



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:19 AM BST

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 Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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) : 2.13.1

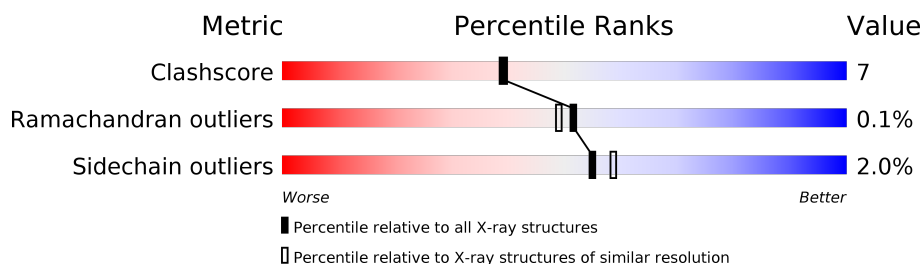
1 Overall quality at a glance

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	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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	
1	B	472	
1	C	472	
2	D	2	
3	E	5	

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	E	3	X	-	-	-

2 Entry composition

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.

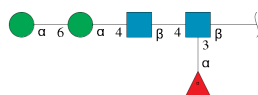
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	63	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	64	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	51	0	0
			3715	2374	627	700	14			

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



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

- Molecule 3 is an oligosaccharide called 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.



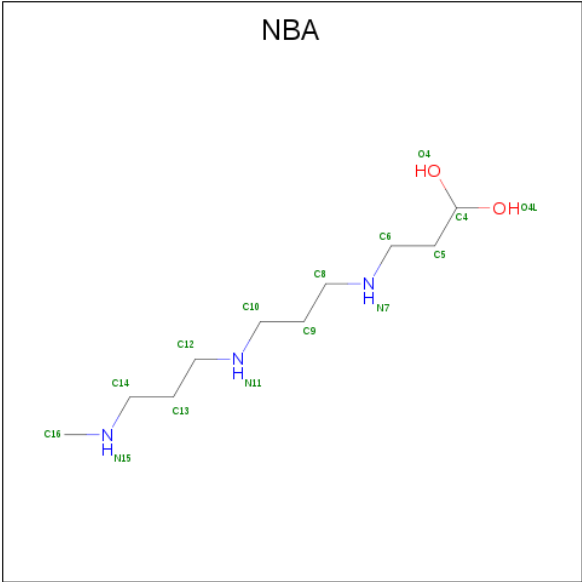
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



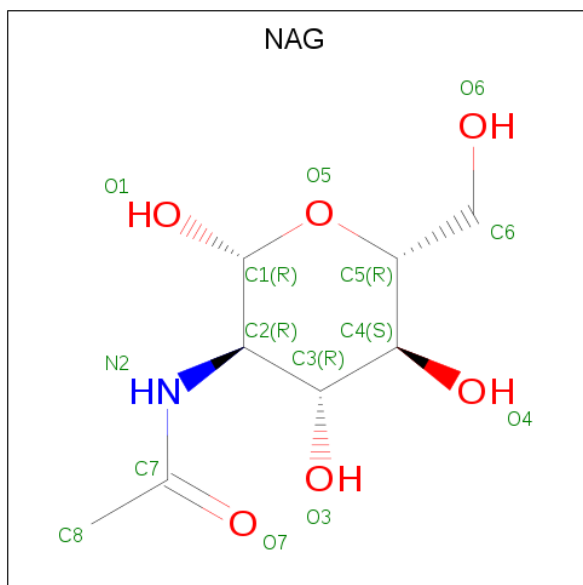
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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	A	1	Total	C	N	O	0	0
			14	10	3	1		
5	B	1	Total	C	N	O	0	0
			14	10	3	1		
5	C	1	Total	C	N	O	0	0
			14	10	3	1		

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

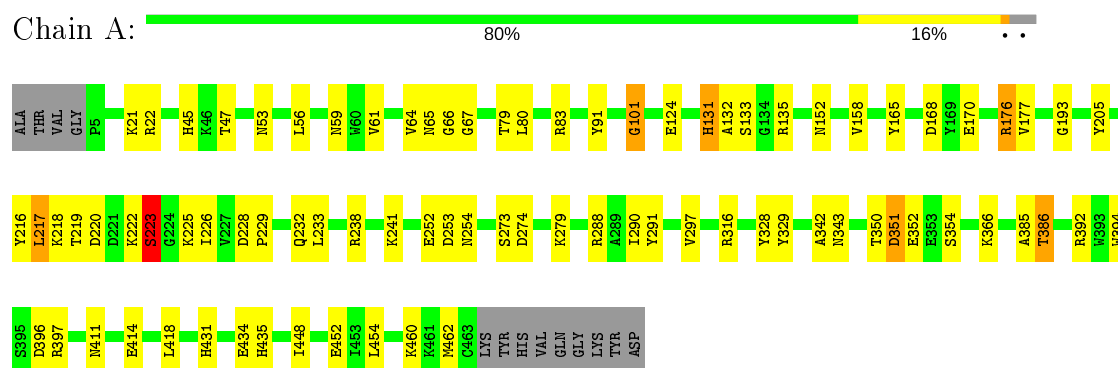
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	239	Total	O	0	0
			239	239		
7	B	269	Total	O	0	0
			269	269		
7	C	283	Total	O	0	0
			283	283		

3 Residue-property plots [i](#)

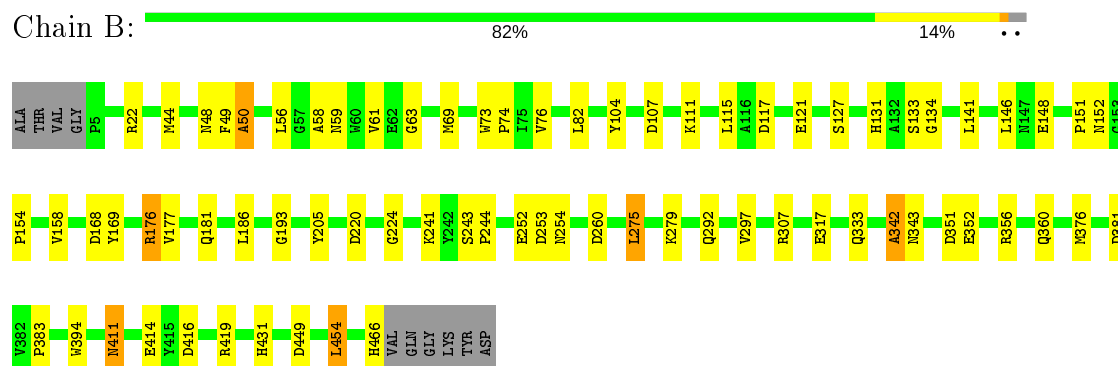
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

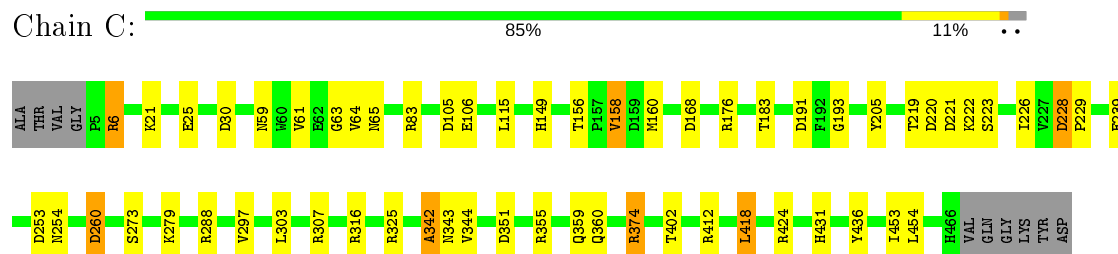
- Molecule 1: POLYAMINE OXIDASE



- Molecule 1: POLYAMINE OXIDASE



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

Chain D:  100%

MAG1
MAG2

- Molecule 3: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -D-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  20%  80%

MAG1
MAG2
MAN3
MAN4
FCA5

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

There are no bond length outliers.

All (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
1	A	101	GLY	N-CA-C	8.08	133.31	113.10
1	A	176	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	392	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	176	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	C	288	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	A	83	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	C	6	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	A	316	ARG	NE-CZ-NH1	7.27	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	LEU	CA-CB-CG	6.72	130.75	115.30
1	A	22	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	386	THR	N-CA-CB	-6.50	97.94	110.30
1	A	176	ARG	CB-CG-CD	-6.44	94.86	111.60
1	C	176	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	454	LEU	CA-CB-CG	6.39	130.01	115.30
1	A	397	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	273	SER	C-N-CA	-6.25	106.07	121.70
1	C	374	ARG	CG-CD-NE	-6.22	98.74	111.80
1	C	176	ARG	CB-CG-CD	-6.19	95.50	111.60
1	C	228	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	C	342	ALA	N-CA-C	6.09	127.45	111.00
1	C	325	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	B	260	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	C	297	VAL	CB-CA-C	-6.04	99.93	111.40
1	B	176	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	376	MET	CG-SD-CE	5.83	109.53	100.20
1	A	297	VAL	CB-CA-C	-5.81	100.36	111.40
1	A	351	ASP	N-CA-CB	-5.77	100.22	110.60
1	B	297	VAL	CB-CA-C	-5.73	100.51	111.40
1	A	288	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	B	44	MET	N-CA-C	-5.61	95.86	111.00
1	B	61	VAL	N-CA-C	-5.60	95.87	111.00
1	C	61	VAL	N-CA-C	-5.54	96.06	111.00
1	B	356	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	186	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	C	83	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	C	260	ASP	CB-CG-OD2	5.39	123.16	118.30
1	B	56	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	B	22	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	233	LEU	CA-CB-CG	-5.30	103.10	115.30
1	C	183	THR	OG1-CB-CG2	-5.29	97.82	110.00
1	B	50	ALA	C-N-CA	-5.25	111.28	122.30
1	C	351	ASP	N-CA-CB	-5.23	101.19	110.60
1	A	61	VAL	N-CA-C	-5.22	96.90	111.00
1	A	223	SER	N-CA-CB	-5.18	102.73	110.50
1	C	158	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	A	396	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	449	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	22	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	288	ARG	CG-CD-NE	-5.02	101.26	111.80
1	C	418	LEU	CA-CB-CG	5.01	126.82	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	342	ALA	CA

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	D	28	0	26	3	1
3	E	60	0	52	6	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
4	C	53	0	31	1	0
5	A	14	0	23	3	0
5	B	14	0	23	2	0
5	C	14	0	23	3	0
6	A	28	0	26	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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:HB3	1:A:223:SER:HB3	1.53	0.88
1:A:411:ASN:OD1	1:A:414:GLU:HG3	1.73	0.88
3:E:1:NAG:C4	3:E:2:NAG:C1	2.52	0.87
1:A:131:HIS:CE1	1:A:133:SER:H	1.94	0.85
2:D:1:NAG:C4	2:D:2:NAG:C1	2.55	0.84
1:C:239:GLU:OE2	1:C:279:LYS:HD2	1.77	0.83
1:B:69:MET:CE	1:B:74:PRO:HD3	2.09	0.82
1:B:131:HIS:HD2	1:B:133:SER:H	1.27	0.82
1:B:69:MET:HE3	1:B:73:TRP:CD1	2.14	0.81
1:B:131:HIS:CD2	1:B:133:SER:H	1.98	0.80
3:E:1:NAG:H3	3:E:5:FCA:O2	1.87	0.75
6:A:601:NAG:C4	6:A:602:NAG:C1	2.67	0.73
1:B:69:MET:HE2	1:B:74:PRO:CD	2.11	0.73
1:B:411:ASN:ND2	1:B:414:GLU:H	1.88	0.72
1:A:220:ASP:OD1	1:A:222:LYS:N	2.23	0.71
1:A:152:ASN:ND2	1:B:394:TRP:HE1	1.88	0.71
1:A:79:THR:HG22	1:A:80:LEU:HD23	1.71	0.71
1:A:219:THR:HG22	1:A:226:ILE:HA	1.73	0.71
5:A:591:NBA:H122	7:A:2080:HOH:O	1.90	0.71
1:A:273:SER:O	1:A:274:ASP:HB2	1.89	0.71
1:B:69:MET:HE3	1:B:73:TRP:CB	2.21	0.70
1:A:131:HIS:ND1	1:A:132:ALA:N	2.39	0.70
1:B:115:LEU:HD11	1:B:148:GLU:OE2	1.94	0.68
1:C:220:ASP:OD2	1:C:222:LYS:N	2.26	0.68
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.28	0.67
1:A:218:LYS:H	1:A:228:ASP:HB2	1.60	0.67
2:D:1:NAG:O4	2:D:2:NAG:C2	2.42	0.66
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.44	0.65
1:A:220:ASP:CG	1:A:223:SER:HB2	2.17	0.65
1:B:69:MET:HE2	1:B:73:TRP:HB3	1.77	0.63
1:B:117:ASP:O	1:B:121:GLU:HG3	1.98	0.63
1:B:69:MET:HE3	1:B:73:TRP:HD1	1.59	0.63
1:C:219:THR:HG22	1:C:226:ILE:HA	1.80	0.63
1:A:229:PRO:O	1:A:232:GLN:NE2	2.31	0.61
1:A:220:ASP:HB3	1:A:223:SER:CB	2.26	0.61
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.99	0.60
1:A:131:HIS:ND1	1:A:133:SER:N	2.35	0.60
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.35	0.60
1:A:431:HIS:H	1:A:431:HIS:CD2	2.18	0.59
1:C:239:GLU:OE2	1:C:279:LYS:CD	2.51	0.59
1:A:253:ASP:O	1:A:254:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:HIS:CE1	1:A:133:SER:HB3	2.37	0.59
1:B:431:HIS:CD2	1:B:431:HIS:H	2.20	0.59
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.85	0.58
1:A:47:THR:O	1:A:53:ASN:HA	2.04	0.58
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.84	0.58
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.38	0.58
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.34	0.58
5:C:591:NBA:HC52	7:C:2263:HOH:O	2.04	0.58
1:B:243:SER:HB2	1:B:244:PRO:CD	2.34	0.57
1:B:360:GLN:NE2	7:B:2204:HOH:O	2.37	0.57
1:B:69:MET:HE3	1:B:73:TRP:CG	2.39	0.57
1:C:431:HIS:H	1:C:431:HIS:CD2	2.22	0.57
1:B:419:ARG:HD3	7:B:2242:HOH:O	2.05	0.57
1:B:69:MET:CE	1:B:73:TRP:HD1	2.18	0.57
1:A:131:HIS:CE1	1:A:133:SER:N	2.70	0.57
1:B:107:ASP:O	1:B:111:LYS:HG3	2.06	0.56
1:B:69:MET:CE	1:B:73:TRP:CD1	2.88	0.56
1:C:21:LYS:O	1:C:25:GLU:HG3	2.06	0.55
1:A:67:GLY:HA3	7:A:2097:HOH:O	2.05	0.55
1:B:411:ASN:HD22	1:B:414:GLU:H	1.54	0.55
1:C:228:ASP:OD1	1:C:229:PRO:HD2	2.07	0.55
2:D:1:NAG:O6	2:D:2:NAG:C1	2.56	0.54
3:E:1:NAG:O4	3:E:2:NAG:C2	2.50	0.53
1:B:49:PHE:O	1:B:50:ALA:HB3	2.09	0.53
1:B:69:MET:CE	1:B:74:PRO:CD	2.81	0.53
1:B:342:ALA:O	1:B:343:ASN:HB2	2.10	0.52
1:C:220:ASP:OD2	1:C:222:LYS:HB3	2.10	0.52
1:C:454:LEU:HD12	1:C:454:LEU:O	2.09	0.52
1:B:275:LEU:HD12	1:B:275:LEU:O	2.10	0.51
1:A:131:HIS:HD2	1:A:135:ARG:CZ	2.24	0.51
6:A:601:NAG:HO4	6:A:602:NAG:C1	2.14	0.50
1:B:131:HIS:HD2	1:B:133:SER:N	2.04	0.50
1:B:131:HIS:HD2	1:B:133:SER:CB	2.25	0.50
1:B:241:LYS:HA	1:B:279:LYS:O	2.12	0.50
1:C:374:ARG:HD2	7:C:2224:HOH:O	2.10	0.50
1:A:131:HIS:ND1	1:A:131:HIS:C	2.65	0.50
1:B:351:ASP:CG	1:B:352:GLU:H	2.14	0.50
1:A:218:LYS:N	1:A:228:ASP:HB2	2.26	0.50
1:C:158:VAL:HG12	7:C:2095:HOH:O	2.12	0.50
3:E:1:NAG:C3	3:E:5:FCA:O2	2.58	0.49
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ALA:O	1:C:343:ASN:HB2	2.13	0.49
1:B:134:GLY:HA2	1:B:181:GLN:OE1	2.13	0.49
1:A:454:LEU:HD12	1:A:454:LEU:O	2.13	0.48
1:C:64:VAL:O	1:C:65:ASN:HB2	2.12	0.48
1:A:219:THR:HG22	1:A:226:ILE:CA	2.42	0.48
5:B:591:NBA:H122	7:B:2091:HOH:O	2.13	0.48
1:B:169:TYR:CE2	5:B:591:NBA:H102	2.49	0.48
1:C:105:ASP:OD2	7:C:2060:HOH:O	2.20	0.47
1:B:63:GLY:HA2	1:B:193:GLY:O	2.14	0.47
1:B:131:HIS:CD2	1:B:133:SER:CB	2.98	0.47
1:C:303:LEU:O	1:C:344:VAL:HA	2.15	0.47
1:C:220:ASP:OD2	1:C:223:SER:N	2.48	0.47
1:B:252:GLU:C	1:B:254:ASN:H	2.18	0.47
1:A:434:GLU:HG2	1:A:435:HIS:CD2	2.50	0.46
1:B:58:ALA:HA	4:B:590:FAD:C4X	2.45	0.46
6:A:601:NAG:O4	6:A:602:NAG:C2	2.54	0.46
1:B:131:HIS:CD2	1:B:133:SER:OG	2.69	0.46
1:B:104:TYR:CZ	1:B:158:VAL:CG2	2.99	0.46
1:A:411:ASN:OD1	1:A:414:GLU:CG	2.55	0.46
1:B:416:ASP:OD2	1:B:466:HIS:HD2	1.99	0.46
3:E:2:NAG:H62	3:E:5:FCA:H5	1.97	0.46
1:A:220:ASP:CB	1:A:223:SER:CB	2.93	0.46
1:A:170:GLU:OE2	5:A:591:NBA:H121	2.16	0.46
1:B:317:GLU:O	1:B:333:GLN:HA	2.16	0.46
1:C:6:ARG:HA	1:C:30:ASP:O	2.16	0.46
1:C:260:ASP:O	1:C:424:ARG:HD3	2.15	0.45
1:A:328:TYR:O	1:A:329:TYR:C	2.54	0.45
1:A:350:THR:HA	1:A:354:SER:OG	2.16	0.45
5:C:591:NBA:H122	7:C:2101:HOH:O	2.15	0.45
1:A:342:ALA:O	1:A:343:ASN:HB2	2.17	0.44
1:B:253:ASP:O	1:B:254:ASN:HB2	2.18	0.44
1:C:253:ASP:O	1:C:254:ASN:HB2	2.17	0.44
1:A:228:ASP:OD1	1:A:229:PRO:HD2	2.18	0.44
1:A:460:LYS:HB3	1:A:462:MET:CE	2.48	0.44
1:B:220:ASP:O	1:B:224:GLY:N	2.48	0.44
1:A:131:HIS:CE1	1:A:133:SER:CB	3.00	0.44
1:A:91:TYR:CD1	1:A:91:TYR:N	2.86	0.44
1:A:448:ILE:O	1:A:452:GLU:HG3	2.18	0.44
1:B:76:VAL:HG13	1:B:82:LEU:HB2	2.00	0.43
1:A:158:VAL:HG12	7:A:2074:HOH:O	2.18	0.43
1:A:290:ILE:HA	1:A:418:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:HIS:HD2	1:B:133:SER:OG	2.02	0.43
5:A:591:NBA:HC52	7:A:2228:HOH:O	2.18	0.43
1:B:151:PRO:HG2	1:B:152:ASN:HD22	1.82	0.43
1:A:66:GLY:HA3	1:A:193:GLY:CA	2.49	0.43
1:A:124:GLU:OE2	7:A:2053:HOH:O	2.21	0.43
1:A:253:ASP:O	1:A:254:ASN:CB	2.63	0.43
1:A:291:TYR:CG	1:B:146:LEU:HA	2.54	0.42
1:C:220:ASP:HB3	1:C:223:SER:OG	2.19	0.42
1:B:292:GLN:NE2	7:B:2156:HOH:O	2.50	0.42
1:B:307:ARG:HG2	1:B:383:PRO:HG3	2.01	0.42
1:C:63:GLY:HA2	1:C:193:GLY:O	2.19	0.42
1:A:223:SER:HB3	1:A:225:LYS:H	1.84	0.42
1:C:402:THR:HG22	4:C:590:FAD:HM83	2.01	0.42
1:C:156:THR:O	1:C:160:MET:HG3	2.19	0.42
1:C:360:GLN:NE2	7:C:2211:HOH:O	2.51	0.42
1:A:253:ASP:OD1	1:A:253:ASP:C	2.58	0.42
1:A:431:HIS:CD2	7:A:2219:HOH:O	2.72	0.42
1:A:228:ASP:HA	1:A:229:PRO:HD3	1.84	0.42
1:B:411:ASN:C	1:B:411:ASN:HD22	2.23	0.42
1:C:453:ILE:HA	1:C:453:ILE:HD13	1.76	0.41
1:C:191:ASP:OD2	1:C:436:TYR:OH	2.33	0.41
1:A:366:LYS:HD2	1:A:385:ALA:HB3	2.02	0.41
1:A:64:VAL:O	1:A:65:ASN:HB2	2.20	0.41
5:C:591:NBA:C12	7:C:2101:HOH:O	2.68	0.41
1:C:355:ARG:O	1:C:359:GLN:HG3	2.20	0.41
1:C:105:ASP:OD2	1:C:106:GLU:N	2.53	0.41
1:A:79:THR:HG22	1:A:80:LEU:CD2	2.45	0.41
1:A:45:HIS:CD2	1:A:56:LEU:HD12	2.56	0.40
1:B:243:SER:CB	1:B:244:PRO:CD	2.96	0.40
1:A:241:LYS:HG2	1:A:279:LYS:HB2	2.03	0.40
1:A:351:ASP:CG	1:A:352:GLU:H	2.25	0.40
1:B:141:LEU:HD22	1:B:176:ARG:HB3	2.02	0.40
1:B:431:HIS:CD2	7:B:2251:HOH:O	2.75	0.40
3:E:1:NAG:O6	3:E:2:NAG:C1	2.70	0.40

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	Percentiles	
1	A	457/472 (97%)	438 (96%)	18 (4%)	1 (0%)	47	44
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%)	51	49

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%)	50	53
1	B	397/404 (98%)	388 (98%)	9 (2%)	50	53
1	C	397/404 (98%)	391 (98%)	6 (2%)	65	69
All	All	1188/1212 (98%)	1164 (98%)	24 (2%)	55	58

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	131	HIS

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Mol	Chain	Res	Type
1	A	165	TYR
1	A	168	ASP
1	A	177	VAL
1	A	205	TYR
1	A	217	LEU
1	A	223	SER
1	A	386	THR
1	B	59	ASN
1	B	127	SER
1	B	154	PRO
1	B	168	ASP
1	B	205	TYR
1	B	275	LEU
1	B	381	ASP
1	B	411	ASN
1	B	454	LEU
1	C	59	ASN
1	C	149	HIS
1	C	168	ASP
1	C	205	TYR
1	C	221	ASP
1	C	418	LEU

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	48	ASN
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	292	GLN
1	B	359	GLN
1	B	360	GLN
1	B	364	GLN
1	B	411	ASN
1	B	431	HIS
1	B	466	HIS
1	C	48	ASN
1	C	360	GLN

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Mol	Chain	Res	Type
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 ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	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	6 (35%)
3	NAG	E	1	1,3	14,14,15	1.29	2 (14%)	17,19,21	1.97	6 (35%)
3	NAG	E	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.86	5 (29%)
3	MAN	E	3	3	11,11,12	0.74	0	15,15,17	3.29	5 (33%)
3	MAN	E	4	3	11,11,12	0.62	0	15,15,17	1.92	3 (20%)
3	FCA	E	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	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	2/2/4/5	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	FCA	E	5	3	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C1	-3.49	1.38	1.43
3	E	5	FCA	C2-C3	-3.46	1.47	1.52
3	E	2	NAG	O5-C1	-2.88	1.39	1.43
3	E	1	NAG	C1-C2	-2.83	1.48	1.52
2	D	2	NAG	C1-C2	-2.79	1.48	1.52
3	E	1	NAG	O5-C5	2.32	1.48	1.43
2	D	1	NAG	O5-C1	-2.10	1.40	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	MAN	O2-C2-C3	10.24	130.65	110.14
3	E	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	E	2	NAG	O5-C5-C6	-5.00	99.36	107.20
3	E	3	MAN	C1-O5-C5	3.97	117.57	112.19
3	E	3	MAN	O2-C2-C1	3.97	117.27	109.15
3	E	1	NAG	O5-C5-C6	-3.89	101.11	107.20
3	E	3	MAN	O5-C5-C6	3.64	112.92	107.20
2	D	1	NAG	C1-O5-C5	3.48	116.90	112.19
2	D	2	NAG	C1-C2-N2	-3.42	104.64	110.49
3	E	2	NAG	O5-C5-C4	-3.39	102.57	110.83
3	E	1	NAG	C1-C2-N2	-3.32	104.82	110.49
2	D	1	NAG	C2-N2-C7	-3.25	118.27	122.90
2	D	1	NAG	O3-C3-C4	3.19	117.72	110.35
3	E	4	MAN	O2-C2-C3	3.00	116.14	110.14
3	E	5	FCA	C3-C4-C5	-2.91	105.24	109.77
3	E	1	NAG	O7-C7-C8	2.84	127.32	122.06
3	E	1	NAG	C8-C7-N2	-2.81	111.34	116.10
3	E	5	FCA	C2-C3-C4	-2.80	106.06	110.89
3	E	4	MAN	C2-C3-C4	-2.75	106.14	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	MAN	O4-C4-C3	2.75	116.70	110.35
3	E	1	NAG	O4-C4-C3	-2.71	104.08	110.35
3	E	2	NAG	C3-C4-C5	2.68	115.02	110.24
2	D	2	NAG	O5-C1-C2	-2.56	107.25	111.29
2	D	2	NAG	C4-C3-C2	2.46	114.62	111.02
2	D	2	NAG	C2-N2-C7	-2.38	119.51	122.90
3	E	5	FCA	O5-C1-C2	-2.38	107.09	110.77
3	E	1	NAG	O5-C5-C4	-2.24	105.37	110.83
3	E	2	NAG	C2-N2-C7	-2.19	119.78	122.90
2	D	2	NAG	C1-O5-C5	2.18	115.14	112.19
3	E	2	NAG	O5-C1-C2	-2.07	108.01	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	3	MAN	C2
3	E	3	MAN	C1

All (10) torsion outliers are listed below:

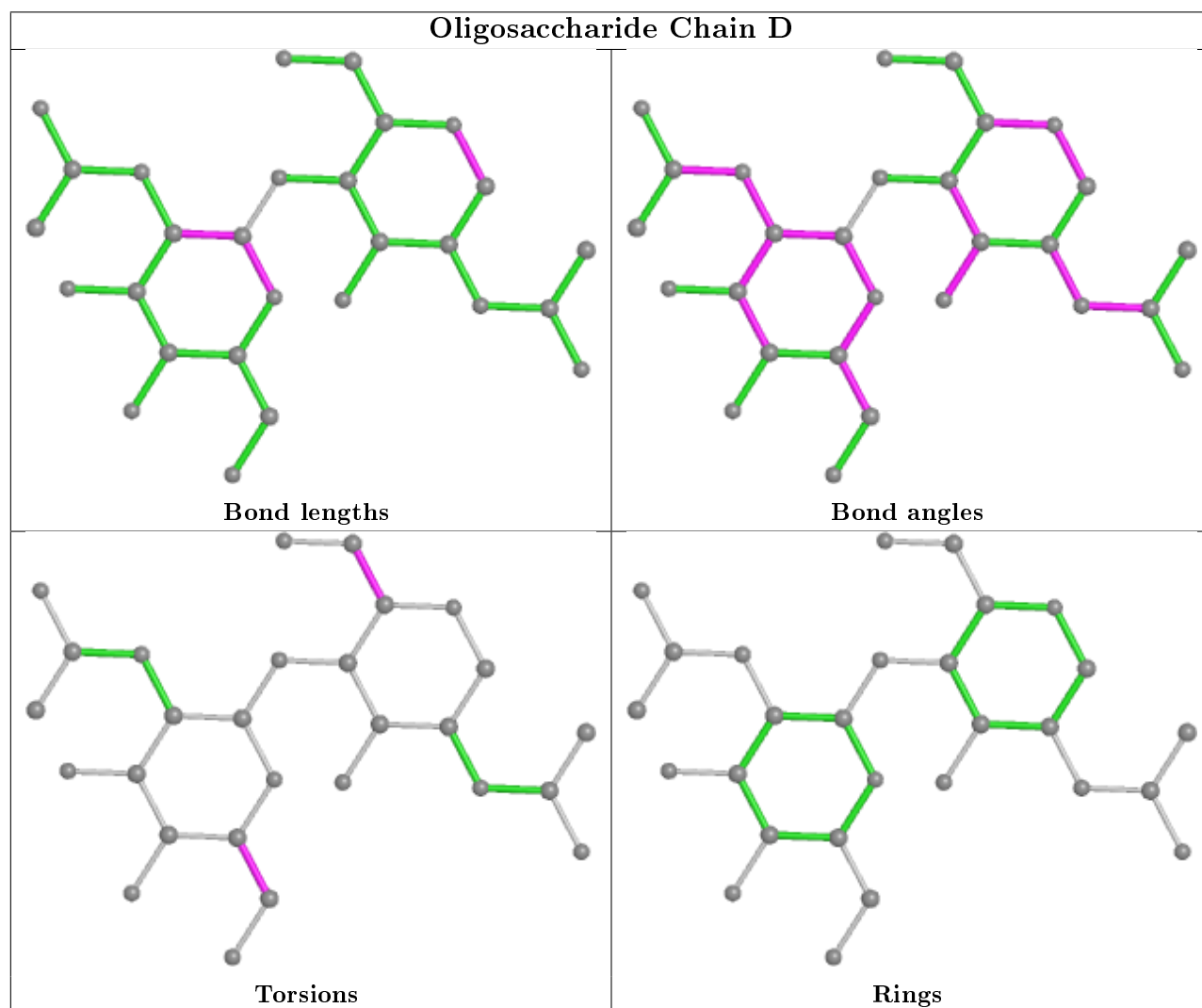
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

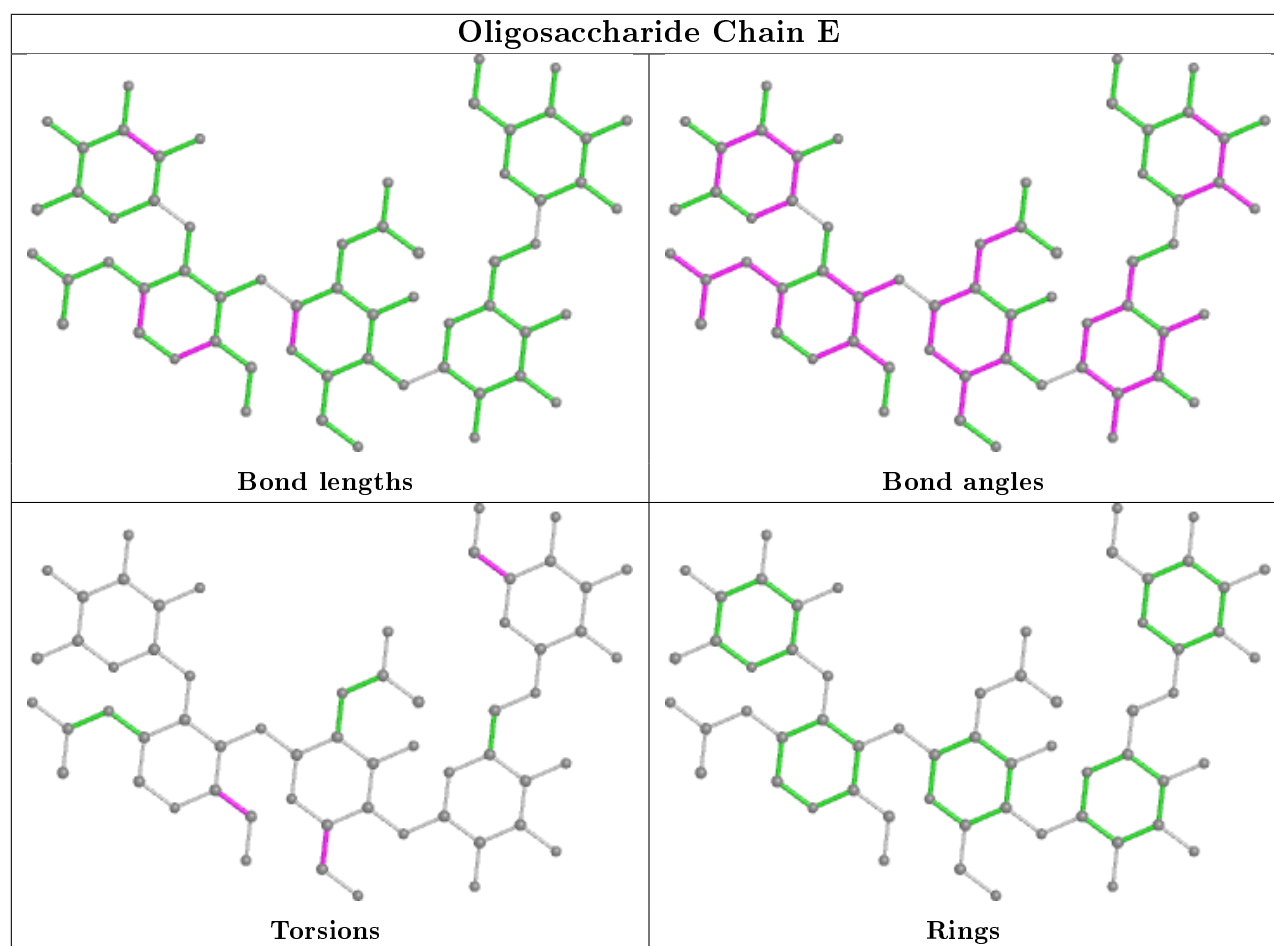
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	3	1
3	E	5	FCA	3	0
3	E	2	NAG	4	0
3	E	1	NAG	5	0
2	D	1	NAG	3	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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NBA	B	591	4	13,13,14	0.58	0	12,12,14	1.81	4 (33%)
6	NAG	A	601	1	14,14,15	1.01	1 (7%)	17,19,21	2.38	6 (35%)
5	NBA	C	591	4	13,13,14	0.56	0	12,12,14	2.11	3 (25%)
5	NBA	A	591	4	13,13,14	0.55	0	12,12,14	1.51	4 (33%)
4	FAD	B	590	5	51,58,58	1.27	4 (7%)	60,89,89	1.91	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	C	590	5	51,58,58	1.36	6 (11%)	60,89,89	2.34	17 (28%)
4	FAD	A	590	5	51,58,58	1.17	5 (9%)	60,89,89	2.72	15 (25%)
6	NAG	A	602	-	14,14,15	0.89	1 (7%)	17,19,21	1.21	2 (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
5	NBA	B	591	4	-	5/11/11/12	-
6	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NBA	C	591	4	-	3/11/11/12	-
5	NBA	A	591	4	-	4/11/11/12	-
4	FAD	B	590	5	-	3/30/50/50	0/6/6/6
4	FAD	C	590	5	-	5/30/50/50	0/6/6/6
4	FAD	A	590	5	-	1/30/50/50	0/6/6/6
6	NAG	A	602	-	-	2/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	590	FAD	C4X-C10	5.03	1.43	1.38
4	B	590	FAD	C4-N3	4.34	1.40	1.33
4	B	590	FAD	C4X-C10	3.95	1.42	1.38
4	C	590	FAD	C4-N3	3.74	1.39	1.33
4	A	590	FAD	C4X-C10	3.40	1.42	1.38
4	A	590	FAD	C4-N3	3.31	1.38	1.33
4	A	590	FAD	C2-N1	-3.24	1.31	1.38
4	B	590	FAD	C4X-N5	2.99	1.37	1.33
4	C	590	FAD	C10-N1	2.98	1.37	1.33
4	C	590	FAD	C4X-N5	2.78	1.37	1.33
4	B	590	FAD	C2-N1	-2.65	1.32	1.38
4	C	590	FAD	C2-N1	-2.64	1.32	1.38
4	A	590	FAD	C4X-N5	2.56	1.37	1.33
6	A	601	NAG	O5-C1	-2.42	1.39	1.43
4	A	590	FAD	C5'-C4'	2.32	1.55	1.51
6	A	602	NAG	O5-C1	-2.11	1.40	1.43
4	C	590	FAD	C4-C4X	2.08	1.44	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	590	FAD	C4-N3-C2	11.89	125.18	115.14
4	C	590	FAD	C4-N3-C2	10.73	124.20	115.14
4	A	590	FAD	C4-C4X-C10	-6.96	115.34	119.95
4	A	590	FAD	C1'-N10-C9A	6.88	123.70	118.29
4	B	590	FAD	C4-N3-C2	6.28	120.45	115.14
4	B	590	FAD	C1'-N10-C10	5.43	123.27	118.41
5	C	591	NBA	C9-C8-N7	-5.28	97.89	112.14
4	A	590	FAD	C4X-C4-N3	-5.16	116.37	123.43
4	C	590	FAD	C4X-C4-N3	-4.94	116.67	123.43
4	A	590	FAD	C4X-C10-N10	-4.91	115.26	120.30
6	A	601	NAG	O5-C5-C6	-4.84	99.62	107.20
4	C	590	FAD	C4-C4X-N5	4.72	123.99	118.60
4	C	590	FAD	C4-C4X-C10	-4.70	116.84	119.95
4	B	590	FAD	O4B-C1B-C2B	-4.58	100.24	106.93
6	A	601	NAG	C1-O5-C5	4.56	118.37	112.19
4	A	590	FAD	C5X-C9A-N10	4.55	121.01	117.72
4	C	590	FAD	C4X-C10-N10	-4.50	115.68	120.30
4	B	590	FAD	C4X-C4-N3	-4.44	117.35	123.43
6	A	601	NAG	C2-N2-C7	-4.21	116.90	122.90
4	A	590	FAD	C4-C4X-N5	3.98	123.15	118.60
4	B	590	FAD	C4A-C5A-N7A	3.97	113.54	109.40
4	B	590	FAD	C9A-N10-C10	-3.95	116.74	121.91
4	C	590	FAD	O4B-C1B-C2B	-3.81	101.35	106.93
5	B	591	NBA	C6-C5-C4	3.73	118.81	112.99
4	A	590	FAD	O4B-C1B-C2B	-3.69	101.53	106.93
4	A	590	FAD	C1'-N10-C10	-3.66	115.13	118.41
5	C	591	NBA	C9-C10-N11	-3.65	102.30	112.14
4	A	590	FAD	O2A-PA-O1A	3.19	128.03	112.24
4	C	590	FAD	C10-C4X-N5	-3.04	119.15	121.26
4	B	590	FAD	C6-C5X-N5	-3.04	115.70	119.05
6	A	601	NAG	C8-C7-N2	-3.03	110.97	116.10
4	C	590	FAD	C1'-N10-C9A	3.03	120.67	118.29
4	A	590	FAD	C5A-C6A-N6A	2.94	124.83	120.35
4	A	590	FAD	C9A-C5X-N5	-2.85	117.91	122.36
6	A	601	NAG	O3-C3-C4	2.73	116.67	110.35
5	A	591	NBA	C9-C10-N11	-2.67	104.94	112.14
6	A	602	NAG	C8-C7-N2	-2.66	111.60	116.10
4	C	590	FAD	C4'-C3'-C2'	2.60	118.77	113.36
4	C	590	FAD	O2'-C2'-C1'	-2.55	103.46	109.59
5	B	591	NBA	C14-C13-C12	-2.52	105.05	114.26
4	C	590	FAD	O3B-C3B-C2B	-2.50	103.73	111.82
5	B	591	NBA	C9-C10-N11	-2.50	105.41	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	590	FAD	C6-C7-C8	-2.45	115.79	119.91
5	C	591	NBA	C12-N11-C10	-2.43	101.99	113.45
6	A	601	NAG	O7-C7-C8	2.42	126.55	122.06
4	B	590	FAD	O2P-P-O1P	2.42	124.18	112.24
4	C	590	FAD	P-O3P-PA	-2.36	124.72	132.83
4	C	590	FAD	O2A-PA-O1A	2.34	123.81	112.24
5	A	591	NBA	C6-C5-C4	-2.30	109.40	112.99
5	A	591	NBA	C12-N11-C10	-2.29	102.67	113.45
4	B	590	FAD	C4'-C3'-C2'	2.28	118.11	113.36
5	B	591	NBA	C9-C8-N7	-2.23	106.12	112.14
4	C	590	FAD	C3B-C2B-C1B	2.20	104.30	100.98
4	B	590	FAD	O2'-C2'-C1'	2.15	114.77	109.59
4	A	590	FAD	C9-C8-C7	2.14	123.52	119.91
4	C	590	FAD	O5'-C5'-C4'	-2.14	103.65	109.36
4	B	590	FAD	O2P-P-O5'	2.14	117.68	107.75
6	A	602	NAG	O7-C7-N2	2.14	125.88	121.95
4	C	590	FAD	C5A-C6A-N6A	2.13	123.59	120.35
4	C	590	FAD	C8M-C8-C9	-2.12	115.26	120.34
4	A	590	FAD	O2P-P-O1P	2.11	122.66	112.24
5	A	591	NBA	C14-C13-C12	-2.02	106.88	114.26

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	NAG	C4-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	A	602	NAG	O5-C5-C6-O6
5	C	591	NBA	N11-C12-C13-C14
5	A	591	NBA	N11-C10-C9-C8
6	A	601	NAG	O5-C5-C6-O6
5	A	591	NBA	N11-C12-C13-C14
5	B	591	NBA	N11-C12-C13-C14
5	B	591	NBA	C12-C13-C14-N15
5	A	591	NBA	C9-C10-N11-C12
5	C	591	NBA	N7-C8-C9-C10
5	B	591	NBA	N7-C8-C9-C10
4	C	590	FAD	C2'-C3'-C4'-O4'
4	B	590	FAD	C2'-C3'-C4'-O4'
4	B	590	FAD	PA-O3P-P-O5'
5	C	591	NBA	N11-C10-C9-C8
5	B	591	NBA	N11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	C	590	FAD	C2'-C3'-C4'-C5'
5	B	591	NBA	C4-C5-C6-N7
4	C	590	FAD	O3'-C3'-C4'-C5'
4	C	590	FAD	O3'-C3'-C4'-O4'
5	A	591	NBA	N7-C8-C9-C10
4	B	590	FAD	O4B-C4B-C5B-O5B
4	C	590	FAD	O4B-C4B-C5B-O5B
4	A	590	FAD	O4B-C4B-C5B-O5B

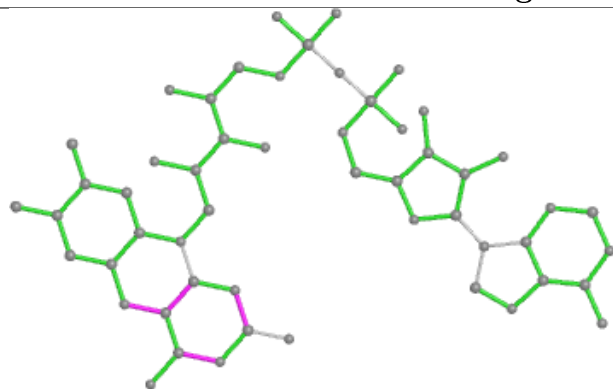
There are no ring outliers.

7 monomers are involved in 14 short contacts:

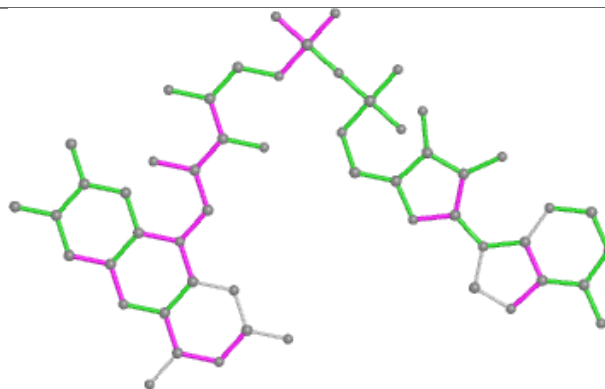
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	591	NBA	2	0
6	A	601	NAG	4	0
5	C	591	NBA	3	0
5	A	591	NBA	3	0
4	B	590	FAD	1	0
4	C	590	FAD	1	0
6	A	602	NAG	4	0

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

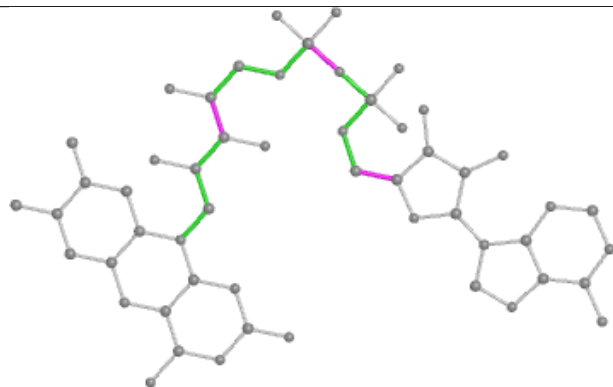
Ligand FAD B 590



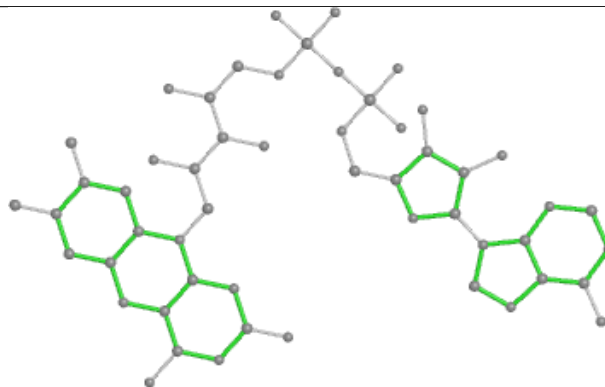
Bond lengths



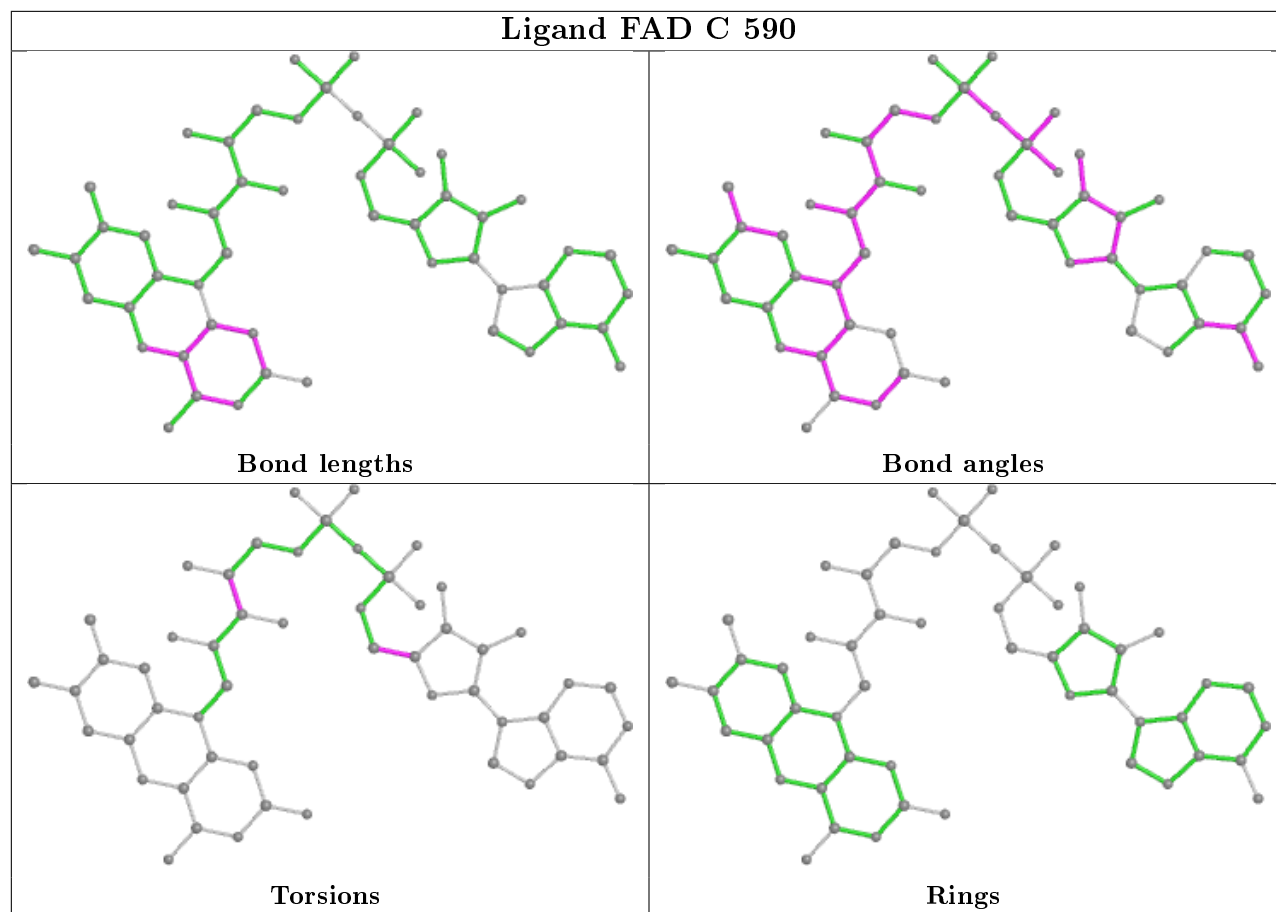
Bond angles

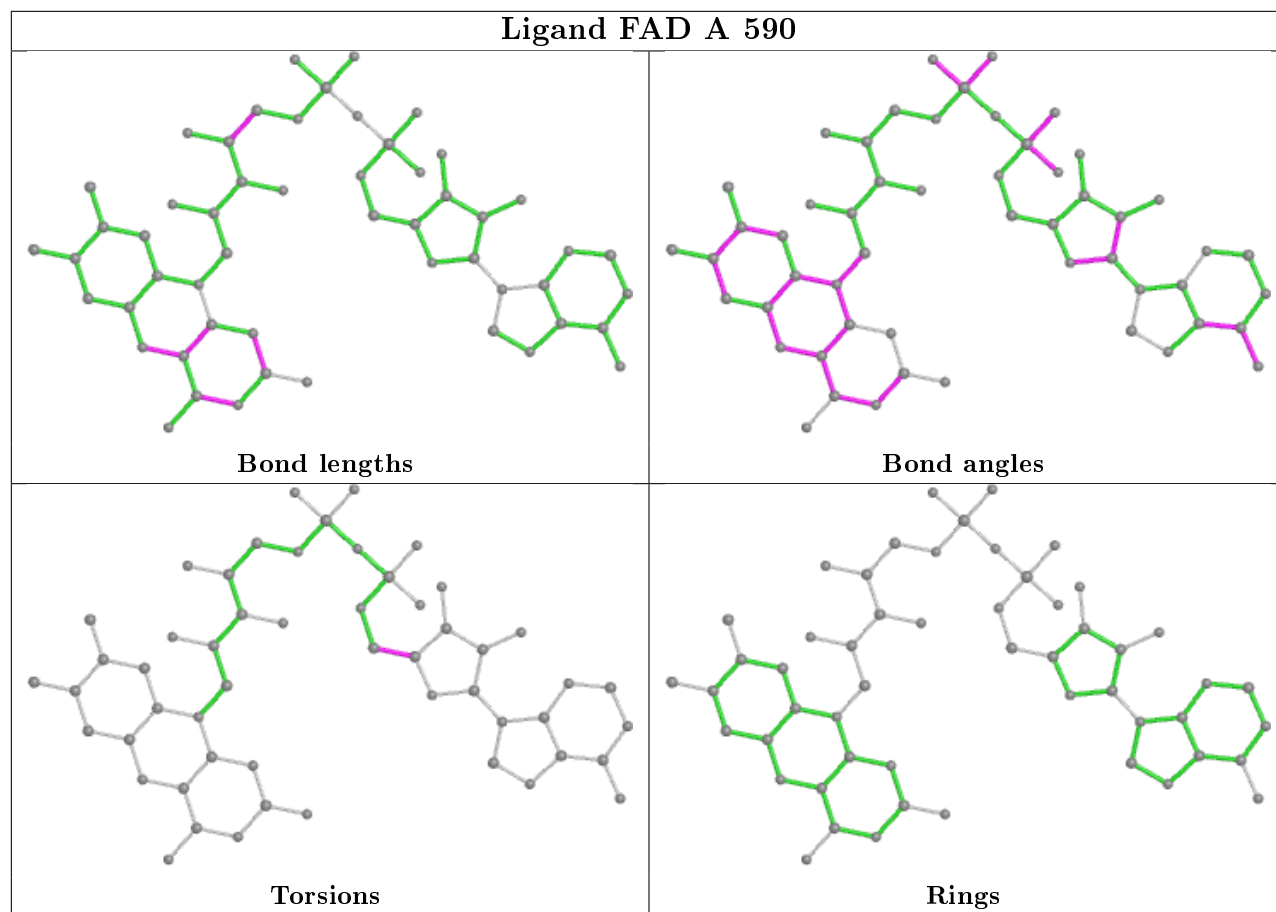


Torsions



Rings





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.