



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2017 – 02:53 PM EST

PDB ID : 5XTN  
Title : Crystal structure of baculoviral sulfhydryl oxidase P33 (C155A, C158A mutant)  
Authors : Kuang, W.; Hu, Z.; Gong, P.  
Deposited on : unknown  
Resolution : 2.54 Å(reported)

This is a Full wwPDB X-ray 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/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 : rb-20030345  
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) : rb-20030345

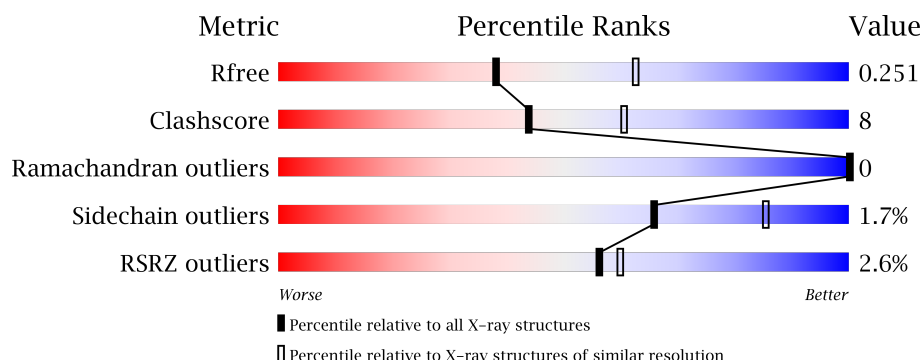
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	293	<div> <div>3%</div> <div>70%12%18%</div> </div>
1	B	293	<div> <div>3%</div> <div>68%14%16%</div> </div>
1	C	293	<div> <div>2%</div> <div>73%13%14%</div> </div>
1	D	293	<div> <div>0%</div> <div>71%15%13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8237 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 FAD-linked sulfhydryl oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1958	1274	314	355	15			
1	B	245	Total	C	N	O	S	0	0	0
			1963	1278	315	356	14			
1	C	253	Total	C	N	O	S	0	0	0
			2021	1312	324	370	15			
1	D	254	Total	C	N	O	S	0	0	0
			2021	1310	326	370	15			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP P41480
A	-32	GLY	-	expression tag	UNP P41480
A	-31	SER	-	expression tag	UNP P41480
A	-30	SER	-	expression tag	UNP P41480
A	-29	HIS	-	expression tag	UNP P41480
A	-28	HIS	-	expression tag	UNP P41480
A	-27	HIS	-	expression tag	UNP P41480
A	-26	HIS	-	expression tag	UNP P41480
A	-25	HIS	-	expression tag	UNP P41480
A	-24	HIS	-	expression tag	UNP P41480
A	-23	SER	-	expression tag	UNP P41480
A	-22	SER	-	expression tag	UNP P41480
A	-21	GLY	-	expression tag	UNP P41480
A	-20	LEU	-	expression tag	UNP P41480
A	-19	VAL	-	expression tag	UNP P41480
A	-18	PRO	-	expression tag	UNP P41480
A	-17	ARG	-	expression tag	UNP P41480
A	-16	GLY	-	expression tag	UNP P41480
A	-15	SER	-	expression tag	UNP P41480
A	-14	HIS	-	expression tag	UNP P41480
A	-13	MET	-	expression tag	UNP P41480

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP P41480
A	-11	SER	-	expression tag	UNP P41480
A	-10	MET	-	expression tag	UNP P41480
A	-9	THR	-	expression tag	UNP P41480
A	-8	GLY	-	expression tag	UNP P41480
A	-7	GLY	-	expression tag	UNP P41480
A	-6	GLN	-	expression tag	UNP P41480
A	-5	GLN	-	expression tag	UNP P41480
A	-4	MET	-	expression tag	UNP P41480
A	-3	GLY	-	expression tag	UNP P41480
A	-2	ARG	-	expression tag	UNP P41480
A	-1	GLY	-	expression tag	UNP P41480
A	0	SER	-	expression tag	UNP P41480
A	155	ALA	CYS	engineered mutation	UNP P41480
A	158	ALA	CYS	engineered mutation	UNP P41480
B	-33	MET	-	initiating methionine	UNP P41480
B	-32	GLY	-	expression tag	UNP P41480
B	-31	SER	-	expression tag	UNP P41480
B	-30	SER	-	expression tag	UNP P41480
B	-29	HIS	-	expression tag	UNP P41480
B	-28	HIS	-	expression tag	UNP P41480
B	-27	HIS	-	expression tag	UNP P41480
B	-26	HIS	-	expression tag	UNP P41480
B	-25	HIS	-	expression tag	UNP P41480
B	-24	HIS	-	expression tag	UNP P41480
B	-23	SER	-	expression tag	UNP P41480
B	-22	SER	-	expression tag	UNP P41480
B	-21	GLY	-	expression tag	UNP P41480
B	-20	LEU	-	expression tag	UNP P41480
B	-19	VAL	-	expression tag	UNP P41480
B	-18	PRO	-	expression tag	UNP P41480
B	-17	ARG	-	expression tag	UNP P41480
B	-16	GLY	-	expression tag	UNP P41480
B	-15	SER	-	expression tag	UNP P41480
B	-14	HIS	-	expression tag	UNP P41480
B	-13	MET	-	expression tag	UNP P41480
B	-12	ALA	-	expression tag	UNP P41480
B	-11	SER	-	expression tag	UNP P41480
B	-10	MET	-	expression tag	UNP P41480
B	-9	THR	-	expression tag	UNP P41480
B	-8	GLY	-	expression tag	UNP P41480
B	-7	GLY	-	expression tag	UNP P41480

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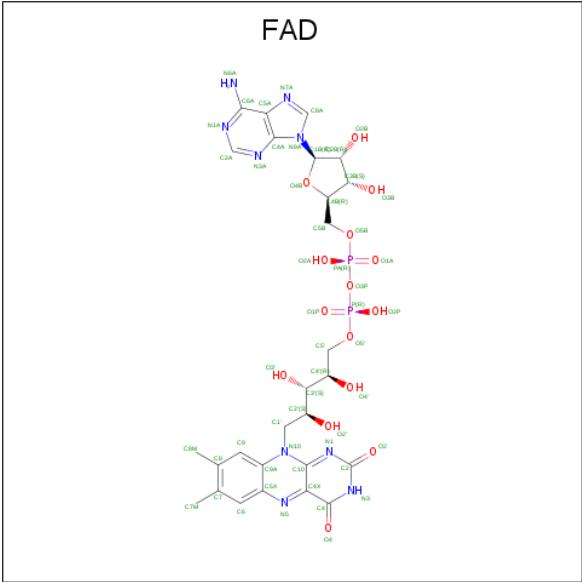
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLN	-	expression tag	UNP P41480
B	-5	GLN	-	expression tag	UNP P41480
B	-4	MET	-	expression tag	UNP P41480
B	-3	GLY	-	expression tag	UNP P41480
B	-2	ARG	-	expression tag	UNP P41480
B	-1	GLY	-	expression tag	UNP P41480
B	0	SER	-	expression tag	UNP P41480
B	155	ALA	CYS	engineered mutation	UNP P41480
B	158	ALA	CYS	engineered mutation	UNP P41480
C	-33	MET	-	initiating methionine	UNP P41480
C	-32	GLY	-	expression tag	UNP P41480
C	-31	SER	-	expression tag	UNP P41480
C	-30	SER	-	expression tag	UNP P41480
C	-29	HIS	-	expression tag	UNP P41480
C	-28	HIS	-	expression tag	UNP P41480
C	-27	HIS	-	expression tag	UNP P41480
C	-26	HIS	-	expression tag	UNP P41480
C	-25	HIS	-	expression tag	UNP P41480
C	-24	HIS	-	expression tag	UNP P41480
C	-23	SER	-	expression tag	UNP P41480
C	-22	SER	-	expression tag	UNP P41480
C	-21	GLY	-	expression tag	UNP P41480
C	-20	LEU	-	expression tag	UNP P41480
C	-19	VAL	-	expression tag	UNP P41480
C	-18	PRO	-	expression tag	UNP P41480
C	-17	ARG	-	expression tag	UNP P41480
C	-16	GLY	-	expression tag	UNP P41480
C	-15	SER	-	expression tag	UNP P41480
C	-14	HIS	-	expression tag	UNP P41480
C	-13	MET	-	expression tag	UNP P41480
C	-12	ALA	-	expression tag	UNP P41480
C	-11	SER	-	expression tag	UNP P41480
C	-10	MET	-	expression tag	UNP P41480
C	-9	THR	-	expression tag	UNP P41480
C	-8	GLY	-	expression tag	UNP P41480
C	-7	GLY	-	expression tag	UNP P41480
C	-6	GLN	-	expression tag	UNP P41480
C	-5	GLN	-	expression tag	UNP P41480
C	-4	MET	-	expression tag	UNP P41480
C	-3	GLY	-	expression tag	UNP P41480
C	-2	ARG	-	expression tag	UNP P41480
C	-1	GLY	-	expression tag	UNP P41480

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P41480
C	155	ALA	CYS	engineered mutation	UNP P41480
C	158	ALA	CYS	engineered mutation	UNP P41480
D	-33	MET	-	initiating methionine	UNP P41480
D	-32	GLY	-	expression tag	UNP P41480
D	-31	SER	-	expression tag	UNP P41480
D	-30	SER	-	expression tag	UNP P41480
D	-29	HIS	-	expression tag	UNP P41480
D	-28	HIS	-	expression tag	UNP P41480
D	-27	HIS	-	expression tag	UNP P41480
D	-26	HIS	-	expression tag	UNP P41480
D	-25	HIS	-	expression tag	UNP P41480
D	-24	HIS	-	expression tag	UNP P41480
D	-23	SER	-	expression tag	UNP P41480
D	-22	SER	-	expression tag	UNP P41480
D	-21	GLY	-	expression tag	UNP P41480
D	-20	LEU	-	expression tag	UNP P41480
D	-19	VAL	-	expression tag	UNP P41480
D	-18	PRO	-	expression tag	UNP P41480
D	-17	ARG	-	expression tag	UNP P41480
D	-16	GLY	-	expression tag	UNP P41480
D	-15	SER	-	expression tag	UNP P41480
D	-14	HIS	-	expression tag	UNP P41480
D	-13	MET	-	expression tag	UNP P41480
D	-12	ALA	-	expression tag	UNP P41480
D	-11	SER	-	expression tag	UNP P41480
D	-10	MET	-	expression tag	UNP P41480
D	-9	THR	-	expression tag	UNP P41480
D	-8	GLY	-	expression tag	UNP P41480
D	-7	GLY	-	expression tag	UNP P41480
D	-6	GLN	-	expression tag	UNP P41480
D	-5	GLN	-	expression tag	UNP P41480
D	-4	MET	-	expression tag	UNP P41480
D	-3	GLY	-	expression tag	UNP P41480
D	-2	ARG	-	expression tag	UNP P41480
D	-1	GLY	-	expression tag	UNP P41480
D	0	SER	-	expression tag	UNP P41480
D	155	ALA	CYS	engineered mutation	UNP P41480
D	158	ALA	CYS	engineered mutation	UNP P41480

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

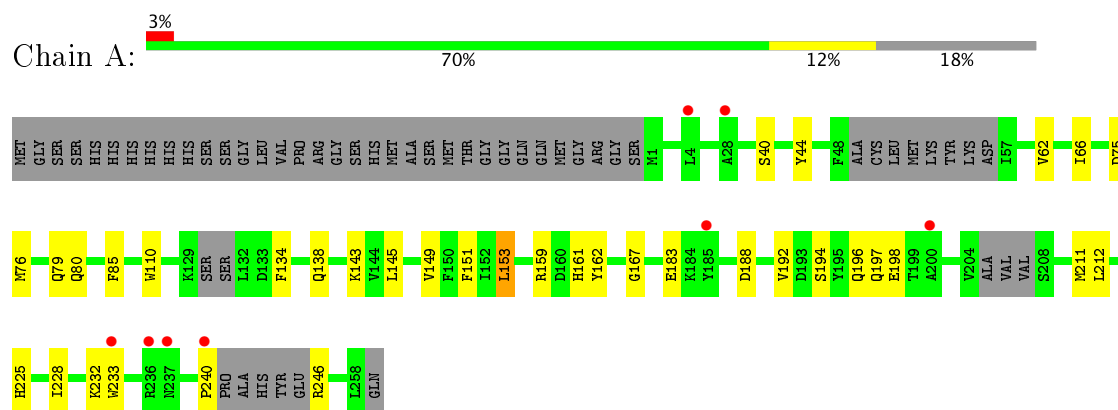
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	14	Total	O	0	0
			14	14		
3	C	18	Total	O	0	0
			18	18		
3	D	21	Total	O	0	0
			21	21		

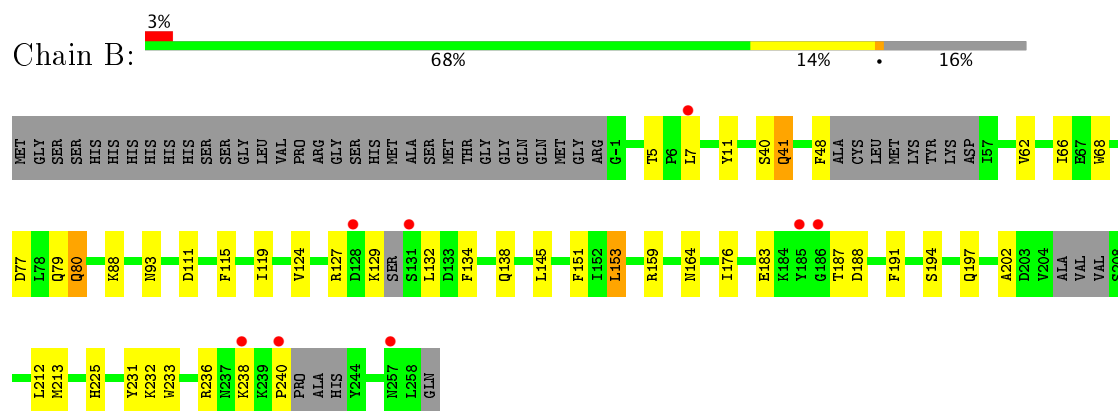
### 3 Residue-property plots

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.

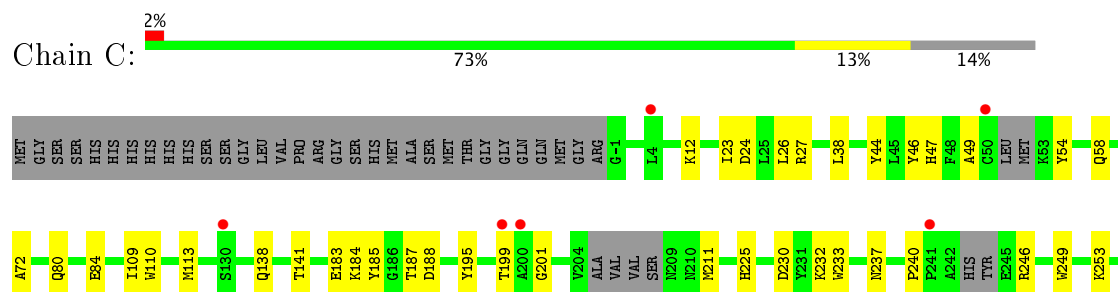
- Molecule 1: FAD-linked sulfhydryl oxidase



- Molecule 1: FAD-linked sulfhydryl oxidase



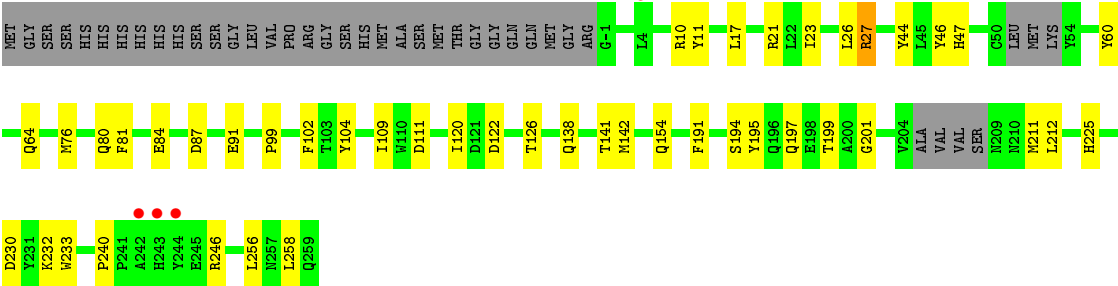
- Molecule 1: FAD-linked sulfhydryl oxidase





L258  
Q259

● Molecule 1: FAD-linked sulfhydryl oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.66Å 153.50Å 75.55Å 90.00° 110.29° 90.00°	Depositor
Resolution (Å)	37.60 – 2.54 43.80 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.4 (37.60-2.54) 98.7 (43.80-2.54)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.216 , 0.254 0.209 , 0.251	Depositor DCC
$R_{free}$ test set	1904 reflections (4.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.1548e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/2003	0.55	0/2711
1	B	0.42	0/2008	0.54	0/2721
1	C	0.46	0/2067	0.58	0/2802
1	D	0.47	0/2068	0.57	0/2806
All	All	0.45	0/8146	0.56	0/11040

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1958	0	1878	29	0
1	B	1963	0	1853	30	0
1	C	2021	0	1910	29	0
1	D	2021	0	1898	37	0
2	A	53	0	30	2	0
2	B	53	0	30	1	0
2	C	53	0	30	4	0
2	D	53	0	30	5	0
3	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	0	0	0
3	C	18	0	0	1	0
3	D	21	0	0	1	0
All	All	8237	0	7659	120	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 8.

All (120) 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:151:PHE:H	1:A:159:ARG:NH1	1.69	0.90
1:A:151:PHE:H	1:A:159:ARG:HH11	1.22	0.85
1:C:47:HIS:NE2	1:C:138:GLN:OE1	2.14	0.80
1:C:23:ILE:HD11	1:C:46:TYR:HE2	1.45	0.79
1:D:256:LEU:CB	1:D:258:LEU:HD13	2.13	0.78
1:D:230:ASP:OD2	1:D:246:ARG:NH2	2.16	0.77
1:C:27:ARG:HG3	1:C:72:ALA:HB3	1.68	0.75
1:C:230:ASP:OD2	1:C:246:ARG:NH2	2.21	0.73
1:D:23:ILE:HD11	1:D:46:TYR:HE2	1.52	0.73
1:C:80:GLN:NE2	3:C:401:HOH:O	2.21	0.72
1:A:232:LYS:NZ	2:A:301:FAD:O4'	2.23	0.71
1:B:5:THR:HG22	1:B:7:LEU:H	1.56	0.70
1:D:27:ARG:HH11	1:D:76:MET:HG3	1.56	0.70
1:D:256:LEU:HB2	1:D:258:LEU:HD13	1.73	0.69
1:D:120:ILE:HD11	1:D:142:MET:HG2	1.75	0.68
1:B:5:THR:HG22	1:B:7:LEU:N	2.09	0.68
1:A:183:GLU:HG3	1:A:188:ASP:HA	1.75	0.68
1:D:233:TRP:CD1	1:D:240:PRO:HB3	2.30	0.67
1:C:24:ASP:OD2	1:C:27:ARG:NH2	2.28	0.67
1:D:27:ARG:NH1	1:D:76:MET:HG3	2.10	0.65
1:C:199:THR:HG21	1:D:195:TYR:HD2	1.60	0.65
1:B:225:HIS:NE2	2:B:301:FAD:O2A	2.21	0.64
1:D:102:PHE:O	3:D:401:HOH:O	2.15	0.64
1:A:246:ARG:NH1	1:B:202:ALA:O	2.31	0.63
1:B:151:PHE:H	1:B:159:ARG:HH22	1.45	0.63
1:D:256:LEU:HB3	1:D:258:LEU:CD1	2.28	0.63
1:C:253:LYS:HG2	1:C:258:LEU:HD11	1.81	0.62
1:D:47:HIS:NE2	1:D:138:GLN:OE1	2.29	0.62
1:A:225:HIS:NE2	2:A:301:FAD:O2A	2.25	0.62
1:D:201:GLY:HA3	1:D:211:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:LYS:HD3	1:C:185:TYR:CE2	2.35	0.62
1:D:256:LEU:HB3	1:D:258:LEU:HD13	1.81	0.61
1:C:23:ILE:HD11	1:C:46:TYR:CE2	2.32	0.61
1:A:233:TRP:CD1	1:A:240:PRO:HB3	2.36	0.60
1:B:183:GLU:HG3	1:B:188:ASP:HA	1.83	0.59
1:D:17:LEU:HD22	1:D:104:TYR:CD2	2.38	0.58
1:A:79:GLN:HG3	1:D:154:GLN:HE21	1.67	0.58
1:A:151:PHE:O	1:A:153:LEU:CD2	2.51	0.58
1:B:115:PHE:CE2	1:B:119:ILE:HD11	2.40	0.57
1:D:80:GLN:O	1:D:84:GLU:HG3	2.04	0.57
1:B:124:VAL:O	1:B:127:ARG:HD3	2.06	0.55
1:A:194:SER:H	1:A:197:GLN:HE21	1.53	0.55
1:D:17:LEU:CD2	1:D:104:TYR:HD2	2.20	0.55
1:C:249:TRP:CE2	1:C:253:LYS:HD2	2.43	0.54
1:D:17:LEU:HD22	1:D:104:TYR:HD2	1.72	0.54
1:B:151:PHE:H	1:B:159:ARG:NH2	2.06	0.54
1:B:194:SER:OG	1:B:197:GLN:HG3	2.07	0.54
1:C:253:LYS:HG2	1:C:258:LEU:CD1	2.37	0.53
1:D:11:TYR:HA	1:D:111:ASP:HB3	1.90	0.53
1:C:232:LYS:NZ	2:C:301:FAD:O4'	2.42	0.53
1:B:129:LYS:HA	1:B:132:LEU:HG	1.91	0.52
1:B:77:ASP:OD1	1:B:79:GLN:HB2	2.10	0.52
1:C:44:TYR:CG	1:C:141:THR:HG23	2.44	0.52
1:A:151:PHE:O	1:A:153:LEU:HD22	2.10	0.51
1:A:196:GLN:OE1	1:A:196:GLN:N	2.44	0.51
1:D:23:ILE:CD1	1:D:46:TYR:HE2	2.22	0.51
1:C:12:LYS:NZ	1:C:49:ALA:O	2.36	0.51
1:B:134:PHE:O	1:B:138:GLN:HG2	2.12	0.50
1:C:233:TRP:CD1	1:C:240:PRO:HB3	2.46	0.49
1:C:201:GLY:HA3	1:C:211:MET:CE	2.42	0.49
1:D:27:ARG:HD3	1:D:81:PHE:CD1	2.46	0.49
1:D:232:LYS:NZ	2:D:301:FAD:O4'	2.43	0.49
1:C:183:GLU:HA	1:C:187:THR:O	2.13	0.49
1:C:80:GLN:O	1:C:84:GLU:HG3	2.13	0.48
1:A:194:SER:H	1:A:197:GLN:NE2	2.11	0.48
1:B:233:TRP:CD1	1:B:240:PRO:HG3	2.49	0.48
1:B:11:TYR:HA	1:B:111:ASP:HB3	1.95	0.48
1:B:212:LEU:HD23	1:B:213:MET:N	2.29	0.48
1:A:62:VAL:O	1:A:66:ILE:HG12	2.14	0.47
1:A:76:MET:HB3	1:A:80:GLN:HB3	1.96	0.47
1:B:62:VAL:O	1:B:66:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:TYR:HD2	1:D:199:THR:HG21	1.79	0.47
1:D:194:SER:OG	1:D:197:GLN:HG3	2.15	0.47
1:B:77:ASP:HB3	1:B:80:GLN:NE2	2.30	0.47
1:D:122:ASP:O	1:D:126:THR:HB	2.15	0.47
2:D:301:FAD:H8A	2:D:301:FAD:H2B	1.82	0.47
1:A:151:PHE:O	1:A:153:LEU:HD23	2.14	0.46
1:D:21:ARG:HG3	1:D:104:TYR:CD2	2.51	0.46
1:A:192:VAL:HG11	1:A:211:MET:CE	2.46	0.46
1:D:44:TYR:CG	1:D:141:THR:HG23	2.51	0.46
1:B:77:ASP:HB3	1:B:80:GLN:HE21	1.81	0.45
1:C:237:ASN:ND2	1:C:237:ASN:O	2.49	0.45
1:A:44:TYR:HB2	1:A:145:LEU:HD21	1.99	0.45
1:B:151:PHE:HD1	1:B:159:ARG:NH2	2.14	0.45
1:A:192:VAL:HG11	1:A:211:MET:HE3	1.98	0.45
1:C:54:TYR:HA	1:C:58:GLN:OE1	2.16	0.45
2:C:301:FAD:H2B	2:C:301:FAD:H8A	1.84	0.45
1:D:109:ILE:CG2	2:D:301:FAD:HM83	2.47	0.45
1:A:110:TRP:HA	1:A:110:TRP:CE3	2.52	0.44
1:C:184:LYS:HD3	1:C:185:TYR:CD2	2.53	0.44
1:A:134:PHE:O	1:A:138:GLN:HG2	2.18	0.43
1:D:191:PHE:HA	1:D:212:LEU:O	2.18	0.43
1:B:48:PHE:HB3	1:B:119:ILE:HD13	1.99	0.43
1:A:194:SER:OG	1:A:197:GLN:HG3	2.19	0.43
1:D:87:ASP:O	1:D:91:GLU:HG3	2.19	0.43
1:A:143:LYS:NZ	1:B:231:TYR:OH	2.50	0.43
1:A:161:HIS:CE1	1:A:228:ILE:HD12	2.55	0.42
1:A:79:GLN:HG3	1:D:154:GLN:NE2	2.33	0.42
1:C:201:GLY:HA3	1:C:211:MET:HE2	2.01	0.42
1:C:113:MET:SD	2:C:301:FAD:HM71	2.59	0.42
1:B:183:GLU:HA	1:B:187:THR:O	2.19	0.42
1:C:26:LEU:HD13	1:C:38:LEU:HB2	2.00	0.42
1:D:60:TYR:O	1:D:64:GLN:HG2	2.18	0.42
1:A:167:GLY:HA2	1:B:164:ASN:O	2.19	0.42
1:C:110:TRP:CH2	1:C:225:HIS:HA	2.55	0.42
1:A:149:VAL:HG22	1:A:162:TYR:CE2	2.55	0.42
1:D:201:GLY:HA3	1:D:211:MET:CE	2.47	0.42
1:D:23:ILE:HD11	1:D:46:TYR:CE2	2.42	0.42
1:A:198:GLU:OE1	1:A:212:LEU:HD23	2.19	0.41
1:B:151:PHE:HB3	1:B:153:LEU:HD23	2.01	0.41
1:B:191:PHE:HA	1:B:212:LEU:O	2.20	0.41
1:B:176:ILE:HG12	1:B:212:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLN:OE1	1:B:145:LEU:HA	2.20	0.41
1:D:99:PRO:HG2	1:D:102:PHE:CZ	2.56	0.41
1:B:119:ILE:HG21	1:B:119:ILE:HD13	1.87	0.41
1:C:183:GLU:HG3	1:C:188:ASP:HA	2.03	0.41
1:D:225:HIS:HB3	2:D:301:FAD:N6A	2.36	0.41
1:C:109:ILE:CG2	2:C:301:FAD:HM83	2.51	0.40
1:A:75:ASP:HB3	2:D:301:FAD:H5'2	2.02	0.40
1:B:68:TRP:HB2	1:B:88:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/293 (78%)	225 (98%)	5 (2%)	0	100	100
1	B	235/293 (80%)	226 (96%)	9 (4%)	0	100	100
1	C	245/293 (84%)	237 (97%)	8 (3%)	0	100	100
1	D	248/293 (85%)	240 (97%)	8 (3%)	0	100	100
All	All	958/1172 (82%)	928 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/267 (78%)	205 (99%)	3 (1%)	71	88
1	B	202/267 (76%)	194 (96%)	8 (4%)	36	59
1	C	208/267 (78%)	208 (100%)	0	100	100
1	D	206/267 (77%)	203 (98%)	3 (2%)	70	87
All	All	824/1068 (77%)	810 (98%)	14 (2%)	66	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	85	PHE
1	A	153	LEU
1	B	40	SER
1	B	41	GLN
1	B	80	GLN
1	B	93	ASN
1	B	153	LEU
1	B	232	LYS
1	B	236	ARG
1	B	238	LYS
1	D	10	ARG
1	D	26	LEU
1	D	27	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	197	GLN
1	B	63	GLN
1	B	71	ASN
1	B	80	GLN
1	B	93	ASN
1	B	237	ASN
1	C	80	GLN
1	C	237	ASN
1	C	257	ASN
1	D	154	GLN



### 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 ⓘ

4 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	$\# Z  > 2$
2	FAD	A	301	-	51,58,58	4.49	21 (41%)	54,89,89	2.52	14 (25%)
2	FAD	B	301	-	51,58,58	4.57	21 (41%)	54,89,89	2.81	16 (29%)
2	FAD	C	301	-	51,58,58	4.49	22 (43%)	54,89,89	2.58	12 (22%)
2	FAD	D	301	-	51,58,58	4.39	22 (43%)	54,89,89	2.46	14 (25%)

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	FAD	A	301	-	-	0/28/50/50	0/6/6/6
2	FAD	B	301	-	-	0/28/50/50	0/6/6/6
2	FAD	C	301	-	-	0/28/50/50	0/6/6/6
2	FAD	D	301	-	-	0/28/50/50	0/6/6/6

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	FAD	C2B-C1B	-14.82	1.30	1.53
2	D	301	FAD	C2B-C1B	-14.53	1.30	1.53
2	A	301	FAD	C2B-C1B	-14.15	1.31	1.53
2	B	301	FAD	C2B-C1B	-13.85	1.31	1.53
2	B	301	FAD	O4B-C4B	-5.83	1.31	1.45
2	C	301	FAD	O4B-C4B	-5.67	1.32	1.45
2	A	301	FAD	O4B-C4B	-5.58	1.32	1.45
2	D	301	FAD	O4B-C4B	-5.38	1.32	1.45
2	A	301	FAD	O3B-C3B	-3.50	1.34	1.43
2	D	301	FAD	O3B-C3B	-3.29	1.35	1.43
2	C	301	FAD	O3B-C3B	-3.26	1.35	1.43
2	D	301	FAD	C5A-C4A	-3.23	1.33	1.40
2	B	301	FAD	C5A-C4A	-3.22	1.33	1.40
2	A	301	FAD	C5A-C4A	-3.11	1.33	1.40
2	B	301	FAD	O3B-C3B	-3.00	1.36	1.43
2	C	301	FAD	C5A-C4A	-2.93	1.33	1.40
2	D	301	FAD	O2'-C2'	-2.87	1.37	1.43
2	C	301	FAD	O2'-C2'	-2.76	1.37	1.43
2	B	301	FAD	O2'-C2'	-2.64	1.37	1.43
2	A	301	FAD	O2'-C2'	-2.61	1.37	1.43
2	A	301	FAD	O4-C4	-2.44	1.18	1.24
2	C	301	FAD	O4-C4	-2.42	1.18	1.24
2	D	301	FAD	O4-C4	-2.37	1.18	1.24
2	B	301	FAD	O4'-C4'	-2.18	1.38	1.43
2	D	301	FAD	O4'-C4'	-2.09	1.38	1.43
2	B	301	FAD	O4-C4	-2.04	1.19	1.24
2	B	301	FAD	P-O5'	2.03	1.67	1.59
2	C	301	FAD	P-O5'	2.04	1.67	1.59
2	C	301	FAD	PA-O5B	2.04	1.67	1.59
2	C	301	FAD	C5'-C4'	2.12	1.54	1.51
2	A	301	FAD	C4X-C10	2.20	1.44	1.41
2	B	301	FAD	C4X-C10	2.20	1.44	1.41
2	D	301	FAD	PA-O5B	2.23	1.68	1.59
2	D	301	FAD	C5'-C4'	2.30	1.55	1.51
2	A	301	FAD	P-O5'	2.31	1.69	1.59
2	D	301	FAD	C2A-N3A	2.36	1.36	1.32
2	C	301	FAD	C8M-C8	2.51	1.56	1.51
2	C	301	FAD	C2A-N3A	2.53	1.36	1.32
2	A	301	FAD	C2A-N3A	2.55	1.36	1.32
2	D	301	FAD	O2B-C2B	2.57	1.48	1.43
2	A	301	FAD	O2B-C2B	2.60	1.48	1.43
2	D	301	FAD	C8M-C8	2.65	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FAD	C8M-C8	2.71	1.56	1.51
2	B	301	FAD	O2B-C2B	2.80	1.49	1.43
2	C	301	FAD	O2B-C2B	3.03	1.49	1.43
2	B	301	FAD	C8M-C8	3.25	1.57	1.51
2	C	301	FAD	C6A-N6A	3.50	1.48	1.34
2	D	301	FAD	C6A-N6A	3.57	1.48	1.34
2	A	301	FAD	C6A-N6A	3.67	1.49	1.34
2	B	301	FAD	C6A-N6A	3.73	1.49	1.34
2	D	301	FAD	C2-N1	4.76	1.47	1.38
2	C	301	FAD	C2-N1	5.22	1.48	1.38
2	D	301	FAD	C2-N3	5.29	1.48	1.38
2	A	301	FAD	C2-N3	5.41	1.48	1.38
2	A	301	FAD	C2-N1	5.54	1.49	1.38
2	C	301	FAD	C2-N3	5.55	1.49	1.38
2	D	301	FAD	C4-C4X	5.61	1.52	1.41
2	B	301	FAD	C2-N1	5.73	1.49	1.38
2	B	301	FAD	C2-N3	5.80	1.49	1.38
2	A	301	FAD	C4-C4X	6.00	1.52	1.41
2	B	301	FAD	C4-C4X	6.26	1.53	1.41
2	C	301	FAD	C4-C4X	6.54	1.53	1.41
2	D	301	FAD	C4-N3	7.40	1.46	1.33
2	C	301	FAD	C4-N3	7.54	1.46	1.33
2	A	301	FAD	C4-N3	7.68	1.46	1.33
2	B	301	FAD	C4-N3	8.14	1.47	1.33
2	D	301	FAD	C9A-N10	8.69	1.50	1.38
2	A	301	FAD	C9A-N10	8.74	1.50	1.38
2	C	301	FAD	C9A-N10	8.77	1.50	1.38
2	B	301	FAD	C9A-N10	9.13	1.50	1.38
2	D	301	FAD	C5X-N5	9.16	1.49	1.35
2	C	301	FAD	C5X-N5	9.32	1.49	1.35
2	D	301	FAD	C4X-N5	9.48	1.47	1.33
2	D	301	FAD	C10-N1	9.49	1.46	1.33
2	A	301	FAD	C4X-N5	9.58	1.47	1.33
2	C	301	FAD	C10-N1	9.73	1.46	1.33
2	C	301	FAD	C4X-N5	9.87	1.47	1.33
2	B	301	FAD	C4X-N5	9.96	1.47	1.33
2	A	301	FAD	C5X-N5	10.21	1.51	1.35
2	B	301	FAD	C5X-N5	10.25	1.51	1.35
2	A	301	FAD	C10-N1	10.50	1.48	1.33
2	B	301	FAD	C10-N1	10.82	1.48	1.33
2	B	301	FAD	O4B-C1B	12.22	1.58	1.41
2	A	301	FAD	O4B-C1B	12.27	1.58	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	FAD	O4B-C1B	12.39	1.58	1.41
2	C	301	FAD	O4B-C1B	12.53	1.58	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FAD	N3A-C2A-N1A	-12.46	118.01	128.86
2	A	301	FAD	N3A-C2A-N1A	-11.21	119.09	128.86
2	C	301	FAD	N3A-C2A-N1A	-11.04	119.25	128.86
2	D	301	FAD	N3A-C2A-N1A	-10.37	119.83	128.86
2	B	301	FAD	C4X-C10-N10	-7.28	115.46	120.52
2	A	301	FAD	C4X-C10-N10	-5.58	116.64	120.52
2	D	301	FAD	C4B-O4B-C1B	-5.44	103.98	109.77
2	C	301	FAD	C4X-C10-N10	-4.95	117.08	120.52
2	C	301	FAD	N6A-C6A-N1A	-4.92	109.01	118.77
2	B	301	FAD	N6A-C6A-N1A	-4.88	109.09	118.77
2	A	301	FAD	N6A-C6A-N1A	-4.86	109.14	118.77
2	A	301	FAD	C4B-O4B-C1B	-4.57	104.90	109.77
2	D	301	FAD	N6A-C6A-N1A	-4.53	109.79	118.77
2	D	301	FAD	C4X-C10-N10	-4.51	117.39	120.52
2	C	301	FAD	C4B-O4B-C1B	-4.45	105.03	109.77
2	D	301	FAD	C4-C4X-C10	-3.74	116.94	119.96
2	B	301	FAD	C4'-C3'-C2'	-3.71	105.42	113.41
2	C	301	FAD	C4-C4X-C10	-3.50	117.13	119.96
2	D	301	FAD	O2B-C2B-C3B	-3.37	101.04	111.83
2	C	301	FAD	C7M-C7-C6	-3.35	111.94	120.34
2	B	301	FAD	C4B-O4B-C1B	-3.35	106.21	109.77
2	B	301	FAD	C4-C4X-C10	-3.05	117.49	119.96
2	A	301	FAD	C7M-C7-C6	-3.00	112.82	120.34
2	A	301	FAD	C4-C4X-C10	-2.99	117.54	119.96
2	B	301	FAD	O2B-C2B-C3B	-2.92	102.46	111.83
2	B	301	FAD	C7M-C7-C6	-2.92	113.03	120.34
2	D	301	FAD	C7M-C7-C6	-2.70	113.56	120.34
2	A	301	FAD	C4'-C3'-C2'	-2.48	108.07	113.41
2	B	301	FAD	C9A-C5X-N5	-2.40	118.67	122.24
2	D	301	FAD	C1'-N10-C10	-2.13	116.32	118.50
2	C	301	FAD	C9A-C5X-N5	-2.13	119.07	122.24
2	A	301	FAD	O3B-C3B-C4B	-2.02	105.19	111.09
2	A	301	FAD	O4B-C4B-C3B	2.01	109.16	105.17
2	A	301	FAD	C4-C4X-N5	2.13	121.01	118.68
2	B	301	FAD	O3'-C3'-C2'	2.25	114.39	108.82
2	B	301	FAD	C4-C4X-N5	2.35	121.25	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FAD	C6-C5X-N5	2.37	121.75	118.97
2	D	301	FAD	C4-C4X-N5	2.44	121.35	118.68
2	D	301	FAD	C4X-N5-C5X	2.49	119.40	116.76
2	D	301	FAD	C1'-N10-C9A	2.55	120.68	118.35
2	A	301	FAD	C4X-N5-C5X	3.25	120.20	116.76
2	A	301	FAD	C7M-C7-C8	3.31	127.67	120.72
2	B	301	FAD	C7M-C7-C8	3.35	127.75	120.72
2	C	301	FAD	C4-C4X-N5	3.51	122.53	118.68
2	D	301	FAD	C7M-C7-C8	3.66	128.39	120.72
2	B	301	FAD	C4X-N5-C5X	4.18	121.18	116.76
2	C	301	FAD	C4X-N5-C5X	4.22	121.22	116.76
2	D	301	FAD	C5A-C6A-N6A	4.24	129.11	120.47
2	C	301	FAD	C7M-C7-C8	4.64	130.45	120.72
2	A	301	FAD	C5A-C6A-N6A	4.80	130.26	120.47
2	C	301	FAD	C4-N3-C2	4.84	119.39	115.16
2	C	301	FAD	C5A-C6A-N6A	4.91	130.47	120.47
2	A	301	FAD	C4-N3-C2	4.93	119.47	115.16
2	B	301	FAD	C5A-C6A-N6A	5.03	130.73	120.47
2	D	301	FAD	C4-N3-C2	5.34	119.83	115.16
2	B	301	FAD	C4-N3-C2	5.49	119.96	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FAD	2	0
2	B	301	FAD	1	0
2	C	301	FAD	4	0
2	D	301	FAD	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	240/293 (81%)	0.24	8 (3%) 47 51	26, 38, 60, 74	0
1	B	245/293 (83%)	0.15	8 (3%) 47 51	25, 38, 66, 78	0
1	C	253/293 (86%)	0.11	6 (2%) 59 62	20, 36, 59, 69	0
1	D	254/293 (86%)	0.07	4 (1%) 72 74	21, 37, 60, 74	0
All	All	992/1172 (84%)	0.14	26 (2%) 56 60	20, 37, 60, 78	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	TYR	4.2
1	B	131	SER	3.8
1	C	130	SER	3.7
1	B	128	ASP	3.5
1	D	242	ALA	3.5
1	B	185	TYR	3.4
1	A	240	PRO	3.3
1	D	243	HIS	3.1
1	A	200	ALA	3.0
1	B	240	PRO	2.9
1	C	199	THR	2.9
1	A	237	ASN	2.8
1	B	238	LYS	2.7
1	C	4	LEU	2.7
1	B	257	ASN	2.7
1	A	236	ARG	2.6
1	A	233	TRP	2.4
1	C	200	ALA	2.3
1	A	185	TYR	2.3
1	D	4	LEU	2.2
1	B	186	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	241	PRO	2.2
1	B	7	LEU	2.2
1	C	50	CYS	2.1
1	A	28	ALA	2.1
1	A	4	LEU	2.0

## 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
2	FAD	C	301	53/53	0.95	0.15	0.27	24,32,38,47	0
2	FAD	D	301	53/53	0.94	0.15	0.01	26,32,40,43	0
2	FAD	B	301	53/53	0.94	0.16	-0.20	28,37,48,56	0
2	FAD	A	301	53/53	0.95	0.15	-0.45	26,38,52,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.