



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 01:57 PM UTC

PDB ID : 3CP8 / pdb_00003cp8
Title : Crystal structure of GidA from Chlorobium tepidum
Authors : Meyer, S.; Scrima, A.; Versees, W.; Wittinghofer, A.
Deposited on : 2008-03-31
Resolution : 3.20 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

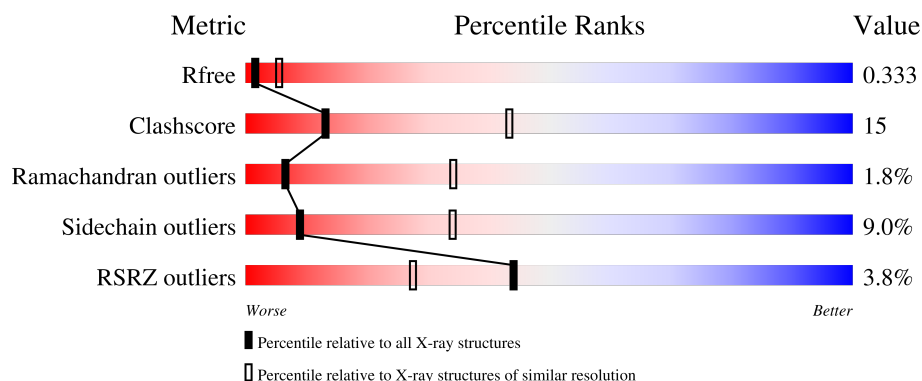
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	641	 6% 65% 27% • 5%
1	B	641	 2% 66% 26% • 5%
1	C	641	 3% 65% 27% • 5%
1	D	641	 2% 59% 24% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18567 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	B	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	C	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	D	552	Total	C	N	O	S	0	0	0
			4243	2658	752	810	23			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8KA85
A	-18	GLY	-	expression tag	UNP Q8KA85
A	-17	SER	-	expression tag	UNP Q8KA85
A	-16	SER	-	expression tag	UNP Q8KA85
A	-15	HIS	-	expression tag	UNP Q8KA85
A	-14	HIS	-	expression tag	UNP Q8KA85
A	-13	HIS	-	expression tag	UNP Q8KA85
A	-12	HIS	-	expression tag	UNP Q8KA85
A	-11	HIS	-	expression tag	UNP Q8KA85
A	-10	HIS	-	expression tag	UNP Q8KA85
A	-9	SER	-	expression tag	UNP Q8KA85
A	-8	SER	-	expression tag	UNP Q8KA85
A	-7	GLY	-	expression tag	UNP Q8KA85
A	-6	LEU	-	expression tag	UNP Q8KA85
A	-5	VAL	-	expression tag	UNP Q8KA85
A	-4	PRO	-	expression tag	UNP Q8KA85
A	-3	ARG	-	expression tag	UNP Q8KA85
A	-2	GLY	-	expression tag	UNP Q8KA85
A	-1	SER	-	expression tag	UNP Q8KA85
A	0	HIS	-	expression tag	UNP Q8KA85

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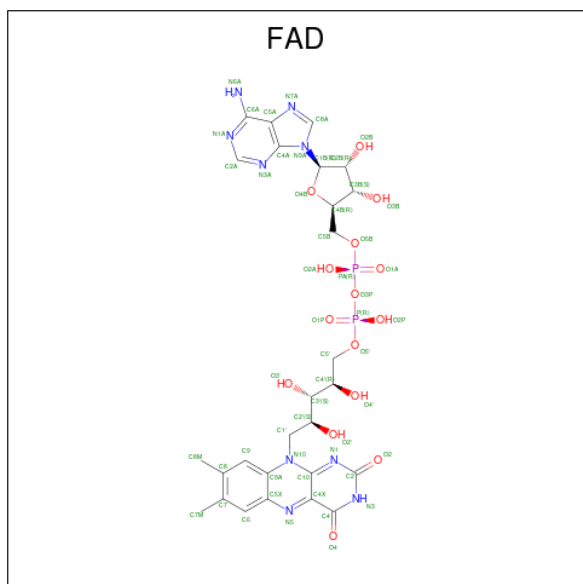
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q8KA85
B	-18	GLY	-	expression tag	UNP Q8KA85
B	-17	SER	-	expression tag	UNP Q8KA85
B	-16	SER	-	expression tag	UNP Q8KA85
B	-15	HIS	-	expression tag	UNP Q8KA85
B	-14	HIS	-	expression tag	UNP Q8KA85
B	-13	HIS	-	expression tag	UNP Q8KA85
B	-12	HIS	-	expression tag	UNP Q8KA85
B	-11	HIS	-	expression tag	UNP Q8KA85
B	-10	HIS	-	expression tag	UNP Q8KA85
B	-9	SER	-	expression tag	UNP Q8KA85
B	-8	SER	-	expression tag	UNP Q8KA85
B	-7	GLY	-	expression tag	UNP Q8KA85
B	-6	LEU	-	expression tag	UNP Q8KA85
B	-5	VAL	-	expression tag	UNP Q8KA85
B	-4	PRO	-	expression tag	UNP Q8KA85
B	-3	ARG	-	expression tag	UNP Q8KA85
B	-2	GLY	-	expression tag	UNP Q8KA85
B	-1	SER	-	expression tag	UNP Q8KA85
B	0	HIS	-	expression tag	UNP Q8KA85
C	-19	MET	-	expression tag	UNP Q8KA85
C	-18	GLY	-	expression tag	UNP Q8KA85
C	-17	SER	-	expression tag	UNP Q8KA85
C	-16	SER	-	expression tag	UNP Q8KA85
C	-15	HIS	-	expression tag	UNP Q8KA85
C	-14	HIS	-	expression tag	UNP Q8KA85
C	-13	HIS	-	expression tag	UNP Q8KA85
C	-12	HIS	-	expression tag	UNP Q8KA85
C	-11	HIS	-	expression tag	UNP Q8KA85
C	-10	HIS	-	expression tag	UNP Q8KA85
C	-9	SER	-	expression tag	UNP Q8KA85
C	-8	SER	-	expression tag	UNP Q8KA85
C	-7	GLY	-	expression tag	UNP Q8KA85
C	-6	LEU	-	expression tag	UNP Q8KA85
C	-5	VAL	-	expression tag	UNP Q8KA85
C	-4	PRO	-	expression tag	UNP Q8KA85
C	-3	ARG	-	expression tag	UNP Q8KA85
C	-2	GLY	-	expression tag	UNP Q8KA85
C	-1	SER	-	expression tag	UNP Q8KA85
C	0	HIS	-	expression tag	UNP Q8KA85
D	-19	MET	-	expression tag	UNP Q8KA85
D	-18	GLY	-	expression tag	UNP Q8KA85

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP Q8KA85
D	-16	SER	-	expression tag	UNP Q8KA85
D	-15	HIS	-	expression tag	UNP Q8KA85
D	-14	HIS	-	expression tag	UNP Q8KA85
D	-13	HIS	-	expression tag	UNP Q8KA85
D	-12	HIS	-	expression tag	UNP Q8KA85
D	-11	HIS	-	expression tag	UNP Q8KA85
D	-10	HIS	-	expression tag	UNP Q8KA85
D	-9	SER	-	expression tag	UNP Q8KA85
D	-8	SER	-	expression tag	UNP Q8KA85
D	-7	GLY	-	expression tag	UNP Q8KA85
D	-6	LEU	-	expression tag	UNP Q8KA85
D	-5	VAL	-	expression tag	UNP Q8KA85
D	-4	PRO	-	expression tag	UNP Q8KA85
D	-3	ARG	-	expression tag	UNP Q8KA85
D	-2	GLY	-	expression tag	UNP Q8KA85
D	-1	SER	-	expression tag	UNP Q8KA85
D	0	HIS	-	expression tag	UNP Q8KA85

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

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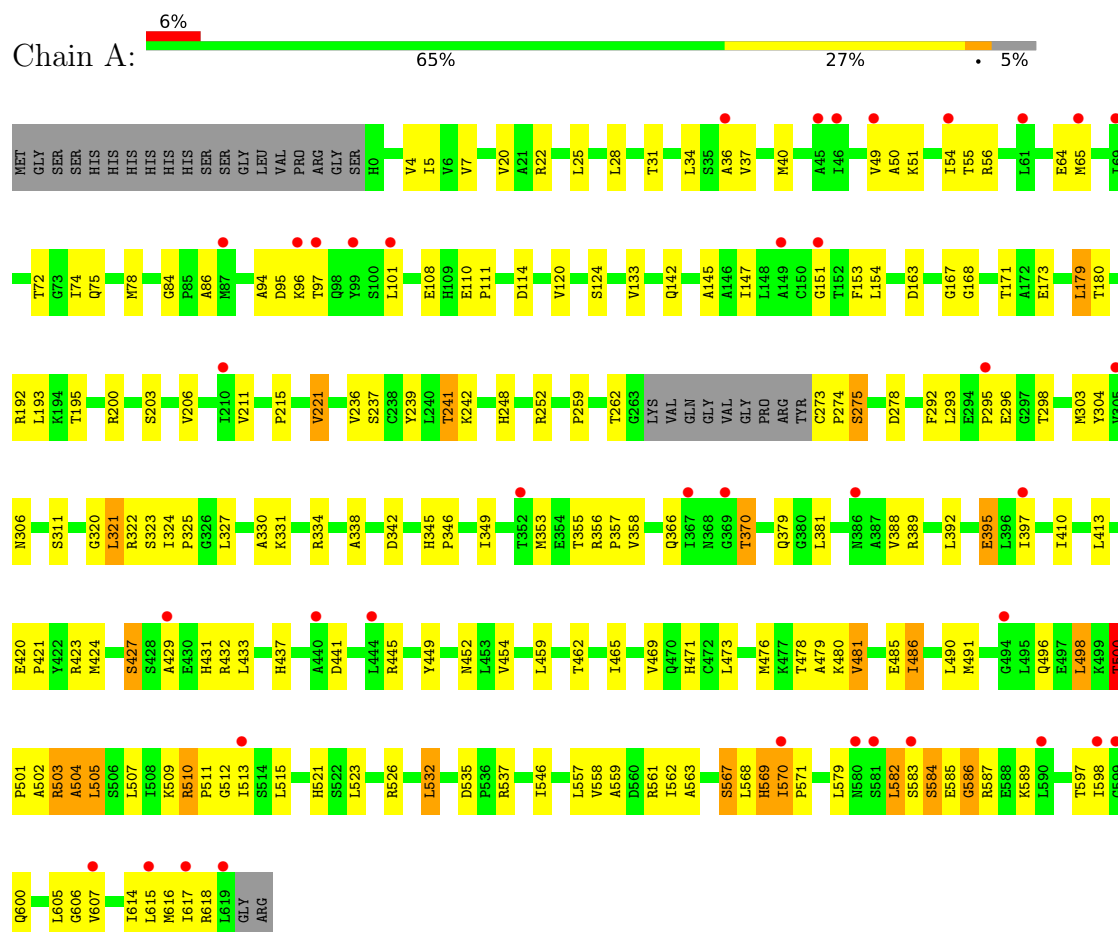
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

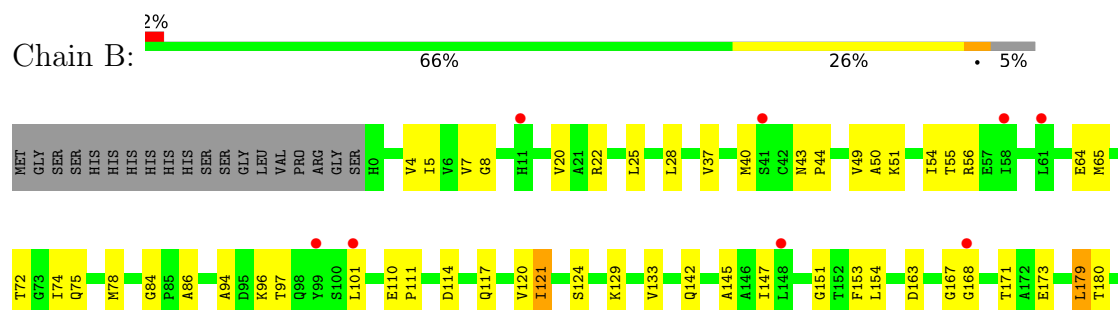
3 Residue-property plots [i](#)

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.

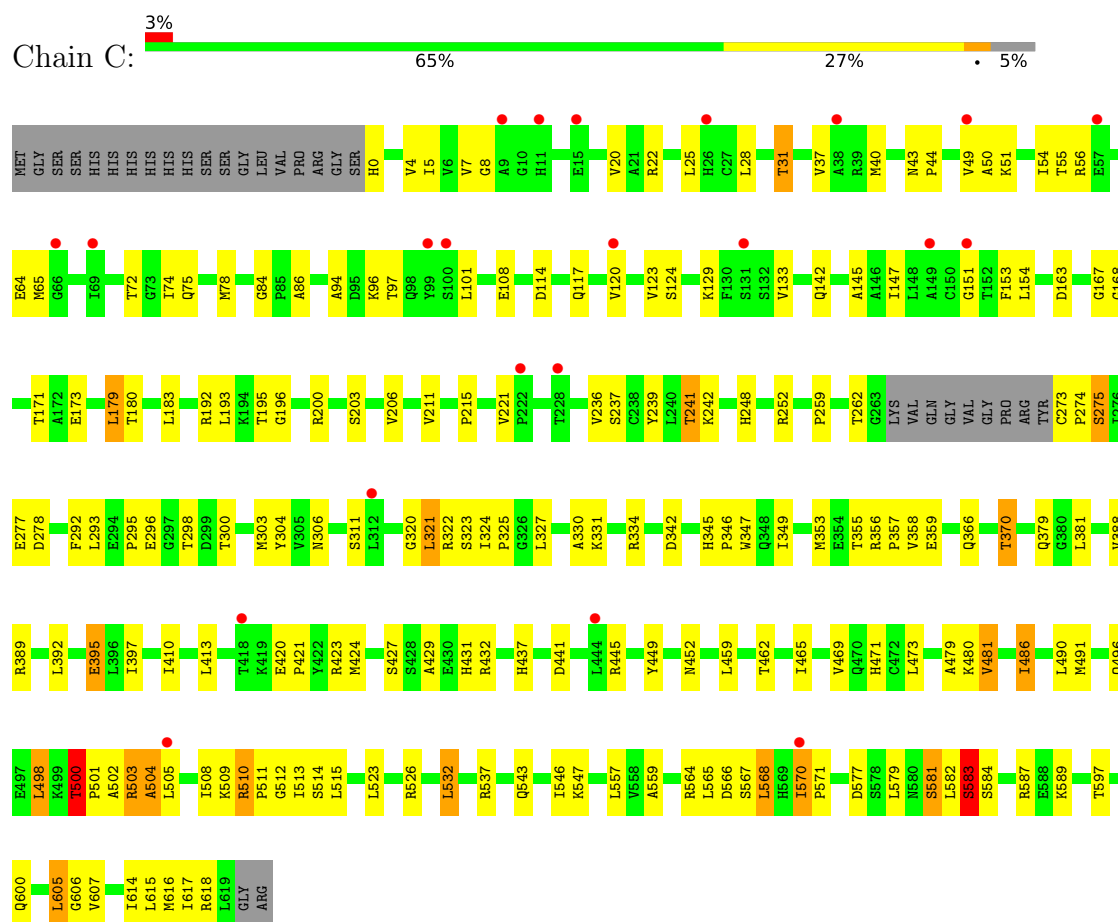
- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



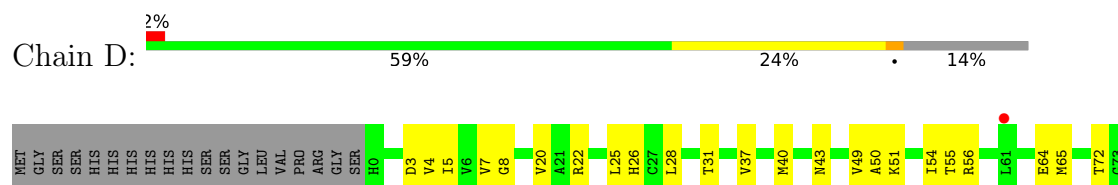
- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



ARG	R503	L413	K303	K194	I74
GLU	A504	E420	Y304	T195	Q75
LYS	L505	P421	Y305	G196	M78
LEU	K509	Y422	N306	R200	G84
LYS	R510	R423	S311	S203	P85
HIS	P511	M424	F425	V206	A86
ARG	G512	F425	T426	V211	A94
PRO	I513	S427	S428	V211	D95
ALA	S514	A429	L321	P215	K96
THR	L515	E430	R322	S223	T97
ILE	H521	F430	S323	P215	Q98
GLY	S522	H431	I324	V221	L101
GLN	L523	R432	P325	G326	E108
ALA	L523	H437	L327	V236	H109
SER	R526	Y449	D342	S237	E110
ARG	L532	D441	K331	Y238	D114
LEU	L532	R445	R334	L240	Q117
GLY	D535	K446	A338	H248	V120
VAL	P536	I447	D342	R252	S124
SER	R537	G448	H345	S258	K129
PRO	V538	Y449	P346	P259	V133
SER	Q543	N452	I349	T262	Q142
ASP	Q543	L459	K353	G263	A145
VAL	I546	T462	E354	LYS	A146
SER	K547	I465	F354	VAL	I147
ILE	L547	I466	T355	GLN	L148
ARG	V557	R468	R356	GLY	A149
ARG	A559	V469	P357	VAL	C150
LEU	D560	Q470	V358	GLY	G151
GLY	ILE	H471	E359	PRO	T152
ARG	ALA	C472	Q366	ARG	F153
LEU	ALA	L473	I367	TYR	L154
GLY	ILE	M476	T370	C273	D163
ARG	PRO	K480	Q379	P274	G167
GLY	ASP	V481	G380	S275	G168
ARG	ASN	E485	E277	I276	T171
ASP	PHE	I486	L381	D278	E173
ASP	ASN	TYR	V388	K279	L179
ASP	TYR	L490	R389	I280	T180
SER	SER	M491	L392	F292	R192
LEU	LEU	Q496	L392	L293	L193
ASN	ASN	E497	E395	E294	
SER	SER	L498	L396	P295	
LEU	LEU	K499	I397	E296	
SER	SER	T500	I410	G297	
SER	SER	P501		T298	
GLU	GLU	A502		D299	
GLY	GLY			T300	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.50Å 71.84Å 171.93Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	44.85 – 3.20 44.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.85-3.20) 99.3 (44.85-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.278 0.325 , 0.333	Depositor DCC
R_{free} test set	2471 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18567	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 [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	0.60	0/4785	0.91	5/6468 (0.1%)
1	B	0.58	1/4785 (0.0%)	0.91	7/6468 (0.1%)
1	C	0.55	1/4785 (0.0%)	0.90	6/6468 (0.1%)
1	D	0.52	0/4317	0.89	5/5836 (0.1%)
All	All	0.57	2/18672 (0.0%)	0.90	23/25240 (0.1%)

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
1	B	0	2
1	C	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	570	ILE	CA-CB	7.79	1.58	1.54
1	B	479	ALA	N-CA	5.91	1.53	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	570	ILE	N-CA-C	6.49	120.78	112.67
1	B	479	ALA	N-CA-C	6.24	118.35	110.24
1	B	179	LEU	N-CA-C	6.18	118.01	111.28
1	C	583	SER	N-CA-C	5.99	123.56	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	479	ALA	N-CA-C	5.63	118.00	110.35

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	582	LEU	Peptide
1	B	582	LEU	Peptide
1	B	583	SER	Peptide
1	C	582	LEU	Peptide
1	C	583	SER	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	4704	0	4748	152	0
1	B	4704	0	4748	144	0
1	C	4704	0	4748	138	0
1	D	4243	0	4269	135	0
2	A	53	0	31	10	0
2	B	53	0	31	13	0
2	C	53	0	31	12	0
2	D	53	0	31	11	0
All	All	18567	0	18637	555	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 15.

The worst 5 of 555 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:500:THR:HB	1:B:501:PRO:CD	1.73	1.18
1:C:500:THR:HB	1:C:501:PRO:CD	1.73	1.18
1:A:500:THR:HB	1:A:501:PRO:CD	1.73	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:THR:HB	1:D:501:PRO:CD	1.70	1.16
1:C:370:THR:HG21	1:C:379:GLN:HE22	1.10	1.15

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	607/641 (95%)	545 (90%)	50 (8%)	12 (2%)	6	31
1	B	607/641 (95%)	552 (91%)	43 (7%)	12 (2%)	6	31
1	C	607/641 (95%)	553 (91%)	44 (7%)	10 (2%)	7	36
1	D	548/641 (86%)	505 (92%)	34 (6%)	9 (2%)	7	36
All	All	2369/2564 (92%)	2155 (91%)	171 (7%)	43 (2%)	6	34

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	THR
1	B	500	THR
1	C	500	THR
1	C	504	ALA
1	D	500	THR

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	515/539 (96%)	469 (91%)	46 (9%)	9	34
1	B	515/539 (96%)	467 (91%)	48 (9%)	8	33
1	C	515/539 (96%)	468 (91%)	47 (9%)	9	34
1	D	462/539 (86%)	422 (91%)	40 (9%)	9	36
All	All	2007/2156 (93%)	1826 (91%)	181 (9%)	9	34

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	358	VAL
1	D	37	VAL
1	C	395	GLU
1	C	523	LEU
1	D	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	600	GLN
1	D	142	GLN
1	C	93	GLN
1	D	437	HIS
1	D	11	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

4 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	B	622	-	58,58,58	1.24	6 (10%)	85,89,89	1.81	23 (27%)
2	FAD	A	622	-	58,58,58	1.21	6 (10%)	85,89,89	1.83	22 (25%)
2	FAD	D	622	-	58,58,58	1.32	8 (13%)	85,89,89	1.78	22 (25%)
2	FAD	C	622	-	58,58,58	1.29	7 (12%)	85,89,89	1.80	21 (24%)

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	B	622	-	-	14/34/50/50	0/5/6/6
2	FAD	A	622	-	-	14/34/50/50	0/5/6/6
2	FAD	D	622	-	-	14/34/50/50	0/5/6/6
2	FAD	C	622	-	-	15/34/50/50	0/5/6/6

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	622	FAD	C2A-N3A	3.40	1.40	1.33
2	B	622	FAD	C4X-N5	3.37	1.38	1.30
2	D	622	FAD	C4X-N5	3.34	1.38	1.30
2	C	622	FAD	C4X-N5	3.33	1.38	1.30
2	A	622	FAD	C4X-N5	3.28	1.37	1.30

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	FAD	N3A-C2A-N1A	-5.39	120.43	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	622	FAD	N3A-C2A-N1A	-5.15	120.78	128.58
2	D	622	FAD	N3A-C2A-N1A	-5.05	120.94	128.58
2	A	622	FAD	C5X-C9A-N10	5.05	122.53	117.97
2	B	622	FAD	C5X-C9A-N10	5.01	122.49	117.97

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

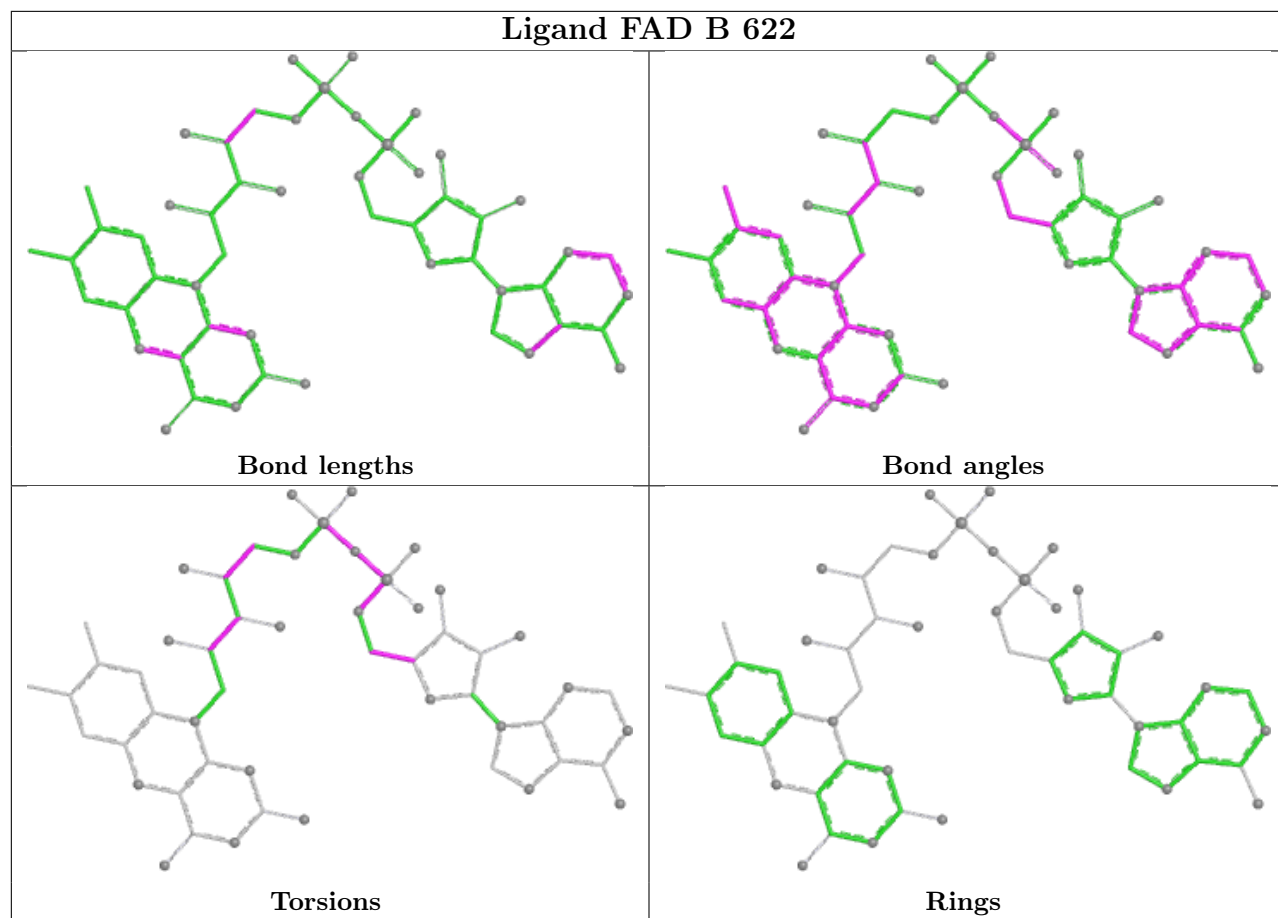
Mol	Chain	Res	Type	Atoms
2	A	622	FAD	C5B-O5B-PA-O1A
2	A	622	FAD	O4B-C4B-C5B-O5B
2	A	622	FAD	C1'-C2'-C3'-O3'
2	A	622	FAD	C1'-C2'-C3'-C4'
2	A	622	FAD	O2'-C2'-C3'-O3'

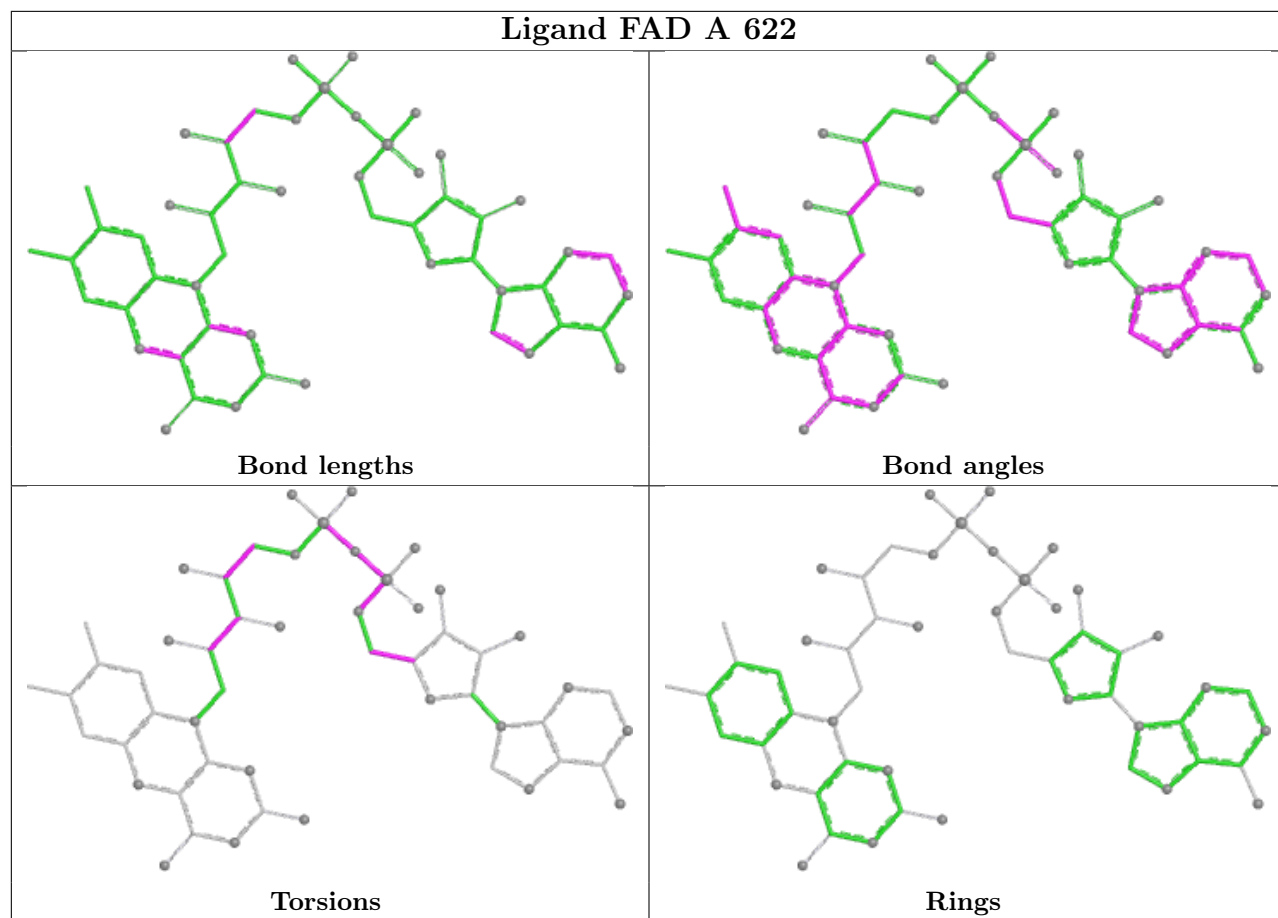
There are no ring outliers.

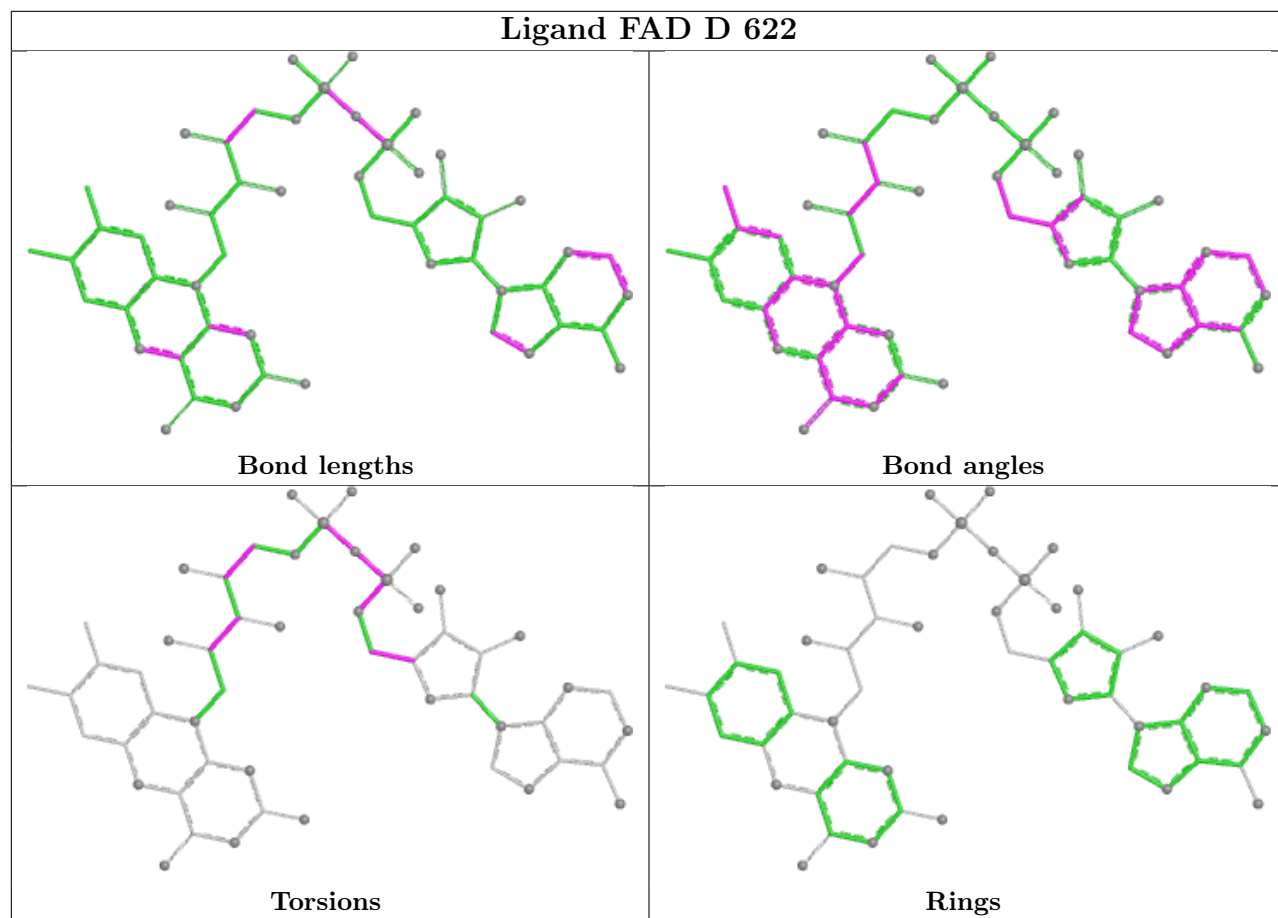
4 monomers are involved in 46 short contacts:

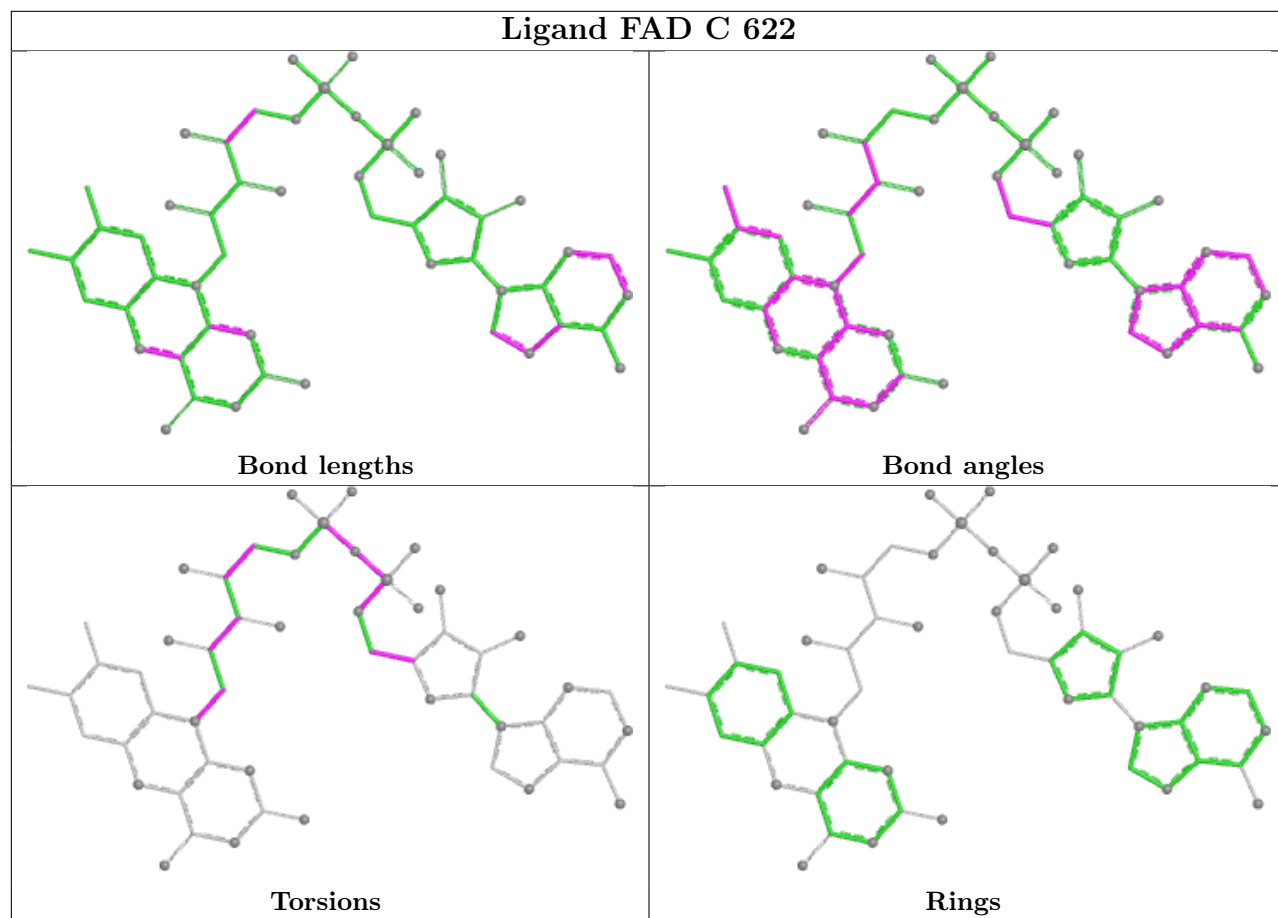
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	622	FAD	13	0
2	A	622	FAD	10	0
2	D	622	FAD	11	0
2	C	622	FAD	12	0

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	611/641 (95%)	0.67	39 (6%) 25 16	123, 126, 129, 133	0
1	B	611/641 (95%)	0.55	16 (2%) 57 37	123, 126, 129, 134	0
1	C	611/641 (95%)	0.57	22 (3%) 46 28	117, 126, 129, 133	0
1	D	552/641 (86%)	0.51	13 (2%) 59 40	123, 126, 129, 134	0
All	All	2385/2564 (93%)	0.58	90 (3%) 44 27	117, 126, 129, 134	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	SER	4.1
1	A	619	LEU	4.0
1	A	570	ILE	3.5
1	C	57	GLU	3.1
1	D	447	ILE	3.1

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](#)

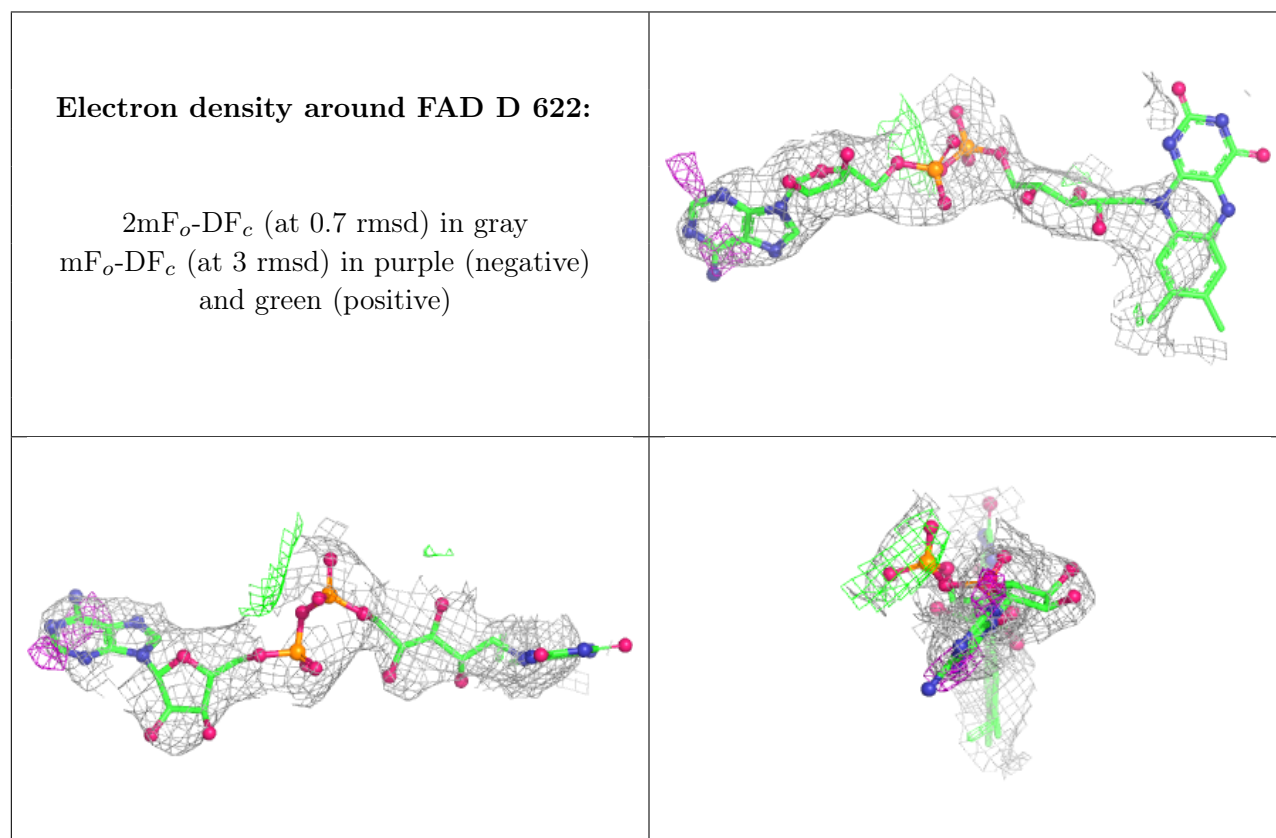
There are no oligosaccharides in this entry.

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.

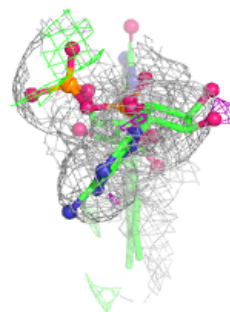
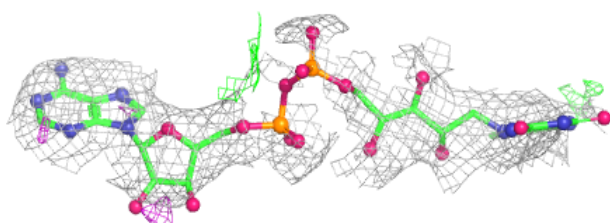
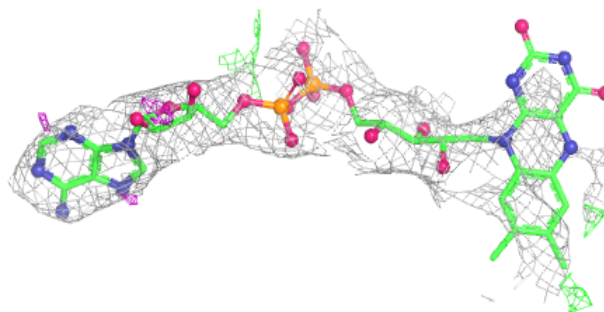
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	D	622	53/53	0.85	0.13	81,87,251,251	0
2	FAD	C	622	53/53	0.87	0.13	81,86,251,251	0
2	FAD	B	622	53/53	0.88	0.13	81,86,251,251	0
2	FAD	A	622	53/53	0.90	0.12	82,86,251,251	0

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.

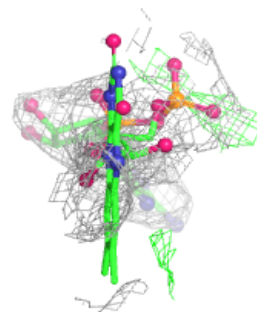
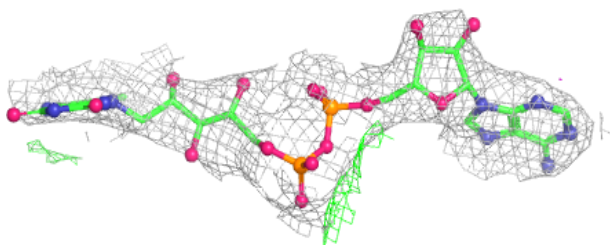
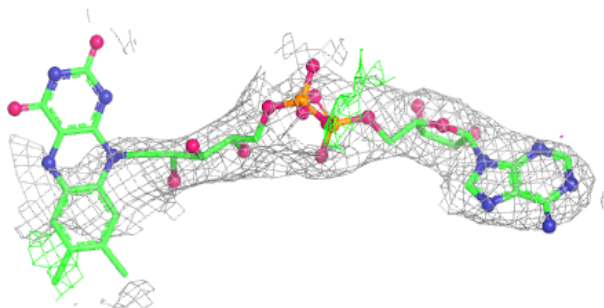


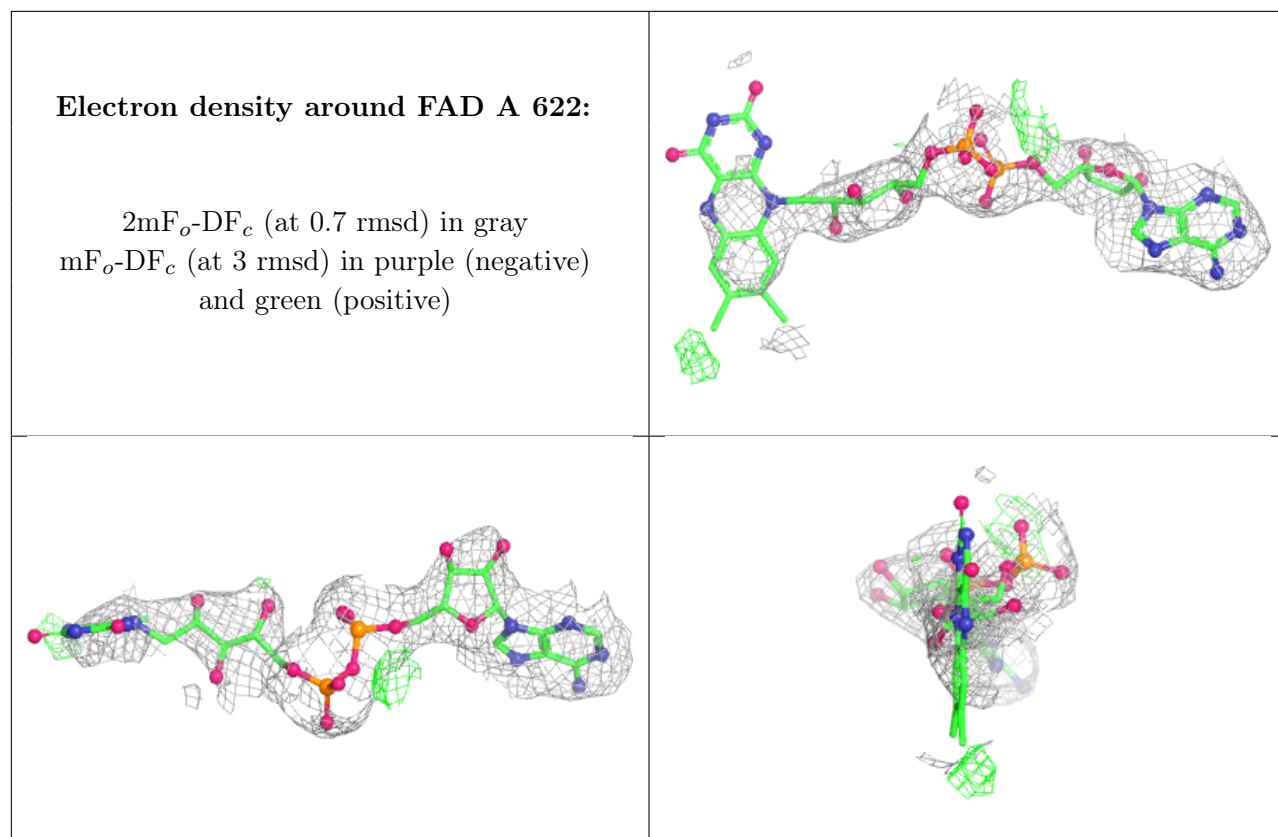
Electron density around FAD C 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD B 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.