



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:08 pm BST

PDB ID : 1EAG  
Title : Secreted aspartic proteinase (SAP2) from *Candida albicans* complexed with A70450  
Authors : Cutfield, J.F.; Cutfield, S.M.  
Deposited on : 1996-05-31  
Resolution : 2.10 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](mailto: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.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

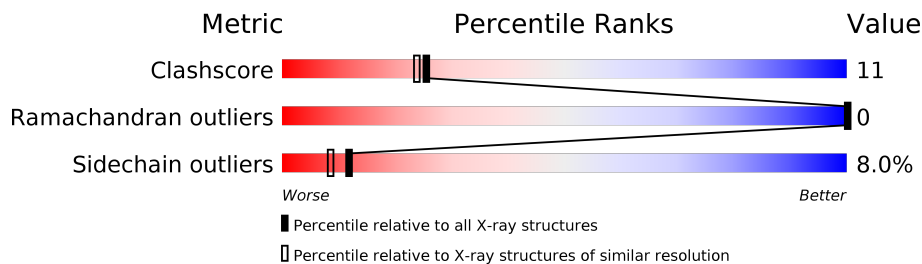
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	342	 72%      22%      5% ..

## 2 Entry composition [i](#)

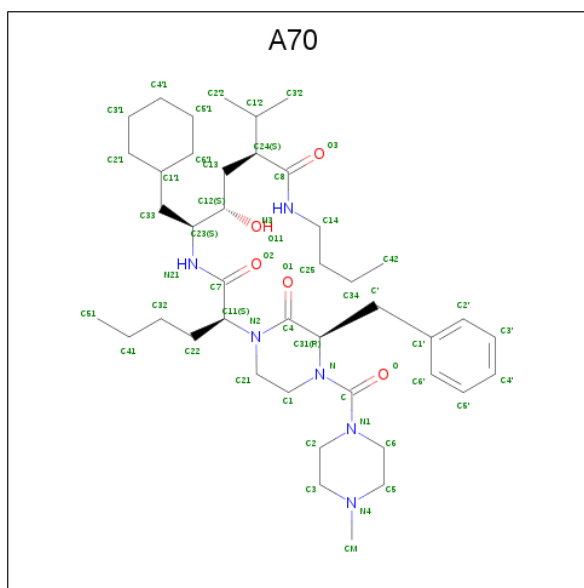
There are 3 unique types of molecules in this entry. The entry contains 2710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASPARTIC PROTEINASE (SAP2 GENE PRODUCT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2538	1581	412	541	4	0	0	0

- Molecule 2 is N-ethyl-N-[(4-methylpiperazin-1-yl)carbonyl]-D-phenylalanyl-N-[(1S,2S,4R)-4-(butylcarbonyl)-1-(cyclohexylmethyl)-2-hydroxy-5-methylhexyl]-L-norleucinamide (three-letter code: A70) (formula:  $C_{42}H_{70}N_6O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	53	42	6	5	0	0

- Molecule 3 is water.

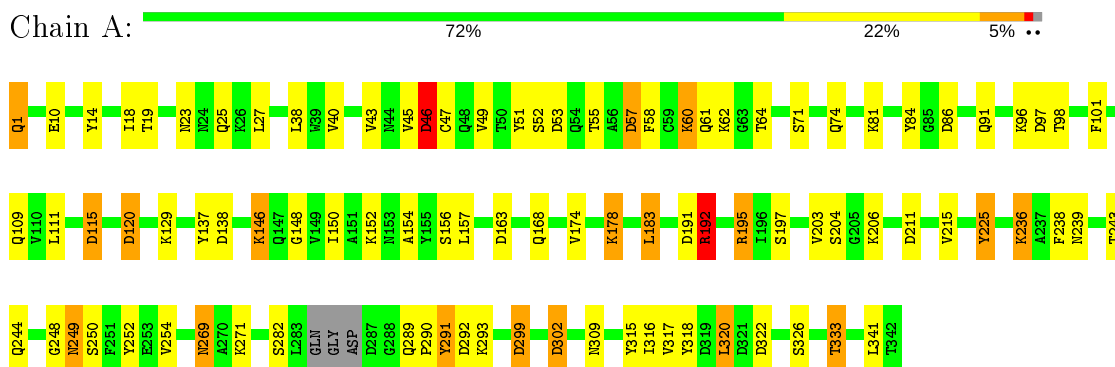
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		

### 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. 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. 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.

Note EDS was not executed.

- Molecule 1: ASPARTIC PROTEINASE (SAP2 GENE PRODUCT)



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.20Å 76.20Å 126.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.195 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 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: A70

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	0.55	0/2575	1.60	34/3503 (1.0%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	NE-CZ-NH1	-14.61	113.00	120.30
1	A	192	ARG	NE-CZ-NH2	9.33	124.96	120.30
1	A	163	ASP	CB-CG-OD2	-9.27	109.96	118.30
1	A	252	TYR	CB-CG-CD2	-8.31	116.01	121.00
1	A	333	THR	CB-CA-C	-8.29	89.20	111.60
1	A	195	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	A	192	ARG	CD-NE-CZ	-7.95	112.47	123.60
1	A	86	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	302	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	51	TYR	CA-CB-CG	-7.12	99.88	113.40
1	A	115	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	A	53	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	291	TYR	CA-CB-CG	6.62	125.97	113.40
1	A	195	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	86	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	A	57	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	A	269	ASN	CA-CB-CG	-6.15	99.88	113.40
1	A	46	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	A	19	THR	N-CA-CB	5.92	121.54	110.30
1	A	53	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	84	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	A	197	SER	CB-CA-C	-5.57	99.52	110.10
1	A	211	ASP	CB-CA-C	-5.48	99.43	110.40
1	A	163	ASP	CB-CG-OD1	5.38	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	TYR	CB-CA-C	-5.36	99.69	110.40
1	A	178	LYS	N-CA-C	5.33	125.39	111.00
1	A	183	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	254	VAL	N-CA-CB	5.29	123.14	111.50
1	A	46	ASP	CA-CB-CG	-5.29	101.76	113.40
1	A	322	ASP	CB-CA-C	-5.17	100.06	110.40
1	A	236	LYS	N-CA-CB	-5.15	101.33	110.60
1	A	14	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	55	THR	N-CA-CB	5.10	119.98	110.30
1	A	120	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2538	0	2447	51	0
2	A	53	0	70	3	0
3	A	119	0	0	2	0
All	All	2710	0	2517	54	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 11.

All (54) 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:A:1:GLN:HA	1:A:1:GLN:OE1	1.52	1.05
1:A:244:GLN:HE21	1:A:248:GLY:HA2	1.37	0.89
1:A:1:GLN:CA	1:A:1:GLN:OE1	2.18	0.84
1:A:244:GLN:NE2	1:A:248:GLY:HA2	2.01	0.74
1:A:290:PRO:HB2	1:A:293:LYS:HG2	1.71	0.71
1:A:23:ASN:HD21	1:A:25:GLN:NE2	1.93	0.67
1:A:1:GLN:HG3	3:A:412:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:OE1	1:A:290:PRO:HD2	1.96	0.64
1:A:47:CYS:HB3	1:A:58:PHE:CE2	2.32	0.64
1:A:243:THR:O	1:A:250:SER:HA	1.98	0.63
2:A:343:A70:C1	2:A:343:A70:H21	2.29	0.63
1:A:244:GLN:HE21	1:A:248:GLY:CA	2.13	0.60
1:A:156:SER:HA	1:A:316:ILE:O	2.07	0.54
1:A:249:ASN:N	1:A:249:ASN:ND2	2.54	0.54
1:A:27:LEU:HD22	1:A:40:VAL:CG1	2.40	0.52
1:A:148:GLY:HA2	3:A:425:HOH:O	2.09	0.52
1:A:138:ASP:OD2	1:A:146:LYS:HD2	2.10	0.52
1:A:249:ASN:N	1:A:249:ASN:HD22	2.07	0.52
1:A:206:LYS:HB2	1:A:206:LYS:NZ	2.25	0.51
1:A:43:VAL:HA	1:A:64:THR:HB	1.92	0.50
1:A:225:TYR:CD2	1:A:299:ASP:HB3	2.46	0.50
1:A:238:PHE:O	1:A:239:ASN:HB2	2.12	0.49
1:A:57:ASP:HB2	1:A:60:LYS:HG3	1.94	0.49
1:A:156:SER:OG	1:A:174:VAL:HG22	2.14	0.48
1:A:292:ASP:N	1:A:292:ASP:OD1	2.47	0.47
1:A:57:ASP:O	1:A:61:GLN:NE2	2.48	0.47
1:A:157:LEU:N	1:A:316:ILE:O	2.45	0.46
1:A:317:VAL:HB	1:A:326:SER:HB2	1.97	0.45
1:A:293:LYS:HD3	1:A:293:LYS:HA	1.54	0.45
1:A:195:ARG:HA	1:A:215:VAL:O	2.17	0.45
1:A:290:PRO:O	1:A:293:LYS:HB2	2.15	0.45
1:A:244:GLN:HA	1:A:250:SER:HA	1.99	0.44
1:A:45:VAL:HG22	1:A:46:ASP:N	2.32	0.44
1:A:49:VAL:O	1:A:49:VAL:HG12	2.17	0.44
1:A:97:ASP:OD1	1:A:98:THR:N	2.37	0.44
1:A:18:ILE:HG22	1:A:101:PHE:HB3	1.98	0.44
2:A:343:A70:H11	2:A:343:A70:H21	2.00	0.44
1:A:129:LYS:HE3	1:A:137:TYR:O	2.18	0.43
1:A:46:ASP:N	1:A:115:ASP:O	2.44	0.43
1:A:178:LYS:HB3	1:A:315:TYR:CD1	2.54	0.42
1:A:96:LYS:HA	1:A:109:GLN:O	2.20	0.42
1:A:192:ARG:H	1:A:192:ARG:HG2	1.66	0.42
1:A:174:VAL:HG23	1:A:341:LEU:HD21	2.02	0.41
1:A:154:ALA:HA	1:A:318:TYR:O	2.20	0.41
1:A:243:THR:HG22	1:A:244:GLN:N	2.36	0.41
1:A:320:LEU:HD23	1:A:320:LEU:N	2.35	0.41
1:A:81:LYS:NZ	1:A:91:GLN:HE21	2.18	0.41
1:A:150:ILE:HD12	1:A:152:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD23	1:A:111:LEU:HB3	2.02	0.41
1:A:10:GLU:OE2	1:A:62:LYS:HE2	2.21	0.41
2:A:343:A70:C6'	2:A:343:A70:H22	2.51	0.40
1:A:23:ASN:ND2	1:A:25:GLN:HE21	2.17	0.40
1:A:43:VAL:HA	1:A:64:THR:CB	2.51	0.40
1:A:203:VAL:O	1:A:204:SER:HB2	2.20	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	335/342 (98%)	321 (96%)	14 (4%)	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	286/288 (99%)	263 (92%)	23 (8%)	12 8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	46	ASP
1	A	52	SER
1	A	60	LYS
1	A	71	SER
1	A	74	GLN
1	A	120	ASP
1	A	146	LYS
1	A	168	GLN
1	A	183	LEU
1	A	191	ASP
1	A	192	ARG
1	A	236	LYS
1	A	249	ASN
1	A	269	ASN
1	A	271	LYS
1	A	282	SER
1	A	291	TYR
1	A	299	ASP
1	A	302	ASP
1	A	309	ASN
1	A	320	LEU
1	A	333	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	25	GLN
1	A	91	GLN
1	A	131	ASN
1	A	244	GLN
1	A	249	ASN
1	A	295	GLN
1	A	309	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](#)

1 ligand is 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	A70	A	343	-	56,56,56	0.81	2 (3%)	65,75,75	2.13	18 (27%)

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	A70	A	343	-	-	5/52/88/88	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	343	A70	O-C	2.24	1.26	1.22
2	A	343	A70	C31-C4	2.15	1.56	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	343	A70	C2-C3-N4	8.52	120.43	110.80
2	A	343	A70	C5-N4-C3	4.62	115.98	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	343	A70	O1-C4-N2	4.51	129.53	123.03
2	A	343	A70	C22-C11-N2	-4.06	108.02	112.65
2	A	343	A70	O-C-N	-3.92	118.96	122.60
2	A	343	A70	O1-C4-C31	-3.80	111.81	120.30
2	A	343	A70	C24-C8-N3	-3.49	110.59	116.24
2	A	343	A70	C11-N2-C4	3.09	121.73	118.64
2	A	343	A70	O3-C8-C24	-3.03	118.07	121.73
2	A	343	A70	O2-C7-N21	3.01	128.51	122.93
2	A	343	A70	C6-N1-C2	2.98	118.36	112.62
2	A	343	A70	C12-C23-N21	2.95	115.61	109.92
2	A	343	A70	C14-N3-C8	-2.45	118.22	122.59
2	A	343	A70	C3-C2-N1	2.44	115.67	110.44
2	A	343	A70	CM-N4-C3	2.38	114.22	110.66
2	A	343	A70	C4'-C3'-C2'	-2.19	116.85	120.19
2	A	343	A70	C1-N-C31	2.05	120.12	115.80
2	A	343	A70	C1'-C'-C31	-2.00	108.47	113.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	343	A70	O-C-N1-C6
2	A	343	A70	O3-C8-N3-C14
2	A	343	A70	C22-C32-C41-C51
2	A	343	A70	C13-C24-C8-O3
2	A	343	A70	C12-C13-C24-C8

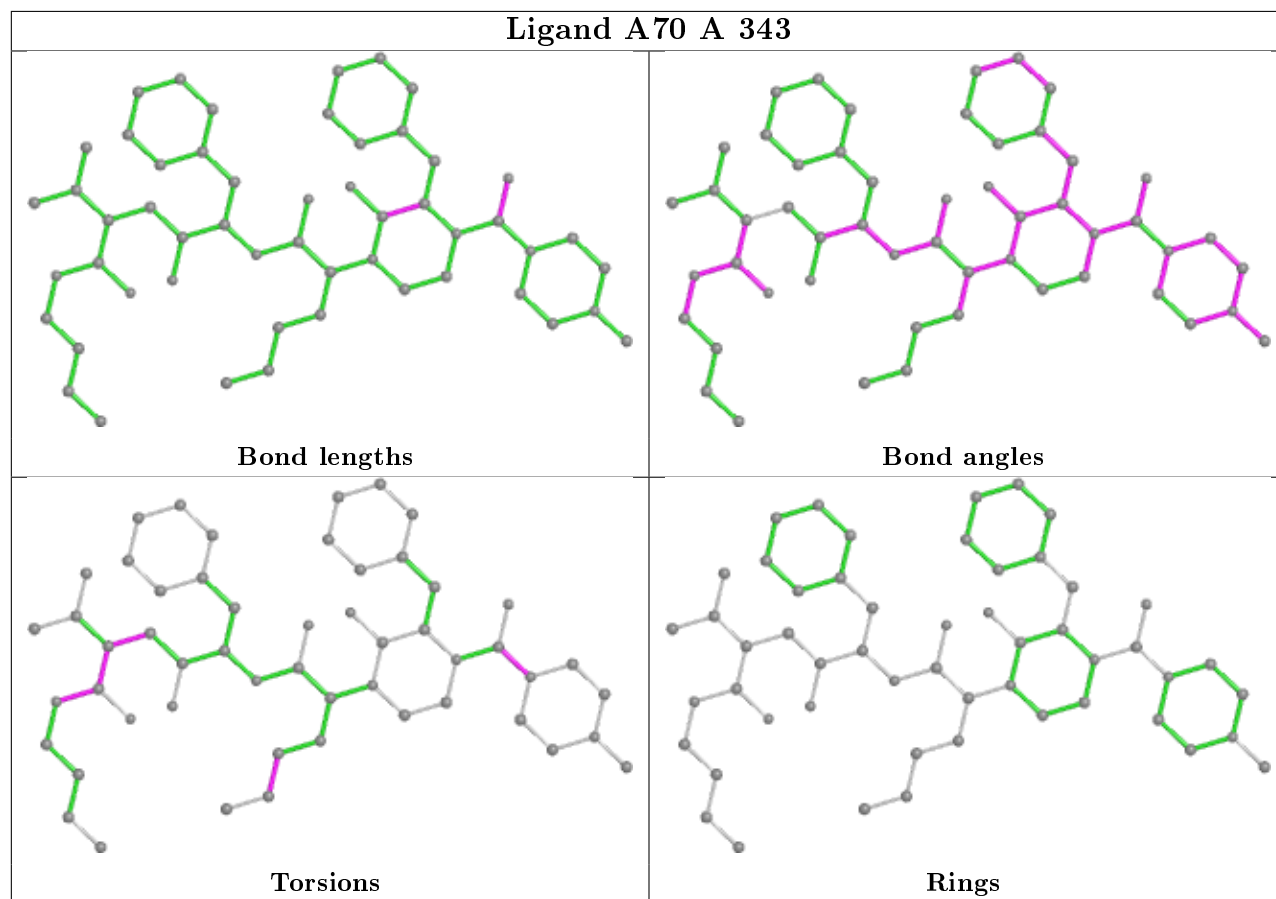
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	343	A70	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.