WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 5, 2023 – 06:41 am GMT

PDB ID	:	1H82
Title	:	STRUCTURE OF POLYAMINE OXIDASE IN COMPLEX WITH GUAZATINE
Authors	:	Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on	:	2001-01-24
Resolution	:	1.90 Å(reported)

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

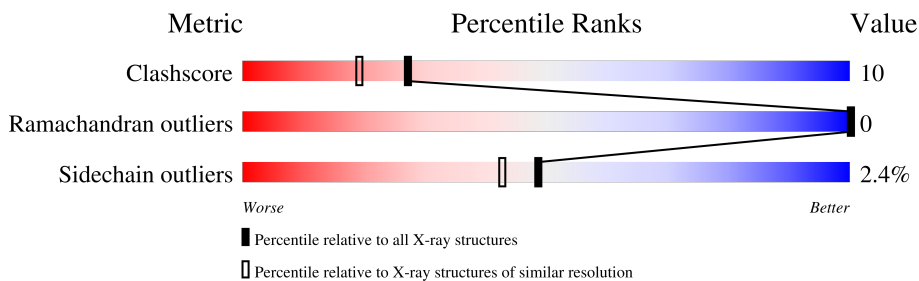|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		2.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	77% 19% • •
1	B	472	76% 20% • •
1	C	472	81% 15% • •
2	D	2	100%
2	E	2	100%
3	F	5	40% 60%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	1	-	-	X	-
3	MAN	F	3	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 12210 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.
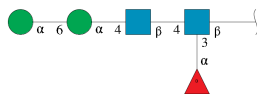
- Molecule 1 is a protein called POLYAMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	54	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	41	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			
2	E	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	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

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

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 N-{8-[(8-{[(E)-AMINO(IMINO)METHYL]AMINO}OCTYL)AMINO]OCTYL}GUANIDINE (three-letter code: GZZ) (formula: $C_{18}H_{41}N_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 25	C 18	N 7	0	0
5	B	1	Total 25	C 18	N 7	0	0
5	C	1	Total 25	C 18	N 7	0	0

• Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	234	Total 234	O 234	0	0
6	B	243	Total 243	O 243	0	0
6	C	269	Total 269	O 269	0	0

3 Residue-property plots ⓘ

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.
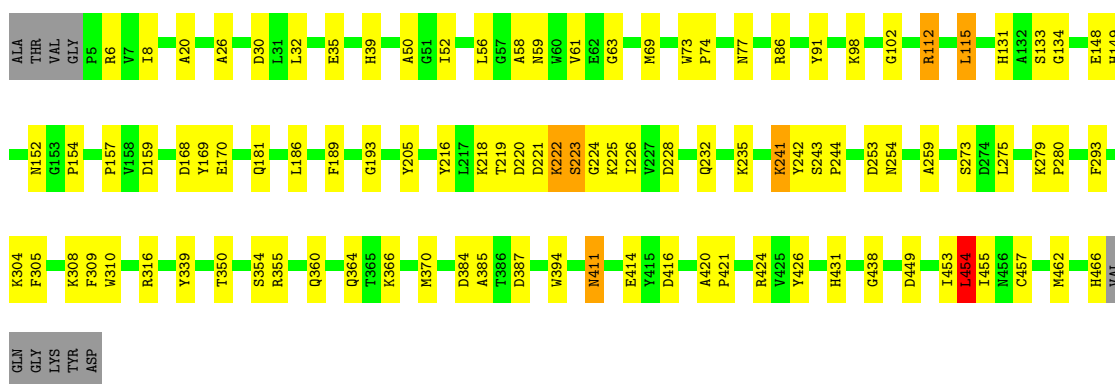
Note EDS was not executed.
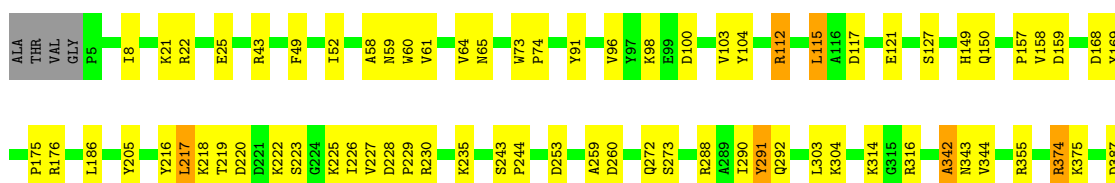
• Molecule 1: POLYAMINE OXIDASE

Chain A:
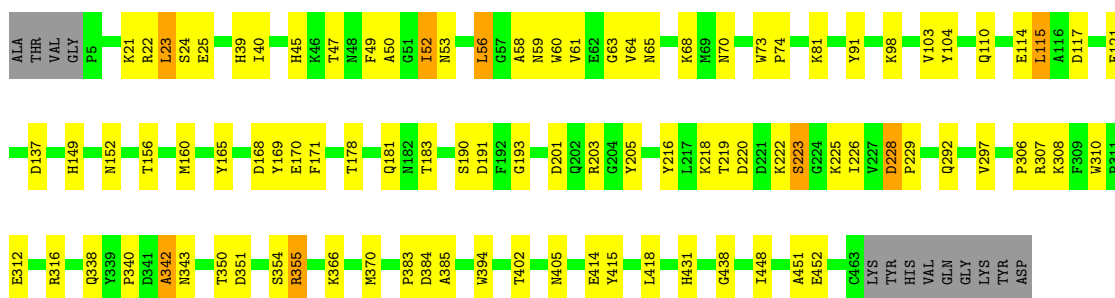
• Molecule 1: POLYAMINE OXIDASE

Chain B:

• Molecule 1: POLYAMINE OXIDASE

Chain C:

R412 L418 R424 H431 E434 G438 L454 H466 VAL GLN GLY LYS TYR ASP

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

Chain D: 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 40%   60%

NAG1 NAG2 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	184.97Å 184.97Å 282.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	94.3 (50.00-1.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.199 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12210	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: GZZ, MAN, FAD, NAG, FCA

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	0.66	0/3775	1.17	13/5116 (0.3%)
1	B	0.66	0/3808	1.18	17/5160 (0.3%)
1	C	0.68	0/3808	1.17	16/5160 (0.3%)
All	All	0.67	0/11391	1.17	46/15436 (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	A	1	0
1	C	0	1
All	All	1	1

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	355	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	A	342	ALA	N-CA-C	8.13	132.95	111.00
1	C	112	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	112	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	C	115	LEU	CB-CG-CD1	-6.55	99.86	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	341	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	291	TYR	Sidechain

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	66	0
1	B	3715	0	3614	87	0
1	C	3715	0	3614	55	0
2	D	28	0	26	2	0
2	E	28	0	26	4	0
3	F	60	0	53	8	0
4	A	53	0	31	4	0
4	B	53	0	31	2	0
4	C	53	0	31	2	0
5	A	25	0	39	7	0
5	B	25	0	39	4	0
5	C	25	0	39	2	0
6	A	234	0	0	5	0
6	B	243	0	0	5	0
6	C	269	0	0	9	0
All	All	12210	0	11128	221	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 10.

The worst 5 of 221 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:C:272:GLN:HA	6:C:2151:HOH:O	1.25	1.28
1:A:220:ASP:HB3	1:A:223:SER:HB2	1.25	1.12
1:A:308:LYS:HZ3	1:A:312:GLU:HG3	0.94	1.10
1:C:219:THR:HG22	1:C:226:ILE:HA	1.43	1.00
1:B:220:ASP:HB3	1:B:223:SER:HB2	1.44	0.98

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%)	437 (96%)	20 (4%)	0	100	100
1	B	460/472 (98%)	441 (96%)	19 (4%)	0	100	100
1	C	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
All	All	1377/1416 (97%)	1321 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	384 (98%)	10 (2%)	47	41
1	B	397/404 (98%)	388 (98%)	9 (2%)	50	45
1	C	397/404 (98%)	387 (98%)	10 (2%)	47	41
All	All	1188/1212 (98%)	1159 (98%)	29 (2%)	49	43

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	205	TYR
1	C	217	LEU
1	B	411	ASN
1	C	168	ASP
1	B	293	PHE

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

Mol	Chain	Res	Type
1	C	360	GLN
1	C	431	HIS
1	B	152	ASN
1	B	292	GLN
1	B	360	GLN

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 ⓘ

9 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	2,1	14,14,15	0.95	2 (14%)	17,19,21	1.62	5 (29%)
2	NAG	D	2	2	14,14,15	0.91	0	17,19,21	1.79	4 (23%)
2	NAG	E	1	2,1	14,14,15	1.26	3 (21%)	17,19,21	2.42	4 (23%)
2	NAG	E	2	2	14,14,15	0.97	1 (7%)	17,19,21	1.41	3 (17%)
3	NAG	F	1	3,1	14,14,15	1.30	2 (14%)	17,19,21	2.02	6 (35%)
3	NAG	F	2	3	14,14,15	0.99	1 (7%)	17,19,21	1.63	4 (23%)
3	MAN	F	3	3	11,11,12	0.66	0	15,15,17	2.60	3 (20%)
3	MAN	F	4	3	11,11,12	0.60	0	15,15,17	1.55	3 (20%)
3	FCA	F	5	3	10,10,11	1.21	1 (10%)	14,14,16	1.66	5 (35%)

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

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-2.90	1.39	1.43
3	F	2	NAG	O5-C1	-2.87	1.39	1.43
2	E	1	NAG	O5-C1	-2.87	1.39	1.43
3	F	5	FCA	C2-C3	-2.57	1.48	1.52
3	F	1	NAG	C1-C2	-2.34	1.48	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	MAN	O2-C2-C3	8.85	127.86	110.14
2	E	1	NAG	C2-N2-C7	-6.49	113.67	122.90
3	F	1	NAG	C1-C2-N2	-5.09	101.79	110.49
2	D	2	NAG	C2-N2-C7	-4.87	115.97	122.90
3	F	2	NAG	C2-N2-C7	-4.70	116.21	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	3	MAN	C1

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6

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

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	2	0
3	F	2	NAG	6	0
2	E	1	NAG	4	0
3	F	5	FCA	3	0
2	D	1	NAG	2	0
3	F	1	NAG	7	0
2	E	2	NAG	4	0

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

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
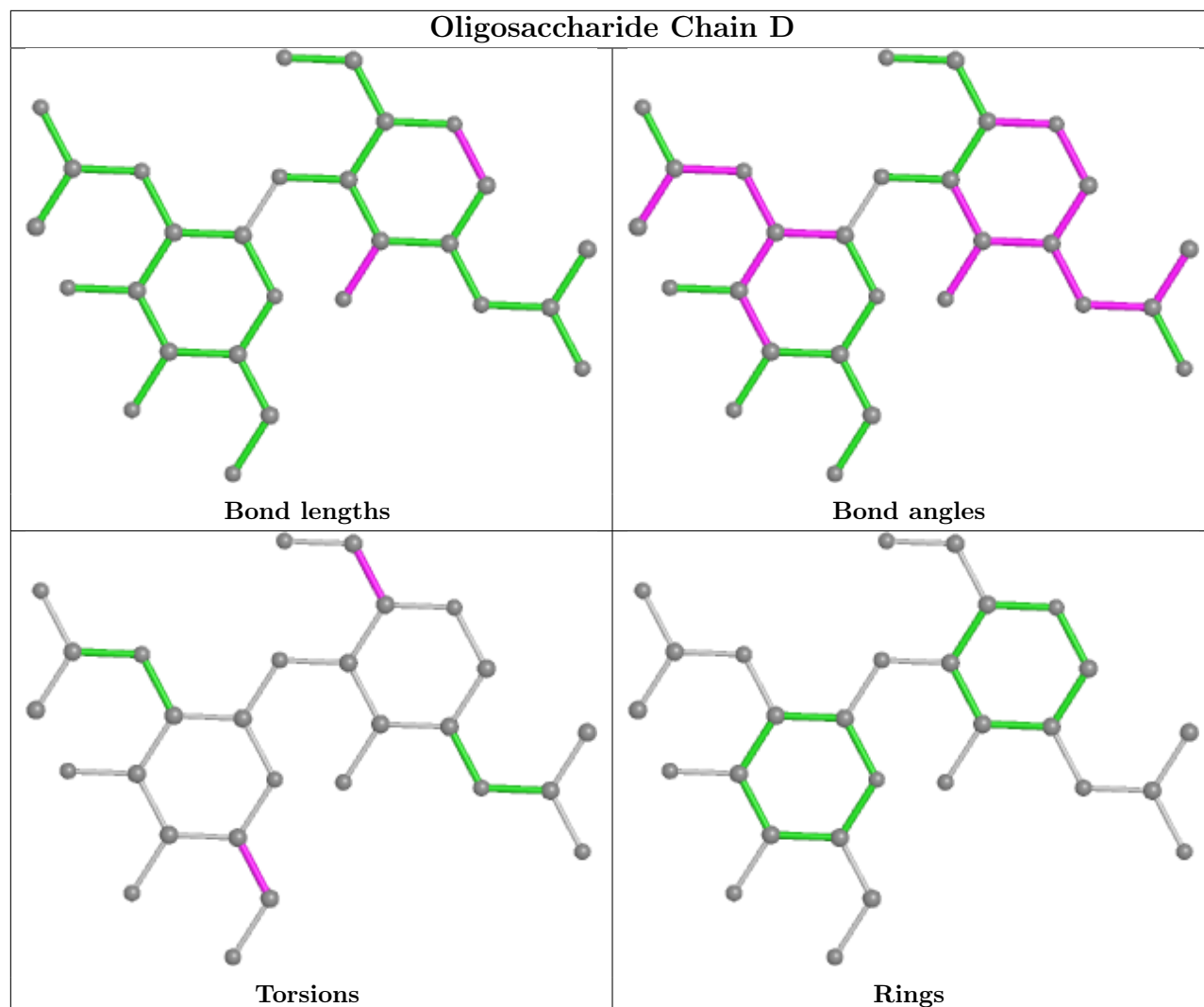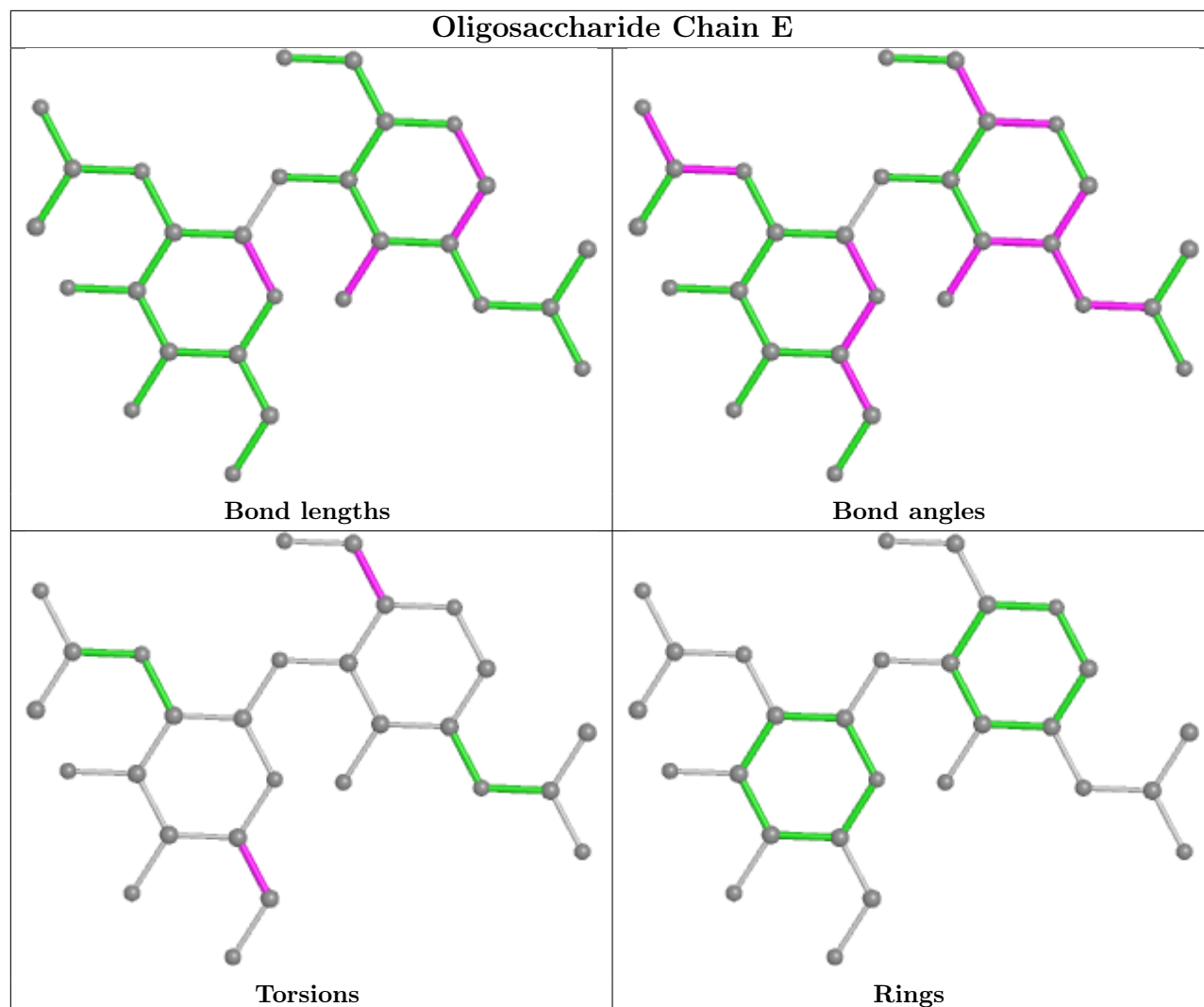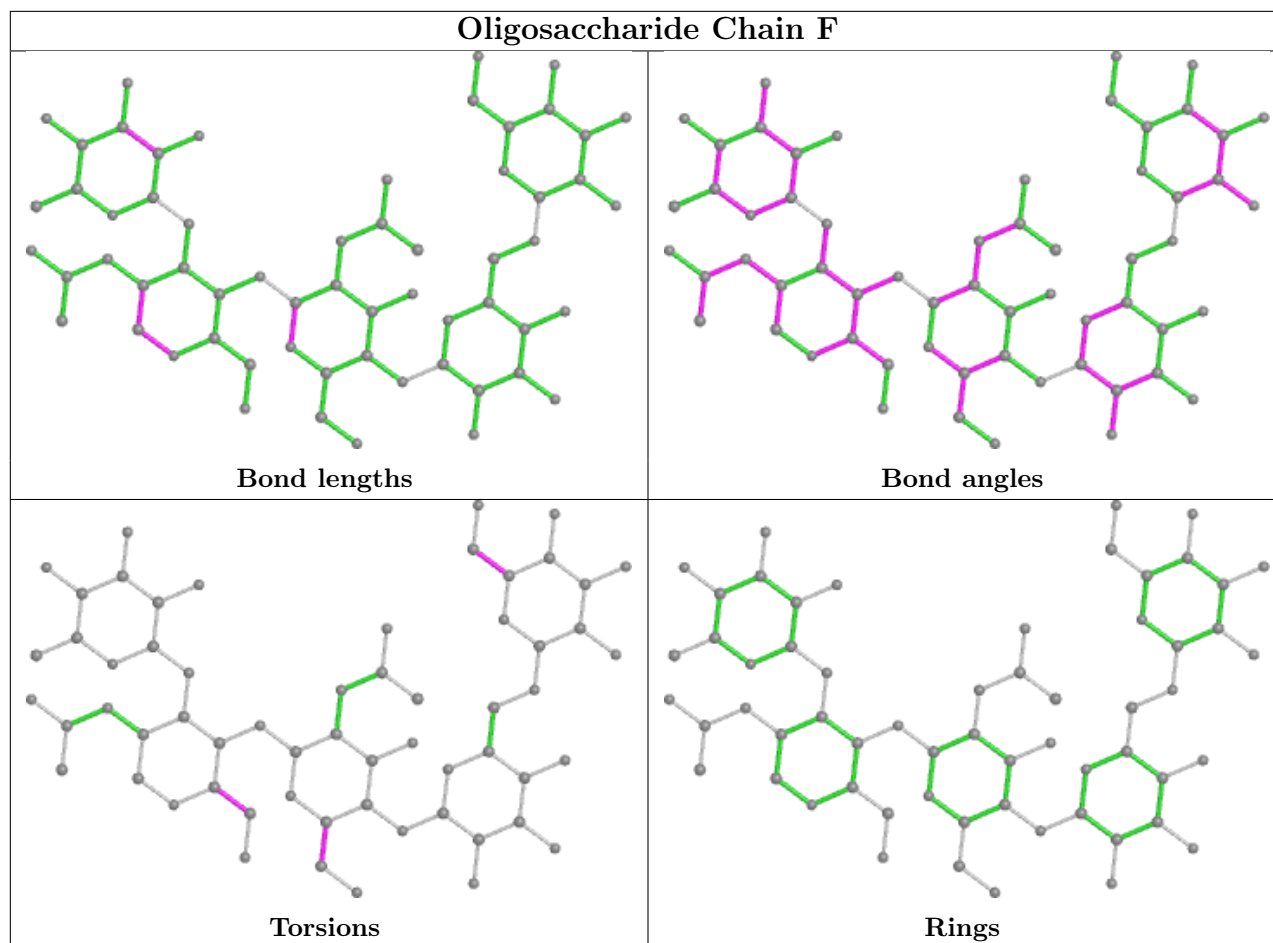
5.6 Ligand geometry ⓘ

6 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	GZZ	B	590	-	24,24,24	1.13	2 (8%)	23,25,25	1.63	4 (17%)
5	GZZ	A	590	-	24,24,24	0.92	2 (8%)	23,25,25	1.47	5 (21%)
4	FAD	A	579	-	53,58,58	0.81	1 (1%)	68,89,89	1.37	7 (10%)
4	FAD	B	579	-	53,58,58	0.91	1 (1%)	68,89,89	1.27	7 (10%)
5	GZZ	C	590	-	24,24,24	1.09	2 (8%)	23,25,25	1.37	5 (21%)
4	FAD	C	579	-	53,58,58	1.06	1 (1%)	68,89,89	1.38	8 (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	GZZ	B	590	-	-	14/22/22/22	-
5	GZZ	A	590	-	-	12/22/22/22	-
4	FAD	A	579	-	-	4/30/50/50	0/6/6/6
4	FAD	B	579	-	-	9/30/50/50	0/6/6/6
5	GZZ	C	590	-	-	10/22/22/22	-
4	FAD	C	579	-	-	1/30/50/50	0/6/6/6

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	579	FAD	C4X-N5	3.63	1.37	1.30
5	B	590	GZZ	C8-N9	3.11	1.57	1.46
5	B	590	GZZ	C10-N9	2.92	1.56	1.46
5	C	590	GZZ	C8-N9	2.86	1.56	1.46
5	C	590	GZZ	C10-N9	2.83	1.56	1.46

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	579	FAD	C9A-C5X-N5	-4.85	117.16	122.43
4	C	579	FAD	C4-C4X-N5	3.87	123.74	118.23
4	C	579	FAD	C9A-C5X-N5	-3.84	118.26	122.43
4	B	579	FAD	C5A-C6A-N6A	3.82	126.16	120.35
5	A	590	GZZ	NE1-CZ1-NH1	-3.64	114.29	120.70

There are no chirality outliers.

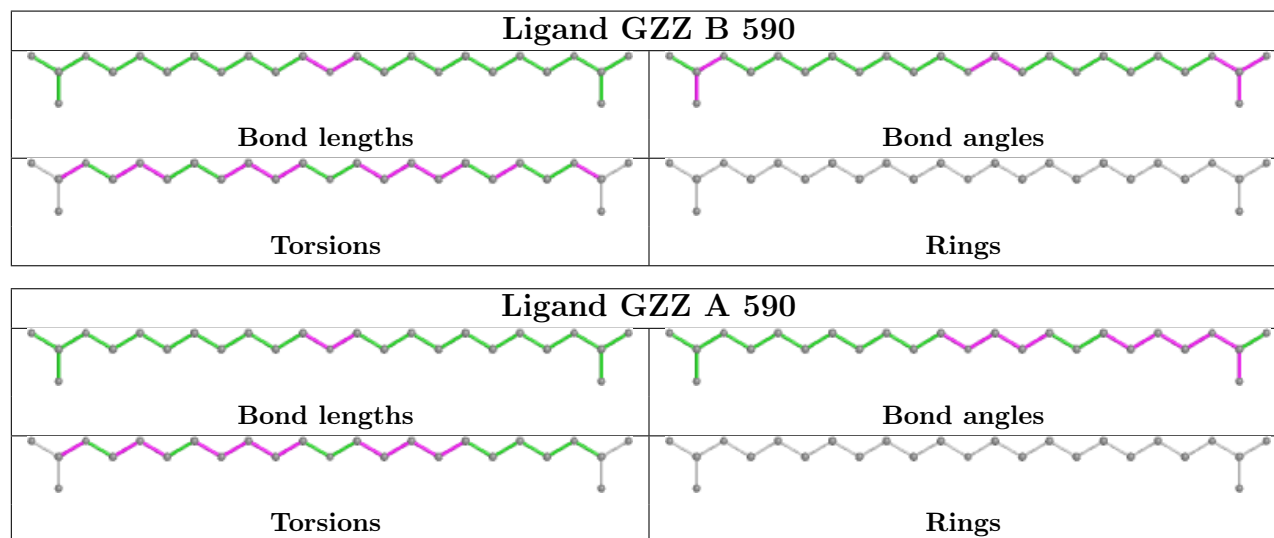5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	579	FAD	C5B-O5B-PA-O1A
5	A	590	GZZ	NH3-CZ2-NE2-C17
5	B	590	GZZ	NH3-CZ2-NE2-C17
5	C	590	GZZ	NH3-CZ2-NE2-C17
5	C	590	GZZ	C6-C7-C8-N9

There are no ring outliers.
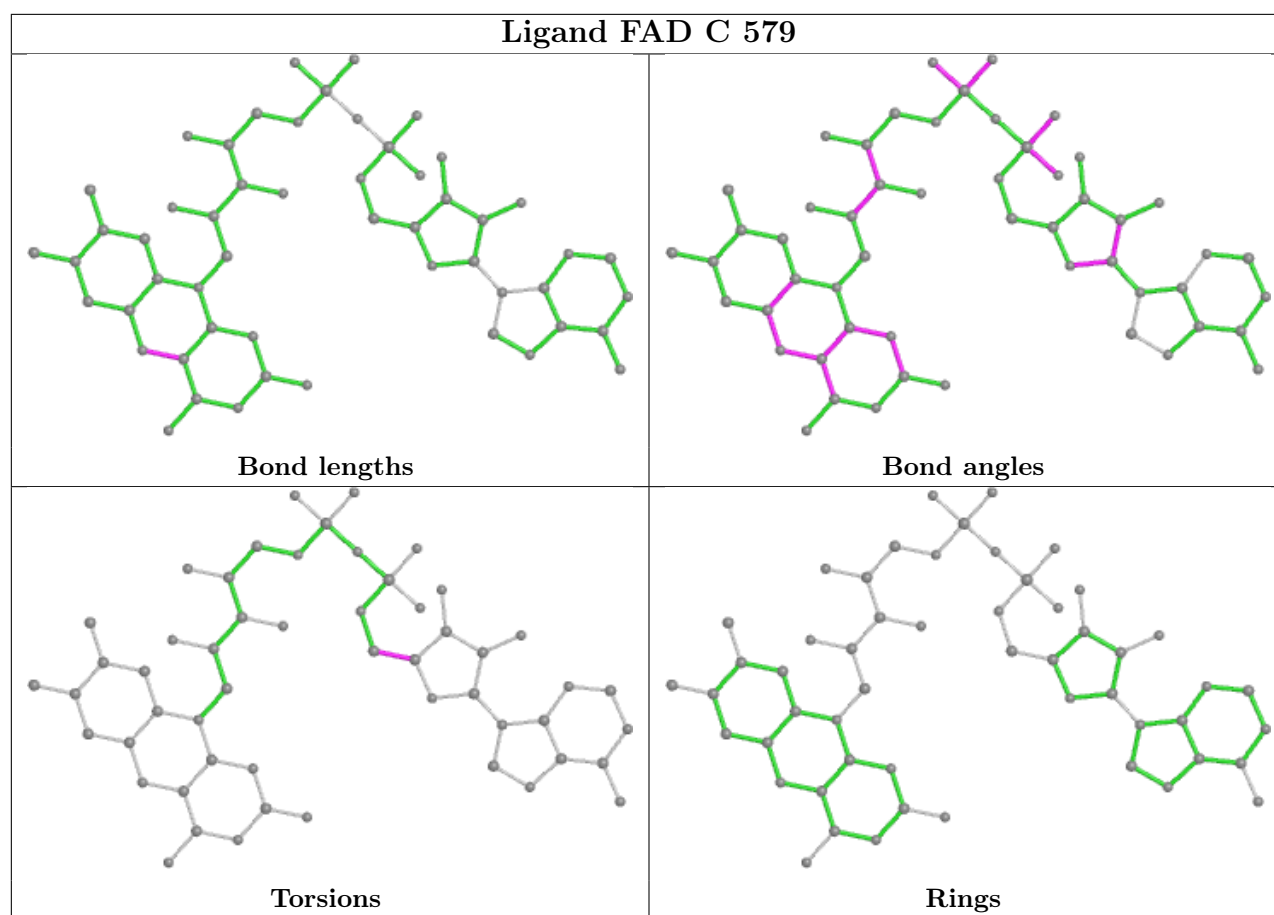
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	590	GZZ	4	0
5	A	590	GZZ	7	0
4	A	579	FAD	4	0
4	B	579	FAD	2	0
5	C	590	GZZ	2	0
4	C	579	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and 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 GZZ B 590

Bond lengths — Bond angles — Torsions — Rings

Ligand GZZ A 590

Bond lengths — Bond angles — Torsions — Rings

Ligand FAD A 579

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 579	
Bond lengths	Bond angles
Torsions	Rings

Ligand GZZ C 590	
Bond lengths	Bond angles
Torsions	Rings

wwPDB X-ray Structure Validation Summary Report

Ligand FAD C 579

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.