



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:23 AM UTC

PDB ID : 1NDH / pdb_00001ndh
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

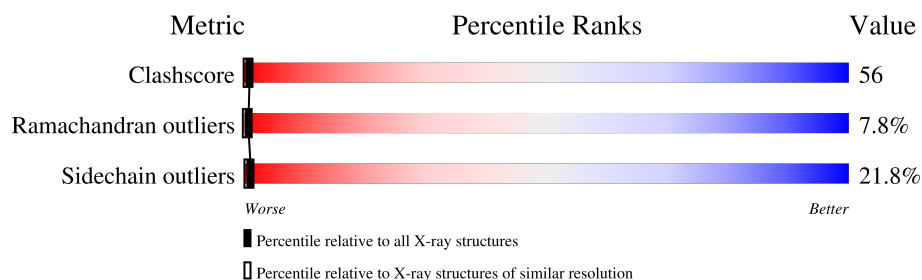
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	272	25% 36% 24% 14%

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 [i](#)

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.

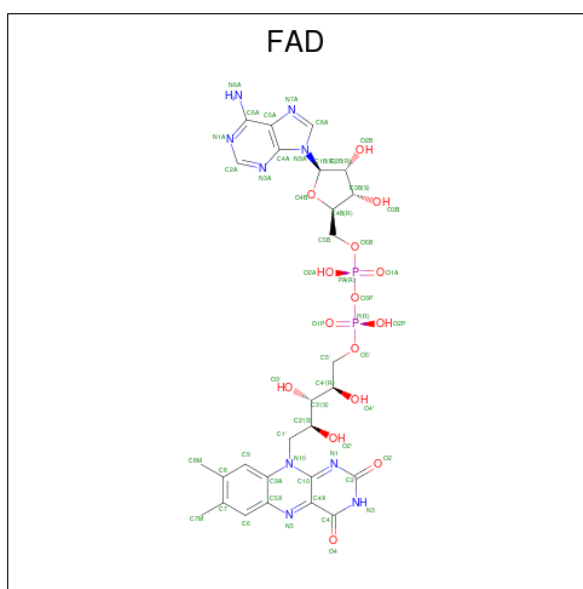
- Molecule 1 is a protein called CYTOCHROME B5 REDUCTASE.

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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is water.

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

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	1.46	13/2217 (0.6%)	2.93	244/3006 (8.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	LEU	CA-C	8.29	1.63	1.52
1	A	239	GLU	C-O	7.78	1.27	1.23
1	A	27	ASP	CA-C	7.25	1.62	1.52
1	A	192	GLU	C-O	6.96	1.32	1.24
1	A	203	ARG	CD-NE	-6.55	1.37	1.46
1	A	115	GLY	C-N	6.17	1.46	1.34
1	A	142	THR	C-N	-6.12	1.25	1.33
1	A	196	LEU	N-CA	5.58	1.52	1.46
1	A	91	LYS	N-CA	-5.40	1.39	1.46
1	A	141	LYS	C-N	-5.33	1.26	1.33
1	A	63	ARG	N-CA	5.25	1.52	1.46
1	A	196	LEU	CA-C	5.11	1.59	1.52
1	A	90	PRO	CA-C	-5.01	1.44	1.52

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	CD-NE-CZ	32.29	169.61	124.40
1	A	25	ASN	CA-CB-CG	-19.93	92.67	112.60
1	A	77	VAL	CA-C-N	13.84	143.24	122.47
1	A	77	VAL	C-N-CA	13.84	143.24	122.47
1	A	199	GLU	CB-CG-CD	13.65	135.80	112.60
1	A	78	ASP	CA-CB-CG	-13.38	99.22	112.60
1	A	26	HIS	N-CA-C	-13.11	96.63	111.71
1	A	191	PRO	O-C-N	12.09	138.96	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	GLU	O-C-N	11.61	138.03	122.59
1	A	144	LYS	CA-C-O	-11.43	104.13	120.13
1	A	25	ASN	OD1-CG-ND2	11.37	133.97	122.60
1	A	272	PHE	CA-CB-CG	11.11	124.91	113.80
1	A	186	ASP	N-CA-CB	11.04	125.79	110.56
1	A	185	LYS	CA-C-O	-10.81	109.56	120.70
1	A	78	ASP	CA-C-O	10.48	134.62	120.47
1	A	76	PHE	CA-C-N	10.47	140.82	121.97
1	A	76	PHE	C-N-CA	10.47	140.82	121.97
1	A	91	LYS	CA-C-O	10.39	131.75	120.32
1	A	198	ASN	CB-CA-C	10.14	126.81	110.88
1	A	90	PRO	O-C-N	9.98	135.10	122.22
1	A	60	LEU	O-C-N	9.82	134.53	123.04
1	A	243	LEU	CA-C-N	9.82	137.71	122.78
1	A	243	LEU	C-N-CA	9.82	137.71	122.78
1	A	194	GLU	CA-C-O	9.72	131.03	120.82
1	A	57	ASP	CA-CB-CG	9.63	122.23	112.60
1	A	197	ARG	N-CA-C	-9.57	99.92	111.69
1	A	28	THR	N-CA-CB	-9.41	95.89	110.56
1	A	141	LYS	CA-C-N	9.36	139.41	121.54
1	A	141	LYS	C-N-CA	9.36	139.41	121.54
1	A	142	THR	CA-C-N	9.22	138.57	121.97
1	A	142	THR	C-N-CA	9.22	138.57	121.97
1	A	234	PRO	O-C-N	9.12	125.50	121.31
1	A	23	VAL	CB-CA-C	9.09	124.04	111.31
1	A	69	SER	CA-C-O	-9.09	111.61	121.88
1	A	156	THR	N-CA-CB	-8.95	96.96	110.30
1	A	196	LEU	CA-C-O	8.90	129.04	119.34
1	A	246	GLY	N-CA-C	-8.84	94.31	112.34
1	A	232	HIS	CA-CB-CG	-8.71	105.09	113.80
1	A	260	GLU	CA-CB-CG	8.71	131.51	114.10
1	A	195	GLU	CB-CA-C	8.66	127.66	110.42
1	A	225	ASN	CA-C-N	8.63	138.02	121.54
1	A	225	ASN	C-N-CA	8.63	138.02	121.54
1	A	60	LEU	CA-C-N	-8.50	111.12	122.94
1	A	60	LEU	C-N-CA	-8.50	111.12	122.94
1	A	223	PHE	O-C-N	8.49	133.00	122.14
1	A	196	LEU	CA-C-N	8.41	134.96	120.58
1	A	196	LEU	C-N-CA	8.41	134.96	120.58
1	A	244	MET	CG-SD-CE	8.37	119.31	100.90
1	A	139	VAL	CB-CA-C	8.36	125.00	111.29
1	A	71	ASP	CA-CB-CG	8.34	120.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	LYS	N-CA-C	-8.32	96.78	110.17
1	A	145	SER	N-CA-C	8.30	121.93	108.32
1	A	139	VAL	O-C-N	8.23	132.85	122.57
1	A	188	LEU	CB-CA-C	-8.20	95.63	109.65
1	A	9	ASN	CA-C-O	-8.12	112.33	119.72
1	A	92	PHE	CB-CA-C	8.09	126.10	110.17
1	A	172	HIS	CA-CB-CG	-8.07	105.73	113.80
1	A	188	LEU	N-CA-CB	8.00	121.72	109.97
1	A	61	VAL	CB-CA-C	7.99	122.81	110.50
1	A	24	VAL	CA-C-O	7.96	131.66	121.15
1	A	217	TRP	CA-C-O	-7.95	112.44	121.19
1	A	139	VAL	CA-C-N	7.90	131.66	120.53
1	A	139	VAL	C-N-CA	7.90	131.66	120.53
1	A	78	ASP	N-CA-C	7.89	122.66	107.44
1	A	267	GLU	CB-CG-CD	7.88	126.00	112.60
1	A	245	CYS	O-C-N	-7.82	112.19	122.59
1	A	9	ASN	O-C-N	7.78	130.97	121.79
1	A	143	VAL	CA-C-N	7.75	137.17	122.60
1	A	143	VAL	C-N-CA	7.75	137.17	122.60
1	A	196	LEU	N-CA-C	-7.69	101.56	113.02
1	A	124	GLY	O-C-N	7.67	129.08	122.64
1	A	142	THR	N-CA-CB	7.66	123.43	110.49
1	A	139	VAL	N-CA-C	-7.59	93.55	109.34
1	A	24	VAL	N-CA-C	-7.55	103.87	110.74
1	A	88	THR	N-CA-CB	-7.49	100.76	112.08
1	A	223	PHE	CA-C-N	7.41	135.31	121.97
1	A	223	PHE	C-N-CA	7.41	135.31	121.97
1	A	202	ALA	N-CA-CB	7.35	121.68	110.28
1	A	245	CYS	CA-C-O	7.34	131.00	120.51
1	A	25	ASN	N-CA-C	7.34	126.42	110.80
1	A	57	ASP	CB-CA-C	7.32	122.48	111.80
1	A	183	THR	CB-CA-C	7.29	126.11	110.07
1	A	203	ARG	NE-CZ-NH1	-7.29	114.21	121.50
1	A	249	PRO	CA-C-N	7.23	135.34	121.54
1	A	249	PRO	C-N-CA	7.23	135.34	121.54
1	A	76	PHE	O-C-N	7.20	132.16	122.59
1	A	143	VAL	CA-C-O	7.19	129.77	120.78
1	A	35	LEU	N-CA-C	-7.18	101.87	110.13
1	A	77	VAL	CA-CB-CG1	7.12	122.51	110.40
1	A	244	MET	N-CA-CB	7.12	123.87	111.40
1	A	113	PHE	CA-CB-CG	7.08	120.88	113.80
1	A	224	VAL	N-CA-C	7.05	124.00	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	TYR	O-C-N	7.03	131.64	123.41
1	A	52	LEU	N-CA-C	-7.01	97.98	109.40
1	A	245	CYS	N-CA-CB	-7.00	98.66	110.49
1	A	18	LEU	O-C-N	6.98	131.60	123.02
1	A	76	PHE	CA-C-O	-6.93	110.60	120.51
1	A	60	LEU	CA-C-O	-6.90	112.82	120.69
1	A	168	ASP	O-C-N	6.89	126.81	121.23
1	A	80	VAL	CA-CB-CG1	6.87	122.08	110.40
1	A	115	GLY	N-CA-C	6.87	126.35	112.34
1	A	82	LYS	N-CA-C	6.77	119.94	108.90
1	A	209	THR	N-CA-CB	6.70	123.12	111.13
1	A	156	THR	CB-CA-C	6.65	125.12	112.76
1	A	186	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	87	ASP	CA-CB-CG	-6.62	105.98	112.60
1	A	268	ARG	NE-CZ-NH1	6.61	128.11	121.50
1	A	16	LEU	O-C-N	6.55	131.75	123.23
1	A	247	PRO	N-CA-C	-6.54	102.72	110.70
1	A	248	PRO	CB-CA-C	6.53	118.89	110.92
1	A	192	GLU	CA-C-N	6.51	133.98	121.54
1	A	192	GLU	C-N-CA	6.51	133.98	121.54
1	A	92	PHE	CA-C-N	6.48	127.94	119.84
1	A	92	PHE	C-N-CA	6.48	127.94	119.84
1	A	144	LYS	CA-CB-CG	6.46	127.03	114.10
1	A	230	ARG	O-C-N	6.46	129.07	122.09
1	A	121	VAL	O-C-N	6.46	130.05	123.07
1	A	182	GLN	CB-CA-C	6.41	121.75	110.85
1	A	103	GLU	CA-CB-CG	6.39	126.89	114.10
1	A	264	HIS	O-C-N	6.35	127.63	121.28
1	A	106	LYS	CA-C-O	-6.29	113.75	121.11
1	A	260	GLU	CG-CD-OE2	6.24	132.76	118.40
1	A	146	VAL	CA-C-N	6.21	128.10	122.20
1	A	146	VAL	C-N-CA	6.21	128.10	122.20
1	A	185	LYS	CG-CD-CE	6.19	125.54	111.30
1	A	91	LYS	CA-C-N	6.19	136.89	121.80
1	A	91	LYS	C-N-CA	6.19	136.89	121.80
1	A	182	GLN	CB-CG-CD	6.18	123.10	112.60
1	A	202	ALA	N-CA-C	-6.18	104.65	111.82
1	A	58	GLY	N-CA-C	6.17	124.19	115.30
1	A	254	ALA	N-CA-C	-6.15	97.69	110.80
1	A	16	LEU	CA-C-O	-6.14	114.07	120.70
1	A	223	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	194	GLU	N-CA-C	-6.08	104.56	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	HIS	CA-C-O	-6.08	114.88	121.20
1	A	133	ASP	O-C-N	6.03	131.17	122.13
1	A	97	LYS	CG-CD-CE	5.98	125.06	111.30
1	A	44	LEU	CB-CA-C	5.97	120.46	110.55
1	A	203	ARG	CB-CA-C	-5.95	99.55	109.55
1	A	131	ARG	NE-CZ-NH2	-5.95	113.85	119.20
1	A	233	LEU	CB-CA-C	5.92	118.14	109.08
1	A	28	THR	O-C-N	5.92	129.72	123.03
1	A	61	VAL	O-C-N	5.92	129.43	123.10
1	A	195	GLU	N-CA-C	-5.91	98.21	110.80
1	A	168	ASP	CA-C-O	-5.90	115.45	119.29
1	A	73	ASP	CA-C-O	-5.89	115.04	121.87
1	A	43	GLY	CA-C-N	-5.88	115.29	122.64
1	A	43	GLY	C-N-CA	-5.88	115.29	122.64
1	A	212	ARG	CA-C-O	-5.88	114.49	120.84
1	A	155	ILE	CA-CB-CG2	5.87	120.48	110.50
1	A	86	LYS	CA-C-N	-5.86	110.41	121.66
1	A	86	LYS	C-N-CA	-5.86	110.41	121.66
1	A	144	LYS	N-CA-C	5.86	120.47	112.68
1	A	18	LEU	CA-C-O	-5.84	113.71	120.49
1	A	196	LEU	CB-CA-C	5.84	120.26	110.44
1	A	170	ASP	CB-CA-C	5.82	120.39	110.56
1	A	192	GLU	CB-CA-C	5.82	122.00	110.42
1	A	22	GLU	CA-C-O	-5.81	114.09	120.43
1	A	24	VAL	CB-CA-C	5.78	119.57	111.94
1	A	93	PRO	N-CA-CB	-5.76	97.20	103.25
1	A	241	LEU	CA-C-O	-5.75	114.41	120.80
1	A	40	HIS	CA-CB-CG	5.74	119.54	113.80
1	A	32	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	8	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	93	PRO	N-CA-C	5.73	124.27	112.47
1	A	226	GLU	N-CA-CB	5.72	120.15	110.49
1	A	257	PRO	N-CA-C	-5.71	106.09	113.57
1	A	51	TYR	O-C-N	5.70	130.63	123.23
1	A	17	ARG	N-CA-CB	5.67	119.42	110.23
1	A	58	GLY	CA-C-O	5.66	126.49	119.25
1	A	191	PRO	N-CA-C	-5.66	100.81	112.47
1	A	51	TYR	CA-C-O	-5.63	114.62	120.70
1	A	37	SER	O-C-N	5.62	127.78	121.32
1	A	140	ILE	O-C-N	5.62	127.39	121.89
1	A	238	GLU	CA-CB-CG	5.62	125.33	114.10
1	A	74	LYS	N-CA-CB	5.60	120.01	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLY	CA-C-N	-5.60	111.98	122.73
1	A	222	GLY	C-N-CA	-5.60	111.98	122.73
1	A	17	ARG	O-C-N	5.59	129.64	123.16
1	A	114	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	158	MET	O-C-N	5.58	128.11	122.09
1	A	69	SER	N-CA-C	-5.57	102.66	110.35
1	A	26	HIS	CA-CB-CG	5.56	119.36	113.80
1	A	5	ILE	CA-C-O	-5.55	113.79	121.51
1	A	197	ARG	CD-NE-CZ	5.55	132.17	124.40
1	A	26	HIS	N-CA-CB	5.55	118.77	110.22
1	A	73	ASP	CB-CA-C	5.47	120.90	109.68
1	A	133	ASP	CA-C-O	-5.47	113.38	119.67
1	A	255	CYS	N-CA-C	-5.46	99.16	110.80
1	A	135	LYS	N-CA-CB	5.46	119.71	110.49
1	A	262	VAL	O-C-N	5.45	129.51	122.26
1	A	9	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	73	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	55	ARG	N-CA-C	-5.40	98.96	108.20
1	A	212	ARG	CD-NE-CZ	5.40	131.96	124.40
1	A	203	ARG	CA-CB-CG	5.37	124.84	114.10
1	A	213	ALA	CA-C-O	-5.37	115.68	120.19
1	A	156	THR	CA-CB-CG2	5.36	119.61	110.50
1	A	131	ARG	N-CA-C	-5.36	102.23	110.32
1	A	268	ARG	NH1-CZ-NH2	-5.34	112.35	119.30
1	A	99	SER	CA-CB-OG	5.34	121.78	111.10
1	A	184	GLU	CA-C-N	5.34	127.70	120.44
1	A	184	GLU	C-N-CA	5.34	127.70	120.44
1	A	260	GLU	CA-C-N	5.34	128.82	120.82
1	A	260	GLU	C-N-CA	5.34	128.82	120.82
1	A	245	CYS	CA-CB-SG	-5.33	102.14	114.40
1	A	245	CYS	N-CA-C	5.33	122.16	110.80
1	A	72	ASP	N-CA-C	-5.32	105.93	112.90
1	A	27	ASP	CA-C-N	5.31	132.40	122.74
1	A	27	ASP	C-N-CA	5.31	132.40	122.74
1	A	132	PRO	CA-C-N	5.30	132.22	122.79
1	A	132	PRO	C-N-CA	5.30	132.22	122.79
1	A	138	PRO	CA-C-O	5.29	127.83	121.48
1	A	11	ASP	O-C-N	5.28	129.33	122.42
1	A	28	THR	N-CA-C	5.27	118.58	110.42
1	A	68	VAL	N-CA-CB	-5.23	102.93	111.98
1	A	191	PRO	N-CA-CB	5.23	108.74	103.25
1	A	74	LYS	CG-CD-CE	5.22	123.32	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ALA	CA-C-N	5.21	130.92	122.48
1	A	34	ALA	C-N-CA	5.21	130.92	122.48
1	A	170	ASP	CA-CB-CG	-5.19	107.41	112.60
1	A	202	ALA	CA-C-O	-5.19	114.00	119.97
1	A	190	ARG	O-C-N	5.19	125.10	120.48
1	A	35	LEU	CA-C-O	-5.19	113.83	121.46
1	A	204	PHE	CA-CB-CG	-5.18	108.62	113.80
1	A	163	ARG	NH1-CZ-NH2	5.17	126.03	119.30
1	A	101	TYR	CA-C-O	5.17	125.90	120.42
1	A	199	GLU	CA-CB-CG	5.16	124.42	114.10
1	A	142	THR	N-CA-C	-5.14	99.84	110.80
1	A	83	VAL	N-CA-C	-5.14	101.18	108.58
1	A	93	PRO	CA-CB-CG	-5.12	94.77	104.50
1	A	244	MET	CA-CB-CG	5.10	124.30	114.10
1	A	226	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	163	ARG	NE-CZ-NH2	-5.07	114.63	119.20
1	A	227	GLU	CB-CA-C	-5.07	102.38	110.79
1	A	157	PRO	N-CA-C	-5.05	106.51	113.53
1	A	6	THR	CA-CB-CG2	5.05	119.08	110.50
1	A	167	LYS	N-CA-C	-5.03	105.92	111.71
1	A	142	THR	CA-CB-CG2	5.03	119.05	110.50
1	A	97	LYS	N-CA-C	5.03	116.61	111.03
1	A	167	LYS	CA-CB-CG	5.03	124.15	114.10
1	A	121	VAL	N-CA-CB	5.02	119.71	111.58
1	A	195	GLU	O-C-N	5.02	129.27	122.59
1	A	244	MET	O-C-N	-5.00	116.97	123.32

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	2169	241	0
2	A	53	0	31	11	0
3	A	48	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2259	0	2200	247	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 56.

All (247) 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: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:185:LYS:HZ1	1:A:186:ASP:HB2	0.97	1.05
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
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:247:PRO:C	1:A:249:PRO:HD2	2.06	0.80
1:A:35:LEU:HD11	1:A:77:VAL:HB	1.62	0.80
1:A:141:LYS:HZ3	1:A:143:VAL:HG13	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:ASP:C	1:A:77:VAL:HG22	2.08	0.78
1:A:32:ARG:HH21	1:A:79:LEU:CD2	1.97	0.78
1:A:191:PRO:C	1:A:193:LEU:N	2.41	0.78
1:A:76:PHE:C	1:A:78:ASP:H	1.81	0.77
1:A:127:LYS:HB3	1:A:140:ILE:HA	1.67	0.76
1:A:142:THR:C	1:A:144:LYS:H	1.90	0.76
1:A:84:TYR:HE2	1:A:103:GLU:HB3	1.50	0.76
1:A:183:THR:OG1	1:A:185:LYS:HD2	1.86	0.75
1:A:191:PRO:C	1:A:193:LEU:H	1.92	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:185:LYS:HZ1	1:A:186:ASP:CB	1.90	0.74
1:A:24:VAL:HG22	1:A:28:THR:HB	1.68	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:158:MET:CE	1:A:244:MET:HB2	2.19	0.72
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:223:PHE:CD1	1:A:224:VAL:N	2.58	0.71
1:A:244:MET:HE2	1:A:248:PRO:HB3	1.72	0.70
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:158:MET:HE1	1:A:244:MET:HB2	1.84	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:134:LYS:HD3	1:A:134:LYS:C	2.28	0.59
1:A:26:HIS:O	1:A:27:ASP:HB2	2.03	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:25:ASN:C	1:A:27:ASP:N	2.51	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:106:LYS:HG2	1:A:109:ASP:CG	2.30	0.57
1:A:25:ASN:O	1:A:26:HIS:C	2.44	0.57
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:250:MET:O	1:A:251:ILE:C	2.52	0.53
2:A:273:FAD:H5'1	2:A:273:FAD:HO2'	1.71	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:84:TYR:CD1	1:A:84:TYR:C	2.89	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
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:245:CYS:C	1:A:256:LEU:HG	2.36	0.50
1:A:66:THR:HG21	1:A:157:PRO:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:LYS:HD3	1:A:185:LYS:C	2.33	0.49
1:A:194:GLU:C	1:A:196:LEU:H	2.17	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:194:GLU:C	1:A:196:LEU:N	2.70	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:254:ALA:C	1:A:255:CYS:O	2.57	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:226:GLU:CD	1:A:261:ARG:HE	2.22	0.47
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.78	0.47
1:A:235:PRO:HB2	1:A:237:GLU:CD	2.40	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:196:LEU:CD1	1:A:196:LEU:C	2.88	0.47
1:A:142:THR:H	1:A:143:VAL:HG13	1.80	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:247:PRO:C	1:A:249:PRO:CD	2.84	0.46
1:A:247:PRO:HG2	1:A:247:PRO:O	2.16	0.46
1:A:248:PRO:O	1:A:249:PRO:C	2.58	0.46
1:A:50:ILE:HD12	1:A:50:ILE:C	2.40	0.46
1:A:236:PRO:O	1:A:238:GLU:N	2.48	0.46
1:A:25:ASN:C	1:A:27:ASP:H	2.21	0.46
1:A:84:TYR:C	1:A:84:TYR:HD1	2.24	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HA	1:A:270:PHE:O	2.16	0.45
1:A:56:ILE:HG12	1:A:101:TYR:CD2	2.52	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:151:GLY:HA3	1:A:247:PRO:CB	2.48	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: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:181:ASN:C	1:A:182:GLN:NE2	2.77	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:132:PRO:CG	1:A:133:ASP:N	2.78	0.43
1:A:156:THR:HG21	2:A:273:FAD:C4	2.48	0.43
1:A:166:MET:HE1	1:A:203:ARG:HB3	2.00	0.43
1:A:232:HIS:C	1:A:233:LEU:HD22	2.45	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:29:ARG:NE	1:A:103:GLU:OE1	2.53	0.42
1:A:196:LEU:C	1:A:196:LEU:HD13	2.44	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:69:SER:OG	1:A:77:VAL:C	2.64	0.41
1:A:82:LYS:HB2	1:A:82:LYS:HZ3	1.85	0.41
1:A:239:GLU:N	1:A:240:PRO:CD	2.83	0.41
1:A:229:ILE:HD12	1:A:258:ASN:CB	2.47	0.41
1:A:149:ILE:HD12	1:A:245:CYS:O	2.20	0.41
1:A:210:VAL:O	1:A:221:GLN:HA	2.21	0.41
1:A:120:LEU:C	1:A:120:LEU:HD23	2.46	0.41
1:A:42:LEU:HB2	1:A:77:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:C	1:A:238:GLU:N	2.79	0.40
1:A:237:GLU:CD	1:A:237:GLU:H	2.28	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:76:PHE:C	1:A:78:ASP:N	2.63	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 [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	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

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Mol	Chain	Res	Type
1	A	254	ALA
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%)	187 (78%)	52 (22%)	1 0

All (52) 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

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Mol	Chain	Res	Type
1	A	134	LYS
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	203	ARG
1	A	206	LEU
1	A	212	ARG
1	A	223	PHE
1	A	225	ASN
1	A	227	GLU
1	A	241	LEU
1	A	243	LEU
1	A	249	PRO
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	48	GLN
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	117	ASN
1	A	123	GLN
1	A	182	GLN
1	A	198	ASN
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 oligosaccharides 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	-	58,58,58	2.40	15 (25%)	85,89,89	2.10	24 (28%)

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	10/34/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	273	FAD	PA-O3P	8.77	1.69	1.59
2	A	273	FAD	O2'-C2'	6.09	1.56	1.43
2	A	273	FAD	C9A-N10	-5.87	1.31	1.41
2	A	273	FAD	O3'-C3'	5.66	1.57	1.43
2	A	273	FAD	C4'-C3'	-4.90	1.44	1.53
2	A	273	FAD	C1'-C2'	4.28	1.58	1.52
2	A	273	FAD	C6-C7	-3.42	1.35	1.39
2	A	273	FAD	O2-C2	-2.63	1.19	1.24
2	A	273	FAD	O4'-C4'	-2.39	1.38	1.43
2	A	273	FAD	C2A-N3A	-2.22	1.30	1.33
2	A	273	FAD	PA-O1A	-2.18	1.43	1.50
2	A	273	FAD	O4-C4	-2.16	1.19	1.23
2	A	273	FAD	C4-N3	-2.14	1.34	1.38
2	A	273	FAD	C2A-N1A	2.13	1.37	1.33
2	A	273	FAD	P-O1P	-2.04	1.43	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	273	FAD	O2'-C2'-C3'	-6.08	95.02	109.25
2	A	273	FAD	P-O5'-C5'	5.81	154.63	121.35
2	A	273	FAD	C4B-O4B-C1B	-4.38	99.80	109.47
2	A	273	FAD	C6-C5X-N5	-4.22	111.44	118.44
2	A	273	FAD	O4'-C4'-C3'	-4.21	99.41	109.25
2	A	273	FAD	O5'-C5'-C4'	4.10	120.31	109.36
2	A	273	FAD	O3'-C3'-C2'	4.08	118.19	108.93
2	A	273	FAD	C5X-N5-C4X	-3.97	111.66	118.09
2	A	273	FAD	C9A-C5X-N5	3.94	126.64	122.45
2	A	273	FAD	O3'-C3'-C4'	3.81	117.59	108.93
2	A	273	FAD	O2A-PA-O1A	3.20	127.32	112.44
2	A	273	FAD	C4A-N9A-C1B	-3.16	119.25	126.63
2	A	273	FAD	C2A-N1A-C6A	2.99	123.65	118.73
2	A	273	FAD	O2B-C2B-C1B	-2.80	100.45	110.10
2	A	273	FAD	C1'-C2'-C3'	2.69	116.96	109.66
2	A	273	FAD	C1B-N9A-C8A	2.69	133.06	127.09
2	A	273	FAD	C2B-C1B-N9A	-2.61	106.83	113.30
2	A	273	FAD	C8M-C8-C7	-2.60	115.44	120.76
2	A	273	FAD	C5A-C4A-N3A	2.56	130.24	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	273	FAD	C8M-C8-C9	2.48	123.94	119.57
2	A	273	FAD	C4-N3-C2	-2.18	121.77	125.64
2	A	273	FAD	N3A-C2A-N1A	-2.17	125.30	128.58
2	A	273	FAD	O4'-C4'-C5'	2.14	114.72	109.99
2	A	273	FAD	C6-C5X-C9A	2.08	121.90	119.05

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	PA-O3P-P-O2P

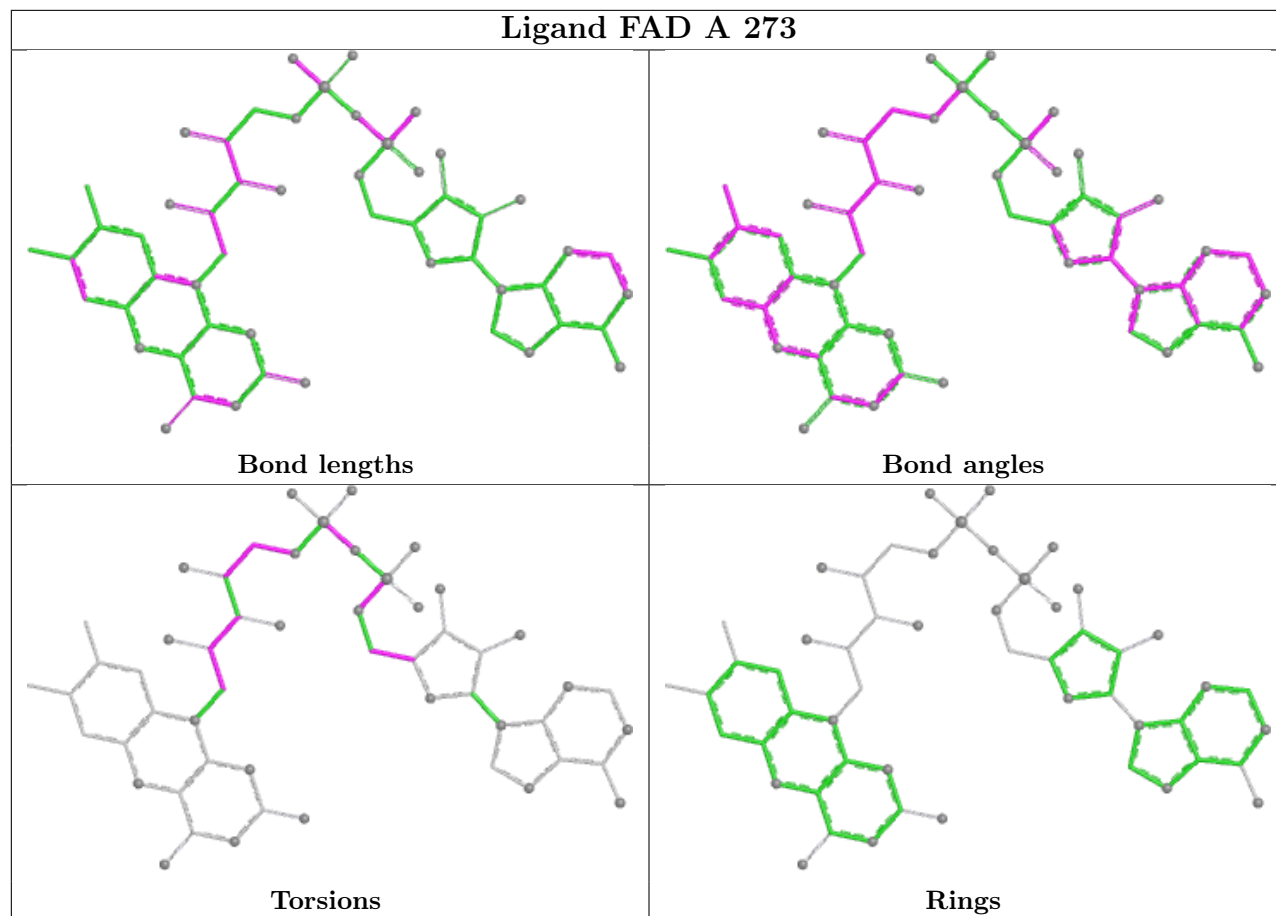
There are no ring outliers.

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 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

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.