



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:28 am BST

PDB ID : 2F99
Title : Crystal structure of the polyketide cyclase AknH with bound substrate and product analogue: implications for catalytic mechanism and product stereoselectivity.
Authors : Kallio, P.; Sultana, A.; Neimi, J.; Mantsala, P.; Schneider, G.
Deposited on : 2005-12-05
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

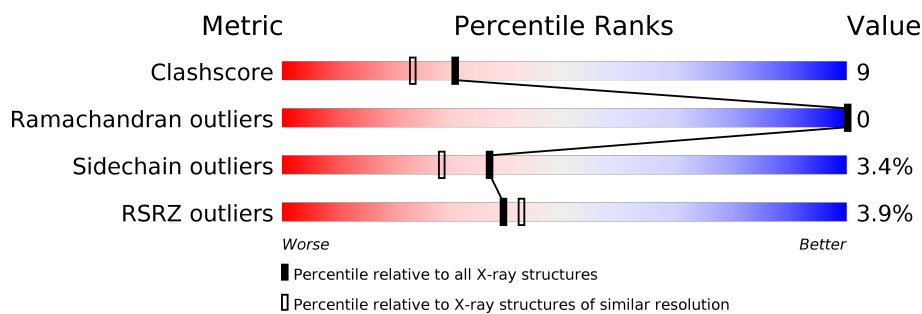
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	153	<div> <div>3%</div> <div>75%</div> <div>16%</div> <div>8%</div> </div>
1	B	153	<div> <div>%</div> <div>80%</div> <div>10%</div> <div>8%</div> </div>
1	C	153	<div> <div>7%</div> <div>78%</div> <div>12%</div> <div>8%</div> </div>
1	D	153	<div> <div>3%</div> <div>79%</div> <div>12%</div> <div>7%</div> </div>

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	SO4	B	1283	-	-	X	-
3	AKV	A	1335	X	-	X	-
3	AKV	B	1334	X	-	-	-
3	AKV	C	1333	X	-	-	-
3	AKV	D	1336	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5316 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 Aklanonic Acid methyl Ester Cyclase, AknH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	4	0
			1165	736	208	216	5			
1	B	141	Total	C	N	O	S	0	5	0
			1168	736	211	216	5			
1	C	140	Total	C	N	O	S	0	4	0
			1154	730	204	215	5			
1	D	143	Total	C	N	O	S	0	7	0
			1195	750	217	223	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	INITIATING METHIONINE	GB 7800671
A	-7	ALA	-	CLONING ARTIFACT	GB 7800671
A	-6	HIS	-	EXPRESSION TAG	GB 7800671
A	-5	HIS	-	EXPRESSION TAG	GB 7800671
A	-4	HIS	-	EXPRESSION TAG	GB 7800671
A	-3	HIS	-	EXPRESSION TAG	GB 7800671
A	-2	HIS	-	EXPRESSION TAG	GB 7800671
A	-1	HIS	-	EXPRESSION TAG	GB 7800671
A	0	HIS	-	EXPRESSION TAG	GB 7800671
A	1	ARG	-	CLONING ARTIFACT	GB 7800671
B	-8	MET	-	INITIATING METHIONINE	GB 7800671
B	-7	ALA	-	CLONING ARTIFACT	GB 7800671
B	-6	HIS	-	EXPRESSION TAG	GB 7800671
B	-5	HIS	-	EXPRESSION TAG	GB 7800671
B	-4	HIS	-	EXPRESSION TAG	GB 7800671
B	-3	HIS	-	EXPRESSION TAG	GB 7800671
B	-2	HIS	-	EXPRESSION TAG	GB 7800671
B	-1	HIS	-	EXPRESSION TAG	GB 7800671
B	0	HIS	-	EXPRESSION TAG	GB 7800671
B	1	ARG	-	CLONING ARTIFACT	GB 7800671
C	-8	MET	-	INITIATING METHIONINE	GB 7800671

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	CLONING ARTIFACT	GB 7800671
C	-6	HIS	-	EXPRESSION TAG	GB 7800671
C	-5	HIS	-	EXPRESSION TAG	GB 7800671
C	-4	HIS	-	EXPRESSION TAG	GB 7800671
C	-3	HIS	-	EXPRESSION TAG	GB 7800671
C	-2	HIS	-	EXPRESSION TAG	GB 7800671
C	-1	HIS	-	EXPRESSION TAG	GB 7800671
C	0	HIS	-	EXPRESSION TAG	GB 7800671
C	1	ARG	-	CLONING ARTIFACT	GB 7800671
D	-8	MET	-	INITIATING METHIONINE	GB 7800671
D	-7	ALA	-	CLONING ARTIFACT	GB 7800671
D	-6	HIS	-	EXPRESSION TAG	GB 7800671
D	-5	HIS	-	EXPRESSION TAG	GB 7800671
D	-4	HIS	-	EXPRESSION TAG	GB 7800671
D	-3	HIS	-	EXPRESSION TAG	GB 7800671
D	-2	HIS	-	EXPRESSION TAG	GB 7800671
D	-1	HIS	-	EXPRESSION TAG	GB 7800671
D	0	HIS	-	EXPRESSION TAG	GB 7800671
D	1	ARG	-	CLONING ARTIFACT	GB 7800671

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



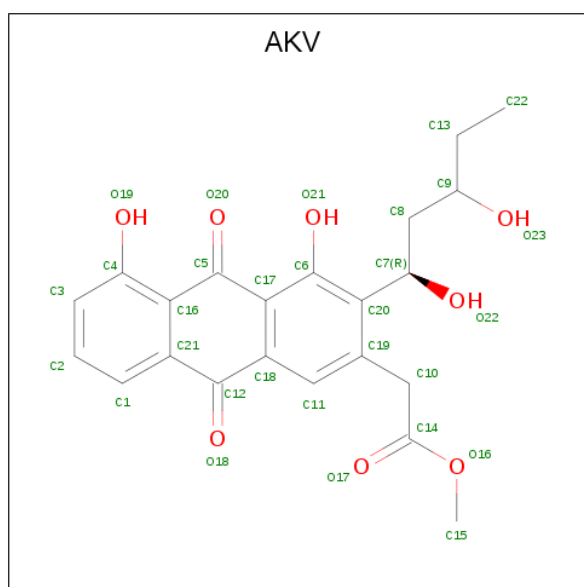
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is {3-[(1R,3S)-1,3-DIHYDROXYPENTYL]-4,5,9,10-TETRAHYDROXY-2-ANTHRYL}ACETATE (three-letter code: AKV) (formula: C₂₂H₂₂O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			30	22	8		
3	B	1	Total	C	O	0	0
			30	22	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			30	22	8		
3	D	1	Total	C	O	0	0
			30	22	8		

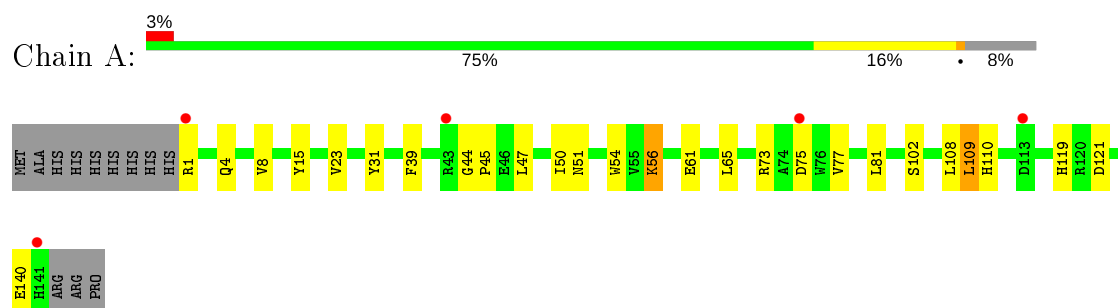
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	95	Total	O		0	0
			95	95			
4	B	147	Total	O		0	0
			147	147			
4	C	85	Total	O		0	0
			85	85			
4	D	132	Total	O		0	0
			132	132			

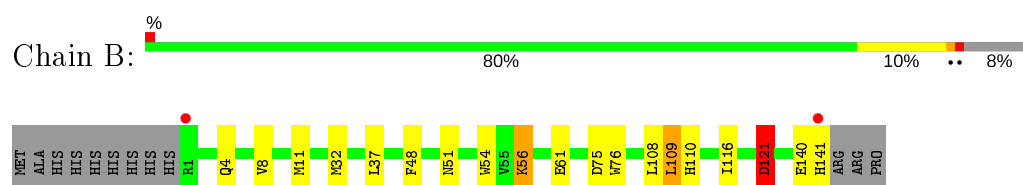
3 Residue-property plots [i](#)

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

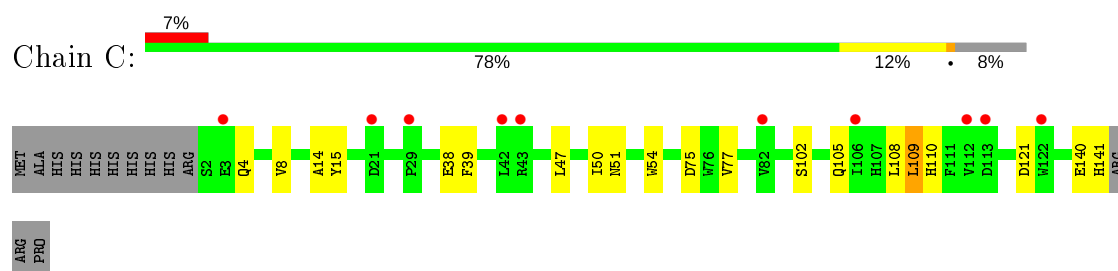
- Molecule 1: Aklanonic Acid methyl Ester Cyclase, AknH



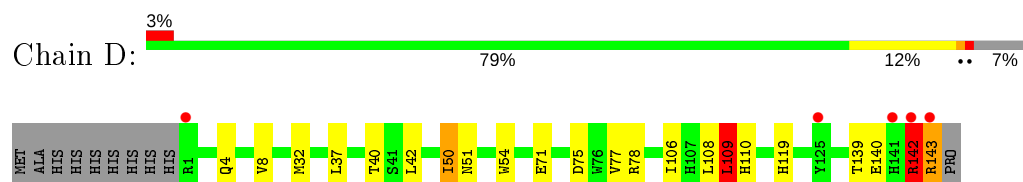
- Molecule 1: Aklanonic Acid methyl Ester Cyclase, AknH



- Molecule 1: Aklanonic Acid methyl Ester Cyclase, AknH



- Molecule 1: Aklanonic Acid methyl Ester Cyclase, AknH



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	151.74Å 151.74Å 108.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.52 – 1.90 37.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (84.52-1.90) 100.0 (37.94-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.207 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5316	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: AKV, SO4

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	0/1217	0.57	1/1649 (0.1%)
1	B	0.43	0/1227	0.61	2/1662 (0.1%)
1	C	0.40	0/1206	0.56	1/1635 (0.1%)
1	D	0.44	0/1263	0.60	1/1710 (0.1%)
All	All	0.42	0/4913	0.59	5/6656 (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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	109	LEU	CA-CB-CG	6.02	129.15	115.30
1	B	121	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	109	LEU	CA-CB-CG	5.59	128.15	115.30
1	C	109	LEU	CA-CB-CG	5.41	127.73	115.30
1	B	109	LEU	CA-CB-CG	5.30	127.50	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	142	ARG	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	1165	0	1110	18	0
1	B	1168	0	1113	18	0
1	C	1154	0	1094	17	0
1	D	1195	0	1134	25	0
2	A	10	0	0	0	0
2	B	15	0	0	2	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	30	0	18	9	0
3	B	30	0	19	8	0
3	C	30	0	18	7	0
3	D	30	0	19	4	0
4	A	95	0	0	5	0
4	B	147	0	0	2	0
4	C	85	0	0	3	0
4	D	132	0	0	3	0
All	All	5316	0	4525	87	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 9.

All (87) 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)
3:B:1334:AKV:H153	4:B:1478:HOH:O	1.33	1.19
1:D:142:ARG:H	1:D:142:ARG:HD2	1.12	1.10
3:C:1333:AKV:O22	3:C:1333:AKV:H102	1.58	1.03
3:A:1335:AKV:O22	3:A:1335:AKV:H102	1.59	1.03
1:B:11[A]:MET:SD	1:B:116:ILE:HD13	2.00	1.01
1:D:143:ARG:HE	1:D:143:ARG:C	1.67	0.97
1:D:142:ARG:N	1:D:142:ARG:HD2	1.80	0.96
3:B:1334:AKV:O22	3:B:1334:AKV:H102	1.66	0.91
1:D:142:ARG:H	1:D:142:ARG:CD	1.79	0.91
1:D:143:ARG:NE	1:D:143:ARG:C	2.30	0.84
1:D:139:THR:HG21	1:D:143:ARG:HA	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1336:AKV:O22	3:D:1336:AKV:H102	1.81	0.80
1:D:142:ARG:HG3	1:D:142:ARG:HH11	1.47	0.79
1:B:110:HIS:HE1	4:B:1481:HOH:O	1.66	0.76
1:A:4:GLN:HE22	1:A:75:ASP:HA	1.51	0.75
1:B:51:ASN:ND2	3:B:1334:AKV:O23	2.19	0.75
3:B:1334:AKV:C10	3:B:1334:AKV:O22	2.30	0.73
1:C:110:HIS:HE1	4:C:1417:HOH:O	1.71	0.73
1:A:140:GLU:OE1	1:B:110:HIS:HD2	1.74	0.71
1:B:141:HIS:ND1	2:B:1283:SO4:O4	2.26	0.69
1:D:142:ARG:NH1	1:D:142:ARG:HG3	2.06	0.69
3:A:1335:AKV:C15	4:A:1395:HOH:O	2.41	0.69
1:C:140:GLU:OE1	1:D:110:HIS:HD2	1.75	0.69
1:D:110:HIS:HE1	4:D:1468:HOH:O	1.76	0.68
3:C:1333:AKV:O22	3:C:1333:AKV:C10	2.36	0.66
1:C:110:HIS:HD2	1:D:140:GLU:OE1	1.80	0.65
1:D:40:THR:OG1	1:D:42:LEU:HG	1.95	0.65
1:D:71:GLU:OE2	1:D:78:ARG:HD2	1.97	0.63
1:A:110:HIS:HE1	4:A:1430:HOH:O	1.83	0.62
1:A:8:VAL:HG21	1:A:77:VAL:HG11	1.82	0.61
3:A:1335:AKV:C10	3:A:1335:AKV:O22	2.41	0.60
1:C:54:TRP:CG	3:C:1333:AKV:H131	2.36	0.60
1:C:4:GLN:HE22	1:C:75:ASP:HA	1.67	0.60
1:D:106:ILE:HD11	4:D:1453:HOH:O	2.02	0.59
1:B:32:MET:HE1	1:B:37:LEU:HD21	1.84	0.59
1:B:121:ASP:OD1	3:B:1334:AKV:O17	2.20	0.59
1:B:4:GLN:HE22	1:B:75:ASP:HA	1.68	0.59
1:B:32:MET:CE	1:B:37:LEU:HD21	2.33	0.58
1:C:39:PHE:CZ	3:C:1333:AKV:H82	2.38	0.58
1:A:56:LYS:HG3	1:A:61:GLU:HA	1.84	0.58
1:C:105:GLN:HB3	4:C:1387:HOH:O	2.05	0.57
1:A:54:TRP:CE3	3:A:1335:AKV:H81	2.40	0.57
1:D:32[A]:MET:CE	1:D:37:LEU:HG	2.36	0.55
1:A:54:TRP:CD2	3:A:1335:AKV:H81	2.42	0.55
3:D:1336:AKV:O22	3:D:1336:AKV:C10	2.54	0.55
1:A:110:HIS:HD2	1:B:140:GLU:OE1	1.89	0.55
1:D:32[A]:MET:HE2	1:D:37:LEU:HD21	1.88	0.54
1:B:141:HIS:CE1	2:B:1283:SO4:O4	2.60	0.54
3:A:1335:AKV:H151	4:A:1395:HOH:O	2.06	0.52
3:A:1335:AKV:H153	4:A:1395:HOH:O	2.08	0.52
1:D:4:GLN:HE22	1:D:75:ASP:HA	1.73	0.52
1:C:39:PHE:CE1	3:C:1333:AKV:H82	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:HB2	4:A:1430:HOH:O	2.11	0.51
1:A:31:TYR:HB3	1:A:44:GLY:HA2	1.94	0.49
1:C:39:PHE:CG	3:C:1333:AKV:H132	2.48	0.49
1:D:142:ARG:CG	1:D:142:ARG:HH11	2.21	0.48
1:D:42:LEU:HD12	1:D:50:ILE:HG12	1.96	0.48
1:A:102[A]:SER:OG	1:C:102[A]:SER:OG	2.18	0.48
1:A:47:LEU:O	1:A:50:ILE:HG22	2.13	0.48
1:C:121:ASP:OD1	3:C:1333:AKV:H152	2.13	0.48
1:C:38:GLU:HG2	1:C:141:HIS:HD2	1.78	0.48
1:D:54:TRP:CD1	3:D:1336:AKV:H131	2.49	0.47
1:B:54:TRP:CD2	3:B:1334:AKV:H81	2.49	0.47
3:B:1334:AKV:O22	3:B:1334:AKV:O23	2.29	0.47
1:D:51[A]:ASN:HD21	3:D:1336:AKV:H153	1.80	0.47
1:D:109:LEU:HD13	1:D:119:HIS:CD2	2.51	0.46
1:C:47:LEU:O	1:C:50:ILE:HG22	2.15	0.46
3:A:1335:AKV:O22	3:A:1335:AKV:O23	2.30	0.45
1:B:54:TRP:CG	3:B:1334:AKV:H131	2.52	0.44
1:B:11[B]:MET:HG3	1:B:48:PHE:CZ	2.53	0.44
1:C:14:ALA:HB3	4:C:1407:HOH:O	2.17	0.44
1:D:32[A]:MET:HE1	1:D:37:LEU:HG	1.99	0.43
1:C:15:TYR:OH	1:C:51:ASN:ND2	2.51	0.43
1:B:8:VAL:O	1:B:11[B]:MET:HB3	2.19	0.43
1:D:8:VAL:HG21	1:D:77:VAL:HG11	2.01	0.43
1:A:65:LEU:HD13	1:A:81:LEU:HD13	2.00	0.42
1:A:23:VAL:HG23	1:A:45:PRO:HB3	2.01	0.42
1:B:56:LYS:HG3	1:B:61:GLU:HA	2.02	0.42
1:D:75:ASP:HB2	4:D:1467:HOH:O	2.20	0.41
1:A:39:PHE:CD1	3:A:1335:AKV:H132	2.55	0.41
1:C:8:VAL:HG21	1:C:77:VAL:HG11	2.03	0.41
1:A:15:TYR:OH	1:A:51:ASN:ND2	2.54	0.41
1:B:8:VAL:O	1:B:11[A]:MET:HB2	2.22	0.40
1:A:109:LEU:HD13	1:A:119:HIS:CD2	2.56	0.40
1:B:76:TRP:CZ3	1:B:110:HIS:HB2	2.56	0.40
1:A:65:LEU:HD22	1:A:81:LEU:HB3	2.03	0.40

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	143/153 (94%)	141 (99%)	2 (1%)	0	100	100
1	B	144/153 (94%)	141 (98%)	3 (2%)	0	100	100
1	C	142/153 (93%)	140 (99%)	2 (1%)	0	100	100
1	D	148/153 (97%)	146 (99%)	2 (1%)	0	100	100
All	All	577/612 (94%)	568 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	123/130 (95%)	118 (96%)	5 (4%)	30	21
1	B	124/130 (95%)	120 (97%)	4 (3%)	39	30
1	C	122/130 (94%)	120 (98%)	2 (2%)	62	60
1	D	128/130 (98%)	123 (96%)	5 (4%)	32	23
All	All	497/520 (96%)	481 (97%)	16 (3%)	37	30

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	56	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	ARG
1	A	108	LEU
1	A	121	ASP
1	B	56	LYS
1	B	108	LEU
1	B	109	LEU
1	B	121	ASP
1	C	108	LEU
1	C	109	LEU
1	D	50	ILE
1	D	108	LEU
1	D	109	LEU
1	D	142	ARG
1	D	143	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	51	ASN
1	A	110	HIS
1	B	4	GLN
1	B	110	HIS
1	C	4	GLN
1	C	51	ASN
1	C	110	HIS
1	C	141	HIS
1	D	4	GLN
1	D	110	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

15 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	SO4	A	1279	-	4,4,4	0.14	0	6,6,6	0.06	0
3	AKV	B	1334	-	31,32,32	2.93	15 (48%)	43,47,47	2.45	12 (27%)
2	SO4	C	1280	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	B	1278	-	4,4,4	0.14	0	6,6,6	0.15	0
3	AKV	C	1333	-	31,32,32	2.58	11 (35%)	43,47,47	1.68	6 (13%)
2	SO4	D	1281	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	C	1285	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	B	1286	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	B	1283	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	D	1276	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	D	1284	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	1282	-	4,4,4	0.14	0	6,6,6	0.08	0
3	AKV	A	1335	-	31,32,32	2.49	10 (32%)	43,47,47	1.71	5 (11%)
3	AKV	D	1336	-	31,32,32	2.39	10 (32%)	43,47,47	1.67	4 (9%)
2	SO4	C	1277	-	4,4,4	0.13	0	6,6,6	0.07	0

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	AKV	B	1334	-	1/1/5/5	8/16/32/32	0/3/3/3
3	AKV	A	1335	-	1/1/5/5	12/16/32/32	0/3/3/3
3	AKV	D	1336	-	1/1/5/5	7/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AKV	C	1333	-	1/1/5/5	7/16/32/32	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1334	AKV	C8-C7	-5.53	1.44	1.53
3	B	1334	AKV	O16-C14	5.49	1.50	1.33
3	C	1333	AKV	C10-C14	-5.39	1.41	1.51
3	B	1334	AKV	C10-C14	-5.15	1.41	1.51
3	D	1336	AKV	C20-C19	5.04	1.51	1.40
3	A	1335	AKV	O23-C9	-5.01	1.28	1.43
3	A	1335	AKV	C10-C14	-5.00	1.41	1.51
3	D	1336	AKV	C10-C14	-4.85	1.42	1.51
3	C	1333	AKV	O23-C9	-4.79	1.29	1.43
3	D	1336	AKV	O23-C9	-4.79	1.29	1.43
3	C	1333	AKV	C8-C7	-4.68	1.45	1.53
3	B	1334	AKV	O23-C9	-4.62	1.29	1.43
3	B	1334	AKV	C21-C12	-4.54	1.38	1.48
3	A	1335	AKV	C8-C7	-4.54	1.46	1.53
3	C	1333	AKV	C21-C12	-4.51	1.38	1.48
3	B	1334	AKV	C20-C19	4.49	1.49	1.40
3	B	1334	AKV	C21-C16	-4.44	1.34	1.41
3	A	1335	AKV	C8-C9	-4.36	1.42	1.52
3	C	1333	AKV	C18-C12	-4.35	1.39	1.48
3	D	1336	AKV	O16-C14	4.29	1.46	1.33
3	A	1335	AKV	O16-C14	4.25	1.46	1.33
3	D	1336	AKV	C8-C9	-4.14	1.43	1.52
3	A	1335	AKV	C21-C12	-3.99	1.40	1.48
3	A	1335	AKV	C20-C19	3.99	1.48	1.40
3	C	1333	AKV	C8-C9	-3.97	1.43	1.52
3	D	1336	AKV	C21-C12	-3.91	1.40	1.48
3	C	1333	AKV	C20-C19	3.90	1.48	1.40
3	B	1334	AKV	C18-C12	-3.85	1.40	1.48
3	A	1335	AKV	C18-C12	-3.84	1.40	1.48
3	C	1333	AKV	O16-C14	3.72	1.44	1.33
3	D	1336	AKV	C18-C12	-3.61	1.40	1.48
3	C	1333	AKV	C17-C5	-3.44	1.39	1.47
3	B	1334	AKV	C8-C9	-3.28	1.45	1.52
3	A	1335	AKV	C16-C5	-3.14	1.40	1.47
3	C	1333	AKV	C16-C5	-3.12	1.40	1.47
3	A	1335	AKV	C17-C5	-3.00	1.40	1.47
3	B	1334	AKV	C16-C4	-2.98	1.36	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1334	AKV	C17-C5	-2.92	1.40	1.47
3	D	1336	AKV	C8-C7	-2.86	1.48	1.53
3	D	1336	AKV	C16-C5	-2.84	1.40	1.47
3	D	1336	AKV	C17-C5	-2.80	1.41	1.47
3	B	1334	AKV	C1-C21	-2.80	1.35	1.39
3	B	1334	AKV	C11-C18	-2.78	1.35	1.39
3	B	1334	AKV	O21-C6	-2.50	1.31	1.37
3	C	1333	AKV	C10-C19	-2.35	1.48	1.51
3	B	1334	AKV	C10-C19	-2.30	1.48	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1334	AKV	O16-C14-C10	8.82	123.67	111.45
3	A	1335	AKV	O16-C14-C10	7.75	122.19	111.45
3	B	1334	AKV	C8-C7-C20	7.56	124.95	111.35
3	C	1333	AKV	O16-C14-C10	6.25	120.11	111.45
3	D	1336	AKV	O16-C14-C10	5.95	119.70	111.45
3	B	1334	AKV	O23-C9-C8	5.24	121.06	109.18
3	C	1333	AKV	O23-C9-C8	5.16	120.88	109.18
3	D	1336	AKV	O23-C9-C8	4.90	120.28	109.18
3	A	1335	AKV	O23-C9-C8	4.50	119.38	109.18
3	C	1333	AKV	C8-C7-C20	4.36	119.20	111.35
3	D	1336	AKV	C8-C9-C13	3.78	121.48	112.34
3	B	1334	AKV	O22-C7-C8	-3.75	101.00	108.78
3	D	1336	AKV	C8-C7-C20	3.67	117.95	111.35
3	A	1335	AKV	C8-C7-C20	3.19	117.10	111.35
3	B	1334	AKV	C3-C4-C16	2.91	123.91	120.17
3	B	1334	AKV	C4-C16-C5	2.84	124.95	120.59
3	B	1334	AKV	C21-C16-C4	-2.78	115.83	118.41
3	B	1334	AKV	C19-C10-C14	2.60	119.75	113.72
3	A	1335	AKV	C8-C9-C13	2.47	118.31	112.34
3	B	1334	AKV	C18-C12-C21	2.42	121.66	117.60
3	C	1333	AKV	C8-C9-C13	2.39	118.12	112.34
3	C	1333	AKV	C15-O16-C14	-2.36	108.32	116.11
3	B	1334	AKV	O17-C14-C10	-2.16	114.36	121.91
3	B	1334	AKV	O20-C5-C17	-2.12	118.00	121.43
3	A	1335	AKV	O23-C9-C13	2.10	119.02	109.06
3	C	1333	AKV	O23-C9-C13	2.06	118.82	109.06
3	B	1334	AKV	O18-C12-C21	-2.01	117.96	120.91

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1334	AKV	C9
3	C	1333	AKV	C9
3	A	1335	AKV	C9
3	D	1336	AKV	C9

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1334	AKV	C6-C20-C7-C8
3	C	1333	AKV	C7-C8-C9-O23
3	A	1335	AKV	C10-C14-O16-C15
3	A	1335	AKV	O22-C7-C8-C9
3	A	1335	AKV	C7-C8-C9-C13
3	A	1335	AKV	C22-C13-C9-O23
3	D	1336	AKV	C6-C20-C7-C8
3	D	1336	AKV	C19-C20-C7-C8
3	D	1336	AKV	C7-C8-C9-O23
3	D	1336	AKV	C22-C13-C9-O23
3	A	1335	AKV	O17-C14-O16-C15
3	C	1333	AKV	C10-C14-O16-C15
3	C	1333	AKV	O17-C14-O16-C15
3	D	1336	AKV	O17-C14-O16-C15
3	B	1334	AKV	C10-C14-O16-C15
3	B	1334	AKV	O17-C14-O16-C15
3	D	1336	AKV	C10-C14-O16-C15
3	A	1335	AKV	C14-C10-C19-C11
3	A	1335	AKV	C6-C20-C7-O22
3	B	1334	AKV	C14-C10-C19-C11
3	B	1334	AKV	C22-C13-C9-O23
3	C	1333	AKV	C22-C13-C9-O23
3	C	1333	AKV	C6-C20-C7-C8
3	A	1335	AKV	C6-C20-C7-C8
3	B	1334	AKV	C19-C20-C7-C8
3	C	1333	AKV	C19-C20-C7-C8
3	A	1335	AKV	C19-C20-C7-C8
3	B	1334	AKV	C19-C20-C7-O22
3	C	1333	AKV	C19-C20-C7-O22
3	A	1335	AKV	C19-C20-C7-O22
3	D	1336	AKV	C19-C20-C7-O22
3	B	1334	AKV	C14-C10-C19-C20
3	A	1335	AKV	C14-C10-C19-C20
3	A	1335	AKV	C22-C13-C9-C8

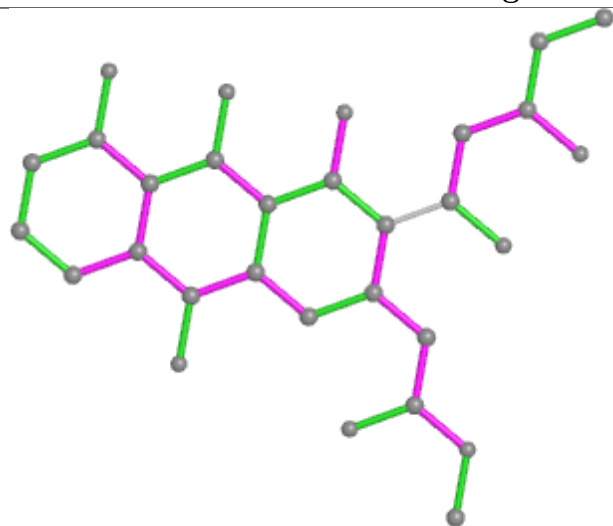
There are no ring outliers.

5 monomers are involved in 30 short contacts:

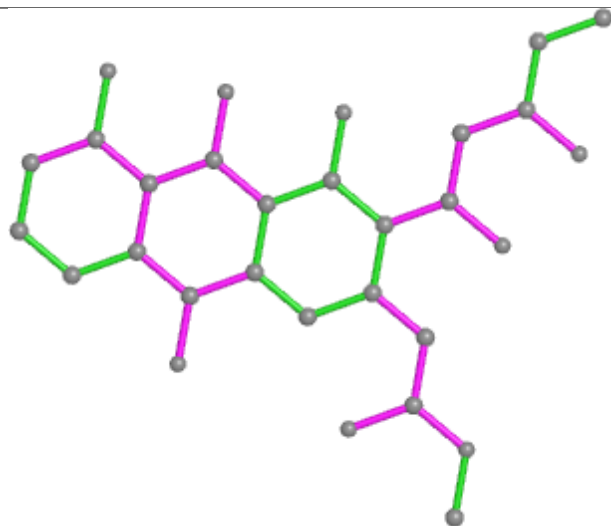
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1334	AKV	8	0
3	C	1333	AKV	7	0
2	B	1283	SO4	2	0
3	A	1335	AKV	9	0
3	D	1336	AKV	4	0

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.

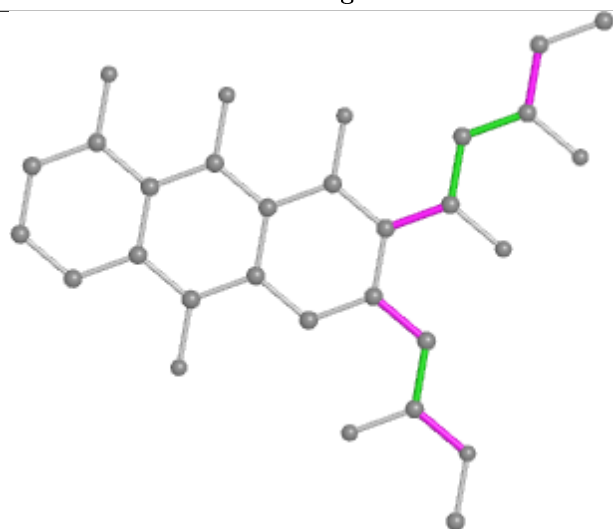
Ligand AKV B 1334



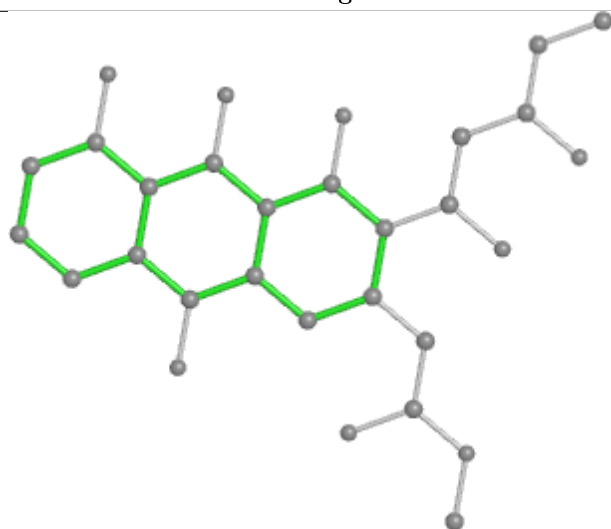
Bond lengths



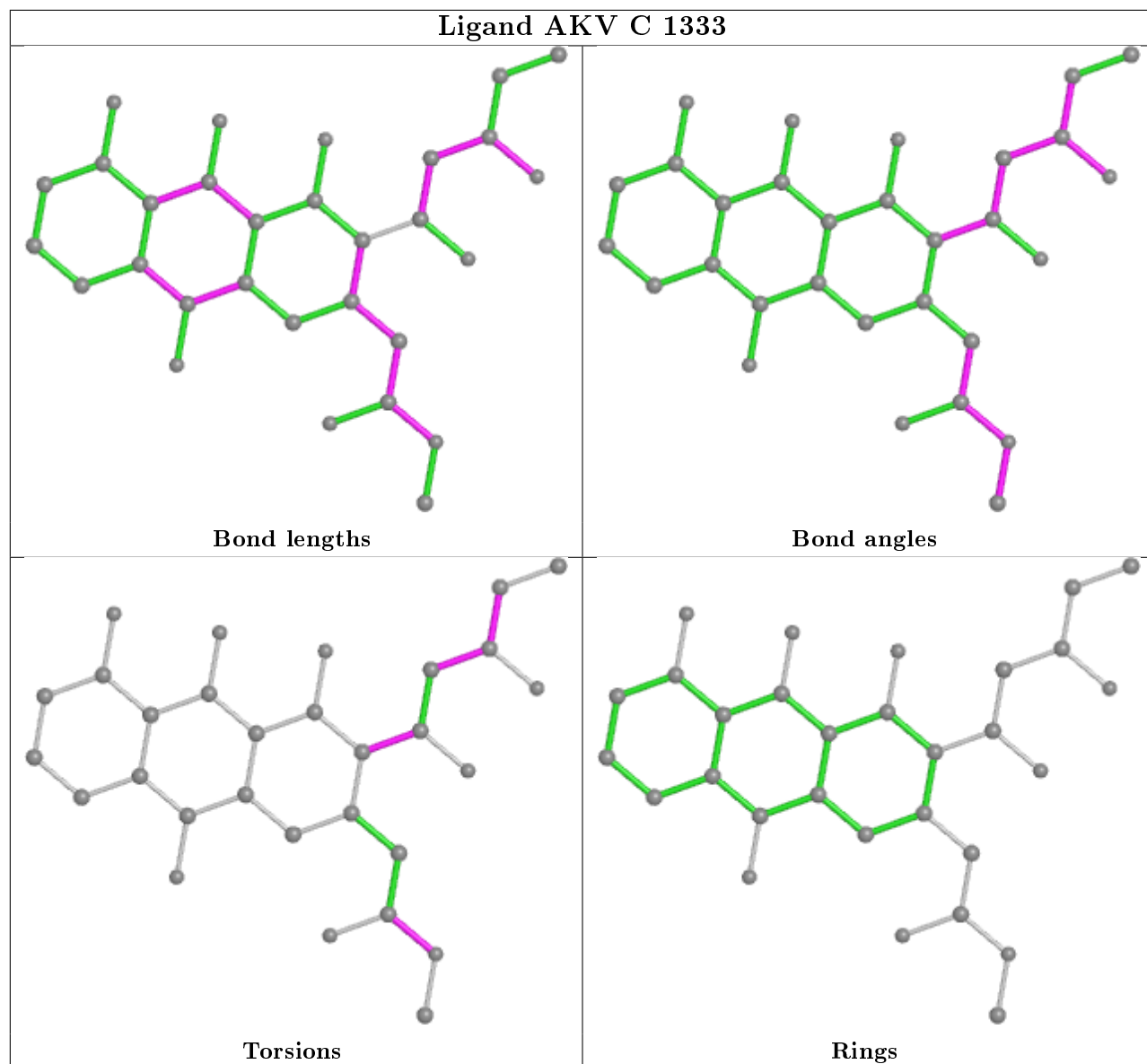
Bond angles



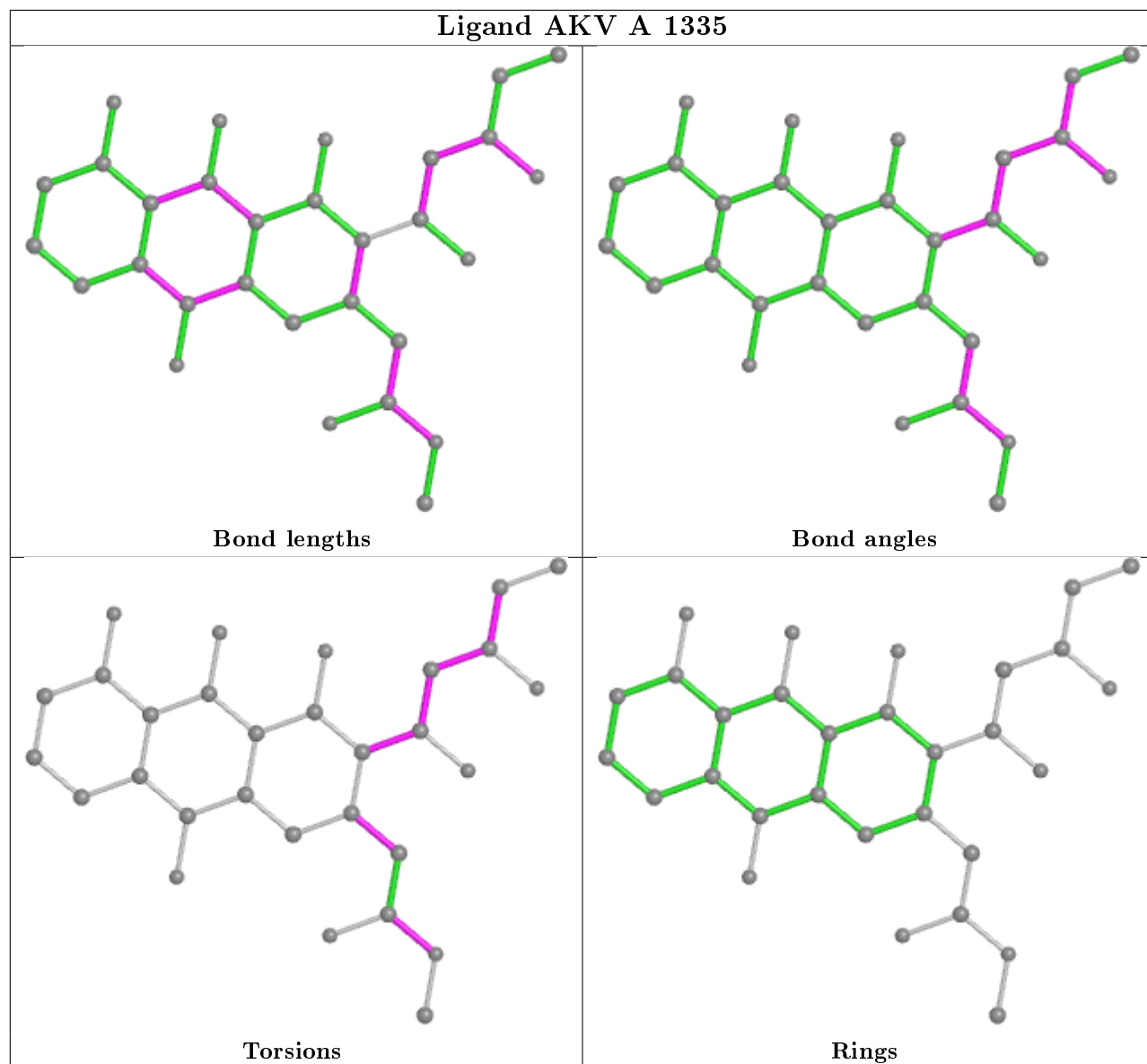
Torsions

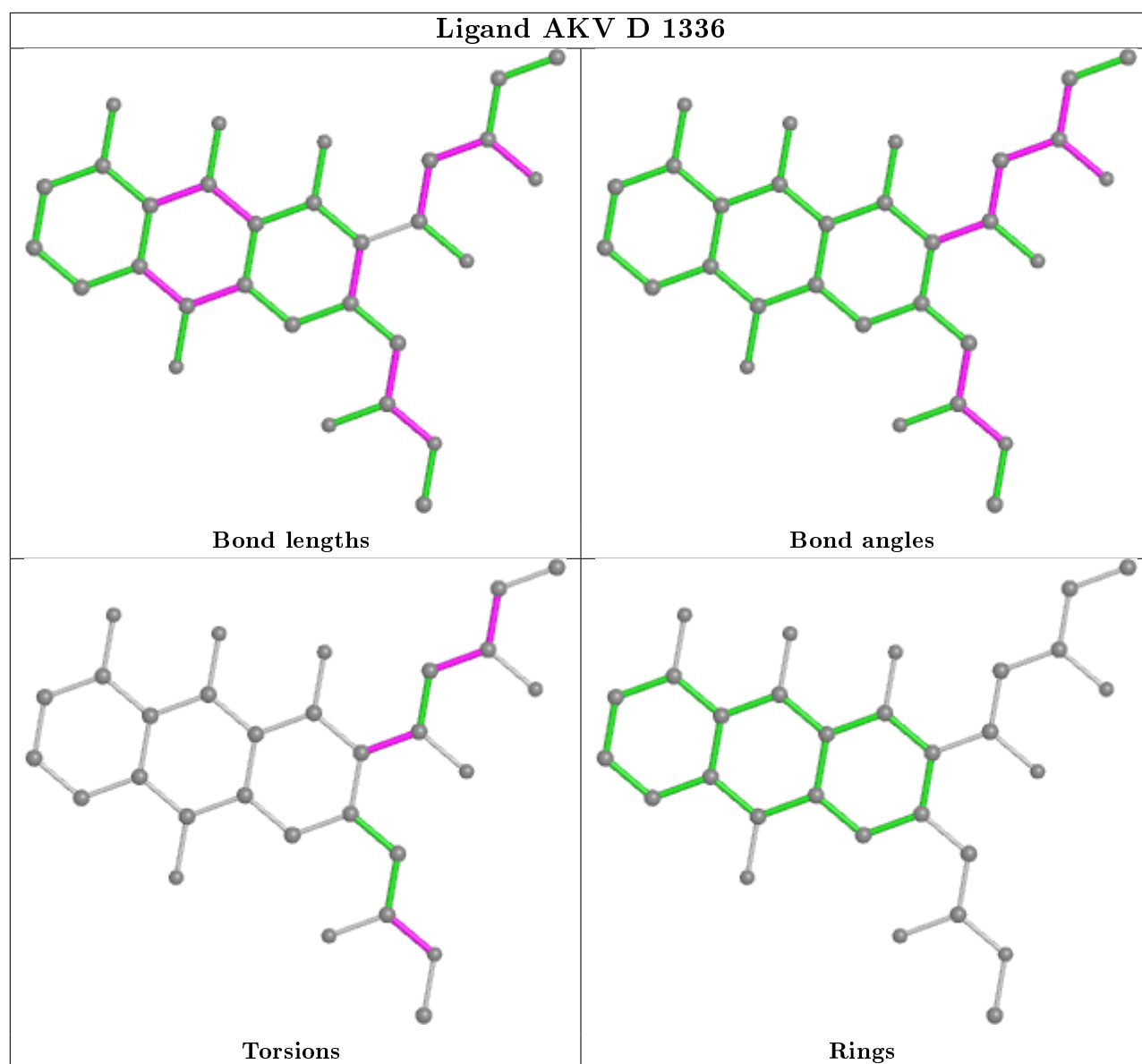


Rings



Ligand AKV A 1335





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, 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	141/153 (92%)	0.16	5 (3%) 44 47	17, 30, 42, 53	2 (1%)
1	B	141/153 (92%)	0.01	2 (1%) 75 77	19, 25, 31, 46	1 (0%)
1	C	140/153 (91%)	0.44	10 (7%) 16 17	25, 30, 34, 42	6 (4%)
1	D	143/153 (93%)	0.16	5 (3%) 44 47	18, 23, 31, 58	5 (3%)
All	All	565/612 (92%)	0.19	22 (3%) 39 42	17, 27, 39, 58	14 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ARG	6.7
1	D	1	ARG	6.0
1	D	143	ARG	6.0
1	D	142	ARG	3.9
1	B	1	ARG	3.9
1	D	141	HIS	3.7
1	B	141	HIS	3.7
1	C	106	ILE	3.1
1	C	113	ASP	2.9
1	C	82	VAL	2.9
1	A	113	ASP	2.8
1	A	43	ARG	2.5
1	C	42	LEU	2.3
1	C	43	ARG	2.3
1	C	122	TRP	2.3
1	C	3	GLU	2.3
1	C	112	VAL	2.2
1	C	29	PRO	2.1
1	A	75	ASP	2.1
1	C	21	ASP	2.1
1	D	125	TYR	2.1
1	A	141	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

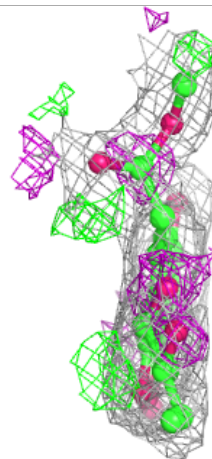
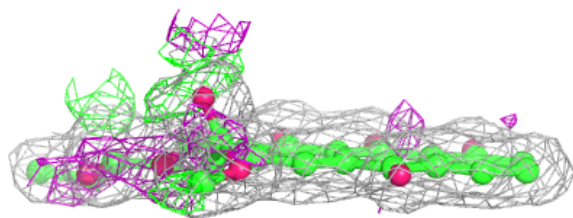
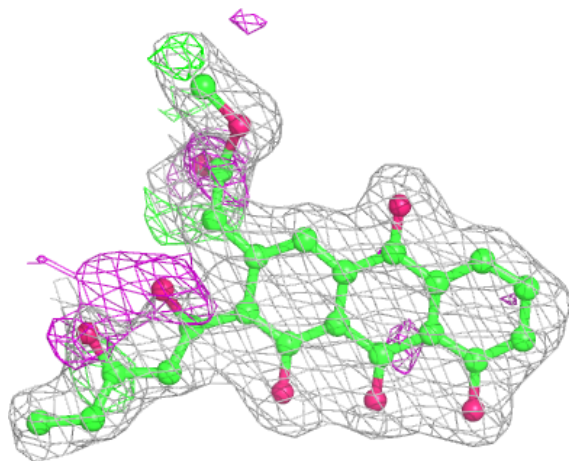
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AKV	B	1334	30/30	0.81	0.14	31,31,38,39	0
3	AKV	A	1335	30/30	0.81	0.15	28,29,39,41	0
3	AKV	C	1333	30/30	0.85	0.14	29,29,37,39	0
3	AKV	D	1336	30/30	0.86	0.15	32,33,39,39	0
2	SO4	A	1279	5/5	0.88	0.19	74,74,74,74	5
2	SO4	A	1282	5/5	0.89	0.25	58,58,59,59	5
2	SO4	C	1285	5/5	0.89	0.21	52,52,52,53	5
2	SO4	B	1283	5/5	0.90	0.18	67,67,68,68	5
2	SO4	B	1278	5/5	0.91	0.24	56,56,57,57	5
2	SO4	D	1276	5/5	0.92	0.24	52,52,52,52	5
2	SO4	D	1284	5/5	0.92	0.19	53,53,54,54	5
2	SO4	B	1286	5/5	0.94	0.14	45,45,46,46	5
2	SO4	D	1281	5/5	0.95	0.22	52,52,53,53	5
2	SO4	C	1280	5/5	0.96	0.12	46,47,47,47	5
2	SO4	C	1277	5/5	0.96	0.23	55,55,55,56	5

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.

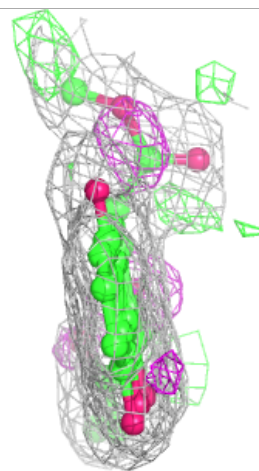
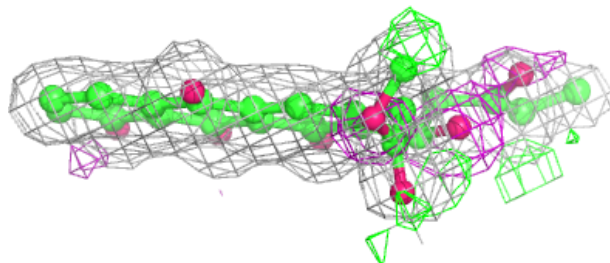
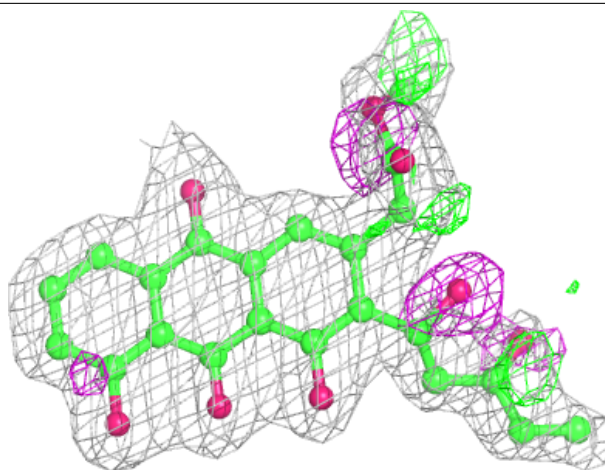
Electron density around AKV B 1334:

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



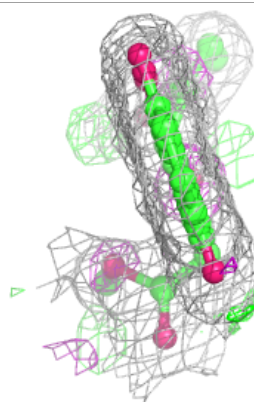
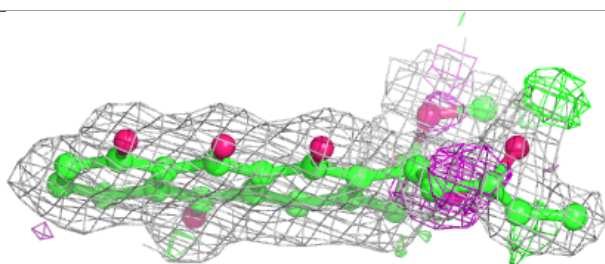
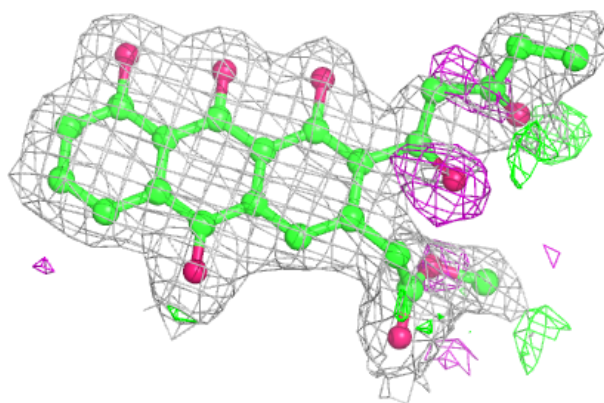
Electron density around AKV A 1335:

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

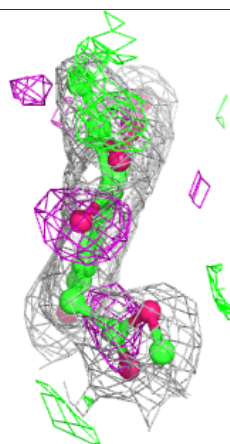
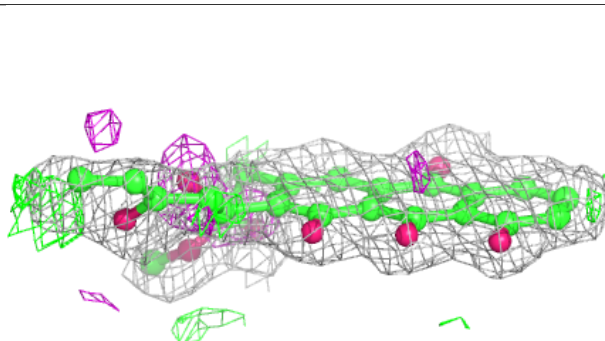
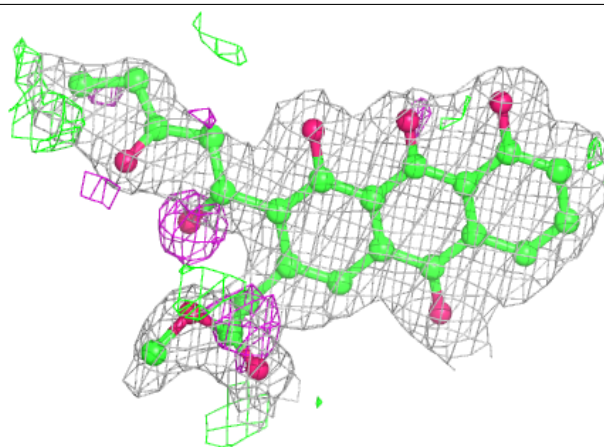


Electron density around AKV C 1333:

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

**Electron density around AKV D 1336:**

$2mF_o-DF_c$ (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.