



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:06 PM UTC

PDB ID : 2IPI / pdb_00002ipi
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)

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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

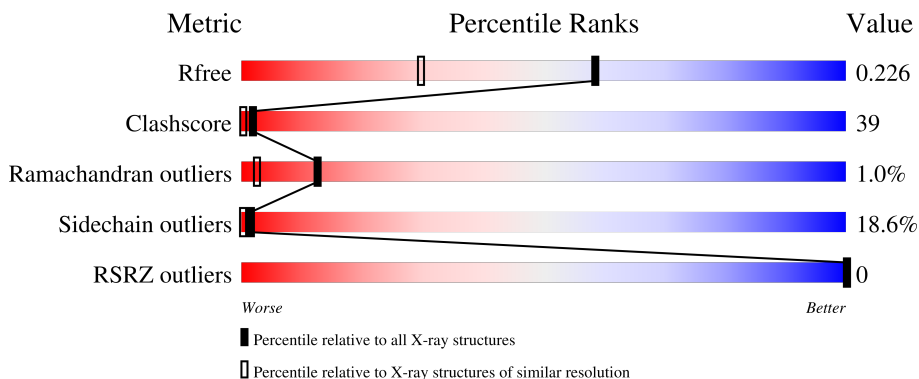
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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	 42% 40% 12% • 6%
1	B	521	 36% 45% 12% • 6%
1	C	521	 41% 41% 11% • 6%
1	D	521	 39% 41% 13% • 6%

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 [i](#)

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
			Total	C	N	O	S			
1	A	492	3836	2423	693	712	8	67	2	0
1	B	492	3823	2415	690	710	8	67	0	0
1	C	492	3828	2418	690	712	8	55	1	0
1	D	492	3823	2415	690	710	8	70	0	0

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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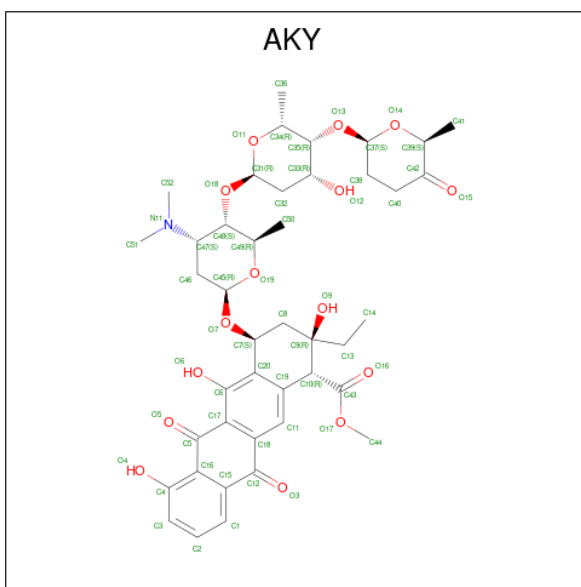
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q0PCD7
B	-15	HIS	-	expression tag	UNP Q0PCD7
B	-14	HIS	-	expression tag	UNP Q0PCD7
B	-13	HIS	-	expression tag	UNP Q0PCD7
B	-12	HIS	-	expression tag	UNP Q0PCD7
B	-11	HIS	-	expression tag	UNP Q0PCD7
B	-10	HIS	-	expression tag	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

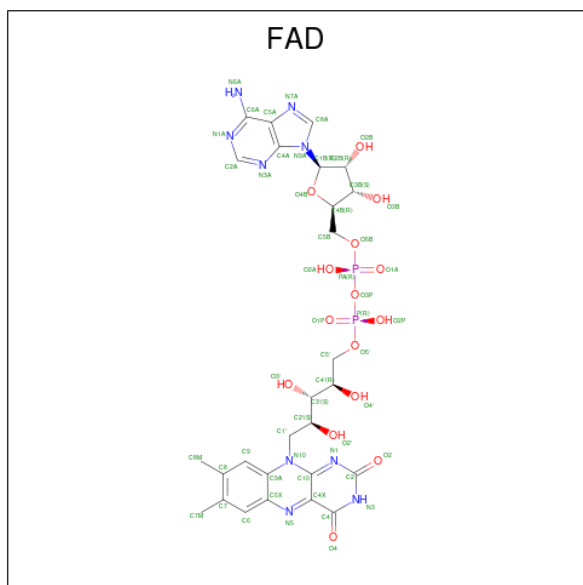
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q0PCD7
D	-11	HIS	-	expression tag	UNP Q0PCD7
D	-10	HIS	-	expression tag	UNP Q0PCD7
D	-9	ARG	-	cloning artifact	UNP Q0PCD7
D	-8	SER	-	cloning artifact	UNP Q0PCD7
D	-7	ALA	-	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 (CCD ID: AKY) (formula: C₄₂H₅₃NO₁₅).





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

- Molecule 4 is water.

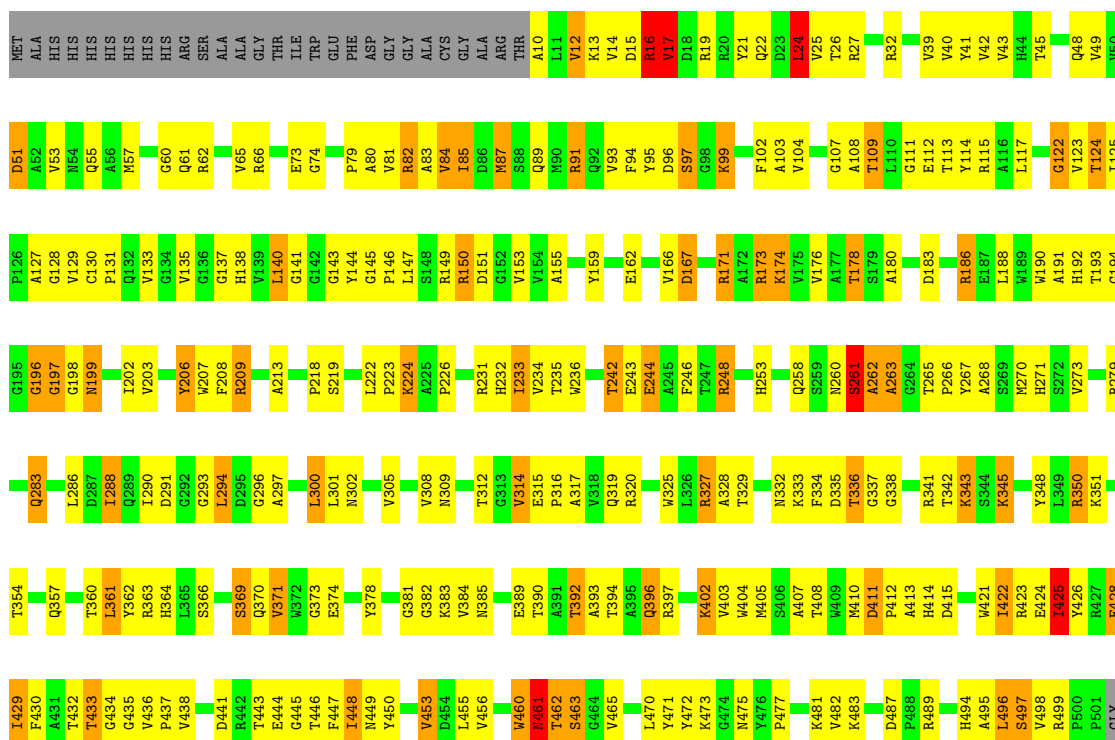
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total	O	0	0
			274	274		
4	B	212	Total	O	0	0
			212	212		
4	C	317	Total	O	0	0
			317	317		
4	D	206	Total	O	0	0
			206	206		

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.

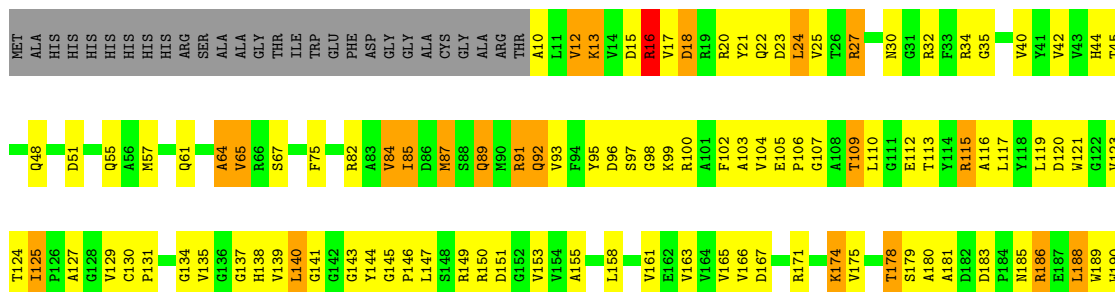
- Molecule 1: Aclacinomycin oxidoreductase (AknOx)

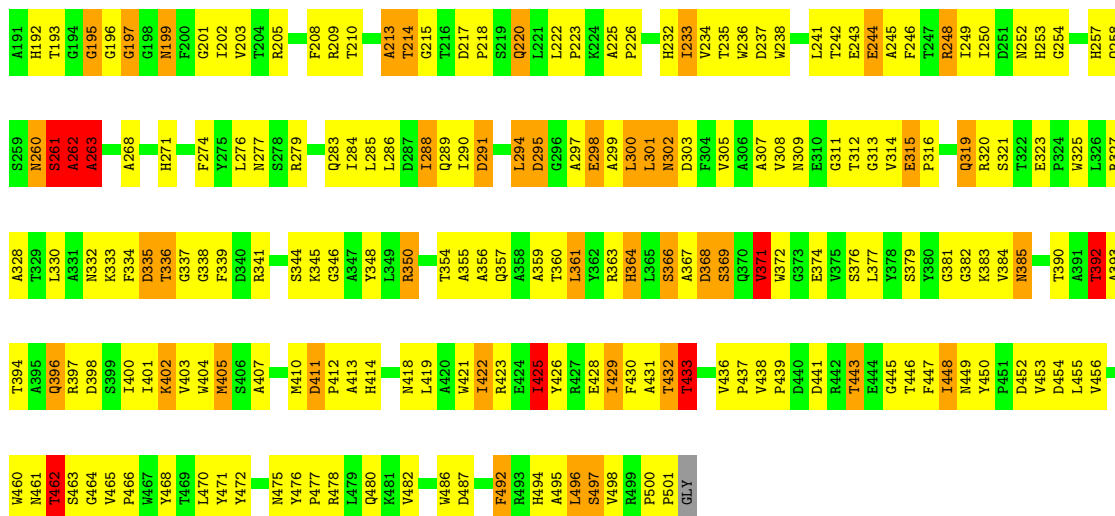
Chain A:  42% 40% 12% • 6%



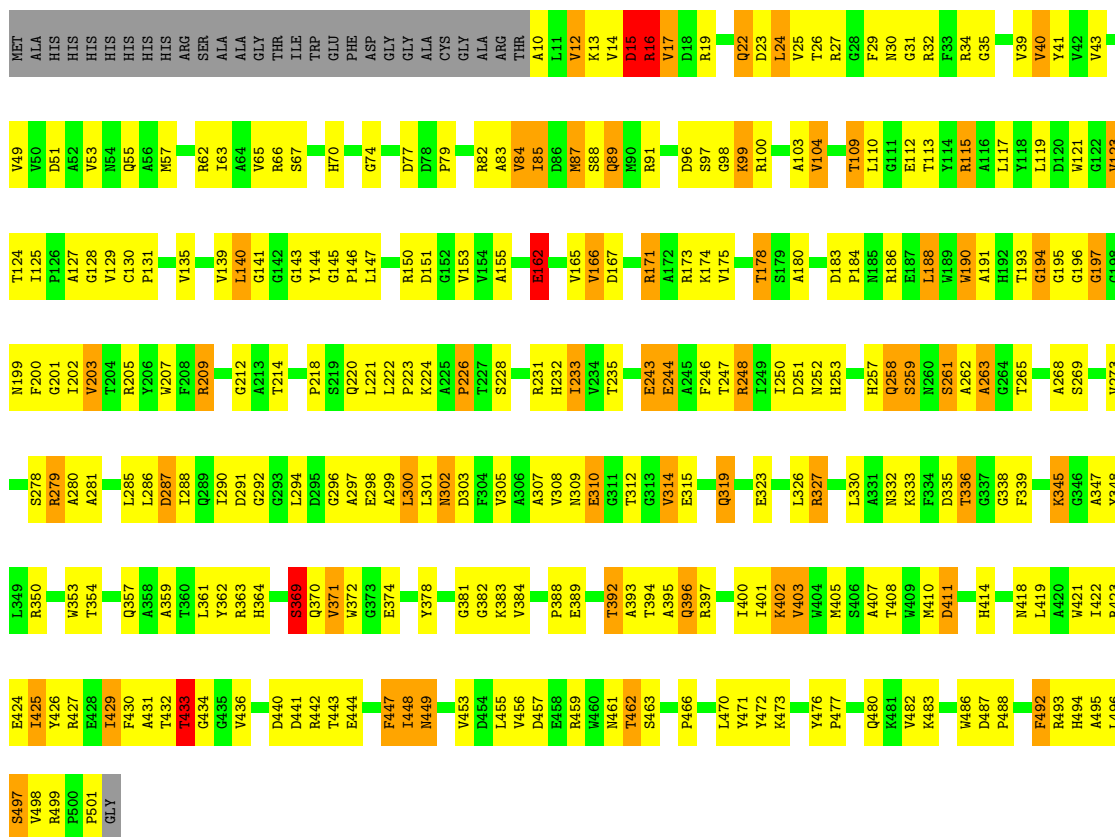
- Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain B:  36% 45% 12% • 6%





• Molecule 1: Aclacinomycin oxidoreductase (AknOx)



• Molecule 1: Aclacinomycin oxidoreductase (AknOx)



V482	V483	V484	V485	V486	V487	V488	V489	V490	V491	V492	V493	V494	V495	V496	V497	V498	V499	P500	P501	GLY																																		
R341	T342	K343	S344	K345	R350	K351	P352	W353	T354	A355	A356	Q357	L361	Y362	R363	H364	L365	D368	S369	G370	V371	W372	G373	E374	V375	S376	D377	Y378	S379	Y380	G381	G382	K383	V384	N385	T392	A393	T394	A395	Q396	R397	D398	S399	I400	W401	K402	V403	M405	S406	A407	T408	W409	M410	D411
Y267	A268	S269	M270	V273	F274	S278	R279	I284	L285	L286	D287	I288	Q289	I290	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	S344	K345	R350	K351	P352	W353	T354	A355	A356	Q357	L361	Y362	R363	H364	L365	D368	S369	G370	V371	W372	G373	E374	V375	S376	D377	Y378	S379	Y380	G381	G382	K383	V384	N385	T392	A393	T394	A395	Q396	R397	D398	S399	I400	W401	K402	V403	M405	S406	A407	T408	W409	M410	D411
P412	A413	H414	D415	D416	A417	N418	L419	A420	W421	I422	R423	E424	L425	Y426	R427	E428	I429	F430	A431	T432	T433	G434	G435	V436	F437	V438	P439	D440	D441	R442	T443	E444	G445	T446	F447	I448	M449	V453	D454	L455	V456	W460	N461	T462	V465	P466	T469	L470	Y471	Y472	R478	L479	Q480	K481
V42	T45	Q48	D51	Q55	A56	M57	A58	I63	A64	V65	R66	S67	G68	G69	H70	D78	V81	R82	A83	V84	I85	D86	M87	S88	Q89	M90	R91	D96	S97	G98	K99	R100	A103	V104	A108	T109	E112	T113	Y114	R115	A116	H117	Y118	L119	V123	T124	I125							
R126	A127	G128	V129	C130	P131	Q132	V133	G134	V135	H138	V139	L140	G143	Y144	G145	P146	L147	S148	R149	R150	D151	G152	V153	V154	A155	E162	V163	V166	D167	R171	A172	R173	K174	V175	V176	A177	T178	S179	A180	D183	E187	L188	W189	W190	A191	H192	T193	G194	G195	R196	G197	G198		
N199	F200	G201	I202	T204	R205	Y206	W207	F208	R209	A213	T214	G215	T216	D217	G218	S219	Q220	L221	L222	P223	K224	A225	P226	T227	S228	T229	L230	R231	H232	I233	V234	T235	W238	T242	E243	E244	A245	F246	T247	R248	I249	N252	H253	G254	H257	Q258	S261	A263	G264	T265	P266			

4 Data and refinement statistics i

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	9546 reflections (3.87%)	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 , 55.4	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 [i](#)

5.1 Standard geometry [i](#)

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	0.51	1/3946 (0.0%)	1.48	48/5386 (0.9%)
1	B	0.53	1/3927 (0.0%)	1.54	47/5361 (0.9%)
1	C	0.56	2/3935 (0.1%)	1.61	51/5372 (0.9%)
1	D	0.51	0/3927	1.52	50/5361 (0.9%)
All	All	0.53	4/15735 (0.0%)	1.54	196/21480 (0.9%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	GLN	C-N	6.32	1.43	1.33
1	B	258	GLN	C-N	5.75	1.42	1.33
1	C	258	GLN	C-N	5.51	1.41	1.33
1	C	259	SER	C-N	-5.27	1.26	1.33

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	GLY	CA-C-N	18.66	140.69	119.98
1	C	196	GLY	C-N-CA	18.66	140.69	119.98
1	D	196	GLY	CA-C-N	13.20	147.28	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	GLY	C-N-CA	13.20	147.28	121.41
1	C	197	GLY	N-CA-C	11.88	126.98	112.73

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 [i](#)

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	284	2
1	B	3823	0	3679	306	0
1	C	3828	0	3688	317	0
1	D	3823	0	3684	282	0
2	A	58	0	48	13	0
3	A	53	0	29	3	0
3	B	53	0	28	6	0
3	C	53	0	30	9	0
3	D	53	0	30	13	0
4	A	274	0	0	53	0
4	B	212	0	0	50	1
4	C	317	0	0	61	1
4	D	206	0	0	41	0
All	All	16589	0	14913	1166	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 39.

The worst 5 of 1166 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:HM82	0.99	1.29
1:C:130:CYS:SG	3:C:801:FAD:C6	2.25	1.25
1:C:392:THR:HG21	1:C:397:ARG:HH21	1.23	1.02

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry 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%)	21 8
1	D	490/521 (94%)	448 (91%)	37 (8%)	5 (1%)	12 2
All	All	1963/2084 (94%)	1812 (92%)	132 (7%)	19 (1%)	12 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%)	318 (81%)	73 (19%)	1	0
1	B	389/408 (95%)	317 (82%)	72 (18%)	1	0
1	C	390/408 (96%)	321 (82%)	69 (18%)	2	0
1	D	389/408 (95%)	312 (80%)	77 (20%)	1	0
All	All	1559/1632 (96%)	1268 (81%)	291 (19%)	1	0

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	129	VAL
1	D	453	VAL
1	D	174	LYS
1	D	320	ARG
1	B	199	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	357	GLN
1	D	258	GLN
1	C	364	HIS
1	D	30	ASN
1	D	283	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 [i](#)

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
2	AKY	A	601[A]	-	62,64,64	1.97	16 (25%)	87,98,98	1.96	22 (25%)
3	FAD	B	801	1	58,58,58	1.85	15 (25%)	85,89,89	1.99	28 (32%)
3	FAD	D	801	1	58,58,58	1.88	23 (39%)	85,89,89	1.96	22 (25%)
3	FAD	C	801	1	58,58,58	1.79	15 (25%)	85,89,89	2.04	28 (32%)
3	FAD	A	801	1	58,58,58	1.59	11 (18%)	85,89,89	1.83	22 (25%)

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	AKY	A	601[A]	-	7/7/18/18	6/25/105/105	0/7/7/7
3	FAD	B	801	1	1/1/9/9	10/34/50/50	0/6/6/6
3	FAD	D	801	1	-	11/34/50/50	0/6/6/6
3	FAD	C	801	1	-	12/34/50/50	0/6/6/6
3	FAD	A	801	1	-	9/34/50/50	0/6/6/6

The worst 5 of 80 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601[A]	AKY	O19-C49-C50	6.35	120.83	106.74
3	B	801	FAD	C5A-C4A-N3A	-5.78	118.75	126.72
3	A	801	FAD	C4'-C3'-C2'	-5.73	104.03	113.57
3	B	801	FAD	N3A-C2A-N1A	-5.67	120.00	128.58
3	C	801	FAD	N3A-C2A-N1A	-5.50	120.26	128.58

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601[A]	AKY	C31
2	A	601[A]	AKY	C33
2	A	601[A]	AKY	C49
2	A	601[A]	AKY	C39
2	A	601[A]	AKY	C35

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'

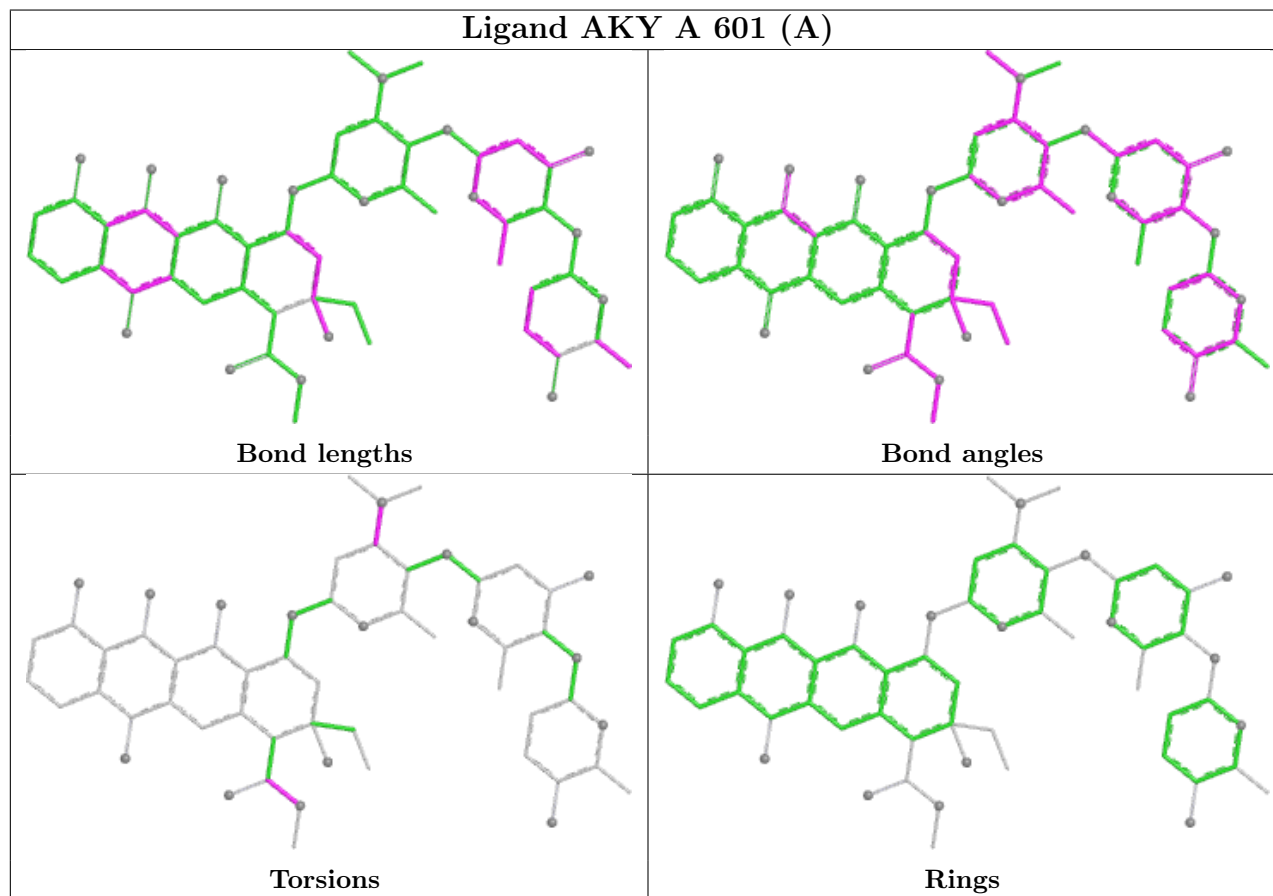
There are no ring outliers.

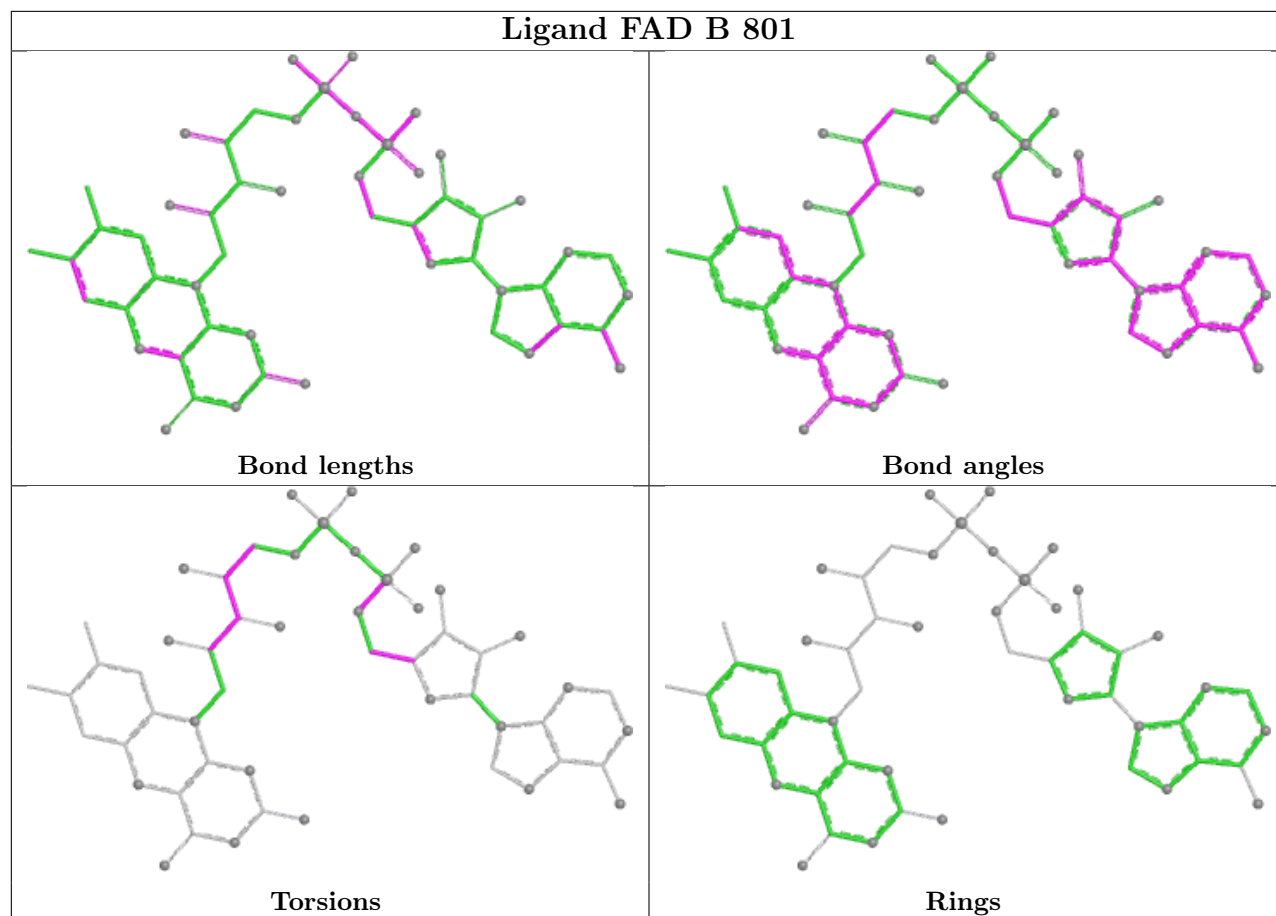
5 monomers are involved in 44 short contacts:

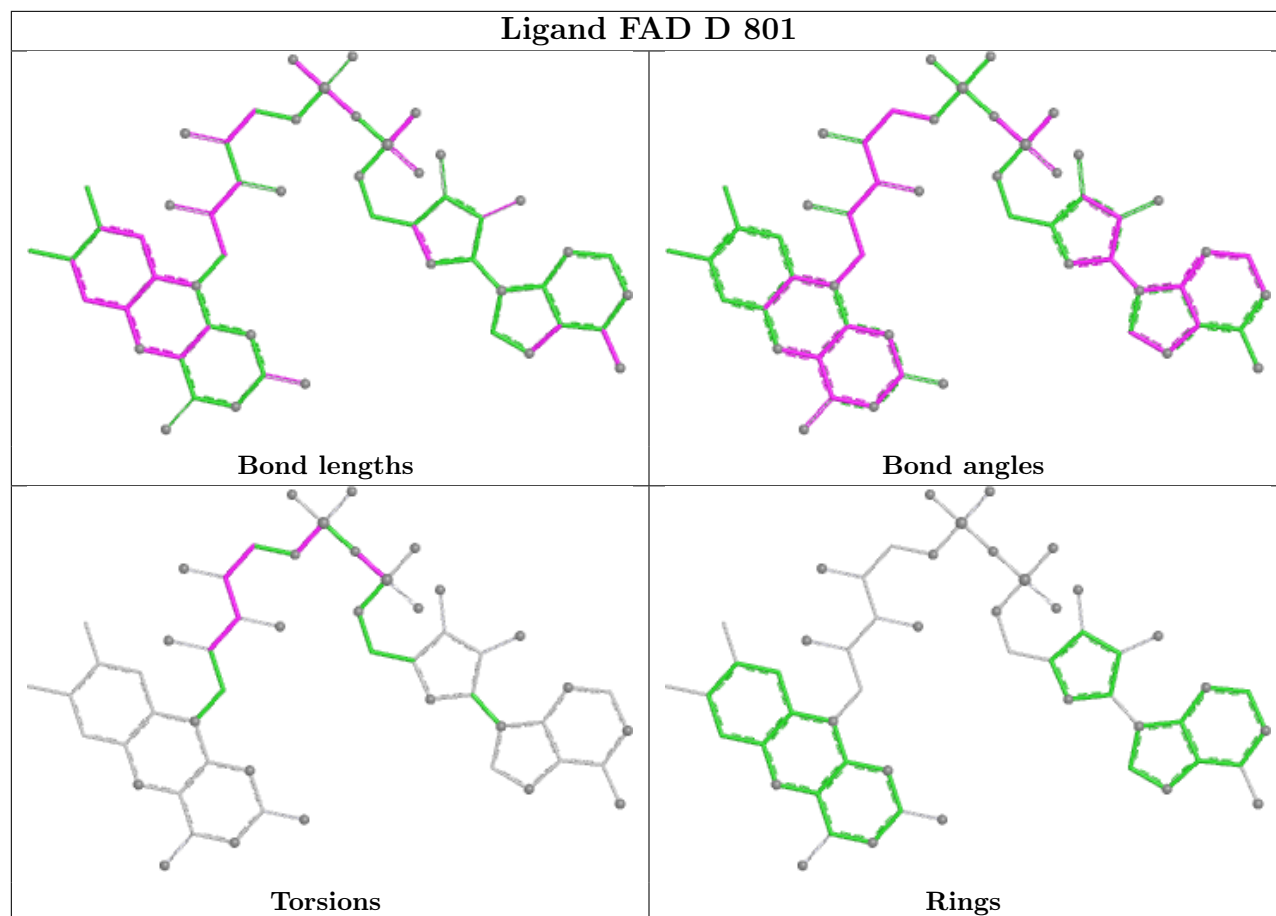
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601[A]	AKY	13	0
3	B	801	FAD	6	0
3	D	801	FAD	13	0
3	C	801	FAD	9	0
3	A	801	FAD	3	0

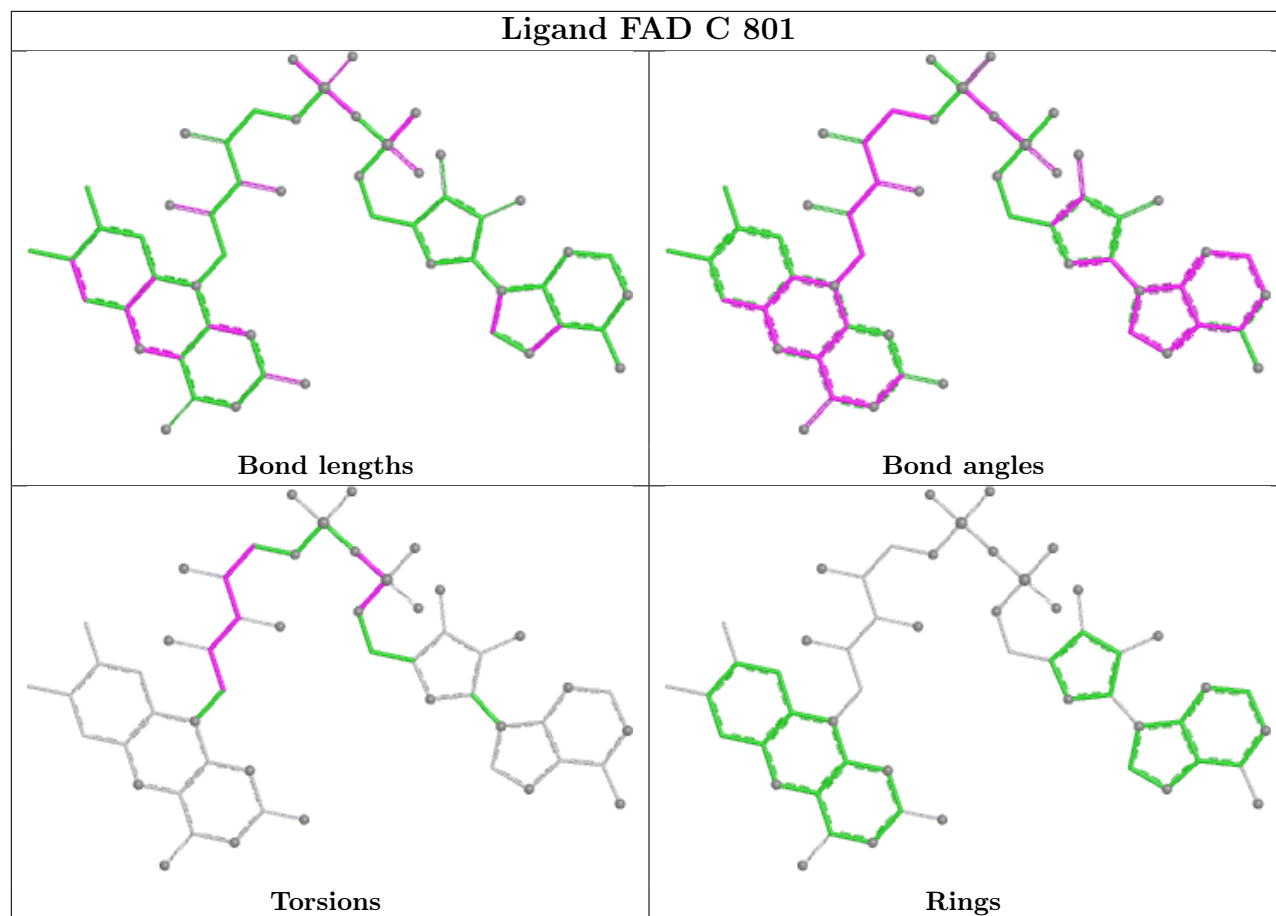
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

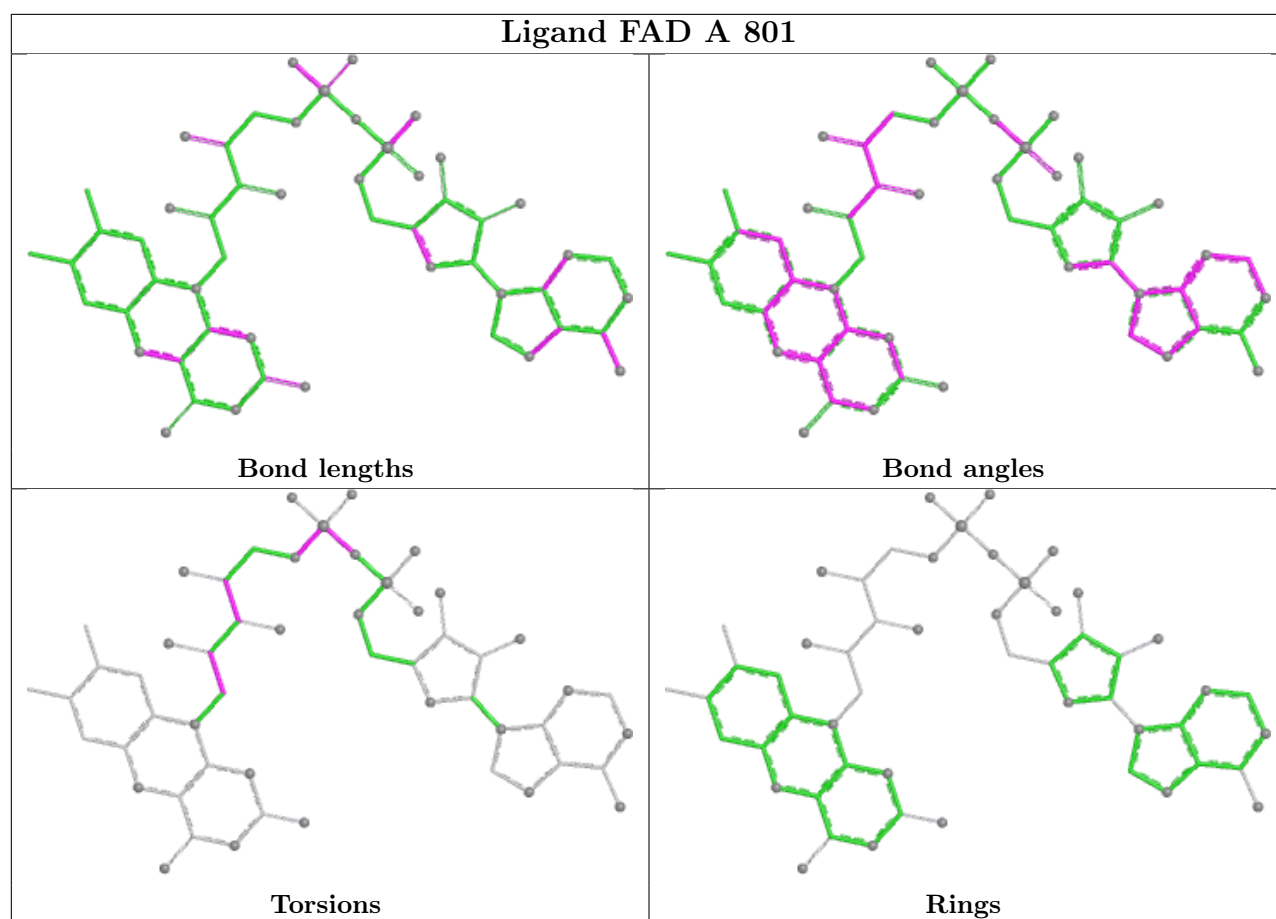
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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	492/521 (94%)	-1.09	0 100 100	3, 16, 30, 39	16 (3%)
1	B	492/521 (94%)	-1.07	0 100 100	6, 17, 30, 39	14 (2%)
1	C	492/521 (94%)	-1.11	0 100 100	5, 16, 29, 40	13 (2%)
1	D	492/521 (94%)	-1.07	0 100 100	4, 16, 31, 43	15 (3%)
All	All	1968/2084 (94%)	-1.09	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 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(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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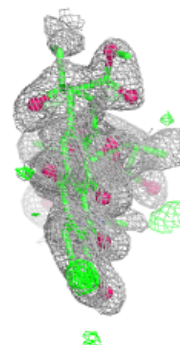
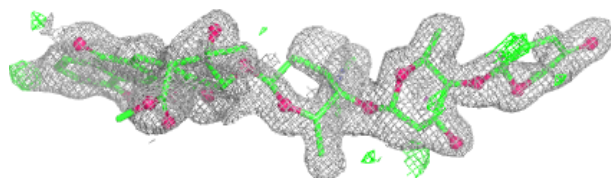
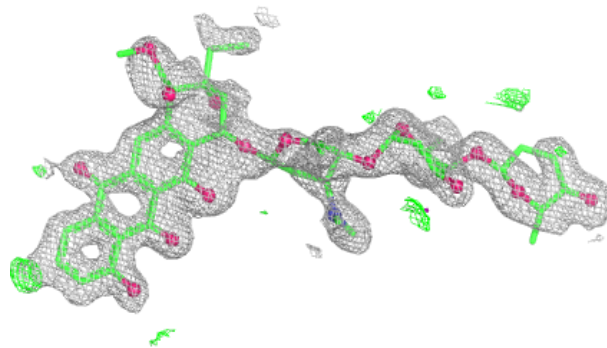
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	D	801	53/53	0.99	0.03	4,11,26,42	0

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.

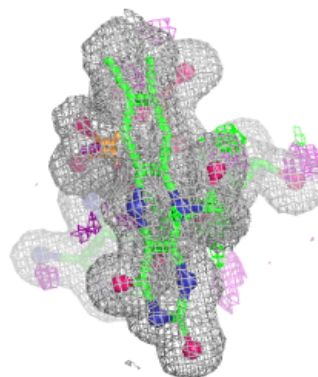
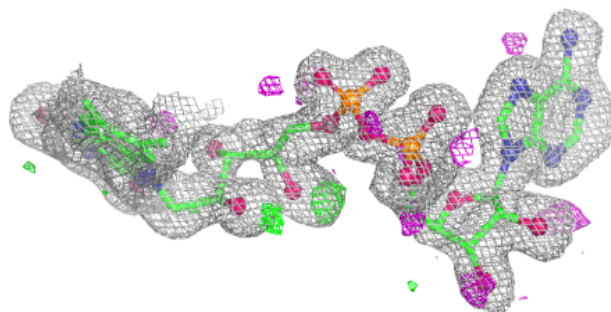
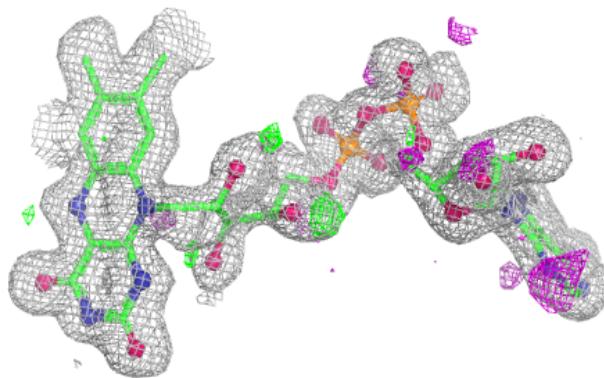
Electron density around AKY A 601 (A):

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

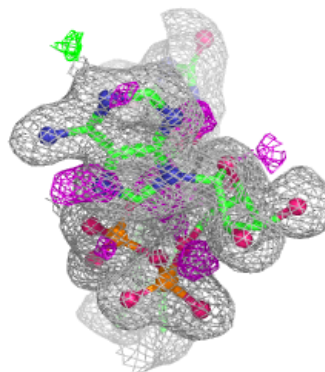
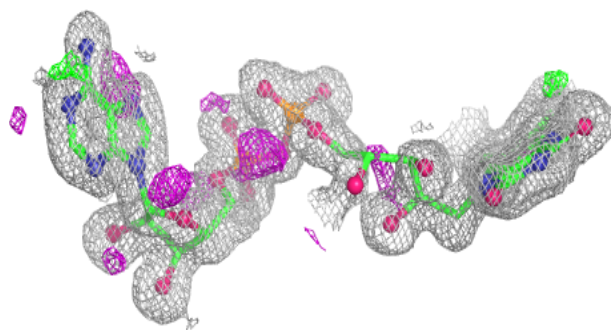
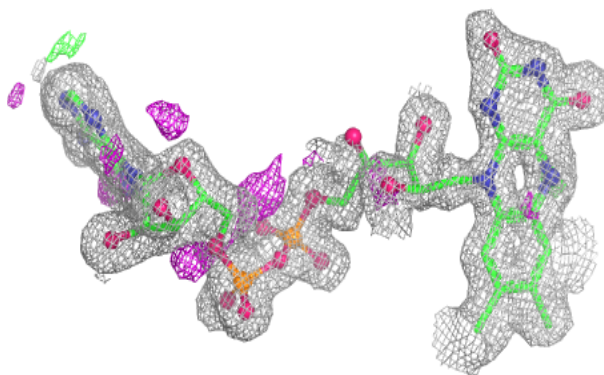


Electron density around FAD A 801:

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

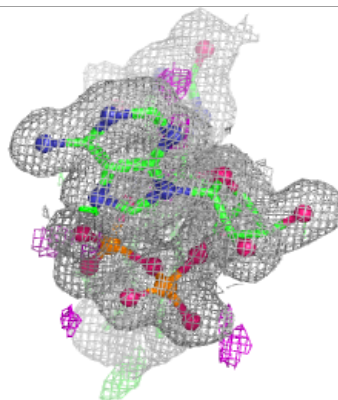
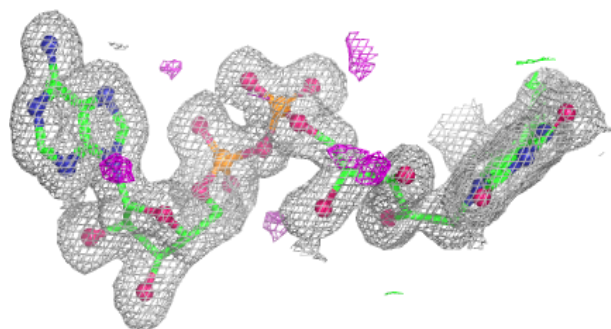
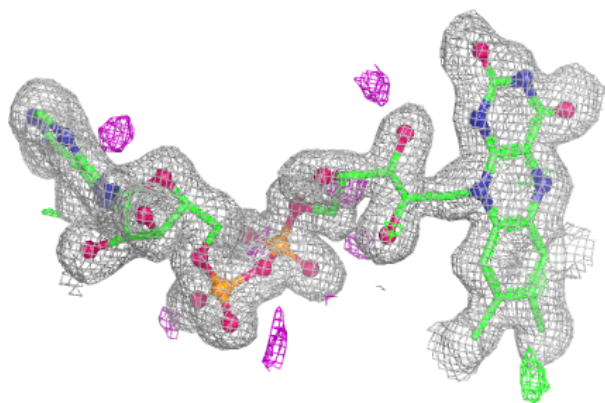
**Electron density around FAD B 801:**

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

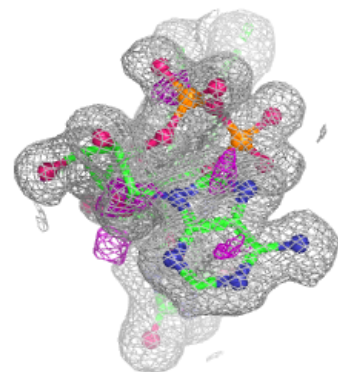
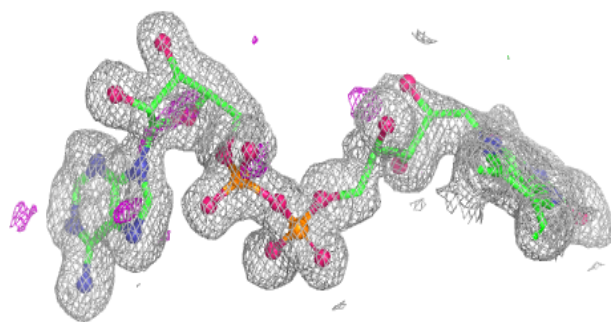
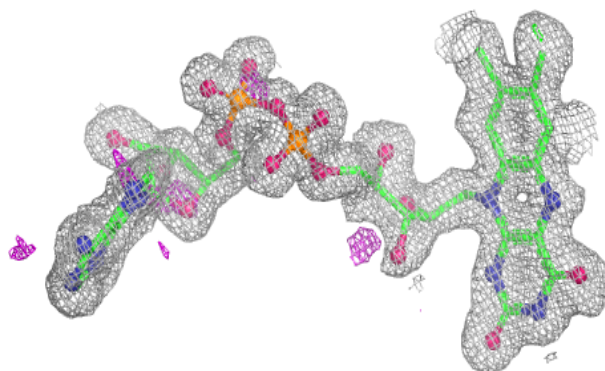


Electron density around FAD C 801:

$2mF_o-DF_c$ (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

There are no such residues in this entry.