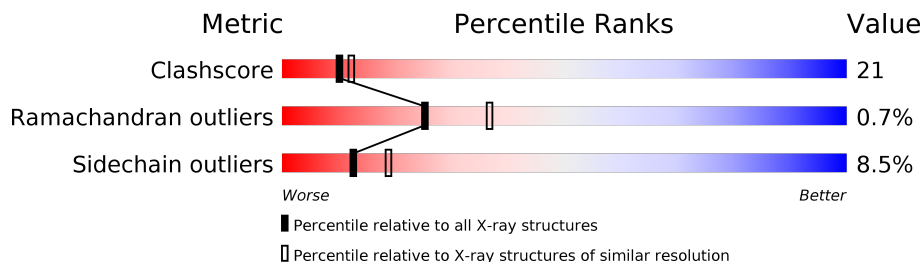
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
























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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	154	 71% 24% . .
1	2	154	 70% 25% . .
1	3	154	 72% 23% . .
1	4	154	 66% 29% . .
1	A	154	 71% 25% . .
1	B	154	 71% 24% . .
1	C	154	 70% 25% . .

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Mol	Chain	Length	Quality of chain
1	D	154	 71% 25% . .
1	E	154	 71% 24% . .
1	F	154	 69% 26% . .
1	G	154	 69% 26% . .
1	H	154	 73% 22% . .
1	I	154	 71% 24% . .
1	J	154	 70% 25% . .
1	K	154	 69% 27% . .
1	L	154	 71% 24% . .
1	M	154	 69% 26% . .
1	N	154	 70% 25% . .
1	O	154	 66% 29% . .
1	P	154	 69% 26% . .
1	Q	154	 71% 25% . .
1	R	154	 70% 25% . .
1	S	154	 71% 24% . .
1	T	154	 70% 25% . .
1	U	154	 70% 25% . .
1	V	154	 69% 26% . .
1	W	154	 73% 23% . .
1	X	154	 68% 27% . .
1	Y	154	 71% 24% . .
1	Z	154	 70% 25% . .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36150 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 RIBOFLAVIN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	B	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	C	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	D	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	E	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	F	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	G	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	H	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	I	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	J	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	K	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	L	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	M	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	N	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	O	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	P	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	R	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	S	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	T	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	U	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	V	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	W	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	X	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	Y	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	Z	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	1	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	2	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	3	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	4	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



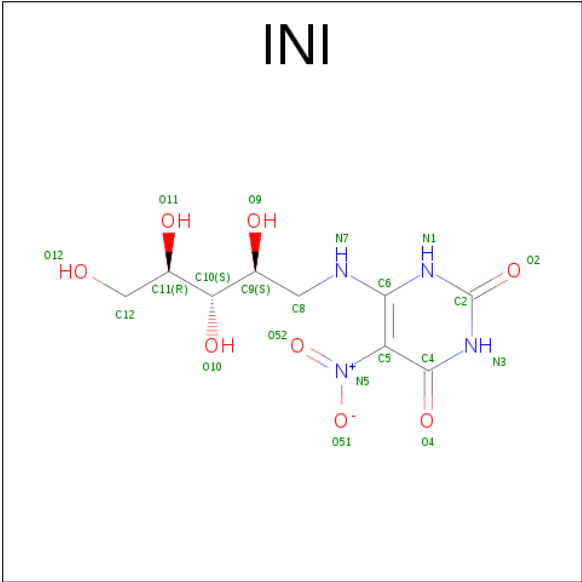
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	T	1	Total	O	P	0	0
			5	4	1		
2	U	1	Total	O	P	0	0
			5	4	1		
2	V	1	Total	O	P	0	0
			5	4	1		
2	W	1	Total	O	P	0	0
			5	4	1		
2	X	1	Total	O	P	0	0
			5	4	1		
2	Y	1	Total	O	P	0	0
			5	4	1		
2	Z	1	Total	O	P	0	0
			5	4	1		
2	1	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		
2	3	1	Total	O	P	0	0
			5	4	1		
2	4	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 5-NITRO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: INI) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>4</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	9	4	8		
3	B	1	Total	C	N	O	0	0
			21	9	4	8		
3	C	1	Total	C	N	O	0	0
			21	9	4	8		
3	D	1	Total	C	N	O	0	0
			21	9	4	8		
3	E	1	Total	C	N	O	0	0
			21	9	4	8		
3	F	1	Total	C	N	O	0	0
			21	9	4	8		
3	G	1	Total	C	N	O	0	0
			21	9	4	8		
3	H	1	Total	C	N	O	0	0
			21	9	4	8		
3	I	1	Total	C	N	O	0	0
			21	9	4	8		
3	J	1	Total	C	N	O	0	0
			21	9	4	8		
3	K	1	Total	C	N	O	0	0
			21	9	4	8		
3	L	1	Total	C	N	O	0	0
			21	9	4	8		
3	M	1	Total	C	N	O	0	0
			21	9	4	8		
3	N	1	Total	C	N	O	0	0
			21	9	4	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	1	Total	C	N	O	0	0
			21	9	4	8		
3	P	1	Total	C	N	O	0	0
			21	9	4	8		
3	Q	1	Total	C	N	O	0	0
			21	9	4	8		
3	R	1	Total	C	N	O	0	0
			21	9	4	8		
3	S	1	Total	C	N	O	0	0
			21	9	4	8		
3	T	1	Total	C	N	O	0	0
			21	9	4	8		
3	U	1	Total	C	N	O	0	0
			21	9	4	8		
3	V	1	Total	C	N	O	0	0
			21	9	4	8		
3	W	1	Total	C	N	O	0	0
			21	9	4	8		
3	X	1	Total	C	N	O	0	0
			21	9	4	8		
3	Y	1	Total	C	N	O	0	0
			21	9	4	8		
3	Z	1	Total	C	N	O	0	0
			21	9	4	8		
3	1	1	Total	C	N	O	0	0
			21	9	4	8		
3	2	1	Total	C	N	O	0	0
			21	9	4	8		
3	3	1	Total	C	N	O	0	0
			21	9	4	8		
3	4	1	Total	C	N	O	0	0
			21	9	4	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	35	Total	O	0	0
			35	35		
4	2	35	Total	O	0	0
			35	35		
4	3	32	Total	O	0	0
			32	32		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	4	35	Total 35	O 35	0	0
4	A	38	Total 38	O 38	0	0
4	B	31	Total 31	O 31	0	0
4	C	36	Total 36	O 36	0	0
4	D	35	Total 35	O 35	0	0
4	E	35	Total 35	O 35	0	0
4	F	35	Total 35	O 35	0	0
4	G	38	Total 38	O 38	0	0
4	H	35	Total 35	O 35	0	0
4	I	31	Total 31	O 31	0	0
4	J	34	Total 34	O 34	0	0
4	K	39	Total 39	O 39	0	0
4	L	35	Total 35	O 35	0	0
4	M	35	Total 35	O 35	0	0
4	N	32	Total 32	O 32	0	0
4	O	36	Total 36	O 36	0	0
4	P	38	Total 38	O 38	0	0
4	Q	32	Total 32	O 32	0	0
4	R	34	Total 34	O 34	0	0
4	S	32	Total 32	O 32	0	0
4	T	34	Total 34	O 34	0	0

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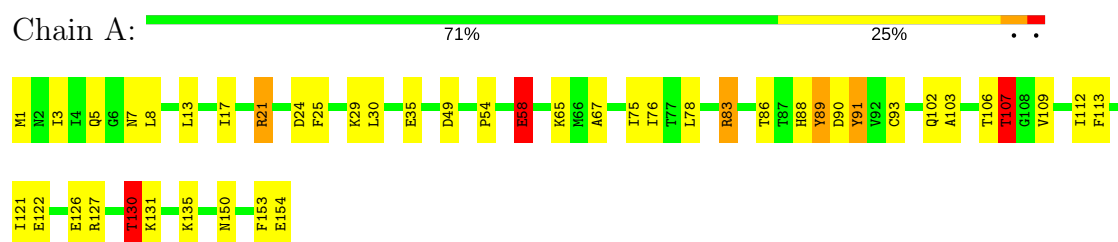
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	U	36	Total 36	O 36	0	0
4	V	39	Total 39	O 39	0	0
4	W	35	Total 35	O 35	0	0
4	X	33	Total 33	O 33	0	0
4	Y	37	Total 37	O 37	0	0
4	Z	38	Total 38	O 38	0	0

### 3 Residue-property plots

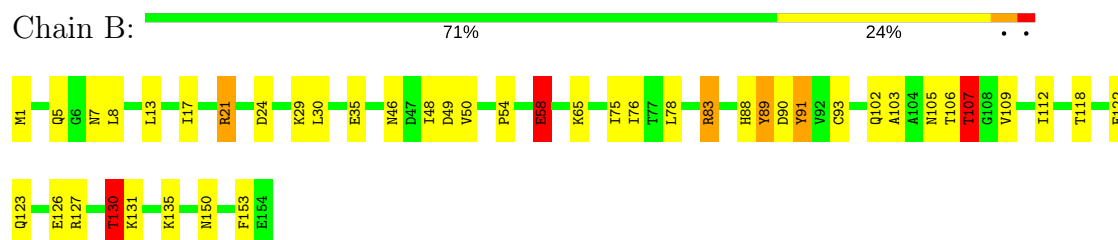
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

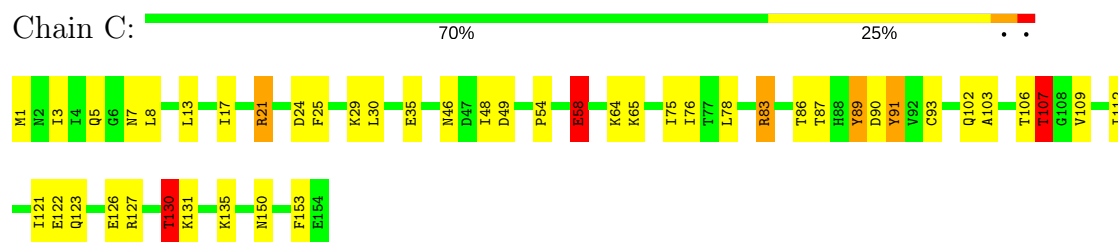
#### • Molecule 1: RIBOFLAVIN SYNTHASE



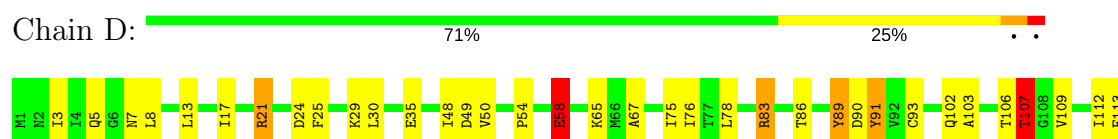
#### • Molecule 1: RIBOFLAVIN SYNTHASE

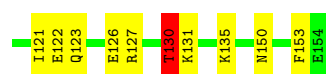


#### • Molecule 1: RIBOFLAVIN SYNTHASE



#### • Molecule 1: RIBOFLAVIN SYNTHASE





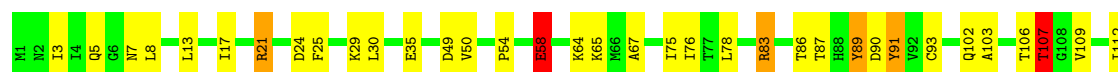
● Molecule 1: RIBOFLAVIN SYNTHASE

Chain E: 71% 24%



● Molecule 1: RIBOFLAVIN SYNTHASE

Chain F: 69% 26%



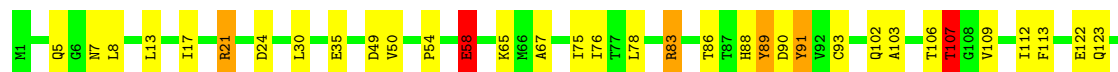
● Molecule 1: RIBOFLAVIN SYNTHASE

Chain G: 69% 26%



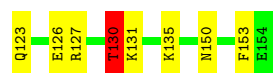
● Molecule 1: RIBOFLAVIN SYNTHASE

Chain H: 73% 22%

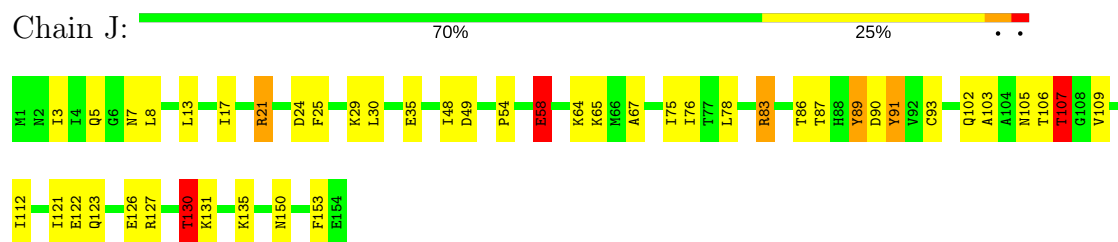


● Molecule 1: RIBOFLAVIN SYNTHASE

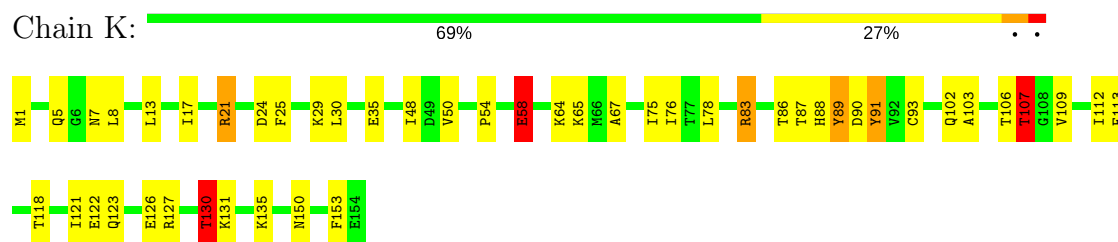
Chain I: 71% 24%



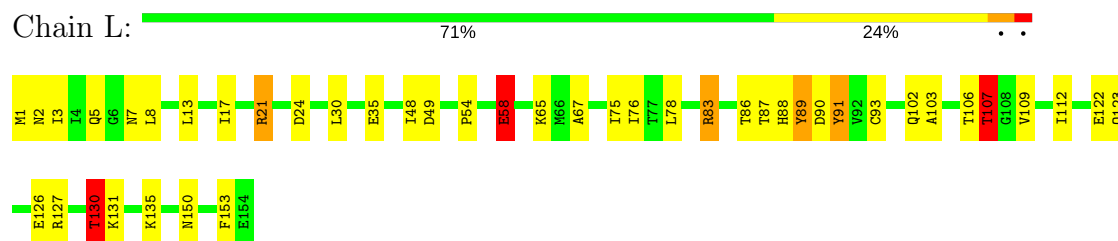
- Molecule 1: RIBOFLAVIN SYNTHASE



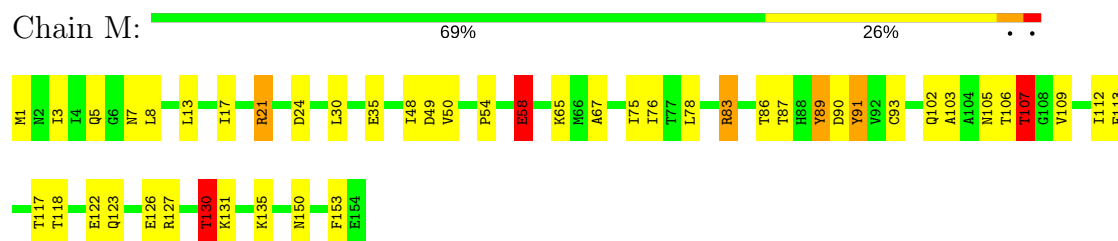
- Molecule 1: RIBOFLAVIN SYNTHASE



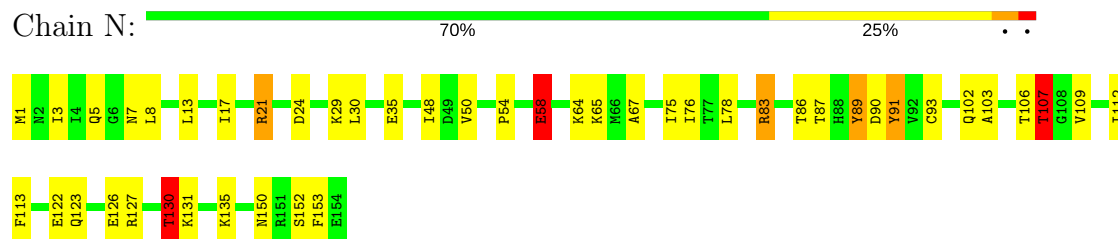
- Molecule 1: RIBOFLAVIN SYNTHASE



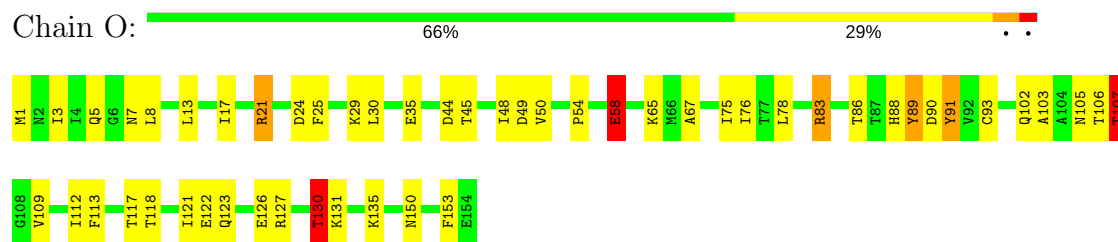
- Molecule 1: RIBOFLAVIN SYNTHASE



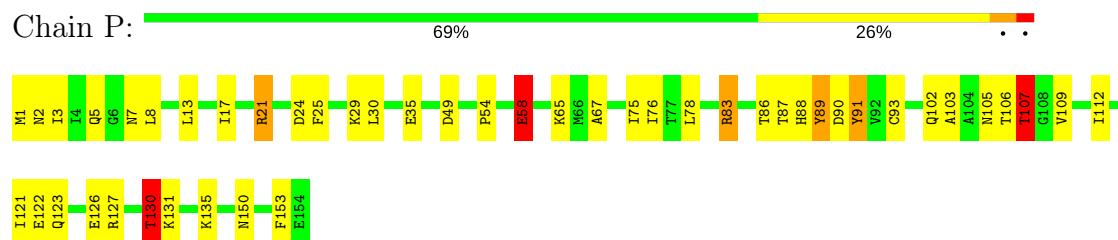
- Molecule 1: RIBOFLAVIN SYNTHASE



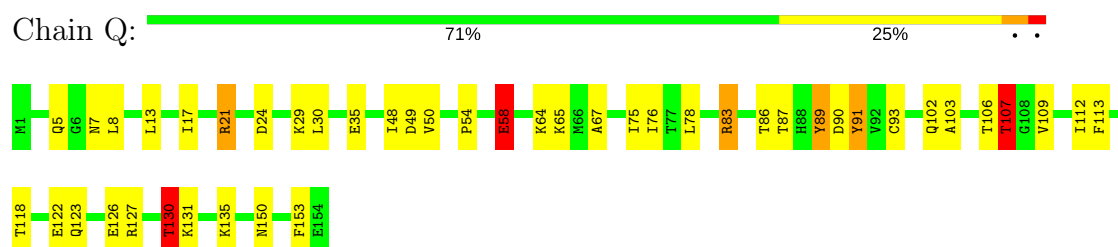
- Molecule 1: RIBOFLAVIN SYNTHASE



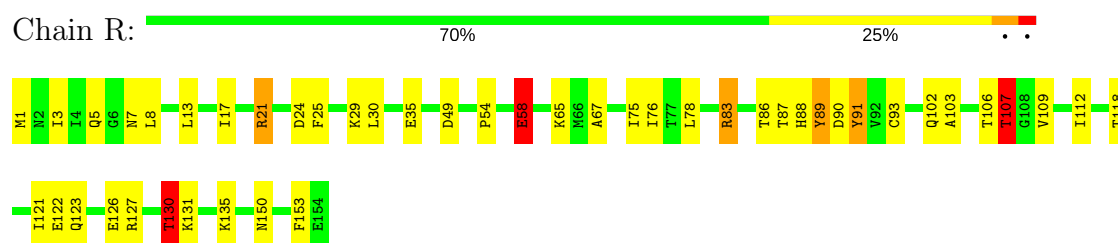
• Molecule 1: RIBOFLAVIN SYNTHASE



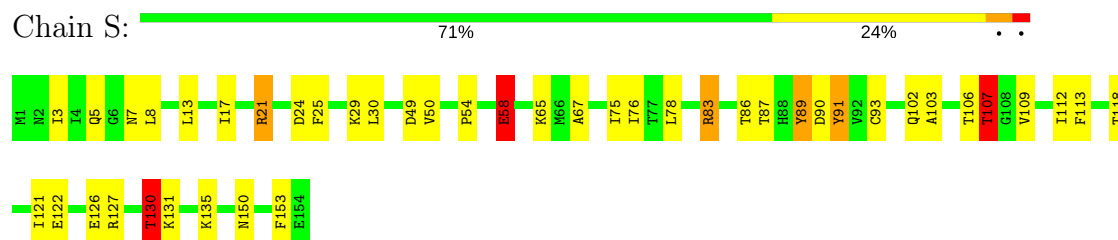
• Molecule 1: RIBOFLAVIN SYNTHASE



• Molecule 1: RIBOFLAVIN SYNTHASE

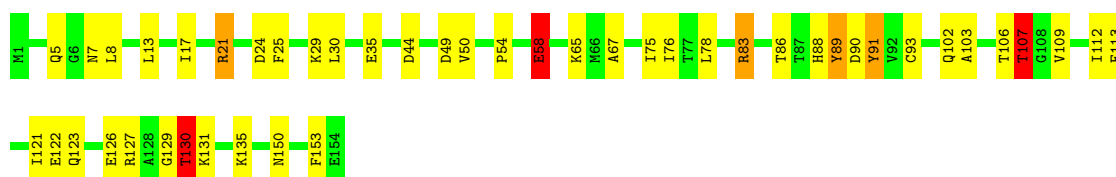


• Molecule 1: RIBOFLAVIN SYNTHASE



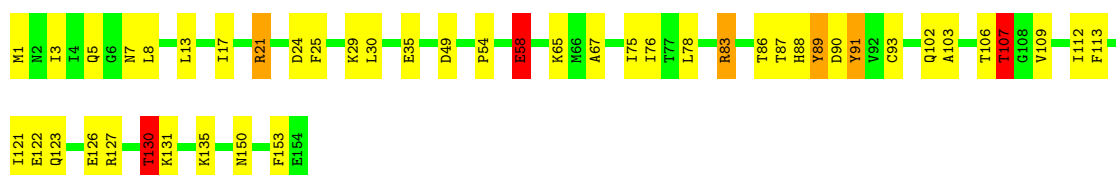
• Molecule 1: RIBOFLAVIN SYNTHASE





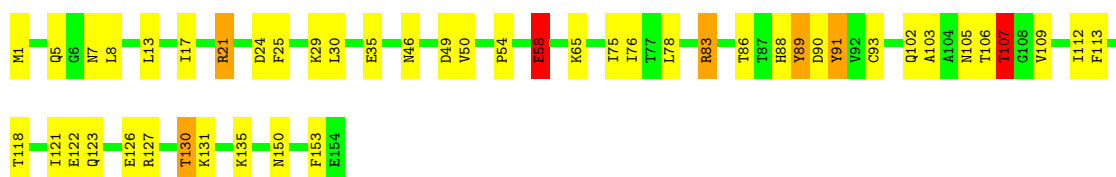
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain U: 70% 25%



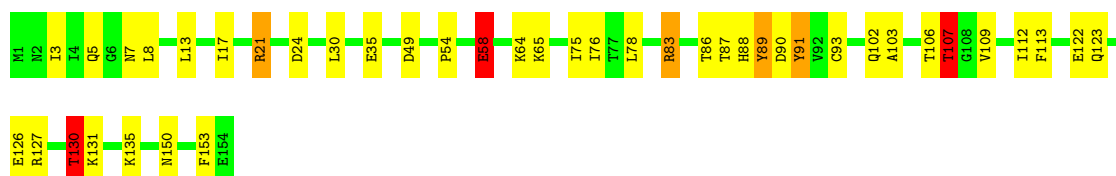
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain V: 69% 26%



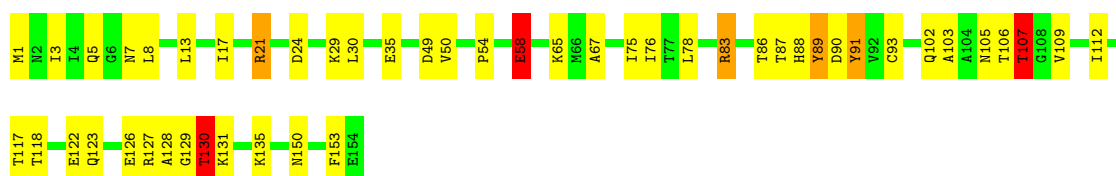
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain W: 73% 23%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain X: 68% 27%

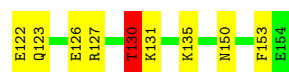


• Molecule 1: RIBOFLAVIN SYNTHASE

Chain Y: 71% 24%

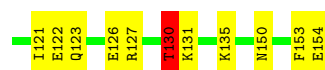
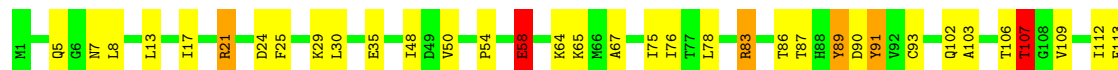






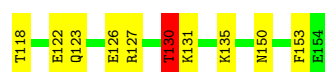
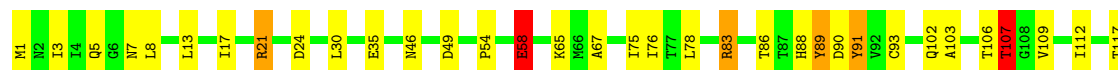
● Molecule 1: RIBOFLAVIN SYNTHASE

Chain Z: 70% 25%



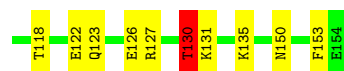
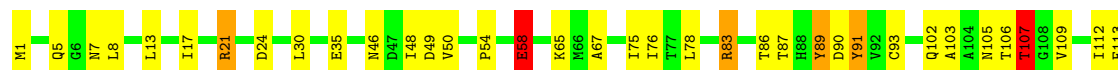
● Molecule 1: RIBOFLAVIN SYNTHASE

Chain 1: 71% 24%



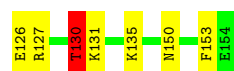
● Molecule 1: RIBOFLAVIN SYNTHASE

Chain 2: 70% 25%



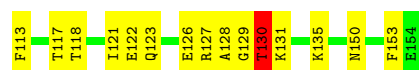
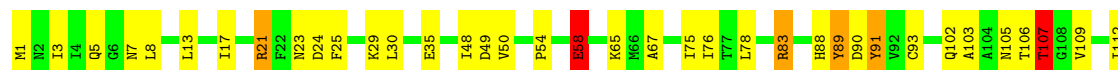
● Molecule 1: RIBOFLAVIN SYNTHASE

Chain 3: 72% 23%



● Molecule 1: RIBOFLAVIN SYNTHASE

Chain 4: 66% 29%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.90Å 192.60Å 168.60Å 90.00° 134.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.237 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: PO4, INI

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	1	0.69	0/1159	1.38	7/1569 (0.4%)
1	2	0.69	0/1159	1.38	7/1569 (0.4%)
1	3	0.69	0/1159	1.38	7/1569 (0.4%)
1	4	0.69	0/1159	1.38	7/1569 (0.4%)
1	A	0.69	0/1159	1.38	7/1569 (0.4%)
1	B	0.69	0/1159	1.38	7/1569 (0.4%)
1	C	0.69	0/1159	1.38	7/1569 (0.4%)
1	D	0.69	0/1159	1.38	7/1569 (0.4%)
1	E	0.69	0/1159	1.38	7/1569 (0.4%)
1	F	0.69	0/1159	1.38	7/1569 (0.4%)
1	G	0.69	0/1159	1.38	7/1569 (0.4%)
1	H	0.69	0/1159	1.38	7/1569 (0.4%)
1	I	0.69	0/1159	1.38	7/1569 (0.4%)
1	J	0.69	0/1159	1.38	7/1569 (0.4%)
1	K	0.69	0/1159	1.38	7/1569 (0.4%)
1	L	0.69	0/1159	1.38	7/1569 (0.4%)
1	M	0.69	0/1159	1.38	7/1569 (0.4%)
1	N	0.69	0/1159	1.38	7/1569 (0.4%)
1	O	0.69	0/1159	1.38	7/1569 (0.4%)
1	P	0.69	0/1159	1.38	7/1569 (0.4%)
1	Q	0.69	0/1159	1.38	7/1569 (0.4%)
1	R	0.69	0/1159	1.38	7/1569 (0.4%)
1	S	0.69	0/1159	1.38	7/1569 (0.4%)
1	T	0.69	0/1159	1.38	7/1569 (0.4%)
1	U	0.69	0/1159	1.38	7/1569 (0.4%)
1	V	0.69	0/1159	1.38	6/1569 (0.4%)
1	W	0.69	0/1159	1.38	7/1569 (0.4%)
1	X	0.69	0/1159	1.38	7/1569 (0.4%)
1	Y	0.69	0/1159	1.38	7/1569 (0.4%)
1	Z	0.69	0/1159	1.38	7/1569 (0.4%)
All	All	0.69	0/34770	1.38	209/47070 (0.4%)

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
1	1	0	2
1	2	0	2
1	3	0	2
1	4	0	2
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
1	Z	0	2
All	All	0	60

There are no bond length outliers.

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	21	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	Q	21	ARG	NE-CZ-NH1	9.31	124.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	21	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	L	21	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	C	21	ARG	NE-CZ-NH1	9.25	124.93	120.30

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	ARG	Sidechain
1	A	91	TYR	Sidechain
1	B	83	ARG	Sidechain
1	B	91	TYR	Sidechain
1	C	83	ARG	Sidechain

## 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	1	1144	0	1157	67	0
1	2	1144	0	1157	75	0
1	3	1144	0	1157	66	0
1	4	1144	0	1157	93	0
1	A	1144	0	1157	64	1
1	B	1144	0	1157	66	0
1	C	1144	0	1157	83	0
1	D	1144	0	1157	82	0
1	E	1144	0	1157	78	0
1	F	1144	0	1157	89	0
1	G	1144	0	1157	86	1
1	H	1144	0	1157	61	0
1	I	1144	0	1157	69	0
1	J	1144	0	1157	80	0
1	K	1144	0	1157	85	0
1	L	1144	0	1157	65	0
1	M	1144	0	1157	70	0
1	N	1144	0	1157	71	1
1	O	1144	0	1157	91	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1144	0	1157	66	0
1	Q	1144	0	1157	74	0
1	R	1144	0	1156	81	0
1	S	1144	0	1155	72	0
1	T	1144	0	1157	79	1
1	U	1144	0	1156	75	0
1	V	1144	0	1156	73	0
1	W	1144	0	1157	67	0
1	X	1144	0	1157	82	0
1	Y	1144	0	1157	87	0
1	Z	1144	0	1157	81	1
2	1	5	0	0	0	0
2	2	5	0	0	0	0
2	3	5	0	0	0	0
2	4	5	0	0	0	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
2	U	5	0	0	0	0
2	V	5	0	0	0	0
2	W	5	0	0	0	0
2	X	5	0	0	0	0
2	Y	5	0	0	0	0
2	Z	5	0	0	0	0
3	1	21	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	21	0	14	1	0
3	3	21	0	14	5	0
3	4	21	0	14	1	0
3	A	21	0	14	3	0
3	B	21	0	14	1	0
3	C	21	0	14	1	0
3	D	21	0	14	1	0
3	E	21	0	14	3	0
3	F	21	0	14	1	0
3	G	21	0	14	3	0
3	H	21	0	14	4	0
3	I	21	0	14	2	0
3	J	21	0	14	1	0
3	K	21	0	14	2	0
3	L	21	0	14	3	0
3	M	21	0	14	1	0
3	N	21	0	14	2	0
3	O	21	0	14	3	0
3	P	21	0	14	1	0
3	Q	21	0	14	1	0
3	R	21	0	14	2	0
3	S	21	0	14	1	0
3	T	21	0	14	3	0
3	U	21	0	14	3	0
3	V	21	0	14	1	0
3	W	21	0	14	5	0
3	X	21	0	14	2	0
3	Y	21	0	14	1	0
3	Z	21	0	14	3	0
4	1	35	0	0	6	2
4	2	35	0	0	6	0
4	3	32	0	0	2	0
4	4	35	0	0	6	1
4	A	38	0	0	6	0
4	B	31	0	0	6	1
4	C	36	0	0	6	0
4	D	35	0	0	6	0
4	E	35	0	0	1	0
4	F	35	0	0	6	0
4	G	38	0	0	6	1
4	H	35	0	0	6	0
4	I	31	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	34	0	0	6	1
4	K	39	0	0	2	0
4	L	35	0	0	6	1
4	M	35	0	0	6	0
4	N	32	0	0	2	0
4	O	36	0	0	6	1
4	P	38	0	0	6	0
4	Q	32	0	0	5	0
4	R	34	0	0	11	0
4	S	32	0	0	5	0
4	T	34	0	0	6	1
4	U	36	0	0	6	0
4	V	39	0	0	6	0
4	W	35	0	0	6	0
4	X	33	0	0	6	0
4	Y	37	0	0	3	0
4	Z	38	0	0	3	1
All	All	36150	0	35125	1447	9

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 21.

The worst 5 of 1447 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:V:5:GLN:HE21	1:W:21:ARG:NH2	1.05	1.47
1:X:5:GLN:HE21	1:Y:21:ARG:NH2	1.09	1.47
1:C:5:GLN:NE2	1:D:21:ARG:HH22	1.13	1.46
1:2:5:GLN:HE21	1:3:21:ARG:NH2	1.06	1.45
1:K:21:ARG:HH22	1:O:5:GLN:NE2	1.15	1.45

The worst 5 of 9 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)
1:O:44:ASP:CA	4:1:930:HOH:O[3_555]	1.02	1.18
4:L:405:HOH:O	4:T:665:HOH:O[3_454]	1.30	0.90
1:A:154:GLU:OE2	4:4:1035:HOH:O[4_556]	1.65	0.55
1:O:44:ASP:N	4:1:930:HOH:O[3_555]	1.70	0.50
1:O:45:THR:CG2	4:Z:928:HOH:O[3_555]	1.80	0.40



## 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	1	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	2	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	3	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	4	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	A	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	B	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	C	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	D	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	25	37
1	E	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	F	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	G	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	H	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	I	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	J	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	K	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	L	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	M	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	N	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	O	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	P	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	Q	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	R	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	S	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	T	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	U	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	X	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	25	37
1	Y	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
1	Z	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
All	All	4560/4620 (99%)	4438 (97%)	92 (2%)	30 (1%)	25	37

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	TYR
1	B	89	TYR
1	C	89	TYR
1	D	89	TYR
1	E	89	TYR

### 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	1	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	2	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	3	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	4	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	A	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	B	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	C	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	D	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	E	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	F	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	G	118/118 (100%)	108 (92%)	10 (8%)	12	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	I	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	J	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	K	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	L	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	M	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	N	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	O	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	P	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	Q	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	R	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	S	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	T	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	U	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	V	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	W	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	X	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	Y	118/118 (100%)	108 (92%)	10 (8%)	12	19
1	Z	118/118 (100%)	108 (92%)	10 (8%)	12	19
All	All	3540/3540 (100%)	3240 (92%)	300 (8%)	12	19

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	90	ASP
1	Q	122	GLU
1	2	122	GLU
1	N	135	LYS
1	P	30	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	102	GLN

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Mol	Chain	Res	Type
1	Q	148	ASN
1	2	148	ASN
1	O	5	GLN
1	P	46	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

60 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$
3	INI	1	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	1	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	2	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	2	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	3	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	3	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	4	200	-	17,21,21	2.89	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	4	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	A	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	A	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	B	200	-	17,21,21	2.89	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	B	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	C	200	-	17,21,21	2.89	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	C	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	D	200	-	17,21,21	2.87	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	D	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	E	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	E	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	F	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	F	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	G	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	G	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	H	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	H	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	I	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	I	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	J	200	-	17,21,21	2.89	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	J	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	K	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	K	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	L	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	L	500	-	4,4,4	0.90	0	6,6,6	0.36	0
3	INI	M	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	M	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	N	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	N	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	O	200	-	17,21,21	2.89	8 (47%)	20,29,29	4.33	12 (60%)
2	PO4	O	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	P	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	P	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	Q	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	Q	500	-	4,4,4	0.88	0	6,6,6	0.35	0
3	INI	R	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.30	12 (60%)
2	PO4	R	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	S	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	S	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	T	200	-	17,21,21	2.87	8 (47%)	20,29,29	4.32	12 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	T	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	U	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	U	500	-	4,4,4	0.90	0	6,6,6	0.36	0
3	INI	V	200	-	17,21,21	2.87	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	V	500	-	4,4,4	0.90	0	6,6,6	0.35	0
3	INI	W	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	W	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	X	200	-	17,21,21	2.89	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	X	500	-	4,4,4	0.88	0	6,6,6	0.35	0
3	INI	Y	200	-	17,21,21	2.87	8 (47%)	20,29,29	4.32	12 (60%)
2	PO4	Y	500	-	4,4,4	0.89	0	6,6,6	0.35	0
3	INI	Z	200	-	17,21,21	2.88	8 (47%)	20,29,29	4.31	12 (60%)
2	PO4	Z	500	-	4,4,4	0.89	0	6,6,6	0.35	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
3	INI	1	200	-	-	0/15/19/19	0/1/1/1
2	PO4	1	500	-	-	0/0/0/0	0/0/0/0
3	INI	2	200	-	-	0/15/19/19	0/1/1/1
2	PO4	2	500	-	-	0/0/0/0	0/0/0/0
3	INI	3	200	-	-	0/15/19/19	0/1/1/1
2	PO4	3	500	-	-	0/0/0/0	0/0/0/0
3	INI	4	200	-	-	0/15/19/19	0/1/1/1
2	PO4	4	500	-	-	0/0/0/0	0/0/0/0
3	INI	A	200	-	-	0/15/19/19	0/1/1/1
2	PO4	A	500	-	-	0/0/0/0	0/0/0/0
3	INI	B	200	-	-	0/15/19/19	0/1/1/1
2	PO4	B	500	-	-	0/0/0/0	0/0/0/0
3	INI	C	200	-	-	0/15/19/19	0/1/1/1
2	PO4	C	500	-	-	0/0/0/0	0/0/0/0
3	INI	D	200	-	-	0/15/19/19	0/1/1/1
2	PO4	D	500	-	-	0/0/0/0	0/0/0/0
3	INI	E	200	-	-	0/15/19/19	0/1/1/1
2	PO4	E	500	-	-	0/0/0/0	0/0/0/0
3	INI	F	200	-	-	0/15/19/19	0/1/1/1
2	PO4	F	500	-	-	0/0/0/0	0/0/0/0
3	INI	G	200	-	-	0/15/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	G	500	-	-	0/0/0/0	0/0/0/0
3	INI	H	200	-	-	0/15/19/19	0/1/1/1
2	PO4	H	500	-	-	0/0/0/0	0/0/0/0
3	INI	I	200	-	-	0/15/19/19	0/1/1/1
2	PO4	I	500	-	-	0/0/0/0	0/0/0/0
3	INI	J	200	-	-	0/15/19/19	0/1/1/1
2	PO4	J	500	-	-	0/0/0/0	0/0/0/0
3	INI	K	200	-	-	0/15/19/19	0/1/1/1
2	PO4	K	500	-	-	0/0/0/0	0/0/0/0
3	INI	L	200	-	-	0/15/19/19	0/1/1/1
2	PO4	L	500	-	-	0/0/0/0	0/0/0/0
3	INI	M	200	-	-	0/15/19/19	0/1/1/1
2	PO4	M	500	-	-	0/0/0/0	0/0/0/0
3	INI	N	200	-	-	0/15/19/19	0/1/1/1
2	PO4	N	500	-	-	0/0/0/0	0/0/0/0
3	INI	O	200	-	-	0/15/19/19	0/1/1/1
2	PO4	O	500	-	-	0/0/0/0	0/0/0/0
3	INI	P	200	-	-	0/15/19/19	0/1/1/1
2	PO4	P	500	-	-	0/0/0/0	0/0/0/0
3	INI	Q	200	-	-	0/15/19/19	0/1/1/1
2	PO4	Q	500	-	-	0/0/0/0	0/0/0/0
3	INI	R	200	-	-	0/15/19/19	0/1/1/1
2	PO4	R	500	-	-	0/0/0/0	0/0/0/0
3	INI	S	200	-	-	0/15/19/19	0/1/1/1
2	PO4	S	500	-	-	0/0/0/0	0/0/0/0
3	INI	T	200	-	-	0/15/19/19	0/1/1/1
2	PO4	T	500	-	-	0/0/0/0	0/0/0/0
3	INI	U	200	-	-	0/15/19/19	0/1/1/1
2	PO4	U	500	-	-	0/0/0/0	0/0/0/0
3	INI	V	200	-	-	0/15/19/19	0/1/1/1
2	PO4	V	500	-	-	0/0/0/0	0/0/0/0
3	INI	W	200	-	-	0/15/19/19	0/1/1/1
2	PO4	W	500	-	-	0/0/0/0	0/0/0/0
3	INI	X	200	-	-	0/15/19/19	0/1/1/1
2	PO4	X	500	-	-	0/0/0/0	0/0/0/0
3	INI	Y	200	-	-	0/15/19/19	0/1/1/1
2	PO4	Y	500	-	-	0/0/0/0	0/0/0/0
3	INI	Z	200	-	-	0/15/19/19	0/1/1/1
2	PO4	Z	500	-	-	0/0/0/0	0/0/0/0

The worst 5 of 240 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	200	INI	C6-N1	2.56	1.38	1.34
3	S	200	INI	C6-N1	2.57	1.38	1.34
3	Z	200	INI	C6-N1	2.57	1.39	1.34
3	F	200	INI	C6-N1	2.58	1.39	1.34
3	P	200	INI	C6-N1	2.58	1.39	1.34

The worst 5 of 360 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	200	INI	O11-C11-C10	-5.83	94.61	109.09
3	S	200	INI	O11-C11-C10	-5.82	94.64	109.09
3	W	200	INI	O11-C11-C10	-5.82	94.64	109.09
3	M	200	INI	O11-C11-C10	-5.82	94.65	109.09
3	3	200	INI	O11-C11-C10	-5.82	94.65	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	200	INI	2	0
3	2	200	INI	1	0
3	3	200	INI	5	0
3	4	200	INI	1	0
3	A	200	INI	3	0
3	B	200	INI	1	0
3	C	200	INI	1	0
3	D	200	INI	1	0
3	E	200	INI	3	0
3	F	200	INI	1	0
3	G	200	INI	3	0
3	H	200	INI	4	0
3	I	200	INI	2	0
3	J	200	INI	1	0
3	K	200	INI	2	0
3	L	200	INI	3	0
3	M	200	INI	1	0
3	N	200	INI	2	0
3	O	200	INI	3	0
3	P	200	INI	1	0
3	Q	200	INI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	200	INI	2	0
3	S	200	INI	1	0
3	T	200	INI	3	0
3	U	200	INI	3	0
3	V	200	INI	1	0
3	W	200	INI	5	0
3	X	200	INI	2	0
3	Y	200	INI	1	0
3	Z	200	INI	3	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.