wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:48 AM GMT

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.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

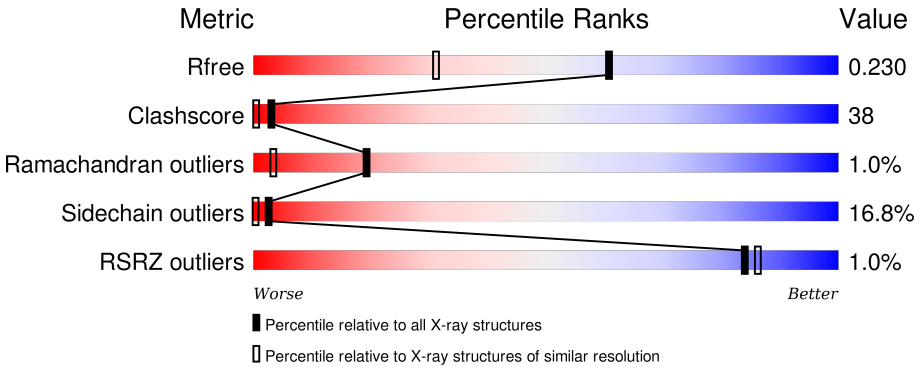
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	44% 39% 11% 6%
1	B	521	37% 45% 11% 6%
1	C	521	44% 41% 9% 6%
1	D	521	41% 41% 11% 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 crite-

ria:

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
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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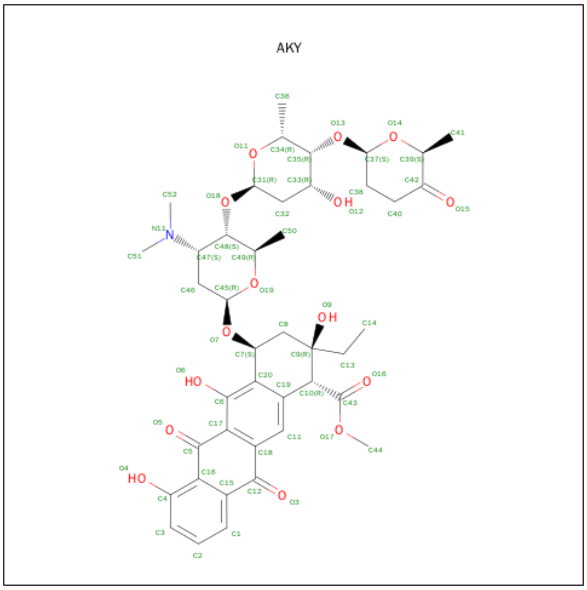
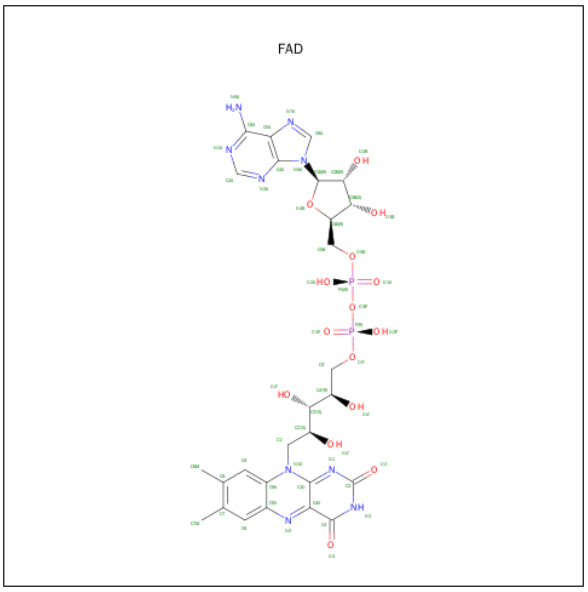
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-11	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-10	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-9	ARG	-	CLONING ARTIFACT	UNP Q0PCD7
D	-8	SER	-	CLONING ARTIFACT	UNP Q0PCD7
D	-7	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
D	-6	ALA	-	CLONING ARTIFACT	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-TRIDEOXY-4-O-{2,6-DIDEOXY-4-O-[(2S,6S)-6-METHYL-5-OXOTETRAHYDRO-2H-PYRAN-2-YL]-ALPHA-D-LYXO-HEXOPYRANOSYL}-3-(DIMETHYLAMINO)-D-RIBO-HEXOPYRANOSYL]OXY}-1,2,3,4,6,11-HEXAHYDROTETRACENE-1-CARBOXYLATE (three-letter code: AKY) (formula: $C_{42}H_{53}NO_{15}$).



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: $C_{27}H_{33}N_9O_{15}P_2$).



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

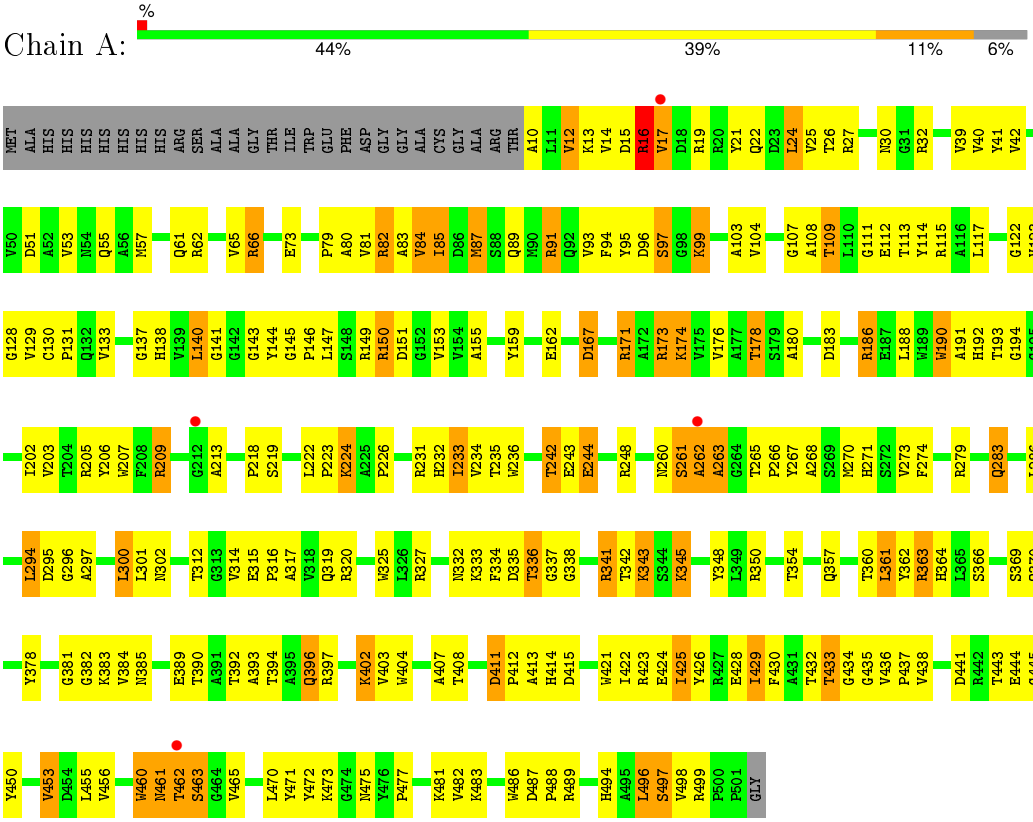
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total	O	0	0
			274	274		
4	B	212	Total	O	0	0
			212	212		
4	C	317	Total	O	0	0
			317	317		
4	D	206	Total	O	0	0
			206	206		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

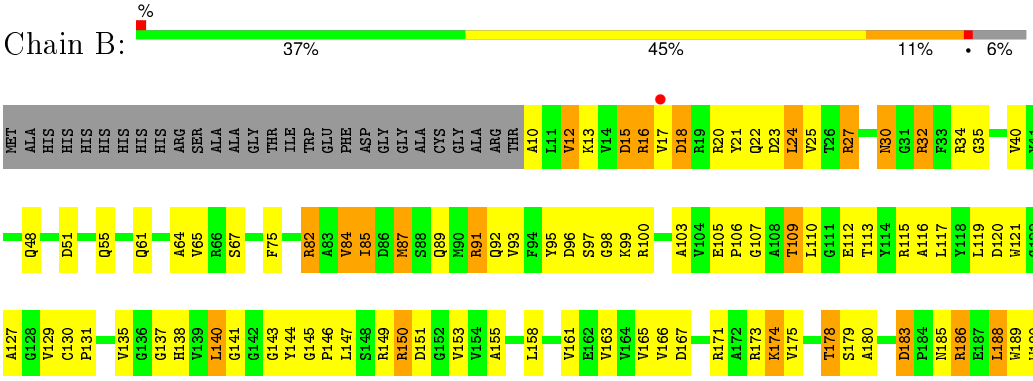
- Molecule 1: Aclacinomycin oxidoreductase (AknOx)

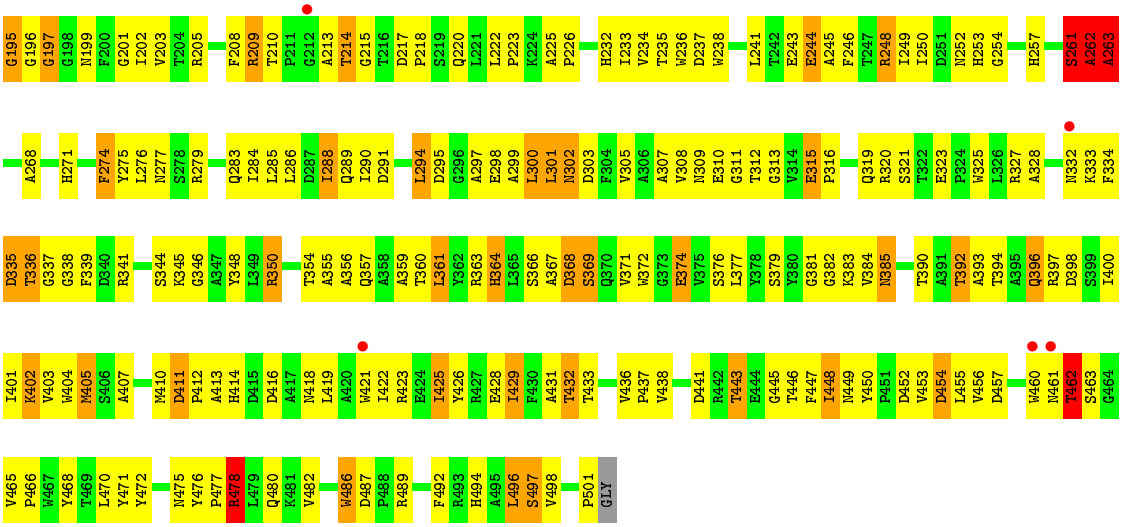
Chain A:



- Molecule 1: Aclacinomycin oxidoreductase (AknOx)

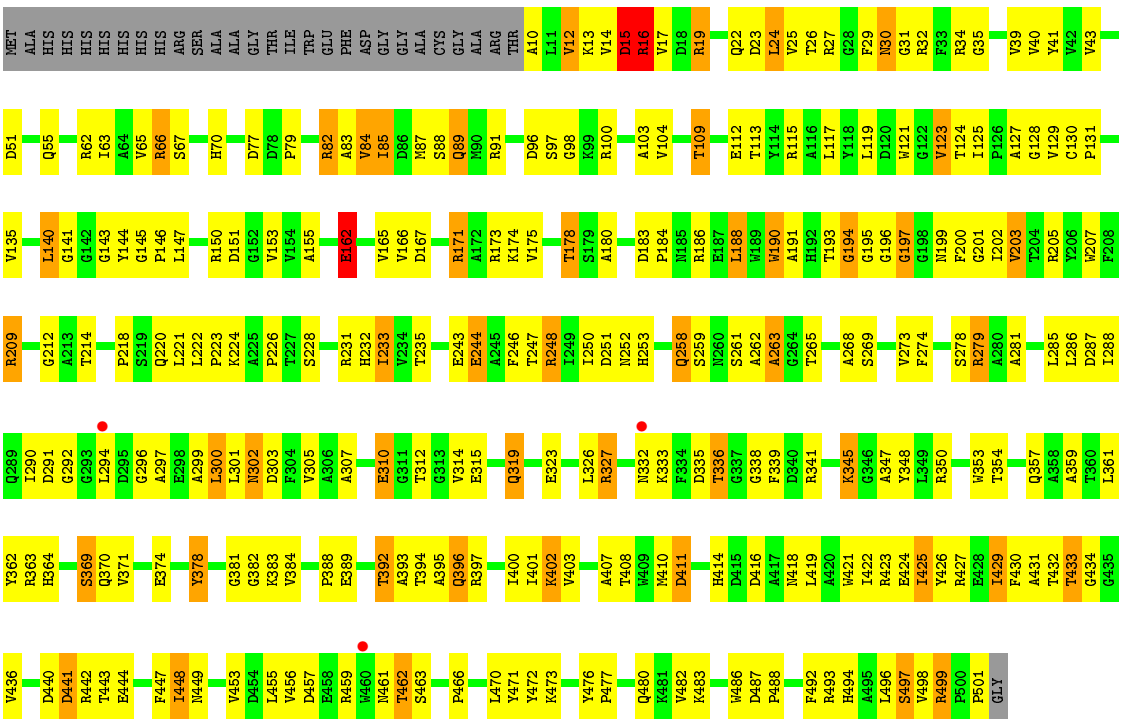
Chain B:





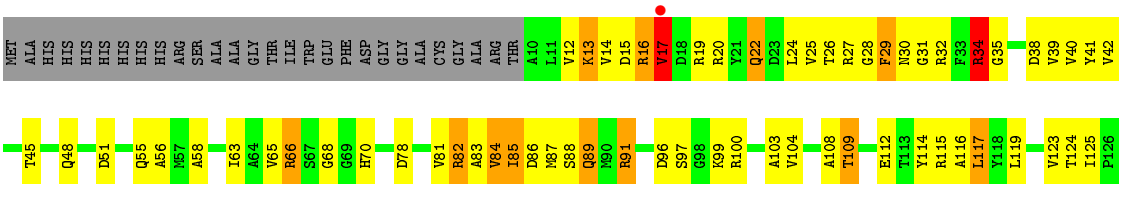
• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

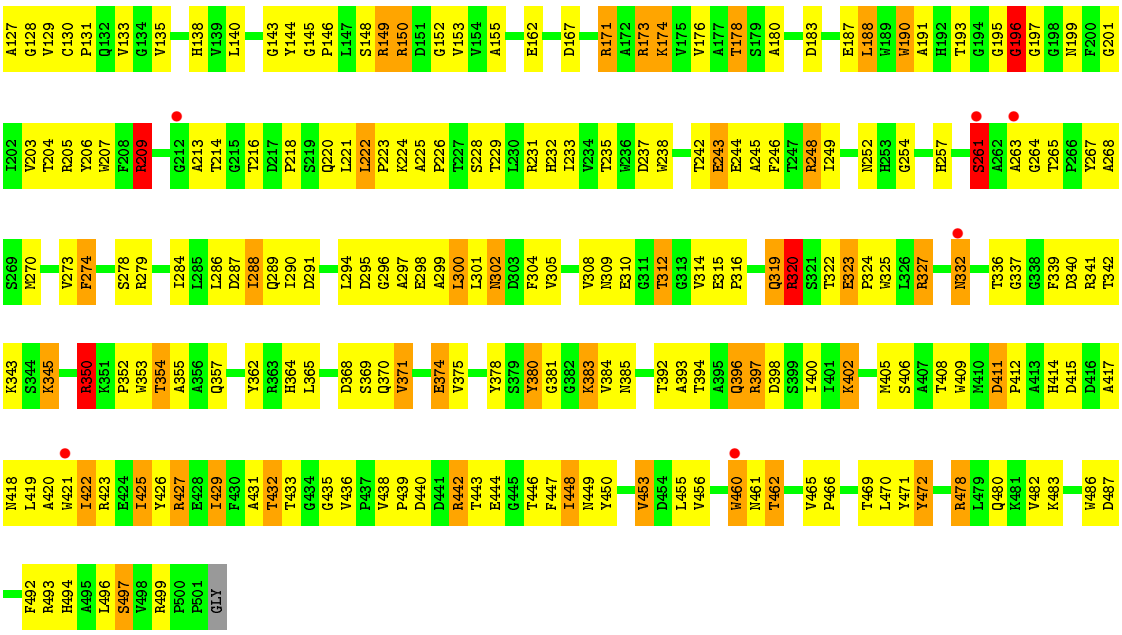
Chain C:



• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain D:




A127 G128 V129 C130 P131 Q132 V133 G134 V135 H138 Y139 L140 G143 Y144 G145 P146 L147 S148 R149 R150 D151 G152 V153 Y154 A155 E162 D167 R171 A172 R173 K174 Y175 V176 A177 T178 S179 A180 D183 E187 L188 W189 W190 A191 H192 T193 G194 G195 G196 G197 G198 N199 F200 G201
I202 V203 T204 R205 Y206 W207 P208 R209 G212 A213 T214 G215 T216 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 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 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 I401 K402 M405 S406 A407 T408 W409 M410 D411 P412 A413 H414 D415 D416 A417
N418 L419 A420 W421 I422 R423 E424 I425 Y426 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
F492 R493 H494 A495 L496 S497 V498 R499 P500 P501 GLY

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 19.76 – 1.67	Depositor EDS
% Data completeness (in resolution range)	95.9 (20.00-1.65) 98.5 (19.76-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 1.67Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.185 , 0.242 0.182 , 0.230	Depositor DCC
R_{free} test set	9545 reflections (4.04%)	DCC
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.0	EDS
Estimated twinning fraction	0.129 for -h-l,k,h 0.129 for l,k,-h-l 0.135 for h,-k,-h-l 0.128 for -h-l,-k,l 0.430 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.14$	Xtriage
Outliers	0 of 246725 reflections	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: AKY, 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	0.40	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(^{o})	Ideal(^{o})
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 (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	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%)	24 5
1	B	490/521 (94%)	456 (93%)	27 (6%)	7 (1%)	14 1
1	C	491/521 (94%)	449 (91%)	39 (8%)	3 (1%)	30 9
1	D	490/521 (94%)	448 (91%)	37 (8%)	5 (1%)	19 3
All	All	1963/2084 (94%)	1812 (92%)	132 (7%)	19 (1%)	19 3

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%)	2 0
1	B	389/408 (95%)	323 (83%)	66 (17%)	2 0
1	C	390/408 (96%)	327 (84%)	63 (16%)	3 0
1	D	389/408 (95%)	323 (83%)	66 (17%)	2 0
All	All	1559/1632 (96%)	1296 (83%)	263 (17%)	2 0

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

Mol	Chain	Res	Type
1	B	405	MET
1	C	123	VAL
1	D	354	THR
1	B	429	ILE
1	B	497	SER

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

Mol	Chain	Res	Type
1	B	364	HIS
1	C	89	GLN
1	D	319	GLN
1	B	494	HIS
1	C	199	ASN

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 carbohydrates 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	2.07	15 (24%)	83,98,98	2.04	20 (24%)
3	FAD	A	801	1	48,58,58	1.59	9 (18%)	54,89,89	2.22	14 (25%)
3	FAD	B	801	1	48,58,58	1.72	15 (31%)	54,89,89	2.41	12 (22%)
3	FAD	C	801	1	48,58,58	1.68	11 (22%)	54,89,89	2.68	18 (33%)
3	FAD	D	801	1	48,58,58	1.76	16 (33%)	54,89,89	2.33	14 (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	0/25/105/105	0/7/7/7
3	FAD	A	801	1	-	0/30/50/50	0/6/6/6
3	FAD	B	801	1	1/1/9/9	0/30/50/50	0/6/6/6
3	FAD	C	801	1	-	0/30/50/50	0/6/6/6
3	FAD	D	801	1	-	0/30/50/50	0/6/6/6

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[A]	AKY	C32-C33	-7.78	1.40	1.52
2	A	601[A]	AKY	C41-C39	-5.59	1.34	1.51
2	A	601[A]	AKY	C32-C31	-4.73	1.41	1.51
3	B	801	FAD	P-O1P	-4.02	1.36	1.51
3	C	801	FAD	P-O1P	-3.55	1.38	1.51

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	801	FAD	N3A-C2A-N1A	-11.62	120.00	128.89
3	C	801	FAD	N3A-C2A-N1A	-11.28	120.26	128.89
3	D	801	FAD	N3A-C2A-N1A	-10.92	120.53	128.89
3	A	801	FAD	N3A-C2A-N1A	-7.43	123.21	128.89
2	A	601[A]	AKY	C14-C13-C9	-6.09	104.45	115.00

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601[A]	AKY	C33
2	A	601[A]	AKY	C31
2	A	601[A]	AKY	C39
2	A	601[A]	AKY	C37
2	A	601[A]	AKY	C34

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 46 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.34	4 (0%)	87	88	3, 16, 31, 39	14 (2%)
1	B	492/521 (94%)	-0.33	6 (1%)	81	83	7, 17, 30, 39	14 (2%)
1	C	492/521 (94%)	-0.37	3 (0%)	90	90	7, 16, 30, 40	12 (2%)
1	D	492/521 (94%)	-0.31	7 (1%)	78	80	4, 17, 32, 43	15 (3%)
All	All	1968/2084 (94%)	-0.34	20 (1%)	84	86	3, 16, 31, 43	55 (2%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	VAL	4.2
1	D	263	ALA	3.9
1	D	212	GLY	3.4
1	B	17	VAL	3.3
1	B	460	TRP	3.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	AKY	A	601[A]	58/58	0.88	0.12	1.15	10,20,34,38	58
3	FAD	B	801	53/53	0.97	0.07	0.12	4,14,23,36	0
3	FAD	A	801	53/53	0.97	0.07	0.03	7,14,19,24	0
3	FAD	C	801	53/53	0.97	0.07	-0.15	3,11,25,37	0
3	FAD	D	801	53/53	0.98	0.06	-0.63	4,11,26,42	0

6.5 Other polymers (i)

There are no such residues in this entry.