Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 09:10 PM EST

PDB ID	:	1NDH
Title	:	CRYSTAL STRUCTURE OF NADH-CYTOCHROME B5 REDUCTASE FROM PIG LIVER AT 2.4 ANGSTROMS RESOLUTION
Authors	:	Nishida, H.; Miki, K.
Deposited on	:	1994-10-31
Resolution	:	2.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
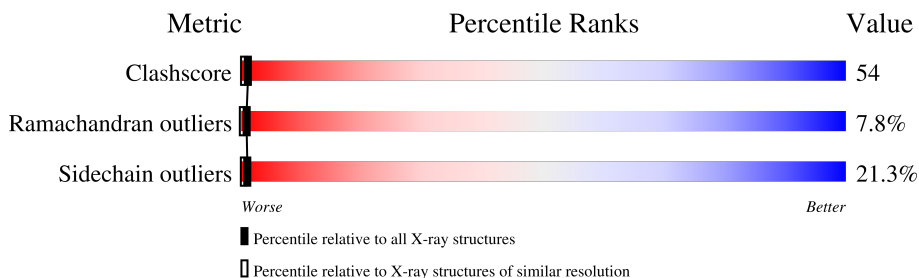http://www.wwpdb.org/validation/2017/FAQs#types.

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 2.10 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	Percentile Ranks	Value
Clashscore		54
Ramachandran outliers		7.8%
Sidechain outliers		21.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	272	33% 38% 17% 12% •

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	273	X	-	-	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2259 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 CYTOCHROME B5 REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2158	1386	371	389	12	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	VAL	ILE	conflict	UNP P83686
A	25	ASN	SER	conflict	UNP P83686
A	137	SER	ASP	conflict	UNP P83686
A	212	ARG	LYS	conflict	UNP P83686
A	260	GLU	ASP	conflict	UNP P83686

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

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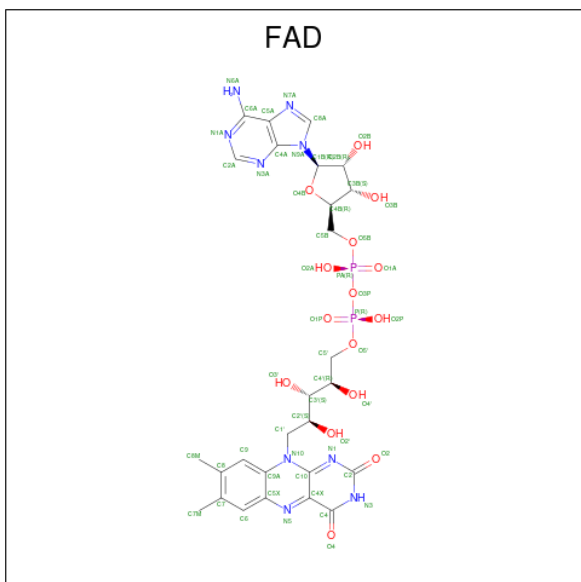
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: CYTOCHROME B5 REDUCTASE

Chain A:
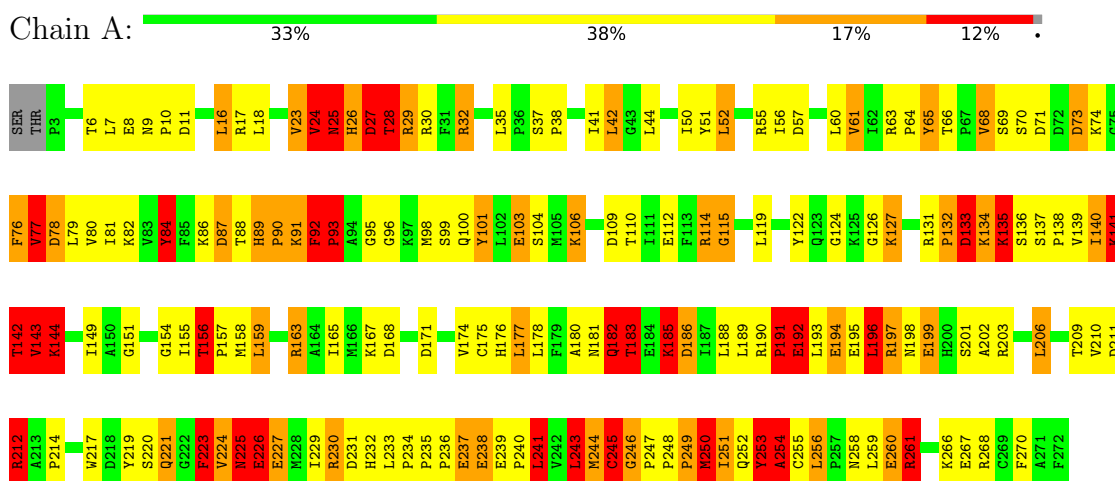
4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.90Å 73.10Å 48.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.223 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2259	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.11	2/2217 (0.1%)	2.40	141/3006 (4.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLY	C-N	6.17	1.46	1.34
1	A	203	ARG	CD-NE	-5.51	1.37	1.46

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	CD-NE-CZ	32.86	169.61	123.60
1	A	268	ARG	NE-CZ-NH1	15.61	128.11	120.30
1	A	131	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	A	203	ARG	NE-CZ-NH1	-12.17	114.21	120.30
1	A	244	MET	CG-SD-CE	11.95	119.31	100.20
1	A	163	ARG	NE-CZ-NH2	-11.33	114.63	120.30
1	A	114	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	A	191	PRO	O-C-N	10.16	138.96	122.70
1	A	57	ASP	CB-CG-OD2	9.84	127.15	118.30
1	A	55	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	A	192	GLU	O-C-N	9.58	138.03	122.70
1	A	25	ASN	CA-CB-CG	-9.42	92.67	113.40
1	A	71	ASP	CB-CG-OD1	9.11	126.50	118.30
1	A	122	TYR	CB-CG-CD2	8.71	126.23	121.00
1	A	195	GLU	CB-CA-C	8.63	127.66	110.40
1	A	77	VAL	C-N-CA	8.61	143.24	121.70
1	A	212	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	A	186	ASP	N-CA-CB	8.44	125.79	110.60
1	A	55	ARG	NE-CZ-NH1	8.37	124.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	ALA	N-CA-CB	8.27	121.68	110.10
1	A	260	GLU	CA-CB-CG	8.23	131.51	113.40
1	A	198	ASN	CB-CA-C	8.20	126.81	110.40
1	A	197	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	32	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	A	199	GLU	CB-CG-CD	8.00	135.80	114.20
1	A	192	GLU	CA-C-N	-7.90	99.81	117.20
1	A	92	PHE	CB-CA-C	7.85	126.10	110.40
1	A	90	PRO	O-C-N	7.75	135.10	122.70
1	A	77	VAL	CA-CB-CG1	7.74	122.51	110.90
1	A	188	LEU	CB-CA-C	-7.67	95.63	110.20
1	A	76	PHE	C-N-CA	7.65	140.82	121.70
1	A	144	LYS	CA-C-O	-7.61	104.13	120.10
1	A	28	THR	N-CA-CB	-7.59	95.89	110.30
1	A	197	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	246	GLY	N-CA-C	-7.51	94.31	113.10
1	A	80	VAL	CA-CB-CG1	7.45	122.08	110.90
1	A	60	LEU	O-C-N	7.40	134.53	122.70
1	A	78	ASP	CA-C-N	-7.39	100.93	117.20
1	A	244	MET	N-CA-CB	7.37	123.87	110.60
1	A	186	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	260	GLU	CG-CD-OE2	7.23	132.76	118.30
1	A	139	VAL	CB-CA-C	7.16	125.00	111.40
1	A	141	LYS	C-N-CA	7.08	139.41	121.70
1	A	32	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	A	156	THR	N-CA-CB	-7.02	96.96	110.30
1	A	78	ASP	CA-C-O	6.91	134.62	120.10
1	A	142	THR	N-CA-CB	6.91	123.43	110.30
1	A	142	THR	C-N-CA	6.75	138.57	121.70
1	A	209	THR	N-CA-CB	6.75	123.12	110.30
1	A	23	VAL	CB-CA-C	6.65	124.04	111.40
1	A	245	CYS	N-CA-CB	-6.63	98.66	110.60
1	A	245	CYS	CA-CB-SG	-6.59	102.14	114.00
1	A	231	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	225	ASN	C-N-CA	6.53	138.02	121.70
1	A	245	CYS	O-C-N	-6.48	112.19	123.20
1	A	244	MET	CA-CB-CG	6.47	124.30	113.30
1	A	139	VAL	N-CA-C	-6.46	93.55	111.00
1	A	78	ASP	CA-CB-CG	-6.45	99.22	113.40
1	A	223	PHE	O-C-N	6.44	133.00	122.70
1	A	268	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	A	243	LEU	C-N-CA	6.41	137.71	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	A	206	LEU	CA-CB-CG	6.36	129.92	115.30
1	A	139	VAL	O-C-N	6.35	132.85	122.70
1	A	112	GLU	OE1-CD-OE2	6.25	130.80	123.30
1	A	57	ASP	OD1-CG-OD2	-6.23	111.46	123.30
1	A	144	LYS	CA-CB-CG	6.20	127.03	113.40
1	A	143	VAL	C-N-CA	6.19	137.17	121.70
1	A	68	VAL	CG1-CB-CG2	6.17	120.77	110.90
1	A	114	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	103	GLU	CA-CB-CG	6.13	126.89	113.40
1	A	197	ARG	CD-NE-CZ	6.12	132.17	123.60
1	A	261	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	168	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	91	LYS	C-N-CA	6.08	136.89	121.70
1	A	57	ASP	CB-CA-C	6.04	122.48	110.40
1	A	163	ARG	NH1-CZ-NH2	6.02	126.03	119.40
1	A	61	VAL	CB-CA-C	6.00	122.81	111.40
1	A	212	ARG	CD-NE-CZ	5.97	131.96	123.60
1	A	241	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	171	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	76	PHE	O-C-N	5.92	132.16	122.70
1	A	71	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	84	TYR	CB-CG-CD1	5.84	124.50	121.00
1	A	122	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	192	GLU	CB-CA-C	5.80	122.00	110.40
1	A	212	ARG	NH1-CZ-NH2	-5.75	113.07	119.40
1	A	144	LYS	CA-C-N	5.75	129.85	117.20
1	A	25	ASN	N-CA-C	5.71	126.42	111.00
1	A	182	GLN	CB-CA-C	5.67	121.75	110.40
1	A	188	LEU	N-CA-CB	5.66	121.72	110.40
1	A	250	MET	CA-CB-CG	5.66	122.92	113.30
1	A	16	LEU	O-C-N	5.66	131.75	122.70
1	A	29	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	65	TYR	O-C-N	5.59	131.64	122.70
1	A	231	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	18	LEU	O-C-N	5.56	131.60	122.70
1	A	91	LYS	CA-C-O	5.55	131.75	120.10
1	A	131	ARG	NH1-CZ-NH2	5.52	125.47	119.40
1	A	24	VAL	CA-C-O	5.50	131.66	120.10
1	A	249	PRO	C-N-CA	5.46	135.34	121.70
1	A	223	PHE	C-N-CA	5.44	135.31	121.70
1	A	139	VAL	CA-C-N	-5.43	105.24	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	CB-CA-C	-5.43	99.55	110.40
1	A	238	GLU	CA-CB-CG	5.42	125.33	113.40
1	A	27	ASP	CA-C-N	-5.41	105.29	117.20
1	A	44	LEU	CB-CA-C	5.40	120.46	110.20
1	A	183	THR	CB-CA-C	5.38	126.11	111.60
1	A	101	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	186	ASP	OD1-CG-OD2	-5.35	113.14	123.30
1	A	26	HIS	N-CA-C	-5.32	96.63	111.00
1	A	226	GLU	N-CA-CB	5.31	120.15	110.60
1	A	196	LEU	C-N-CA	5.30	134.96	121.70
1	A	115	GLY	N-CA-C	5.30	126.35	113.10
1	A	133	ASP	O-C-N	5.29	131.17	122.70
1	A	196	LEU	CB-CA-C	5.29	120.26	110.20
1	A	141	LYS	N-CA-C	-5.27	96.78	111.00
1	A	254	ALA	N-CA-CB	5.27	117.47	110.10
1	A	73	ASP	CB-CA-C	5.25	120.90	110.40
1	A	25	ASN	OD1-CG-ND2	5.25	133.97	121.90
1	A	74	LYS	N-CA-CB	5.23	120.01	110.60
1	A	194	GLU	CA-C-O	5.20	131.03	120.10
1	A	203	ARG	CA-CB-CG	5.20	124.84	113.40
1	A	9	ASN	O-C-N	5.20	130.97	121.10
1	A	245	CYS	CA-C-O	5.19	131.00	120.10
1	A	143	VAL	CA-C-N	-5.17	105.82	117.20
1	A	156	THR	CA-CB-CG2	5.15	119.61	112.40
1	A	91	LYS	CA-C-N	-5.14	105.89	117.20
1	A	195	GLU	OE1-CD-OE2	-5.11	117.16	123.30
1	A	253	TYR	CG-CD1-CE1	5.10	125.38	121.30
1	A	260	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	A	135	LYS	N-CA-CB	5.06	119.71	110.60
1	A	87	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	A	188	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	28	THR	CA-C-N	-5.04	106.11	117.20
1	A	51	TYR	CB-CG-CD2	5.04	124.02	121.00
1	A	88	THR	N-CA-CB	-5.02	100.76	110.30
1	A	185	LYS	CA-C-O	-5.02	109.56	120.10
1	A	156	THR	CB-CA-C	5.01	125.12	111.60
1	A	199	GLU	CA-CB-CG	5.01	124.42	113.40
1	A	232	HIS	CA-CB-CG	-5.01	105.09	113.60

There are no chirality outliers.

There are no planarity outliers.

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	2158	0	2166	231	0
2	A	53	0	31	11	0
3	A	48	0	0	2	0
All	All	2259	0	2197	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 54.

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:89:HIS:HB3	1:A:90:PRO:CD	1.60	1.31
1:A:32:ARG:HE	1:A:79:LEU:HD11	0.99	1.14
1:A:89:HIS:HB3	1:A:90:PRO:HD2	1.29	1.13
1:A:185:LYS:HZ1	1:A:186:ASP:HB2	1.06	1.12
1:A:154:GLY:HA3	1:A:248:PRO:HG2	1.33	1.09
1:A:151:GLY:H	1:A:248:PRO:HD2	1.14	1.07
1:A:32:ARG:HH21	1:A:79:LEU:HD21	1.18	1.05
1:A:32:ARG:NE	1:A:79:LEU:HD11	1.76	1.00
1:A:89:HIS:HB3	1:A:90:PRO:HD3	1.44	0.99
1:A:244:MET:SD	1:A:248:PRO:HG3	2.02	0.98
1:A:151:GLY:N	1:A:248:PRO:HD2	1.79	0.97
1:A:185:LYS:HD3	1:A:186:ASP:H	1.30	0.97
2:A:273:FAD:H5'1	2:A:273:FAD:O2'	1.63	0.96
1:A:89:HIS:CB	1:A:90:PRO:CD	2.45	0.94
1:A:185:LYS:NZ	1:A:186:ASP:HB2	1.82	0.93
1:A:126:GLY:HA3	1:A:143:VAL:HA	1.50	0.93
1:A:193:LEU:HG	1:A:196:LEU:HB3	1.52	0.91
1:A:191:PRO:O	1:A:193:LEU:N	2.06	0.89
1:A:41:ILE:HA	1:A:77:VAL:HG21	1.54	0.87
1:A:193:LEU:O	1:A:196:LEU:HG	1.73	0.87
1:A:84:TYR:CE1	1:A:100:GLN:HG2	2.10	0.86
1:A:89:HIS:CB	1:A:90:PRO:HD2	2.06	0.86
1:A:229:ILE:HA	1:A:233:LEU:HD23	1.58	0.84
1:A:66:THR:HB	1:A:156:THR:HG23	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HD3	1:A:186:ASP:N	1.91	0.83
1:A:70:SER:O	1:A:77:VAL:HG13	1.79	0.83
1:A:84:TYR:HE1	1:A:86:LYS:HA	1.44	0.82
1:A:142:THR:O	1:A:144:LYS:N	2.12	0.81
1:A:241:LEU:HD13	1:A:243:LEU:HD11	1.63	0.81
1:A:132:PRO:HG2	1:A:133:ASP:H	1.44	0.81
1:A:35:LEU:HD11	1:A:77:VAL:HB	1.62	0.80
1:A:84:TYR:CE2	1:A:100:GLN:HA	2.17	0.79
1:A:183:THR:CB	1:A:185:LYS:HD2	2.13	0.79
1:A:32:ARG:HH21	1:A:79:LEU:CD2	1.97	0.78
1:A:127:LYS:HB3	1:A:140:ILE:HA	1.67	0.76
1:A:84:TYR:HE2	1:A:103:GLU:HB3	1.50	0.76
1:A:247:PRO:C	1:A:249:PRO:HD2	2.06	0.76
1:A:183:THR:OG1	1:A:185:LYS:HD2	1.86	0.75
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.52	0.75
1:A:84:TYR:CZ	1:A:100:GLN:HG2	2.21	0.75
1:A:24:VAL:HG22	1:A:28:THR:HB	1.68	0.74
1:A:73:ASP:C	1:A:77:VAL:HG22	2.08	0.74
1:A:156:THR:HG21	2:A:273:FAD:O4	1.87	0.73
1:A:223:PHE:CZ	1:A:247:PRO:HD3	2.23	0.73
1:A:32:ARG:HE	1:A:79:LEU:CD1	1.92	0.73
1:A:76:PHE:C	1:A:78:ASP:H	1.81	0.72
1:A:158:MET:CE	1:A:244:MET:HB2	2.19	0.72
1:A:191:PRO:C	1:A:193:LEU:N	2.41	0.72
1:A:142:THR:C	1:A:144:LYS:H	1.90	0.71
1:A:224:VAL:O	1:A:226:GLU:N	2.24	0.71
1:A:42:LEU:H	1:A:77:VAL:CG1	2.03	0.71
1:A:42:LEU:H	1:A:77:VAL:HG11	1.55	0.71
1:A:141:LYS:HZ3	1:A:143:VAL:HG13	1.53	0.71
1:A:223:PHE:CD1	1:A:224:VAL:N	2.58	0.71
1:A:26:HIS:CE1	1:A:189:LEU:H	2.09	0.70
2:A:273:FAD:H4B	2:A:273:FAD:C8A	2.22	0.70
1:A:189:LEU:HA	1:A:192:GLU:OE1	1.91	0.70
1:A:132:PRO:CG	1:A:133:ASP:H	2.04	0.69
1:A:191:PRO:C	1:A:193:LEU:H	1.92	0.69
1:A:37:SER:HB2	1:A:38:PRO:CD	2.23	0.68
1:A:191:PRO:O	1:A:193:LEU:CA	2.43	0.67
1:A:76:PHE:O	1:A:78:ASP:N	2.25	0.67
1:A:223:PHE:HD1	1:A:224:VAL:N	1.93	0.67
1:A:76:PHE:CD2	1:A:79:LEU:HD13	2.30	0.67
1:A:84:TYR:CE2	1:A:103:GLU:HB3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:CYS:O	1:A:256:LEU:HG	1.94	0.66
1:A:154:GLY:HA3	1:A:248:PRO:CG	2.18	0.66
1:A:229:ILE:HD12	1:A:258:ASN:HB3	1.78	0.66
1:A:63:ARG:HB3	2:A:273:FAD:O3'	1.96	0.65
1:A:183:THR:HG23	1:A:185:LYS:HE2	1.77	0.65
1:A:225:ASN:HB2	1:A:227:GLU:HG2	1.79	0.65
1:A:229:ILE:HA	1:A:233:LEU:CD2	2.26	0.65
1:A:212:ARG:HH11	1:A:212:ARG:HG2	1.60	0.65
1:A:252:GLN:O	1:A:253:TYR:HB2	1.96	0.64
1:A:25:ASN:ND2	3:A:299:HOH:O	2.29	0.64
1:A:141:LYS:HA	1:A:143:VAL:CG1	2.27	0.64
1:A:250:MET:O	1:A:252:GLN:N	2.30	0.64
1:A:255:CYS:SG	1:A:256:LEU:N	2.70	0.63
1:A:32:ARG:NH2	1:A:79:LEU:HD21	2.03	0.63
1:A:151:GLY:H	1:A:248:PRO:CD	2.03	0.62
1:A:66:THR:HB	1:A:156:THR:CG2	2.30	0.62
1:A:191:PRO:O	1:A:193:LEU:HA	2.00	0.62
1:A:244:MET:SD	1:A:248:PRO:CG	2.86	0.61
1:A:212:ARG:NH1	1:A:212:ARG:O	2.34	0.61
1:A:25:ASN:C	1:A:27:ASP:N	2.51	0.60
1:A:50:ILE:HG13	1:A:65:TYR:O	2.02	0.60
1:A:185:LYS:CD	1:A:186:ASP:H	2.09	0.60
1:A:224:VAL:HG13	1:A:225:ASN:N	2.15	0.60
1:A:217:TRP:CE2	1:A:219:TYR:HB2	2.37	0.60
1:A:217:TRP:CZ2	1:A:219:TYR:HB2	2.37	0.60
1:A:181:ASN:O	1:A:210:VAL:HA	2.02	0.59
1:A:84:TYR:CE1	1:A:86:LYS:HA	2.34	0.59
1:A:26:HIS:O	1:A:27:ASP:HB2	2.03	0.59
1:A:235:PRO:HB2	1:A:237:GLU:OE1	2.03	0.59
1:A:73:ASP:O	1:A:77:VAL:HG22	2.02	0.59
1:A:158:MET:HE1	1:A:244:MET:HB2	1.84	0.58
1:A:11:ASP:O	1:A:114:ARG:NH2	2.37	0.58
1:A:27:ASP:HA	3:A:300:HOH:O	2.03	0.58
1:A:182:GLN:O	1:A:211:ASP:HB2	2.03	0.58
1:A:193:LEU:O	1:A:196:LEU:HB3	2.04	0.58
1:A:65:TYR:CE1	2:A:273:FAD:H3'	2.38	0.58
1:A:30:ARG:HG2	1:A:30:ARG:NH1	2.18	0.58
1:A:223:PHE:O	1:A:225:ASN:ND2	2.37	0.58
1:A:224:VAL:HG22	1:A:258:ASN:OD1	2.05	0.57
1:A:76:PHE:HD2	1:A:79:LEU:HD13	1.71	0.56
1:A:106:LYS:HG2	1:A:109:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:MET:O	1:A:252:GLN:HG2	2.05	0.56
1:A:87:ASP:HB2	1:A:93:PRO:O	2.05	0.56
1:A:26:HIS:CD2	1:A:28:THR:HG21	2.41	0.56
1:A:52:LEU:HD22	1:A:65:TYR:CD2	2.41	0.56
1:A:214:PRO:HD2	1:A:217:TRP:HB2	1.87	0.56
1:A:156:THR:HG22	1:A:157:PRO:HD3	1.88	0.56
1:A:241:LEU:HD13	1:A:243:LEU:CD1	2.34	0.56
2:A:273:FAD:C8A	2:A:273:FAD:C4B	2.83	0.56
1:A:244:MET:CE	1:A:248:PRO:HB3	2.37	0.55
1:A:84:TYR:CE2	1:A:103:GLU:CB	2.89	0.55
1:A:182:GLN:NE2	1:A:182:GLN:N	2.55	0.55
1:A:183:THR:CA	1:A:185:LYS:HD2	2.37	0.55
1:A:149:ILE:O	1:A:244:MET:O	2.25	0.54
1:A:37:SER:HB2	1:A:38:PRO:HD2	1.89	0.54
1:A:17:ARG:HA	1:A:110:THR:HG22	1.89	0.54
1:A:50:ILE:HD11	1:A:65:TYR:HB2	1.89	0.54
1:A:252:GLN:O	1:A:253:TYR:CB	2.55	0.54
1:A:134:LYS:HD3	1:A:134:LYS:C	2.28	0.54
1:A:246:GLY:N	1:A:256:LEU:HD21	2.23	0.54
1:A:106:LYS:HE3	1:A:109:ASP:OD2	2.07	0.54
1:A:26:HIS:HD2	1:A:28:THR:HG21	1.73	0.54
1:A:185:LYS:CD	1:A:186:ASP:N	2.68	0.54
1:A:91:LYS:O	1:A:92:PHE:O	2.26	0.53
1:A:37:SER:CB	1:A:38:PRO:CD	2.85	0.53
1:A:50:ILE:HD13	1:A:52:LEU:HD13	1.91	0.53
1:A:182:GLN:N	1:A:182:GLN:HE21	2.06	0.53
1:A:183:THR:HG23	1:A:185:LYS:CE	2.39	0.53
1:A:194:GLU:O	1:A:196:LEU:N	2.37	0.53
1:A:193:LEU:O	1:A:196:LEU:CG	2.52	0.53
1:A:84:TYR:CE1	1:A:86:LYS:HG3	2.44	0.53
1:A:106:LYS:HG2	1:A:109:ASP:CG	2.30	0.52
2:A:273:FAD:H5'1	2:A:273:FAD:HO2'	1.71	0.52
1:A:25:ASN:O	1:A:26:HIS:C	2.44	0.52
1:A:233:LEU:HD22	1:A:233:LEU:N	2.24	0.52
2:A:273:FAD:H4B	2:A:273:FAD:H8A	1.92	0.51
1:A:248:PRO:N	1:A:249:PRO:HD2	2.26	0.51
1:A:76:PHE:O	1:A:78:ASP:CA	2.59	0.50
1:A:84:TYR:CE2	1:A:103:GLU:HG2	2.46	0.50
1:A:224:VAL:CG2	1:A:258:ASN:OD1	2.60	0.50
1:A:217:TRP:NE1	1:A:220:SER:O	2.37	0.50
1:A:230:ARG:NH1	1:A:230:ARG:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HB2	1:A:81:ILE:CD1	2.42	0.50
1:A:151:GLY:HA3	1:A:247:PRO:HB2	1.94	0.50
1:A:193:LEU:O	1:A:196:LEU:CB	2.60	0.50
1:A:66:THR:HG21	1:A:157:PRO:HA	1.94	0.50
1:A:185:LYS:NZ	1:A:186:ASP:CB	2.67	0.50
1:A:10:PRO:HA	1:A:115:GLY:O	2.11	0.49
1:A:159:LEU:HD13	1:A:163:ARG:NH1	2.27	0.49
1:A:223:PHE:HE2	1:A:247:PRO:HG3	1.77	0.49
1:A:190:ARG:HB3	1:A:191:PRO:HD3	1.94	0.49
1:A:246:GLY:CA	1:A:256:LEU:HD11	2.42	0.49
1:A:224:VAL:CG1	1:A:225:ASN:N	2.75	0.49
1:A:149:ILE:HB	1:A:244:MET:O	2.14	0.48
1:A:16:LEU:O	1:A:110:THR:HA	2.13	0.48
1:A:250:MET:O	1:A:251:ILE:C	2.52	0.48
1:A:165:ILE:HD12	1:A:175:CYS:SG	2.54	0.47
1:A:190:ARG:N	1:A:191:PRO:CD	2.77	0.47
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.78	0.47
1:A:225:ASN:O	1:A:258:ASN:ND2	2.48	0.47
1:A:32:ARG:HA	1:A:79:LEU:HD12	1.97	0.47
1:A:92:PHE:HB3	1:A:93:PRO:HD2	1.96	0.47
1:A:176:HIS:CD2	1:A:234:PRO:HG3	2.49	0.47
1:A:191:PRO:HD2	1:A:192:GLU:OE1	2.13	0.47
1:A:142:THR:O	1:A:144:LYS:CA	2.62	0.46
1:A:7:LEU:HG	1:A:42:LEU:HD22	1.95	0.46
1:A:141:LYS:HA	1:A:143:VAL:HG12	1.96	0.46
1:A:248:PRO:N	1:A:249:PRO:CD	2.79	0.46
1:A:84:TYR:CD1	1:A:84:TYR:C	2.89	0.46
1:A:247:PRO:HG2	1:A:247:PRO:O	2.16	0.46
1:A:236:PRO:O	1:A:238:GLU:N	2.48	0.46
1:A:144:LYS:O	1:A:174:VAL:HG12	2.17	0.45
1:A:84:TYR:CZ	1:A:100:GLN:HA	2.51	0.45
1:A:132:PRO:CG	1:A:133:ASP:N	2.78	0.45
1:A:245:CYS:C	1:A:256:LEU:HG	2.36	0.45
1:A:96:GLY:O	1:A:100:GLN:HG3	2.16	0.45
1:A:183:THR:CG2	1:A:185:LYS:HD2	2.46	0.45
1:A:91:LYS:HB2	2:A:273:FAD:N1A	2.32	0.45
1:A:137:SER:HA	1:A:138:PRO:HD3	1.79	0.45
1:A:243:LEU:HA	1:A:270:PHE:O	2.16	0.45
1:A:185:LYS:HD3	1:A:185:LYS:C	2.33	0.45
1:A:194:GLU:C	1:A:196:LEU:H	2.17	0.45
1:A:56:ILE:HG12	1:A:101:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:C	1:A:196:LEU:N	2.70	0.45
1:A:193:LEU:HA	1:A:193:LEU:HD12	1.89	0.44
1:A:255:CYS:SG	1:A:259:LEU:HD12	2.58	0.44
1:A:6:THR:O	1:A:8:GLU:N	2.50	0.44
1:A:124:GLY:O	1:A:127:LYS:HE3	2.17	0.44
1:A:26:HIS:CE1	1:A:189:LEU:N	2.84	0.44
1:A:247:PRO:HB2	1:A:249:PRO:HD2	1.99	0.44
1:A:141:LYS:NZ	1:A:143:VAL:HG13	2.29	0.43
1:A:151:GLY:HA3	1:A:247:PRO:CB	2.48	0.43
1:A:226:GLU:CD	1:A:261:ARG:HE	2.22	0.43
1:A:98:MET:O	1:A:98:MET:HG3	2.18	0.43
1:A:155:ILE:HD11	1:A:177:LEU:HD11	2.00	0.43
1:A:254:ALA:C	1:A:255:CYS:O	2.57	0.43
1:A:84:TYR:HD2	1:A:103:GLU:HB2	1.82	0.43
1:A:225:ASN:CB	1:A:227:GLU:HG2	2.48	0.43
1:A:193:LEU:HG	1:A:196:LEU:CB	2.36	0.43
2:A:273:FAD:O2'	2:A:273:FAD:C5'	2.41	0.43
1:A:183:THR:HG23	1:A:185:LYS:HD2	2.01	0.43
1:A:84:TYR:HA	1:A:99:SER:HB2	2.00	0.43
1:A:156:THR:HG21	2:A:273:FAD:C4	2.48	0.43
1:A:196:LEU:CD1	1:A:196:LEU:C	2.88	0.43
1:A:235:PRO:HB2	1:A:237:GLU:CD	2.40	0.42
1:A:95:GLY:HA3	1:A:100:GLN:NE2	2.34	0.42
1:A:69:SER:OG	1:A:78:ASP:HA	2.19	0.42
1:A:84:TYR:CD2	1:A:103:GLU:HB2	2.54	0.42
1:A:90:PRO:HB2	1:A:91:LYS:HG2	2.02	0.42
1:A:229:ILE:CA	1:A:233:LEU:HD23	2.37	0.42
1:A:30:ARG:NH1	1:A:30:ARG:CG	2.82	0.42
1:A:248:PRO:O	1:A:249:PRO:C	2.58	0.42
1:A:29:ARG:NE	1:A:103:GLU:OE1	2.53	0.42
1:A:247:PRO:C	1:A:249:PRO:CD	2.84	0.42
1:A:76:PHE:CE2	1:A:79:LEU:HD13	2.54	0.42
1:A:156:THR:N	1:A:157:PRO:HD2	2.35	0.42
1:A:151:GLY:HA2	1:A:180:ALA:O	2.20	0.41
1:A:239:GLU:N	1:A:240:PRO:CD	2.83	0.41
1:A:25:ASN:C	1:A:27:ASP:H	2.21	0.41
1:A:229:ILE:HD12	1:A:258:ASN:CB	2.47	0.41
1:A:50:ILE:HD12	1:A:50:ILE:C	2.40	0.41
1:A:149:ILE:HD12	1:A:245:CYS:O	2.20	0.41
1:A:84:TYR:C	1:A:84:TYR:HD1	2.24	0.41
1:A:210:VAL:O	1:A:221:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HB2	1:A:77:VAL:HG12	2.02	0.40
1:A:185:LYS:HZ2	1:A:186:ASP:N	2.18	0.40
1:A:50:ILE:O	1:A:64:PRO:HA	2.20	0.40
1:A:70:SER:N	1:A:73:ASP:OD2	2.49	0.40
1:A:73:ASP:O	1:A:77:VAL:CG2	2.68	0.40
1:A:183:THR:OG1	1:A:185:LYS:HG3	2.22	0.40
1:A:246:GLY:CA	1:A:256:LEU:HD21	2.52	0.40
1:A:251:ILE:O	1:A:252:GLN:NE2	2.55	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	268/272 (98%)	228 (85%)	19 (7%)	21 (8%)	1	0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	77	VAL
1	A	92	PHE
1	A	93	PRO
1	A	132	PRO
1	A	142	THR
1	A	143	VAL
1	A	192	GLU
1	A	224	VAL
1	A	225	ASN
1	A	250	MET
1	A	251	ILE
1	A	254	ALA

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Mol	Chain	Res	Type
1	A	226	GLU
1	A	253	TYR
1	A	25	ASN
1	A	135	LYS
1	A	191	PRO
1	A	237	GLU
1	A	89	HIS
1	A	245	CYS

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	239/241 (99%)	188 (79%)	51 (21%)	1	0

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	24	VAL
1	A	25	ASN
1	A	28	THR
1	A	42	LEU
1	A	52	LEU
1	A	61	VAL
1	A	68	VAL
1	A	82	LYS
1	A	84	TYR
1	A	92	PHE
1	A	93	PRO
1	A	104	SER
1	A	106	LYS
1	A	119	LEU
1	A	127	LYS
1	A	133	ASP
1	A	134	LYS

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Mol	Chain	Res	Type
1	A	135	LYS
1	A	136	SER
1	A	140	ILE
1	A	141	LYS
1	A	142	THR
1	A	143	VAL
1	A	144	LYS
1	A	156	THR
1	A	159	LEU
1	A	167	LYS
1	A	177	LEU
1	A	178	LEU
1	A	182	GLN
1	A	183	THR
1	A	185	LYS
1	A	196	LEU
1	A	197	ARG
1	A	199	GLU
1	A	201	SER
1	A	206	LEU
1	A	212	ARG
1	A	221	GLN
1	A	223	PHE
1	A	225	ASN
1	A	227	GLU
1	A	241	LEU
1	A	243	LEU
1	A	250	MET
1	A	256	LEU
1	A	260	GLU
1	A	261	ARG
1	A	266	LYS
1	A	267	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	59	ASN
1	A	117	ASN
1	A	123	GLN
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	221	GLN
1	A	232	HIS
1	A	252	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	273	-	53,58,58	2.18	16 (30%)	68,89,89	2.24	25 (36%)

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	273	-	1/1/9/9	10/30/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	273	FAD	O2'-C2'	6.02	1.56	1.43
2	A	273	FAD	O3'-C3'	5.95	1.57	1.43
2	A	273	FAD	C9A-N10	-5.77	1.31	1.41
2	A	273	FAD	C4'-C3'	-4.57	1.44	1.53
2	A	273	FAD	C1'-C2'	4.23	1.58	1.52
2	A	273	FAD	O4B-C1B	3.25	1.45	1.41
2	A	273	FAD	C6-C7	-3.15	1.35	1.39
2	A	273	FAD	O2-C2	-2.75	1.19	1.24
2	A	273	FAD	O4'-C4'	-2.37	1.38	1.43
2	A	273	FAD	C4A-N3A	-2.32	1.32	1.35
2	A	273	FAD	C2B-C1B	-2.28	1.50	1.53
2	A	273	FAD	O4-C4	-2.17	1.19	1.23
2	A	273	FAD	PA-O1A	-2.16	1.43	1.50
2	A	273	FAD	C4-N3	-2.15	1.34	1.38
2	A	273	FAD	C2A-N1A	2.05	1.37	1.33
2	A	273	FAD	P-O1P	-2.02	1.43	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	273	FAD	O2'-C2'-C3'	-5.79	95.02	109.10
2	A	273	FAD	P-O5'-C5'	5.62	154.63	121.68
2	A	273	FAD	C1B-N9A-C4A	-4.21	119.25	126.64
2	A	273	FAD	C5A-C6A-N6A	4.14	126.64	120.35
2	A	273	FAD	O5'-C5'-C4'	4.10	120.31	109.36
2	A	273	FAD	C6-C5X-N5	-4.05	111.44	118.51
2	A	273	FAD	O4'-C4'-C3'	-3.99	99.41	109.10
2	A	273	FAD	O3'-C3'-C2'	3.88	118.19	108.81
2	A	273	FAD	C9A-C5X-N5	3.87	126.64	122.43
2	A	273	FAD	C5X-N5-C4X	-3.86	111.66	118.07
2	A	273	FAD	O3'-C3'-C4'	3.64	117.59	108.81
2	A	273	FAD	O2A-PA-O1A	3.05	127.32	112.24
2	A	273	FAD	C2A-N1A-C6A	2.86	123.65	118.75
2	A	273	FAD	O2B-C2B-C1B	-2.82	100.45	110.85
2	A	273	FAD	O4B-C1B-C2B	-2.78	102.87	106.93
2	A	273	FAD	C5A-C6A-N1A	-2.67	114.31	120.35
2	A	273	FAD	C4A-C5A-N7A	2.61	112.12	109.40
2	A	273	FAD	C8M-C8-C7	-2.58	115.44	120.74
2	A	273	FAD	C1'-C2'-C3'	2.57	116.96	109.79
2	A	273	FAD	C8M-C8-C9	2.41	123.94	119.49
2	A	273	FAD	P-O3P-PA	-2.25	125.09	132.83
2	A	273	FAD	N3A-C2A-N1A	-2.16	125.30	128.68

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	273	FAD	O4'-C4'-C5'	2.14	114.72	109.92
2	A	273	FAD	C4-N3-C2	-2.10	121.77	125.64
2	A	273	FAD	C6-C5X-C9A	2.09	121.90	118.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	273	FAD	C4B

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	273	FAD	C5B-O5B-PA-O1A
2	A	273	FAD	O4B-C4B-C5B-O5B
2	A	273	FAD	C3B-C4B-C5B-O5B
2	A	273	FAD	N10-C1'-C2'-C3'
2	A	273	FAD	C1'-C2'-C3'-O3'
2	A	273	FAD	O4'-C4'-C5'-O5'
2	A	273	FAD	O2'-C2'-C3'-O3'
2	A	273	FAD	C3'-C4'-C5'-O5'
2	A	273	FAD	C4'-C5'-O5'-P
2	A	273	FAD	C5B-O5B-PA-O3P

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	273	FAD	11	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 then 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.

Ligand FAD A 273

Bond lengths

Bond angles

Torsions

Rings
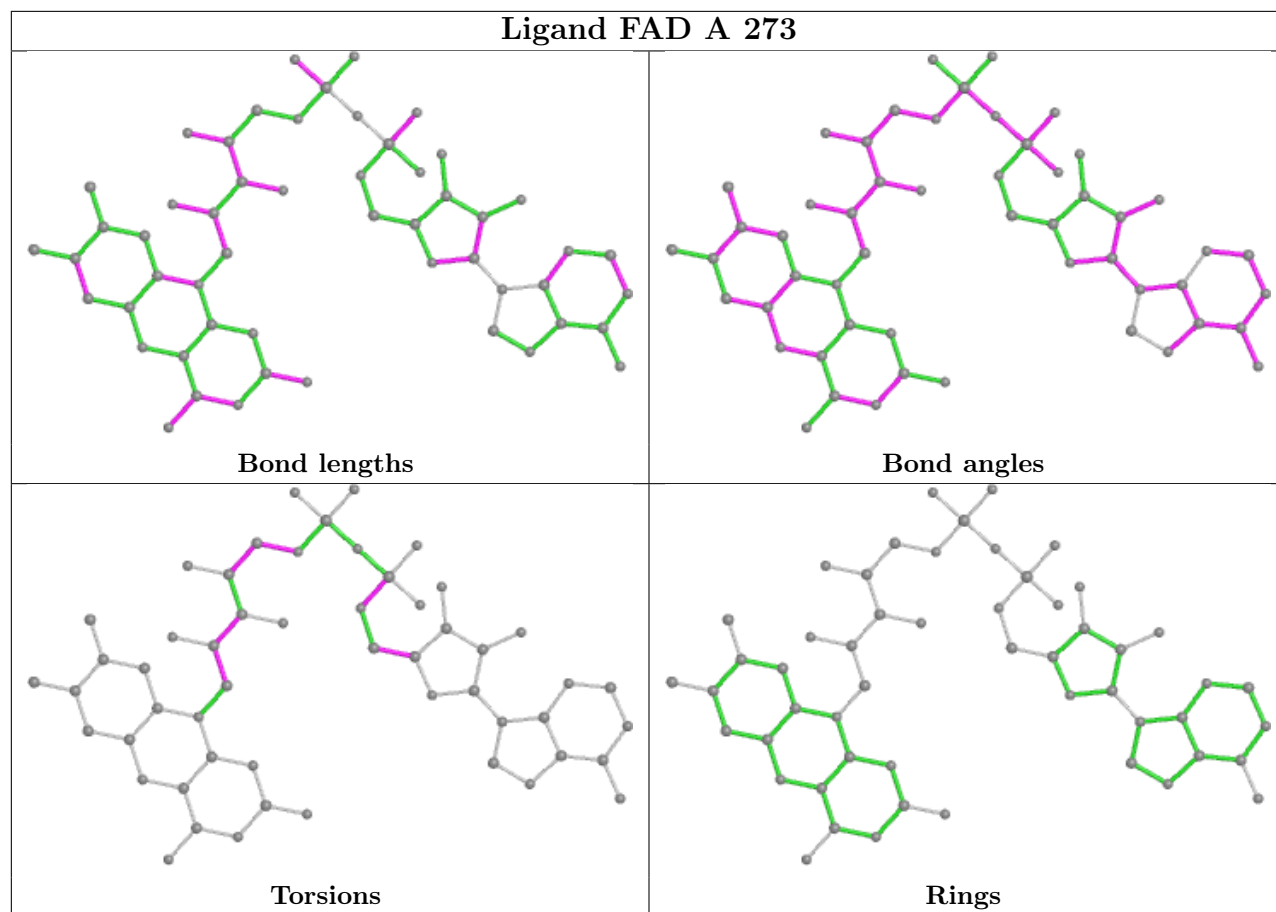
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.