



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:07 pm GMT

PDB ID : 4Z2R  
Title : Crystal Structure of 2-hydroxybiphenyl 3-monooxygenase from *Pseudomonas azelaica*  
Authors : Kanteev, M.; Bregman-Cohen, A.; Fishman, A.  
Deposited on : 2015-03-30  
Resolution : 2.30 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 : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

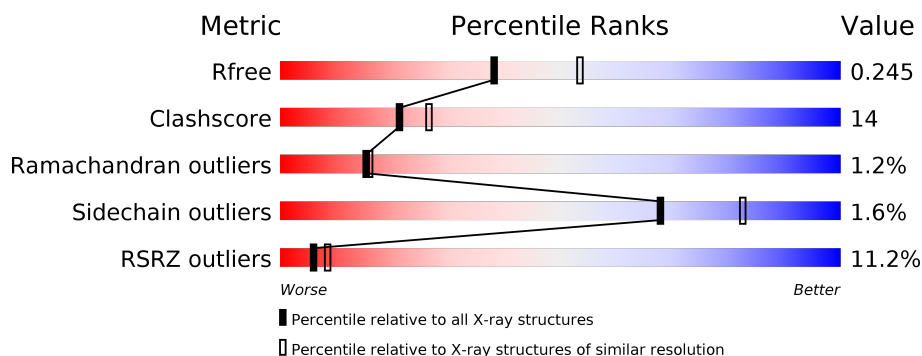
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	592	<div> <div>11%</div> <div>67%</div> <div>27%</div> <div>• •</div> </div>
1	B	592	<div> <div>10%</div> <div>71%</div> <div>22%</div> <div>• 5%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	601	X	-	-	-
2	FAD	B	601	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9421 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.

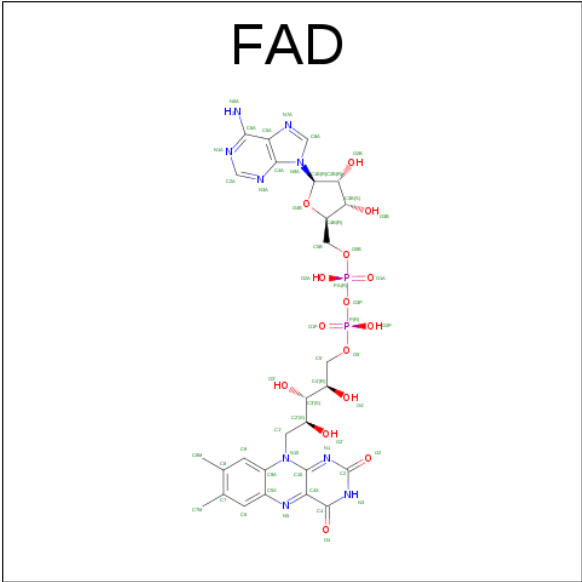
- Molecule 1 is a protein called 2-hydroxybiphenyl-3-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4350	2748	764	818	20			
1	B	563	Total	C	N	O	S	0	0	0
			4329	2734	761	814	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP O06647
A	-4	HIS	-	expression tag	UNP O06647
A	-3	HIS	-	expression tag	UNP O06647
A	-2	HIS	-	expression tag	UNP O06647
A	-1	HIS	-	expression tag	UNP O06647
A	0	HIS	-	expression tag	UNP O06647
A	1	HIS	-	expression tag	UNP O06647
B	-5	MET	-	initiating methionine	UNP O06647
B	-4	HIS	-	expression tag	UNP O06647
B	-3	HIS	-	expression tag	UNP O06647
B	-2	HIS	-	expression tag	UNP O06647
B	-1	HIS	-	expression tag	UNP O06647
B	0	HIS	-	expression tag	UNP O06647
B	1	HIS	-	expression tag	UNP O06647

- 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	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	325	Total	O	0	0
			325	325		
3	B	311	Total	O	0	0
			311	311		

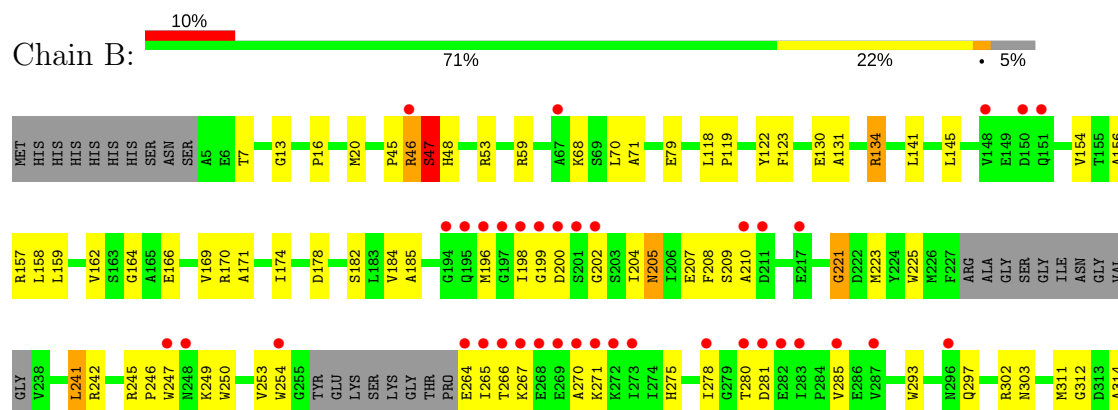
### 3 Residue-property plots [i](#)

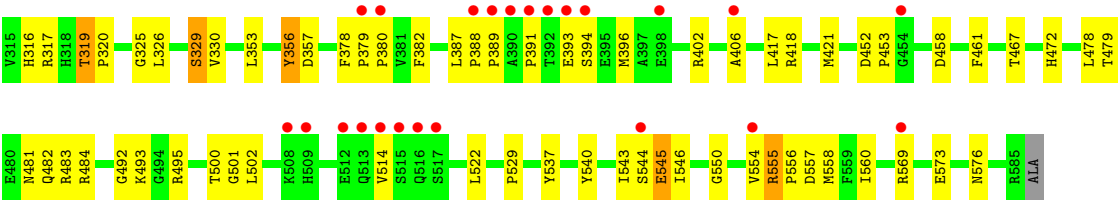
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 2-hydroxybiphenyl-3-monooxygenase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.35Å 131.49Å 79.16Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	29.27 – 2.30 37.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.27-2.30) 97.0 (37.68-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.234 , 0.258 0.222 , 0.245	Depositor DCC
$R_{free}$ test set	3408 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.92	9/4445 (0.2%)	0.90	20/6024 (0.3%)
1	B	0.95	7/4423 (0.2%)	0.92	17/5994 (0.3%)
All	All	0.94	16/8868 (0.2%)	0.91	37/12018 (0.3%)

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	A	0	2
1	B	0	1
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	PRO	N-CD	9.14	1.60	1.47
1	A	299	TYR	CD1-CE1	-6.67	1.29	1.39
1	A	359	GLU	CD-OE1	-6.11	1.19	1.25
1	B	164	GLY	C-N	5.95	1.47	1.34
1	A	253	VAL	CB-CG2	-5.81	1.40	1.52
1	B	316	HIS	C-N	-5.63	1.21	1.34
1	B	325	GLY	C-N	-5.54	1.21	1.34
1	A	301	VAL	CB-CG1	-5.53	1.41	1.52
1	A	148	VAL	CB-CG2	-5.46	1.41	1.52
1	B	221	GLY	C-N	-5.40	1.21	1.34
1	B	253	VAL	CB-CG2	-5.26	1.41	1.52
1	B	555	ARG	C-N	-5.25	1.24	1.34
1	A	72	VAL	C-N	-5.11	1.24	1.34
1	A	299	TYR	CD2-CE2	-5.05	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	LEU	C-N	-5.03	1.22	1.34
1	B	356	TYR	CD1-CE1	-5.00	1.31	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ARG	O-C-N	-9.86	106.92	122.70
1	A	71	ALA	N-CA-CB	8.71	122.29	110.10
1	A	239	ALA	CB-CA-C	-8.18	97.84	110.10
1	B	554	VAL	CB-CA-C	7.98	126.57	111.40
1	B	394	SER	N-CA-CB	7.57	121.86	110.50
1	A	72	VAL	C-N-CD	-7.31	104.51	120.60
1	A	195	GLN	CB-CA-C	-7.30	95.79	110.40
1	B	170	ARG	CA-C-N	7.18	133.00	117.20
1	A	19	ALA	O-C-N	-7.17	111.23	122.70
1	B	70	LEU	CB-CA-C	-7.11	96.69	110.20
1	A	77	MET	O-C-N	-6.91	111.45	123.20
1	B	555	ARG	N-CA-CB	-6.65	98.63	110.60
1	B	267	LYS	CB-CA-C	6.59	123.58	110.40
1	B	207	GLU	CB-CA-C	6.57	123.54	110.40
1	B	478	LEU	O-C-N	-6.40	112.46	122.70
1	A	77	MET	N-CA-CB	-6.16	99.52	110.60
1	B	555	ARG	O-C-N	6.05	132.60	121.10
1	A	70	LEU	CB-CA-C	-6.02	98.76	110.20
1	A	240	ALA	N-CA-CB	-5.99	101.72	110.10
1	A	263	PRO	N-CA-CB	5.92	110.41	103.30
1	B	393	GLU	N-CA-C	5.90	126.94	111.00
1	A	171	ALA	CB-CA-C	5.83	118.85	110.10
1	B	131	ALA	N-CA-C	-5.78	95.39	111.00
1	A	453	PRO	C-N-CA	-5.72	110.28	122.30
1	B	170	ARG	C-N-CA	5.69	135.92	121.70
1	B	522	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	171	ALA	N-CA-CB	-5.65	102.19	110.10
1	A	53	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	293	TRP	CB-CA-C	5.49	121.37	110.40
1	B	208	PHE	N-CA-CB	5.46	120.44	110.60
1	A	403	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	77	MET	N-CA-C	5.21	125.06	111.00
1	B	156	ALA	CB-CA-C	5.14	117.81	110.10
1	A	53	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	134	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	116	CYS	O-C-N	5.05	130.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ALA	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	ARG	Sidechain
1	A	77	MET	Mainchain
1	B	402	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	A	4350	0	4293	136	0
1	B	4329	0	4277	101	0
2	A	53	0	30	7	0
2	B	53	0	30	7	0
3	A	325	0	0	4	0
3	B	311	0	0	0	0
All	All	9421	0	8630	237	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 14.

All (237) 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:197:GLY:O	1:A:198:ILE:HG22	1.58	1.00
1:B:544:SER:O	1:B:545:GLU:HB2	1.58	0.97
1:B:7:THR:O	1:B:171:ALA:HA	1.64	0.97
1:A:217:GLU:HA	1:A:217:GLU:OE1	1.70	0.92
1:B:154:VAL:HG21	1:B:174:ILE:HG13	1.54	0.89
1:B:46:ARG:NH2	2:B:601:FAD:O2'	2.07	0.85
1:A:266:THR:HG21	1:A:270:ALA:HB2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASN:O	1:A:206:ILE:HG13	1.79	0.82
1:A:492:GLY:C	1:A:493:LYS:HG2	2.02	0.80
1:A:492:GLY:O	1:A:493:LYS:CG	2.32	0.78
1:B:118:LEU:CD2	1:B:123:PHE:HB2	2.14	0.77
1:A:243:MET:SD	1:A:246:PRO:HD3	2.25	0.77
1:A:244:ILE:O	1:A:245:ARG:HD3	1.85	0.76
1:A:37:ARG:HD3	1:A:143:GLU:HB2	1.67	0.74
1:A:143:GLU:O	1:A:143:GLU:HG3	1.88	0.73
1:A:206:ILE:HD12	1:A:254:TRP:HH2	1.54	0.72
1:A:386:SER:HB2	1:A:402:ARG:HH21	1.56	0.71
1:A:492:GLY:O	1:A:493:LYS:HG2	1.91	0.71
1:A:48:HIS:CE1	1:A:242:ARG:HD2	2.25	0.71
1:A:266:THR:CG2	1:A:270:ALA:HB2	2.19	0.71
1:A:569:ARG:O	1:A:573:GLU:HG3	1.92	0.70
1:A:154:VAL:HG21	1:A:174:ILE:HG13	1.73	0.69
1:A:205:ASN:O	1:A:206:ILE:CG1	2.40	0.69
1:A:206:ILE:HD12	1:A:254:TRP:CH2	2.27	0.69
1:A:20:MET:HG2	1:A:330:VAL:HG13	1.74	0.69
1:B:46:ARG:NH2	2:B:601:FAD:HO2'	1.90	0.68
1:A:244:ILE:HB	1:A:249:LYS:HB3	1.75	0.68
1:B:157:ARG:HD2	1:B:166:GLU:OE2	1.94	0.68
1:A:266:THR:HG23	1:A:269:GLU:HG3	1.76	0.68
1:B:45:PRO:HB2	1:B:242:ARG:NH2	2.08	0.68
1:A:46:ARG:NH2	2:A:601:FAD:O2'	2.27	0.68
1:B:45:PRO:HB2	1:B:242:ARG:HH22	1.57	0.68
1:B:264:GLU:O	1:B:265:ILE:HG13	1.95	0.67
1:B:46:ARG:HG2	2:B:601:FAD:C6	2.26	0.66
1:B:280:THR:OG1	1:B:281:ASP:N	2.28	0.66
1:A:495:ARG:HD3	1:A:521:GLU:OE2	1.97	0.65
1:B:278:ILE:HD11	1:B:280:THR:O	1.97	0.64
1:A:46:ARG:O	1:A:47:SER:C	2.35	0.64
1:B:312:GLY:HA2	1:B:329:SER:OG	1.96	0.64
1:A:205:ASN:HB3	1:A:251:ILE:HD11	1.80	0.64
1:A:326:LEU:HD23	1:A:326:LEU:C	2.18	0.64
1:A:198:ILE:O	1:A:199:GLY:C	2.37	0.64
1:A:511:ALA:HB1	1:A:522:LEU:HD22	1.79	0.63
1:B:48:HIS:NE2	1:B:242:ARG:HD2	2.13	0.63
1:A:47:SER:HB2	1:A:120:GLN:OE1	1.98	0.63
1:A:16:PRO:HD2	2:A:601:FAD:O2P	1.98	0.63
1:A:197:GLY:O	1:A:198:ILE:CG2	2.42	0.63
1:A:47:SER:OG	1:A:326:LEU:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:O	1:A:143:GLU:CG	2.48	0.62
1:A:46:ARG:HG2	2:A:601:FAD:C6	2.30	0.61
1:A:492:GLY:O	1:A:493:LYS:CB	2.48	0.61
1:A:326:LEU:HD23	1:A:326:LEU:O	2.01	0.60
1:A:206:ILE:HG22	1:A:206:ILE:O	2.02	0.59
1:B:417:LEU:HD11	1:B:421:MET:HE3	1.85	0.59
1:A:226:MET:O	1:A:238:VAL:HG13	2.02	0.59
1:A:244:ILE:O	1:A:245:ARG:CD	2.51	0.59
1:B:20:MET:HG2	1:B:330:VAL:HG13	1.84	0.58
1:A:147:HIS:HB3	1:A:156:ALA:HB2	1.84	0.58
1:A:285:VAL:HG12	1:A:286:GLU:N	2.17	0.58
1:B:544:SER:O	1:B:545:GLU:CB	2.42	0.58
1:A:243:MET:SD	1:A:243:MET:O	2.62	0.57
1:A:58:LEU:HD13	1:A:67:ALA:HB2	1.85	0.57
1:B:145:LEU:HD12	1:B:157:ARG:HG2	1.87	0.57
1:B:198:ILE:O	1:B:198:ILE:HG22	2.04	0.57
1:A:557:ASP:O	1:A:558:MET:HB2	2.05	0.56
1:B:154:VAL:HG21	1:B:174:ILE:CG1	2.33	0.56
1:B:379:PRO:HB2	1:B:380:PRO:HD3	1.86	0.56
1:A:311:MET:HB3	1:A:356:TYR:OH	2.06	0.56
1:B:48:HIS:CE1	1:B:242:ARG:HD2	2.41	0.56
1:A:212:LEU:HD21	1:A:278:ILE:HD12	1.88	0.55
1:A:39:ARG:NH2	3:A:711:HOH:O	2.38	0.55
1:B:46:ARG:CZ	2:B:601:FAD:O2'	2.53	0.55
1:B:303:ASN:OD1	1:B:357:ASP:HB2	2.06	0.55
1:A:198:ILE:O	1:A:198:ILE:HG23	2.07	0.55
1:B:278:ILE:HD12	1:B:280:THR:H	1.72	0.55
1:A:154:VAL:HG21	1:A:174:ILE:CG1	2.37	0.53
1:A:379:PRO:HB2	1:A:380:PRO:HD3	1.91	0.53
1:B:130:GLU:O	1:B:134:ARG:HG3	2.07	0.53
1:B:202:GLY:HA3	1:B:293:TRP:O	2.09	0.53
1:B:546:ILE:HD12	1:B:550:GLY:HA3	1.90	0.53
1:A:84:THR:HG21	1:A:400:LEU:HD11	1.91	0.53
1:A:555:ARG:HD3	1:A:561:ALA:HB2	1.91	0.53
1:B:145:LEU:HD11	1:B:159:LEU:HB2	1.91	0.53
1:B:326:LEU:HD23	1:B:326:LEU:C	2.29	0.53
1:A:425:ILE:HD11	3:A:876:HOH:O	2.09	0.53
1:B:204:ILE:CG2	1:B:254:TRP:CE2	2.93	0.52
1:A:285:VAL:CG1	1:A:286:GLU:N	2.73	0.52
1:B:16:PRO:HD2	2:B:601:FAD:O2P	2.10	0.52
1:A:245:ARG:HB2	1:A:249:LYS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:HA2	2:A:601:FAD:O4B	2.10	0.52
1:B:45:PRO:O	1:B:46:ARG:O	2.28	0.51
1:B:418:ARG:O	1:B:418:ARG:HD3	2.10	0.51
1:B:543:ILE:CG2	1:B:544:SER:N	2.72	0.51
1:B:452:ASP:OD2	1:B:453:PRO:O	2.28	0.51
1:B:543:ILE:O	1:B:544:SER:C	2.49	0.51
1:A:266:THR:HG23	1:A:269:GLU:CG	2.40	0.51
1:B:417:LEU:HD21	1:B:421:MET:HE1	1.91	0.50
1:A:399:ALA:HA	1:A:402:ARG:NH1	2.26	0.50
1:B:182:SER:HB3	1:B:185:ALA:HB3	1.92	0.50
1:A:208:PHE:CD2	1:A:274:ILE:HD13	2.46	0.50
1:A:198:ILE:O	1:A:199:GLY:O	2.30	0.50
1:B:241:LEU:C	1:B:241:LEU:HD12	2.32	0.50
1:A:204:ILE:O	1:A:204:ILE:HG23	2.12	0.49
1:B:196:MET:HG3	1:B:297:GLN:OE1	2.11	0.49
1:A:7:THR:O	1:A:171:ALA:HA	2.11	0.49
1:A:151:GLN:O	1:A:151:GLN:HG2	2.11	0.49
1:B:458:ASP:OD2	1:B:461:PHE:HD2	1.95	0.49
1:B:467:THR:HA	1:B:560:ILE:HD12	1.95	0.49
1:A:46:ARG:O	1:A:47:SER:O	2.30	0.49
1:B:241:LEU:CD2	1:B:278:ILE:HG22	2.42	0.49
1:A:338:TRP:CE3	1:A:556:PRO:HG2	2.48	0.49
1:B:500:THR:OG1	1:B:501:GLY:N	2.46	0.48
1:B:540:TYR:O	1:B:544:SER:HB3	2.13	0.48
1:A:108:GLU:HG3	1:A:114:ARG:NH2	2.29	0.48
1:B:569:ARG:O	1:B:573:GLU:HG3	2.14	0.48
1:A:117:ASP:OD2	1:A:117:ASP:C	2.52	0.48
1:A:385:LEU:HD21	1:A:417:LEU:HD22	1.95	0.48
1:B:484:ARG:HD2	1:B:537:TYR:OH	2.12	0.48
1:A:198:ILE:O	1:A:198:ILE:CG2	2.61	0.48
1:B:205:ASN:N	1:B:205:ASN:ND2	2.62	0.48
1:B:46:ARG:O	1:B:47:SER:C	2.51	0.48
1:B:544:SER:OG	1:B:545:GLU:N	2.47	0.48
1:A:367:ILE:HG13	1:A:368:VAL:N	2.28	0.48
1:A:515:SER:HB2	1:A:520:ILE:O	2.14	0.48
1:A:157:ARG:HG3	3:A:942:HOH:O	2.12	0.48
1:A:387:LEU:HD11	1:A:399:ALA:CB	2.44	0.47
1:B:492:GLY:O	1:B:493:LYS:HB2	2.14	0.47
1:A:206:ILE:HD13	1:A:270:ALA:HB1	1.96	0.47
1:B:302:ARG:HA	1:B:357:ASP:OD1	2.14	0.47
1:A:64:GLU:HG2	1:A:68:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PRO:O	1:A:46:ARG:O	2.32	0.47
1:B:387:LEU:HD11	1:B:396:MET:CE	2.44	0.47
1:B:557:ASP:O	1:B:558:MET:HB2	2.15	0.47
1:A:458:ASP:OD2	3:A:701:HOH:O	2.20	0.47
1:B:158:LEU:HD11	1:B:169:VAL:HG21	1.95	0.47
1:B:502:LEU:HD11	1:B:529:PRO:HD2	1.97	0.47
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.66	0.47
1:B:204:ILE:HG21	1:B:254:TRP:CE2	2.49	0.47
1:A:144:TYR:HB3	2:A:601:FAD:N1A	2.30	0.47
1:A:205:ASN:C	1:A:206:ILE:HG13	2.35	0.46
1:A:245:ARG:HB2	1:A:249:LYS:HB2	1.97	0.46
1:A:213:SER:O	1:A:217:GLU:HB2	2.15	0.46
1:B:479:THR:HA	1:B:483:ARG:O	2.15	0.46
1:A:553:LEU:HB3	1:A:562:PHE:HB3	1.97	0.46
1:B:245:ARG:HB2	1:B:249:LYS:HB2	1.98	0.46
1:B:382:PHE:HE2	1:B:391:PRO:HD2	1.80	0.46
1:B:388:PRO:O	1:B:389:PRO:C	2.53	0.46
1:A:130:GLU:O	1:A:134:ARG:HG3	2.16	0.45
1:B:46:ARG:NE	2:B:601:FAD:O2'	2.50	0.45
1:A:246:PRO:HA	1:A:247:TRP:HA	1.42	0.45
1:B:319:THR:HB	1:B:320:PRO:HD2	1.97	0.45
1:A:141:LEU:HD13	1:A:162:VAL:HG23	1.98	0.45
1:B:246:PRO:HA	1:B:247:TRP:HA	1.62	0.45
1:A:178:ASP:OD2	1:A:184:VAL:HG23	2.17	0.45
1:B:119:PRO:HD2	1:B:122:TYR:CD2	2.52	0.45
1:B:198:ILE:HA	1:B:199:GLY:HA2	1.56	0.45
1:B:417:LEU:CD1	1:B:421:MET:HE3	2.46	0.45
1:A:154:VAL:O	1:A:170:ARG:HD2	2.16	0.45
1:B:387:LEU:CD1	1:B:396:MET:SD	3.05	0.45
1:A:436:LEU:HB3	1:A:463:TYR:CD1	2.52	0.45
1:A:323:GLY:O	1:A:327:ASN:ND2	2.50	0.45
1:A:544:SER:O	1:A:545:GLU:HB2	2.16	0.45
1:A:245:ARG:HD2	1:A:245:ARG:HA	1.57	0.44
1:A:24:LEU:O	1:A:28:LEU:HD12	2.17	0.44
1:A:303:ASN:OD1	1:A:357:ASP:HB2	2.18	0.44
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.87	0.44
1:B:502:LEU:CD1	1:B:529:PRO:HD2	2.48	0.44
1:B:141:LEU:HD13	1:B:162:VAL:HG23	2.00	0.44
1:A:397:ALA:O	1:A:401:VAL:HG23	2.17	0.44
1:B:281:ASP:C	1:B:281:ASP:OD1	2.56	0.44
1:A:385:LEU:HD23	1:A:403:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:HA	1:A:43:PRO:HD2	1.84	0.43
1:A:204:ILE:HD12	1:A:264:GLU:HB3	2.00	0.43
1:B:178:ASP:OD2	1:B:184:VAL:HG23	2.18	0.43
1:B:154:VAL:CG2	1:B:174:ILE:HG13	2.37	0.43
1:A:145:LEU:HD11	1:A:159:LEU:HB2	1.99	0.43
1:A:206:ILE:HG12	1:A:290:ILE:HG12	2.00	0.43
1:A:418:ARG:O	1:A:418:ARG:HD3	2.19	0.43
1:A:58:LEU:CD1	1:A:67:ALA:HB2	2.48	0.43
1:A:91:PHE:CE1	1:A:400:LEU:CD2	3.02	0.43
1:B:225:TRP:CZ3	1:B:378:PHE:CE1	3.07	0.43
1:A:278:ILE:HG22	1:A:280:THR:HG22	2.00	0.43
1:A:422:ASP:O	1:A:425:ILE:HG22	2.19	0.43
1:B:205:ASN:HD22	1:B:205:ASN:N	2.16	0.43
1:B:225:TRP:CZ3	1:B:378:PHE:CZ	3.07	0.43
1:B:379:PRO:N	1:B:380:PRO:CD	2.82	0.43
1:B:266:THR:CG2	1:B:270:ALA:HB2	2.49	0.42
1:B:210:ALA:HB2	1:B:285:VAL:HG22	2.01	0.42
1:A:302:ARG:HA	1:A:357:ASP:OD1	2.19	0.42
1:B:514:VAL:HG22	1:B:576:ASN:HB2	2.01	0.42
1:A:120:GLN:HG3	1:A:326:LEU:HD12	2.01	0.42
1:A:75:GLU:CD	1:A:75:GLU:H	2.22	0.42
1:B:118:LEU:O	1:B:118:LEU:HD23	2.19	0.42
1:B:241:LEU:HD11	1:B:250:TRP:CE3	2.54	0.42
1:A:47:SER:HB3	1:A:326:LEU:HD12	2.02	0.42
1:B:13:GLY:HA2	2:B:601:FAD:O4B	2.18	0.42
1:A:139:ARG:HG3	1:A:142:THR:OG1	2.20	0.42
1:B:53:ARG:NH2	1:B:472:HIS:CD2	2.87	0.42
1:B:555:ARG:HA	1:B:556:PRO:HD3	1.78	0.42
1:A:392:THR:HG23	1:A:395:GLU:OE1	2.19	0.42
1:B:387:LEU:HD13	1:B:391:PRO:HG3	2.01	0.42
1:B:225:TRP:HZ3	1:B:378:PHE:CE1	2.36	0.42
1:B:271:LYS:HE3	1:B:275:HIS:NE2	2.35	0.42
1:A:182:SER:HB3	1:A:185:ALA:HB3	2.02	0.41
1:A:86:LEU:CD2	1:A:212:LEU:HD13	2.49	0.41
1:A:144:TYR:OH	1:A:147:HIS:HD2	2.02	0.41
1:A:147:HIS:HA	1:A:156:ALA:HA	2.00	0.41
1:B:417:LEU:HG	1:B:421:MET:CE	2.49	0.41
1:B:68:LYS:HA	1:B:71:ALA:HB3	2.02	0.41
1:B:79:GLU:O	1:B:221:GLY:HA3	2.20	0.41
1:A:218:HIS:CD2	1:A:219:ARG:HG2	2.55	0.41
1:A:398:GLU:HG3	1:A:402:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:C	1:A:326:LEU:CD2	2.88	0.41
1:A:555:ARG:CD	1:A:561:ALA:HB2	2.49	0.41
1:B:481:ASN:O	1:B:482:GLN:HB2	2.20	0.41
1:A:432:HIS:NE2	1:A:436:LEU:HD22	2.36	0.41
1:A:83:ALA:HB2	1:A:90:GLU:HA	2.02	0.41
1:A:144:TYR:OH	1:A:146:GLY:HA2	2.20	0.41
1:A:217:GLU:OE1	1:A:217:GLU:CA	2.50	0.41
1:A:243:MET:SD	1:A:243:MET:C	2.99	0.41
1:A:206:ILE:CD1	1:A:254:TRP:HH2	2.28	0.41
1:A:458:ASP:OD1	1:A:458:ASP:C	2.58	0.41
1:B:223:MET:HE2	1:B:225:TRP:HE1	1.85	0.41
1:B:314:ALA:O	1:B:317:ARG:NH2	2.53	0.41
1:A:398:GLU:HG3	1:A:402:ARG:HH11	1.85	0.41
1:B:311:MET:HB3	1:B:356:TYR:OH	2.21	0.40
1:A:393:GLU:HG2	1:A:393:GLU:H	1.67	0.40
1:A:91:PHE:CE1	1:A:400:LEU:HD21	2.57	0.40
1:A:46:ARG:NH2	2:A:601:FAD:O4'	2.54	0.40
1:A:312:GLY:HA3	2:A:601:FAD:O1P	2.22	0.40
1:B:209:SER:O	1:B:210:ALA:HB2	2.20	0.40
1:A:379:PRO:N	1:A:380:PRO:CD	2.84	0.40
1:A:446:PHE:HA	1:A:447:PRO:HD3	1.73	0.40
1:A:508:LYS:HD2	1:A:508:LYS:HA	1.94	0.40
1:B:200:ASP:OD1	1:B:200:ASP:O	2.40	0.40
1:B:387:LEU:HA	1:B:387:LEU:HD23	1.80	0.40
1:B:225:TRP:HZ3	1:B:378:PHE:CZ	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	560/592 (95%)	524 (94%)	27 (5%)	9 (2%)	11 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	557/592 (94%)	512 (92%)	41 (7%)	4 (1%)	25	30
All	All	1117/1184 (94%)	1036 (93%)	68 (6%)	13 (1%)	15	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	206	ILE
1	B	46	ARG
1	A	47	SER
1	A	198	ILE
1	A	199	GLY
1	A	493	LYS
1	B	47	SER
1	B	406	ALA
1	B	545	GLU
1	A	6	GLU
1	A	391	PRO
1	A	73	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/473 (96%)	446 (99%)	6 (1%)	73	86
1	B	451/473 (95%)	443 (98%)	8 (2%)	64	79
All	All	903/946 (96%)	889 (98%)	14 (2%)	68	82

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

Mol	Chain	Res	Type
1	A	47	SER
1	A	143	GLU
1	A	196	MET

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Mol	Chain	Res	Type
1	A	245	ARG
1	A	277	ILE
1	A	319	THR
1	B	47	SER
1	B	59	ARG
1	B	205	ASN
1	B	241	LEU
1	B	319	THR
1	B	329	SER
1	B	353	LEU
1	B	495	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	205	ASN
1	B	147	HIS
1	B	205	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	601	-	51,58,58	2.39	16 (31%)	54,89,89	2.95	17 (31%)
2	FAD	B	601	-	51,58,58	2.32	17 (33%)	54,89,89	2.94	19 (35%)

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	601	-	1/1/9/9	0/28/50/50	0/6/6/6
2	FAD	B	601	-	1/1/9/9	0/28/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C1'-N10	-4.42	1.43	1.48
2	A	601	FAD	C2B-C1B	-4.01	1.47	1.53
2	B	601	FAD	C1'-N10	-3.88	1.44	1.48
2	B	601	FAD	C2B-C1B	-3.73	1.47	1.53
2	B	601	FAD	O2B-C2B	-2.50	1.37	1.43
2	B	601	FAD	O3'-C3'	-2.39	1.37	1.43
2	A	601	FAD	O2B-C2B	-2.34	1.37	1.43
2	A	601	FAD	O3'-C3'	-2.22	1.37	1.43
2	A	601	FAD	O3B-C3B	-2.15	1.38	1.43
2	B	601	FAD	O4B-C4B	-2.07	1.40	1.45
2	B	601	FAD	O3B-C3B	-2.05	1.38	1.43
2	B	601	FAD	O4'-C4'	-2.03	1.38	1.43
2	A	601	FAD	C2-N3	2.09	1.42	1.38
2	A	601	FAD	C6A-N6A	2.09	1.42	1.34
2	B	601	FAD	C6A-N6A	2.19	1.43	1.34
2	A	601	FAD	C2A-N3A	2.39	1.36	1.32
2	B	601	FAD	C2A-N3A	2.42	1.36	1.32
2	A	601	FAD	O2'-C2'	2.46	1.48	1.43
2	A	601	FAD	C4-C4X	2.55	1.46	1.41
2	B	601	FAD	O2'-C2'	2.78	1.49	1.43
2	B	601	FAD	C4-C4X	2.93	1.46	1.41
2	A	601	FAD	C9A-N10	3.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C4-N3	3.10	1.38	1.33
2	A	601	FAD	C4-N3	3.54	1.39	1.33
2	B	601	FAD	C9A-N10	4.01	1.44	1.38
2	A	601	FAD	C2'-C3'	4.04	1.61	1.53
2	B	601	FAD	C2-N1	4.18	1.46	1.38
2	B	601	FAD	C2'-C3'	4.31	1.62	1.53
2	A	601	FAD	C2-N1	4.31	1.46	1.38
2	B	601	FAD	C4X-C10	5.83	1.51	1.41
2	A	601	FAD	C4X-C10	6.17	1.51	1.41
2	B	601	FAD	C5X-N5	8.04	1.47	1.35
2	A	601	FAD	C5X-N5	8.94	1.49	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	N3A-C2A-N1A	-10.17	120.00	128.86
2	A	601	FAD	N3A-C2A-N1A	-10.01	120.14	128.86
2	B	601	FAD	O5'-P-O1P	-6.47	83.14	109.25
2	A	601	FAD	O5'-P-O1P	-6.20	84.23	109.25
2	A	601	FAD	C4X-C10-N10	-5.57	116.66	120.52
2	B	601	FAD	O2P-P-O5'	-5.06	84.26	108.14
2	A	601	FAD	O2P-P-O5'	-4.89	85.07	108.14
2	B	601	FAD	C4X-C10-N10	-4.31	117.53	120.52
2	B	601	FAD	C4X-C4-N3	-4.08	117.68	123.48
2	A	601	FAD	C4X-C4-N3	-3.99	117.80	123.48
2	A	601	FAD	C4-C4X-C10	-3.21	117.37	119.96
2	A	601	FAD	C4A-C5A-N7A	-2.73	106.77	109.41
2	B	601	FAD	C4B-O4B-C1B	-2.48	107.13	109.77
2	B	601	FAD	C4A-C5A-N7A	-2.29	107.19	109.41
2	B	601	FAD	C1'-N10-C10	-2.13	116.32	118.50
2	A	601	FAD	C1B-N9A-C4A	-2.07	123.07	126.64
2	B	601	FAD	C4-C4X-C10	-2.02	118.33	119.96
2	B	601	FAD	C4-C4X-N5	2.10	120.98	118.68
2	A	601	FAD	C4-C4X-N5	2.31	121.21	118.68
2	A	601	FAD	C4X-N5-C5X	2.39	119.29	116.76
2	B	601	FAD	C1'-N10-C9A	2.75	120.87	118.35
2	A	601	FAD	C1'-C2'-C3'	2.96	118.29	109.82
2	B	601	FAD	C1'-C2'-C3'	2.98	118.34	109.82
2	A	601	FAD	O3'-C3'-C2'	3.18	116.69	108.82
2	B	601	FAD	C4X-N5-C5X	3.28	120.23	116.76
2	B	601	FAD	O3'-C3'-C4'	3.40	117.25	108.82
2	A	601	FAD	O3'-C3'-C4'	3.43	117.32	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O3'-C3'-C2'	3.72	118.02	108.82
2	A	601	FAD	O2'-C2'-C1'	3.86	118.71	109.79
2	B	601	FAD	O2'-C2'-C3'	4.06	119.16	109.09
2	B	601	FAD	O2'-C2'-C1'	4.41	119.98	109.79
2	B	601	FAD	C4'-C3'-C2'	4.69	123.50	113.41
2	A	601	FAD	O2'-C2'-C3'	4.72	120.81	109.09
2	A	601	FAD	C4'-C3'-C2'	5.23	124.67	113.41
2	B	601	FAD	C4-N3-C2	10.52	124.36	115.16
2	A	601	FAD	C4-N3-C2	10.82	124.62	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	FAD	C3'
2	B	601	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	7	0
2	B	601	FAD	7	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	566/592 (95%)	0.70	65 (11%) 5 8	7, 22, 58, 126	0
1	B	563/592 (95%)	0.76	61 (10%) 6 9	9, 22, 70, 126	0
All	All	1129/1184 (95%)	0.73	126 (11%) 6 8	7, 22, 65, 126	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	ILE	15.4
1	A	198	ILE	10.7
1	B	392	THR	10.3
1	B	200	ASP	9.3
1	A	197	GLY	9.0
1	B	199	GLY	8.7
1	B	202	GLY	8.0
1	A	199	GLY	7.9
1	A	196	MET	7.7
1	A	200	ASP	6.7
1	B	265	ILE	6.6
1	B	194	GLY	6.3
1	B	201	SER	6.3
1	A	282	GLU	6.1
1	B	196	MET	5.8
1	A	256	TYR	5.8
1	B	390	ALA	5.6
1	B	388	PRO	5.5
1	A	264	GLU	5.4
1	B	393	GLU	5.2
1	A	202	GLY	5.0
1	B	197	GLY	5.0
1	A	195	GLN	5.0
1	A	516	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	268	GLU	4.9
1	A	388	PRO	4.9
1	B	264	GLU	4.8
1	B	569	ARG	4.8
1	B	282	GLU	4.7
1	A	265	ILE	4.7
1	B	268	GLU	4.5
1	B	270	ALA	4.4
1	B	210	ALA	4.3
1	B	266	THR	4.3
1	A	194	GLY	4.2
1	A	391	PRO	4.1
1	B	195	GLN	4.1
1	B	267	LYS	4.1
1	B	389	PRO	4.0
1	A	281	ASP	4.0
1	B	509	HIS	4.0
1	B	151	GLN	3.9
1	B	516	GLN	3.9
1	A	201	SER	3.9
1	B	281	ASP	3.9
1	A	296	ASN	3.8
1	A	263	PRO	3.8
1	B	391	PRO	3.8
1	B	271	LYS	3.8
1	A	272	LYS	3.6
1	A	390	ALA	3.5
1	B	283	ILE	3.4
1	A	270	ALA	3.4
1	B	254	TRP	3.3
1	B	454	GLY	3.3
1	B	398	GLU	3.2
1	A	148	VAL	3.2
1	A	151	GLN	3.2
1	A	392	THR	3.2
1	A	254	TRP	3.2
1	B	211	ASP	3.2
1	B	296	ASN	3.1
1	A	389	PRO	3.1
1	B	269	GLU	3.1
1	A	144	TYR	3.1
1	B	394	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	517	SER	3.1
1	A	295	ILE	3.1
1	A	248	ASN	3.0
1	A	285	VAL	3.0
1	A	267	LYS	2.9
1	B	247	TRP	2.9
1	B	513	GLN	2.9
1	A	210	ALA	2.8
1	B	287	VAL	2.8
1	B	67	ALA	2.8
1	A	238	VAL	2.8
1	A	271	LYS	2.7
1	A	495	ARG	2.7
1	B	272	LYS	2.7
1	A	237	GLY	2.7
1	B	248	ASN	2.6
1	B	406	ALA	2.6
1	B	285	VAL	2.5
1	A	249	LYS	2.5
1	B	150	ASP	2.5
1	A	255	GLY	2.5
1	A	253	VAL	2.5
1	A	387	LEU	2.5
1	A	266	THR	2.4
1	A	330	VAL	2.4
1	B	278	ILE	2.4
1	A	239	ALA	2.4
1	A	386	SER	2.4
1	A	385	LEU	2.3
1	A	211	ASP	2.3
1	A	246	PRO	2.3
1	B	217	GLU	2.3
1	A	269	GLU	2.3
1	B	379	PRO	2.3
1	A	286	GLU	2.2
1	A	98	ALA	2.2
1	B	273	ILE	2.2
1	A	217	GLU	2.2
1	B	544	SER	2.2
1	B	280	THR	2.2
1	A	409	GLU	2.2
1	B	554	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	512	GLU	2.1
1	B	148	VAL	2.1
1	A	156	ALA	2.1
1	A	456	VAL	2.1
1	B	514	VAL	2.1
1	A	46	ARG	2.1
1	A	143	GLU	2.1
1	A	536	THR	2.1
1	B	515	SER	2.1
1	A	169	VAL	2.1
1	B	380	PRO	2.0
1	A	569	ARG	2.0
1	B	46	ARG	2.0
1	B	508	LYS	2.0
1	A	444	ALA	2.0
1	A	509	HIS	2.0
1	A	205	ASN	2.0
1	A	512	GLU	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(Å <sup>2</sup> )	Q<0.9
2	FAD	B	601	53/53	0.91	0.17	0.02	17,29,44,46	0
2	FAD	A	601	53/53	0.93	0.16	-0.23	18,27,41,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.