



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:27 AM UTC

PDB ID : 1MBB / pdb_00001mbb
Title : OXIDOREDUCTASE
Authors : Benson, T.E.; Lees, W.J.; Walsh, C.T.; Hogle, J.M.
Deposited on : 1995-11-07
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

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

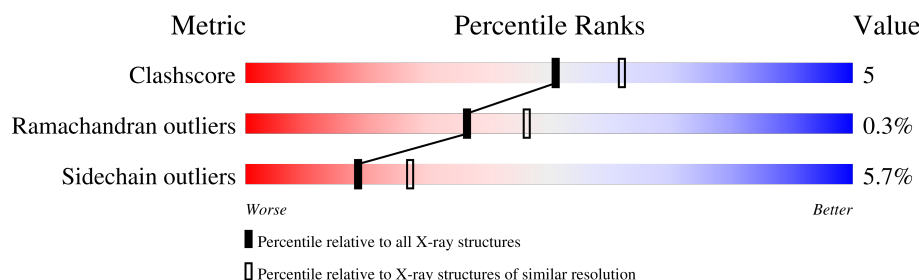
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	63% 32% . ..

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	EEB	A	402	X	-	-	-

2 Entry composition [i](#)

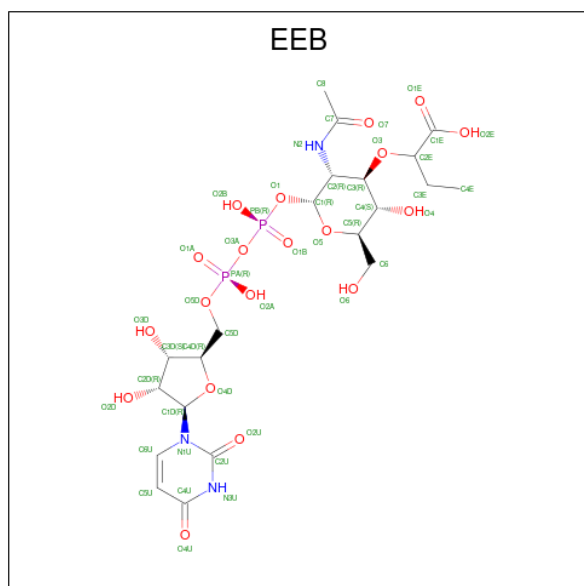
There are 4 unique types of molecules in this entry. The entry contains 2871 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 URIDINE-DIPHOSPHATE-3(N-ACETYLGLUCOSAMINYL)BUTYRIC ACID (CCD ID: EEB) (formula: $C_{21}H_{33}N_3O_{19}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			45	21	3	19	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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.

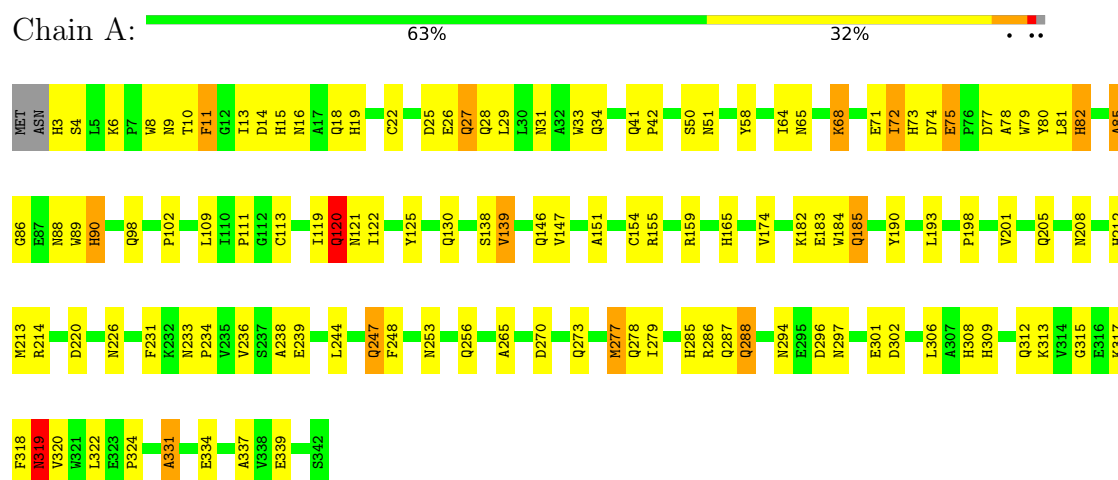
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	119	Total O 119 119	0	0

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 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	50.00Å 50.00Å 264.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.9 (12.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.238 , 0.324	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2871	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: EEB, 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	1.02	13/2716 (0.5%)	1.98	96/3695 (2.6%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	309	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	15	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	285	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	308	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	73	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	212	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	19	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	3	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	90	HIS	CD2-NE2	-5.48	1.31	1.37
1	A	82	HIS	CD2-NE2	-5.23	1.32	1.37
1	A	308	HIS	CG-ND1	-5.15	1.32	1.38
1	A	15	HIS	CG-ND1	-5.12	1.32	1.38

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ASN	OD1-CG-ND2	-11.58	111.02	122.60
1	A	185	GLN	OE1-CD-NE2	-9.65	112.95	122.60
1	A	34	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	A	31	ASN	OD1-CG-ND2	-9.35	113.25	122.60
1	A	312	GLN	OE1-CD-NE2	-9.00	113.60	122.60
1	A	205	GLN	OE1-CD-NE2	-8.84	113.76	122.60
1	A	25	ASP	CA-CB-CG	8.67	121.27	112.60
1	A	322	LEU	N-CA-C	8.55	122.78	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	GLN	OE1-CD-NE2	-8.45	114.15	122.60
1	A	65	ASN	OD1-CG-ND2	-8.44	114.16	122.60
1	A	27	GLN	OE1-CD-NE2	-8.09	114.52	122.60
1	A	9	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	A	120	GLN	OE1-CD-NE2	-7.87	114.73	122.60
1	A	288	GLN	OE1-CD-NE2	-7.65	114.95	122.60
1	A	297	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	A	146	GLN	OE1-CD-NE2	-7.59	115.01	122.60
1	A	4	SER	N-CA-C	7.47	120.57	109.59
1	A	201	VAL	N-CA-C	7.46	119.44	109.37
1	A	51	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	34	GLN	CG-CD-NE2	7.33	127.39	116.40
1	A	331	ALA	N-CA-C	7.19	126.12	110.80
1	A	233	ASN	OD1-CG-ND2	-7.05	115.55	122.60
1	A	73	HIS	CA-CB-CG	7.00	120.80	113.80
1	A	319	ASN	CB-CG-ND2	6.92	126.79	116.40
1	A	247	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	A	278	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	122	ILE	N-CA-C	6.71	118.09	109.30
1	A	88	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	A	226	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	A	41	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	A	302	ASP	CA-CB-CG	6.55	119.16	112.60
1	A	16	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	A	98	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	A	294	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	256	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	185	GLN	CG-CD-NE2	6.40	126.01	116.40
1	A	198	PRO	N-CA-C	6.25	121.96	113.84
1	A	285	HIS	CB-CG-CD2	-6.23	123.11	131.20
1	A	205	GLN	CG-CD-NE2	6.21	125.71	116.40
1	A	121	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	A	72	ILE	N-CA-CB	-6.17	103.90	111.67
1	A	9	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	190	TYR	N-CA-C	6.10	119.19	109.24
1	A	119	ILE	N-CA-C	6.07	116.73	110.36
1	A	287	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	A	85	ALA	N-CA-C	5.99	118.60	111.71
1	A	165	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	6	LYS	N-CA-C	5.84	121.58	113.45
1	A	277	MET	CA-CB-CG	-5.84	102.41	114.10
1	A	120	GLN	CG-CD-NE2	5.84	125.16	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	A	74	ASP	N-CA-C	5.82	119.02	109.76
1	A	248	PHE	CA-C-N	5.78	125.46	119.05
1	A	248	PHE	C-N-CA	5.78	125.46	119.05
1	A	286	ARG	N-CA-C	5.73	119.53	112.54
1	A	334	GLU	N-CA-C	5.70	118.60	110.10
1	A	18	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	A	317	LYS	N-CA-C	5.67	117.14	111.07
1	A	130	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	A	125	TYR	N-CA-C	5.63	118.96	111.30
1	A	238	ALA	N-CA-C	5.63	118.14	111.33
1	A	68	LYS	N-CA-C	5.62	118.84	109.96
1	A	9	ASN	CB-CG-ND2	5.62	124.83	116.40
1	A	253	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	155	ARG	N-CA-C	5.52	118.81	111.30
1	A	15	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	A	236	VAL	O-C-N	-5.51	117.56	122.69
1	A	75	GLU	O-C-N	-5.45	117.12	121.80
1	A	22	CYS	N-CA-C	5.42	117.06	108.67
1	A	33	TRP	CB-CG-CD1	-5.40	118.80	126.90
1	A	147	VAL	N-CA-C	5.40	117.17	108.85
1	A	19	HIS	CA-CB-CG	5.39	119.19	113.80
1	A	41	GLN	N-CA-C	5.38	117.72	110.29
1	A	138	SER	N-CA-C	5.34	117.80	109.52
1	A	31	ASN	CB-CG-ND2	5.33	124.40	116.40
1	A	14	ASP	CA-C-O	5.30	126.57	120.84
1	A	256	GLN	CG-CD-NE2	5.28	124.32	116.40
1	A	77	ASP	N-CA-C	5.24	119.38	112.89
1	A	78	ALA	N-CA-C	5.17	116.93	108.76
1	A	139	VAL	CB-CA-C	-5.17	103.81	110.84
1	A	320	VAL	CA-C-O	5.17	126.06	120.53
1	A	79	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	247	GLN	CB-CA-C	-5.17	100.75	110.67
1	A	297	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	312	GLN	CG-CD-NE2	5.10	124.05	116.40
1	A	8	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	296	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	220	ASP	CA-C-O	-5.05	115.27	119.76
1	A	33	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	A	270	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	89	TRP	CE2-CD2-CG	-5.04	101.16	107.20
1	A	308	HIS	CB-CG-CD2	-5.03	124.67	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	TRP	CG-CD2-CE3	5.02	138.92	133.90
1	A	208	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	212	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	A	79	TRP	CG-CD2-CE3	5.01	138.91	133.90

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	2654	0	2614	25	0
2	A	45	0	27	2	0
3	A	53	0	31	3	0
4	A	119	0	0	1	0
All	All	2871	0	2672	28	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 5.

All (28) 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:72:ILE:HG12	1:A:81:LEU:HD22	1.81	0.62
2:A:402:EEB:HE42	3:A:401:FAD:C5X	2.34	0.57
1:A:324:PRO:HG2	1:A:337:ALA:HB1	1.88	0.55
3:A:401:FAD:O5B	3:A:401:FAD:H8A	2.06	0.55
1:A:71:GLU:HB2	1:A:82:HIS:HB3	1.91	0.52
1:A:234:PRO:HD3	1:A:265:ALA:HB2	1.91	0.52
1:A:75:GLU:HG3	1:A:80:TYR:CE1	2.45	0.52
1:A:244:LEU:HD21	1:A:318:PHE:HB3	1.92	0.51
1:A:279:ILE:HD12	1:A:306:LEU:HA	1.91	0.51
1:A:120:GLN:O	1:A:159:ARG:HA	2.11	0.51
1:A:214:ARG:NH2	3:A:401:FAD:O4	2.44	0.50
1:A:85:ALA:O	1:A:113:CYS:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:OG1	1:A:50:SER:HA	2.12	0.49
1:A:231:PHE:HA	1:A:324:PRO:HA	1.95	0.49
1:A:68:LYS:HE2	1:A:86:GLY:O	2.14	0.48
1:A:11:PHE:HB3	1:A:13:ILE:HG12	1.96	0.47
1:A:151:ALA:O	1:A:154:CYS:HB2	2.16	0.45
1:A:26:GLU:HG3	1:A:174:VAL:HG11	1.98	0.45
1:A:315:GLY:O	1:A:319:ASN:HA	2.18	0.44
1:A:75:GLU:O	1:A:182:LYS:NZ	2.50	0.44
1:A:214:ARG:NH1	4:A:563:HOH:O	2.50	0.43
1:A:90:HIS:HD2	1:A:109:LEU:H	1.65	0.43
1:A:313:LYS:HA	1:A:313:LYS:HD3	1.76	0.42
1:A:109:LEU:O	1:A:111:PRO:HD3	2.20	0.42
2:A:402:EEB:HE31	2:A:402:EEB:H3	1.76	0.41
1:A:42:PRO:HB2	1:A:58:TYR:OH	2.20	0.41
1:A:102:PRO:HB2	1:A:184:TRP:CD1	2.56	0.41
1:A:193:LEU:HG	1:A:213:MET:HE1	2.02	0.41

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	338/342 (99%)	320 (95%)	17 (5%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	ALA

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%)	266 (94%)	16 (6%)	18	27

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	27	GLN
1	A	28	GLN
1	A	29	LEU
1	A	64	ILE
1	A	120	GLN
1	A	139	VAL
1	A	183	GLU
1	A	185	GLN
1	A	239	GLU
1	A	247	GLN
1	A	277	MET
1	A	288	GLN
1	A	301	GLU
1	A	319	ASN
1	A	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	51	ASN
1	A	82	HIS
1	A	90	HIS
1	A	98	GLN
1	A	256	GLN
1	A	287	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 ⓘ

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	1.92	12 (20%)	85,89,89	2.28	19 (22%)
2	EEB	A	402	-	46,47,47	2.39	15 (32%)	62,70,70	3.33	18 (29%)

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	-	-	3/34/50/50	0/6/6/6
2	EEB	A	402	-	1/1/14/15	11/36/73/73	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	EEB	O3-C2E	-7.79	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	EEB	PA-O3A	-7.74	1.51	1.59
3	A	401	FAD	C8A-N7A	7.24	1.45	1.31
3	A	401	FAD	C5A-N7A	6.20	1.50	1.39
2	A	402	EEB	C3E-C2E	-5.38	1.37	1.51
3	A	401	FAD	P-O3P	4.77	1.64	1.59
2	A	402	EEB	C6U-N1U	4.03	1.47	1.38
2	A	402	EEB	PB-O3A	-3.50	1.55	1.59
3	A	401	FAD	C4X-N5	3.50	1.38	1.30
2	A	402	EEB	C4-C3	3.31	1.61	1.52
3	A	401	FAD	C5A-C4A	-3.03	1.33	1.39
3	A	401	FAD	C5A-C6A	2.75	1.48	1.41
3	A	401	FAD	C4-N3	-2.71	1.33	1.38
3	A	401	FAD	C9A-C5X	-2.55	1.37	1.41
2	A	402	EEB	C5U-C4U	2.51	1.49	1.43
3	A	401	FAD	C2A-N3A	-2.47	1.29	1.33
2	A	402	EEB	PB-O1	-2.47	1.51	1.59
3	A	401	FAD	C4A-N3A	2.46	1.39	1.34
3	A	401	FAD	PA-O3P	-2.41	1.56	1.59
2	A	402	EEB	O1E-C1E	2.38	1.29	1.22
2	A	402	EEB	O2D-C2D	-2.37	1.37	1.43
2	A	402	EEB	O7-C7	-2.36	1.18	1.23
2	A	402	EEB	C3D-C2D	-2.32	1.47	1.53
2	A	402	EEB	C5D-C4D	2.29	1.58	1.51
2	A	402	EEB	C4U-N3U	-2.25	1.34	1.38
2	A	402	EEB	O3-C3	-2.09	1.38	1.43
3	A	401	FAD	C4X-C4	2.09	1.52	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	EEB	C3-C2-N2	13.72	132.79	110.91
3	A	401	FAD	C4A-N9A-C8A	11.49	117.80	105.74
2	A	402	EEB	O3-C2E-C3E	10.48	123.97	106.90
2	A	402	EEB	C2-N2-C7	8.97	144.11	123.11
3	A	401	FAD	N9A-C8A-N7A	-8.91	101.30	113.94
2	A	402	EEB	C4E-C3E-C2E	8.68	125.95	113.47
2	A	402	EEB	C8-C7-N2	-5.09	107.68	116.12
3	A	401	FAD	C8M-C8-C9	4.76	127.95	119.57
2	A	402	EEB	O3-C3-C4	4.74	119.27	107.23
2	A	402	EEB	O7-C7-N2	4.49	129.91	121.98
3	A	401	FAD	C1B-N9A-C8A	-4.40	117.33	127.09
3	A	401	FAD	C6A-C5A-N7A	4.39	140.55	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	FAD	C6A-C5A-C4A	-4.18	111.48	117.18
2	A	402	EEB	O4U-C4U-C5U	-4.02	118.23	125.16
2	A	402	EEB	O1-C1-C2	4.01	115.66	108.40
2	A	402	EEB	C1-C2-N2	-3.84	104.47	110.92
3	A	401	FAD	C8M-C8-C7	-3.78	113.05	120.76
2	A	402	EEB	O3D-C3D-C4D	3.74	121.82	111.08
3	A	401	FAD	C9A-C5X-N5	-3.54	118.69	122.45
2	A	402	EEB	C5U-C4U-N3U	3.42	119.60	114.80
3	A	401	FAD	C4-C4X-N5	3.02	122.38	118.21
3	A	401	FAD	O4-C4-C4X	-2.97	118.68	126.53
3	A	401	FAD	C10-N1-C2	2.92	123.17	116.85
2	A	402	EEB	O5-C1-O1	2.84	115.07	111.36
3	A	401	FAD	C5A-C4A-N3A	2.80	130.56	126.72
2	A	402	EEB	C5D-C4D-C3D	-2.77	105.23	115.21
2	A	402	EEB	C5U-C6U-N1U	-2.75	117.37	121.84
2	A	402	EEB	O2E-C1E-C2E	2.61	119.50	112.71
3	A	401	FAD	N10-C10-N1	2.60	126.15	118.51
2	A	402	EEB	O5D-PA-O1A	-2.52	98.94	108.94
2	A	402	EEB	O2D-C2D-C1D	2.49	118.68	110.10
3	A	401	FAD	C5X-C9A-N10	2.32	120.06	117.97
3	A	401	FAD	C4A-C5A-N7A	-2.28	107.97	110.58
3	A	401	FAD	N3A-C4A-N9A	-2.21	123.41	127.17
3	A	401	FAD	C5A-N7A-C8A	2.07	106.71	103.45
3	A	401	FAD	C4X-C4-N3	2.02	118.39	113.25
3	A	401	FAD	C2B-C1B-N9A	2.01	118.30	113.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	402	EEB	C2E

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	EEB	C5D-O5D-PA-O1A
2	A	402	EEB	C3E-C2E-O3-C3
3	A	401	FAD	N10-C1'-C2'-O2'
3	A	401	FAD	N10-C1'-C2'-C3'
2	A	402	EEB	O1E-C1E-C2E-C3E
2	A	402	EEB	PB-O3A-PA-O5D
2	A	402	EEB	O2E-C1E-C2E-C3E
2	A	402	EEB	C1E-C2E-C3E-C4E

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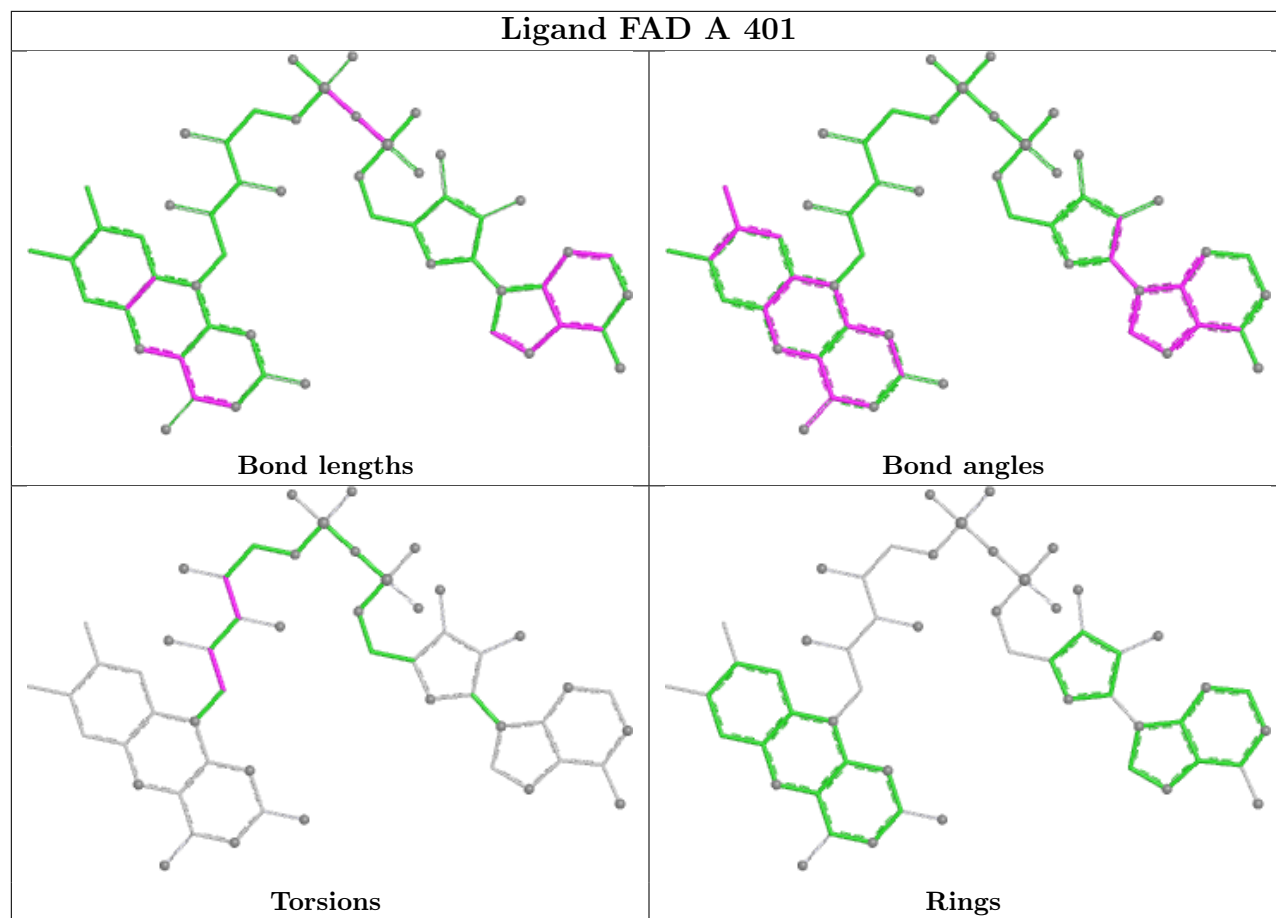
Mol	Chain	Res	Type	Atoms
2	A	402	EEB	PB-O3A-PA-O1A
2	A	402	EEB	O2E-C1E-C2E-O3
2	A	402	EEB	C1-O1-PB-O2B
3	A	401	FAD	C2'-C3'-C4'-O4'
2	A	402	EEB	O3-C2E-C3E-C4E
2	A	402	EEB	C1E-C2E-O3-C3

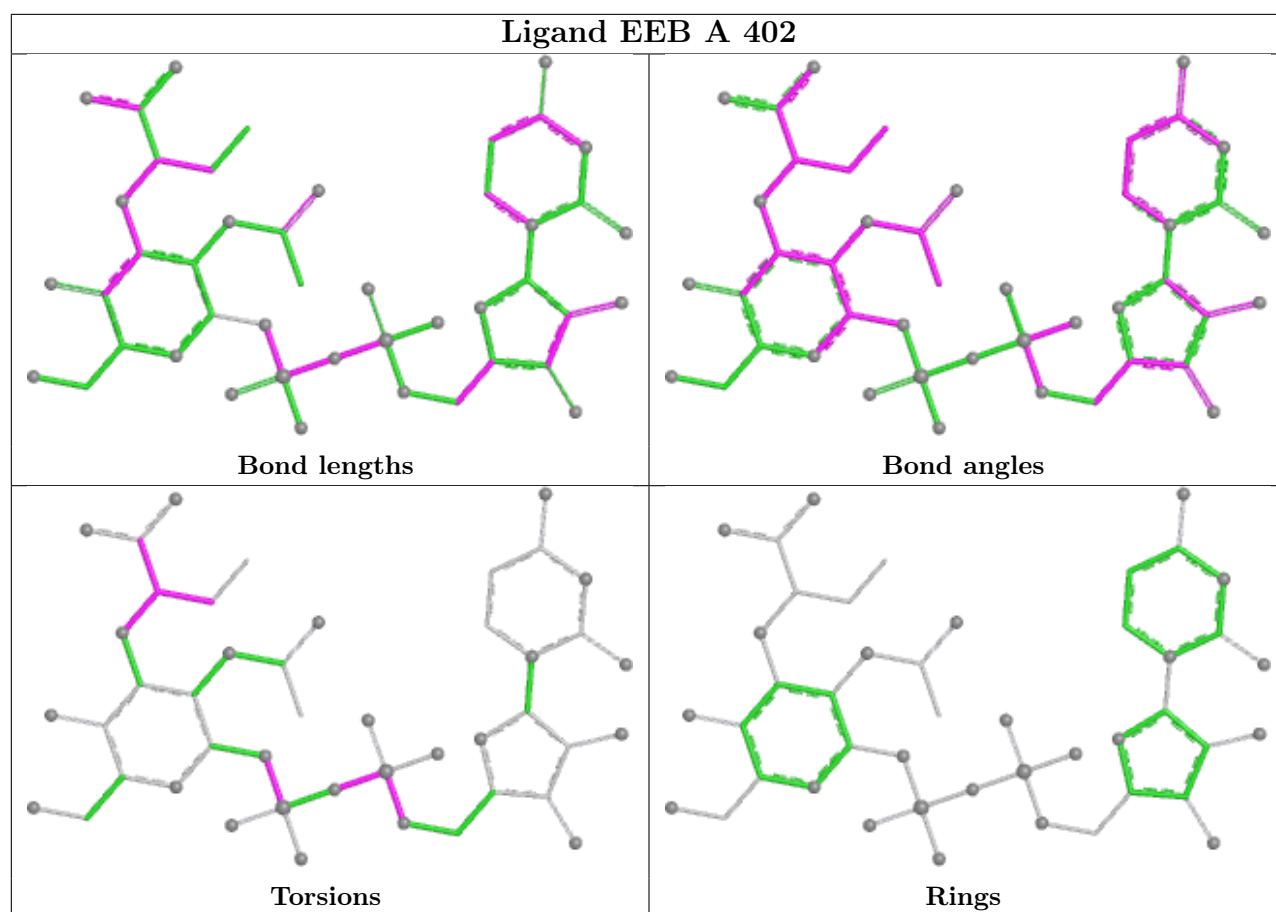
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	FAD	3	0
2	A	402	EEB	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.