



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:17 AM UTC

PDB ID : 1XDI / pdb_00001xdi
Title : Crystal structure of LpdA (Rv3303c) from Mycobacterium tuberculosis
Authors : Argyrou, A.; Vetting, M.W.; Blanchard, J.S.
Deposited on : 2004-09-06
Resolution : 2.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

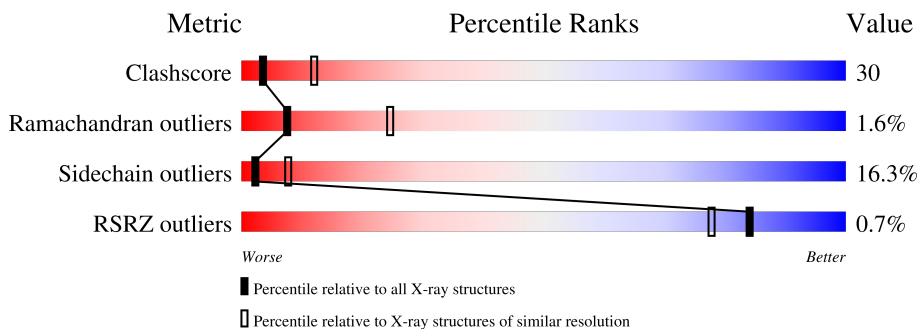
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	% 50% 31% 10% • 8%
1	B	499	42% 37% 11% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6925 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.

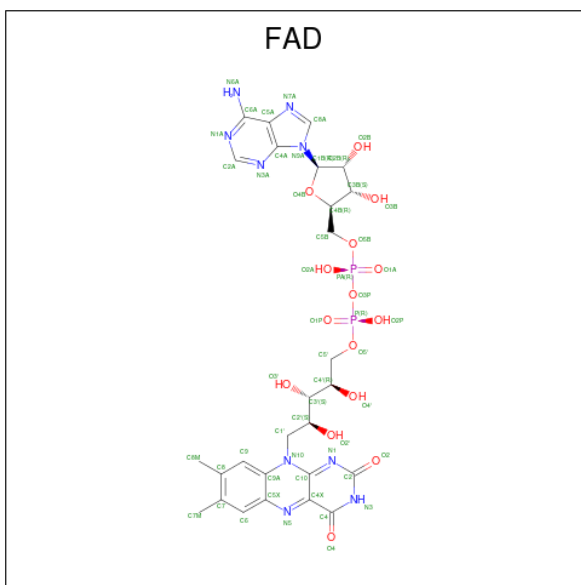
- Molecule 1 is a protein called Rv3303c-lpdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3356	2101	607	635	13			
1	B	459	Total	C	N	O	S	0	0	0
			3356	2101	607	635	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	HIS	-	expression tag	UNP O53355
A	495	HIS	-	expression tag	UNP O53355
A	496	HIS	-	expression tag	UNP O53355
A	497	HIS	-	expression tag	UNP O53355
A	498	HIS	-	expression tag	UNP O53355
A	499	HIS	-	expression tag	UNP O53355
B	494	HIS	-	expression tag	UNP O53355
B	495	HIS	-	expression tag	UNP O53355
B	496	HIS	-	expression tag	UNP O53355
B	497	HIS	-	expression tag	UNP O53355
B	498	HIS	-	expression tag	UNP O53355
B	499	HIS	-	expression tag	UNP O53355

- 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
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

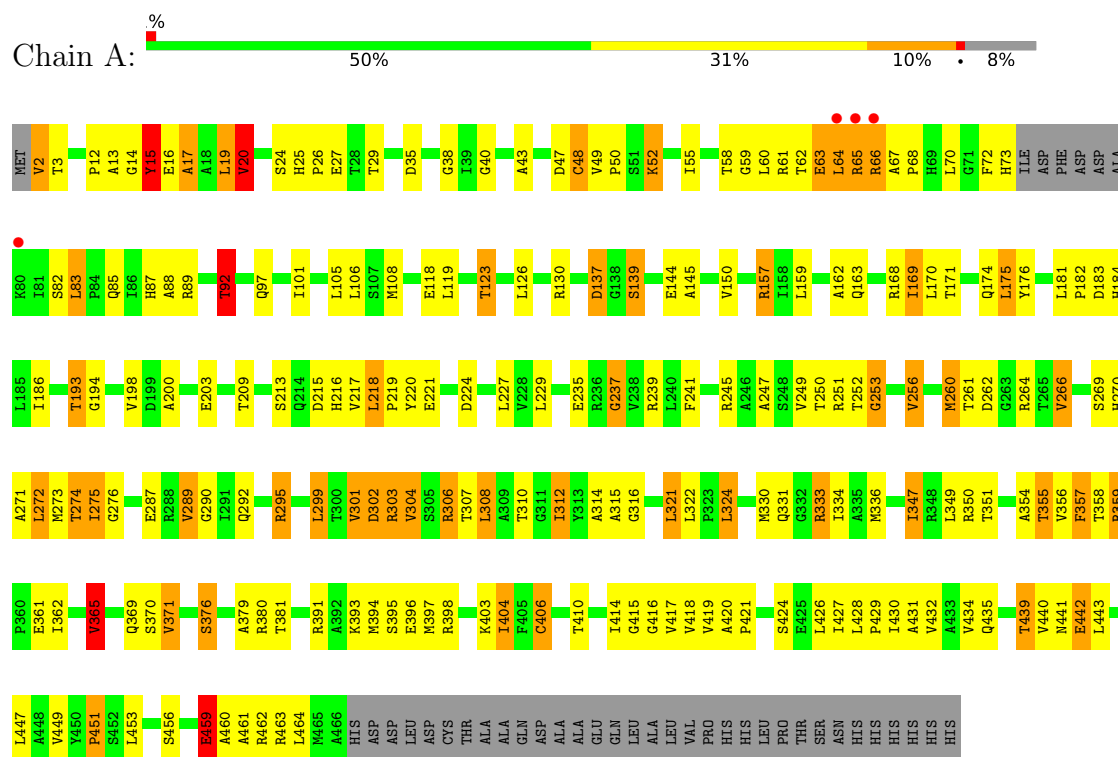
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 57 57	0	0
3	B	50	Total O 50 50	0	0

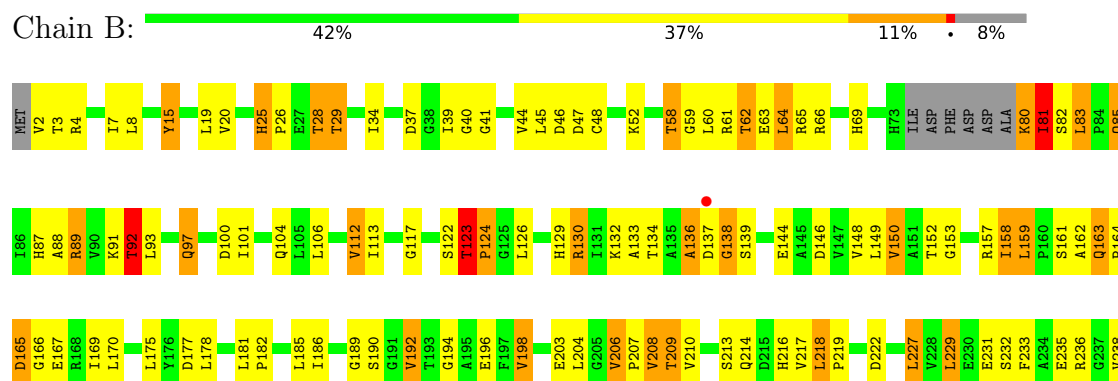
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Rv3303c-lpdA



• Molecule 1: Rv3303c-lpdA



R239	A309	R391	R463
L240	T310	A392	L464
F241	G311	S395	M465
K242	T312	E396	A466
N243	Y313	M397	HIS
	A314	R398	ASP
			LEU
S248	G320	F401	ASP
V249	L321	V402	ASP
T250	L322	K403	CYS
R251	P323	I404	THR
T252		F405	ALA
G253	V327		ALA
A254			GLN
G255	M330	R408	ASP
V256	Q331	S409	ALA
L257	G332	T410	ALA
V258	R333	G411	ALA
T259		V412	GLU
M260	M336	V413	GLN
T261	Y337	I414	LEU
D262	H338	G415	ALA
G263	A339		LEU
R264	L340	S424	VAL
T265	G341	E425	PRO
V266	E342	L426	HIS
		I427	HIS
H270	P346	L428	LEU
A271	T347	P429	PRO
L272	R348		THR
M273	L349	V432	SER
T274	R350	A433	ASN
T275			HIS
G276	T355	M436	HIS
S277	V356	R437	HIS
V278	F357	I438	HIS
P279	T358	T439	HIS
N280		V440	HIS
T281		M441	
		E442	
G285	G366	L443	
L286	V367	A444	
E287	P368	Q445	
R288	Q369	T446	
V289	S370	L447	
	V371	A448	
	I372	V449	
Q292	D373	Y450	
L293	A374	P451	
G294	G375	S452	
R295	S376	L453	
		S454	
L299	V377	G455	
T300	A378	S456	
V301	A379	I457	
D302	R380	T458	
R303	T381	E459	
V304	I382	A460	
S305	M383	A461	
R306	L384	R462	
T307			
L308	A390		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	244.20Å 244.20Å 104.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.81 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.81) 99.7 (50.00-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.31 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.276 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6925	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	5/3404 (0.1%)	1.48	43/4637 (0.9%)
1	B	1.14	4/3404 (0.1%)	1.52	58/4637 (1.3%)
All	All	1.13	9/6808 (0.1%)	1.50	101/9274 (1.1%)

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLU	CA-C	-8.46	1.42	1.52
1	B	383	MET	SD-CE	8.46	2.00	1.79
1	A	16	GLU	N-CA	-6.24	1.39	1.46
1	A	312	ILE	CA-CB	5.57	1.60	1.53
1	A	434	VAL	CA-CB	-5.54	1.48	1.54

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	THR	CA-C-N	12.81	134.32	119.47
1	B	123	THR	C-N-CA	12.81	134.32	119.47
1	A	303	ARG	N-CA-C	-11.51	99.22	113.38
1	A	17	ALA	N-CA-C	-10.95	99.75	113.55
1	B	25	HIS	CA-C-N	10.88	130.56	119.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3356	0	3454	197	0
1	B	3356	0	3454	229	0
2	A	53	0	31	5	0
2	B	53	0	31	3	0
3	A	57	0	0	4	0
3	B	50	0	0	4	0
All	All	6925	0	6970	407	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 30.

The worst 5 of 407 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:B:249:VAL:HG21	1:B:273:MET:HE1	1.24	1.14
1:B:275:ILE:HG22	1:B:276:GLY:H	1.03	1.14
1:A:275:ILE:HG22	1:A:276:GLY:H	1.00	1.13
1:B:308:LEU:H	1:B:308:LEU:HD12	1.16	1.11
1:B:392:ALA:HA	1:B:397:MET:HE3	1.24	1.09

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	455/499 (91%)	418 (92%)	30 (7%)	7 (2%)	8	26
1	B	455/499 (91%)	413 (91%)	34 (8%)	8 (2%)	6	22
All	All	910/998 (91%)	831 (91%)	64 (7%)	15 (2%)	7	24

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	64	LEU
1	A	253	GLY
1	A	261	THR
1	A	275	ILE

5.3.2 Protein sidechains [i](#)

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	352/386 (91%)	295 (84%)	57 (16%)	2	8
1	B	352/386 (91%)	294 (84%)	58 (16%)	2	7
All	All	704/772 (91%)	589 (84%)	115 (16%)	2	8

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	THR

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Mol	Chain	Res	Type
1	B	432	VAL
1	B	92	THR
1	B	409	SER
1	B	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	HIS
1	B	87	HIS
1	B	441	ASN
1	B	270	HIS
1	B	338	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	999	-	58,58,58	2.16	17 (29%)	85,89,89	1.74	19 (22%)
2	FAD	B	999	-	58,58,58	2.26	14 (24%)	85,89,89	1.81	18 (21%)

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	999	-	-	6/34/50/50	0/6/6/6
2	FAD	B	999	-	-	6/34/50/50	0/6/6/6

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	FAD	C4A-N3A	6.93	1.47	1.34
2	B	999	FAD	C4X-N5	6.52	1.44	1.30
2	A	999	FAD	C4X-N5	5.60	1.42	1.30
2	A	999	FAD	C5A-C4A	-5.38	1.29	1.39
2	B	999	FAD	C9A-N10	5.18	1.50	1.41

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	FAD	C5A-C4A-N9A	6.10	112.45	105.81
2	A	999	FAD	C5A-C4A-N9A	5.78	112.11	105.81
2	B	999	FAD	N3A-C4A-N9A	-5.39	118.00	127.17
2	A	999	FAD	N3A-C4A-N9A	-5.36	118.05	127.17
2	A	999	FAD	C4A-N9A-C8A	-4.76	100.74	105.74

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

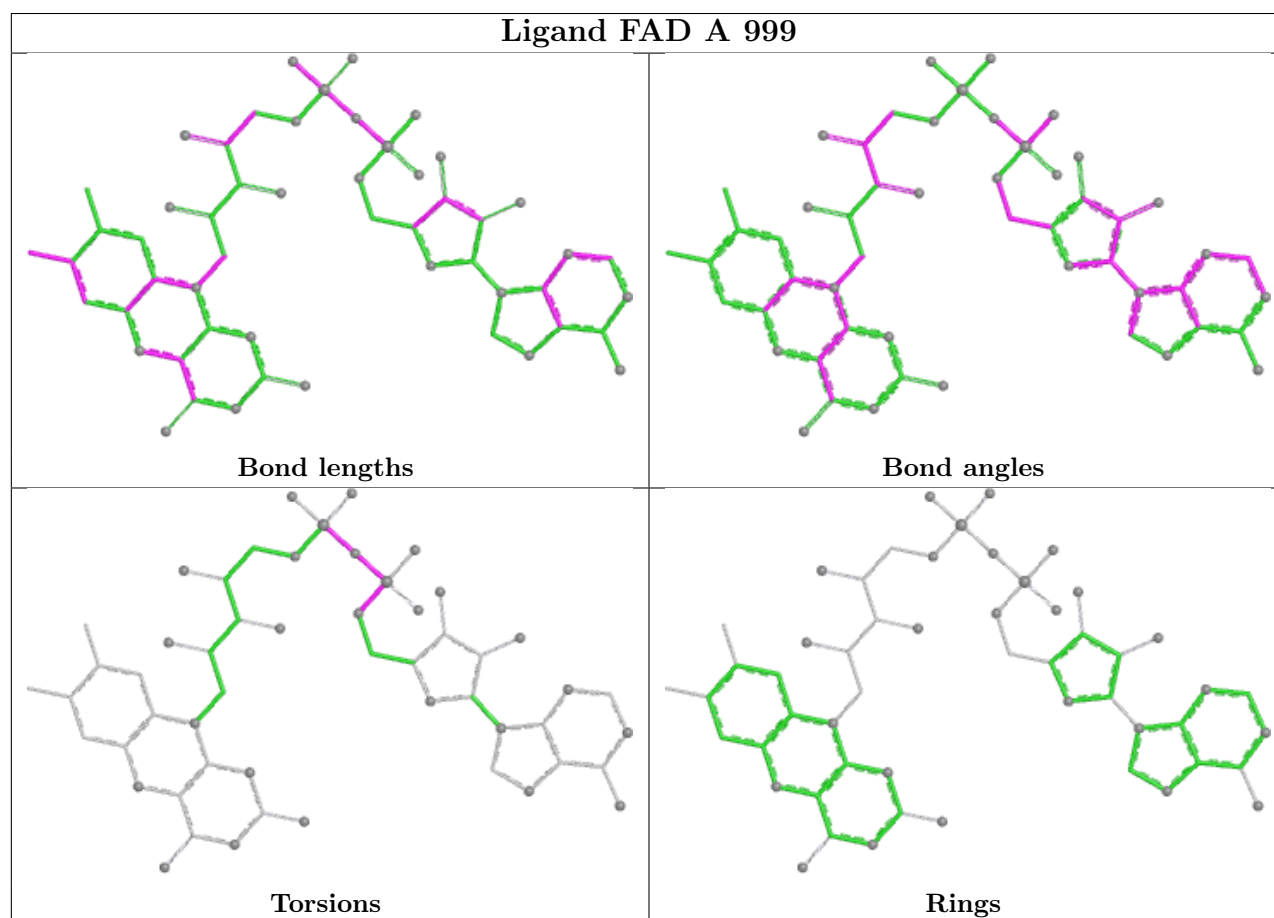
Mol	Chain	Res	Type	Atoms
2	A	999	FAD	C5B-O5B-PA-O1A
2	A	999	FAD	P-O3P-PA-O1A
2	A	999	FAD	PA-O3P-P-O5'
2	B	999	FAD	PA-O3P-P-O5'
2	A	999	FAD	C5B-O5B-PA-O2A

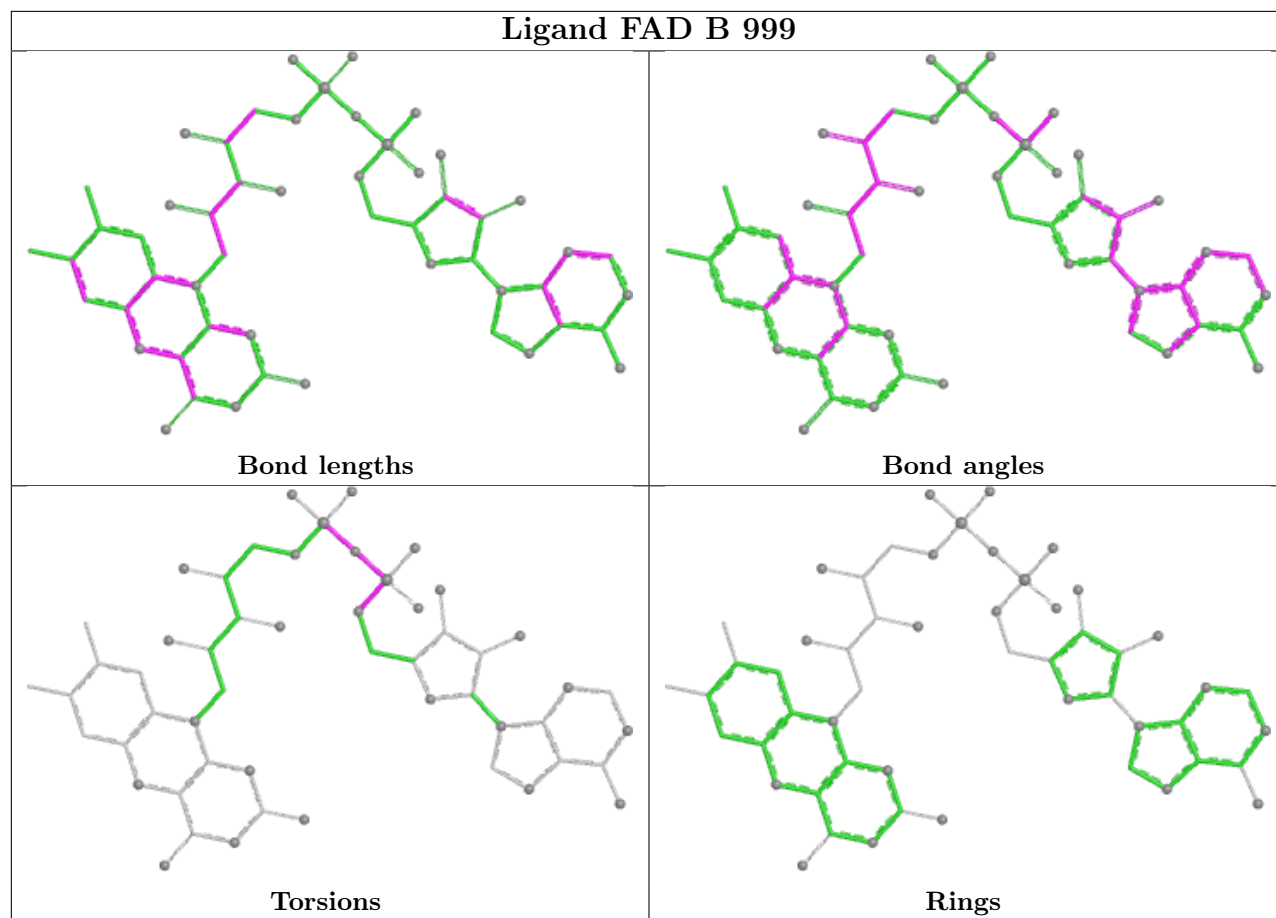
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	FAD	5	0
2	B	999	FAD	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/499 (91%)	-0.48	4 (0%) 81 74	1, 12, 34, 61	0
1	B	459/499 (91%)	-0.41	2 (0%) 88 84	1, 12, 37, 51	0
All	All	918/998 (91%)	-0.45	6 (0%) 84 78	1, 12, 36, 61	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	ASP	3.0
1	A	80	LYS	2.7
1	B	374	ALA	2.2
1	A	65	ARG	2.1
1	A	64	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

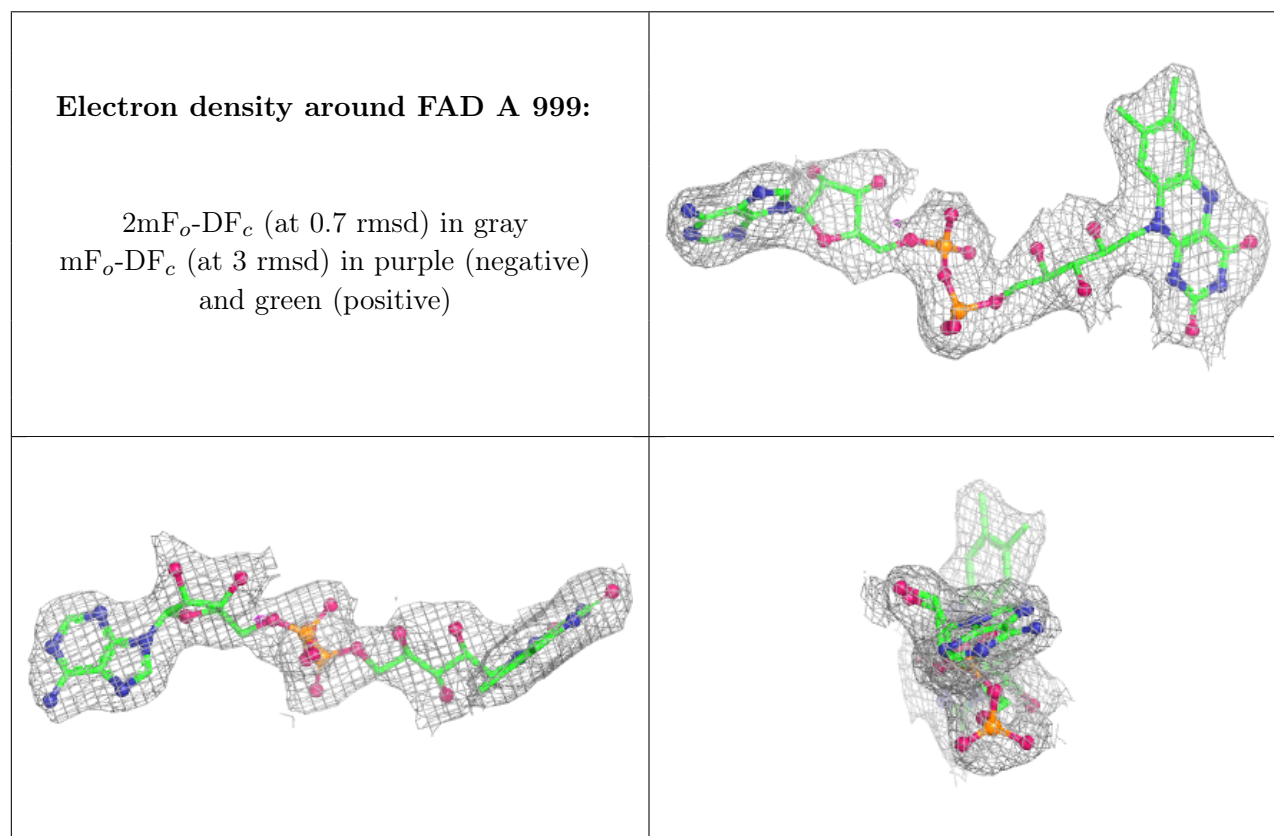
There are no oligosaccharides in this entry.

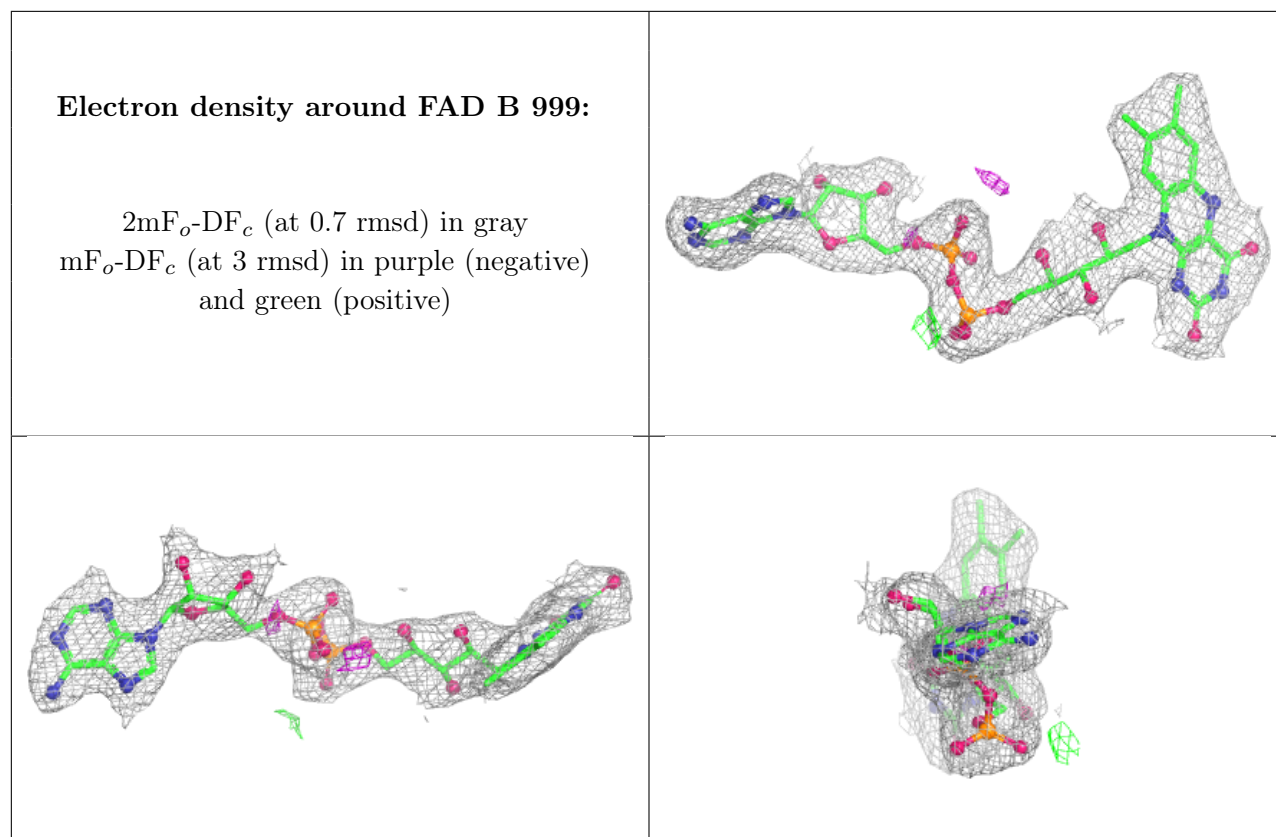
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	999	53/53	0.98	0.06	1,6,10,12	0
2	FAD	B	999	53/53	0.98	0.05	1,8,12,12	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.