



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:47 PM GMT

PDB ID : 1H84  
Title : COVALENT ADDUCT BETWEEN POLYAMINE OXIDASE AND N1ethyl  
N11((cycloheptyl)methyl)4,8diazoundecane at pH 4.6  
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 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

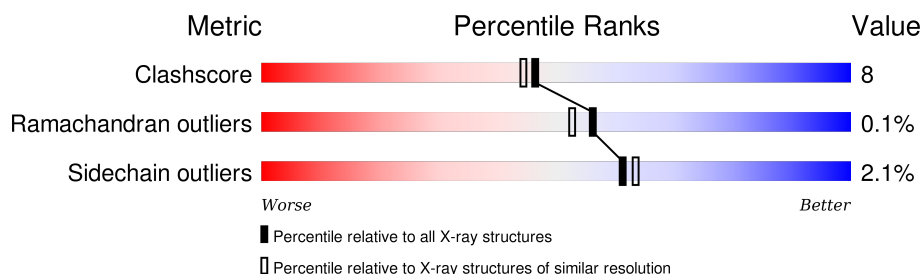
# 1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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  $\geq 3$ , 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	<div> <div style="width: 78%;"></div> <div style="width: 18%;"></div> <div style="width: 4%;"></div> </div> <div>78% 18% ..</div>
1	B	472	<div> <div style="width: 81%;"></div> <div style="width: 16%;"></div> <div style="width: 3%;"></div> </div> <div>81% 16% ..</div>
1	C	472	<div> <div style="width: 82%;"></div> <div style="width: 15%;"></div> <div style="width: 3%;"></div> </div> <div>82% 15% ..</div>

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	NAG	C	601	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MAN	C	604	X	-	-	-

## 2 Entry composition [i](#)

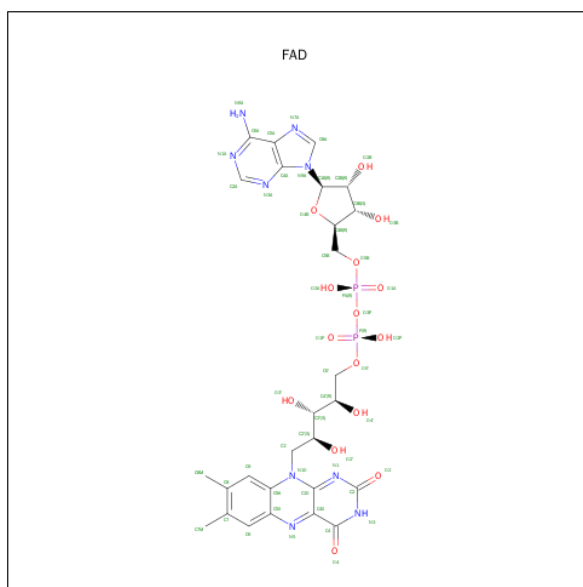
There are 7 unique types of molecules in this entry. The entry contains 12174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

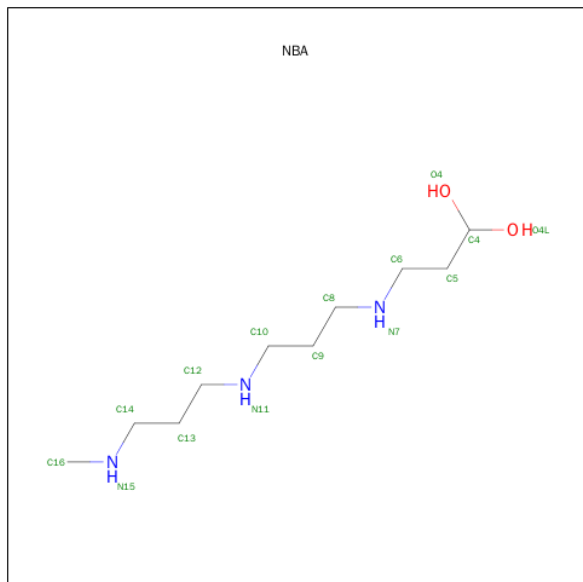
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	56	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	54	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	56	0	0
			3715	2374	627	700	14			

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



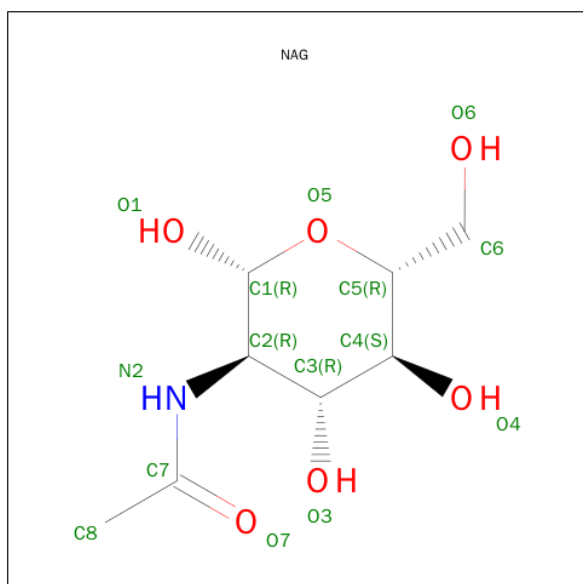
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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		
4	C	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 (2-MER).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	235	Total	O	0	0
			235	235		
7	B	245	Total	O	0	0
			245	245		
7	C	263	Total	O	0	0
			263	263		



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.04Å 184.04Å 280.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.5 (20.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, $R_{free}$	0.189 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: 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	0.57	0/3775	1.27	21/5116 (0.4%)
1	B	0.55	0/3808	1.23	18/5160 (0.3%)
1	C	0.57	0/3808	1.25	25/5160 (0.5%)
All	All	0.57	0/11391	1.25	64/15436 (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
6	C	1	0

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ARG	NE-CZ-NH2	-12.83	113.89	120.30
1	B	355	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	C	355	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	C	307	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	A	355	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	B	135	ARG	NE-CZ-NH1	-8.51	116.04	120.30
1	A	307	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	C	86	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	C	176	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	228	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	C	374	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	115	LEU	CB-CG-CD1	-7.15	98.84	111.00
1	B	170	GLU	OE1-CD-OE2	-6.98	114.93	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	397	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	101	GLY	N-CA-C	6.87	130.26	113.10
1	C	115	LEU	CB-CG-CD2	-6.76	99.50	111.00
1	C	316	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	340	PRO	C-N-CA	-6.36	105.81	121.70
1	C	230	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	297	VAL	CB-CA-C	-6.19	99.64	111.40
1	C	22	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	135	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	454	LEU	CB-CG-CD1	-5.98	100.84	111.00
1	C	325	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	316	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	308	LYS	CD-CE-NZ	5.92	125.32	111.70
1	B	115	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	B	355	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	C	288	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	381	ASP	N-CA-C	-5.82	95.27	111.00
1	C	61	VAL	N-CA-C	-5.72	95.55	111.00
1	B	412	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	260	ASP	CB-CG-OD2	5.72	123.44	118.30
1	C	22	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	351	ASP	N-CA-CB	-5.67	100.39	110.60
1	B	316	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	88	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	22	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	424	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	61	VAL	N-CA-C	-5.56	95.99	111.00
1	C	38	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	374	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	454	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	230	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	307	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	A	397	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	38	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	88	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	454	LEU	CB-CG-CD1	5.35	120.10	111.00
1	A	351	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	342	ALA	N-CA-C	5.33	125.40	111.00
1	A	397	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	297	VAL	CB-CA-C	-5.28	101.36	111.40
1	C	158	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	A	176	ARG	CB-CG-CD	-5.27	97.90	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	VAL	CB-CA-C	-5.24	101.45	111.40
1	C	397	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	362	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	61	VAL	N-CA-C	-5.17	97.05	111.00
1	A	386	THR	N-CA-CB	-5.16	100.49	110.30
1	A	60	TRP	CB-CA-C	-5.15	100.10	110.40
1	C	105	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	397	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	186	LEU	CB-CG-CD2	-5.03	102.44	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	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	3585	51	0
1	B	3715	0	3614	60	0
1	C	3715	0	3614	42	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
3	A	14	0	23	1	0
3	B	14	0	23	0	0
3	C	14	0	23	1	0
4	A	28	0	26	4	0
4	B	28	0	26	3	0
4	C	14	0	12	6	0
5	C	24	0	22	8	0
6	C	22	0	19	0	0
7	A	235	0	0	1	0
7	B	245	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	263	0	0	2	0
All	All	12174	0	11080	165	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 8.

All (165) 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:HE2	1:B:74:PRO:HD3	1.29	1.12
1:B:69:MET:CE	1:B:73:TRP:HB3	1.86	1.05
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.42	1.00
1:B:69:MET:CE	1:B:74:PRO:HD3	1.92	0.99
1:C:131:HIS:CD2	1:C:133:SER:H	1.87	0.90
5:C:601:NAG:C4	4:C:602:NAG:C1	2.50	0.90
1:C:91:TYR:OH	1:C:314:LYS:HE2	1.74	0.85
1:A:273:SER:O	1:A:274:ASP:HB2	1.78	0.83
1:B:411:ASN:ND2	1:B:414:GLU:H	1.75	0.82
4:B:601:NAG:C4	4:B:602:NAG:C1	2.62	0.78
1:B:131:HIS:CD2	1:B:133:SER:H	2.02	0.77
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.82	0.76
1:C:131:HIS:HD2	1:C:133:SER:H	1.30	0.74
1:B:131:HIS:HD2	1:B:133:SER:H	1.35	0.73
4:A:601:NAG:C4	4:A:602:NAG:C1	2.66	0.73
1:A:431:HIS:H	1:A:431:HIS:CD2	2.09	0.67
1:C:117:ASP:O	1:C:121:GLU:HG3	1.94	0.67
5:C:601:NAG:O4	4:C:602:NAG:C2	2.43	0.66
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.43	0.66
5:C:601:NAG:H3	5:C:603:FCA:O2	1.97	0.65
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.29	0.64
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.32	0.64
4:A:601:NAG:HO4	4:A:602:NAG:C1	2.09	0.63
1:C:412:ARG:NH1	1:C:434:GLU:OE1	2.29	0.63
1:C:431:HIS:H	1:C:431:HIS:CD2	2.18	0.62
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.81	0.62
1:B:69:MET:HE3	1:B:73:TRP:CB	2.25	0.61
1:B:411:ASN:HD22	1:B:414:GLU:H	1.46	0.61
4:B:601:NAG:O4	4:B:602:NAG:C2	2.48	0.61
1:A:98:LYS:HG2	1:A:104:TYR:CE1	2.37	0.60
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.00	0.60
1:A:21:LYS:O	1:A:25:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:HIS:HD2	1:C:133:SER:OG	1.85	0.59
1:C:220:ASP:OD2	1:C:222:LYS:N	2.36	0.59
1:B:342:ALA:O	1:B:343:ASN:HB2	2.03	0.58
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.85	0.58
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.40	0.57
1:C:91:TYR:CZ	1:C:314:LYS:HE2	2.40	0.57
1:C:253:ASP:O	1:C:254:ASN:HB2	2.05	0.57
1:B:220:ASP:O	1:B:224:GLY:N	2.37	0.56
1:C:412:ARG:HD3	1:C:434:GLU:OE1	2.05	0.56
1:B:431:HIS:CD2	1:B:431:HIS:H	2.23	0.56
1:B:69:MET:HE2	1:B:73:TRP:HB3	1.86	0.55
1:C:220:ASP:HB3	1:C:223:SER:OG	2.07	0.55
1:C:158:VAL:HG12	7:C:2073:HOH:O	2.05	0.55
1:C:131:HIS:CD2	1:C:133:SER:OG	2.60	0.55
1:B:449:ASP:O	1:B:453:ILE:HG13	2.06	0.55
1:A:111:LYS:O	1:A:115:LEU:HG	2.07	0.54
1:C:131:HIS:HD2	1:C:133:SER:N	2.03	0.54
1:C:366:LYS:HD2	1:C:385:ALA:HB3	1.89	0.54
1:B:411:ASN:HD21	1:B:414:GLU:HG3	1.73	0.54
1:C:342:ALA:O	1:C:343:ASN:HB2	2.08	0.54
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.73	0.54
1:A:220:ASP:HB3	1:A:223:SER:OG	2.08	0.53
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.90	0.53
1:B:26:ALA:HB2	1:B:455:ILE:HD13	1.91	0.53
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.56	0.52
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.91	0.52
1:A:253:ASP:O	1:A:254:ASN:HB2	2.08	0.52
1:C:219:THR:HA	1:C:225:LYS:O	2.09	0.52
1:B:451:ALA:O	1:B:455:ILE:HG13	2.10	0.51
5:C:601:NAG:HO4	4:C:602:NAG:C1	2.12	0.51
1:C:131:HIS:HD2	1:C:133:SER:CB	2.24	0.51
1:B:243:SER:HB2	1:B:244:PRO:CD	2.40	0.51
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.46	0.51
1:A:63:GLY:HA2	1:A:193:GLY:O	2.10	0.51
1:B:457:CYS:HA	1:B:462:MET:O	2.12	0.50
1:A:220:ASP:OD1	1:A:222:LYS:N	2.36	0.49
1:C:306:PRO:HD3	1:C:386:THR:HG23	1.94	0.49
1:B:411:ASN:C	1:B:411:ASN:HD22	2.16	0.49
1:C:170:GLU:OE2	3:C:591:NBA:H122	2.13	0.49
1:B:419:ARG:HD3	7:B:2219:HOH:O	2.13	0.49
1:A:218:LYS:H	1:A:228:ASP:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:HIS:HA	1:B:206:GLU:OE2	2.13	0.48
1:C:402:THR:CB	2:C:590:FAD:HM83	2.44	0.48
1:C:6:ARG:HA	1:C:30:ASP:O	2.13	0.48
1:C:218:LYS:H	1:C:228:ASP:HB2	1.78	0.48
1:A:47:THR:O	1:A:53:ASN:HA	2.13	0.48
1:A:219:THR:HG22	1:A:226:ILE:HA	1.96	0.48
1:B:219:THR:HG22	1:B:226:ILE:HA	1.95	0.47
1:A:49:PHE:O	1:A:50:ALA:HB3	2.13	0.47
1:B:220:ASP:HB3	1:B:223:SER:OG	2.14	0.47
1:A:414:GLU:HG3	1:A:414:GLU:O	2.13	0.47
1:B:131:HIS:HD2	1:B:133:SER:OG	1.98	0.47
1:C:402:THR:HB	2:C:590:FAD:HM83	1.96	0.47
4:B:601:NAG:O6	4:B:602:NAG:C1	2.63	0.47
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.62	0.47
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.46	0.47
1:B:141:LEU:HD22	1:B:176:ARG:HB3	1.97	0.46
1:A:64:VAL:HG12	1:A:65:ASN:N	2.30	0.46
1:A:370:MET:HE2	1:A:384:ASP:HA	1.98	0.46
1:B:360:GLN:NE2	7:B:2188:HOH:O	2.49	0.46
5:C:601:NAG:C3	5:C:603:FCA:O2	2.63	0.46
1:A:143:MET:SD	1:A:147:ASN:ND2	2.89	0.46
1:B:411:ASN:ND2	1:B:414:GLU:HG3	2.31	0.45
1:A:156:THR:O	1:A:160:MET:HG3	2.16	0.45
5:C:601:NAG:O6	4:C:602:NAG:C1	2.64	0.45
5:C:603:FCA:H5	4:C:602:NAG:H62	1.98	0.45
4:A:601:NAG:H4	4:A:602:NAG:C1	2.46	0.45
1:B:69:MET:HE1	1:B:74:PRO:HD3	1.88	0.45
1:B:411:ASN:HD21	1:B:414:GLU:H	1.60	0.45
1:B:104:TYR:CZ	1:B:158:VAL:CG2	3.00	0.45
1:A:98:LYS:HG2	1:A:104:TYR:CD1	2.52	0.45
1:A:300:LYS:HB3	1:A:346:LEU:HD11	1.98	0.45
5:C:601:NAG:H4	4:C:602:NAG:C1	2.42	0.44
1:B:131:HIS:CD2	1:B:133:SER:OG	2.71	0.44
1:A:370:MET:HE1	1:A:383:PRO:O	2.18	0.44
1:B:220:ASP:CG	1:B:223:SER:HG	2.21	0.44
1:B:273:SER:O	1:B:274:ASP:HB2	2.18	0.44
1:C:131:HIS:CD2	1:C:133:SER:CB	3.00	0.44
1:B:344:VAL:HG12	1:B:345:LEU:N	2.32	0.44
1:A:82:LEU:HA	1:A:82:LEU:HD23	1.81	0.44
1:A:20:ALA:HB3	1:A:216:TYR:OH	2.19	0.43
1:C:63:GLY:HA2	1:C:193:GLY:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:O	1:B:424:ARG:HD3	2.18	0.43
1:C:438:GLY:O	2:C:590:FAD:H1'2	2.18	0.43
1:A:158:VAL:HG13	1:A:159:ASP:N	2.34	0.43
1:B:69:MET:CE	1:B:73:TRP:CB	2.77	0.43
1:A:273:SER:O	1:A:274:ASP:CB	2.45	0.43
1:A:377:PHE:HB3	1:A:380:LYS:HG3	2.01	0.43
1:A:460:LYS:HB3	1:A:462:MET:CE	2.49	0.43
1:A:100:ASP:OD1	1:A:375:LYS:HE2	2.19	0.43
1:C:338:GLN:OE1	1:C:338:GLN:N	2.51	0.43
1:C:101:GLY:HA3	1:C:378:PRO:HG3	2.00	0.43
1:A:58:ALA:HA	2:A:590:FAD:C4X	2.49	0.42
1:C:105:ASP:OD2	1:C:107:ASP:N	2.51	0.42
1:A:213:ALA:O	1:A:217:LEU:HB2	2.18	0.42
1:B:80:LEU:O	1:B:81:LYS:HB2	2.19	0.42
1:B:351:ASP:CG	1:B:352:GLU:H	2.22	0.42
1:A:402:THR:HB	2:A:590:FAD:HM83	2.00	0.42
1:B:26:ALA:CB	1:B:455:ILE:HD13	2.49	0.42
1:A:253:ASP:OD1	1:A:253:ASP:C	2.58	0.42
1:A:350:THR:HA	1:A:354:SER:OG	2.19	0.42
1:A:23:LEU:HD13	1:A:451:ALA:HB1	2.01	0.42
3:A:591:NBA:HC52	7:A:2228:HOH:O	2.19	0.42
1:B:57:GLY:HA2	2:B:590:FAD:C7M	2.50	0.42
1:C:381:ASP:HB3	7:C:2206:HOH:O	2.20	0.42
1:B:311:PRO:HB2	1:B:316:ARG:HD2	2.01	0.42
1:C:91:TYR:CD1	1:C:91:TYR:N	2.87	0.42
1:B:69:MET:CE	1:B:73:TRP:CD1	3.03	0.42
1:B:145:ARG:O	1:B:149:HIS:N	2.51	0.42
1:B:104:TYR:CZ	1:B:158:VAL:HG23	2.55	0.41
1:B:69:MET:CE	1:B:74:PRO:CD	2.81	0.41
1:B:21:LYS:HB2	1:B:216:TYR:CE2	2.55	0.41
1:B:131:HIS:HD2	1:B:133:SER:N	2.12	0.41
1:B:220:ASP:O	1:B:224:GLY:HA2	2.21	0.41
1:A:218:LYS:N	1:A:228:ASP:HB2	2.36	0.41
1:C:351:ASP:CG	1:C:352:GLU:H	2.22	0.41
1:A:328:TYR:O	1:A:329:TYR:C	2.58	0.41
1:B:317:GLU:O	1:B:333:GLN:HA	2.21	0.41
1:B:332:TRP:CZ3	1:B:347:VAL:HB	2.56	0.41
1:B:52:ILE:HD12	1:B:339:TYR:CD2	2.55	0.41
1:C:454:LEU:HD12	1:C:454:LEU:O	2.21	0.41
4:A:601:NAG:O6	4:A:602:NAG:C1	2.69	0.41
1:A:220:ASP:OD1	1:A:220:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LYS:O	1:C:227:VAL:N	2.47	0.41
1:C:303:LEU:O	1:C:344:VAL:HA	2.21	0.41
1:A:177:VAL:HG12	1:A:177:VAL:O	2.21	0.41
1:B:57:GLY:HA2	2:B:590:FAD:HM72	2.03	0.41
1:A:271:LEU:HA	1:A:271:LEU:HD23	1.85	0.41
1:C:239:GLU:OE2	1:C:279:LYS:HD2	2.21	0.40
1:A:136:ASP:N	1:A:136:ASP:OD1	2.48	0.40
1:B:220:ASP:O	1:B:224:GLY:CA	2.70	0.40
1:C:64:VAL:O	1:C:65:ASN:HB2	2.20	0.40
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.82	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	440 (96%)	16 (4%)	1 (0%)	52	48
1	B	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
1	C	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
All	All	1377/1416 (97%)	1326 (96%)	50 (4%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

### 5.3.2 Protein sidechains ⓘ

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%)	58	60
1	B	397/404 (98%)	386 (97%)	11 (3%)	51	50
1	C	397/404 (98%)	392 (99%)	5 (1%)	76	79
All	All	1188/1212 (98%)	1163 (98%)	25 (2%)	61	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	52	ILE
1	A	59	ASN
1	A	168	ASP
1	A	205	TYR
1	A	217	LEU
1	A	384	ASP
1	A	386	THR
1	A	434	GLU
1	B	59	ASN
1	B	105	ASP
1	B	154	PRO
1	B	157	PRO
1	B	168	ASP
1	B	205	TYR
1	B	238	ARG
1	B	411	ASN
1	B	434	GLU
1	B	454	LEU
1	B	466	HIS
1	C	59	ASN
1	C	105	ASP
1	C	115	LEU
1	C	127	SER
1	C	205	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	152	ASN
1	A	360	GLN
1	A	431	HIS
1	B	131	HIS
1	B	150	GLN
1	B	152	ASN
1	B	360	GLN
1	B	411	ASN
1	B	431	HIS
1	B	435	HIS
1	C	48	ASN
1	C	131	HIS
1	C	152	ASN
1	C	292	GLN
1	C	360	GLN
1	C	431	HIS

### 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 ⓘ

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	$\# Z  > 2$
5	NAG	C	601	1,5,4	14,14,15	1.01	1 (7%)	15,19,21	1.59	5 (33%)
5	FCA	C	603	5	10,10,11	1.23	1 (10%)	14,14,16	2.11	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	C	604	4,6	11,11,12	0.74	0	14,15,17	3.20	5 (35%)
6	MAN	C	605	6	11,11,12	0.51	0	14,15,17	1.71	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
5	NAG	C	601	1,5,4	-	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	4,6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	605	6	-	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)
5	C	603	FCA	C2-C3	-2.85	1.48	1.52
5	C	601	NAG	C1-C2	-2.19	1.49	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	605	MAN	C1-C2-C3	-3.92	104.91	109.54
5	C	603	FCA	O5-C1-C2	-3.66	104.92	110.86
6	C	605	MAN	C2-C3-C4	-3.27	105.48	111.04
5	C	601	NAG	C8-C7-N2	-3.07	110.23	116.11
5	C	601	NAG	O4-C4-C3	-2.99	103.61	110.34
5	C	603	FCA	C3-C4-C5	-2.96	104.72	109.72
5	C	603	FCA	O3-C3-C4	-2.67	104.33	110.34
5	C	603	FCA	C2-C3-C4	-2.19	107.32	111.04
5	C	603	FCA	O2-C2-C1	-2.12	104.95	109.21
5	C	601	NAG	O5-C5-C6	-2.10	102.80	107.35
6	C	604	MAN	O5-C5-C6	2.20	112.11	107.35
5	C	601	NAG	C1-O5-C5	2.27	115.13	112.25
6	C	604	MAN	O4-C4-C3	2.33	115.58	110.34
5	C	601	NAG	O7-C7-C8	2.36	126.39	122.06
6	C	604	MAN	O2-C2-C1	2.57	114.35	109.21
6	C	604	MAN	C1-O5-C5	2.60	115.55	112.25
6	C	605	MAN	O2-C2-C3	3.08	116.32	110.12
5	C	603	FCA	C1-O5-C5	3.25	117.40	112.38
6	C	604	MAN	O2-C2-C3	10.57	131.38	110.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	604	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	NAG	7	0
5	C	603	FCA	3	0

## 5.6 Ligand geometry

11 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	48,58,58	1.04	3 (6%)	54,89,89	2.48	12 (22%)
3	NBA	A	591	2	13,13,14	0.74	0	12,12,14	1.65	2 (16%)
4	NAG	A	601	1,4	14,14,15	0.92	0	15,19,21	1.60	4 (26%)
4	NAG	A	602	4	14,14,15	0.89	1 (7%)	15,19,21	1.60	2 (13%)
2	FAD	B	590	3	48,58,58	0.92	2 (4%)	54,89,89	2.05	7 (12%)
3	NBA	B	591	2	13,13,14	0.55	0	12,12,14	2.11	6 (50%)
4	NAG	B	601	1,4	14,14,15	1.22	2 (14%)	15,19,21	1.80	3 (20%)
4	NAG	B	602	4	14,14,15	0.90	1 (7%)	15,19,21	1.21	1 (6%)
2	FAD	C	590	3	48,58,58	1.11	2 (4%)	54,89,89	2.48	10 (18%)
3	NBA	C	591	2	13,13,14	0.61	0	12,12,14	1.59	2 (16%)
4	NAG	C	602	5,6	14,14,15	1.02	1 (7%)	15,19,21	1.42	4 (26%)

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	-	0/30/50/50	0/6/6/6
3	NBA	A	591	2	-	0/11/11/12	0/0/0/0
4	NAG	A	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	602	4	-	0/6/23/26	0/1/1/1
2	FAD	B	590	3	-	0/30/50/50	0/6/6/6
3	NBA	B	591	2	-	0/11/11/12	0/0/0/0
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	-	0/30/50/50	0/6/6/6
3	NBA	C	591	2	-	0/11/11/12	0/0/0/0
4	NAG	C	602	5,6	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	NAG	C1-C2	-3.06	1.48	1.52
4	C	602	NAG	O5-C1	-2.85	1.38	1.43
2	A	590	FAD	C10-N10	-2.61	1.36	1.39
4	B	602	NAG	O5-C1	-2.50	1.39	1.43
4	B	601	NAG	O5-C1	-2.37	1.39	1.43
4	A	602	NAG	O5-C1	-2.13	1.40	1.43
2	B	590	FAD	C4X-N5	2.21	1.36	1.33
2	A	590	FAD	C4X-N5	2.34	1.37	1.33
2	C	590	FAD	C4X-N5	3.13	1.38	1.33
2	B	590	FAD	C4-N3	3.74	1.40	1.33
2	C	590	FAD	C4-N3	3.89	1.40	1.33
2	A	590	FAD	C4-N3	4.09	1.40	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	590	FAD	C4X-C10-N10	-10.04	114.61	120.52
2	C	590	FAD	C4-C4X-C10	-7.91	114.88	119.94
2	A	590	FAD	C4X-C10-N10	-7.58	116.05	120.52
2	B	590	FAD	C4X-C10-N10	-7.01	116.39	120.52
2	A	590	FAD	C4X-C4-N3	-6.23	115.08	123.59
2	B	590	FAD	C4X-C4-N3	-5.83	115.61	123.59
4	B	601	NAG	C2-N2-C7	-4.94	116.70	123.04
2	A	590	FAD	C4-C4X-C10	-4.86	116.83	119.94
4	A	602	NAG	C2-N2-C7	-4.46	117.31	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	591	NBA	C9-C8-N7	-4.39	101.00	111.96
3	C	591	NBA	C9-C8-N7	-3.95	102.10	111.96
3	B	591	NBA	C12-N11-C10	-3.78	99.96	113.35
2	C	590	FAD	C4X-C4-N3	-3.12	119.32	123.59
3	B	591	NBA	C9-C8-N7	-3.06	104.32	111.96
3	B	591	NBA	C16-N15-C14	-3.01	103.41	112.23
2	A	590	FAD	C9A-C5X-N5	-2.96	117.97	122.36
4	C	602	NAG	C2-N2-C7	-2.95	119.24	123.04
4	A	601	NAG	O5-C5-C6	-2.89	101.09	107.35
2	A	590	FAD	C4X-N5-C5X	-2.87	113.46	116.76
4	C	602	NAG	O5-C5-C6	-2.87	101.14	107.35
2	C	590	FAD	C4X-N5-C5X	-2.59	113.79	116.76
3	B	591	NBA	C14-C13-C12	-2.55	103.83	114.31
4	A	602	NAG	C8-C7-N2	-2.52	111.28	116.11
2	B	590	FAD	C1'-N10-C9A	-2.38	116.19	118.86
3	B	591	NBA	C10-C9-C8	-2.28	104.96	114.31
2	B	590	FAD	C4X-N5-C5X	-2.25	114.17	116.76
3	C	591	NBA	C12-N11-C10	-2.14	105.78	113.35
4	C	602	NAG	C3-C2-N2	-2.10	105.54	110.56
3	A	591	NBA	C8-N7-C6	-2.05	106.08	113.35
2	C	590	FAD	P-O3P-PA	-2.03	127.02	132.73
2	A	590	FAD	O5B-PA-O1A	-2.02	101.77	109.62
2	B	590	FAD	O3'-C3'-C4'	-2.01	103.67	108.75
2	A	590	FAD	O4'-C4'-C3'	2.04	114.14	109.02
4	A	601	NAG	O3-C3-C2	2.08	113.23	109.11
3	B	591	NBA	C5-C6-N7	2.10	117.22	111.96
2	C	590	FAD	O2P-P-O1P	2.18	124.36	112.53
4	B	601	NAG	O3-C3-C4	2.21	115.32	110.34
2	A	590	FAD	C6-C5X-C9A	2.27	121.97	118.98
2	A	590	FAD	C4-C4X-N5	2.39	121.62	118.72
2	A	590	FAD	C5X-C9A-N10	2.51	119.53	117.62
4	C	602	NAG	C3-C4-C5	2.55	114.64	110.20
4	B	601	NAG	C1-O5-C5	2.57	115.51	112.25
4	B	602	NAG	C1-O5-C5	2.64	115.60	112.25
2	C	590	FAD	O2A-PA-O1A	2.75	127.45	112.53
4	A	601	NAG	O3-C3-C4	2.76	116.55	110.34
4	A	601	NAG	C1-O5-C5	3.14	116.23	112.25
2	B	590	FAD	N3A-C2A-N1A	3.35	131.46	128.89
2	C	590	FAD	C4-C4X-N5	3.81	123.35	118.72
2	C	590	FAD	N3A-C2A-N1A	4.14	132.06	128.89
2	A	590	FAD	C1'-N10-C9A	5.81	125.39	118.86
2	C	590	FAD	C4-N3-C2	8.54	122.62	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	590	FAD	C4-N3-C2	8.60	122.68	115.25
2	A	590	FAD	C4-N3-C2	9.86	123.77	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	590	FAD	2	0
3	A	591	NBA	1	0
4	A	601	NAG	4	0
4	A	602	NAG	4	0
2	B	590	FAD	2	0
4	B	601	NAG	3	0
4	B	602	NAG	3	0
2	C	590	FAD	3	0
3	C	591	NBA	1	0
4	C	602	NAG	6	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.