



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:52 AM UTC

PDB ID : 1H86 / pdb_00001h86
Title : COVALENT ADDUCT BETWEEN POLYAMINE OXIDASE AND N1ethyl
N11((cycloheptyl)methyl)4,8diazaundecane 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

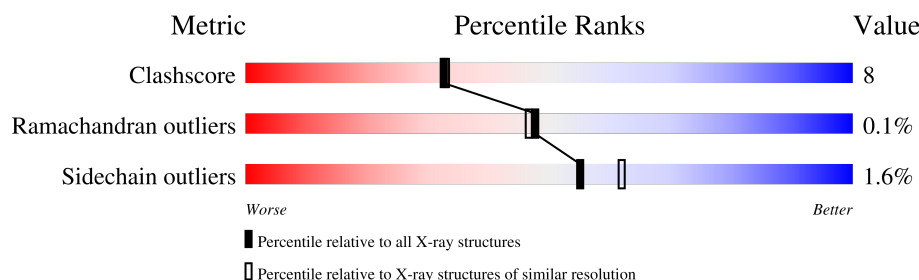
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	76% 18% . .
1	B	472	80% 16% . .
1	C	472	82% 15% ..
2	D	2	100%
3	E	5	20% 80%

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 [i](#)

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called POLYAMINE OXIDASE.

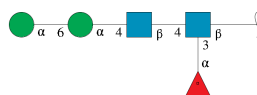
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	63	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	64	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	51	0	0
			3715	2374	627	700	14			

- Molecule 2 is 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.



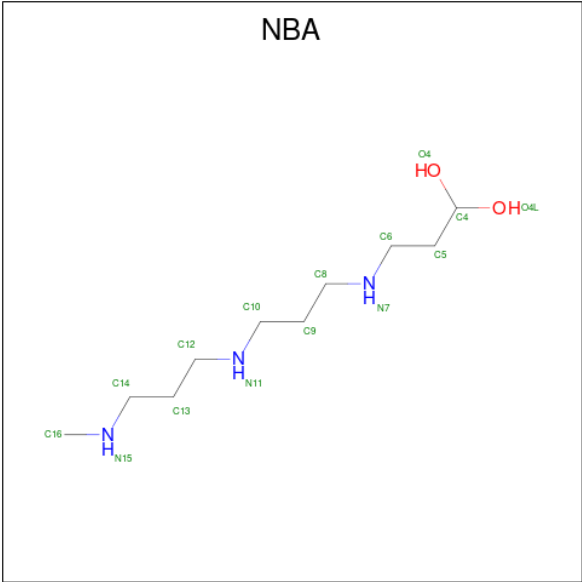
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



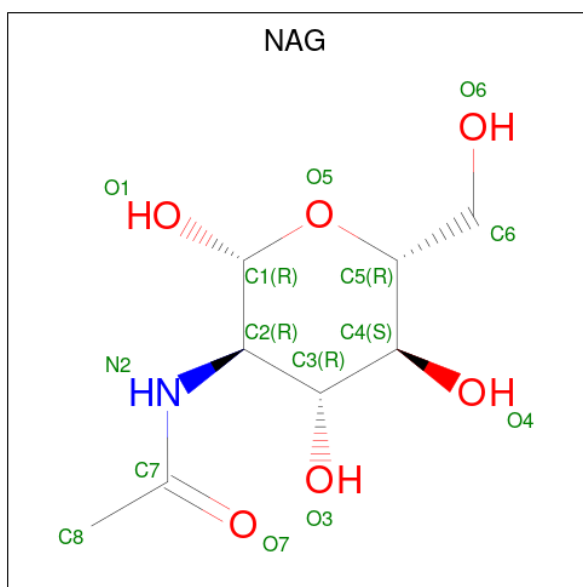
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is 3-[(3-{[3-(METHYLAMINO)PROPYL]AMINO}PROPYL)AMINO]PROPA NE-1,1-DIOL (CCD ID: 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 (CCD ID: 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

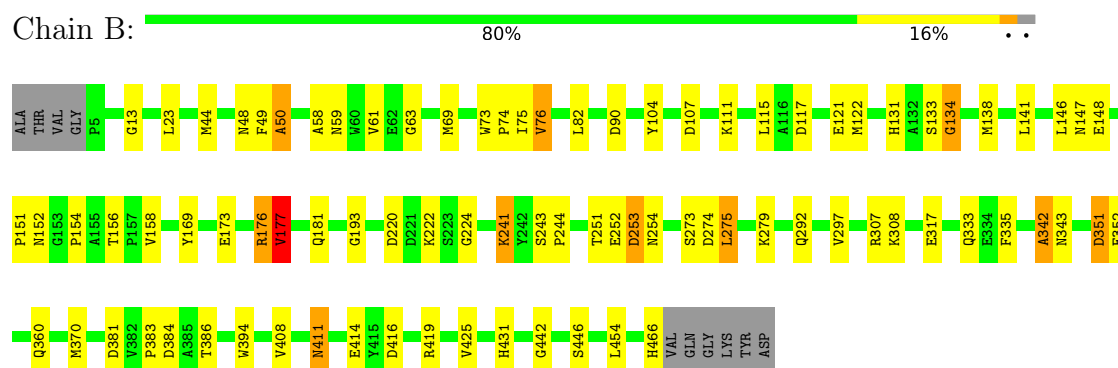
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

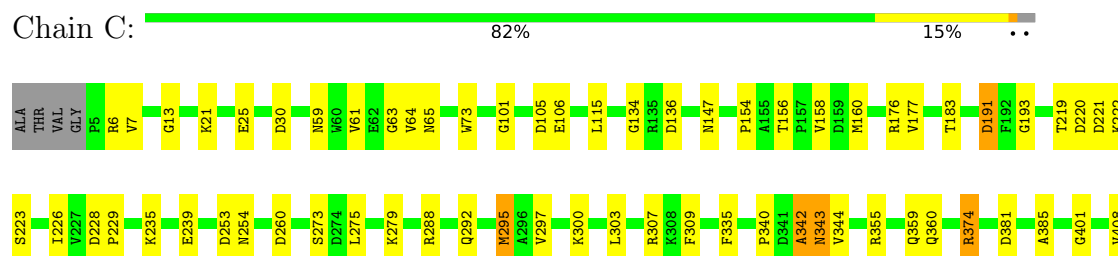
• Molecule 1: POLYAMINE OXIDASE



• Molecule 1: POLYAMINE OXIDASE



• Molecule 1: POLYAMINE OXIDASE





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

Chain D:  100%



- 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 E:  20%  80%



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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FCA, MAN, NBA, FAD

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	0.72	0/3775	1.60	42/5116 (0.8%)
1	B	0.72	0/3808	1.62	38/5160 (0.7%)
1	C	0.75	1/3808 (0.0%)	1.61	43/5160 (0.8%)
All	All	0.73	1/11391 (0.0%)	1.61	123/15436 (0.8%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	MET	SD-CE	5.00	1.92	1.79

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	ALA	N-CA-C	23.44	139.24	111.11
1	C	342	ALA	N-CA-C	13.47	127.45	111.82
1	C	273	SER	CA-C-N	-11.48	106.07	123.17
1	C	273	SER	C-N-CA	-11.48	106.07	123.17
1	C	420	ALA	N-CA-C	10.72	122.76	109.57
1	A	177	VAL	N-CA-CB	-8.75	102.59	112.21
1	A	101	GLY	N-CA-C	8.49	133.31	113.18
1	C	147	ASN	N-CA-C	8.32	120.43	111.36
1	C	409	GLY	CA-C-N	-8.26	112.52	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	GLY	C-N-CA	-8.26	112.52	122.93
1	A	386	THR	N-CA-CB	-8.01	97.94	110.44
1	B	61	VAL	N-CA-C	-7.81	95.87	107.51
1	C	61	VAL	N-CA-C	-7.69	96.06	107.51
1	B	351	ASP	CB-CA-C	-7.56	107.84	116.54
1	B	177	VAL	N-CA-CB	-7.33	102.24	112.35
1	B	90	ASP	N-CA-C	7.23	120.03	111.71
1	B	176	ARG	CA-C-N	-7.17	113.32	121.85
1	B	176	ARG	C-N-CA	-7.17	113.32	121.85
1	A	176	ARG	CB-CG-CD	-7.15	94.86	111.30
1	A	61	VAL	N-CA-C	-7.12	96.90	107.51
1	A	343	ASN	CB-CA-C	-7.03	101.75	111.73
1	A	385	ALA	N-CA-C	-6.99	100.64	110.50
1	A	273	SER	N-CA-C	6.87	121.83	113.17
1	C	176	ARG	CB-CG-CD	-6.87	95.50	111.30
1	C	297	VAL	CB-CA-C	-6.86	99.93	110.50
1	A	273	SER	CA-C-N	-6.84	112.89	124.31
1	A	273	SER	C-N-CA	-6.84	112.89	124.31
1	A	297	VAL	CB-CA-C	-6.83	100.36	110.33
1	A	409	GLY	N-CA-C	-6.81	106.30	113.58
1	B	273	SER	CA-C-N	-6.77	113.11	123.47
1	B	273	SER	C-N-CA	-6.77	113.11	123.47
1	B	134	GLY	N-CA-C	-6.55	106.28	115.32
1	A	205	TYR	N-CA-C	-6.54	104.19	111.71
1	B	297	VAL	CB-CA-C	-6.49	100.51	110.50
1	B	13	GLY	N-CA-C	-6.46	102.72	112.41
1	A	224	GLY	N-CA-C	-6.45	106.42	115.32
1	C	340	PRO	CA-C-N	-6.39	111.99	122.54
1	C	340	PRO	C-N-CA	-6.39	111.99	122.54
1	B	253	ASP	N-CA-C	-6.33	105.94	113.21
1	B	156	THR	N-CA-C	-6.31	102.13	110.40
1	C	13	GLY	N-CA-C	-6.28	102.99	112.41
1	A	381	ASP	N-CA-C	-6.20	97.60	108.20
1	B	274	ASP	N-CA-C	6.18	120.77	113.23
1	A	73	TRP	N-CA-C	6.16	121.13	112.75
1	C	176	ARG	CA-C-N	-6.13	113.56	122.69
1	C	176	ARG	C-N-CA	-6.13	113.56	122.69
1	A	156	THR	N-CA-C	-6.11	102.18	110.36
1	A	351	ASP	N-CA-CB	-6.08	100.22	110.49
1	A	27	GLY	CA-C-N	-6.07	115.24	122.22
1	A	27	GLY	C-N-CA	-6.07	115.24	122.22
1	B	147	ASN	CA-C-N	-6.04	113.13	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASN	C-N-CA	-6.04	113.13	122.49
1	C	374	ARG	CG-CD-NE	-6.03	98.74	112.00
1	C	335	PHE	N-CA-C	5.99	120.40	112.25
1	B	408	VAL	N-CA-C	-5.99	101.81	109.30
1	B	44	MET	N-CA-C	-5.97	95.86	107.62
1	C	275	LEU	CA-C-N	-5.95	115.29	122.90
1	C	275	LEU	C-N-CA	-5.95	115.29	122.90
1	A	23	LEU	N-CA-C	-5.94	104.72	111.14
1	A	182	ASN	N-CA-C	5.90	120.10	113.02
1	B	386	THR	N-CA-C	-5.89	105.75	113.17
1	B	222	LYS	N-CA-C	5.86	117.47	111.14
1	C	177	VAL	N-CA-C	-5.85	107.28	112.90
1	C	191	ASP	CB-CA-C	-5.82	101.01	110.79
1	B	75	ILE	CA-C-O	5.77	127.29	121.17
1	B	351	ASP	N-CA-C	5.76	117.07	108.31
1	A	275	LEU	N-CA-C	-5.76	105.08	111.36
1	C	183	THR	OG1-CB-CG2	-5.74	97.82	109.30
1	C	307	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	C	7	VAL	CB-CA-C	-5.72	101.98	110.33
1	C	412	ARG	N-CA-CB	5.71	119.01	110.22
1	C	412	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	C	409	GLY	N-CA-C	-5.69	107.13	113.79
1	B	241	LYS	N-CA-C	-5.68	100.44	109.59
1	B	335	PHE	N-CA-C	5.65	120.51	111.81
1	A	244	PRO	N-CA-C	-5.62	107.12	114.03
1	A	236	VAL	CB-CA-C	-5.60	104.13	111.81
1	C	101	GLY	N-CA-C	5.60	119.06	111.72
1	B	134	GLY	CA-C-O	5.59	125.32	119.06
1	A	386	THR	OG1-CB-CG2	5.57	120.43	109.30
1	A	26	ALA	CA-C-N	-5.57	113.77	122.51
1	A	26	ALA	C-N-CA	-5.57	113.77	122.51
1	C	273	SER	O-C-N	-5.54	114.78	122.76
1	A	106	GLU	N-CA-C	5.54	117.31	111.28
1	B	76	VAL	CB-CA-C	-5.53	104.78	112.02
1	A	226	ILE	N-CA-C	-5.50	101.62	108.89
1	B	50	ALA	CA-C-N	-5.49	111.28	121.93
1	B	50	ALA	C-N-CA	-5.49	111.28	121.93
1	C	136	ASP	CB-CA-C	-5.46	101.33	110.56
1	A	26	ALA	N-CA-C	-5.42	106.64	113.20
1	A	298	TYR	N-CA-CB	-5.41	102.61	110.84
1	A	380	LYS	CA-C-N	-5.41	115.81	122.84
1	A	380	LYS	C-N-CA	-5.41	115.81	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	TRP	N-CA-C	5.37	120.05	112.75
1	A	210	TYR	CA-C-N	-5.34	112.71	120.29
1	A	210	TYR	C-N-CA	-5.34	112.71	120.29
1	C	343	ASN	CB-CA-C	-5.27	104.46	111.63
1	C	300	LYS	CA-C-N	-5.27	115.80	122.43
1	C	300	LYS	C-N-CA	-5.27	115.80	122.43
1	C	381	ASP	N-CA-C	-5.25	98.74	107.99
1	C	408	VAL	CA-C-N	-5.25	117.19	123.44
1	C	408	VAL	C-N-CA	-5.25	117.19	123.44
1	B	425	VAL	CB-CA-C	-5.23	103.81	110.98
1	B	122	MET	N-CA-C	-5.22	105.76	111.82
1	A	95	ASN	N-CA-CB	-5.20	103.81	111.51
1	B	173	GLU	N-CA-C	-5.20	102.22	108.25
1	A	49	PHE	N-CA-C	-5.15	99.57	108.69
1	A	122	MET	N-CA-C	-5.15	105.84	111.82
1	B	147	ASN	N-CA-C	5.14	117.78	111.82
1	C	292	GLN	CA-CB-CG	-5.14	103.83	114.10
1	B	446	SER	N-CA-C	-5.13	105.87	111.82
1	C	288	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	36	ALA	N-CA-C	5.11	116.85	111.28
1	C	309	PHE	N-CA-C	-5.10	106.19	114.09
1	C	385	ALA	CA-C-N	-5.05	113.53	122.26
1	C	385	ALA	C-N-CA	-5.05	113.53	122.26
1	B	442	GLY	N-CA-C	-5.04	106.32	112.77
1	B	308	LYS	CA-C-N	-5.04	112.92	121.18
1	B	308	LYS	C-N-CA	-5.04	112.92	121.18
1	B	23	LEU	N-CA-C	-5.02	105.88	111.36
1	C	134	GLY	N-CA-C	-5.02	108.40	115.32
1	A	74	PRO	N-CA-C	-5.01	106.88	113.65
1	A	194	ASP	N-CA-C	5.00	119.23	113.18

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	65	0
1	B	3715	0	3614	66	1
1	C	3715	0	3614	31	0
2	D	28	0	26	3	1
3	E	60	0	52	6	0
4	A	53	0	31	1	0
4	B	53	0	31	1	0
4	C	53	0	31	0	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	3	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	173	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 8.

All (173) 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:HE3	1:B:73:TRP:HB3	1.34	1.07
1:B:69:MET:HE1	1:B:73:TRP:HD1	1.22	1.02
1:B:69:MET:HE1	1:B:73:TRP:CD1	1.94	1.01
1:B:69:MET:CE	1:B:73:TRP:HB3	1.97	0.94
1:A:460:LYS:HB3	1:A:462:MET:HE3	1.51	0.92
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:131:HIS:CD2	1:B:133:SER:H	1.98	0.80
1:B:69:MET:HE3	1:B:74:PRO:HD3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1.70	0.73
1:B:411:ASN:ND2	1:B:414:GLU:H	1.88	0.72
1:A:152:ASN:ND2	1:B:394:TRP:HE1	1.88	0.71
1:A:220:ASP:OD1	1:A:222:LYS:N	2.23	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:A:131:HIS:ND1	1:A:132:ALA:N	2.39	0.70
1:A:220:ASP:CG	1:A:223:SER:HB2	2.17	0.69
1:B:69:MET:HE2	1:B:74:PRO:CD	2.22	0.68
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:C:460:LYS:HB3	1:C:462:MET:HE2	1.76	0.66
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.44	0.65
1:B:69:MET:HE2	1:B:74:PRO:CG	2.27	0.64
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.79	0.64
1:B:117:ASP:O	1:B:121:GLU:HG3	1.98	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:292:GLN:OE1	1:B:138:MET:HE2	2.01	0.60
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.99	0.60
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.35	0.60
1:A:131:HIS:ND1	1:A:133:SER:N	2.35	0.60
1:A:431:HIS:CD2	1:A:431:HIS:H	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
1:A:131:HIS:CE1	1:A:133:SER:HB3	2.37	0.59
1:B:431:HIS:H	1:B:431:HIS:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:A:131:HIS:ND1	1:A:131:HIS:C	2.65	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:351:ASP:CG	1:B:352:GLU:H	2.14	0.53
1:B:49:PHE:O	1:B:50:ALA:HB3	2.09	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:252:GLU:C	1:B:254:ASN:H	2.18	0.51
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
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: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
1:A:328:TYR:O	1:A:329:TYR:C	2.54	0.49
1:B:69:MET:CE	1:B:73:TRP:CB	2.83	0.49
1:B:370:MET:HE2	1:B:384:ASP:HA	1.95	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:434:GLU:HG2	1:A:435:HIS:CD2	2.50	0.46
1:B:411:ASN:HD22	1:B:411:ASN:C	2.23	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:170:GLU:OE2	5:A:591:NBA:H121	2.16	0.46
1:A:220:ASP:CB	1:A:223:SER:CB	2.93	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:253:ASP:OD1	1:A:253:ASP:C	2.58	0.45
1:A:351:ASP:CG	1:A:352:GLU:H	2.25	0.45
1:B:351:ASP:CG	1:B:352:GLU:N	2.75	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:B:69:MET:CE	1:B:74:PRO:CD	2.81	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:B:252:GLU:C	1:B:254:ASN:N	2.75	0.44
1:B:220:ASP:O	1:B:224:GLY:N	2.48	0.44
1:A:91:TYR:CD1	1:A:91:TYR:N	2.86	0.44
1:A:131:HIS:CE1	1:A:133:SER:CB	3.00	0.44
1:A:448:ILE:O	1:A:452:GLU:HG3	2.18	0.44
1:B:251:THR:OG1	1:B:253:ASP:OD1	2.35	0.43
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
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:A:454:LEU:HD12	1:A:454:LEU:C	2.44	0.43
1:B:151:PRO:HG2	1:B:152:ASN:HD22	1.82	0.43
1:C:454:LEU:HD12	1:C:454:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:275:LEU:HD12	1:B:275:LEU:C	2.44	0.42
1:C:220:ASP:HB3	1:C:223:SER:OG	2.19	0.42
1:C:295:MET:HE3	1:C:401:GLY:C	2.44	0.42
1:A:57:GLY:HA2	4:A:590:FAD:HM73	2.01	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:B:69:MET:HE1	1:B:73:TRP:CG	2.48	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: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: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:C:453:ILE:HD13	1:C:453:ILE:HA	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
5:C:591:NBA:C12	7:C:2101:HOH:O	2.68	0.41
1:A:38:ASP:OD1	1:A:38:ASP:C	2.63	0.41
1:C:355:ARG:O	1:C:359:GLN:HG3	2.20	0.41
1:A:64:VAL:O	1:A:65:ASN:HB2	2.20	0.41
1:A:79:THR:HG22	1:A:80:LEU:CD2	2.45	0.41
1:B:69:MET:HE1	1:B:73:TRP:HB3	1.94	0.41
1:C:105:ASP:OD2	1:C:106:GLU:N	2.53	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: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
1:C:235:LYS:NZ	1:C:253:ASP:OD2	2.44	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

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%)	438 (96%)	18 (4%)	1 (0%)	43	42
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%)	48	46

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%)	387 (98%)	7 (2%)	51	58
1	B	397/404 (98%)	390 (98%)	7 (2%)	51	58
1	C	397/404 (98%)	392 (99%)	5 (1%)	61	68
All	All	1188/1212 (98%)	1169 (98%)	19 (2%)	55	62

All (19) 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	154	PRO
1	A	177	VAL
1	A	217	LEU
1	A	223	SER
1	A	386	THR
1	B	59	ASN
1	B	154	PRO
1	B	177	VAL
1	B	275	LEU
1	B	381	ASP
1	B	411	ASN
1	B	454	LEU
1	C	59	ASN
1	C	115	LEU
1	C	154	PRO
1	C	221	ASP
1	C	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	149	HIS
1	A	152	ASN
1	A	359	GLN
1	A	360	GLN
1	A	431	HIS
1	A	435	HIS
1	A	459	GLN
1	B	131	HIS
1	B	152	ASN
1	B	292	GLN
1	B	360	GLN
1	B	364	GLN
1	B	411	ASN
1	B	431	HIS
1	B	435	HIS
1	B	437	ASN
1	B	466	HIS
1	C	215	GLN
1	C	360	GLN
1	C	431	HIS

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Mol	Chain	Res	Type
1	C	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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	0	17,19,21	1.71	3 (17%)
2	NAG	D	2	2	14,14,15	1.33	2 (14%)	17,19,21	2.08	6 (35%)
3	NAG	E	1	1,3	14,14,15	1.35	2 (14%)	17,19,21	1.95	6 (35%)
3	NAG	E	2	3	14,14,15	0.91	1 (7%)	17,19,21	1.77	5 (29%)
3	MAN	E	3	3	11,11,12	0.74	0	15,15,17	3.12	5 (33%)
3	MAN	E	4	3	11,11,12	0.62	0	15,15,17	1.70	3 (20%)
3	FCA	E	5	3	10,10,11	1.34	1 (10%)	14,14,16	1.42	2 (14%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	FCA	C2-C3	-3.31	1.47	1.52
2	D	2	NAG	O5-C1	-3.30	1.38	1.43
3	E	1	NAG	C1-C2	-3.11	1.48	1.52
2	D	2	NAG	C1-C2	-3.07	1.48	1.52
3	E	2	NAG	O5-C1	-2.72	1.39	1.43
3	E	1	NAG	O5-C5	2.41	1.48	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	MAN	O2-C2-C3	9.90	130.65	110.15
2	D	2	NAG	O5-C5-C6	-4.46	98.98	107.66
3	E	4	MAN	C1-C2-C3	-4.44	103.18	109.64
3	E	2	NAG	O5-C5-C6	-4.27	99.36	107.66
3	E	3	MAN	C1-O5-C5	4.02	117.57	112.19
2	D	2	NAG	C1-C2-N2	-3.67	104.64	110.43
3	E	1	NAG	C1-C2-N2	-3.56	104.82	110.43
2	D	1	NAG	C1-O5-C5	3.52	116.90	112.19
3	E	3	MAN	O2-C2-C1	3.52	117.27	109.22
2	D	1	NAG	C2-N2-C7	-3.45	118.27	122.90
3	E	2	NAG	O5-C5-C4	-3.39	102.57	110.83
3	E	1	NAG	O5-C5-C6	-3.37	101.11	107.66
2	D	1	NAG	O3-C3-C4	3.12	117.72	110.38
3	E	5	FCA	C3-C4-C5	-3.01	105.24	109.81
3	E	1	NAG	O7-C7-C8	2.96	127.32	122.05
3	E	4	MAN	O2-C2-C3	2.89	116.14	110.15
3	E	1	NAG	C8-C7-N2	-2.88	111.34	116.12
3	E	5	FCA	C2-C3-C4	-2.73	106.06	110.86
3	E	3	MAN	O5-C5-C6	2.70	112.92	107.66
3	E	4	MAN	C2-C3-C4	-2.69	106.14	110.86
3	E	3	MAN	O4-C4-C3	2.68	116.70	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	O4-C4-C3	-2.67	104.08	110.38
3	E	2	NAG	C3-C4-C5	2.64	115.02	110.23
2	D	2	NAG	O5-C1-C2	-2.61	107.25	111.29
2	D	2	NAG	C2-N2-C7	-2.53	119.51	122.90
2	D	2	NAG	C4-C3-C2	2.46	114.62	111.02
3	E	2	NAG	C2-N2-C7	-2.33	119.78	122.90
3	E	1	NAG	O5-C5-C4	-2.24	105.37	110.83
2	D	2	NAG	C1-O5-C5	2.21	115.14	112.19
3	E	2	NAG	O5-C1-C2	-2.12	108.01	111.29

All (2) chirality outliers are listed below:

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

All (10) torsion outliers are listed below:

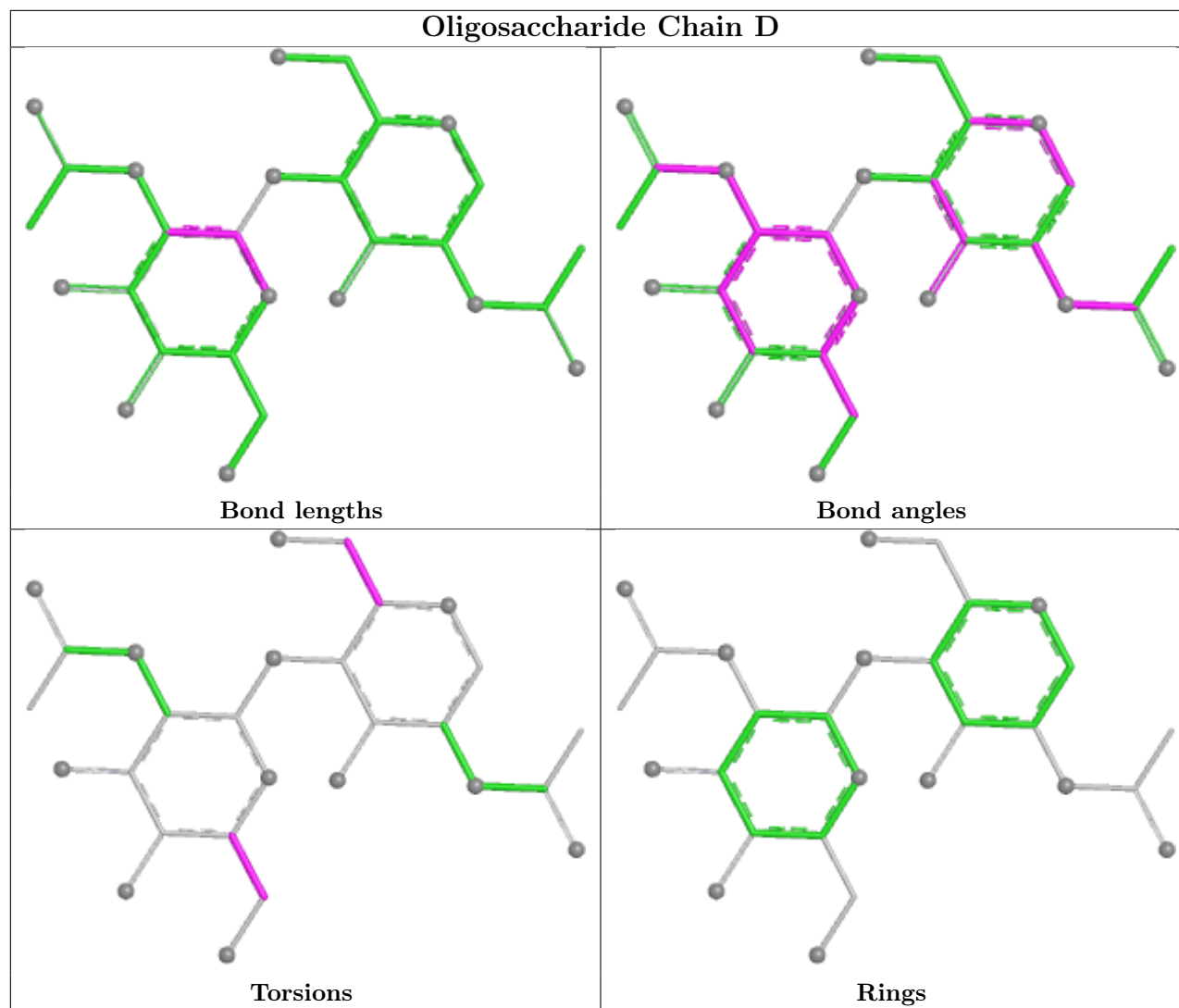
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

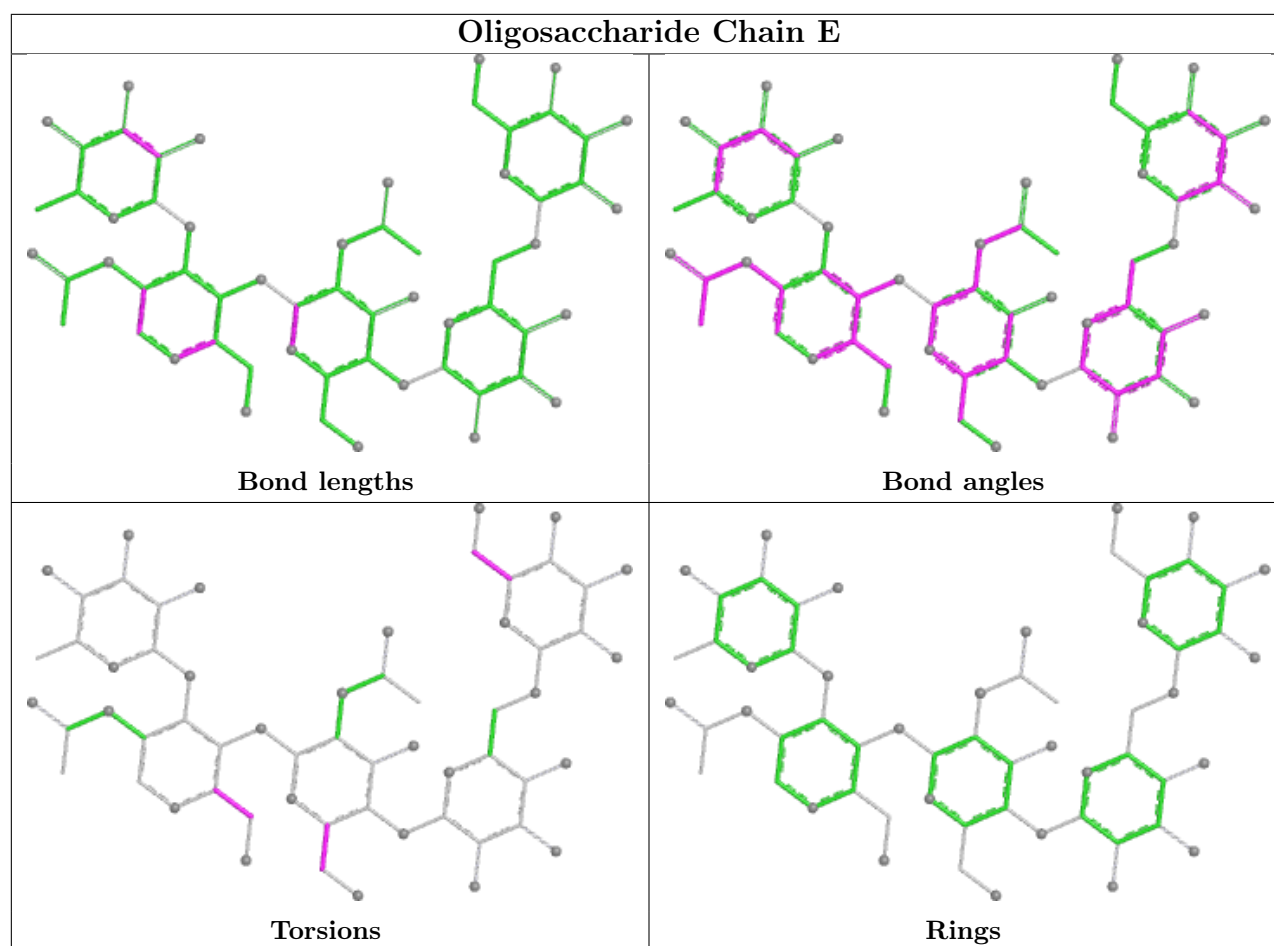
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	5	0
3	E	5	FCA	3	0
3	E	2	NAG	4	0
2	D	2	NAG	3	1
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
4	FAD	B	590	5	58,58,58	1.07	3 (5%)	85,89,89	1.56	20 (23%)
5	NBA	A	591	4	13,13,14	0.55	0	12,12,14	1.51	4 (33%)
5	NBA	C	591	4	13,13,14	0.56	0	12,12,14	2.10	3 (25%)
5	NBA	B	591	4	13,13,14	0.58	0	12,12,14	1.84	4 (33%)
4	FAD	A	590	5	58,58,58	0.92	4 (6%)	85,89,89	1.47	16 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	601	1	14,14,15	1.00	1 (7%)	17,19,21	2.34	6 (35%)
4	FAD	C	590	5	58,58,58	1.07	5 (8%)	85,89,89	1.35	12 (14%)
6	NAG	A	602	-	14,14,15	0.89	0	17,19,21	1.23	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
4	FAD	B	590	5	-	4/34/50/50	0/6/6/6
5	NBA	A	591	4	-	4/11/11/12	-
5	NBA	C	591	4	-	3/11/11/12	-
5	NBA	B	591	4	-	5/11/11/12	-
4	FAD	A	590	5	-	3/34/50/50	0/6/6/6
6	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	FAD	C	590	5	-	5/34/50/50	0/6/6/6
6	NAG	A	602	-	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	590	FAD	P-O3P	3.92	1.63	1.59
4	B	590	FAD	PA-O3P	3.39	1.63	1.59
4	B	590	FAD	C4X-N5	3.17	1.37	1.30
4	C	590	FAD	C4X-N5	3.03	1.37	1.30
4	A	590	FAD	PA-O3P	2.97	1.62	1.59
4	A	590	FAD	C4X-N5	2.89	1.37	1.30
4	A	590	FAD	C5'-C4'	2.40	1.55	1.51
4	C	590	FAD	P-O3P	2.36	1.62	1.59
6	A	601	NAG	O5-C1	-2.29	1.39	1.43
4	C	590	FAD	PA-O3P	2.25	1.61	1.59
4	A	590	FAD	C2-N1	-2.16	1.31	1.36
4	C	590	FAD	C6-C7	2.11	1.42	1.39
4	C	590	FAD	C9A-C5X	2.08	1.44	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	591	NBA	C9-C8-N7	-5.28	97.89	112.07
6	A	601	NAG	C1-O5-C5	4.62	118.37	112.19
6	A	601	NAG	C2-N2-C7	-4.48	116.90	122.90
4	A	590	FAD	C9A-C5X-N5	-4.28	117.91	122.45
4	C	590	FAD	C4-C4X-N5	4.19	123.99	118.21
6	A	601	NAG	O5-C5-C6	-4.13	99.62	107.66
5	B	591	NBA	C6-C5-C4	3.86	118.81	112.95
4	B	590	FAD	O2-C2-N1	-3.73	115.61	121.80
5	C	591	NBA	C9-C10-N11	-3.64	102.30	112.07
4	A	590	FAD	C4-C4X-N5	3.58	123.15	118.21
4	A	590	FAD	C5X-C9A-N10	3.37	121.01	117.97
4	A	590	FAD	O2A-PA-O1A	3.35	128.03	112.44
4	B	590	FAD	C10-N1-C2	3.33	124.06	116.85
4	C	590	FAD	O3P-PA-O1A	-3.20	101.08	110.70
4	C	590	FAD	C4'-C3'-C2'	3.13	118.77	113.57
6	A	601	NAG	C8-C7-N2	-3.10	110.97	116.12
4	B	590	FAD	O4B-C1B-C2B	-2.98	100.24	106.62
4	B	590	FAD	C4-N3-C2	-2.92	120.45	125.64
4	C	590	FAD	C10-N1-C2	2.80	122.92	116.85
4	C	590	FAD	C10-C4X-N5	-2.77	119.15	124.81
4	B	590	FAD	O2-C2-N3	2.75	123.86	118.58
4	B	590	FAD	C4'-C3'-C2'	2.73	118.11	113.57
4	B	590	FAD	C5A-C4A-N9A	-2.73	102.84	105.81
6	A	602	NAG	C8-C7-N2	-2.72	111.60	116.12
6	A	601	NAG	O3-C3-C4	2.67	116.67	110.38
4	A	590	FAD	O2P-P-O3P	-2.66	100.09	107.27
5	A	591	NBA	C9-C10-N11	-2.66	104.94	112.07
4	A	590	FAD	C6-C7-C8	-2.65	115.79	119.69
4	B	590	FAD	C9A-N10-C10	-2.63	116.74	120.75
4	C	590	FAD	O2P-P-O3P	-2.63	100.17	107.27
4	A	590	FAD	C9-C8-C7	2.61	123.52	119.69
4	B	590	FAD	C4A-C5A-N7A	2.59	113.54	110.58
4	B	590	FAD	C4X-C10-N1	-2.56	118.32	124.59
5	B	591	NBA	C14-C13-C12	-2.56	105.05	114.15
4	B	590	FAD	O2P-P-O3P	-2.55	100.39	107.27
6	A	601	NAG	O7-C7-C8	2.53	126.55	122.05
4	B	590	FAD	O2P-P-O1P	2.52	124.18	112.44
4	C	590	FAD	O3B-C3B-C2B	-2.52	103.73	111.82
5	B	591	NBA	C9-C10-N11	-2.48	105.41	112.07
4	B	590	FAD	O4B-C1B-N9A	-2.46	103.36	108.09
4	C	590	FAD	O4B-C1B-C2B	-2.46	101.35	106.62
4	B	590	FAD	O3P-PA-O1A	-2.45	103.34	110.70
4	C	590	FAD	C8M-C8-C9	-2.45	115.26	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	590	FAD	O2A-PA-O1A	2.44	123.81	112.44
4	A	590	FAD	C7M-C7-C6	2.43	123.85	119.57
4	B	590	FAD	C4A-N9A-C8A	2.42	108.28	105.74
5	C	591	NBA	C12-N11-C10	-2.41	101.99	113.40
4	A	590	FAD	O4B-C1B-C2B	-2.37	101.53	106.62
4	A	590	FAD	C5A-N7A-C8A	2.35	107.15	103.45
5	A	591	NBA	C6-C5-C4	-2.34	109.40	112.95
4	B	590	FAD	C10-C4X-N5	-2.33	120.06	124.81
4	A	590	FAD	N9A-C8A-N7A	-2.29	110.69	113.94
5	A	591	NBA	C12-N11-C10	-2.27	102.67	113.40
4	B	590	FAD	O2A-PA-O3P	2.27	113.40	107.27
4	B	590	FAD	O2P-P-O5'	2.23	117.68	107.57
4	A	590	FAD	C8M-C8-C9	-2.23	115.65	119.57
4	B	590	FAD	C4X-C10-N10	2.22	119.66	116.48
5	B	591	NBA	C9-C8-N7	-2.22	106.12	112.07
4	A	590	FAD	C2B-C1B-N9A	2.21	118.79	113.30
6	A	602	NAG	O7-C7-N2	2.21	125.88	121.98
4	A	590	FAD	O2P-P-O1P	2.20	122.66	112.44
4	A	590	FAD	O3P-PA-O1A	-2.16	104.20	110.70
4	A	590	FAD	C4A-C5A-N7A	-2.14	108.13	110.58
4	C	590	FAD	O5'-C5'-C4'	-2.14	103.65	109.36
4	B	590	FAD	O4-C4-C4X	-2.05	121.12	126.53
5	A	591	NBA	C14-C13-C12	-2.04	106.88	114.15
4	C	590	FAD	C5X-N5-C4X	-2.02	114.83	118.09

There are no chirality outliers.

All (28) 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
5	A	591	NBA	N11-C10-C9-C8
5	C	591	NBA	N11-C12-C13-C14
6	A	602	NAG	O5-C5-C6-O6
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	A	591	NBA	C9-C10-N11-C12
5	B	591	NBA	C12-C13-C14-N15
5	C	591	NBA	N7-C8-C9-C10
4	C	590	FAD	C2'-C3'-C4'-O4'
5	B	591	NBA	N7-C8-C9-C10

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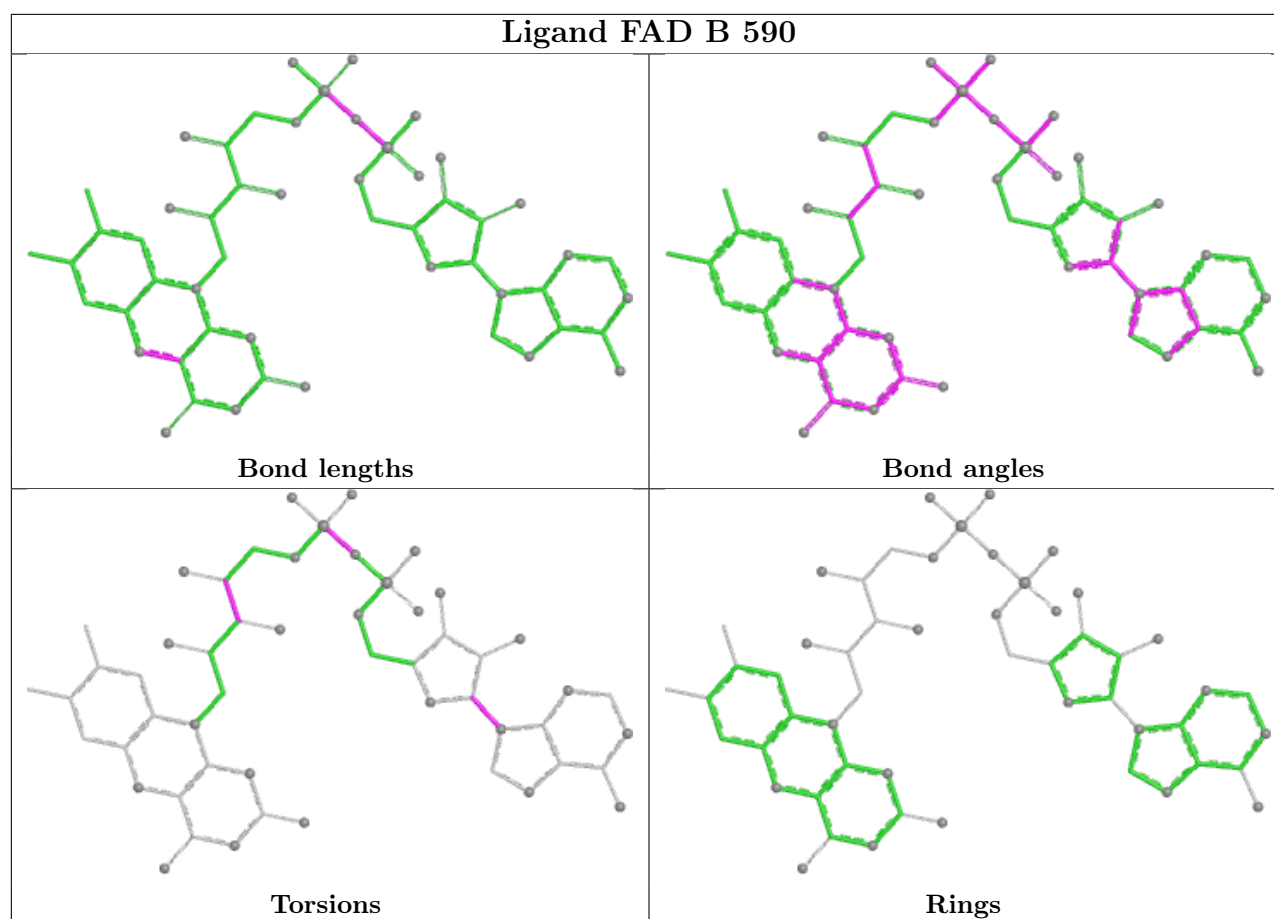
Mol	Chain	Res	Type	Atoms
4	B	590	FAD	C2'-C3'-C4'-O4'
4	B	590	FAD	PA-O3P-P-O5'
5	C	591	NBA	N11-C10-C9-C8
5	B	591	NBA	N11-C10-C9-C8
4	C	590	FAD	C2'-C3'-C4'-C5'
4	C	590	FAD	O3'-C3'-C4'-C5'
5	B	591	NBA	C4-C5-C6-N7
4	C	590	FAD	O3'-C3'-C4'-O4'
4	A	590	FAD	C2B-C1B-N9A-C8A
5	A	591	NBA	N7-C8-C9-C10
4	A	590	FAD	O3'-C3'-C4'-O4'
4	A	590	FAD	O3'-C3'-C4'-C5'
4	B	590	FAD	C2B-C1B-N9A-C8A
4	C	590	FAD	C2B-C1B-N9A-C8A
4	B	590	FAD	O3'-C3'-C4'-O4'

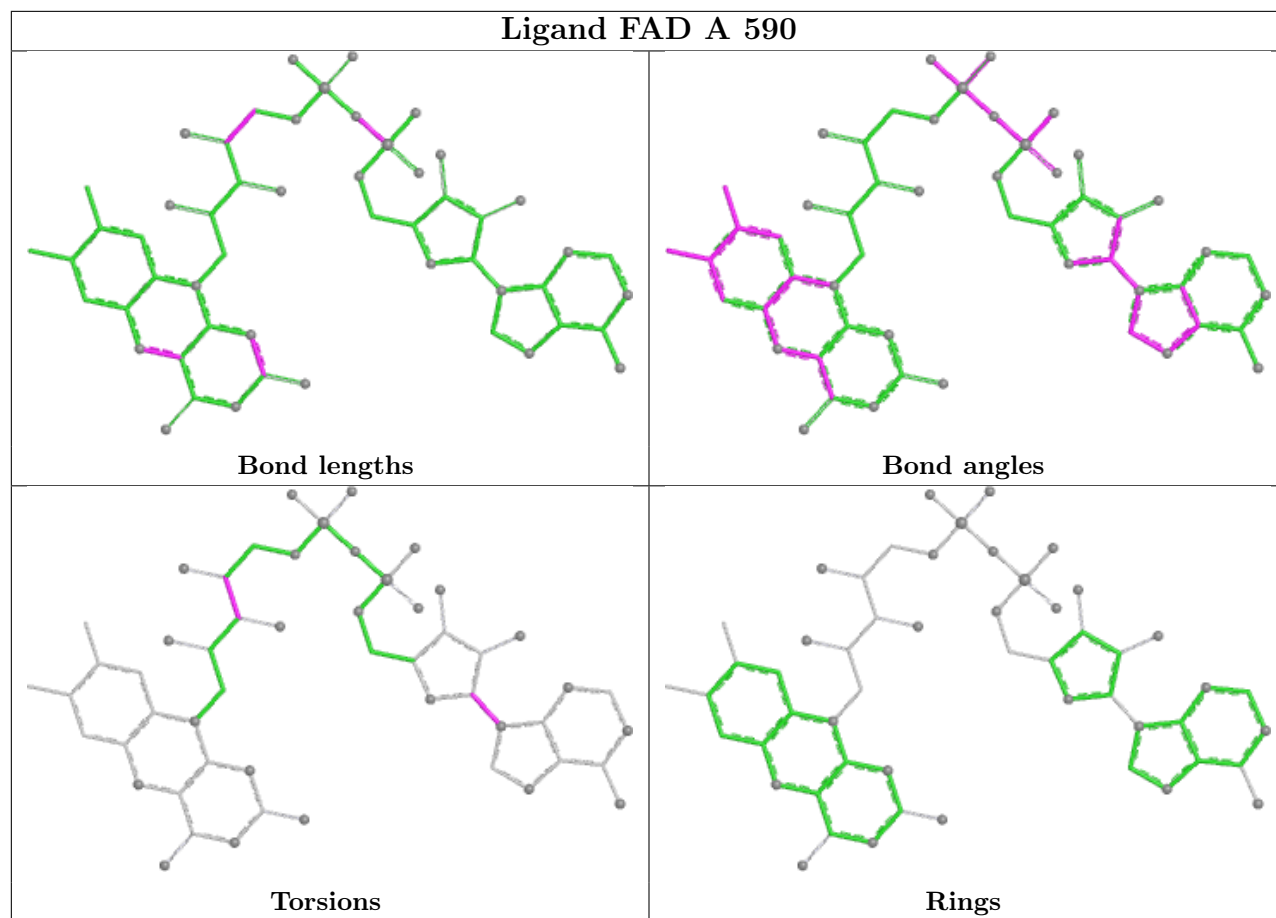
There are no ring outliers.

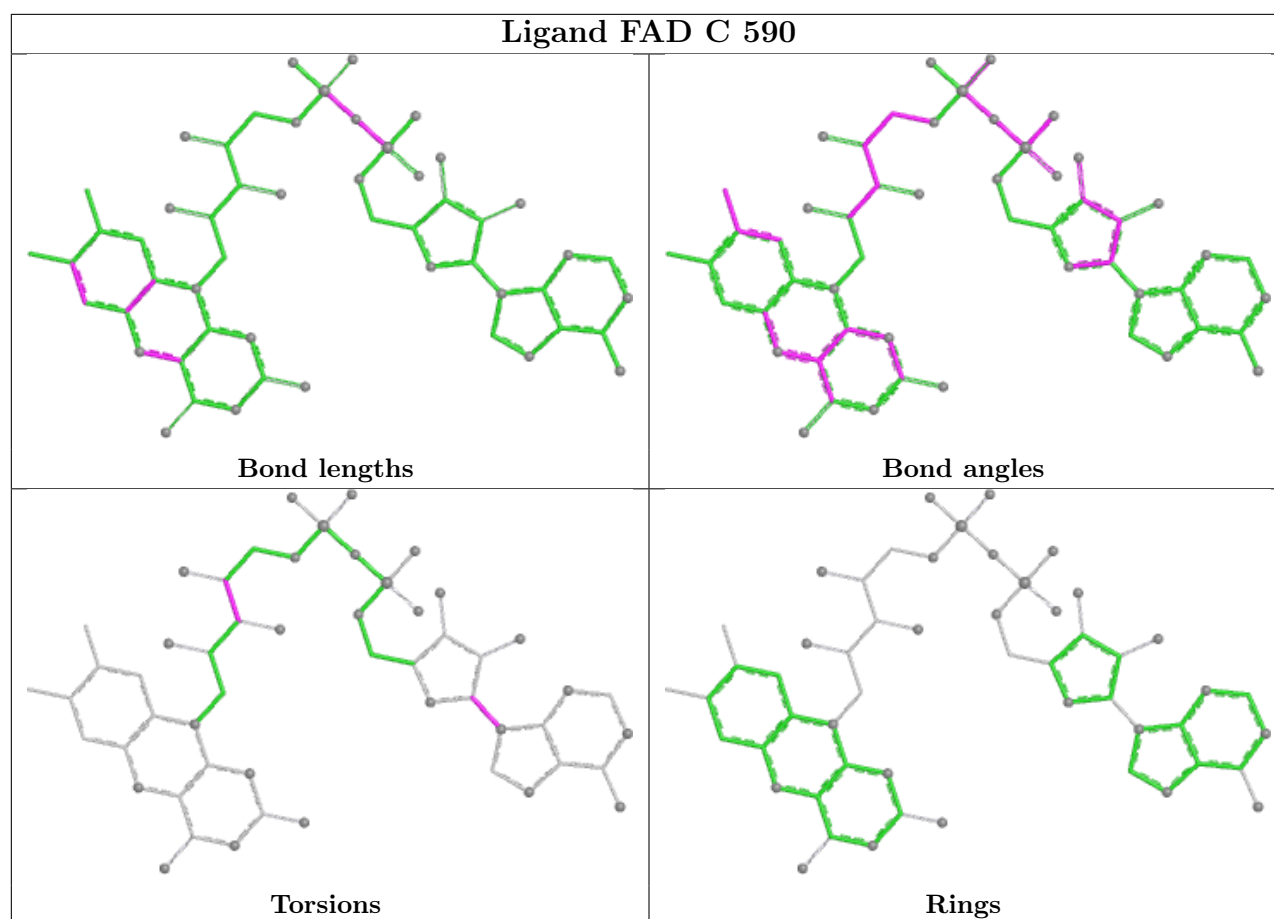
7 monomers are involved in 13 short contacts:

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







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.