



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:09 PM UTC

PDB ID : 1MBT / pdb_00001mbt
Title : OXIDOREDUCTASE
Authors : Benson, T.E.; Walsh, C.T.; Hogle, J.M.
Deposited on : 1995-11-28
Resolution : 3.00 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 ⓘ 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

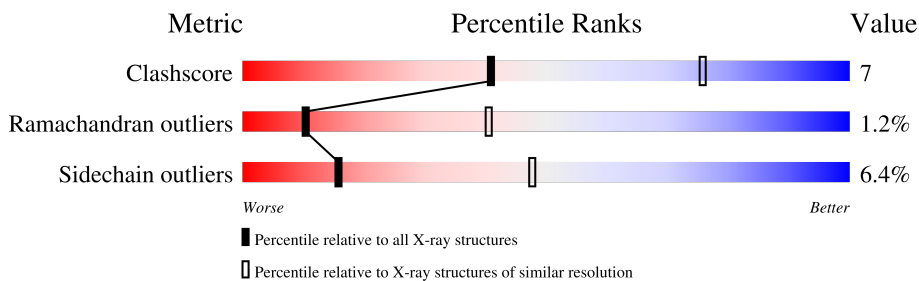
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	342	 57% 35% 7% ..

2 Entry composition [i](#)

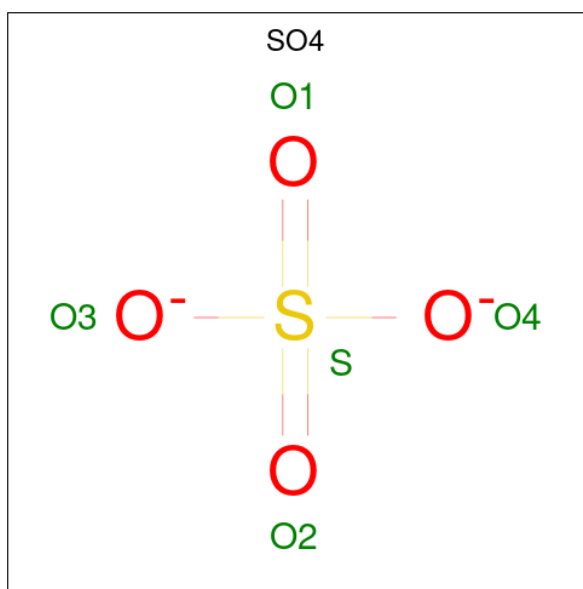
There are 4 unique types of molecules in this entry. The entry contains 2716 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 URIDINE DIPHOSPHO-N-ACETYLENOLPYRUVYLGLUCOSAMINE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2654	1685	465	495	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is water.

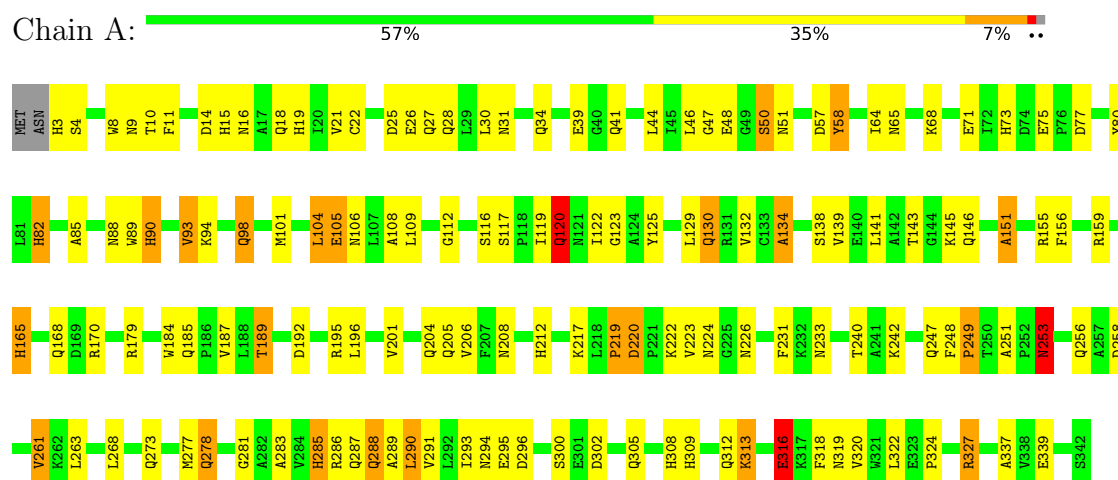
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0

3 Residue-property plots [i](#)

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: URIDINE DIPHOSPHO-N-ACETYLENOLPYRUVYLGLUCOSAMINE REDUCTASE



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	50.40 Å 79.10 Å 90.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.00	Depositor
% Data completeness (in resolution range)	95.9 (12.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.209 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2716	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SO4

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	1.01	12/2716 (0.4%)	2.10	118/3695 (3.2%)

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	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	90	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	82	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	165	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	3	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	285	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	19	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	308	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	309	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	82	HIS	CG-ND1	-5.23	1.32	1.38

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLN	OE1-CD-NE2	-10.39	112.21	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	GLN	OE1-CD-NE2	-10.22	112.38	122.60
1	A	253	ASN	OD1-CG-ND2	-10.00	112.60	122.60
1	A	168	GLN	OE1-CD-NE2	-9.44	113.16	122.60
1	A	146	GLN	OE1-CD-NE2	-9.19	113.41	122.60
1	A	226	ASN	OD1-CG-ND2	-9.00	113.60	122.60
1	A	88	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	A	287	GLN	OE1-CD-NE2	-8.77	113.83	122.60
1	A	288	GLN	OE1-CD-NE2	-8.73	113.87	122.60
1	A	204	GLN	OE1-CD-NE2	-8.70	113.90	122.60
1	A	9	ASN	OD1-CG-ND2	-8.60	114.00	122.60
1	A	185	GLN	OE1-CD-NE2	-8.48	114.12	122.60
1	A	34	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	A	312	GLN	OE1-CD-NE2	-8.28	114.32	122.60
1	A	286	ARG	N-CA-C	8.11	119.75	111.07
1	A	68	LYS	N-CA-C	7.92	121.24	110.55
1	A	305	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	A	253	ASN	N-CA-C	7.70	122.39	109.76
1	A	322	LEU	N-CA-C	7.64	121.31	110.23
1	A	77	ASP	N-CA-C	7.58	119.63	111.36
1	A	319	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	A	286	ARG	O-C-N	-7.38	114.47	122.07
1	A	256	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	A	201	VAL	N-CA-C	7.22	119.23	108.54
1	A	253	ASN	CB-CG-ND2	7.20	127.20	116.40
1	A	294	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	A	18	GLN	OE1-CD-NE2	-7.15	115.45	122.60
1	A	27	GLN	OE1-CD-NE2	-7.10	115.50	122.60
1	A	205	GLN	OE1-CD-NE2	-7.10	115.50	122.60
1	A	247	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	285	HIS	CB-CG-ND1	6.94	133.11	122.70
1	A	28	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	208	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	A	273	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	98	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	A	285	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	A	316	GLU	CB-CG-CD	6.64	123.89	112.60
1	A	217	LYS	N-CA-C	6.61	119.82	111.69
1	A	156	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	220	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	165	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	A	65	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	A	316	GLU	CA-CB-CG	6.50	127.10	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASP	N-CA-C	6.42	118.53	108.96
1	A	4	SER	N-CA-C	6.41	119.00	109.59
1	A	287	GLN	CG-CD-NE2	6.33	125.89	116.40
1	A	51	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	145	LYS	N-CA-C	6.30	124.21	110.80
1	A	143	THR	O-C-N	-6.29	115.26	121.93
1	A	226	ASN	CB-CG-ND2	6.29	125.84	116.40
1	A	105	GLU	N-CA-C	6.26	121.69	111.37
1	A	130	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	263	LEU	O-C-N	-6.20	115.97	123.16
1	A	224	ASN	N-CA-C	6.14	118.77	108.02
1	A	308	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	A	104	LEU	N-CA-C	6.07	120.84	113.38
1	A	75	GLU	O-C-N	-6.06	116.78	121.14
1	A	16	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	93	VAL	O-C-N	-5.98	116.03	121.89
1	A	261	VAL	N-CA-C	5.95	116.49	108.17
1	A	58	TYR	N-CA-C	5.91	118.29	109.25
1	A	120	GLN	CG-CD-NE2	5.90	125.25	116.40
1	A	251	ALA	O-C-N	-5.85	116.34	121.31
1	A	219	PRO	N-CA-C	5.80	119.60	110.50
1	A	212	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	278	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	A	312	GLN	CG-CD-NE2	5.75	125.03	116.40
1	A	50	SER	N-CA-C	5.75	123.05	110.80
1	A	125	TYR	N-CA-C	5.69	119.41	111.90
1	A	8	TRP	CE2-CD2-CG	-5.68	100.38	107.20
1	A	168	GLN	CG-CD-NE2	5.68	124.92	116.40
1	A	89	TRP	CE2-CD2-CG	-5.67	100.40	107.20
1	A	196	LEU	N-CA-C	5.66	118.46	109.24
1	A	14	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	251	ALA	CA-C-O	-5.63	115.13	119.46
1	A	26	GLU	N-CA-C	5.61	117.84	111.11
1	A	327	ARG	CA-CB-CG	-5.61	102.89	114.10
1	A	313	LYS	CA-CB-CG	-5.58	102.93	114.10
1	A	201	VAL	N-CA-CB	-5.55	104.73	110.95
1	A	249	PRO	N-CA-C	5.55	123.90	112.47
1	A	89	TRP	CG-CD2-CE3	5.54	139.44	133.90
1	A	129	LEU	N-CA-C	5.53	117.75	111.11
1	A	233	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	312	GLN	N-CA-C	5.53	117.11	111.14
1	A	48	GLU	N-CA-C	5.50	119.98	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ASP	N-CA-C	5.50	118.99	112.72
1	A	47	GLY	O-C-N	-5.47	118.79	121.85
1	A	204	GLN	CG-CD-NE2	5.39	124.49	116.40
1	A	57	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	8	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	A	185	GLN	O-C-N	-5.33	116.91	121.23
1	A	151	ALA	N-CA-C	5.32	122.13	110.80
1	A	256	GLN	CG-CD-NE2	5.27	124.31	116.40
1	A	141	LEU	N-CA-C	5.26	117.76	111.71
1	A	138	SER	N-CA-C	5.25	117.37	109.23
1	A	185	GLN	CG-CD-NE2	5.24	124.26	116.40
1	A	68	LYS	O-C-N	-5.24	116.88	122.85
1	A	189	THR	N-CA-C	5.23	119.75	112.90
1	A	30	LEU	N-CA-C	5.22	116.66	111.07
1	A	184	TRP	N-CA-C	5.19	117.22	109.59
1	A	293	ILE	N-CA-C	5.19	117.24	109.20
1	A	309	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	A	165	HIS	N-CA-C	5.17	121.81	110.80
1	A	106	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	134	ALA	N-CA-C	5.16	116.76	111.03
1	A	251	ALA	N-CA-C	-5.16	101.79	109.42
1	A	290	LEU	N-CA-CB	-5.15	102.61	110.33
1	A	224	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	85	ALA	N-CA-C	5.10	118.28	111.75
1	A	34	GLN	CG-CD-NE2	5.09	124.03	116.40
1	A	15	HIS	CB-CG-CD2	-5.09	124.59	131.20
1	A	22	CYS	CB-CA-C	-5.08	102.66	111.30
1	A	101	MET	N-CA-C	5.08	119.70	108.27
1	A	302	ASP	CA-CB-CG	5.05	117.66	112.60
1	A	31	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	226	ASN	N-CA-C	5.03	115.94	108.60
1	A	289	ALA	N-CA-C	5.03	121.50	110.80
1	A	3	HIS	CB-CG-CD2	-5.02	124.68	131.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	PHE	Peptide

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	2654	0	2614	34	0
2	A	5	0	0	0	0
3	A	53	0	31	2	0
4	A	4	0	0	1	0
All	All	2716	0	2645	35	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 7.

All (35) 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:324:PRO:HG2	1:A:337:ALA:HB1	1.73	0.70
1:A:120:GLN:HE22	1:A:327:ARG:HH11	1.39	0.69
1:A:268:LEU:HD13	1:A:320:VAL:HG21	1.78	0.65
3:A:401:FAD:O5B	3:A:401:FAD:H8A	2.07	0.55
1:A:219:PRO:HG2	1:A:291:VAL:HG11	1.89	0.54
1:A:104:LEU:HD21	1:A:132:VAL:HG21	1.89	0.54
1:A:313:LYS:HA	1:A:316:GLU:HG3	1.91	0.53
1:A:71:GLU:HB2	1:A:82:HIS:HB3	1.91	0.53
1:A:318:PHE:HB2	1:A:320:VAL:HG22	1.91	0.52
1:A:220:ASP:CG	1:A:222:LYS:HG2	2.35	0.52
1:A:117:SER:HB2	1:A:122:ILE:HG12	1.92	0.50
1:A:187:VAL:HG12	1:A:189:THR:HG22	1.92	0.50
1:A:21:VAL:HG23	4:A:503:HOH:O	2.10	0.50
1:A:90:HIS:CE1	1:A:94:LYS:HD2	2.46	0.50
1:A:134:ALA:HB2	1:A:179:ARG:HB2	1.93	0.50
1:A:222:LYS:HG3	1:A:223:VAL:N	2.27	0.49
1:A:123:GLY:HA3	1:A:159:ARG:HH12	1.77	0.49
1:A:112:GLY:HA3	3:A:401:FAD:O5'	2.11	0.49
1:A:278:GLN:HG2	1:A:283:ALA:HB2	1.95	0.48
1:A:80:TYR:CZ	1:A:179:ARG:HG3	2.49	0.47
1:A:105:GLU:HG3	1:A:206:VAL:HB	1.96	0.47
1:A:253:ASN:HB2	1:A:261:VAL:HG13	1.97	0.46
1:A:90:HIS:CD2	1:A:109:LEU:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:HIS:HD2	1:A:288:GLN:HB2	1.83	0.43
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.84	0.43
1:A:93:VAL:HG11	1:A:108:ALA:HB2	2.00	0.43
1:A:231:PHE:HB2	1:A:290:LEU:HD11	2.01	0.42
1:A:281:GLY:HA3	1:A:296:ASP:O	2.19	0.42
1:A:10:THR:OG1	1:A:50:SER:HA	2.18	0.42
1:A:44:LEU:HB2	1:A:58:TYR:OH	2.20	0.42
1:A:192:ASP:HA	1:A:195:ARG:NH1	2.35	0.42
1:A:119:ILE:HG21	1:A:327:ARG:HH12	1.86	0.41
1:A:120:GLN:NE2	1:A:327:ARG:HD2	2.36	0.41
1:A:195:ARG:HG3	1:A:195:ARG:NH1	2.37	0.40
1:A:119:ILE:CG2	1:A:327:ARG:HH12	2.34	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	338/342 (99%)	306 (90%)	28 (8%)	4 (1%)	10	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ALA
1	A	130	GLN
1	A	170	ARG
1	A	249	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	282/284 (99%)	264 (94%)	18 (6%)	16	48

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	39	GLU
1	A	46	LEU
1	A	64	ILE
1	A	98	GLN
1	A	116	SER
1	A	120	GLN
1	A	139	VAL
1	A	155	ARG
1	A	165	HIS
1	A	240	THR
1	A	242	LYS
1	A	253	ASN
1	A	277	MET
1	A	295	GLU
1	A	300	SER
1	A	316	GLU
1	A	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	90	HIS
1	A	120	GLN
1	A	121	ASN
1	A	256	GLN
1	A	278	GLN
1	A	285	HIS

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Mol	Chain	Res	Type
1	A	305	GLN
1	A	309	HIS

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 ⓘ

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	$\# Z > 2$
3	FAD	A	401	-	58,58,58	1.89	12 (20%)	85,89,89	2.32	21 (24%)
2	SO4	A	600	-	4,4,4	0.36	0	6,6,6	0.17	0

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
3	FAD	A	401	-	-	7/34/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	FAD	C8A-N7A	7.20	1.45	1.31
3	A	401	FAD	C5A-N7A	5.86	1.49	1.39
3	A	401	FAD	P-O3P	4.78	1.64	1.59
3	A	401	FAD	C4X-N5	3.83	1.39	1.30
3	A	401	FAD	PA-O3P	-2.99	1.56	1.59
3	A	401	FAD	C4A-N3A	2.93	1.39	1.34
3	A	401	FAD	C5A-C4A	-2.76	1.34	1.39
3	A	401	FAD	C5A-C6A	2.61	1.48	1.41
3	A	401	FAD	C4-N3	-2.52	1.34	1.38
3	A	401	FAD	C4X-C4	2.25	1.52	1.44
3	A	401	FAD	C2A-N3A	-2.16	1.30	1.33
3	A	401	FAD	C9A-C5X	-2.08	1.37	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	FAD	C4A-N9A-C8A	11.64	117.96	105.74
3	A	401	FAD	N9A-C8A-N7A	-9.01	101.15	113.94
3	A	401	FAD	C8M-C8-C9	4.52	127.53	119.57
3	A	401	FAD	C1B-N9A-C8A	-4.43	117.27	127.09
3	A	401	FAD	C6A-C5A-N7A	4.34	140.46	132.09
3	A	401	FAD	C6A-C5A-C4A	-4.12	111.55	117.18
3	A	401	FAD	C9A-C5X-N5	-4.11	118.09	122.45
3	A	401	FAD	C8M-C8-C7	-3.68	113.24	120.76
3	A	401	FAD	C4-C4X-N5	3.22	122.66	118.21
3	A	401	FAD	O4-C4-C4X	-3.18	118.13	126.53
3	A	401	FAD	C10-N1-C2	2.89	123.10	116.85
3	A	401	FAD	C5A-C4A-N3A	2.73	130.47	126.72
3	A	401	FAD	C5X-C9A-N10	2.63	120.34	117.97
3	A	401	FAD	N10-C10-N1	2.53	125.97	118.51
3	A	401	FAD	C4A-C5A-N7A	-2.27	107.99	110.58
3	A	401	FAD	C4X-C10-N10	-2.22	113.31	116.48
3	A	401	FAD	C9A-N10-C10	2.22	124.13	120.75
3	A	401	FAD	C4X-C4-N3	2.11	118.63	113.25
3	A	401	FAD	C5A-N7A-C8A	2.04	106.66	103.45
3	A	401	FAD	N3A-C4A-N9A	-2.04	123.70	127.17
3	A	401	FAD	C2B-C1B-N9A	2.01	118.29	113.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

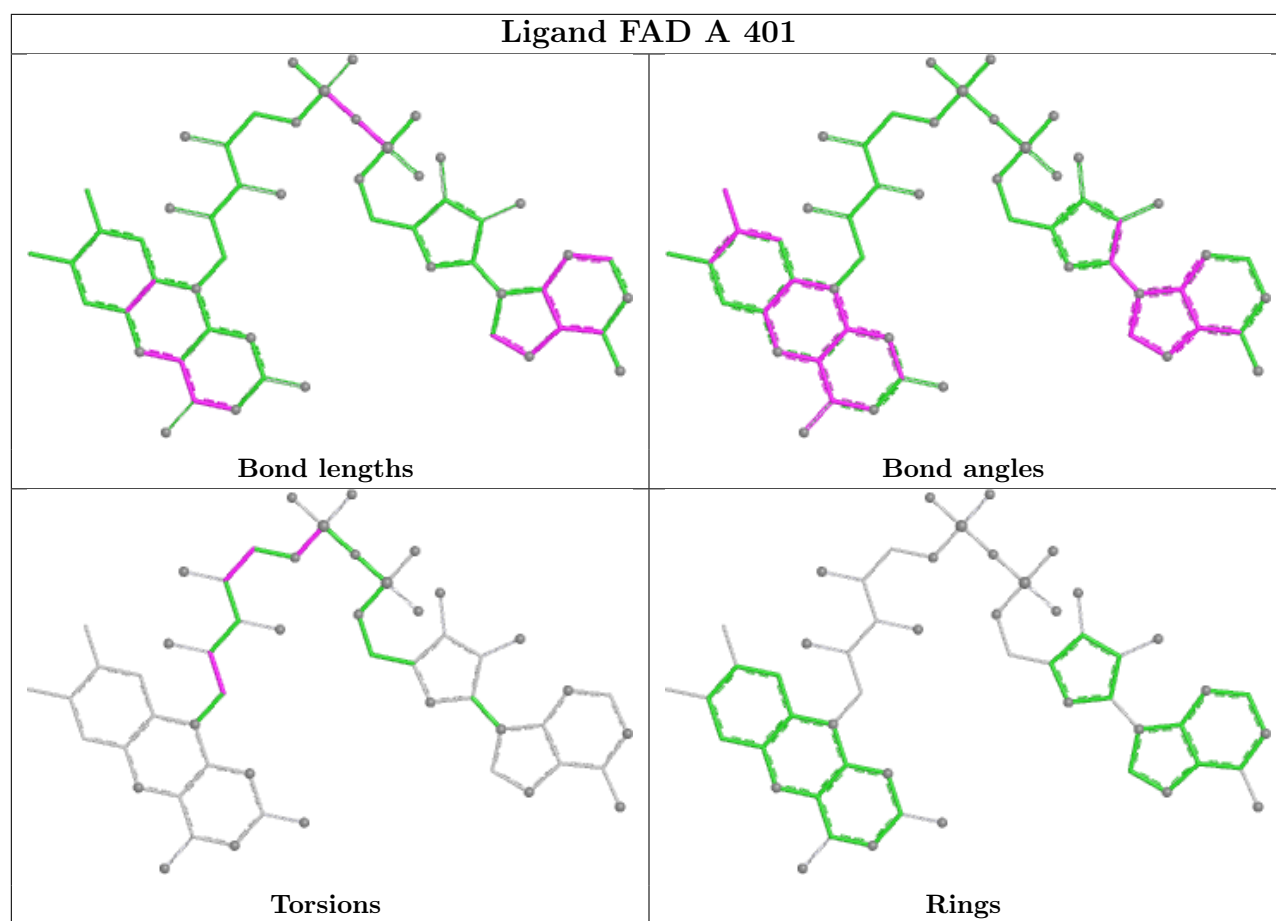
Mol	Chain	Res	Type	Atoms
3	A	401	FAD	N10-C1'-C2'-O2'
3	A	401	FAD	N10-C1'-C2'-C3'
3	A	401	FAD	C3'-C4'-C5'-O5'
3	A	401	FAD	C5'-O5'-P-O1P
3	A	401	FAD	C5'-O5'-P-O2P
3	A	401	FAD	O4'-C4'-C5'-O5'
3	A	401	FAD	C5'-O5'-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	FAD	2	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.