



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:31 am GMT

PDB ID : 1H86
Title : COVALENT ADDUCT BETWEEN POLYAMINE OXIDASE AND N1ethyl
N11((cycloheptyl)methyl)4,8diazoundecane 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

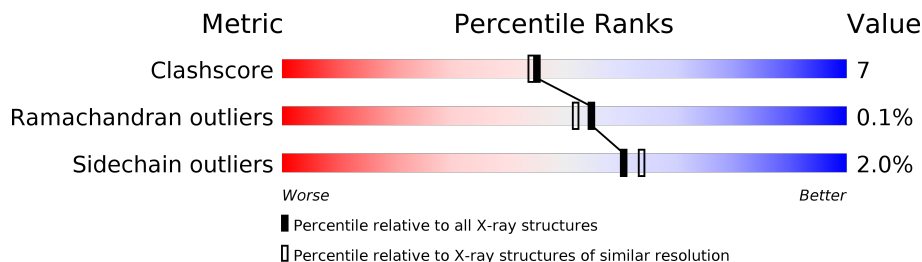
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	
1	B	472	
1	C	472	

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
6	MAN	C	604	X	-	-	-

2 Entry composition [i](#)

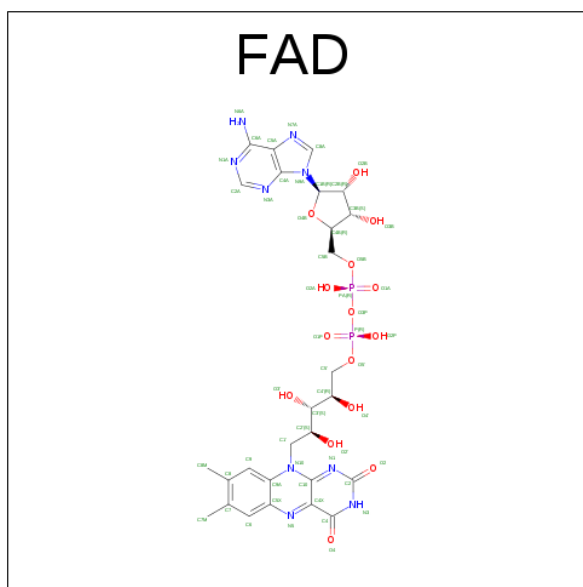
There are 7 unique types of molecules in this entry. The entry contains 12222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

- Molecule 1 is a protein called POLYAMINE OXIDASE.

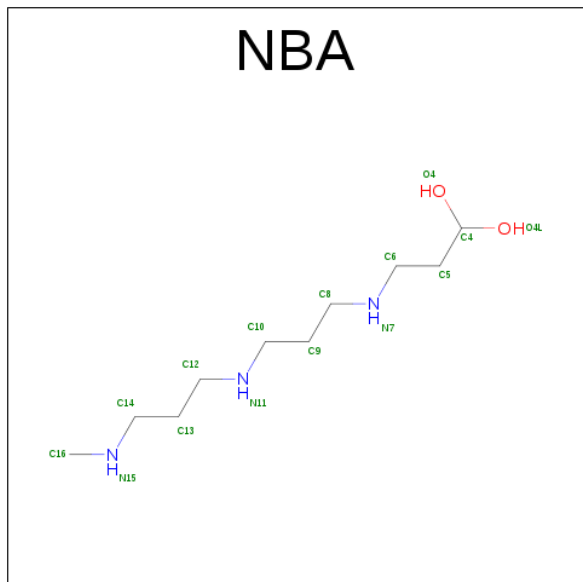
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	63	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	64	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	51	0	0
			3715	2374	627	700	14			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



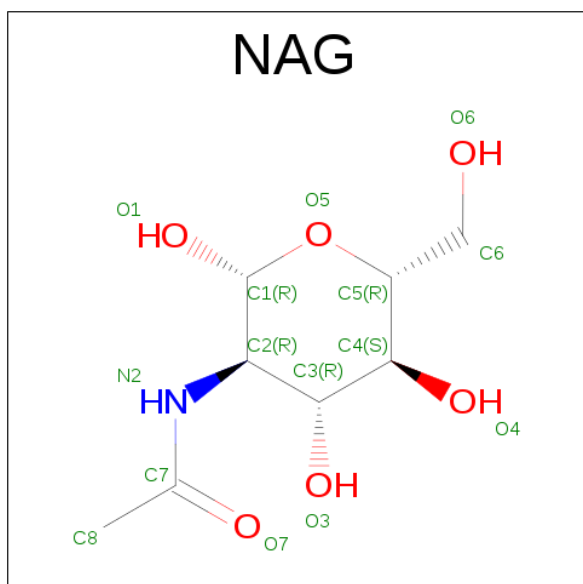
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-[(3-{[3-(METHYLAMINO)PROPYL]AMINO}PROPYL)AMINO]PROPANE-1,1-DIOL (three-letter code: NBA) (formula: $C_{10}H_{25}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	10	3	1		
3	B	1	Total	C	N	O	0	0
			14	10	3	1		
3	C	1	Total	C	N	O	0	0
			14	10	3	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	3	Total	C	N	O	0	0
			36	20	1	15		

- Molecule 7 is water.

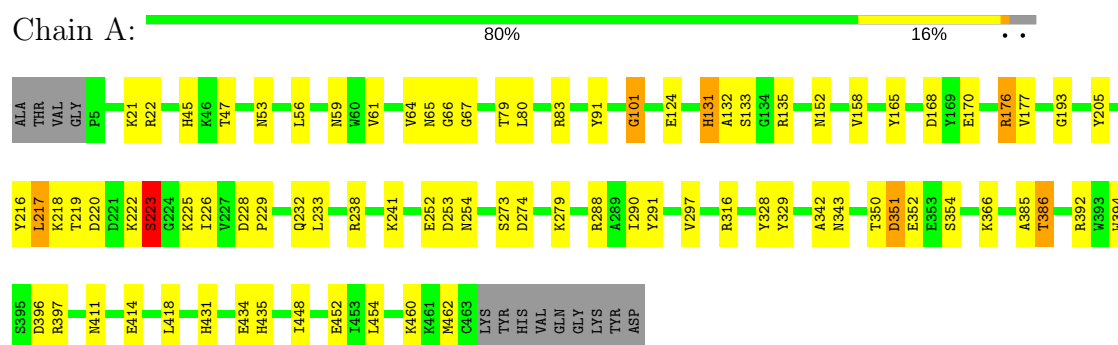
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	239	Total	O	0	0
			239	239		
7	B	269	Total	O	0	0
			269	269		
7	C	283	Total	O	0	0
			283	283		

3 Residue-property plots

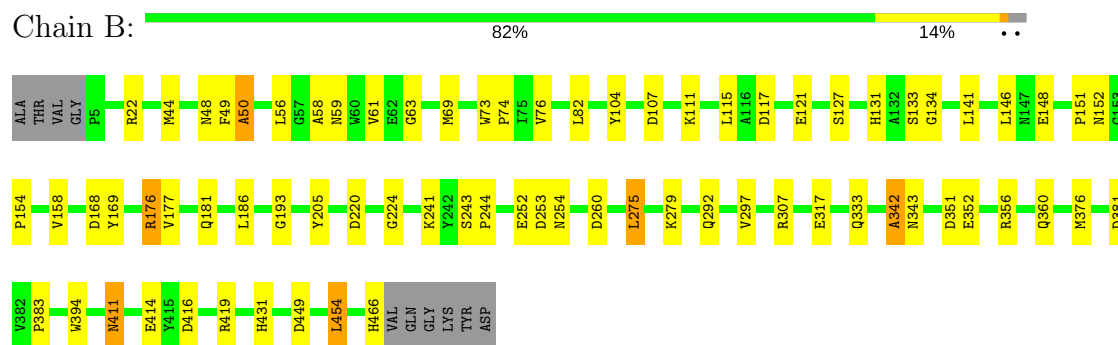
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

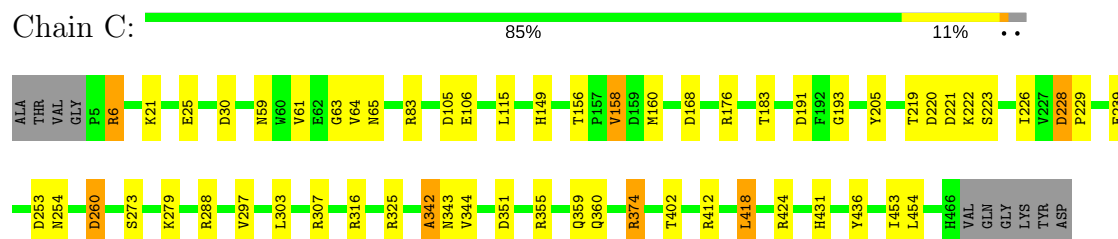
• Molecule 1: POLYAMINE OXIDASE



• Molecule 1: POLYAMINE OXIDASE



• Molecule 1: POLYAMINE OXIDASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.29Å 184.29Å 279.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.9 (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: FCA, NBA, NAG, FAD, MAN

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	0.60	0/3775	1.28	18/5116 (0.4%)
1	B	0.62	0/3808	1.26	14/5160 (0.3%)
1	C	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	B	1	0
6	C	2	0
All	All	3	0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	ALA	N-CA-C	10.46	139.24	111.00
1	C	307	ARG	NE-CZ-NH1	-9.05	115.77	120.30
1	C	412	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	C	316	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	C	176	ARG	NE-CZ-NH2	-8.22	116.19	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	342	ALA	CA
6	C	604	MAN	C2,C1

There are no planarity outliers.

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	3684	0	3585	61	0
1	B	3715	0	3614	59	1
1	C	3715	0	3614	28	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
3	A	14	0	23	3	0
3	B	14	0	23	2	0
3	C	14	0	23	3	0
4	A	28	0	26	4	0
4	B	28	0	26	3	1
5	C	24	0	22	6	0
6	C	36	0	30	4	0
7	A	239	0	0	6	0
7	B	269	0	0	5	0
7	C	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)
4:A:601:NAG:O4	4: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	4:B:602: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	Percentiles	
1	A	457/472 (97%)	438 (96%)	18 (4%)	1 (0%)	51	48
1	B	460/472 (98%)	446 (97%)	14 (3%)	0	100	100
1	C	460/472 (98%)	441 (96%)	19 (4%)	0	100	100
All	All	1377/1416 (97%)	1325 (96%)	51 (4%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

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	394/404 (98%)	385 (98%)	9 (2%)	56	58
1	B	397/404 (98%)	388 (98%)	9 (2%)	56	58
1	C	397/404 (98%)	391 (98%)	6 (2%)	70	74
All	All	1188/1212 (98%)	1164 (98%)	24 (2%)	60	64

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

Mol	Chain	Res	Type
1	B	127	SER
1	B	205	TYR
1	C	221	ASP
1	B	154	PRO
1	B	168	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	292	GLN
1	B	359	GLN
1	B	466	HIS
1	B	152	ASN
1	C	48	ASN

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 ⓘ

5 carbohydrates 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	$\# Z > 2$
5	NAG	C	601	1,5,6	14,14,15	1.32	2 (14%)	15,19,21	1.76	4 (26%)
6	NAG	C	602	5,6	14,14,15	0.92	1 (7%)	15,19,21	1.27	3 (20%)
5	FCA	C	603	5	9,10,11	1.52	1 (11%)	13,14,16	1.56	3 (23%)
6	MAN	C	604	6	11,11,12	0.72	0	13,15,17	3.44	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	C	605	6	11,11,12	0.60	0	13,15,17	1.95	3 (23%)

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
5	NAG	C	601	1,5,6	-	0/6/23/26	0/1/1/1
6	NAG	C	602	5,6	-	0/6/23/26	0/1/1/1
5	FCA	C	603	5	-	0/0/17/20	0/1/1/1
6	MAN	C	604	6	2/2/4/5	0/2/19/22	0/1/1/1
6	MAN	C	605	6	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	FCA	C2-C3	-3.81	1.47	1.52
5	C	601	NAG	C1-C2	-3.13	1.48	1.52
6	C	602	NAG	O5-C1	-2.81	1.39	1.43
5	C	601	NAG	O5-C5	2.23	1.48	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	605	MAN	C1-C2-C3	-5.11	103.18	109.65
5	C	601	NAG	C1-C2-N2	-3.32	104.82	110.49
5	C	601	NAG	O4-C4-C3	-2.89	104.08	110.36
5	C	603	FCA	C3-C4-C5	-2.83	105.24	109.68
5	C	603	FCA	C2-C3-C4	-2.76	106.06	110.88

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	604	MAN	C2
6	C	604	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	NAG	5	0
6	C	602	NAG	4	0
5	C	603	FCA	3	0

5.6 Ligand geometry

10 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	FAD	A	590	3	51,58,58	1.03	4 (7%)	54,89,89	2.78	15 (27%)
3	NBA	A	591	2	13,13,14	0.54	0	12,12,14	1.62	3 (25%)
4	NAG	A	601	1	14,14,15	1.01	1 (7%)	15,19,21	2.17	5 (33%)
4	NAG	A	602	-	14,14,15	0.89	1 (7%)	15,19,21	1.24	2 (13%)
2	FAD	B	590	3	51,58,58	1.12	3 (5%)	54,89,89	1.74	10 (18%)
3	NBA	B	591	2	13,13,14	0.56	0	12,12,14	1.82	5 (41%)
4	NAG	B	601	1,4	14,14,15	1.09	1 (7%)	15,19,21	1.80	3 (20%)
4	NAG	B	602	4	14,14,15	1.35	2 (14%)	15,19,21	1.83	5 (33%)
2	FAD	C	590	3	51,58,58	1.14	4 (7%)	54,89,89	2.38	13 (24%)
3	NBA	C	591	2	13,13,14	0.55	0	12,12,14	2.26	3 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	590	3	-	0/28/50/50	0/6/6/6
3	NBA	A	591	2	-	0/11/11/12	0/0/0/0
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	602	-	-	0/6/23/26	0/1/1/1
2	FAD	B	590	3	-	0/28/50/50	0/6/6/6
3	NBA	B	591	2	-	0/11/11/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	602	4	-	0/6/23/26	0/1/1/1
2	FAD	C	590	3	-	0/28/50/50	0/6/6/6
3	NBA	C	591	2	-	0/11/11/12	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	NAG	O5-C1	-3.40	1.38	1.43
2	A	590	FAD	C2-N1	-3.24	1.31	1.38
4	B	602	NAG	C1-C2	-3.09	1.48	1.52
2	B	590	FAD	C2-N1	-2.65	1.32	1.38
2	C	590	FAD	C2-N1	-2.64	1.32	1.38

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	590	FAD	C4X-C10-N10	-7.57	115.26	120.52
2	C	590	FAD	C4X-C10-N10	-6.97	115.68	120.52
2	A	590	FAD	C4-C4X-C10	-5.71	115.34	119.96
3	C	591	NBA	C9-C8-N7	-5.56	97.89	112.06
2	A	590	FAD	C4X-C4-N3	-5.00	116.37	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	591	NBA	3	0
4	A	601	NAG	4	0
4	A	602	NAG	4	0
2	B	590	FAD	1	0
3	B	591	NBA	2	0
4	B	601	NAG	3	0
4	B	602	NAG	3	1
2	C	590	FAD	1	0
3	C	591	NBA	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.