



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:17 PM UTC

PDB ID : 1H82 / pdb_00001h82
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)

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

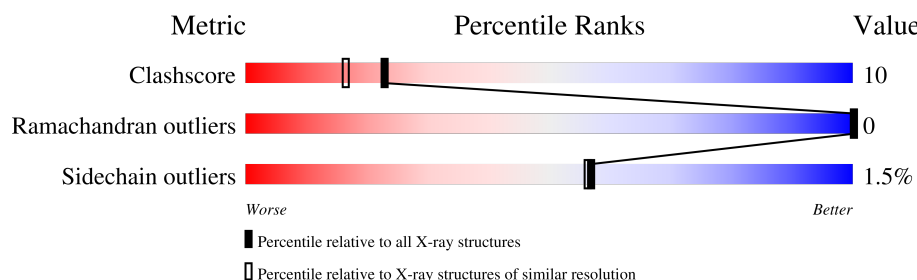
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	
1	B	472	
1	C	472	
2	D	2	
2	E	2	
3	F	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 crite-

ria:

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

2 Entry composition [i](#)

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.

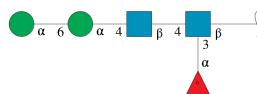
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	54	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	54	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	41	0	0
			3715	2374	627	700	14			

- 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			

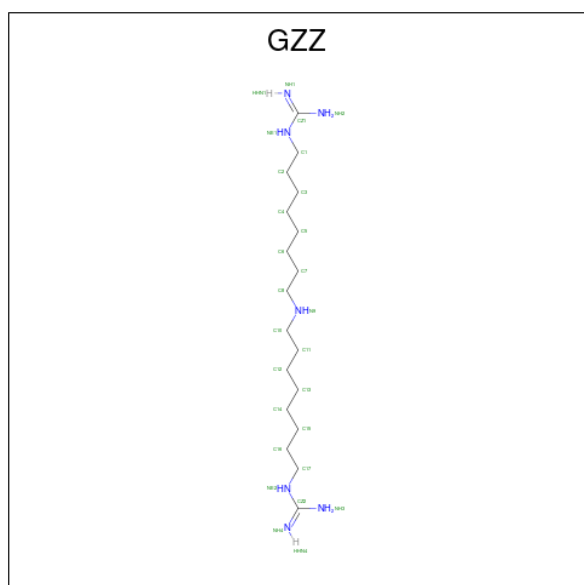
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- # FAD

- Molecule 5 is N-{8-[8-[(E)-AMINO(IMINO)METHYL]AMINO]OCTYL)AMINO]OCTYL}GUANIDINE (CCD ID: GZZ) (formula: C₁₈H₄₁N₇).



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

- Molecule 6 is water.

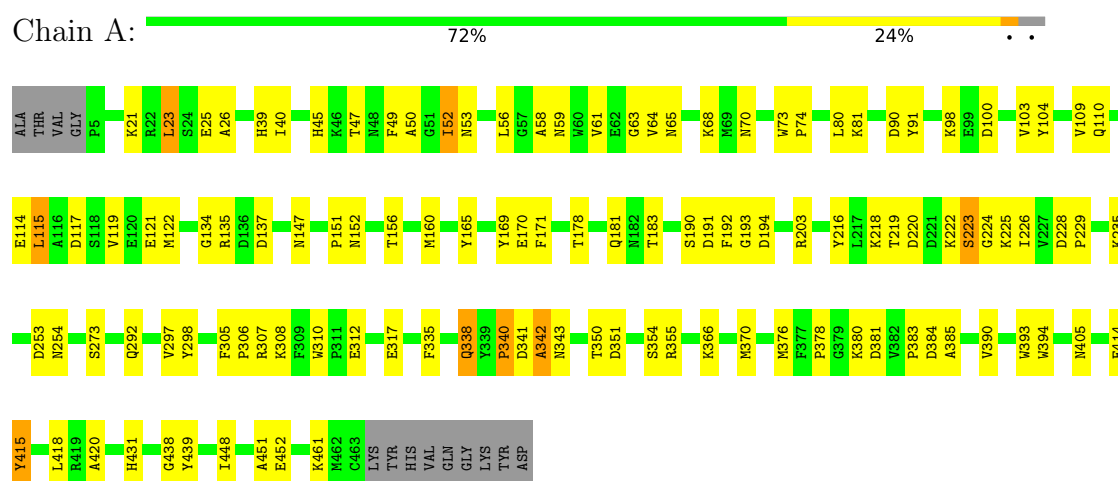
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	237	Total	O	0	0
			237	237		
6	B	242	Total	O	0	0
			242	242		
6	C	267	Total	O	0	0
			267	267		

3 Residue-property plots

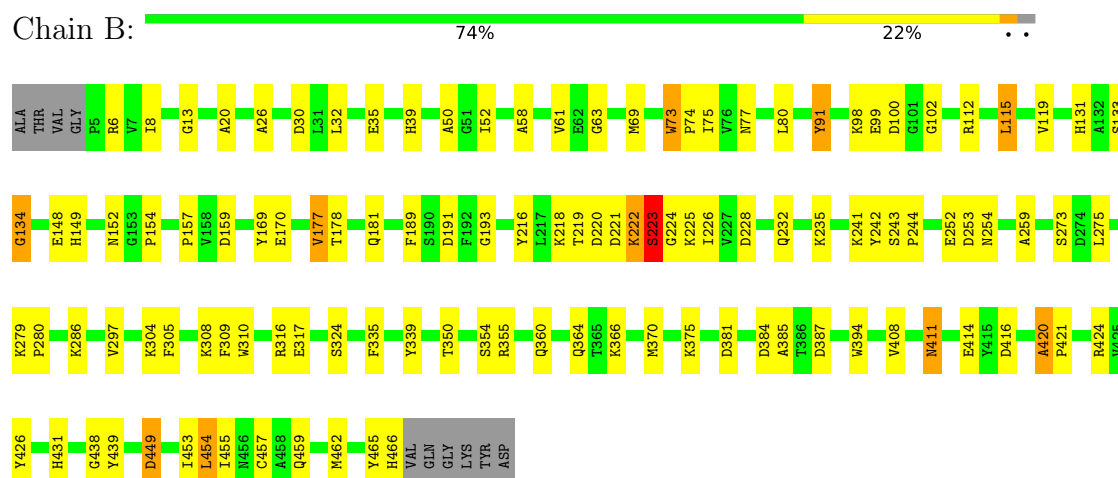
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

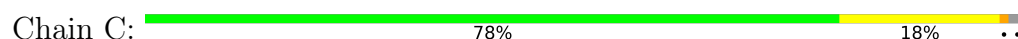
• Molecule 1: POLYAMINE OXIDASE

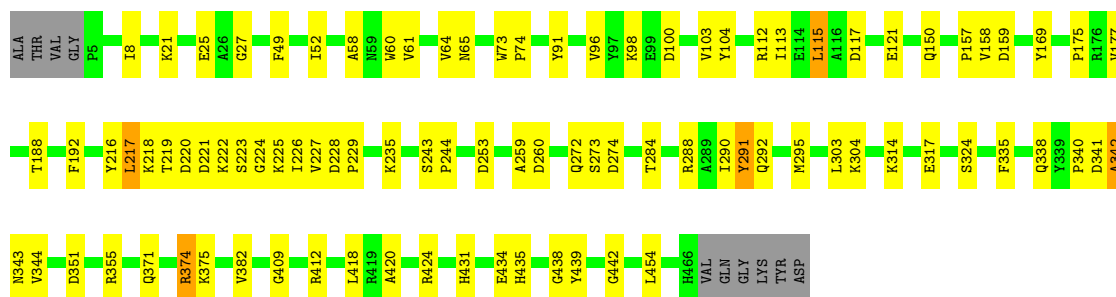


• Molecule 1: POLYAMINE OXIDASE



• 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%

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: FCA, NAG, MAN, GZZ, 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	0.81	0/3775	1.55	44/5116 (0.9%)
1	B	0.79	0/3808	1.52	44/5160 (0.9%)
1	C	0.81	1/3808 (0.0%)	1.47	31/5160 (0.6%)
All	All	0.80	1/11391 (0.0%)	1.51	119/15436 (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	A	1	0
1	C	0	1
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	MET	SD-CE	5.17	1.92	1.79

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ALA	N-CA-C	17.87	132.95	111.33
1	C	342	ALA	N-CA-C	14.05	126.67	111.36
1	B	224	GLY	N-CA-C	-13.36	97.59	115.36
1	C	273	SER	CA-C-N	-10.32	106.93	122.83
1	C	273	SER	C-N-CA	-10.32	106.93	122.83
1	B	223	SER	N-CA-C	-10.00	97.64	112.04
1	B	335	PHE	N-CA-C	9.62	123.44	112.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLY	N-CA-C	-9.45	102.93	115.21
1	B	273	SER	N-CA-C	-9.08	96.28	110.36
1	A	341	ASP	N-CA-C	9.04	124.31	113.28
1	B	100	ASP	N-CA-C	8.88	123.98	112.26
1	A	61	VAL	N-CA-C	-8.53	95.53	107.99
1	C	420	ALA	N-CA-C	8.51	119.38	109.60
1	C	335	PHE	N-CA-C	8.37	122.03	112.57
1	A	273	SER	CA-C-N	-8.34	109.99	122.83
1	A	273	SER	C-N-CA	-8.34	109.99	122.83
1	B	449	ASP	N-CA-C	8.15	120.17	111.28
1	C	439	TYR	N-CA-C	8.12	122.53	110.52
1	A	26	ALA	N-CA-C	-8.04	103.37	113.02
1	A	381	ASP	CA-C-N	-7.94	116.87	122.59
1	A	381	ASP	C-N-CA	-7.94	116.87	122.59
1	B	459	GLN	N-CA-C	7.90	119.89	111.28
1	A	439	TYR	N-CA-C	7.90	122.21	110.52
1	B	273	SER	CA-C-N	-7.75	106.73	121.54
1	B	273	SER	C-N-CA	-7.75	106.73	121.54
1	A	100	ASP	N-CA-C	7.56	122.80	112.90
1	A	390	VAL	CB-CA-C	-7.41	104.04	111.08
1	C	61	VAL	N-CA-C	-7.34	96.57	107.51
1	B	420	ALA	N-CA-C	7.29	117.98	109.60
1	C	224	GLY	N-CA-C	-7.24	105.84	115.40
1	B	61	VAL	N-CA-C	-7.12	96.90	107.51
1	A	223	SER	CB-CA-C	-6.99	99.80	110.92
1	A	297	VAL	CB-CA-C	-6.98	99.25	110.28
1	C	192	PHE	N-CA-C	6.96	121.77	113.28
1	A	305	PHE	CA-C-N	6.64	126.33	119.56
1	A	305	PHE	C-N-CA	6.64	126.33	119.56
1	B	439	TYR	N-CA-C	6.49	120.12	110.52
1	A	340	PRO	CA-C-N	-6.46	110.04	122.06
1	A	340	PRO	C-N-CA	-6.46	110.04	122.06
1	A	338	GLN	N-CA-C	6.37	118.02	111.14
1	B	324	SER	N-CA-C	-6.35	105.49	113.18
1	C	324	SER	N-CA-C	-6.35	105.49	113.18
1	B	222	LYS	N-CA-CB	6.35	120.58	110.73
1	C	274	ASP	N-CA-C	6.32	119.71	112.57
1	B	73	TRP	CA-C-O	6.21	124.34	118.63
1	B	134	GLY	N-CA-C	-6.14	106.85	115.32
1	B	191	ASP	N-CA-C	6.06	119.15	111.69
1	B	317	GLU	N-CA-C	6.06	118.66	111.33
1	A	194	ASP	N-CA-C	6.04	120.49	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ASP	CB-CA-C	6.03	120.51	110.92
1	B	13	GLY	N-CA-C	-6.02	103.38	112.41
1	A	461	LYS	CA-C-N	-5.99	114.33	122.95
1	A	461	LYS	C-N-CA	-5.99	114.33	122.95
1	C	340	PRO	CA-C-N	-5.98	113.08	122.65
1	C	340	PRO	C-N-CA	-5.98	113.08	122.65
1	C	177	VAL	N-CA-CB	-5.92	105.70	112.21
1	B	221	ASP	CA-C-N	-5.90	113.39	122.60
1	B	221	ASP	C-N-CA	-5.90	113.39	122.60
1	A	90	ASP	N-CA-C	5.88	119.55	112.38
1	C	409	GLY	N-CA-C	-5.83	107.34	113.58
1	B	75	ILE	CB-CA-C	-5.78	104.44	112.02
1	C	27	GLY	CA-C-N	-5.76	115.28	122.48
1	C	27	GLY	C-N-CA	-5.76	115.28	122.48
1	C	442	GLY	N-CA-C	-5.71	105.87	112.73
1	C	338	GLN	N-CA-C	5.70	117.30	111.14
1	A	351	ASP	N-CA-CB	-5.69	100.87	110.49
1	C	115	LEU	N-CA-CB	-5.69	101.76	110.01
1	A	135	ARG	N-CA-C	5.68	119.31	112.38
1	B	178	THR	N-CA-C	5.67	119.49	109.96
1	C	284	THR	N-CA-C	5.52	118.00	111.33
1	C	371	GLN	CB-CA-C	-5.44	101.76	110.79
1	A	151	PRO	N-CA-C	-5.43	109.03	114.68
1	A	381	ASP	N-CA-C	-5.40	98.96	108.20
1	B	119	VAL	N-CA-C	-5.39	105.13	110.62
1	A	298	TYR	N-CA-CB	-5.38	102.67	110.84
1	C	435	HIS	CB-CA-C	-5.37	101.41	110.64
1	B	355	ARG	NE-CZ-NH2	-5.35	114.38	119.20
1	C	341	ASP	CB-CA-C	5.35	119.60	110.56
1	B	222	LYS	CA-C-N	-5.35	110.25	121.80
1	B	222	LYS	C-N-CA	-5.35	110.25	121.80
1	C	382	VAL	N-CA-C	5.35	113.16	107.76
1	C	317	GLU	N-CA-C	5.32	117.50	111.11
1	B	177	VAL	N-CA-CB	-5.31	104.00	112.07
1	B	465	TYR	N-CA-C	5.30	120.84	110.56
1	C	288	ARG	CG-CD-NE	-5.27	100.41	112.00
1	A	380	LYS	CA-C-N	-5.26	116.00	122.84
1	A	380	LYS	C-N-CA	-5.26	116.00	122.84
1	C	341	ASP	N-CA-C	5.25	119.38	112.92
1	A	254	ASN	N-CA-C	5.23	123.74	113.29
1	B	75	ILE	CA-C-N	-5.22	113.88	120.56
1	B	75	ILE	C-N-CA	-5.22	113.88	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ASP	CB-CA-C	5.22	119.54	111.13
1	A	165	TYR	N-CA-C	-5.21	105.69	111.36
1	B	80	LEU	CA-C-N	-5.17	115.15	122.34
1	B	80	LEU	C-N-CA	-5.17	115.15	122.34
1	C	113	ILE	CB-CA-C	-5.17	105.09	112.22
1	A	109	VAL	N-CA-C	5.16	115.89	110.62
1	A	341	ASP	CA-C-N	5.16	127.44	120.38
1	A	341	ASP	C-N-CA	5.16	127.44	120.38
1	B	73	TRP	N-CA-C	5.15	119.95	113.25
1	A	192	PHE	N-CA-C	5.15	119.56	113.28
1	A	317	GLU	N-CA-C	5.15	117.28	111.11
1	C	374	ARG	CG-CD-NE	-5.12	100.73	112.00
1	C	351	ASP	N-CA-CB	-5.12	101.84	110.49
1	B	115	LEU	CB-CA-C	-5.11	102.87	110.88
1	A	393	TRP	N-CA-C	5.10	117.57	111.71
1	B	381	ASP	N-CA-CB	5.10	119.08	110.46
1	B	297	VAL	CB-CA-C	-5.09	102.24	110.28
1	A	134	GLY	N-CA-C	-5.08	108.31	115.32
1	A	335	PHE	N-CA-C	5.06	119.60	111.81
1	B	134	GLY	CA-C-O	5.04	124.71	119.06
1	B	273	SER	O-C-N	-5.04	115.95	122.20
1	A	420	ALA	N-CA-C	5.04	116.73	109.48
1	A	147	ASN	CA-C-N	-5.03	114.70	122.49
1	A	147	ASN	C-N-CA	-5.03	114.70	122.49
1	B	91	TYR	N-CA-C	5.01	118.43	112.72
1	B	375	LYS	N-CA-C	-5.00	105.92	112.23
1	B	316	ARG	N-CA-C	5.00	119.09	112.89
1	A	415	TYR	N-CA-C	-5.00	105.83	111.28

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	70	0
1	B	3715	0	3614	90	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	7	0
4	A	53	0	31	3	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	237	0	0	5	0
6	B	242	0	0	5	0
6	C	267	0	0	9	0
All	All	12210	0	11128	227	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.

All (227) 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:602:HOH:O	1.25	1.28
1:A:220:ASP:HB3	1:A:223:SER:HB2	1.25	1.12
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
1:A:308:LYS:HZ2	1:A:312:GLU:HG3	1.28	0.97
3:F:1:NAG:C4	3:F:2:NAG:C1	2.45	0.95
1:A:308:LYS:NZ	1:A:312:GLU:HG3	1.81	0.94
1:B:69:MET:CE	1:B:73:TRP:HB3	1.97	0.93
1:B:69:MET:HE1	1:B:73:TRP:HD1	1.33	0.93
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.51	0.93
1:B:69:MET:HE1	1:B:73:TRP:CD1	2.06	0.91
3:F:1:NAG:H3	3:F:5:FCA:O2	1.72	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:TYR:CZ	6:C:602:HOH:O	2.27	0.87
1:A:220:ASP:CB	1:A:223:SER:HB2	2.06	0.84
2:E:1:NAG:C4	2:E:2:NAG:C1	2.58	0.82
1:C:21:LYS:O	1:C:25:GLU:HG3	1.80	0.81
1:A:169:TYR:O	5:A:502:GZZ:H102	1.81	0.80
1:B:220:ASP:CB	1:B:223:SER:HB2	2.12	0.79
1:B:411:ASN:ND2	1:B:414:GLU:H	1.80	0.77
1:C:216:TYR:CD1	1:C:217:LEU:HD13	2.19	0.77
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.64	0.76
1:B:69:MET:HE2	1:B:74:PRO:CD	2.16	0.75
1:B:220:ASP:HB3	1:B:223:SER:CB	2.15	0.75
1:C:292:GLN:OE1	6:C:601:HOH:O	2.04	0.74
1:B:131:HIS:CD2	1:B:133:SER:H	2.04	0.74
1:A:171:PHE:HD2	5:A:502:GZZ:HC11	1.53	0.74
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.85	0.73
1:A:117:ASP:O	1:A:121:GLU:HG3	1.88	0.73
2:D:1:NAG:C4	2:D:2:NAG:C1	2.67	0.72
1:C:412:ARG:NH1	1:C:434:GLU:OE2	2.21	0.71
1:A:308:LYS:NZ	1:A:310:TRP:O	2.25	0.70
1:B:69:MET:CE	1:B:74:PRO:HD3	2.22	0.69
1:B:223:SER:HB3	1:B:225:LYS:H	1.57	0.69
1:A:431:HIS:CD2	1:A:431:HIS:H	2.08	0.68
1:C:219:THR:HG22	1:C:226:ILE:CA	2.21	0.68
1:C:112:ARG:HD3	1:C:159:ASP:OD1	1.93	0.68
1:A:292:GLN:NE2	1:A:414:GLU:OE2	2.27	0.68
5:B:502:GZZ:HC11	6:B:723:HOH:O	1.93	0.68
1:A:171:PHE:CD2	5:A:502:GZZ:HC11	2.30	0.67
1:C:220:ASP:OD2	1:C:222:LYS:N	2.26	0.67
1:B:50:ALA:HB1	1:B:304:LYS:HD3	1.77	0.67
1:B:69:MET:HE2	1:B:74:PRO:HG3	1.77	0.66
1:B:243:SER:HB2	1:B:244:PRO:CD	2.25	0.66
1:C:216:TYR:CE1	1:C:217:LEU:HD13	2.29	0.66
1:B:242:TYR:CZ	1:B:280:PRO:HD2	2.31	0.66
3:F:1:NAG:HO4	3:F:2:NAG:C1	2.06	0.65
1:A:220:ASP:OD1	1:A:222:LYS:N	2.30	0.65
3:F:1:NAG:O4	3:F:2:NAG:C2	2.44	0.65
5:A:502:GZZ:HC12	6:A:702:HOH:O	1.97	0.65
1:A:355:ARG:NH1	6:A:601:HOH:O	2.04	0.64
1:A:292:GLN:OE1	6:A:602:HOH:O	2.15	0.64
1:C:218:LYS:H	1:C:228:ASP:HB2	1.63	0.64
1:A:47:THR:O	1:A:53:ASN:HA	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.79	0.63
1:B:424:ARG:HG3	6:B:736:HOH:O	1.99	0.63
1:B:360:GLN:NE2	6:B:601:HOH:O	2.31	0.63
1:C:218:LYS:O	1:C:227:VAL:N	2.25	0.63
1:B:218:LYS:H	1:B:228:ASP:HB2	1.62	0.63
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.34	0.63
1:B:131:HIS:HD2	1:B:133:SER:OG	1.82	0.62
1:B:69:MET:HE2	1:B:74:PRO:CG	2.29	0.62
1:C:291:TYR:CE2	6:C:602:HOH:O	2.48	0.61
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.82	0.61
1:B:131:HIS:HD2	1:B:133:SER:H	1.46	0.61
1:B:169:TYR:O	5:B:502:GZZ:H102	1.99	0.61
1:B:308:LYS:HE2	1:B:310:TRP:O	1.99	0.61
1:C:228:ASP:OD1	1:C:229:PRO:HD2	2.01	0.61
1:B:431:HIS:H	1:B:431:HIS:CD2	2.18	0.61
1:B:360:GLN:NE2	1:B:364:GLN:NE2	2.48	0.61
1:A:218:LYS:H	1:A:228:ASP:HB2	1.66	0.61
1:B:387:ASP:HB2	6:B:664:HOH:O	2.00	0.61
1:B:457:CYS:HA	1:B:462:MET:O	2.00	0.61
1:C:431:HIS:H	1:C:431:HIS:CD2	2.17	0.61
1:A:110:GLN:O	1:A:114:GLU:HG3	2.00	0.60
1:A:219:THR:HG22	1:A:226:ILE:HA	1.81	0.60
1:B:370:MET:HG3	1:B:384:ASP:OD2	2.01	0.60
1:B:20:ALA:HB3	1:B:216:TYR:OH	2.01	0.60
1:B:218:LYS:N	1:B:228:ASP:HB2	2.17	0.60
1:C:91:TYR:OH	1:C:314:LYS:HE2	2.01	0.60
1:B:219:THR:HG22	1:B:226:ILE:HA	1.84	0.60
1:A:307:ARG:HA	1:A:343:ASN:ND2	2.18	0.59
1:C:150:GLN:NE2	6:C:607:HOH:O	2.34	0.59
1:B:223:SER:C	1:B:225:LYS:H	2.11	0.59
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.01	0.59
1:B:98:LYS:HG3	1:B:102:GLY:O	2.03	0.58
1:A:58:ALA:HA	4:A:501:FAD:C4X	2.33	0.58
1:A:223:SER:HB3	1:A:225:LYS:H	1.68	0.58
1:B:411:ASN:HD22	1:B:414:GLU:H	1.48	0.58
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.51	0.58
1:B:131:HIS:CD2	1:B:133:SER:OG	2.58	0.57
1:B:454:LEU:C	1:B:454:LEU:HD12	2.29	0.57
1:A:98:LYS:HE3	1:A:103:VAL:O	2.05	0.57
1:C:219:THR:CG2	1:C:226:ILE:HA	2.28	0.57
1:B:223:SER:HB3	1:B:225:LYS:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:TYR:O	5:C:502:GZZ:H102	2.05	0.56
1:B:411:ASN:HD22	1:B:411:ASN:C	2.14	0.56
1:A:307:ARG:HA	1:A:343:ASN:HD21	1.70	0.56
1:C:117:ASP:O	1:C:121:GLU:HG3	2.05	0.56
1:C:303:LEU:O	1:C:344:VAL:HA	2.06	0.55
3:F:1:NAG:O6	3:F:2:NAG:C1	2.54	0.55
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.40	0.55
1:A:342:ALA:O	1:A:343:ASN:HB2	2.05	0.55
1:A:306:PRO:HG2	1:A:383:PRO:HB2	1.88	0.54
1:A:91:TYR:N	1:A:91:TYR:CD1	2.75	0.54
1:B:112:ARG:HD3	1:B:159:ASP:OD1	2.08	0.54
1:B:241:LYS:HA	1:B:279:LYS:O	2.08	0.54
1:A:338:GLN:C	1:A:340:PRO:HD3	2.34	0.53
1:C:291:TYR:OH	6:C:602:HOH:O	2.04	0.53
1:A:81:LYS:O	1:A:203:ARG:NH2	2.42	0.53
1:C:304:LYS:HE2	1:C:342:ALA:O	2.09	0.53
1:B:366:LYS:HD2	1:B:385:ALA:HB3	1.91	0.52
2:E:1:NAG:O4	2:E:2:NAG:C2	2.54	0.52
1:A:63:GLY:HA2	1:A:193:GLY:O	2.09	0.52
1:C:73:TRP:HB3	1:C:74:PRO:HD3	1.91	0.52
1:C:374:ARG:HD2	6:C:639:HOH:O	2.10	0.51
1:B:63:GLY:HA2	1:B:193:GLY:O	2.10	0.51
1:B:438:GLY:O	4:B:501:FAD:H1'2	2.10	0.50
3:F:1:NAG:H4	3:F:2:NAG:C1	2.39	0.50
1:B:131:HIS:HD2	1:B:133:SER:CB	2.25	0.50
1:B:222:LYS:CG	1:B:222:LYS:O	2.59	0.50
1:A:119:VAL:HA	1:A:122:MET:HE3	1.93	0.50
1:B:148:GLU:O	1:B:149:HIS:HB2	2.12	0.50
1:C:355:ARG:NH1	6:C:603:HOH:O	2.18	0.50
1:C:220:ASP:HB3	1:C:223:SER:OG	2.12	0.49
1:B:222:LYS:O	1:B:222:LYS:HG3	2.12	0.49
1:B:243:SER:CB	1:B:244:PRO:CD	2.89	0.49
1:B:223:SER:C	1:B:225:LYS:N	2.69	0.49
1:A:405:ASN:OD1	5:A:502:GZZ:NH1	2.46	0.49
1:A:98:LYS:HE2	1:A:104:TYR:HA	1.95	0.48
1:B:58:ALA:HA	4:B:501:FAD:C4X	2.43	0.48
1:A:64:VAL:HG12	1:A:65:ASN:N	2.28	0.48
1:C:219:THR:HA	1:C:225:LYS:O	2.13	0.48
2:E:1:NAG:H4	2:E:2:NAG:C1	2.41	0.48
1:A:448:ILE:O	1:A:452:GLU:HG3	2.14	0.47
1:B:449:ASP:O	1:B:453:ILE:HG13	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.96	0.47
1:A:370:MET:HE2	1:A:384:ASP:HA	1.96	0.47
1:B:242:TYR:CE2	1:B:280:PRO:HD2	2.50	0.47
1:C:235:LYS:NZ	1:C:253:ASP:OD2	2.31	0.47
1:C:342:ALA:O	1:C:343:ASN:HB2	2.15	0.47
1:A:415:TYR:O	1:A:418:LEU:HB2	2.15	0.47
1:A:49:PHE:N	1:A:52:ILE:O	2.36	0.47
1:A:220:ASP:OD1	1:A:223:SER:N	2.45	0.46
1:A:170:GLU:OE2	5:A:502:GZZ:H101	2.14	0.46
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.62	0.46
1:C:218:LYS:N	1:C:228:ASP:HB2	2.31	0.46
1:C:104:TYR:CZ	1:C:158:VAL:HG23	2.51	0.46
1:B:454:LEU:HD12	1:B:454:LEU:O	2.15	0.46
1:A:115:LEU:HD12	1:A:115:LEU:C	2.42	0.45
5:A:502:GZZ:C1	6:A:702:HOH:O	2.59	0.45
1:B:6:ARG:HA	1:B:30:ASP:O	2.16	0.45
1:B:52:ILE:CD1	1:B:339:TYR:CD2	2.99	0.45
3:F:2:NAG:H62	3:F:5:FCA:H5	1.99	0.45
1:C:219:THR:HA	1:C:227:VAL:HG22	1.98	0.45
1:C:272:GLN:C	6:C:602:HOH:O	2.50	0.45
1:C:96:VAL:O	1:C:103:VAL:HA	2.17	0.45
1:B:91:TYR:N	1:B:91:TYR:CD1	2.85	0.44
1:A:80:LEU:O	1:A:81:LYS:C	2.61	0.44
1:A:178:THR:CG2	1:A:183:THR:HG21	2.48	0.44
1:B:98:LYS:O	1:B:99:GLU:C	2.60	0.44
1:C:8:ILE:HG13	1:C:259:ALA:HB2	1.98	0.44
1:B:8:ILE:HA	1:B:32:LEU:O	2.18	0.44
1:B:170:GLU:OE2	5:B:502:GZZ:H101	2.17	0.44
1:B:189:PHE:CZ	5:B:502:GZZ:H171	2.53	0.44
1:B:360:GLN:NE2	1:B:364:GLN:HE21	2.14	0.44
1:A:45:HIS:HD2	1:A:56:LEU:HD12	1.83	0.44
1:C:223:SER:C	1:C:225:LYS:H	2.24	0.44
1:A:370:MET:HG3	1:A:384:ASP:OD1	2.18	0.43
1:B:421:PRO:HB3	1:B:426:TYR:CD2	2.53	0.43
1:A:49:PHE:O	1:A:50:ALA:HB3	2.18	0.43
1:C:219:THR:CA	1:C:227:VAL:HG22	2.47	0.43
1:A:68:LYS:HD2	1:A:191:ASP:HB3	1.99	0.43
1:B:52:ILE:HD12	1:B:339:TYR:CD2	2.54	0.43
1:B:304:LYS:HG3	1:B:305:PHE:N	2.33	0.43
1:B:73:TRP:CZ2	1:B:77:ASN:HB2	2.53	0.43
1:B:253:ASP:O	1:B:254:ASN:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HA	1:B:275:LEU:HD12	1.78	0.43
1:A:376:MET:C	1:A:378:PRO:HD3	2.44	0.43
1:C:60:TRP:CZ3	5:C:502:GZZ:H112	2.53	0.43
1:B:420:ALA:HA	1:B:421:PRO:HD3	1.81	0.43
1:A:58:ALA:HA	4:A:501:FAD:N5	2.34	0.42
1:A:21:LYS:O	1:A:25:GLU:HG3	2.18	0.42
1:A:253:ASP:C	1:A:253:ASP:OD1	2.61	0.42
1:A:366:LYS:HD2	1:A:385:ALA:HB3	2.00	0.42
1:B:134:GLY:HA2	1:B:181:GLN:OE1	2.20	0.42
1:B:286:LYS:NZ	1:B:420:ALA:O	2.51	0.42
1:C:98:LYS:HG2	1:C:104:TYR:CE1	2.54	0.42
1:C:100:ASP:OD1	1:C:375:LYS:HE2	2.19	0.42
1:C:104:TYR:CZ	1:C:158:VAL:CG2	3.02	0.42
1:A:70:ASN:O	1:A:74:PRO:HD3	2.18	0.42
1:C:219:THR:CA	1:C:225:LYS:O	2.67	0.42
1:A:228:ASP:HA	1:A:229:PRO:HD2	1.91	0.42
1:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	0.42
1:B:308:LYS:HG2	1:B:309:PHE:N	2.33	0.42
1:C:58:ALA:HA	4:C:501:FAD:C4X	2.50	0.42
1:B:6:ARG:O	1:B:259:ALA:HB1	2.20	0.42
1:B:431:HIS:CD2	6:B:699:HOH:O	2.72	0.42
1:C:217:LEU:HD12	1:C:217:LEU:HA	1.90	0.42
1:B:244:PRO:O	1:B:424:ARG:NH1	2.52	0.42
1:C:91:TYR:CD1	1:C:91:TYR:N	2.87	0.42
1:A:438:GLY:O	4:A:501:FAD:H1'2	2.20	0.42
1:B:69:MET:HE1	1:B:73:TRP:HB3	1.92	0.42
1:C:454:LEU:HD12	1:C:454:LEU:O	2.20	0.42
1:A:218:LYS:N	1:A:228:ASP:HB2	2.31	0.41
1:C:243:SER:HB2	1:C:244:PRO:CD	2.50	0.41
1:C:260:ASP:O	1:C:424:ARG:HD3	2.20	0.41
1:A:235:LYS:NZ	1:A:253:ASP:OD2	2.51	0.41
1:B:252:GLU:C	1:B:254:ASN:H	2.28	0.41
2:D:1:NAG:HO4	2:D:2:NAG:C1	2.18	0.41
1:C:290:ILE:HA	1:C:418:LEU:HD21	2.03	0.41
1:B:35:GLU:HG2	1:B:39:HIS:O	2.21	0.41
1:A:156:THR:O	1:A:160:MET:HG3	2.20	0.41
1:A:219:THR:HA	1:A:225:LYS:O	2.21	0.41
1:A:431:HIS:CD2	6:A:730:HOH:O	2.74	0.41
1:C:49:PHE:O	1:C:52:ILE:HG12	2.21	0.41
1:C:438:GLY:O	4:C:501:FAD:H1'2	2.20	0.41
2:E:1:NAG:O6	2:E:2:NAG:C1	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLN:HB3	1:B:235:LYS:HG3	2.02	0.40
1:B:26:ALA:HB2	1:B:455:ILE:HD13	2.03	0.40
1:B:131:HIS:CD2	1:B:133:SER:CB	3.03	0.40
1:C:64:VAL:HG12	1:C:65:ASN:N	2.35	0.40
1:A:39:HIS:HD2	1:A:40:ILE:O	2.05	0.40
1:A:73:TRP:N	1:A:74:PRO:CD	2.85	0.40
1:B:350:THR:HA	1:B:354:SER:OG	2.21	0.40
1:B:416:ASP:OD2	1:B:466:HIS:HD2	2.04	0.40
1:A:350:THR:HA	1:A:354:SER:OG	2.21	0.40
1:A:137:ASP:OD1	1:A:181:GLN:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/472 (97%)	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%)	389 (99%)	5 (1%)	61	61
1	B	397/404 (98%)	390 (98%)	7 (2%)	51	50
1	C	397/404 (98%)	391 (98%)	6 (2%)	57	56
All	All	1188/1212 (98%)	1170 (98%)	18 (2%)	57	56

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	52	ILE
1	A	59	ASN
1	A	115	LEU
1	A	190	SER
1	B	115	LEU
1	B	157	PRO
1	B	177	VAL
1	B	223	SER
1	B	408	VAL
1	B	411	ASN
1	B	454	LEU
1	C	115	LEU
1	C	157	PRO
1	C	175	PRO
1	C	188	THR
1	C	217	LEU
1	C	221	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	152	ASN
1	A	234	ASN
1	A	292	GLN
1	A	359	GLN
1	A	360	GLN
1	A	371	GLN
1	A	431	HIS
1	B	131	HIS
1	B	152	ASN
1	B	359	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	360	GLN
1	B	364	GLN
1	B	411	ASN
1	B	431	HIS
1	B	435	HIS
1	B	466	HIS
1	C	215	GLN
1	C	360	GLN
1	C	431	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.94	0	17,19,21	1.64	5 (29%)
2	NAG	D	2	2	14,14,15	0.92	0	17,19,21	1.84	4 (23%)
2	NAG	E	1	2,1	14,14,15	1.26	3 (21%)	17,19,21	2.49	4 (23%)
2	NAG	E	2	2	14,14,15	0.96	1 (7%)	17,19,21	1.41	3 (17%)
3	NAG	F	1	3,1	14,14,15	1.33	2 (14%)	17,19,21	2.06	6 (35%)
3	NAG	F	2	3	14,14,15	0.97	1 (7%)	17,19,21	1.69	4 (23%)
3	MAN	F	3	3	11,11,12	0.67	0	15,15,17	2.48	3 (20%)
3	MAN	F	4	3	11,11,12	0.60	0	15,15,17	1.40	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FCA	F	5	3	10,10,11	1.19	1 (10%)	14,14,16	1.51	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	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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-2.75	1.39	1.43
3	F	2	NAG	O5-C1	-2.72	1.39	1.43
2	E	1	NAG	O5-C1	-2.72	1.39	1.43
3	F	1	NAG	C1-C2	-2.58	1.48	1.52
3	F	5	FCA	C2-C3	-2.45	1.48	1.52
2	E	1	NAG	C1-C2	-2.25	1.49	1.52
2	E	1	NAG	O3-C3	2.20	1.48	1.43
2	E	2	NAG	O5-C1	-2.16	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	MAN	O2-C2-C3	8.55	127.86	110.15
2	E	1	NAG	C2-N2-C7	-6.89	113.67	122.90
3	F	1	NAG	C1-C2-N2	-5.48	101.79	110.43
2	D	2	NAG	C2-N2-C7	-5.17	115.97	122.90
3	F	2	NAG	C2-N2-C7	-4.99	116.21	122.90
2	E	1	NAG	C1-C2-N2	-4.38	103.52	110.43
2	E	1	NAG	O3-C3-C2	3.84	117.39	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	3.45	116.80	112.19
2	E	2	NAG	C1-O5-C5	3.13	116.39	112.19
3	F	1	NAG	O3-C3-C4	3.08	117.64	110.38
3	F	4	MAN	C1-C2-C3	-2.94	105.36	109.64
2	D	1	NAG	C8-C7-N2	-2.76	111.53	116.12
2	D	2	NAG	C8-C7-N2	-2.76	111.54	116.12
2	E	1	NAG	O5-C5-C6	-2.69	102.42	107.66
3	F	4	MAN	C2-C3-C4	-2.63	106.24	110.86
3	F	2	NAG	C1-C2-N2	-2.62	106.30	110.43
3	F	4	MAN	O2-C2-C3	2.62	115.58	110.15
2	E	2	NAG	O7-C7-N2	2.61	126.59	121.98
3	F	1	NAG	C8-C7-N2	-2.61	111.79	116.12
3	F	1	NAG	O5-C5-C6	-2.55	102.69	107.66
3	F	1	NAG	C3-C4-C5	2.43	114.63	110.23
2	D	1	NAG	C1-C2-N2	-2.41	106.64	110.43
3	F	1	NAG	O4-C4-C3	-2.40	104.71	110.38
3	F	3	MAN	C1-O5-C5	2.40	115.41	112.19
2	D	2	NAG	C1-C2-N2	-2.33	106.75	110.43
3	F	5	FCA	O5-C5-C4	2.20	113.52	109.55
2	D	1	NAG	O3-C3-C2	2.17	113.91	109.40
3	F	3	MAN	O2-C2-C1	2.15	114.14	109.22
2	D	1	NAG	O3-C3-C4	2.09	115.30	110.38
2	D	2	NAG	C4-C3-C2	-2.08	107.97	111.02
2	E	2	NAG	O5-C5-C6	-2.08	103.62	107.66
3	F	2	NAG	O5-C5-C4	-2.08	105.78	110.83
3	F	5	FCA	C1-C2-C3	2.06	112.65	109.64
3	F	5	FCA	C3-C4-C5	-2.05	106.70	109.81
3	F	2	NAG	O5-C5-C6	-2.04	103.69	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	3	MAN	C1

All (14) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

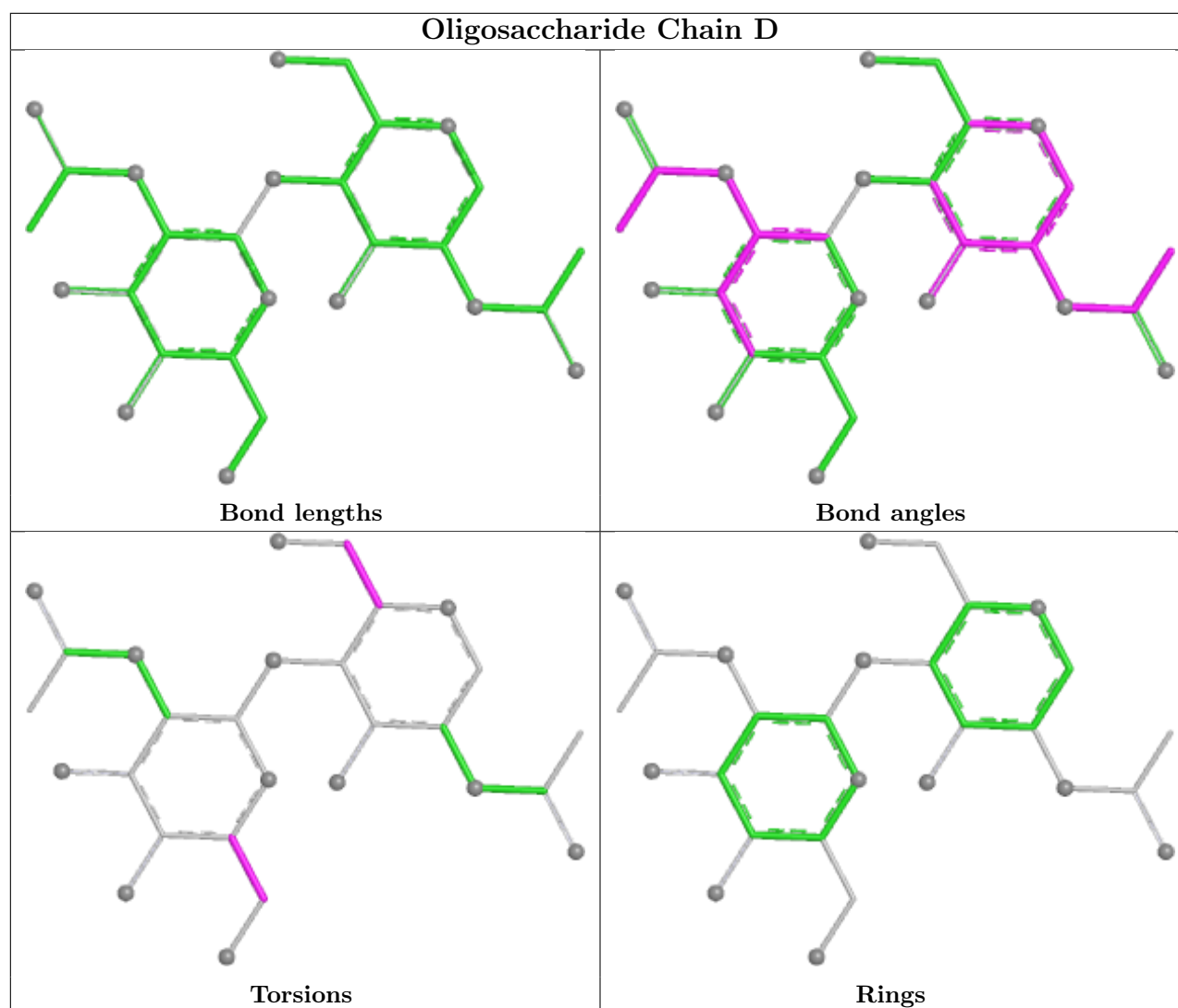
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6

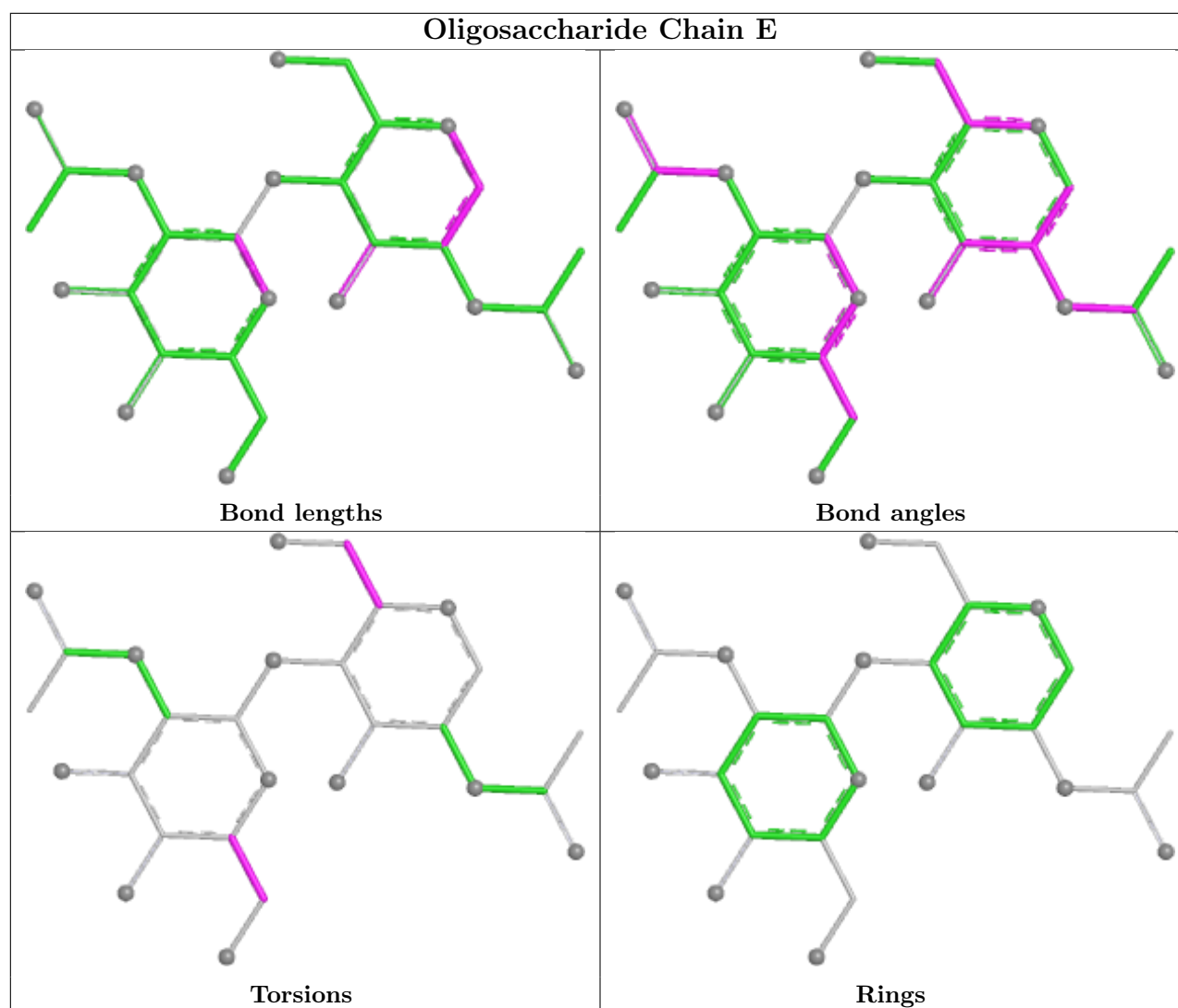
There are no ring outliers.

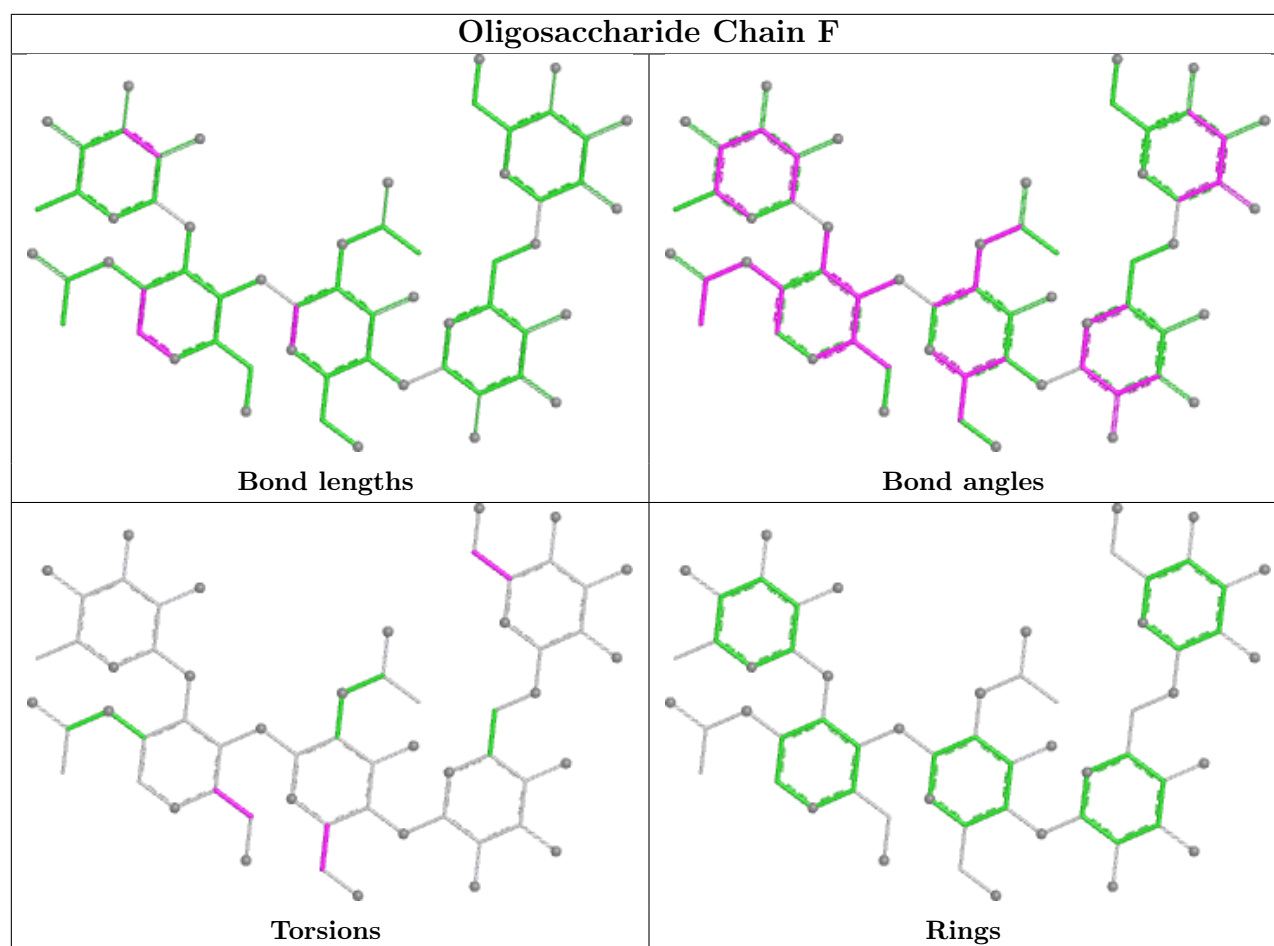
7 monomers are involved in 13 short contacts:

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







5.6 Ligand geometry [i](#)

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	A	502	-	24,24,24	0.94	2 (8%)	23,25,25	1.49	5 (21%)
4	FAD	A	501	-	58,58,58	0.85	2 (3%)	85,89,89	1.26	8 (9%)
5	GZZ	C	502	-	24,24,24	1.11	2 (8%)	23,25,25	1.40	5 (21%)
4	FAD	B	501	-	58,58,58	1.15	3 (5%)	85,89,89	1.21	9 (10%)
5	GZZ	B	502	-	24,24,24	1.15	2 (8%)	23,25,25	1.66	5 (21%)
4	FAD	C	501	-	58,58,58	1.10	5 (8%)	85,89,89	1.28	9 (10%)

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	A	502	-	-	12/22/22/22	-
4	FAD	A	501	-	-	4/34/50/50	0/6/6/6
5	GZZ	C	502	-	-	10/22/22/22	-
4	FAD	B	501	-	-	8/34/50/50	0/6/6/6
5	GZZ	B	502	-	-	14/22/22/22	-
4	FAD	C	501	-	-	1/34/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	FAD	P-O3P	5.15	1.65	1.59
4	B	501	FAD	PA-O3P	3.87	1.63	1.59
4	C	501	FAD	C4X-N5	3.26	1.37	1.30
4	C	501	FAD	PA-O3P	3.18	1.62	1.59
5	B	502	GZZ	C8-N9	3.11	1.57	1.47
5	B	502	GZZ	C10-N9	2.92	1.56	1.47
5	C	502	GZZ	C8-N9	2.86	1.56	1.47
5	C	502	GZZ	C10-N9	2.83	1.56	1.47
4	A	501	FAD	PA-O3P	2.43	1.62	1.59
5	A	502	GZZ	C10-N9	2.41	1.55	1.47
4	C	501	FAD	P-O3P	2.32	1.62	1.59
5	A	502	GZZ	C8-N9	2.19	1.54	1.47
4	B	501	FAD	C4X-N5	2.19	1.35	1.30
4	C	501	FAD	C9-C8	2.08	1.42	1.39
4	A	501	FAD	C4X-N5	2.03	1.35	1.30
4	C	501	FAD	C7M-C7	2.03	1.54	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	FAD	C9A-C5X-N5	-4.99	117.16	122.45
4	C	501	FAD	C4-C4X-N5	4.01	123.74	118.21
4	C	501	FAD	C9A-C5X-N5	-3.95	118.26	122.45
4	B	501	FAD	C4'-C3'-C2'	3.75	119.81	113.57
5	A	502	GZZ	NE1-CZ1-NH1	-3.72	114.29	120.67
5	B	502	GZZ	NE1-CZ1-NH1	-3.60	114.50	120.67
5	B	502	GZZ	NH2-CZ1-NE1	3.45	127.12	119.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	GZZ	C7-C8-N9	3.36	121.08	112.07
4	B	501	FAD	O2A-PA-O3P	3.32	116.25	107.27
4	B	501	FAD	O3P-P-O1P	-3.05	101.52	110.70
4	C	501	FAD	C4'-C3'-C2'	3.00	118.57	113.57
4	A	501	FAD	C10-C4X-N5	-2.95	118.78	124.81
4	A	501	FAD	C4'-C3'-C2'	2.87	118.35	113.57
4	C	501	FAD	C10-C4X-N5	-2.86	118.96	124.81
4	C	501	FAD	O2P-P-O1P	2.85	125.69	112.44
5	C	502	GZZ	NH2-CZ1-NE1	2.84	125.73	119.27
4	A	501	FAD	O2A-PA-O1A	2.73	125.17	112.44
4	A	501	FAD	C6-C5X-C9A	2.67	122.72	119.05
5	C	502	GZZ	NH3-CZ2-NH4	-2.66	112.50	120.07
5	C	502	GZZ	NE1-CZ1-NH1	-2.63	116.16	120.67
4	A	501	FAD	C10-N1-C2	2.53	122.32	116.85
4	C	501	FAD	O2A-PA-O1A	2.42	123.71	112.44
4	B	501	FAD	O2P-P-O5'	2.39	118.39	107.57
5	A	502	GZZ	C10-N9-C8	-2.38	102.13	113.40
5	B	502	GZZ	NE2-CZ2-NH4	-2.33	116.68	120.67
4	B	501	FAD	C10-N1-C2	2.28	121.78	116.85
4	C	501	FAD	O3P-PA-O1A	-2.24	103.95	110.70
4	B	501	FAD	O4B-C1B-C2B	-2.22	101.87	106.62
5	C	502	GZZ	C2-C1-NE1	-2.21	106.00	112.20
5	A	502	GZZ	C6-C7-C8	-2.20	103.39	113.56
5	C	502	GZZ	NH3-CZ2-NE2	2.19	124.23	119.27
4	B	501	FAD	O2P-P-O3P	-2.17	101.41	107.27
4	B	501	FAD	C10-C4X-N5	-2.15	120.42	124.81
4	A	501	FAD	C2B-C1B-N9A	2.12	118.57	113.30
5	A	502	GZZ	C2-C1-NE1	-2.11	106.27	112.20
4	B	501	FAD	O2P-P-O1P	2.10	122.20	112.44
4	C	501	FAD	O3'-C3'-C4'	-2.07	104.22	108.93
5	B	502	GZZ	C16-C17-NE2	-2.03	106.50	112.20
5	A	502	GZZ	C4-C3-C2	-2.02	104.14	114.37
4	A	501	FAD	O3P-PA-O1A	-2.02	104.62	110.70
4	C	501	FAD	O2P-P-O3P	-2.01	101.83	107.27

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	FAD	C5B-O5B-PA-O1A
5	A	502	GZZ	NH3-CZ2-NE2-C17
5	A	502	GZZ	NH4-CZ2-NE2-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	502	GZZ	NH3-CZ2-NE2-C17
5	B	502	GZZ	NH4-CZ2-NE2-C17
5	C	502	GZZ	NH3-CZ2-NE2-C17
5	C	502	GZZ	C6-C7-C8-N9
5	B	502	GZZ	C6-C7-C8-N9
5	C	502	GZZ	N9-C10-C11-C12
5	A	502	GZZ	C6-C7-C8-N9
4	B	501	FAD	C2'-C3'-C4'-C5'
5	A	502	GZZ	N9-C10-C11-C12
5	B	502	GZZ	N9-C10-C11-C12
5	B	502	GZZ	C3-C4-C5-C6
5	C	502	GZZ	C4-C5-C6-C7
4	B	501	FAD	C2'-C3'-C4'-O4'
5	A	502	GZZ	C5-C6-C7-C8
5	C	502	GZZ	C5-C6-C7-C8
5	A	502	GZZ	C14-C15-C16-C17
5	B	502	GZZ	C5-C6-C7-C8
5	A	502	GZZ	C4-C5-C6-C7
5	A	502	GZZ	C10-C11-C12-C13
5	B	502	GZZ	C14-C15-C16-C17
5	B	502	GZZ	C4-C5-C6-C7
5	B	502	GZZ	C1-C2-C3-C4
5	A	502	GZZ	C3-C4-C5-C6
5	B	502	GZZ	C15-C16-C17-NE2
5	A	502	GZZ	C11-C12-C13-C14
5	B	502	GZZ	C11-C12-C13-C14
5	C	502	GZZ	C11-C12-C13-C14
4	B	501	FAD	PA-O3P-P-O5'
4	A	501	FAD	C2'-C3'-C4'-O4'
5	C	502	GZZ	C3-C4-C5-C6
5	C	502	GZZ	C15-C16-C17-NE2
5	C	502	GZZ	C14-C15-C16-C17
5	B	502	GZZ	C10-C11-C12-C13
5	C	502	GZZ	C13-C14-C15-C16
4	B	501	FAD	C5B-O5B-PA-O2A
5	B	502	GZZ	NH1-CZ1-NE1-C1
4	B	501	FAD	O3'-C3'-C4'-C5'
5	A	502	GZZ	C12-C13-C14-C15
4	A	501	FAD	O3'-C3'-C4'-O4'
5	A	502	GZZ	C15-C16-C17-NE2
4	A	501	FAD	O3'-C3'-C4'-C5'
4	B	501	FAD	O3'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

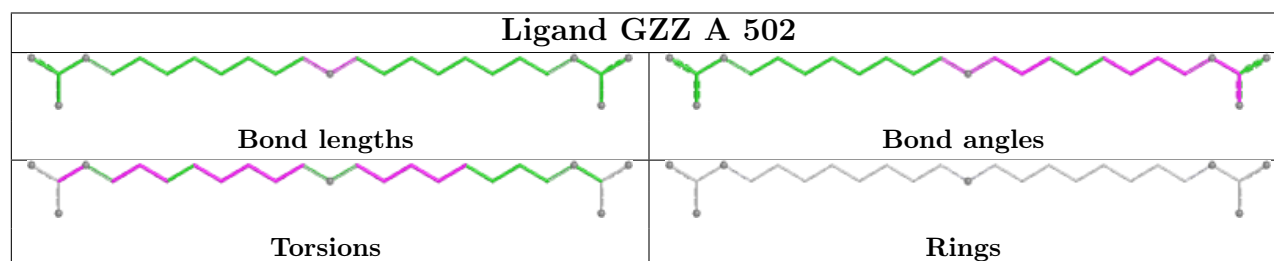
Mol	Chain	Res	Type	Atoms
4	A	501	FAD	O4B-C4B-C5B-O5B
4	B	501	FAD	O4B-C4B-C5B-O5B
5	B	502	GZZ	NH2-CZ1-NE1-C1
4	C	501	FAD	O4B-C4B-C5B-O5B

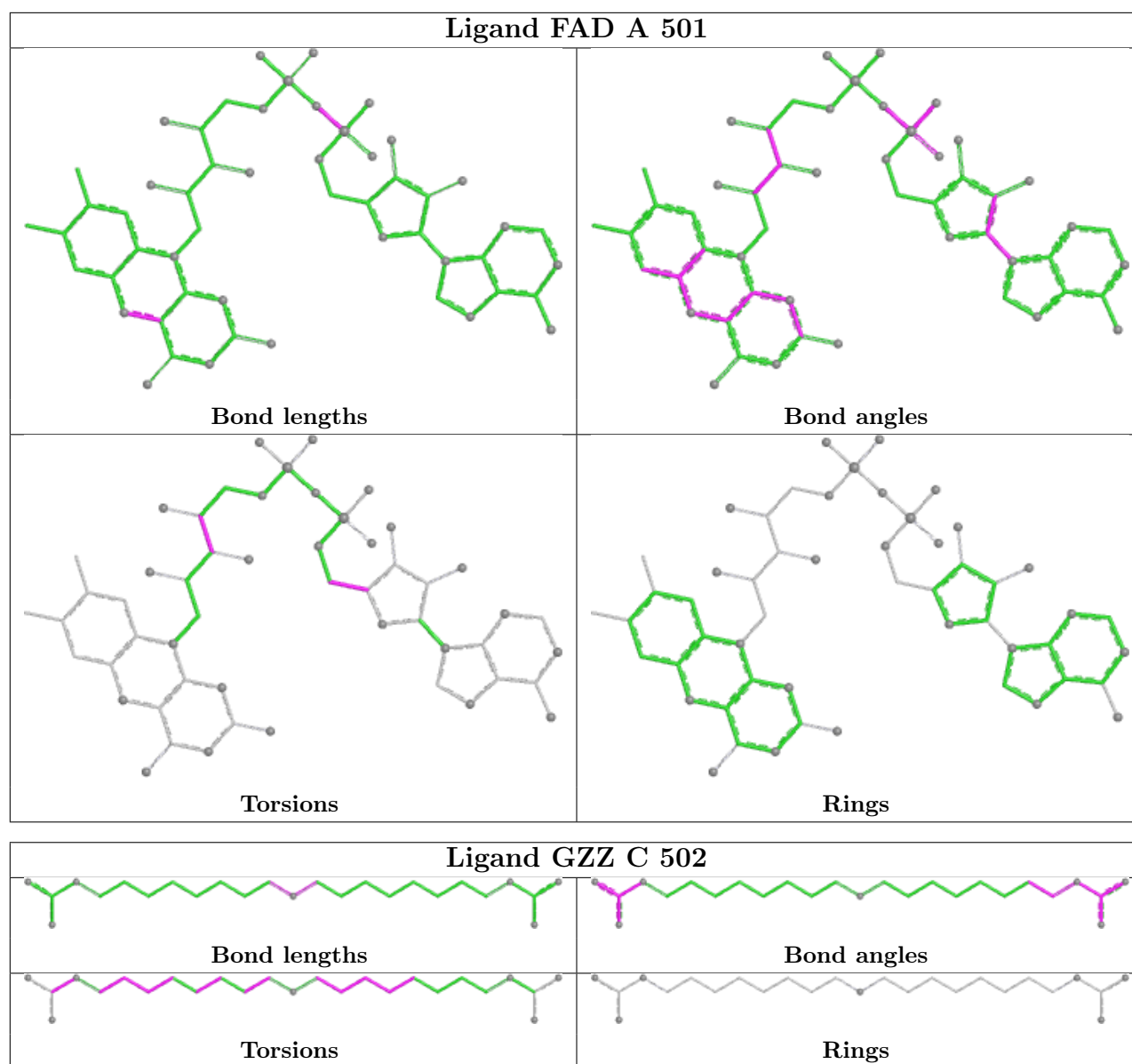
There are no ring outliers.

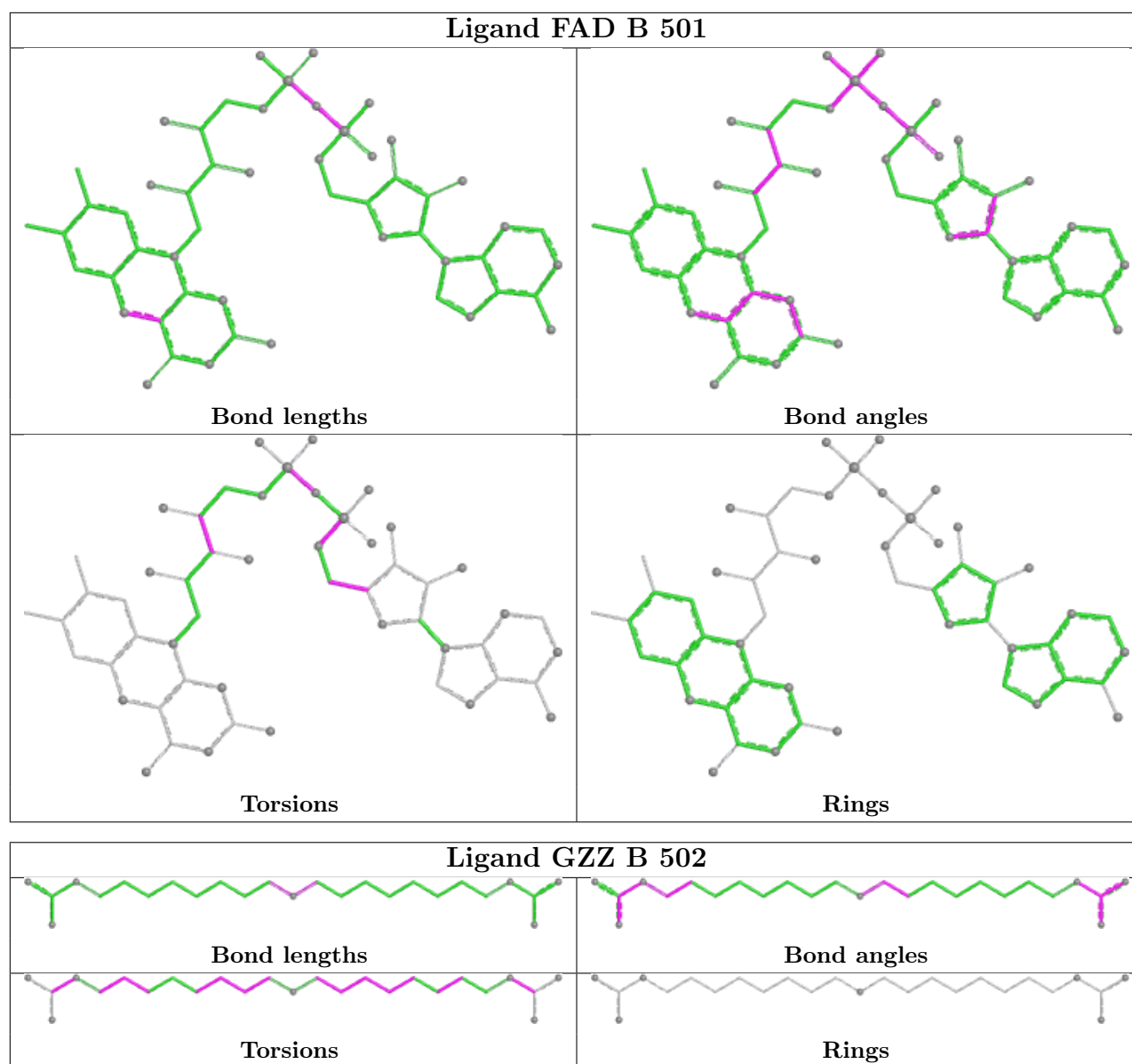
6 monomers are involved in 20 short contacts:

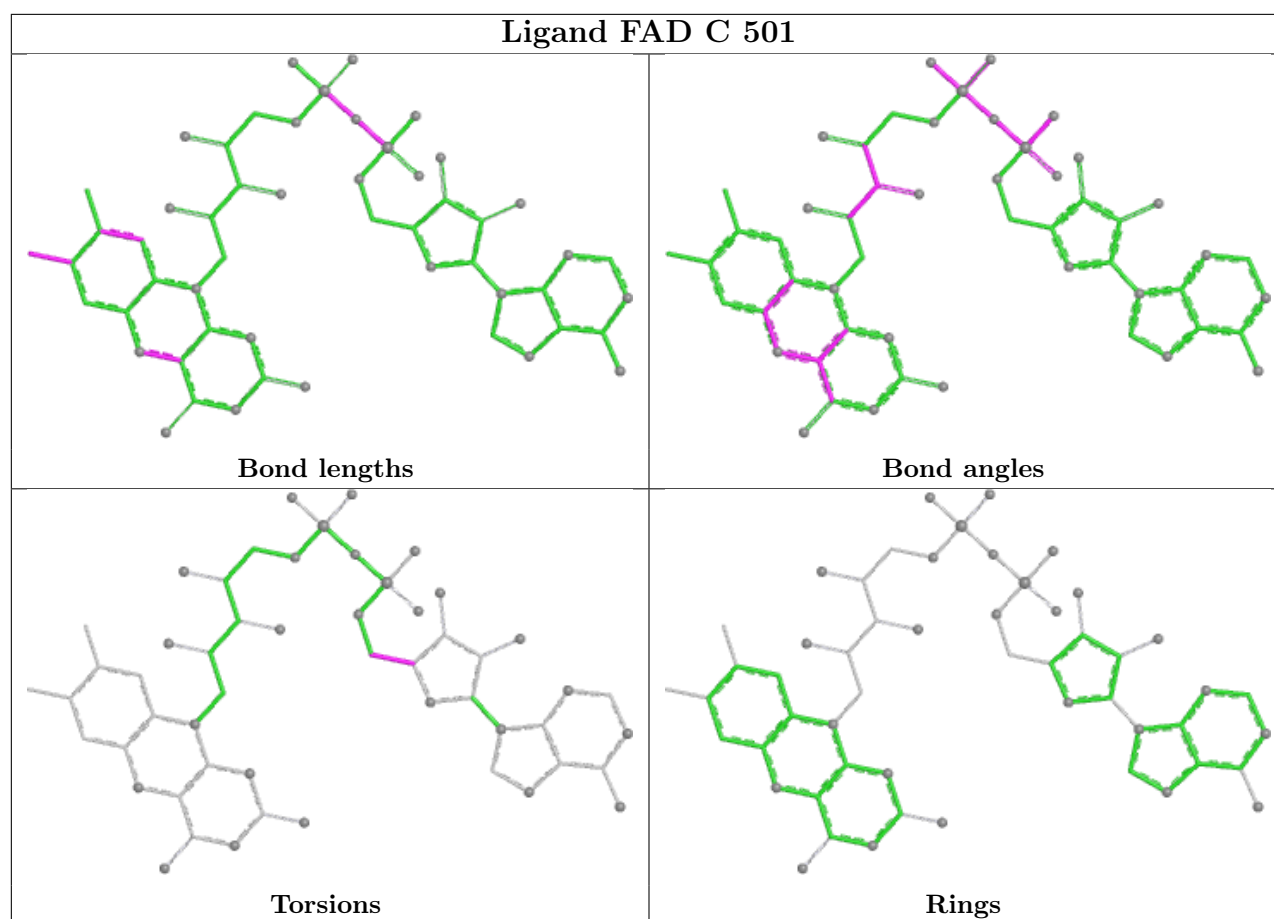
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	GZZ	7	0
4	A	501	FAD	3	0
5	C	502	GZZ	2	0
4	B	501	FAD	2	0
5	B	502	GZZ	4	0
4	C	501	FAD	2	0

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 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.