



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:30 am GMT

PDB ID : 1H81
Title : STRUCTURE OF POLYAMINE OXIDASE IN THE REDUCED STATE
Authors : Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on : 2001-01-24
Resolution : 2.10 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)
Xtrriage (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

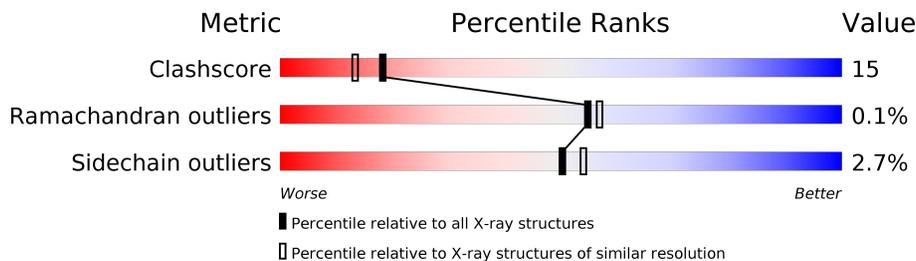
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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 ≥ 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
5	MAN	C	604	X	-	-	-

2 Entry composition [i](#)

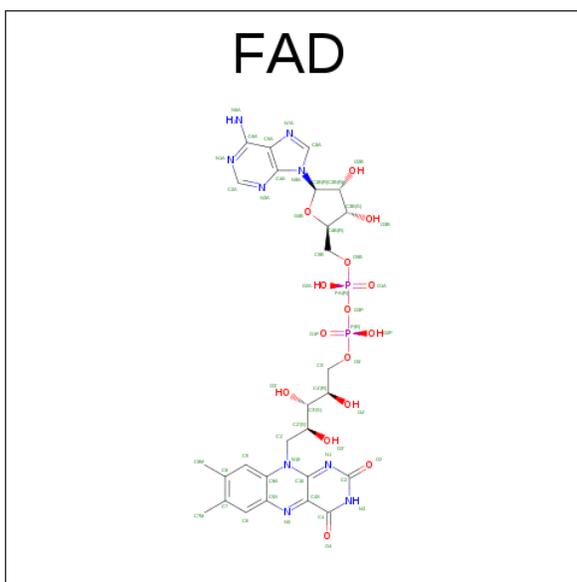
There are 6 unique types of molecules in this entry. The entry contains 12113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

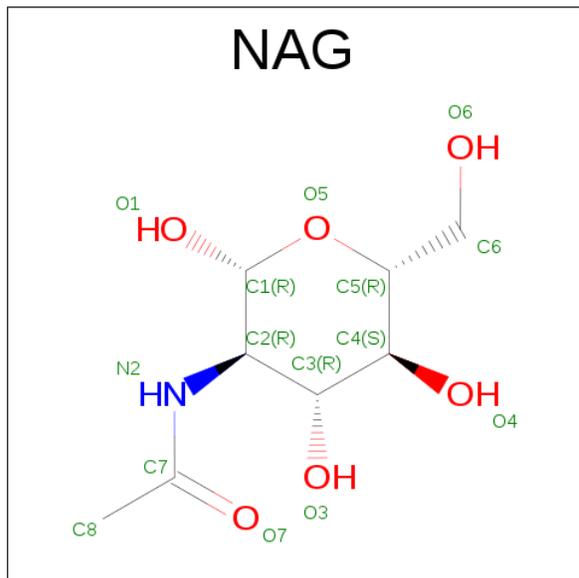
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	Total 3684	C 2353	N 621	O 696	S 14	55	0	0
1	B	462	Total 3715	C 2374	N 627	O 700	S 14	61	0	0
1	C	462	Total 3715	C 2374	N 627	O 700	S 14	50	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	2	Total	C	O	0	0
			22	12	10		

- Molecule 6 is water.

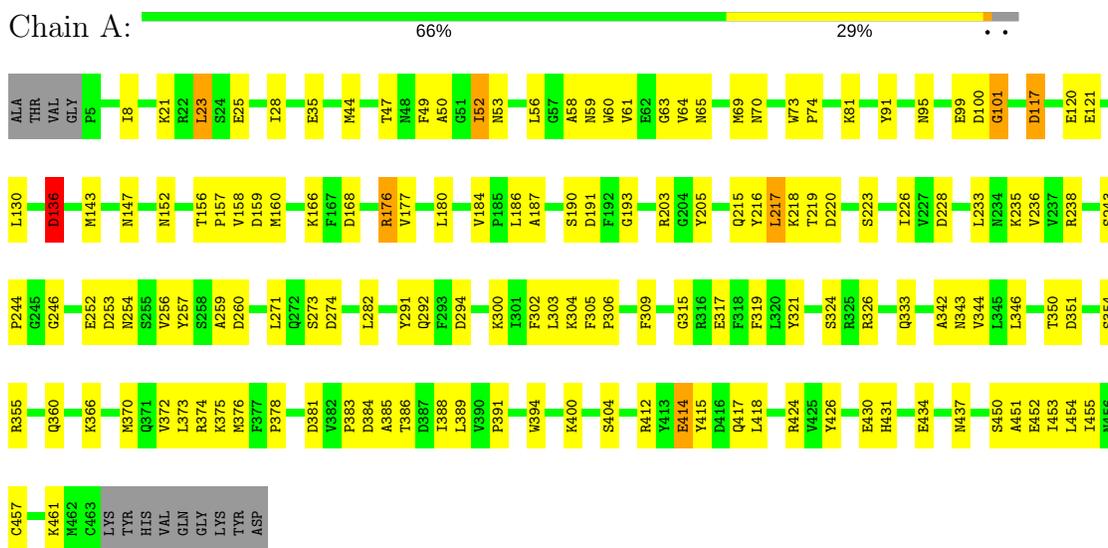
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total 224	O 224	0	0
6	B	245	Total 245	O 245	0	0
6	C	255	Total 255	O 255	0	0

3 Residue-property plots i

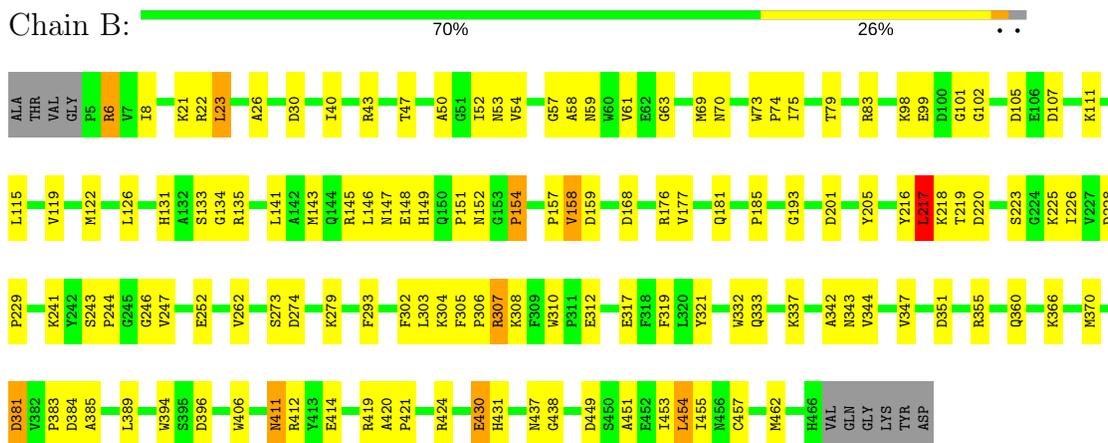
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



ALA	D117	K241	K376
THR	S118	T242	M376
VAL	V119	S243	F377
GLY	E120	P244	P378
PF	E121	G245	P383
R6	M122	G246	D384
V7	S127	K250	A385
I8	S127	T251	L389
K21	H131	E252	R397
R22	A132	D253	T402
L23	S133	N254	N405
S24	S133	S255	R412
E25	R145	V256	L418
A26	L146	Y257	R419
G27	N147	S258	R424
I28	G27	A259	E430
T29	P154	A259	H431
D30	P154	S273	E434
E35	V158	K279	N437
N48	D159	L282	G438
F49	E173	V285	Y439
A50	R176	K286	V440
G51	A187	V287	H441
G57	A187	R288	I455
A58	S190	A289	M456
N59	D191	I290	C457
N60	F192	Y291	K461
V61	G193	Q292	H466
E62	F198	F293	VAL
G63	F198	D294	GLN
V64	Y205	F302	GLY
N65	Y205	L303	LYS
G66	A213	K304	TYR
M69	Y216	R307	ASP
N70	L217	E317	
W73	K218	Q333	
P74	T219	Q338	
Y91	D220	Y339	
V96	D221	P340	
G101	K222	D341	
G102	S223	A342	
V103	G224	R343	
Y104	I226	V344	
D105	V227	R355	
E106	D228	K366	
D107	P229	M370	
R112	R230	R374	
L115	L233		
A116	R238		
	E239		
	I240		

4 Data and refinement statistics

Xtrriage (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	181.77Å 181.77Å 277.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.1 (20.00-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.191 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12113	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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, 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	0.54	0/3775	1.30	16/5116 (0.3%)
1	B	0.53	0/3808	1.26	15/5160 (0.3%)
1	C	0.55	0/3808	1.29	21/5160 (0.4%)
All	All	0.54	0/11391	1.28	52/15436 (0.3%)

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	C	1	0
5	C	1	0
All	All	2	0

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ARG	NE-CZ-NH2	-12.67	113.97	120.30
1	A	117	ASP	CB-CG-OD1	-10.79	108.59	118.30
1	C	230	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	C	145	ARG	NE-CZ-NH2	-10.13	115.24	120.30
1	B	135	ARG	NE-CZ-NH1	-9.11	115.74	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	386	THR	CB
5	C	604	MAN	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	3584	113	0
1	B	3715	0	3614	110	0
1	C	3715	0	3614	99	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	5	0
3	A	28	0	26	3	0
3	B	28	0	26	4	0
3	C	14	0	12	4	0
4	C	24	0	22	6	0
5	C	22	0	18	0	0
6	A	224	0	0	4	0
6	B	245	0	0	10	0
6	C	255	0	0	5	0
All	All	12113	0	11009	326	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 15.

The worst 5 of 326 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:B:69:MET:CE	1:B:73:TRP:HB3	1.81	1.11
1:A:373:LEU:HD23	1:A:376:MET:HE3	1.34	1.08
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.35	1.03
1:A:69:MET:CE	1:A:73:TRP:HB3	1.90	1.02
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.44	0.99

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	457/472 (97%)	437 (96%)	19 (4%)	1 (0%)	51	52
1	B	460/472 (98%)	444 (96%)	16 (4%)	0	100	100
1	C	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
All	All	1377/1416 (97%)	1323 (96%)	53 (4%)	1 (0%)	55	57

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%)	381 (97%)	13 (3%)	43	45
1	B	397/404 (98%)	384 (97%)	13 (3%)	43	45
1	C	397/404 (98%)	391 (98%)	6 (2%)	70	76
All	All	1188/1212 (98%)	1156 (97%)	32 (3%)	50	54

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	ASN
1	B	154	PRO

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Mol	Chain	Res	Type
1	C	217	LEU
1	B	115	LEU
1	B	157	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	360	GLN
1	B	411	ASN
1	C	152	ASN
1	B	152	ASN
1	C	131	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](#)

4 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
4	NAG	C	601	1,3,4	14,14,15	1.10	1 (7%)	15,19,21	2.07	5 (33%)
4	FCA	C	603	4	9,10,11	1.44	1 (11%)	13,14,16	1.91	4 (30%)
5	MAN	C	604	3,5	11,11,12	0.67	0	13,15,17	3.51	3 (23%)
5	MAN	C	605	5	11,11,12	0.54	0	13,15,17	1.21	2 (15%)

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	NAG	C	601	1,3,4	-	0/6/23/26	0/1/1/1
4	FCA	C	603	4	-	0/0/17/20	0/1/1/1
5	MAN	C	604	3,5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	C	605	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	FCA	C2-C3	-3.37	1.48	1.52
4	C	601	NAG	C1-C2	-2.52	1.49	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C1-C2-N2	-4.70	102.45	110.49
4	C	603	FCA	C3-C4-C5	-3.58	104.06	109.68
4	C	601	NAG	C8-C7-N2	-2.85	110.95	116.11
5	C	605	MAN	C2-C3-C4	-2.69	106.18	110.88
4	C	603	FCA	C2-C3-C4	-2.40	106.69	110.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	604	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	6	0
4	C	603	FCA	2	0

5.6 Ligand geometry

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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	579	-	51,58,58	0.95	2 (3%)	54,89,89	2.42	14 (25%)
3	NAG	A	601	1,3	14,14,15	0.90	0	15,19,21	1.75	5 (33%)
3	NAG	A	602	3	14,14,15	0.92	1 (7%)	15,19,21	1.44	2 (13%)
2	FAD	B	579	-	51,58,58	0.87	2 (3%)	54,89,89	1.99	11 (20%)
3	NAG	B	601	1,3	14,14,15	1.14	2 (14%)	15,19,21	1.91	4 (26%)
3	NAG	B	602	3	14,14,15	0.95	1 (7%)	15,19,21	1.64	3 (20%)
2	FAD	C	579	-	51,58,58	1.09	4 (7%)	54,89,89	2.23	10 (18%)
3	NAG	C	602	5,4	14,14,15	1.18	2 (14%)	15,19,21	1.71	3 (20%)

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	579	-	-	0/28/50/50	0/6/6/6
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
2	FAD	B	579	-	-	0/28/50/50	0/6/6/6
3	NAG	B	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3	-	0/6/23/26	0/1/1/1
2	FAD	C	579	-	-	0/28/50/50	0/6/6/6
3	NAG	C	602	5,4	-	0/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	NAG	O5-C1	-3.28	1.38	1.43
2	B	579	FAD	C2-N1	-2.74	1.32	1.38
2	C	579	FAD	C2-N1	-2.67	1.32	1.38
2	A	579	FAD	C2-N1	-2.62	1.33	1.38
3	B	601	NAG	C1-C2	-2.58	1.48	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	579	FAD	C4X-C10-N10	-7.35	115.42	120.52
2	A	579	FAD	C4X-C4-N3	-6.48	114.26	123.48
2	A	579	FAD	C4X-C10-N10	-5.33	116.82	120.52
2	C	579	FAD	C4-C4X-C10	-4.91	115.99	119.96
2	B	579	FAD	C4X-C4-N3	-4.46	117.14	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	FAD	2	0
3	A	601	NAG	3	0
3	A	602	NAG	3	0
2	B	579	FAD	2	0
3	B	601	NAG	4	0
3	B	602	NAG	4	0
2	C	579	FAD	5	0
3	C	602	NAG	4	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 [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.