



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 08:07 AM EST

PDB ID : 2IPI
Title : Crystal Structure of Aclacinomycin Oxidoreductase
Authors : Sultana, A.; Kursula, I.; Schneider, G.; Alexeev, I.; Niemi, J.; Mantsala, P.
Deposited on : 2006-10-12
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

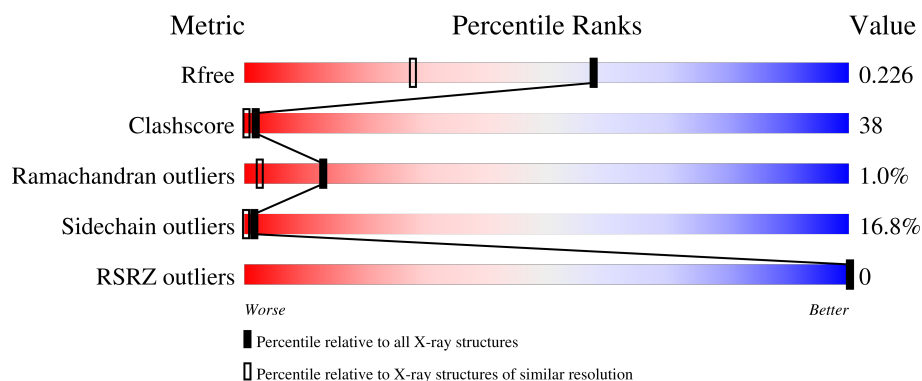
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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	521	
1	B	521	
1	C	521	
1	D	521	

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	AKY	A	601[A]	X	-	-	-
3	FAD	B	801	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16589 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 Aclacinomycin oxidoreductase (AknOx).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	67	2	0
			3836	2423	693	712	8			
1	B	492	Total	C	N	O	S	67	0	0
			3823	2415	690	710	8			
1	C	492	Total	C	N	O	S	55	1	0
			3828	2418	690	712	8			
1	D	492	Total	C	N	O	S	70	0	0
			3823	2415	690	710	8			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q0PCD7
A	-17	ALA	-	cloning artifact	UNP Q0PCD7
A	-16	HIS	-	expression tag	UNP Q0PCD7
A	-15	HIS	-	expression tag	UNP Q0PCD7
A	-14	HIS	-	expression tag	UNP Q0PCD7
A	-13	HIS	-	expression tag	UNP Q0PCD7
A	-12	HIS	-	expression tag	UNP Q0PCD7
A	-11	HIS	-	expression tag	UNP Q0PCD7
A	-10	HIS	-	expression tag	UNP Q0PCD7
A	-9	ARG	-	cloning artifact	UNP Q0PCD7
A	-8	SER	-	cloning artifact	UNP Q0PCD7
A	-7	ALA	-	cloning artifact	UNP Q0PCD7
A	-6	ALA	-	cloning artifact	UNP Q0PCD7
A	-5	GLY	-	cloning artifact	UNP Q0PCD7
A	-4	THR	-	cloning artifact	UNP Q0PCD7
A	-3	ILE	-	cloning artifact	UNP Q0PCD7
A	-2	TRP	-	cloning artifact	UNP Q0PCD7
A	-1	GLU	-	cloning artifact	UNP Q0PCD7
A	0	PHE	-	cloning artifact	UNP Q0PCD7
B	-18	MET	-	initiating methionine	UNP Q0PCD7
B	-17	ALA	-	cloning artifact	UNP Q0PCD7

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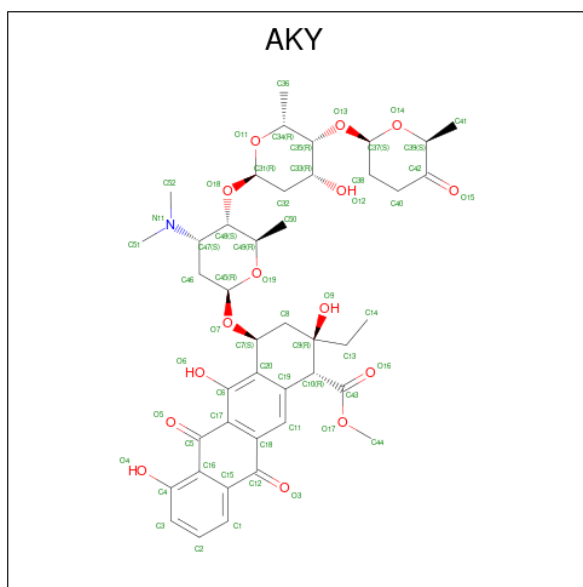
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q0PCD7
B	-15	HIS	-	expression tag	UNP Q0PCD7
B	-14	HIS	-	expression tag	UNP Q0PCD7
B	-13	HIS	-	expression tag	UNP Q0PCD7
B	-12	HIS	-	expression tag	UNP Q0PCD7
B	-11	HIS	-	expression tag	UNP Q0PCD7
B	-10	HIS	-	expression tag	UNP Q0PCD7
B	-9	ARG	-	cloning artifact	UNP Q0PCD7
B	-8	SER	-	cloning artifact	UNP Q0PCD7
B	-7	ALA	-	cloning artifact	UNP Q0PCD7
B	-6	ALA	-	cloning artifact	UNP Q0PCD7
B	-5	GLY	-	cloning artifact	UNP Q0PCD7
B	-4	THR	-	cloning artifact	UNP Q0PCD7
B	-3	ILE	-	cloning artifact	UNP Q0PCD7
B	-2	TRP	-	cloning artifact	UNP Q0PCD7
B	-1	GLU	-	cloning artifact	UNP Q0PCD7
B	0	PHE	-	cloning artifact	UNP Q0PCD7
C	-18	MET	-	initiating methionine	UNP Q0PCD7
C	-17	ALA	-	cloning artifact	UNP Q0PCD7
C	-16	HIS	-	expression tag	UNP Q0PCD7
C	-15	HIS	-	expression tag	UNP Q0PCD7
C	-14	HIS	-	expression tag	UNP Q0PCD7
C	-13	HIS	-	expression tag	UNP Q0PCD7
C	-12	HIS	-	expression tag	UNP Q0PCD7
C	-11	HIS	-	expression tag	UNP Q0PCD7
C	-10	HIS	-	expression tag	UNP Q0PCD7
C	-9	ARG	-	cloning artifact	UNP Q0PCD7
C	-8	SER	-	cloning artifact	UNP Q0PCD7
C	-7	ALA	-	cloning artifact	UNP Q0PCD7
C	-6	ALA	-	cloning artifact	UNP Q0PCD7
C	-5	GLY	-	cloning artifact	UNP Q0PCD7
C	-4	THR	-	cloning artifact	UNP Q0PCD7
C	-3	ILE	-	cloning artifact	UNP Q0PCD7
C	-2	TRP	-	cloning artifact	UNP Q0PCD7
C	-1	GLU	-	cloning artifact	UNP Q0PCD7
C	0	PHE	-	cloning artifact	UNP Q0PCD7
D	-18	MET	-	initiating methionine	UNP Q0PCD7
D	-17	ALA	-	cloning artifact	UNP Q0PCD7
D	-16	HIS	-	expression tag	UNP Q0PCD7
D	-15	HIS	-	expression tag	UNP Q0PCD7
D	-14	HIS	-	expression tag	UNP Q0PCD7
D	-13	HIS	-	expression tag	UNP Q0PCD7

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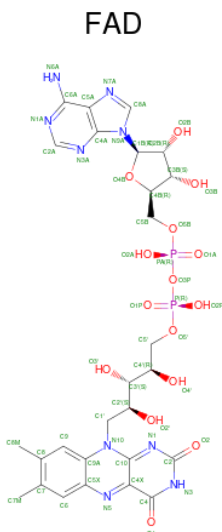
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q0PCD7
D	-11	HIS	-	expression tag	UNP Q0PCD7
D	-10	HIS	-	expression tag	UNP Q0PCD7
D	-9	ARG	-	cloning artifact	UNP Q0PCD7
D	-8	SER	-	cloning artifact	UNP Q0PCD7
D	-7	ALA	-	cloning artifact	UNP Q0PCD7
D	-6	ALA	-	cloning artifact	UNP Q0PCD7
D	-5	GLY	-	cloning artifact	UNP Q0PCD7
D	-4	THR	-	cloning artifact	UNP Q0PCD7
D	-3	ILE	-	cloning artifact	UNP Q0PCD7
D	-2	TRP	-	cloning artifact	UNP Q0PCD7
D	-1	GLU	-	cloning artifact	UNP Q0PCD7
D	0	PHE	-	cloning artifact	UNP Q0PCD7

- Molecule 2 is METHYL (2S,4R)-2-ETHYL-2,5,7-TRIHYDROXY-6,11-DIOXO-4-{[2,3,6-T RIDEOXY-4-O-{2,6-DIDEOXY-4-O-[(2S,6S)-6-METHYL-5-OXOTETRAHYDRO-2H -PY RAN-2-YL]-ALPHA-D-LYXO-HEXOPYRANOSYL}-3-(DIMETHYLAMINO)-D-RIBO-H EXOPYRANOSYL]OXY}-1,2,3,4,6,11-HEXAHYDROTETRACENE-1-C ARBOXYLATE (three-letter code: AKY) (formula: C₄₂H₅₃NO₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			58	42	1	15		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

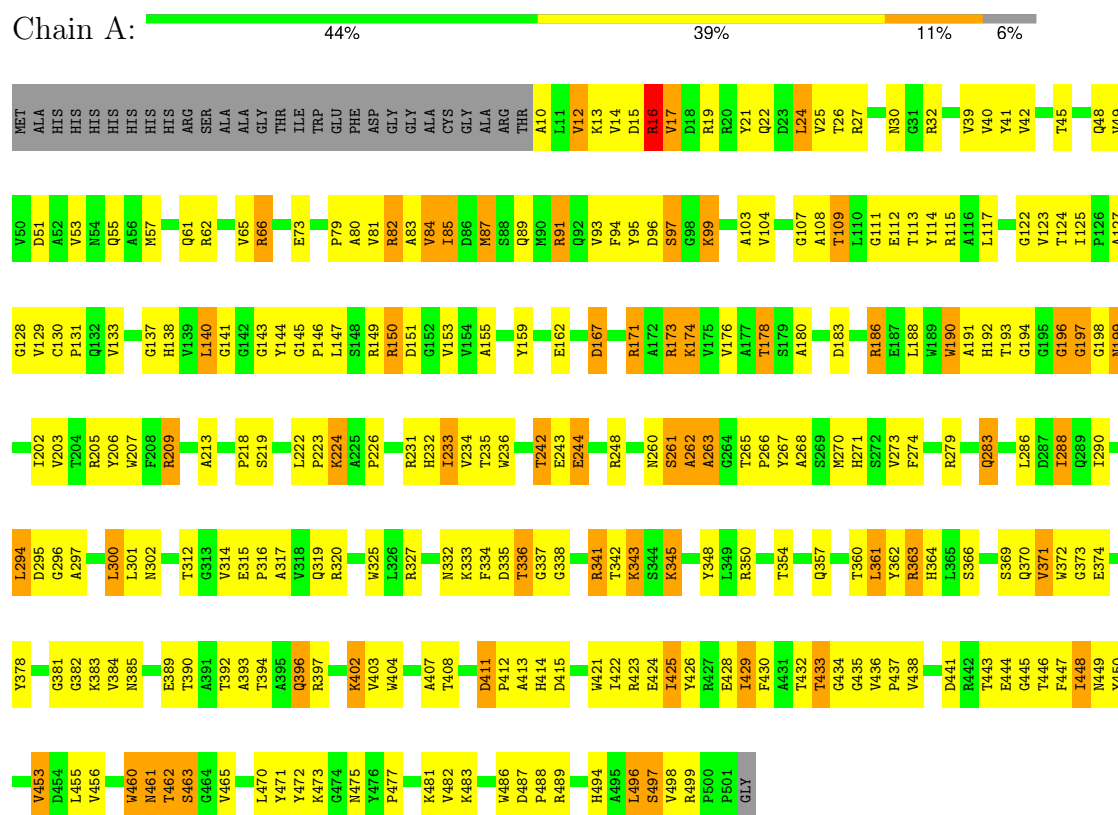
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	274	Total O 274 274	0	0
4	B	212	Total O 212 212	0	0
4	C	317	Total O 317 317	0	0
4	D	206	Total O 206 206	0	0

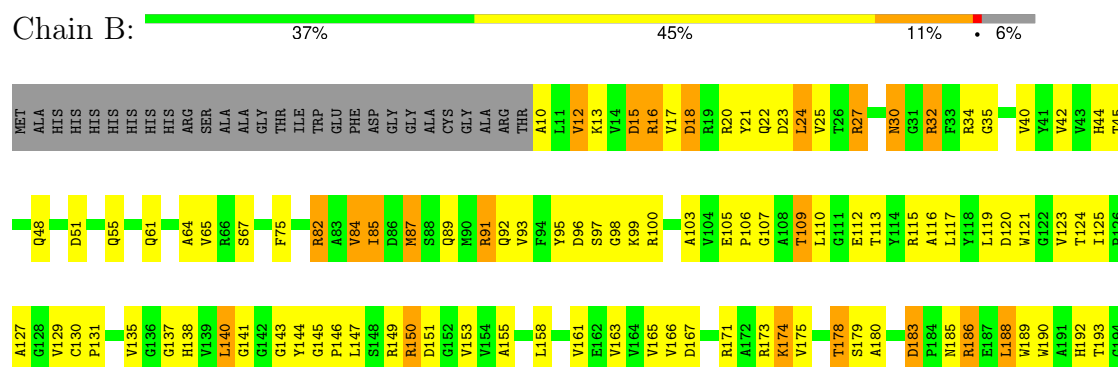
3 Residue-property plots

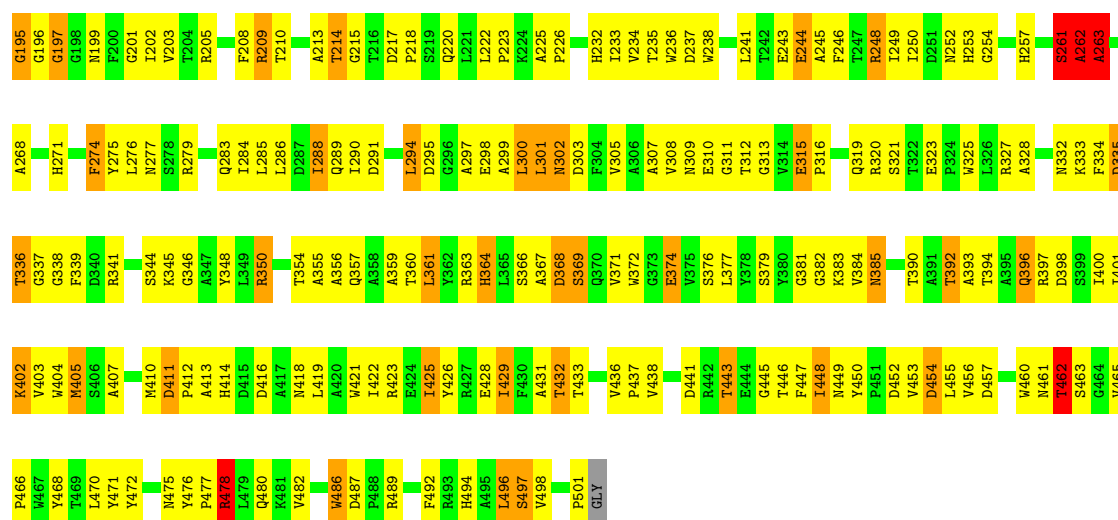
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aclacinomycin oxidoreductase (AknOx)



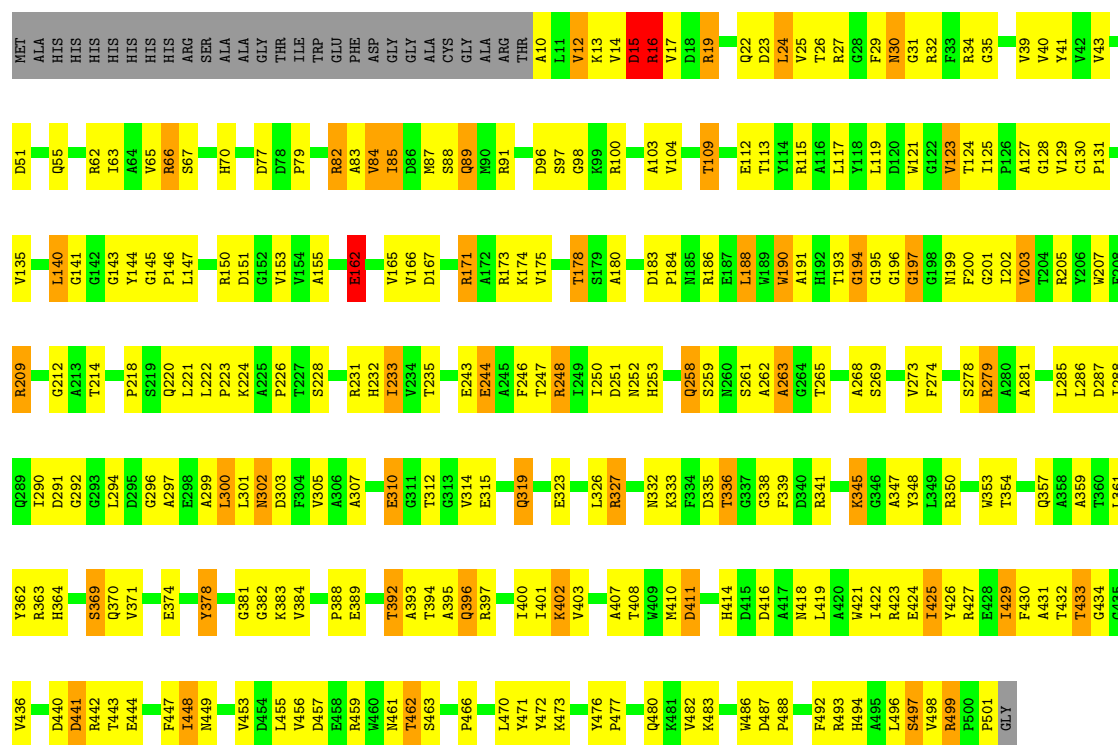
• Molecule 1: Aclacinomycin oxidoreductase (AknOx)





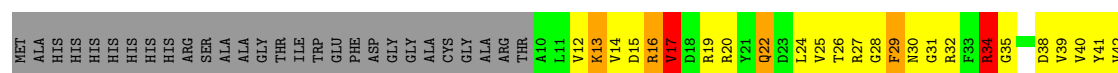
• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain C: 44% 41% 9% 6%



• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain D: 41% 41% 11% 6%



F492	R493	H494	A495	L496	S497	V498	R499	P500	P501	GLY	L419	A420	W421	I422	R423	R424	I425	I426	R427	E428	I429	F430	A431	T432	T433	G434	G435	V436	P437	V438	P439	D440	D441	R442	T443	E444	G445	T446	F447	I448	N449	Y450	V453	D454	L455	V456	W460	N461	T462	V465	P466	T469	L470	Y471	Y472	R478	L479	Q480	K481	V482	K483	W486	D487																																																															
S344	K345	R350	R351	P352	W353	T354	A355	A356	Q357	Y362	R363	H364	L365	D368	S369	Q370	V371	E374	V375	Y378	S379	Y380	G381	G382	K383	V384	N385	T392	A393	T394	A395	Q396	R397	D398	S399	I400	T401	K402	M405	S406	A407	T408	W409	M410	D411	P412	A413	H414	D415	D416	A417	N418	T422	R423	R424	I425	I426	R427	E428	I429	F430	A431	T432	T433	G434	G435	V436	P437	V438	P439	D440	D441	R442	T443	E444	G445	T446	F447	I448	N449	Y450	V453	D454	L455	V456	W460	N461	T462	V465	P466	T469	L470	Y471	Y472	R478	L479	Q480	K481	V482	K483	W486	D487																								
M270	V273	F274	S278	R279	I284	L285	L286	D287	I288	Q289	D291	L294	D295	G296	A297	E298	A299	L300	L301	N302	D303	F304	V305	V308	N309	E310	G311	T312	G313	V314	E315	P316	Q319	R320	S321	T322	E323	P324	W325	L326	R327	N332	T336	G337	G338	F339	D340	R341	T342	K343	T242	E243	E244	A245	F246	T247	R248	I249	N252	H253	G254	H257	S261	A262	A263	G264	T265	F266	Y267	A268	S269	T202	V203	T204	R205	Y206	W207	F208	R209	A213	T214	G215	V216	D217	P218	S219	Q220	L221	L222	P223	K224	A225	P226	T227	S228	T229	L230	R231	H232	I233	V234	T235	W236	D237	W238	T242	E243	E244	A245	F246	T247	R248	I249	N252	H253	G254	H257	S261	A262	A263	G264	T265	F266	Y267	A268	S269
A127	G128	V129	C130	P131	Q132	V133	G134	V135	H138	V139	L140	G143	Y144	G145	P146	I147	S148	R149	R150	D151	G152	V153	V154	A155	E162	D167	R171	A172	R173	K174	W175	V176	A177	T178	S179	A180	D183	E187	L188	W189	W190	A191	H192	T193	G194	G195	Y196	G197	G198	N199	F200	G201																																																																										

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.50Å 266.20Å 68.70Å 90.00° 119.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.67	Depositor EDS
% Data completeness (in resolution range)	95.9 (20.00-1.65) 98.5 (20.00-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.67Å)	Xtriage
Refinement program	REFMAC, SHELXL-97	Depositor
R, R_{free}	0.185 , 0.242 0.182 , 0.226	Depositor DCC
R_{free} test set	9545 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.128 for -h-l,k,h 0.128 for l,k,-h-l 0.130 for h,-k,-h-l 0.128 for -h-l,-k,l 0.430 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16589	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, AKY

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	0.40	0/3946	1.14	19/5386 (0.4%)
1	B	0.41	0/3927	1.17	25/5361 (0.5%)
1	C	0.43	0/3935	1.19	22/5372 (0.4%)
1	D	0.39	0/3927	1.17	28/5361 (0.5%)
All	All	0.41	0/15735	1.16	94/21480 (0.4%)

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	B	0	3
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	ARG	NE-CZ-NH1	-12.09	114.25	120.30
1	D	196	GLY	C-N-CA	11.89	147.28	122.30
1	A	91	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	C	66	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	C	66	ARG	NE-CZ-NH2	-9.66	115.47	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	261	SER	Peptide
1	B	262	ALA	Peptide
1	B	263	ALA	Peptide
1	D	261	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	3836	0	3697	280	2
1	B	3823	0	3678	302	0
1	C	3828	0	3688	309	0
1	D	3823	0	3683	277	0
2	A	58	0	48	13	0
3	A	53	0	29	3	0
3	B	53	0	28	9	0
3	C	53	0	30	9	0
3	D	53	0	30	12	0
4	A	274	0	0	52	0
4	B	212	0	0	50	1
4	C	317	0	0	61	1
4	D	206	0	0	40	0
All	All	16589	0	14911	1146	2

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 38.

The worst 5 of 1146 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:C:130:CYS:SG	3:C:801:FAD:H6	1.28	1.65
1:D:130:CYS:SG	3:D:801:FAD:H6	1.13	1.61
1:D:70:HIS:ND1	3:D:801:FAD:HM83	0.97	1.30
1:C:130:CYS:SG	3:C:801:FAD:C6	2.25	1.25
1:D:70:HIS:CE1	3:D:801:FAD:HM83	1.91	1.05

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LYS:CD	4:C:1070:HOH:O[2_655]	1.75	0.45
1:A:499:ARG:NH2	4:B:820:HOH:O[1_554]	2.18	0.02

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	492/521 (94%)	459 (93%)	29 (6%)	4 (1%)	16	4
1	B	490/521 (94%)	456 (93%)	27 (6%)	7 (1%)	9	1
1	C	491/521 (94%)	449 (91%)	39 (8%)	3 (1%)	22	8
1	D	490/521 (94%)	448 (91%)	37 (8%)	5 (1%)	13	2
All	All	1963/2084 (94%)	1812 (92%)	132 (7%)	19 (1%)	13	2

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ALA
1	B	195	GLY
1	B	214	THR
1	B	368	ASP
1	B	460	TRP

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	391/408 (96%)	323 (83%)	68 (17%)	1	0
1	B	389/408 (95%)	323 (83%)	66 (17%)	1	0
1	C	390/408 (96%)	327 (84%)	63 (16%)	2	0
1	D	389/408 (95%)	323 (83%)	66 (17%)	1	0
All	All	1559/1632 (96%)	1296 (83%)	263 (17%)	1	0

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	302	ASN
1	D	327	ARG
1	D	478	ARG
1	B	289	GLN
1	B	274	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	364	HIS
1	D	289	GLN
1	C	396	GLN
1	D	89	GLN
1	D	357	GLN

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

5 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	801	1	54,58,58	1.64	9 (16%)	71,89,89	1.81	17 (23%)
3	FAD	C	801	1	54,58,58	1.79	14 (25%)	71,89,89	2.09	23 (32%)
3	FAD	B	801	1	54,58,58	1.88	15 (27%)	71,89,89	1.88	19 (26%)
2	AKY	A	601[A]	-	62,64,64	1.97	16 (25%)	87,98,98	1.96	22 (25%)
3	FAD	D	801	1	54,58,58	1.94	22 (40%)	71,89,89	1.84	16 (22%)

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	801	1	-	9/30/50/50	0/6/6/6
3	FAD	C	801	1	-	12/30/50/50	0/6/6/6
3	FAD	B	801	1	1/1/9/9	10/30/50/50	0/6/6/6
2	AKY	A	601[A]	-	7/7/18/18	6/25/105/105	0/7/7/7
3	FAD	D	801	1	-	11/30/50/50	0/6/6/6

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[A]	AKY	C32-C33	-6.61	1.40	1.52
2	A	601[A]	AKY	C41-C39	-5.28	1.34	1.51
3	A	801	FAD	O2-C2	-4.35	1.15	1.24
2	A	601[A]	AKY	O12-C33	4.30	1.52	1.43
3	B	801	FAD	P-O1P	-4.13	1.36	1.50

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	FAD	O4B-C1B-N9A	6.68	117.61	108.75
3	B	801	FAD	N3A-C2A-N1A	-6.39	120.00	128.67
2	A	601[A]	AKY	O19-C49-C50	6.35	120.83	106.74
3	C	801	FAD	N3A-C2A-N1A	-6.20	120.26	128.67
3	D	801	FAD	N3A-C2A-N1A	-6.00	120.53	128.67

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601[A]	AKY	C33
2	A	601[A]	AKY	C37
2	A	601[A]	AKY	C49
2	A	601[A]	AKY	C39
2	A	601[A]	AKY	C34

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[A]	AKY	C10-C43-O17-C44
2	A	601[A]	AKY	C46-C47-N11-C51
2	A	601[A]	AKY	C48-C47-N11-C52
3	A	801	FAD	N10-C1'-C2'-O2'
3	A	801	FAD	N10-C1'-C2'-C3'

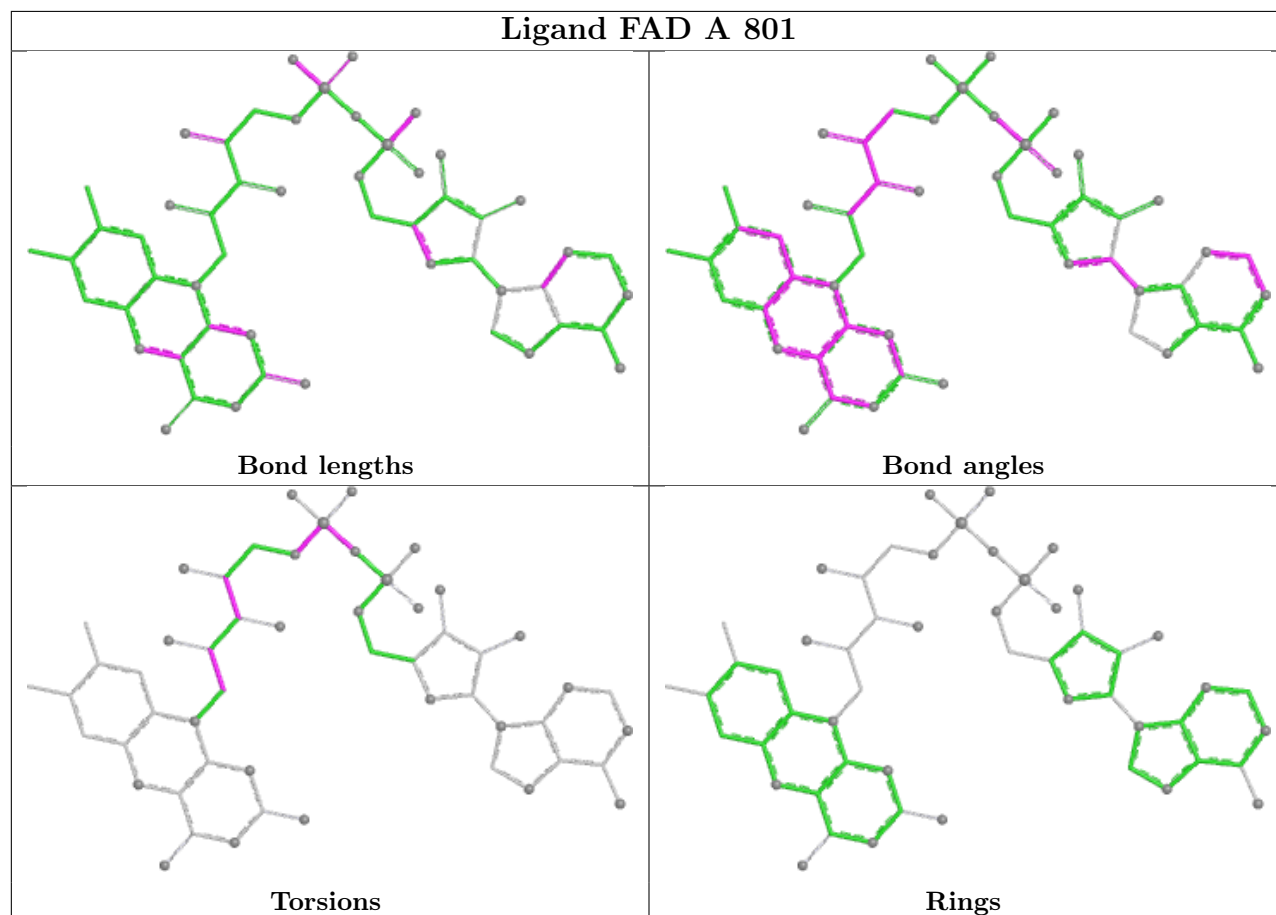
There are no ring outliers.

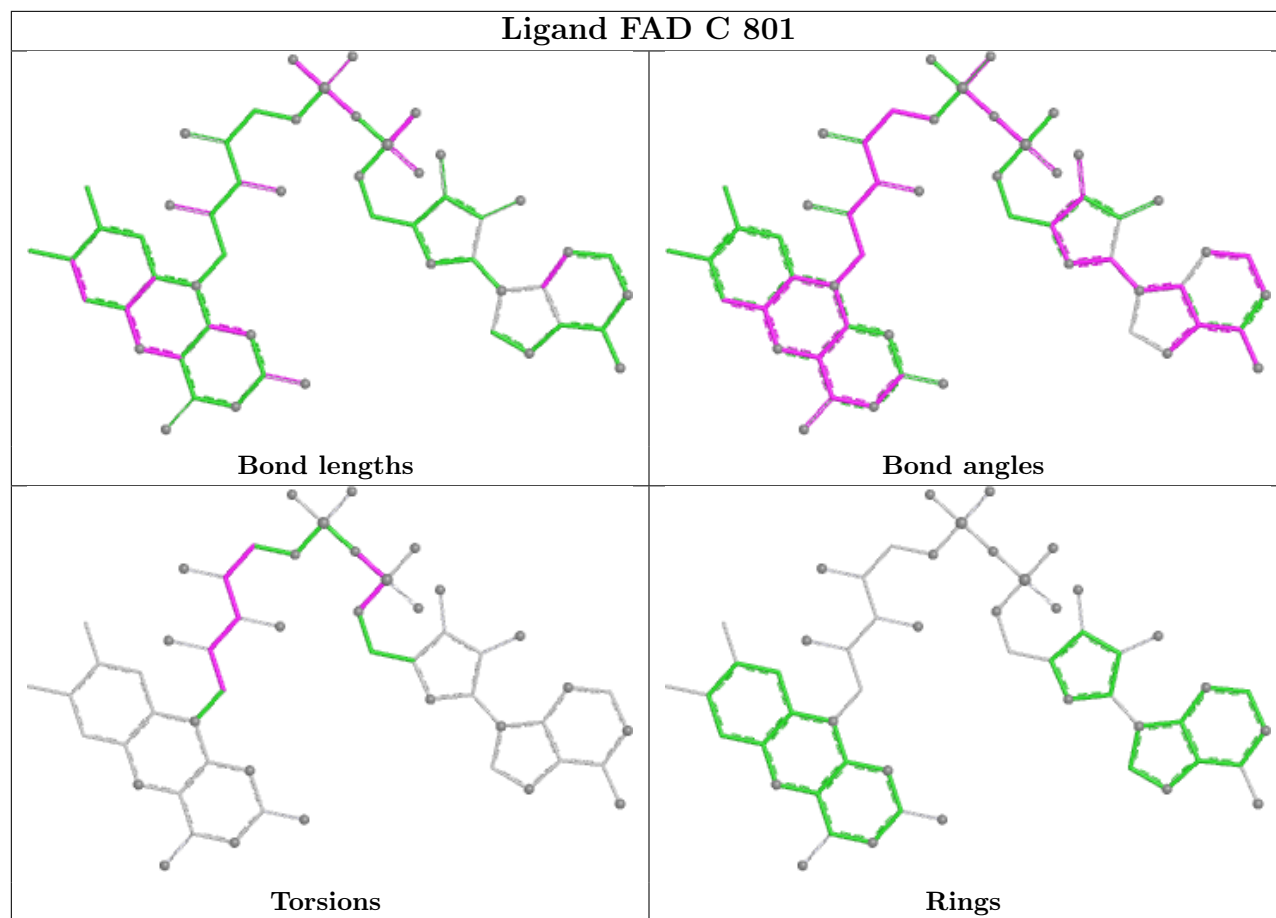
5 monomers are involved in 46 short contacts:

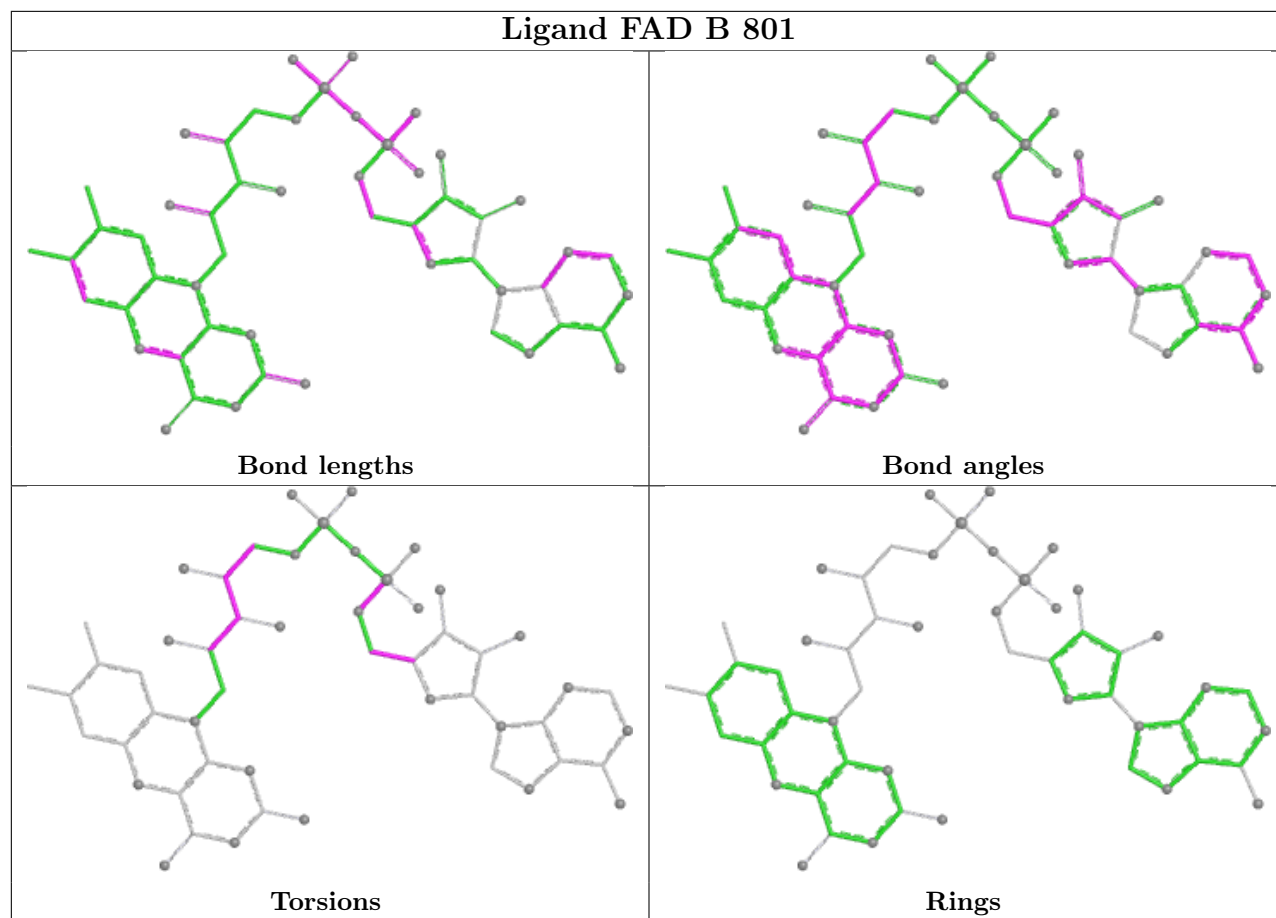
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	FAD	3	0
3	C	801	FAD	9	0
3	B	801	FAD	9	0
2	A	601[A]	AKY	13	0
3	D	801	FAD	12	0

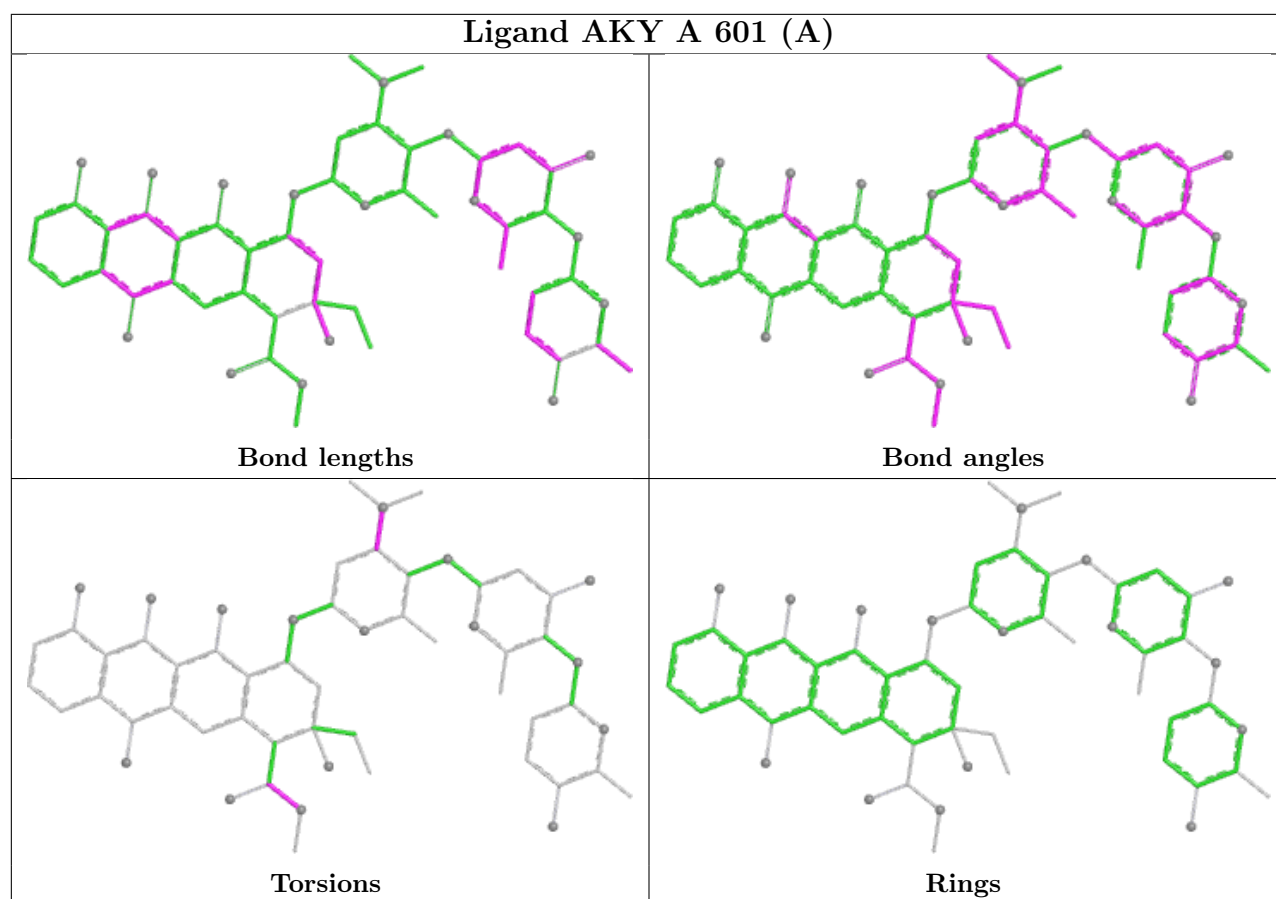
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

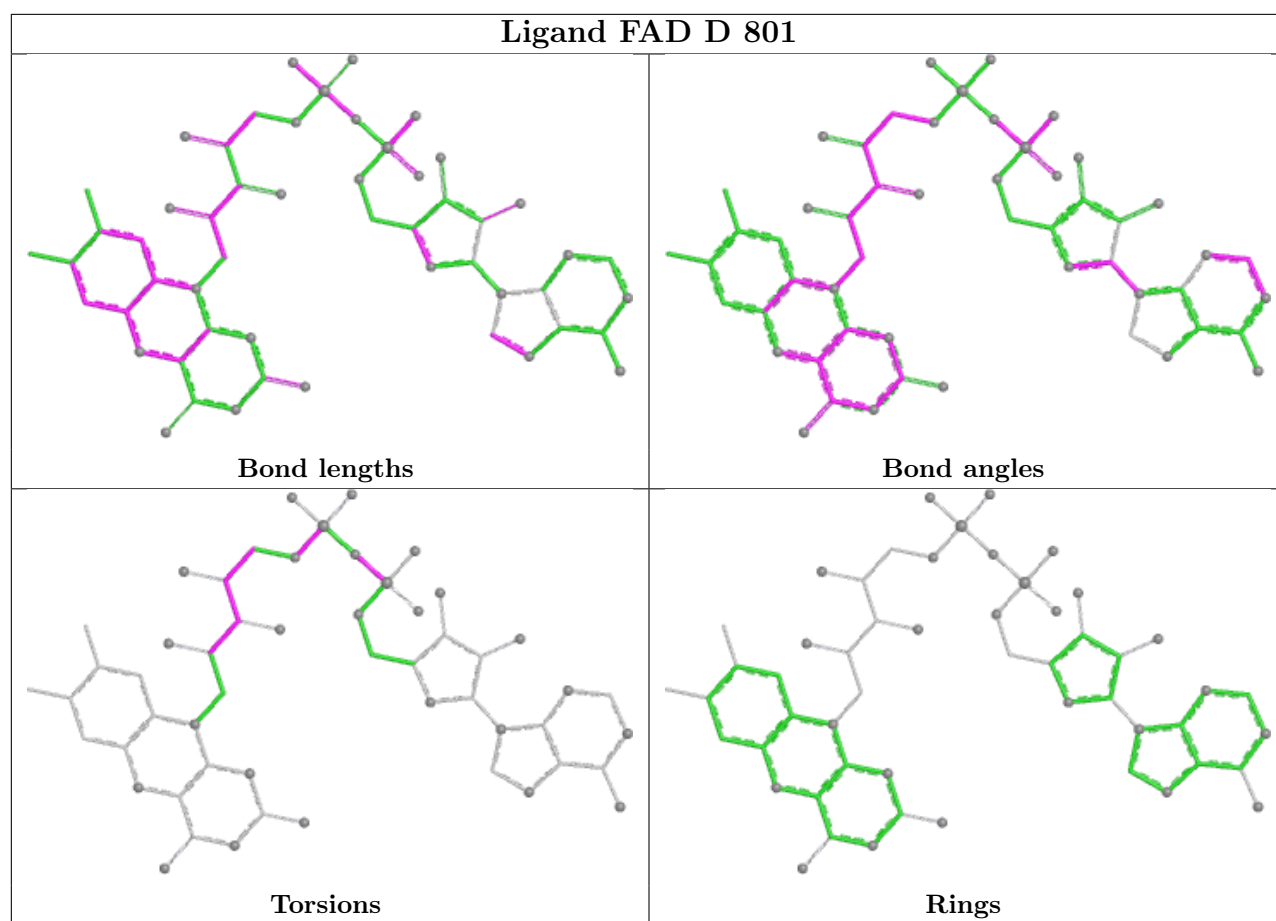
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	492/521 (94%)	-1.15	0 100 100	3, 16, 30, 39	16 (3%)
1	B	492/521 (94%)	-1.13	0 100 100	6, 17, 30, 39	14 (2%)
1	C	492/521 (94%)	-1.17	0 100 100	5, 16, 29, 40	13 (2%)
1	D	492/521 (94%)	-1.13	0 100 100	4, 16, 31, 43	15 (3%)
All	All	1968/2084 (94%)	-1.15	0 100 100	3, 16, 30, 43	58 (2%)

There are no RSRZ outliers to report.

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 monosaccharides 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(Å ²)	Q<0.9
2	AKY	A	601[A]	58/58	0.98	0.05	10,20,34,38	58
3	FAD	A	801	53/53	0.99	0.03	7,14,19,24	0
3	FAD	B	801	53/53	0.99	0.03	4,14,23,36	0
3	FAD	C	801	53/53	0.99	0.03	3,11,25,37	0

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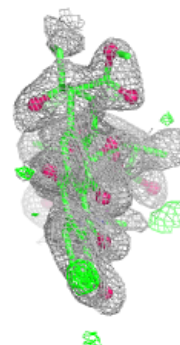
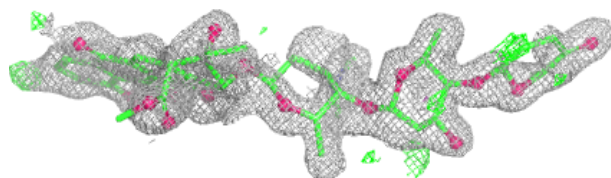
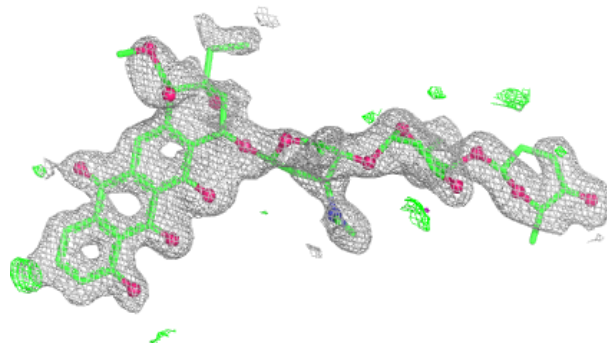
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	D	801	53/53	0.99	0.03	4,11,26,42	0

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.

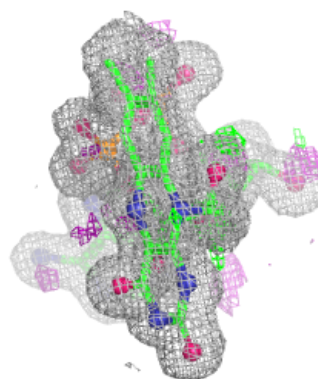
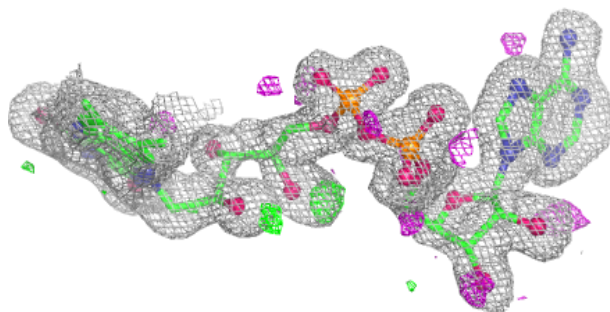
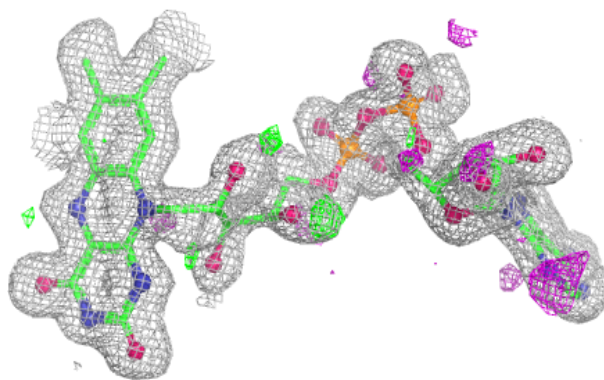
Electron density around AKY A 601 (A):

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

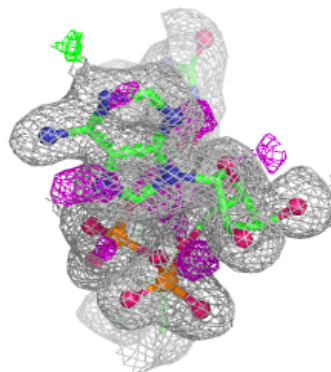
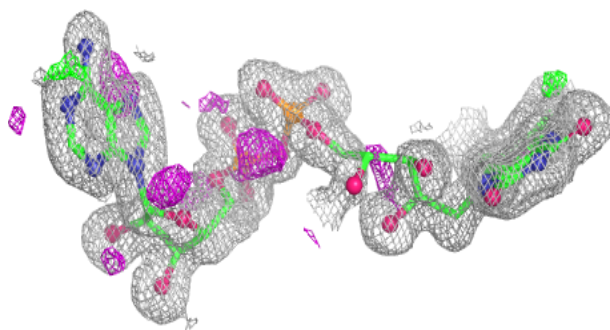
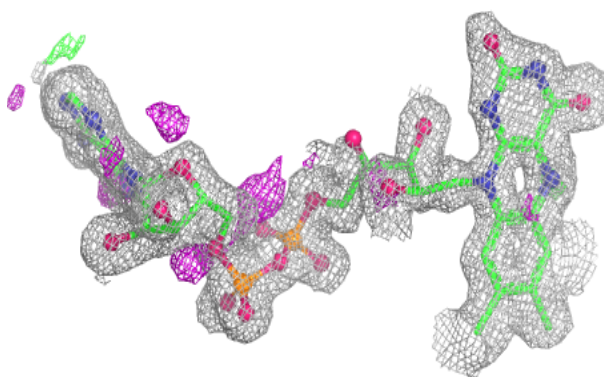


Electron density around FAD A 801:

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

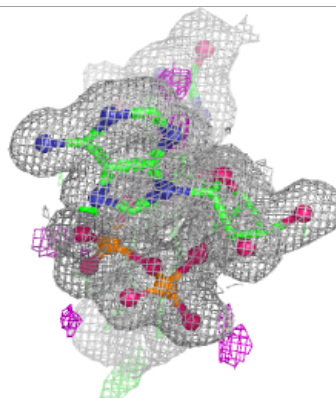
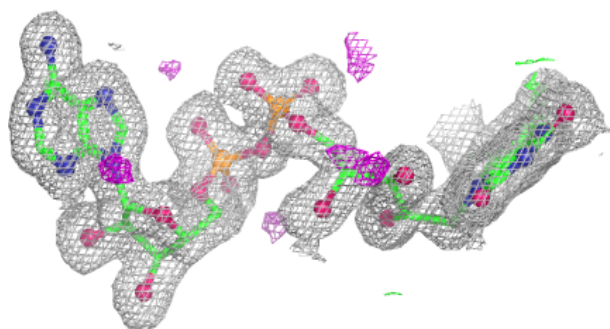
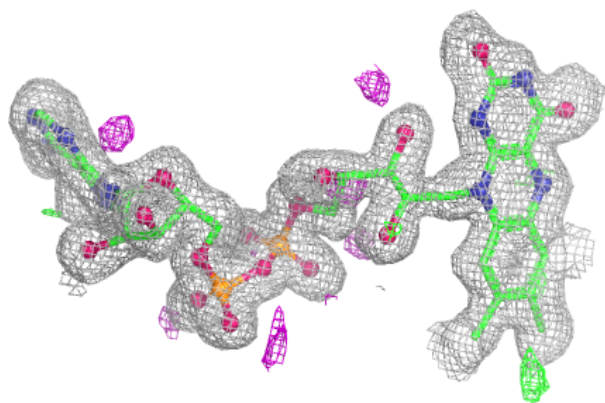
**Electron density around FAD B 801:**

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

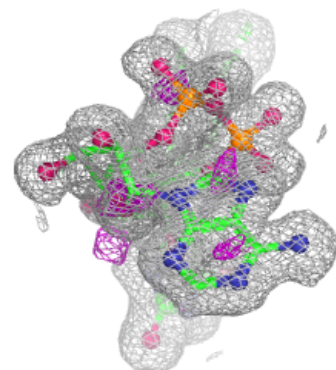
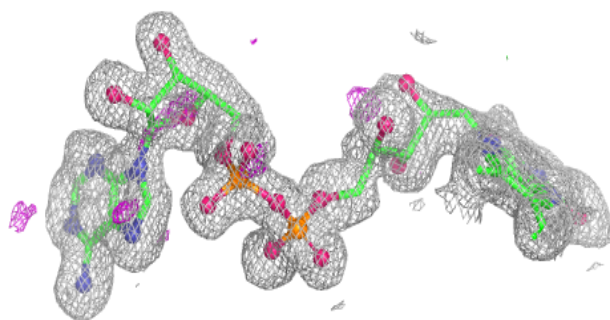
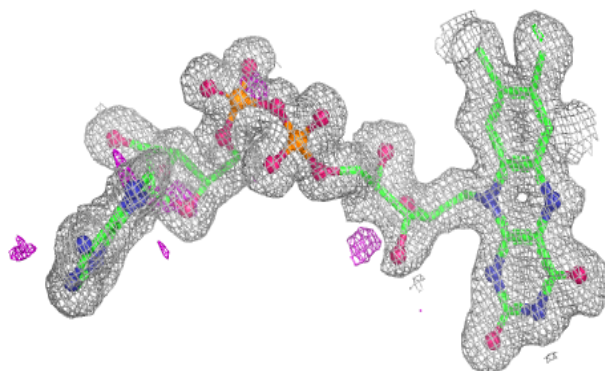


Electron density around FAD C 801:

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

**Electron density around FAD D 801:**

$2mF_o-DF_c$ (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.