

wwPDB X-ray Structure Validation Summary Report (i)

Dec 2, 2023 - 06:24 pm GMT

PDB ID	:	1H86
Title	:	COVALENT ADDUCT BETWEEN POLYAMINE OXIDASE AND N1ethyl
		N11((cycloheptyl)methyl)4,8diazaundecane at pH 7.0
Authors	:	Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on	:	2001-01-24
Resolution	:	2.00 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

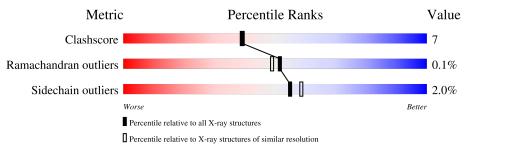
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	А	472	80%	16% ••
1	В	472	82%	14% ••
1	С	472	85%	11% ••
2	D	2	100%	
3	Е	5	20% 80%	

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
3	MAN	Е	3	Х	-	-	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12222 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	459	Total	С	Ν	0	\mathbf{S}	63	0	0
1	А	409	3684	2353	621	696	14	05	0	
1	В	462	Total	С	Ν	0	S	64	0	0
1	D	402	3715	2374	627	700	14	04	0	
1	C	462	Total	С	Ν	0	S	51	0	0
		402	3715	2374	627	700	14	51		0

• Molecule 1 is a protein called POLYAMINE OXIDASE.

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	ŀ	Aton	ns		ZeroOcc	AltConf	Trace
2	D	2	Total 28	C 16	N 2	O 10	0	0	0

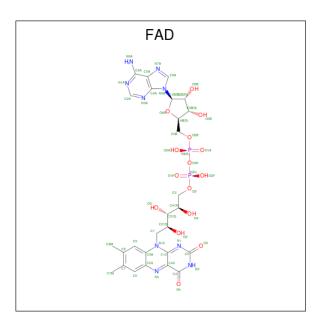
• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-3)]2-ac etamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
3	Е	5	Total 60	С 34	N 2	O 24	0	0	0

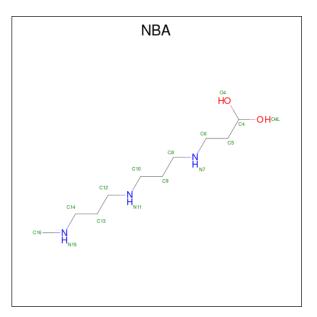
• Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\rm C_{27}H_{33}N_9O_{15}P_2).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
4	Λ	1	Total	С	Ν	Ο	Р	0	0
4	Л	1	53	27	9	15	2	0	0
4	P	1	Total	С	Ν	Ο	Р	0	0
4	D	1	53	27	9	15	2	0	0
4	С	1	Total	С	Ν	Ο	Р	0	0
4	U	1	53	27	9	15	2	0	0

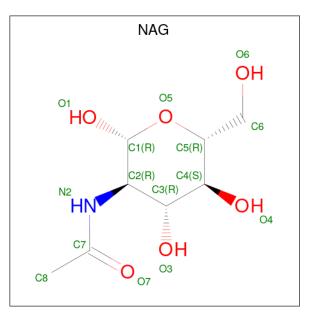
• Molecule 5 is 3-[(3-{[3-(METHYLAMINO)PROPYL]AMINO}PROPYL)AMINO]PROPA NE-1,1-DIOL (three-letter code: NBA) (formula: C₁₀H₂₅N₃O₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C N O 14 10 3 1	0	0
5	В	1	Total C N O 14 10 3 1	0	0
5	С	1	Total C N O 14 10 3 1	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total C N O 14 8 1 5	0	0
6	А	1	Total C N O 14 8 1 5	0	0

• Molecule 7 is water.

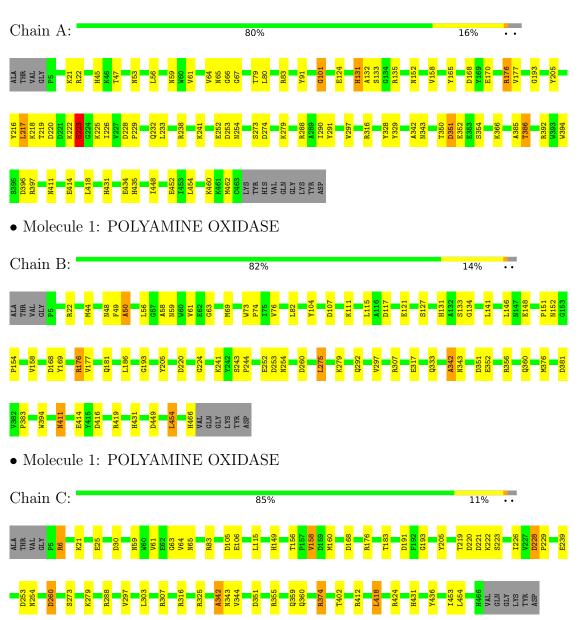
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	239	Total O 239 239	0	0
7	В	269	Total O 269 269	0	0
7	С	283	Total O 283 283	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: POLYAMINE OXIDASE

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose



Chain D:

100%

NAG1 NAG2

 \bullet Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose ose

Chain E:	20%	80%





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	184.29Å 184.29Å 279.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 - 2.00	Depositor
% Data completeness	94.9 (20.00-2.00)	Depositor
(in resolution range)	54.5 (20.00 2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.184 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12222	wwPDB-VP
Average B, all atoms $(Å^2)$	14.0	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: FAD, MAN, FCA, NBA, NAG

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	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.60	0/3775	1.28	18/5116~(0.4%)
1	В	0.62	0/3808	1.26	14/5160~(0.3%)
1	С	0.62	0/3808	1.28	23/5160~(0.4%)
All	All	0.61	0/11391	1.27	55/15436~(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	В	1	0

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	342	ALA	N-CA-C	10.46	139.24	111.00
1	С	307	ARG	NE-CZ-NH1	-9.05	115.77	120.30
1	С	412	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	С	316	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	С	176	ARG	NE-CZ-NH2	-8.22	116.19	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	В	342	ALA	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	А	3684	0	3585	61	0
1	В	3715	0	3614	59	1
1	С	3715	0	3614	28	0
2	D	28	0	26	3	1
3	Е	60	0	52	6	0
4	А	53	0	31	0	0
4	В	53	0	31	1	0
4	С	53	0	31	1	0
5	А	14	0	23	3	0
5	В	14	0	23	2	0
5	С	14	0	23	3	0
6	А	28	0	26	4	0
7	А	239	0	0	6	0
7	В	269	0	0	5	0
7	С	283	0	0	7	0
All	All	12222	0	11079	161	1

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 7.

The worst 5 of 161 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)
6:A:601:NAG:O4	6:A:602:NAG:C1	1.82	1.25
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.25	1.14
1:B:69:MET:CE	1:B:73:TRP:HB3	1.97	0.94
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.49	0.94
1:A:220:ASP:HB3	1:A:223:SER:HB3	1.53	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:ND2	2:D:2:NAG:C8[9_765]	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	Perce	ntiles
1	А	457/472~(97%)	438 (96%)	18 (4%)	1 (0%)	47	44
1	В	460/472~(98%)	446 (97%)	14 (3%)	0	100	100
1	С	460/472~(98%)	441 (96%)	19 (4%)	0	100	100
All	All	1377/1416~(97%)	1325 (96%)	51 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	101	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	394/404~(98%)	385~(98%)	9(2%)	50 53
1	В	397/404~(98%)	388~(98%)	9(2%)	50 53
1	С	397/404 (98%)	391 (98%)	6 (2%)	65 69
All	All	1188/1212 (98%)	1164 (98%)	24 (2%)	55 58

5 of 24 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	275	LEU
1	В	454	LEU

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Mol	Chain	Res	Type
1	В	411	ASN
1	С	59	ASN
1	А	217	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such side chains are listed below:

Mol	Chain	Res	Type
1	С	48	ASN
1	С	431	HIS
1	В	292	GLN
1	В	359	GLN
1	В	360	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

7 monosaccharides 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).

Mal	Mol Type Chain		Res	Link	Bo	Bond lengths			Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	NAG	D	1	2,1	14,14,15	1.09	1 (7%)	17,19,21	1.69	3 (17%)	
2	NAG	D	2	2	14,14,15	1.32	2 (14%)	17,19,21	2.14	<mark>6 (35%)</mark>	
3	NAG	Е	1	1,3	14,14,15	1.29	2 (14%)	17,19,21	1.97	6 (35%)	
3	NAG	Е	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.86	5 (29%)	



Mal	Mol Type Chain	Chain	in Res	Link	Link Bond lengths			Bond angles		
10101	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	MAN	Е	3	3	11,11,12	0.74	0	$15,\!15,\!17$	3.29	5 (33%)
3	MAN	Е	4	3	11,11,12	0.62	0	$15,\!15,\!17$	1.92	3 (20%)
3	FCA	Е	5	3	10,10,11	1.37	1 (10%)	14,14,16	1.53	3 (21%)

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	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	Е	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	2/6/23/26	0/1/1/1
3	MAN	Е	3	3	2/2/4/5	0/2/19/22	0/1/1/1
3	MAN	Е	4	3	-	2/2/19/22	0/1/1/1
3	FCA	Е	5	3	-	-	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	D	2	NAG	O5-C1	-3.49	1.38	1.43
3	Ε	5	FCA	C2-C3	-3.46	1.47	1.52
3	Ε	2	NAG	O5-C1	-2.88	1.39	1.43
3	Е	1	NAG	C1-C2	-2.83	1.48	1.52
2	D	2	NAG	C1-C2	-2.79	1.48	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Ε	3	MAN	O2-C2-C3	10.24	130.65	110.14
3	Е	4	MAN	C1-C2-C3	-5.28	103.18	109.67
2	D	2	NAG	O5-C5-C6	-5.25	98.98	107.20
3	Е	2	NAG	O5-C5-C6	-5.00	99.36	107.20
3	Е	3	MAN	C1-O5-C5	3.97	117.57	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	Ε	3	MAN	C1

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Mol	Chain	Res	Type	Atom
3	Ε	3	MAN	C2

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	Ε	2	NAG	C4-C5-C6-O6
3	Е	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

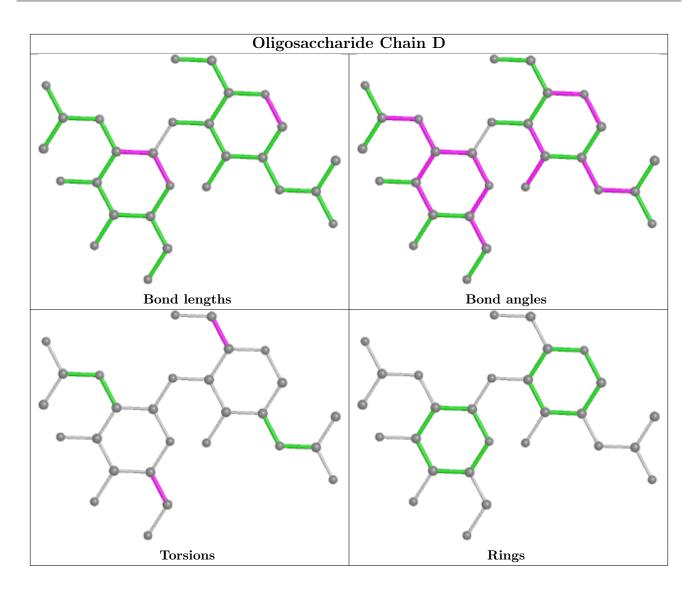
There are no ring outliers.

5 monomers are involved in 10 short contacts:

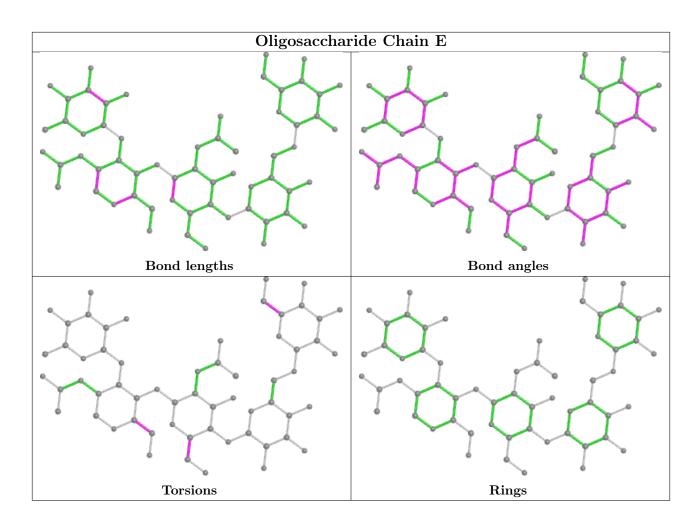
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	0
3	Е	5	FCA	3	0
2	D	2	NAG	3	1
3	Е	1	NAG	5	0
3	Ε	2	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry (i)

8 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		Bo	ond leng	ths	Bond angles			
10101	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	FAD	В	590	5	$53,\!58,\!58$	0.95	1 (1%)	68,89,89	1.63	15 (22%)
6	NAG	А	602	-	14,14,15	0.89	1 (7%)	17,19,21	1.21	2 (11%)
5	NBA	В	591	4	13,13,14	0.58	0	12,12,14	1.81	4 (33%)
6	NAG	А	601	1	14,14,15	1.01	1 (7%)	17,19,21	2.38	<mark>6 (35%)</mark>
5	NBA	А	591	4	13,13,14	0.55	0	12,12,14	1.51	4 (33%)



Mol	Mol Type Chain Res Li		Link	Bo	Bond lengths			Bond angles		
INIOI	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	NBA	С	591	4	13,13,14	0.56	0	12,12,14	2.11	3 (25%)
4	FAD	А	590	5	53,58,58	0.93	3 (5%)	68,89,89	1.52	11 (16%)
4	FAD	С	590	5	53,58,58	1.01	2 (3%)	68,89,89	1.49	13 (19%)

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
4	FAD	В	590	5	-	3/30/50/50	0/6/6/6
6	NAG	А	602	-	-	2/6/23/26	0/1/1/1
5	NBA	В	591	4	-	5/11/11/12	-
6	NAG	А	601	1	-	2/6/23/26	0/1/1/1
5	NBA	А	591	4	-	4/11/11/12	-
5	NBA	С	591	4	-	3/11/11/12	-
4	FAD	А	590	5	-	1/30/50/50	0/6/6/6
4	FAD	С	590	5	_	5/30/50/50	0/6/6/6

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
4	В	590	FAD	C4X-N5	3.53	1.37	1.30
4	С	590	FAD	C4X-N5	3.38	1.37	1.30
4	А	590	FAD	C4X-N5	3.22	1.37	1.30
6	А	601	NAG	O5-C1	-2.42	1.39	1.43
4	А	590	FAD	C5'-C4'	2.32	1.55	1.51

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
5	С	591	NBA	C9-C8-N7	-5.28	97.89	112.14
6	А	601	NAG	O5-C5-C6	-4.84	99.62	107.20
4	В	590	FAD	O4B-C1B-C2B	-4.58	100.24	106.93
6	А	601	NAG	C1-O5-C5	4.56	118.37	112.19
6	А	601	NAG	C2-N2-C7	-4.21	116.90	122.90

There are no chirality outliers.

5 of 25 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
6	А	602	NAG	C4-C5-C6-O6
6	А	601	NAG	C4-C5-C6-O6
6	А	602	NAG	O5-C5-C6-O6
5	А	591	NBA	N11-C10-C9-C8
5	С	591	NBA	N11-C12-C13-C14

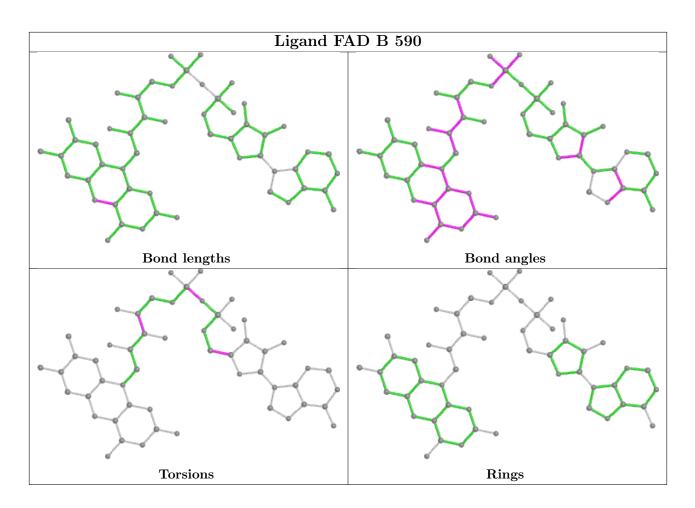
There are no ring outliers.

7 monomers are involved in 14 short contacts:

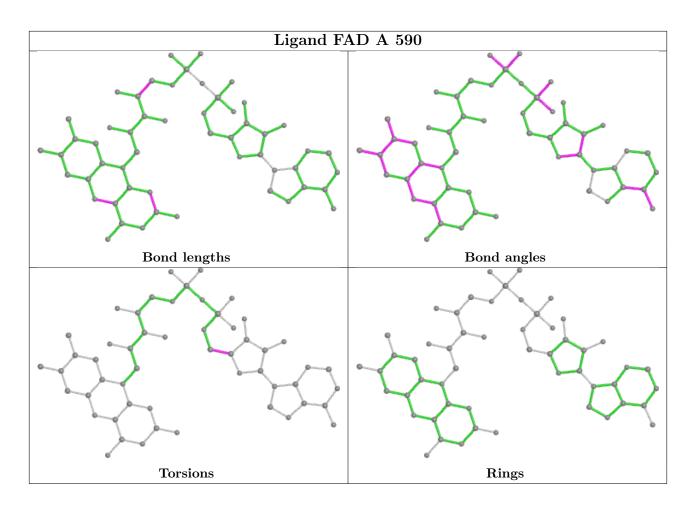
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	590	FAD	1	0
6	А	602	NAG	4	0
5	В	591	NBA	2	0
6	А	601	NAG	4	0
5	А	591	NBA	3	0
5	С	591	NBA	3	0
4	С	590	FAD	1	0

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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



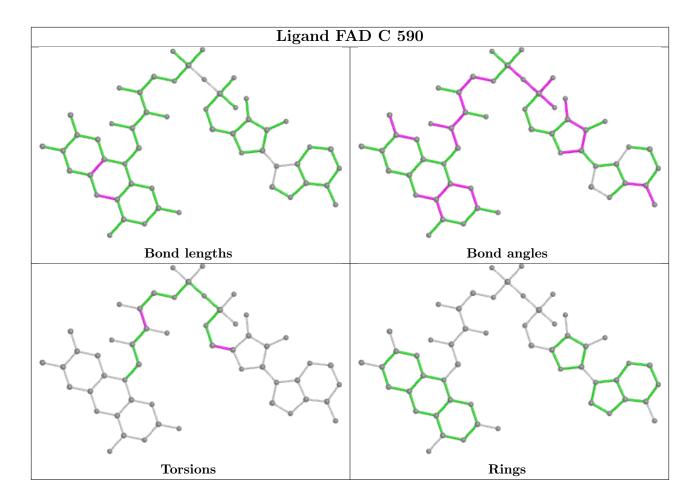












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

