



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:43 am BST

PDB ID : 5YS9  
Title : Crystal structure of acyl-coA oxidase3 from Yarrowia lipolytica  
Authors : Kim, S.; Kim, K.-J.  
Deposited on : 2017-11-13  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

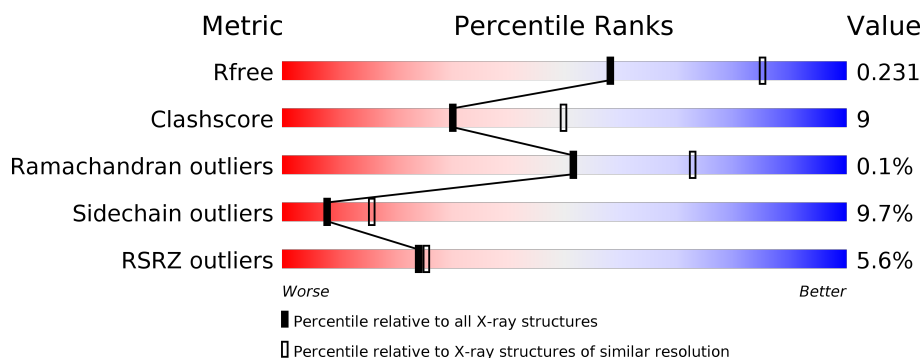
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 respectively. 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	708	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	708	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11129 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.

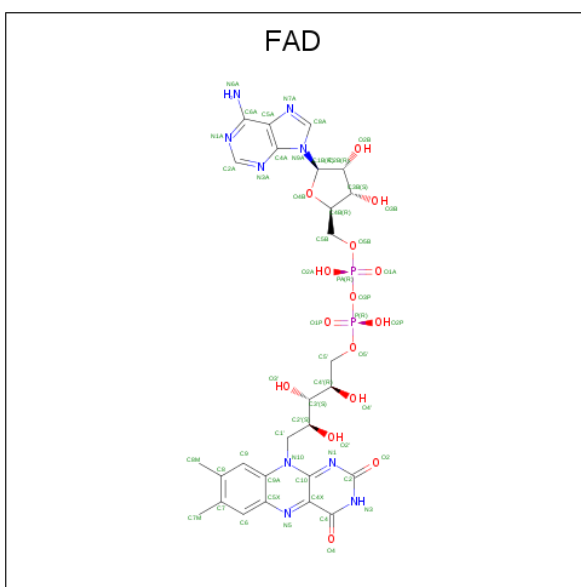
- Molecule 1 is a protein called Acyl-coenzyme A oxidase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	692	Total	C	N	O	S	0	0	0
			5430	3440	942	1021	27			
1	B	691	Total	C	N	O	S	0	0	0
			5425	3437	941	1020	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	701	LEU	-	expression tag	UNP O74936
A	702	GLU	-	expression tag	UNP O74936
A	703	HIS	-	expression tag	UNP O74936
A	704	HIS	-	expression tag	UNP O74936
A	705	HIS	-	expression tag	UNP O74936
A	706	HIS	-	expression tag	UNP O74936
A	707	HIS	-	expression tag	UNP O74936
A	708	HIS	-	expression tag	UNP O74936
B	701	LEU	-	expression tag	UNP O74936
B	702	GLU	-	expression tag	UNP O74936
B	703	HIS	-	expression tag	UNP O74936
B	704	HIS	-	expression tag	UNP O74936
B	705	HIS	-	expression tag	UNP O74936
B	706	HIS	-	expression tag	UNP O74936
B	707	HIS	-	expression tag	UNP O74936
B	708	HIS	-	expression tag	UNP O74936

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

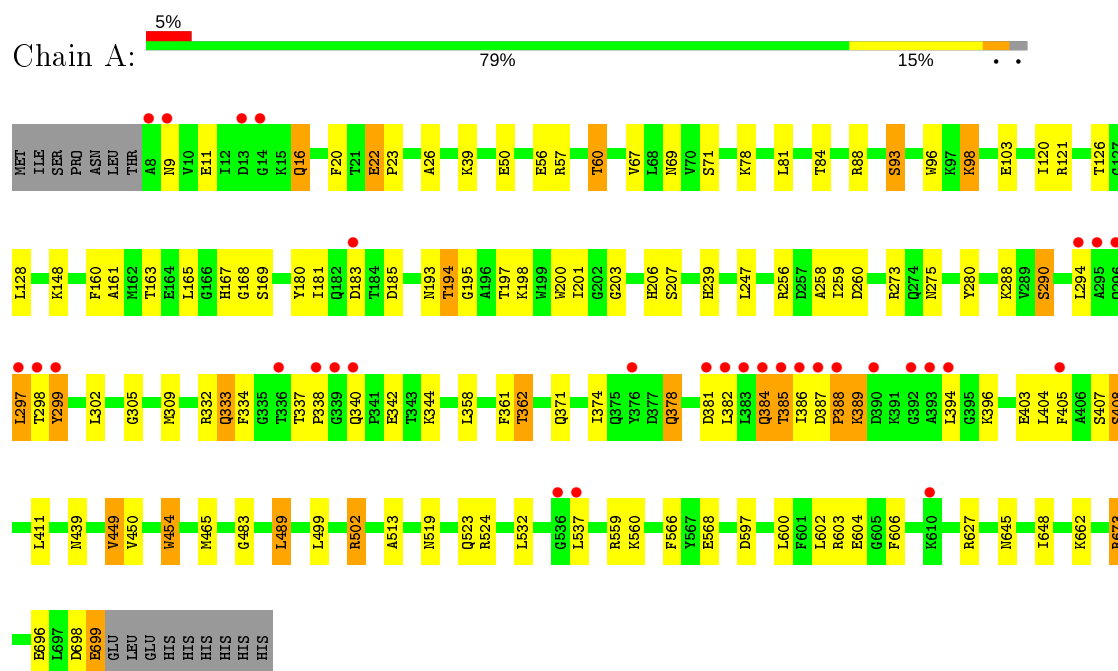
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total O 77 77	0	0
3	B	91	Total O 91 91	0	0

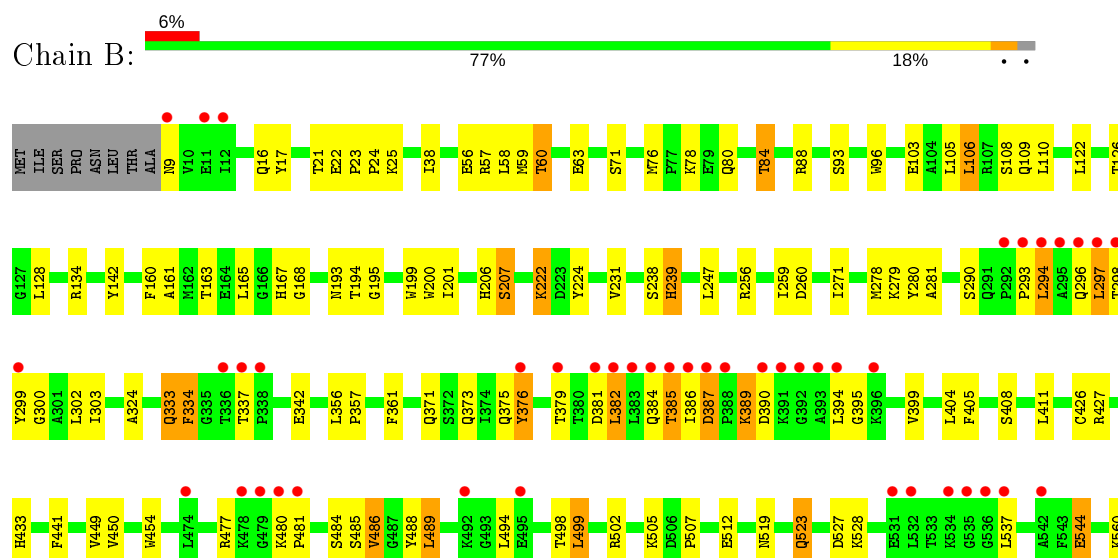
### 3 Residue-property plots [i](#)

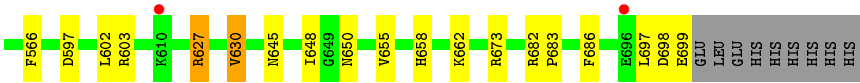
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Acyl-coenzyme A oxidase 3



#### • Molecule 1: Acyl-coenzyme A oxidase 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.82Å 160.82Å 139.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.99 – 2.50 35.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (35.99-2.50) 98.7 (35.96-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.09 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.181 , 0.229 0.185 , 0.231	Depositor DCC
$R_{free}$ test set	3044 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [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	0.73	1/5549 (0.0%)	0.77	1/7508 (0.0%)
1	B	0.71	0/5544	0.79	1/7501 (0.0%)
All	All	0.72	1/11093 (0.0%)	0.78	2/15009 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	PRO	N-CD	5.12	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	ASP	C-N-CD	5.96	140.91	128.40
1	A	387	ASP	C-N-CD	5.88	140.76	128.40

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	5430	0	5344	94	0
1	B	5425	0	5339	113	0
2	A	53	0	31	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	7	0
3	A	77	0	0	4	0
3	B	91	0	0	4	0
All	All	11129	0	10745	201	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 9.

All (201) 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:168:GLY:HA3	2:A:801:FAD:O2P	1.42	1.14
1:B:168:GLY:HA3	2:B:801:FAD:O2P	1.44	1.12
1:A:337:THR:HG22	1:A:338:PRO:HD2	1.30	1.10
1:A:299:TYR:CD2	1:A:302:LEU:HD12	1.89	1.07
1:B:297:LEU:HB3	1:B:299:TYR:HE1	1.20	1.07
1:B:303:ILE:HD11	1:B:405:PHE:CD1	2.02	0.94
1:A:502:ARG:HG3	1:A:502:ARG:HH21	1.32	0.93
1:A:499:LEU:O	1:A:502:ARG:HG3	1.69	0.93
1:B:297:LEU:HB3	1:B:299:TYR:CE1	2.05	0.91
1:A:299:TYR:CD2	1:A:302:LEU:CD1	2.58	0.87
1:B:544:GLU:HG3	3:B:988:HOH:O	1.75	0.87
1:B:76:MET:HG2	1:B:80:GLN:HB3	1.58	0.86
1:B:375:GLN:O	1:B:379:THR:HG23	1.77	0.85
1:A:206:HIS:HD2	3:B:919:HOH:O	1.63	0.81
1:A:299:TYR:HD2	1:A:302:LEU:HD12	1.43	0.81
1:B:648:ILE:HA	1:B:655:VAL:HG23	1.63	0.80
1:B:477:ARG:HH21	1:B:523:GLN:HG3	1.47	0.80
1:B:297:LEU:CB	1:B:299:TYR:HE1	1.93	0.79
1:A:337:THR:CG2	1:A:338:PRO:HD2	2.12	0.79
1:A:168:GLY:CA	2:A:801:FAD:O2P	2.28	0.78
1:B:168:GLY:CA	2:B:801:FAD:O2P	2.28	0.77
1:B:17:TYR:HD1	1:B:21:THR:HG22	1.48	0.77
1:A:193:ASN:HD22	1:A:195:GLY:H	1.31	0.76
1:A:358:LEU:O	1:A:362:THR:HG22	1.85	0.76
1:B:381:ASP:O	1:B:385:THR:HG23	1.85	0.76
1:A:519:ASN:HD21	1:A:523:GLN:HE21	1.34	0.76
1:A:299:TYR:CG	1:A:302:LEU:HD12	2.21	0.75
1:A:299:TYR:HB3	1:A:302:LEU:HD12	1.69	0.75
1:B:627:ARG:O	1:B:630:VAL:HG22	1.87	0.75
1:A:502:ARG:HG3	1:A:502:ARG:NH2	1.96	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASP:O	1:B:389:LYS:HD2	1.87	0.74
1:A:337:THR:HB	1:A:340:GLN:HB2	1.69	0.74
1:A:56:GLU:O	1:A:60:THR:CG2	2.36	0.73
1:A:384:GLN:HE21	1:A:384:GLN:HA	1.52	0.73
1:B:193:ASN:HD22	1:B:195:GLY:H	1.35	0.73
1:B:303:ILE:HD11	1:B:405:PHE:CE1	2.25	0.72
1:A:299:TYR:CB	1:A:302:LEU:HD12	2.20	0.71
1:A:337:THR:HG22	1:A:338:PRO:CD	2.15	0.71
1:B:499:LEU:O	1:B:502:ARG:HD3	1.91	0.71
1:A:299:TYR:HD2	1:A:302:LEU:CD1	2.00	0.70
1:B:294:LEU:O	1:B:294:LEU:HD12	1.92	0.70
1:A:450:VAL:HG23	2:A:801:FAD:HM83	1.75	0.68
1:A:56:GLU:O	1:A:60:THR:HG23	1.93	0.68
1:A:524:ARG:NH1	1:A:604:GLU:OE2	2.26	0.67
1:B:161:ALA:HA	1:B:201:ILE:HD12	1.76	0.67
1:B:280:TYR:CE1	1:B:297:LEU:HD22	2.30	0.67
1:A:405:PHE:O	1:A:408:SER:HB2	1.96	0.65
1:A:193:ASN:ND2	1:A:195:GLY:H	1.94	0.64
1:B:333:GLN:O	1:B:334:PHE:HB2	1.97	0.64
1:A:499:LEU:O	1:A:502:ARG:CG	2.44	0.64
1:A:167:HIS:HE1	1:B:342:GLU:OE2	1.79	0.63
1:A:333:GLN:O	1:A:334:PHE:HB2	1.98	0.63
1:B:206:HIS:O	1:B:239:HIS:HE1	1.82	0.63
1:B:381:ASP:O	1:B:385:THR:CG2	2.47	0.63
1:B:450:VAL:HG23	2:B:801:FAD:HM83	1.82	0.62
1:B:303:ILE:HD11	1:B:405:PHE:HD1	1.60	0.62
1:A:302:LEU:HB3	1:A:405:PHE:CE1	2.35	0.61
1:B:389:LYS:H	1:B:389:LYS:HD3	1.65	0.61
1:B:134:ARG:HG3	1:B:142:TYR:CE1	2.36	0.61
1:A:450:VAL:CG2	2:A:801:FAD:HM83	2.31	0.60
1:A:84:THR:O	1:A:88:ARG:HD3	2.01	0.60
1:B:648:ILE:CA	1:B:655:VAL:HG23	2.30	0.60
1:B:386:ILE:O	1:B:386:ILE:HG22	2.01	0.59
1:A:342:GLU:OE2	1:B:167:HIS:HE1	1.85	0.59
1:B:303:ILE:CD1	1:B:405:PHE:CD1	2.84	0.59
1:B:544:GLU:CG	3:B:988:HOH:O	2.42	0.59
1:A:698:ASP:O	1:A:699:GLU:HB2	2.01	0.59
1:A:298:THR:HG23	1:A:298:THR:O	2.02	0.58
1:B:502:ARG:HH22	1:B:512:GLU:CD	2.06	0.58
1:B:648:ILE:HG22	1:B:655:VAL:HG22	1.85	0.58
1:B:382:LEU:HA	1:B:385:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ARG:NH2	1:B:527:ASP:OD1	2.37	0.58
1:A:502:ARG:CG	1:A:502:ARG:HH21	2.11	0.58
1:B:303:ILE:CD1	1:B:405:PHE:CE1	2.86	0.58
1:B:256:ARG:HB3	1:B:259:ILE:HD12	1.86	0.57
1:B:480:LYS:HB3	1:B:481:PRO:HD2	1.87	0.57
1:A:358:LEU:O	1:A:362:THR:CG2	2.50	0.57
1:B:519:ASN:ND2	1:B:523:GLN:NE2	2.51	0.57
1:A:519:ASN:ND2	1:A:523:GLN:HE21	2.02	0.57
1:B:389:LYS:N	1:B:389:LYS:HD3	2.20	0.57
1:B:502:ARG:NH2	1:B:512:GLU:OE2	2.38	0.56
1:B:519:ASN:ND2	1:B:523:GLN:HE22	2.03	0.56
1:B:168:GLY:HA3	2:B:801:FAD:H5'2	1.88	0.56
1:A:374:ILE:O	1:A:378:GLN:HG2	2.05	0.56
1:B:373:GLN:HE22	1:B:376:TYR:HE1	1.54	0.56
1:A:161:ALA:HA	1:A:201:ILE:HD12	1.87	0.56
1:A:384:GLN:CA	1:A:384:GLN:HE21	2.17	0.56
1:A:299:TYR:CD1	1:A:299:TYR:N	2.73	0.55
1:B:80:GLN:O	1:B:84:THR:HB	2.06	0.55
1:A:294:LEU:O	1:A:297:LEU:HD12	2.07	0.55
1:B:477:ARG:NH1	1:B:527:ASP:OD1	2.40	0.55
1:B:193:ASN:ND2	1:B:195:GLY:H	2.05	0.54
1:B:56:GLU:O	1:B:60:THR:CG2	2.55	0.54
1:A:56:GLU:O	1:A:60:THR:HG22	2.07	0.54
1:B:76:MET:HG2	1:B:80:GLN:CB	2.35	0.54
1:B:450:VAL:CG2	2:B:801:FAD:HM83	2.37	0.53
1:B:373:GLN:NE2	1:B:376:TYR:HE1	2.07	0.53
1:B:650:ASN:HD22	1:B:658:HIS:CD2	2.26	0.53
1:A:332:ARG:HD3	1:A:342:GLU:O	2.08	0.52
1:A:489:LEU:HD12	1:A:519:ASN:HD22	1.73	0.52
1:A:337:THR:CG2	1:A:338:PRO:CD	2.83	0.52
1:A:197:THR:HG22	1:A:198:LYS:O	2.10	0.52
1:B:293:PRO:HG2	1:B:294:LEU:H	1.75	0.52
1:B:389:LYS:N	1:B:389:LYS:CD	2.73	0.52
1:A:384:GLN:NE2	1:A:384:GLN:CA	2.73	0.52
1:B:59:MET:O	1:B:63:GLU:HG3	2.10	0.52
1:B:165:LEU:HD13	1:B:199:TRP:CD2	2.45	0.52
1:A:513:ALA:HB2	1:A:606:PHE:CE2	2.45	0.51
1:B:23:PRO:N	1:B:24:PRO:HD2	2.26	0.51
1:B:200:TRP:HB3	2:B:801:FAD:C9A	2.40	0.51
1:B:105:LEU:O	1:B:109:GLN:HG3	2.11	0.51
1:B:56:GLU:O	1:B:60:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:THR:OG1	2:B:801:FAD:H1'1	2.11	0.51
1:B:519:ASN:HD21	1:B:523:GLN:NE2	2.09	0.51
1:B:489:LEU:HA	1:B:519:ASN:HD22	1.76	0.50
1:B:17:TYR:CD1	1:B:21:THR:HG22	2.38	0.50
1:A:11:GLU:HG3	1:A:16:GLN:HG2	1.93	0.49
1:A:169:SER:HB2	2:A:801:FAD:O2A	2.12	0.49
1:B:648:ILE:HB	1:B:655:VAL:CG2	2.42	0.49
1:A:193:ASN:ND2	1:A:195:GLY:N	2.60	0.49
1:B:22:GLU:N	1:B:23:PRO:CD	2.76	0.48
1:B:488:TYR:CE1	1:B:489:LEU:HD13	2.48	0.48
1:B:207:SER:OG	1:B:260:ASP:OD2	2.29	0.48
1:B:486:VAL:O	1:B:489:LEU:HB2	2.14	0.48
1:A:305:GLY:O	1:A:309:MET:HG3	2.13	0.48
1:A:299:TYR:HB3	1:A:302:LEU:HB2	1.96	0.48
1:B:682:ARG:HB3	1:B:683:PRO:HD3	1.96	0.48
1:B:84:THR:HG23	1:B:88:ARG:NE	2.29	0.48
1:A:180:TYR:O	1:A:181:ILE:HD13	2.14	0.47
1:A:9:ASN:HB3	1:A:16:GLN:OE1	2.14	0.47
1:A:449:VAL:HG13	1:B:427:ARG:NH2	2.30	0.47
1:A:384:GLN:NE2	1:A:384:GLN:HA	2.27	0.47
1:B:299:TYR:CD1	1:B:299:TYR:N	2.83	0.47
1:A:69:ASN:HD21	1:A:71:SER:HB3	1.80	0.47
1:A:256:ARG:HB3	1:A:259:ILE:HD12	1.96	0.47
1:A:532:LEU:HB3	1:A:537:LEU:HD12	1.97	0.47
1:B:57:ARG:NH2	1:B:103:GLU:OE2	2.44	0.46
1:A:185:ASP:OD2	1:A:273:ARG:NH2	2.48	0.46
1:A:382:LEU:O	1:A:386:ILE:HG13	2.16	0.46
1:B:222:LYS:HB3	1:B:224:TYR:CE1	2.50	0.46
1:A:128:LEU:HB3	1:A:160:PHE:CD1	2.51	0.46
1:A:662:LYS:HE2	3:A:966:HOH:O	2.15	0.46
1:B:299:TYR:O	1:B:302:LEU:N	2.48	0.46
1:A:194:THR:HG23	3:A:965:HOH:O	2.15	0.46
1:A:121:ARG:HD2	1:A:258:ALA:O	2.16	0.46
1:A:169:SER:CB	2:A:801:FAD:O2A	2.64	0.46
1:B:389:LYS:HB3	1:B:394:LEU:HD22	1.97	0.46
1:A:93:SER:HA	1:A:96:TRP:CE2	2.51	0.46
1:B:128:LEU:HB3	1:B:160:PHE:CD1	2.50	0.45
1:B:519:ASN:HD21	1:B:523:GLN:HE22	1.63	0.45
1:B:299:TYR:N	1:B:299:TYR:HD1	2.13	0.45
1:B:427:ARG:HB2	1:B:441:PHE:CG	2.51	0.45
1:A:247:LEU:HD12	1:A:247:LEU:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLY:HA2	1:B:376:TYR:HE2	1.81	0.45
1:B:395:GLY:O	1:B:399:VAL:HG23	2.17	0.45
1:A:57:ARG:NH2	1:A:103:GLU:OE2	2.48	0.45
1:B:280:TYR:CD1	1:B:297:LEU:CD2	3.00	0.45
1:B:505:LYS:O	1:B:507:PRO:HD3	2.17	0.44
1:A:22:GLU:N	1:A:23:PRO:CD	2.80	0.44
1:B:297:LEU:O	1:B:299:TYR:CD1	2.70	0.44
1:A:454:TRP:C	1:A:454:TRP:CD1	2.90	0.44
1:B:22:GLU:N	1:B:23:PRO:HD3	2.33	0.44
1:B:280:TYR:CZ	1:B:297:LEU:HD22	2.52	0.43
1:B:84:THR:HG22	3:B:983:HOH:O	2.19	0.43
1:B:93:SER:HA	1:B:96:TRP:CE2	2.54	0.43
1:A:165:LEU:O	1:B:433:HIS:HE1	2.02	0.43
1:A:388:PRO:O	1:A:389:LYS:HB2	2.19	0.43
1:B:682:ARG:HD2	1:B:686:PHE:CD2	2.54	0.43
1:A:673:ARG:NH1	1:B:238:SER:O	2.51	0.43
1:B:523:GLN:HE21	1:B:523:GLN:HB2	1.71	0.43
1:A:167:HIS:HD2	3:A:936:HOH:O	2.02	0.42
1:B:648:ILE:CB	1:B:655:VAL:CG2	2.97	0.42
1:B:300:GLY:CA	1:B:376:TYR:HE2	2.32	0.42
1:B:499:LEU:O	1:B:499:LEU:HD22	2.20	0.42
1:A:120:ILE:HB	1:A:259:ILE:HD11	2.01	0.42
1:A:290:SER:OG	3:A:901:HOH:O	2.21	0.42
1:A:302:LEU:HB3	1:A:405:PHE:HE1	1.82	0.42
1:B:698:ASP:O	1:B:699:GLU:HB2	2.19	0.42
1:A:403:GLU:HG3	1:A:483:GLY:HA3	2.01	0.42
1:B:106:LEU:O	1:B:110:LEU:HG	2.19	0.42
1:B:324:ALA:HB2	1:B:426:CYS:HB3	2.01	0.42
1:A:299:TYR:CD2	1:A:302:LEU:HD11	2.52	0.42
1:B:278:MET:HG2	1:B:281:ALA:O	2.19	0.42
1:A:20:PHE:CD1	1:B:194:THR:HB	2.54	0.42
1:A:280:TYR:HD1	1:A:294:LEU:HD13	1.84	0.41
1:B:498:THR:O	1:B:502:ARG:NH1	2.53	0.41
1:B:356:LEU:N	1:B:357:PRO:CD	2.84	0.41
1:A:203:GLY:HA2	1:A:260:ASP:OD1	2.20	0.41
1:A:163:THR:OG1	2:A:801:FAD:H1'1	2.20	0.41
1:A:439:ASN:OD1	1:A:648:ILE:HG12	2.20	0.41
1:B:231:VAL:HG22	1:B:271:ILE:HG21	2.02	0.41
1:B:280:TYR:CG	1:B:297:LEU:HD21	2.56	0.41
1:B:56:GLU:O	1:B:60:THR:HG22	2.21	0.41
1:A:200:TRP:HB3	2:A:801:FAD:C9A	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ASP:O	1:A:385:THR:HG23	2.20	0.41
1:B:76:MET:CG	1:B:80:GLN:HB3	2.39	0.40
1:A:299:TYR:HD1	1:A:299:TYR:H	1.70	0.40
1:A:98:LYS:HG2	1:A:98:LYS:H	1.56	0.40
1:B:247:LEU:HD12	1:B:247:LEU:C	2.41	0.40
1:B:303:ILE:CD1	1:B:405:PHE:HD1	2.31	0.40
1:A:26:ALA:HB1	1:A:344:LYS:NZ	2.36	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	690/708 (98%)	680 (99%)	10 (1%)	0	100	100
1	B	689/708 (97%)	678 (98%)	10 (2%)	1 (0%)	51	73
All	All	1379/1416 (97%)	1358 (98%)	20 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	334	PHE

### 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	570/586 (97%)	517 (91%)	53 (9%)	9	17
1	B	570/586 (97%)	512 (90%)	58 (10%)	7	14
All	All	1140/1172 (97%)	1029 (90%)	111 (10%)	8	16

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	22	GLU
1	A	39	LYS
1	A	50	GLU
1	A	60	THR
1	A	67	VAL
1	A	78	LYS
1	A	81	LEU
1	A	93	SER
1	A	98	LYS
1	A	126	THR
1	A	148	LYS
1	A	183	ASP
1	A	194	THR
1	A	207	SER
1	A	239	HIS
1	A	275	ASN
1	A	288	LYS
1	A	290	SER
1	A	297	LEU
1	A	299	TYR
1	A	333	GLN
1	A	361	PHE
1	A	362	THR
1	A	371	GLN
1	A	378	GLN
1	A	384	GLN
1	A	385	THR
1	A	389	LYS
1	A	394	LEU
1	A	396	LYS
1	A	404	LEU
1	A	407	SER
1	A	408	SER
1	A	411	LEU

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Mol	Chain	Res	Type
1	A	449	VAL
1	A	454	TRP
1	A	465	MET
1	A	489	LEU
1	A	502	ARG
1	A	559	ARG
1	A	560	LYS
1	A	566	PHE
1	A	568	GLU
1	A	597	ASP
1	A	600	LEU
1	A	602	LEU
1	A	603	ARG
1	A	627	ARG
1	A	645	ASN
1	A	673	ARG
1	A	696	GLU
1	A	699	GLU
1	B	9	ASN
1	B	16	GLN
1	B	25	LYS
1	B	38	ILE
1	B	58	LEU
1	B	60	THR
1	B	71	SER
1	B	78	LYS
1	B	84	THR
1	B	106	LEU
1	B	108	SER
1	B	122	LEU
1	B	126	THR
1	B	207	SER
1	B	222	LYS
1	B	239	HIS
1	B	279	LYS
1	B	290	SER
1	B	294	LEU
1	B	296	GLN
1	B	297	LEU
1	B	298	THR
1	B	333	GLN
1	B	337	THR

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Mol	Chain	Res	Type
1	B	361	PHE
1	B	371	GLN
1	B	376	TYR
1	B	382	LEU
1	B	384	GLN
1	B	385	THR
1	B	389	LYS
1	B	390	ASP
1	B	404	LEU
1	B	408	SER
1	B	411	LEU
1	B	449	VAL
1	B	454	TRP
1	B	484	SER
1	B	485	SER
1	B	486	VAL
1	B	489	LEU
1	B	494	LEU
1	B	499	LEU
1	B	523	GLN
1	B	528	LYS
1	B	537	LEU
1	B	544	GLU
1	B	560	LYS
1	B	566	PHE
1	B	597	ASP
1	B	602	LEU
1	B	603	ARG
1	B	627	ARG
1	B	630	VAL
1	B	645	ASN
1	B	662	LYS
1	B	673	ARG
1	B	697	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	167	HIS
1	A	193	ASN
1	A	206	HIS

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Mol	Chain	Res	Type
1	A	239	HIS
1	A	261	ASN
1	A	275	ASN
1	A	371	GLN
1	A	384	GLN
1	A	425	GLN
1	A	433	HIS
1	A	519	ASN
1	A	561	HIS
1	A	584	ASN
1	A	645	ASN
1	A	664	ASN
1	A	665	GLN
1	B	109	GLN
1	B	167	HIS
1	B	193	ASN
1	B	239	HIS
1	B	261	ASN
1	B	275	ASN
1	B	291	GLN
1	B	318	GLN
1	B	371	GLN
1	B	373	GLN
1	B	375	GLN
1	B	378	GLN
1	B	425	GLN
1	B	433	HIS
1	B	459	ASN
1	B	519	ASN
1	B	523	GLN
1	B	561	HIS
1	B	584	ASN
1	B	645	ASN
1	B	650	ASN
1	B	664	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 ⓘ

2 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	801	-	51,58,58	1.70	6 (11%)	60,89,89	1.96	14 (23%)
2	FAD	B	801	-	51,58,58	1.68	7 (13%)	60,89,89	1.99	11 (18%)

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	801	-	-	5/30/50/50	0/6/6/6
2	FAD	B	801	-	-	9/30/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C4X-C10	8.31	1.47	1.38
2	B	801	FAD	C4X-C10	8.27	1.47	1.38
2	B	801	FAD	C4-C4X	3.20	1.46	1.41
2	A	801	FAD	C4-C4X	3.09	1.46	1.41
2	A	801	FAD	C9A-C5X	3.01	1.48	1.42
2	A	801	FAD	C8-C7	2.96	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C9A-C5X	2.89	1.48	1.42
2	B	801	FAD	C8-C7	2.88	1.48	1.40
2	A	801	FAD	C2-N3	-2.70	1.32	1.38
2	A	801	FAD	C6-C5X	-2.70	1.37	1.41
2	B	801	FAD	C2-N3	-2.61	1.33	1.38
2	B	801	FAD	C6-C5X	-2.34	1.38	1.41
2	B	801	FAD	C5A-C4A	2.01	1.46	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	C4-N3-C2	7.94	121.85	115.14
2	A	801	FAD	C4-N3-C2	7.83	121.75	115.14
2	B	801	FAD	C1'-N10-C9A	5.67	122.75	118.29
2	B	801	FAD	C4-C4X-C10	-4.87	116.73	119.95
2	A	801	FAD	C1'-N10-C9A	4.69	121.98	118.29
2	A	801	FAD	C4-C4X-C10	-4.34	117.08	119.95
2	A	801	FAD	C9A-N10-C10	-3.80	116.94	121.91
2	B	801	FAD	C4X-N5-C5X	3.65	120.42	116.77
2	B	801	FAD	C9A-N10-C10	-3.53	117.28	121.91
2	A	801	FAD	C4X-C4-N3	-3.47	118.68	123.43
2	B	801	FAD	C4X-C4-N3	-3.40	118.78	123.43
2	A	801	FAD	N3A-C2A-N1A	-3.23	123.62	128.68
2	B	801	FAD	C5X-C9A-N10	3.13	119.99	117.72
2	A	801	FAD	C4X-N5-C5X	3.11	119.88	116.77
2	B	801	FAD	C4A-C5A-N7A	-2.98	106.30	109.40
2	A	801	FAD	C1'-N10-C10	2.91	121.01	118.41
2	B	801	FAD	N3A-C2A-N1A	-2.78	124.33	128.68
2	B	801	FAD	C4-C4X-N5	2.66	121.63	118.60
2	A	801	FAD	C5X-C9A-N10	2.54	119.56	117.72
2	A	801	FAD	C4A-C5A-N7A	-2.51	106.78	109.40
2	A	801	FAD	C3B-C2B-C1B	2.44	104.66	100.98
2	A	801	FAD	C4'-C3'-C2'	2.43	118.42	113.36
2	A	801	FAD	C4-C4X-N5	2.28	121.20	118.60
2	B	801	FAD	O5'-C5'-C4'	2.21	115.27	109.36
2	A	801	FAD	O4'-C4'-C5'	-2.17	105.03	109.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	C5'-O5'-P-O1P

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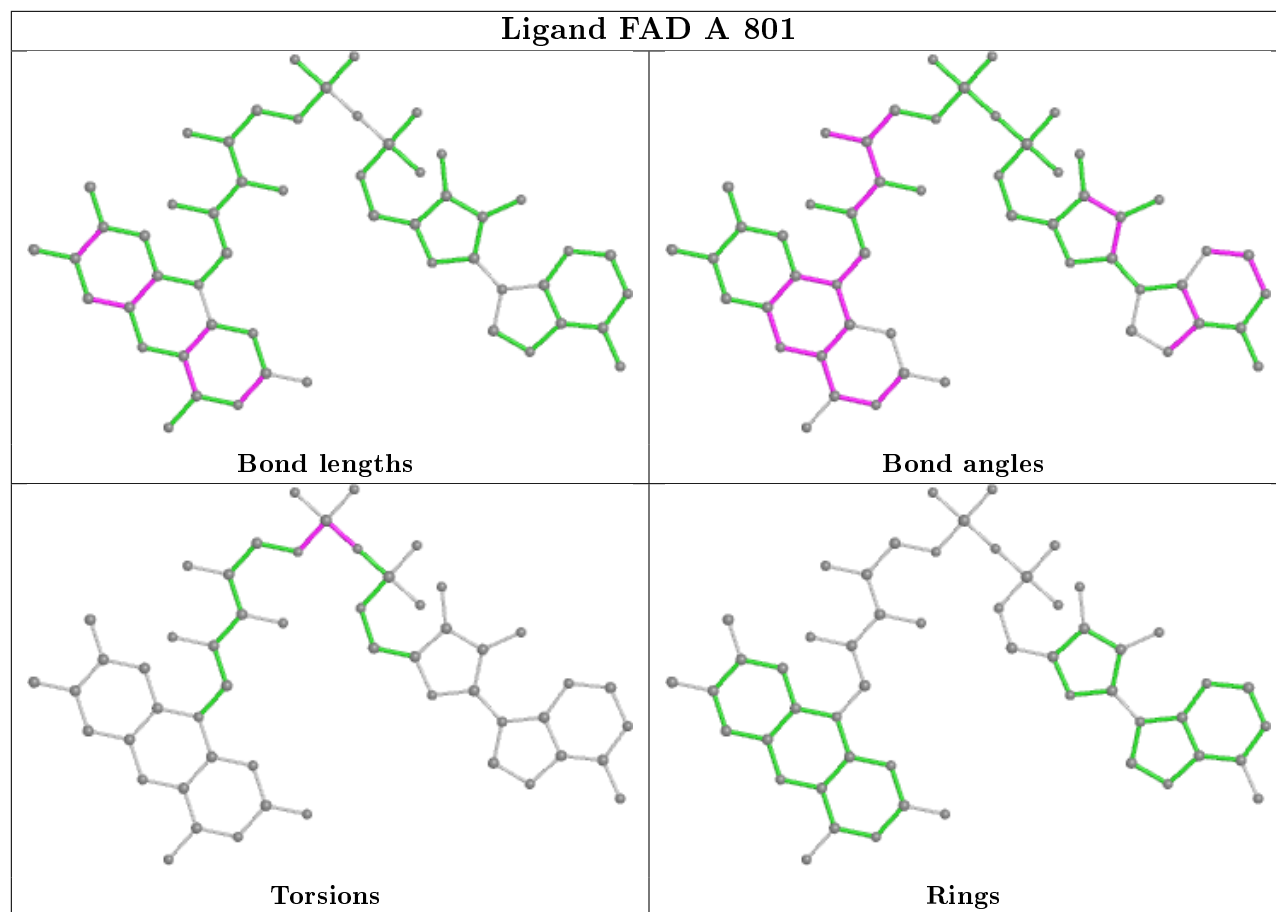
Mol	Chain	Res	Type	Atoms
2	A	801	FAD	C5'-O5'-P-O2P
2	B	801	FAD	C2'-C1'-N10-C10
2	B	801	FAD	C5'-O5'-P-O1P
2	B	801	FAD	C5'-O5'-P-O2P
2	A	801	FAD	PA-O3P-P-O1P
2	B	801	FAD	C5'-O5'-P-O3P
2	B	801	FAD	O3'-C3'-C4'-C5'
2	A	801	FAD	PA-O3P-P-O2P
2	B	801	FAD	O2'-C2'-C3'-C4'
2	B	801	FAD	C2'-C3'-C4'-C5'
2	A	801	FAD	C5'-O5'-P-O3P
2	B	801	FAD	O2'-C2'-C3'-O3'
2	B	801	FAD	C1'-C2'-C3'-O3'

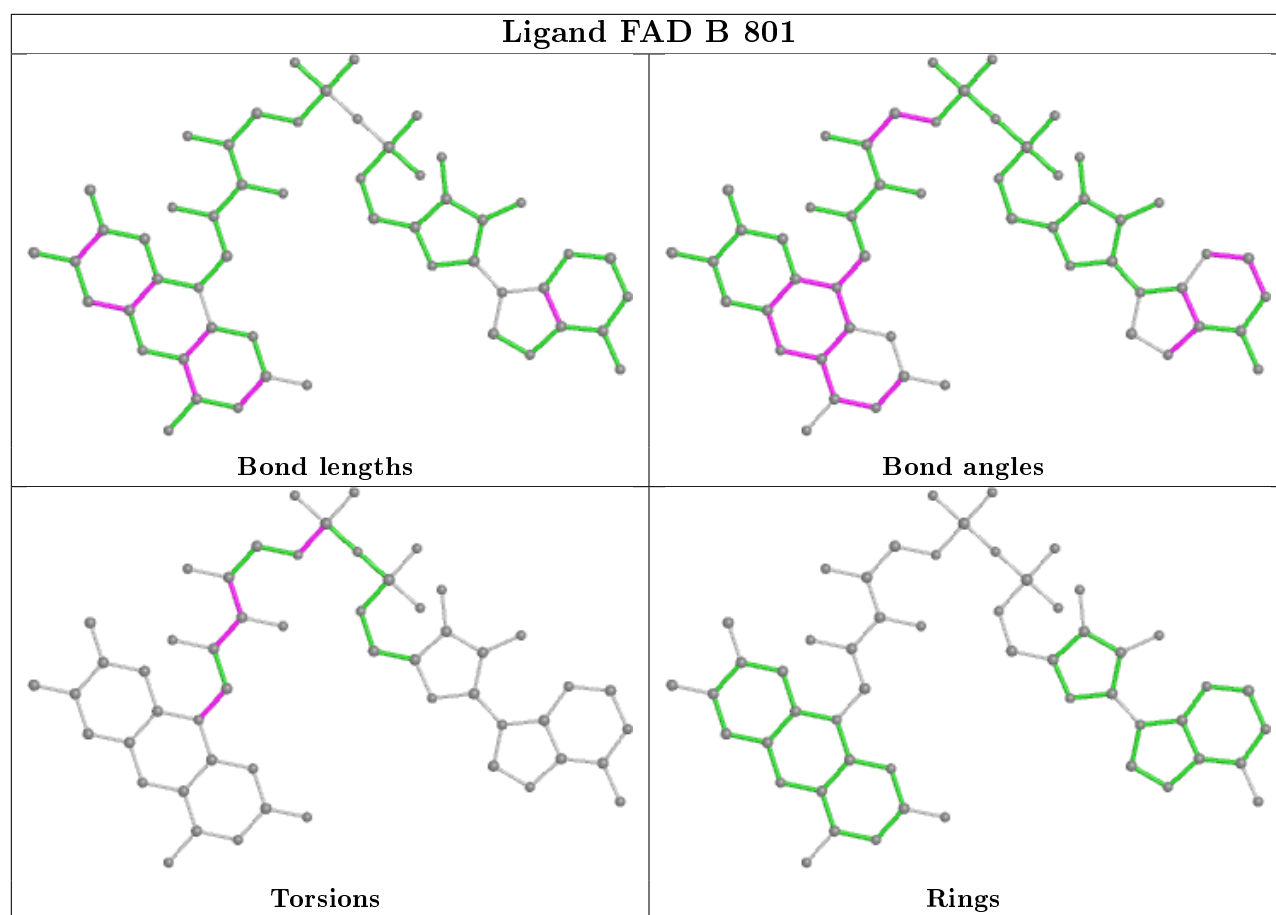
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	8	0
2	B	801	FAD	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	692/708 (97%)	-0.13	32 (4%) 32 34	27, 41, 73, 125	0
1	B	691/708 (97%)	-0.11	46 (6%) 17 18	26, 40, 81, 133	0
All	All	1383/1416 (97%)	-0.12	78 (5%) 24 25	26, 40, 78, 133	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	ALA	9.8
1	B	392	GLY	9.4
1	A	295	ALA	8.6
1	A	297	LEU	7.8
1	B	393	ALA	7.3
1	B	294	LEU	7.2
1	B	297	LEU	7.0
1	A	387	ASP	6.9
1	B	388	PRO	6.7
1	B	383	LEU	6.4
1	B	391	LYS	6.4
1	A	338	PRO	6.3
1	A	296	GLN	6.1
1	B	387	ASP	6.0
1	B	382	LEU	5.5
1	A	393	ALA	5.5
1	B	386	ILE	5.3
1	B	296	GLN	5.1
1	A	299	TYR	5.1
1	B	385	THR	5.0
1	B	293	PRO	4.9
1	B	338	PRO	4.9
1	B	298	THR	4.8
1	A	388	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	385	THR	4.4
1	A	339	GLY	4.2
1	B	474	LEU	4.2
1	A	294	LEU	4.2
1	B	537	LEU	4.2
1	B	534	LYS	4.2
1	A	610	LYS	3.8
1	B	381	ASP	3.7
1	B	536	GLY	3.6
1	A	383	LEU	3.6
1	A	386	ILE	3.6
1	B	394	LEU	3.6
1	B	379	THR	3.6
1	B	376	TYR	3.5
1	A	381	ASP	3.4
1	A	384	GLN	3.3
1	A	14	GLY	3.2
1	A	382	LEU	3.1
1	A	298	THR	3.0
1	B	535	GLY	3.0
1	B	299	TYR	2.9
1	B	12	ILE	2.9
1	B	531	GLU	2.8
1	B	390	ASP	2.7
1	A	340	GLN	2.7
1	B	610	LYS	2.5
1	B	384	GLN	2.4
1	B	478	LYS	2.4
1	A	405	PHE	2.4
1	B	9	ASN	2.4
1	B	481	PRO	2.4
1	A	13	ASP	2.3
1	A	394	LEU	2.3
1	A	392	GLY	2.3
1	A	536	GLY	2.3
1	A	183	ASP	2.2
1	B	532	LEU	2.2
1	A	390	ASP	2.2
1	A	8	ALA	2.2
1	A	537	LEU	2.2
1	B	479	GLY	2.2
1	A	9	ASN	2.2

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	336	THR	2.2
1	B	396	LYS	2.1
1	B	11	GLU	2.1
1	B	480	LYS	2.1
1	B	542	ALA	2.1
1	B	337	THR	2.0
1	A	376	TYR	2.0
1	B	696	GLU	2.0
1	B	292	PRO	2.0
1	B	336	THR	2.0
1	B	495	GLU	2.0
1	B	492	LYS	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](#)

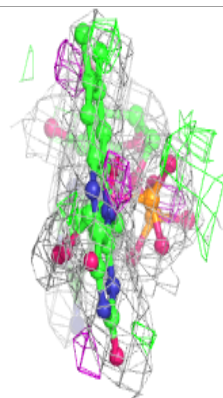
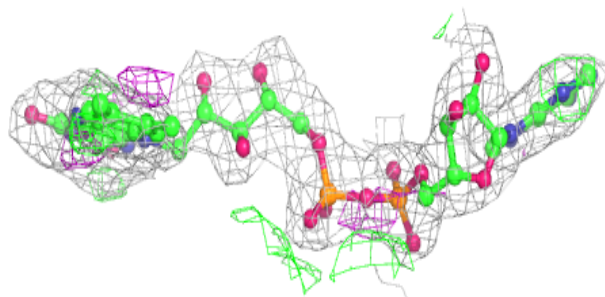
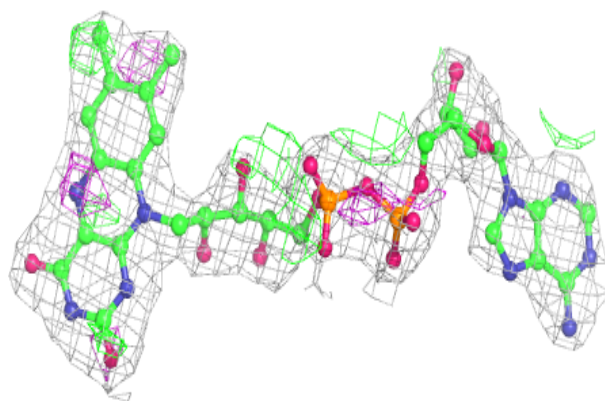
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	801	53/53	0.90	0.16	32,50,65,68	0
2	FAD	A	801	53/53	0.93	0.15	35,45,56,58	0

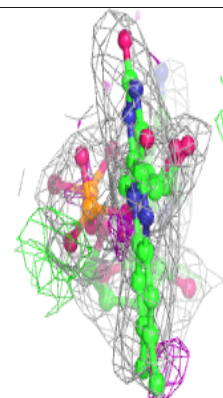
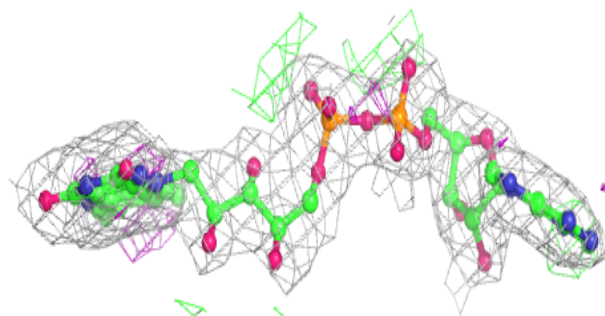
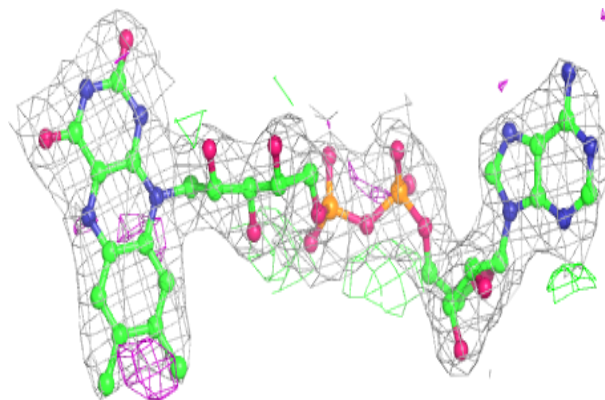
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around FAD B 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD A 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.