wwPDB X-ray Structure Validation Summary Report (i)

May 27, 2020 – 04:50 pm BST

PDB ID	:	1AHU
Title	:	STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH P-CRESOL
Authors	:	Mattevi, A.
Deposited on	:	1997-04-10
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/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:

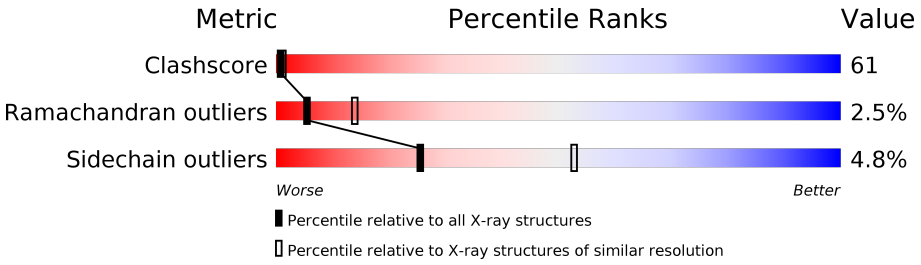
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	26% 56% 16%
1	B	560	25% 57% 16%

2 Entry composition

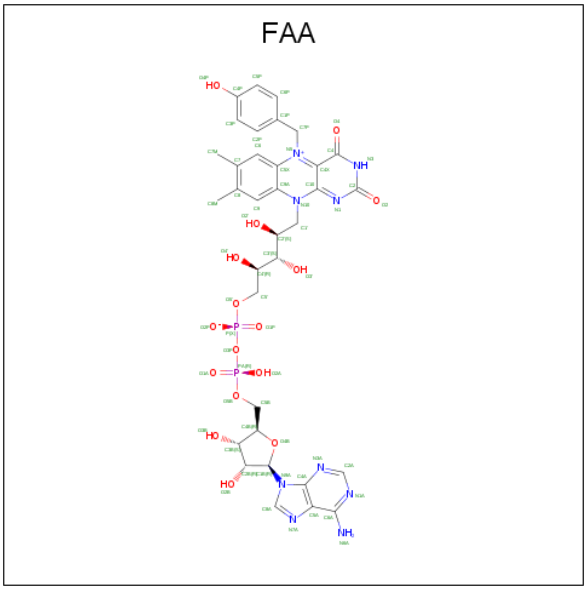
There are 3 unique types of molecules in this entry. The entry contains 9011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	37	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	37	0	0
			4391	2817	751	799	24			

- Molecule 2 is N5-(4-HYDROXYBENZYL)FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAA) (formula: $C_{34}H_{39}N_9O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			61	34	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			61	34	9	16	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	52	Total O 52 52	1	0

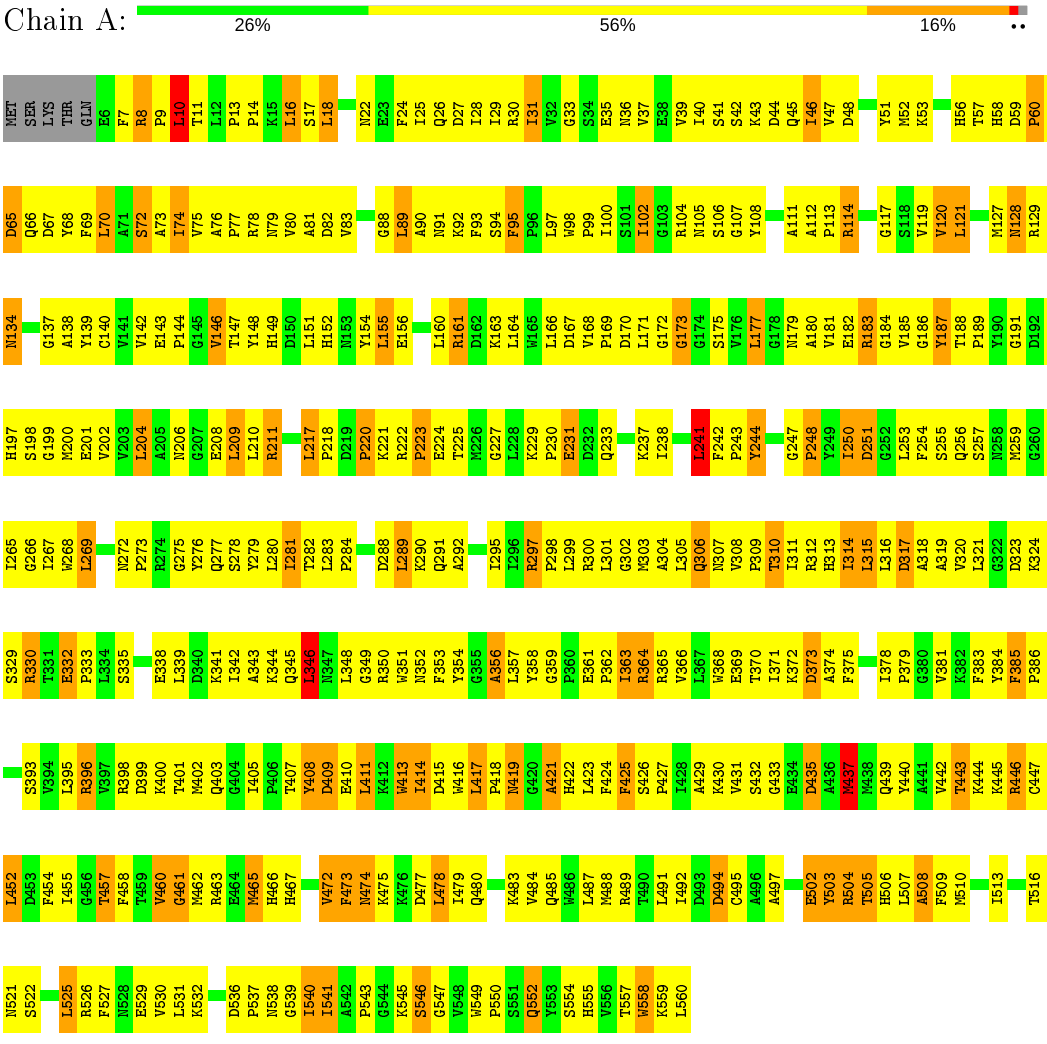
3 Residue-property plots (i)

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.

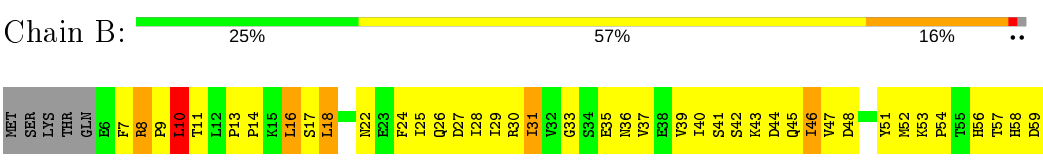
- Molecule 1: VANILLYL-ALCOHOL OXIDASE

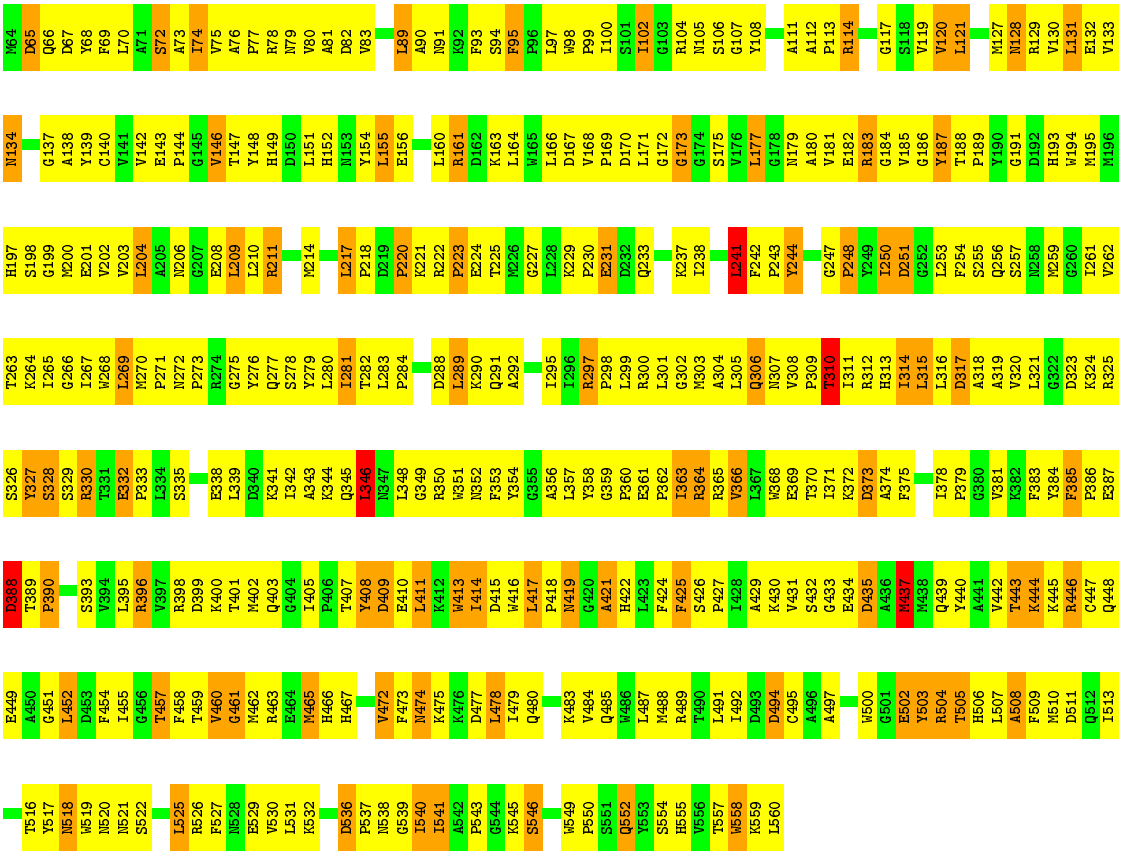
Chain A:



- Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:




M64 D65 Q66 D67 Y68 F69 L70 A71 S72 A73 I74 V75 A76 P77 R78 N79 V80 A81 D82 V83 L89 A90 N91 K92 F93 S94 F95 P96 L97 W98 P99 I100 S101 I102 G103 R104 N105 S106 G107 Y108 A111 A112 P113 R114 G117 S118 V119 V120 L121 M127 N128 R129 V130 L131 E132 V133
N134 G137 A138 Y139 C140 V141 V142 E143 P144 G145 V146 T147 Y148 H149 D150 L151 H152 N153 Y154 L155 E156 L160 R161 D162 K163 L164 W165 L166 D167 V168 P169 D170 L171 G172 G173 G174 S175 V176 L177 G178 N179 A180 V181 E182 R183 G184 V185 G186 Y187 T188 P189 Y190 G191 D192 H193 W194 M195 M196
H197 S198 G199 M200 E201 V202 V203 L204 A205 N206 G207 E208 L209 L210 R211 M214 L217 P218 D219 P220 K221 R222 P223 E224 T225 M226 G227 I228 K229 P230 E231 D232 Q233 K237 I238 L241 F242 P243 Y244 G247 P248 Y249 I250 D251 G252 L253 F254 S255 Q256 S257 N258 M259 G260 I261 V262
T263 K264 I265 G266 I267 W268 L269 M270 P271 N272 P273 R274 G275 Y276 Q277 S278 Y279 L280 I281 T282 L283 P284 D288 L289 K290 Q291 A292 I295 I296 R297 P298 L299 R300 L301 G302 M303 A304 L305 Q306 N307 V308 P309 T310 I311 R312 H313 I314 L315 L316 D317 A318 A319 V320 L321 G322 D323 K324 R325
S326 V327 S328 S329 R330 T331 E332 P333 L334 S335 E338 L339 D340 K341 I342 A343 K344 Q345 L346 N347 L348 G349 R350 W351 N352 F353 Y354 G355 A356 L357 Y358 G359 P360 E361 P362 I363 R364 R365 V366 L367 W368 E369 T370 I371 K372 D373 A374 F375 I378 P379 G380 V381 K382 F383 Y384 F385 P386 E387
D388 T389 P390 S393 V394 L395 R396 V397 R398 D399 K400 T401 M402 Q403 G404 I405 P406 T407 Y408 D409 E410 L411 K412 W413 I414 D415 W416 L417 P418 N419 G420 A421 H422 L423 F424 F425 S426 P427 I428 A429 K430 V431 S432 G433 E434 D435 A436 N437 M438 Q439 Y440 A441 V442 T443 K444 K445 R446 C447 Q448
E449 A450 G451 L452 D453 F454 I455 G456 T457 F458 T459 V460 G461 M462 R463 E464 M465 H466 H467 V472 F473 N474 K475 K476 D477 L478 I479 Q480 K483 V484 Q485 W486 L487 M488 R489 T490 L491 I492 D493 D494 C495 A496 A497 W500 G501 E502 Y503 R504 T505 H506 L507 A508 F509 M510 D511 Q512 I513
T516 Y517 N518 W519 N520 N521 S522 L525 R526 F527 N528 E529 V530 L531 K532 D536 P537 N538 G539 I540 I541 A542 P543 G544 K545 S546 W549 P550 S551 Q552 Y553 S554 H555 V556 T557 W558 K559 L560

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	128.82Å 128.82Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.4 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.97	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.221 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9011	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAA

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	0.73	0/4511	1.74	110/6131 (1.8%)
1	B	0.73	0/4511	1.74	108/6131 (1.8%)
All	All	0.73	0/9022	1.74	218/12262 (1.8%)

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	A	2	0
1	B	2	0
All	All	4	0

There are no bond length outliers.

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	B	330	ARG	NE-CZ-NH1	-11.24	114.68	120.30
1	A	536	ASP	C-N-CD	-9.85	98.92	120.60
1	B	536	ASP	C-N-CD	-9.85	98.93	120.60
1	B	417	LEU	CA-CB-CG	-9.34	93.83	115.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	187	TYR	CA
1	A	332	GLU	CA
1	B	187	TYR	CA

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Mol	Chain	Res	Type	Atom
1	B	332	GLU	CA

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	4391	0	4330	531	0
1	B	4391	0	4330	548	0
2	A	61	0	35	13	0
2	B	61	0	35	13	0
3	A	55	0	0	9	0
3	B	52	0	0	9	0
All	All	9011	0	8730	1058	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 61.

The worst 5 of 1058 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)
2:A:600:FAA:H8A	2:A:600:FAA:H51A	1.21	1.13
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.32	1.11
2:B:600:FAA:H51A	2:B:600:FAA:H8A	1.21	1.10
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.32	1.07
1:A:507:LEU:HA	1:A:510:MET:HE3	1.37	1.06

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	553/560 (99%)	470 (85%)	69 (12%)	14 (2%)	5 14
1	B	553/560 (99%)	470 (85%)	69 (12%)	14 (2%)	5 14
All	All	1106/1120 (99%)	940 (85%)	138 (12%)	28 (2%)	5 14

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	B	44	ASP
1	A	30	ARG
1	A	46	ILE
1	A	328	SER

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	475/482 (98%)	452 (95%)	23 (5%)	25 53
1	B	475/482 (98%)	452 (95%)	23 (5%)	25 53
All	All	950/964 (98%)	904 (95%)	46 (5%)	25 53

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	466	HIS

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Mol	Chain	Res	Type
1	B	65	ASP
1	B	443	THR
1	A	478	LEU
1	B	10	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
1	B	66	GLN
1	B	520	ASN
1	A	552	GLN
1	B	58	HIS

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)

2 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	FAA	B	600	1	59,67,67	1.01	5 (8%)	68,102,102	2.17	8 (11%)
2	FAA	A	600	1	59,67,67	1.02	5 (8%)	68,102,102	2.17	8 (11%)

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	FAA	B	600	1	-	12/34/54/54	0/7/7/7
2	FAA	A	600	1	-	12/34/54/54	0/7/7/7

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAA	C4-N3	3.66	1.39	1.33
2	A	600	FAA	C4-N3	3.64	1.39	1.33
2	A	600	FAA	C2-N1	-2.44	1.33	1.38
2	B	600	FAA	C2-N1	-2.41	1.33	1.38
2	A	600	FAA	C4-C4X	2.09	1.45	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAA	C7P-N5-C5X	-12.44	102.71	120.13
2	B	600	FAA	C7P-N5-C5X	-12.43	102.72	120.13
2	A	600	FAA	C4-N3-C2	7.78	121.72	115.14
2	B	600	FAA	C4-N3-C2	7.74	121.67	115.14
2	B	600	FAA	C4X-C4-N3	-5.50	115.91	123.43

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	FAA	C1P-C7P-N5-C4X
2	B	600	FAA	N10-C1'-C2'-O2'
2	A	600	FAA	C1P-C7P-N5-C4X
2	A	600	FAA	N10-C1'-C2'-O2'
2	B	600	FAA	O3'-C3'-C4'-O4'

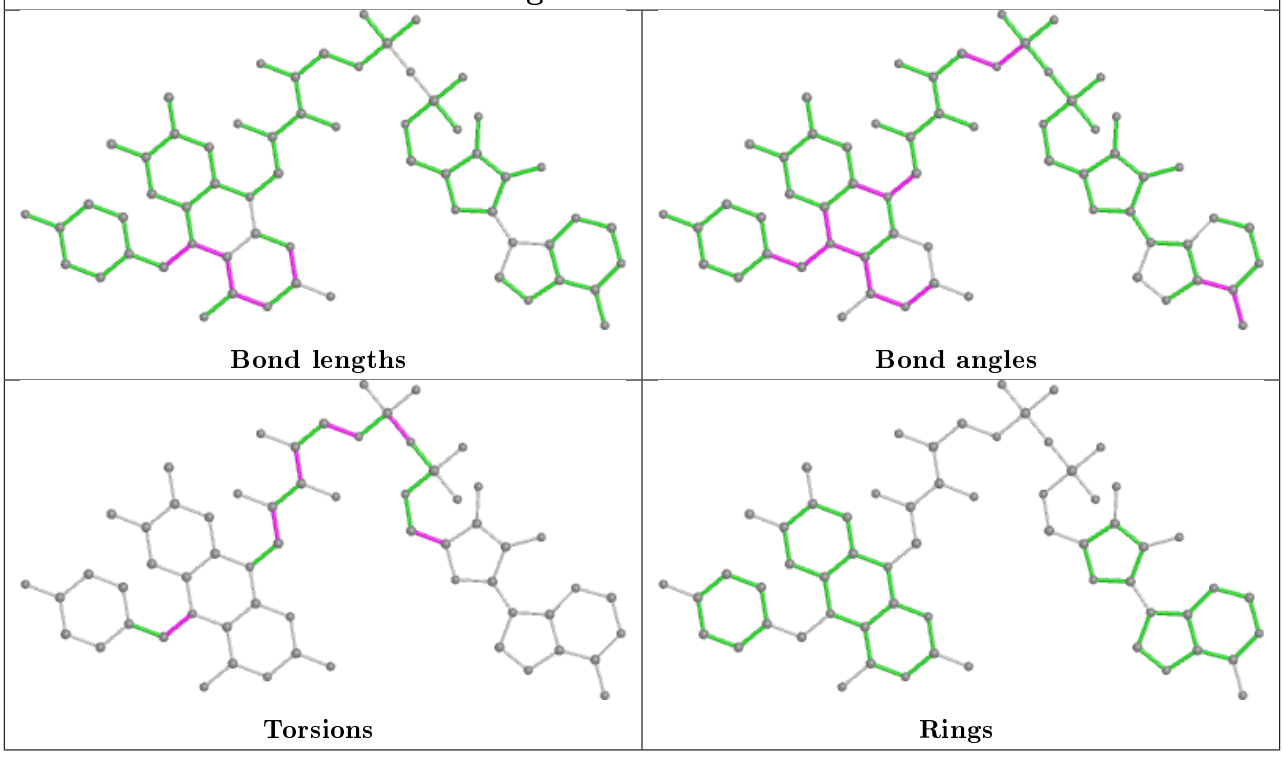
There are no ring outliers.

2 monomers are involved in 26 short contacts:

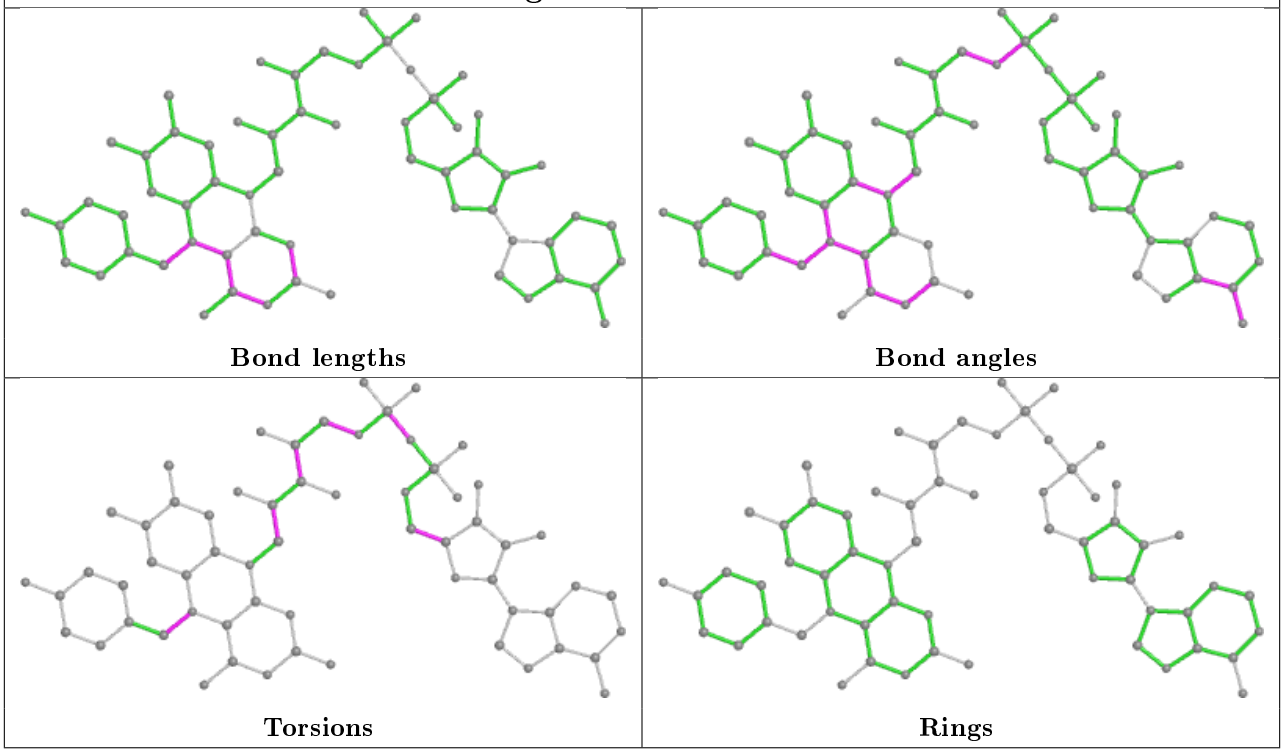
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAA	13	0
2	A	600	FAA	13	0

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 then 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 FAA B 600



Ligand FAA A 600



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.