



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:33 AM UTC

PDB ID : 2BAT / pdb_00002bat
Title : THE STRUCTURE OF THE COMPLEX BETWEEN INFLUENZA VIRUS
NEURAMINIDASE AND SIALIC ACID, THE VIRAL RECEPTOR
Authors : Varghese, J.N.; Colman, P.M.
Deposited on : 1992-08-10
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)
Xtrriage (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

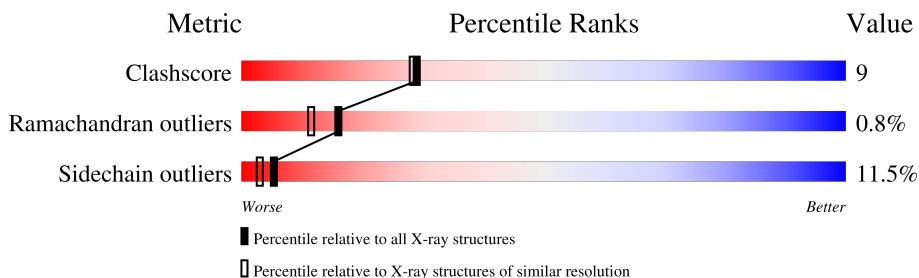
1 Overall quality at a glance

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	388	
2	B	7	
3	C	6	

2 Entry composition [i](#)

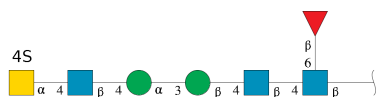
There are 7 unique types of molecules in this entry. The entry contains 3352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEURAMINIDASE N2.

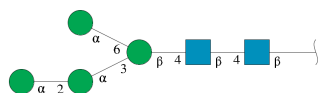
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3022	1866	546	587	23	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-4-O-sulfo-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fuco pyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	7	92	50	4	37	1	38	0	0

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



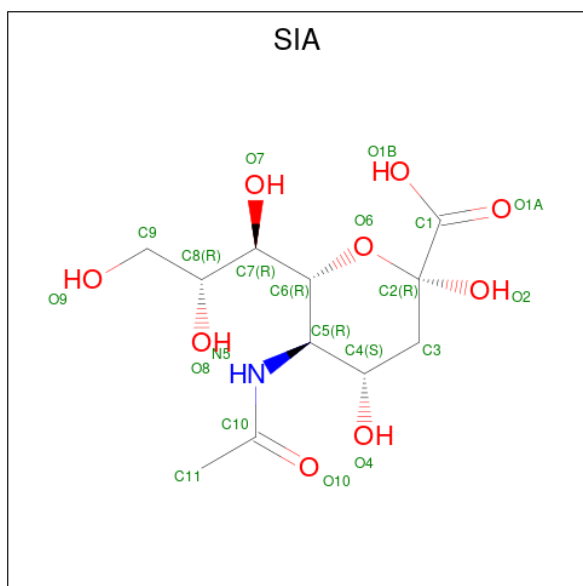
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	6	72	40	2	30	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Ca 1	0	0

- Molecule 7 is water.

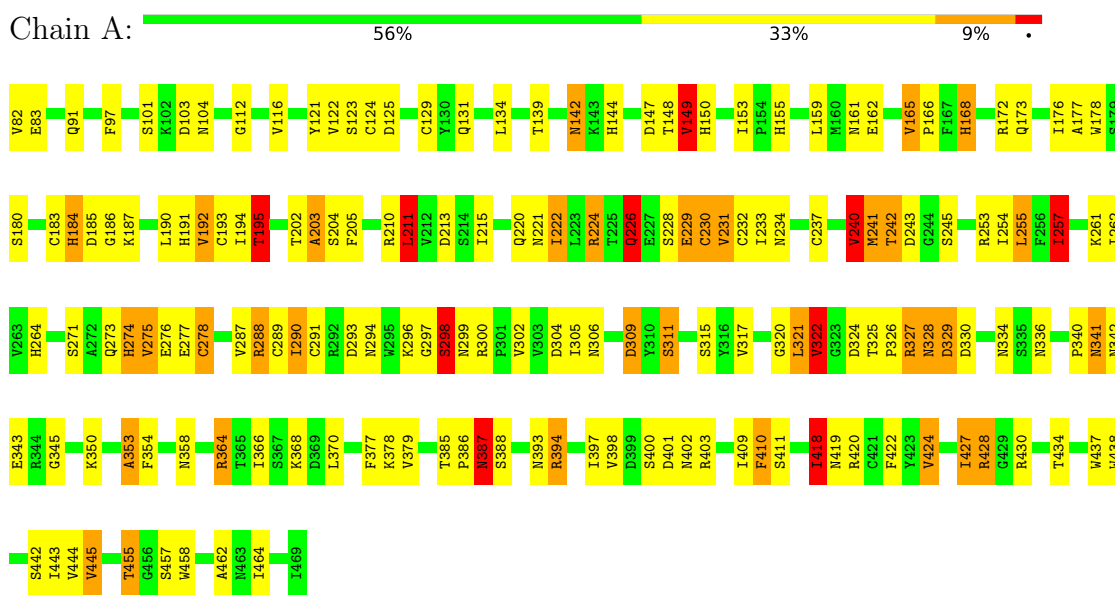
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	116	Total 116	O 116	0	0

3 Residue-property plots

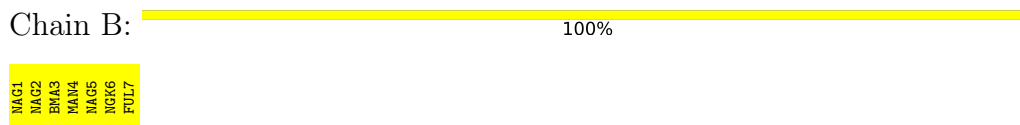
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: NEURAMINIDASE N2



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



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



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.60Å 139.60Å 191.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3352	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NGK, SIA, MAN, BMA, CA, NAG, FUL

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	1.24	20/3092 (0.6%)	2.18	127/4194 (3.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	ILE	CA-CB	8.62	1.65	1.54
1	A	165	VAL	CA-CB	7.75	1.64	1.54
1	A	322	VAL	CA-CB	7.44	1.64	1.54
1	A	240	VAL	CA-CB	7.40	1.63	1.54
1	A	274	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	144	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	150	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	184	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	257	ILE	CA-CB	6.42	1.62	1.54
1	A	168	HIS	CG-ND1	-6.13	1.31	1.38
1	A	427	ILE	CA-CB	6.08	1.64	1.54
1	A	192	VAL	CA-CB	6.03	1.61	1.54
1	A	191	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	264	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	155	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	424	VAL	CA-CB	5.56	1.61	1.54
1	A	168	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	184	HIS	CG-ND1	-5.30	1.32	1.38
1	A	231	VAL	CA-CB	5.27	1.62	1.54
1	A	274	HIS	CG-ND1	-5.06	1.32	1.38

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	CYS	N-CA-CB	-12.49	90.40	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ASP	CA-CB-CG	12.35	124.95	112.60
1	A	397	ILE	N-CA-C	-11.61	102.37	112.12
1	A	298	SER	N-CA-C	-10.85	100.17	113.41
1	A	309	ASP	CA-CB-CG	10.03	122.63	112.60
1	A	229	GLU	N-CA-C	9.92	124.97	110.28
1	A	410	PHE	CA-CB-CG	9.86	123.66	113.80
1	A	271	SER	N-CA-C	9.71	125.41	113.17
1	A	125	ASP	CA-CB-CG	9.58	122.18	112.60
1	A	306	ASN	OD1-CG-ND2	-9.53	113.07	122.60
1	A	142	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	A	387	ASN	OD1-CG-ND2	-8.96	113.64	122.60
1	A	387	ASN	N-CA-C	8.80	123.68	113.38
1	A	290	ILE	N-CA-C	-8.74	95.88	108.11
1	A	455	THR	N-CA-CB	-8.66	97.66	111.43
1	A	353	ALA	O-C-N	-8.38	115.87	123.41
1	A	192	VAL	N-CA-C	-8.31	96.53	108.17
1	A	124	CYS	CB-CA-C	8.30	122.92	110.14
1	A	153	ILE	O-C-N	-8.18	115.99	121.72
1	A	321	LEU	CA-C-O	-7.99	111.95	120.42
1	A	299	ASN	CA-CB-CG	7.99	120.59	112.60
1	A	229	GLU	N-CA-CB	-7.90	98.36	109.97
1	A	149	VAL	CB-CA-C	-7.85	100.00	112.16
1	A	178	TRP	N-CA-C	-7.68	102.12	112.94
1	A	297	GLY	O-C-N	7.35	129.90	123.36
1	A	430	ARG	O-C-N	-7.10	114.48	122.86
1	A	324	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	264	HIS	CB-CG-CD2	-7.08	122.00	131.20
1	A	172	ARG	CG-CD-NE	-7.02	96.56	112.00
1	A	243	ASP	CA-CB-CG	6.97	119.57	112.60
1	A	91	GLN	N-CA-C	-6.92	100.74	110.50
1	A	378	LYS	CB-CG-CD	-6.91	95.40	111.30
1	A	121	TYR	CA-CB-CG	6.84	126.20	113.90
1	A	309	ASP	CB-CA-C	-6.78	98.16	109.55
1	A	306	ASN	CB-CG-ND2	6.75	126.52	116.40
1	A	211	LEU	N-CA-C	-6.69	99.12	109.76
1	A	377	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	103	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	195	THR	OG1-CB-CG2	6.57	122.43	109.30
1	A	300	ARG	CA-C-N	6.54	126.92	119.92
1	A	300	ARG	C-N-CA	6.54	126.92	119.92
1	A	112	GLY	CA-C-O	-6.49	115.25	121.87
1	A	241	MET	CG-SD-CE	-6.49	86.62	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	SER	N-CA-C	-6.45	99.50	109.24
1	A	328	ASN	N-CA-C	6.44	119.26	111.40
1	A	178	TRP	CB-CG-CD1	-6.43	117.25	126.90
1	A	293	ASP	CA-C-O	6.43	127.34	120.46
1	A	150	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	191	HIS	CB-CG-CD2	-6.34	122.95	131.20
1	A	155	HIS	CA-CB-CG	-6.30	107.50	113.80
1	A	147	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	220	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	A	226	GLN	N-CA-C	6.25	124.11	110.80
1	A	320	GLY	N-CA-C	-6.23	107.16	115.32
1	A	394	ARG	CG-CD-NE	-6.22	98.32	112.00
1	A	195	THR	N-CA-CB	6.19	121.65	111.62
1	A	142	ASN	O-C-N	-6.16	116.40	123.42
1	A	358	ASN	OD1-CG-ND2	-6.11	116.50	122.60
1	A	345	GLY	N-CA-C	6.09	119.56	112.50
1	A	83	GLU	CA-CB-CG	6.05	126.21	114.10
1	A	419	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	131	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	A	230	CYS	O-C-N	-5.98	114.28	122.23
1	A	393	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	444	VAL	N-CA-C	-5.94	99.65	108.45
1	A	220	GLN	N-CA-C	5.93	119.73	111.90
1	A	424	VAL	N-CA-C	-5.93	99.52	108.17
1	A	325	THR	CA-C-O	-5.92	114.18	119.86
1	A	434	THR	N-CA-CB	-5.89	101.20	110.46
1	A	173	GLN	CA-CB-CG	-5.87	102.36	114.10
1	A	178	TRP	CG-CD2-CE3	5.87	139.76	133.90
1	A	162	GLU	N-CA-C	-5.86	102.23	110.50
1	A	305	ILE	N-CA-CB	-5.86	104.07	111.46
1	A	264	HIS	CB-CG-ND1	5.80	131.40	122.70
1	A	327	ARG	CA-CB-CG	5.76	125.63	114.10
1	A	221	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	116	VAL	CA-C-O	-5.75	114.21	120.71
1	A	139	THR	N-CA-C	-5.73	101.72	110.14
1	A	278	CYS	N-CA-C	5.73	118.53	110.23
1	A	434	THR	N-CA-C	5.72	120.26	113.28
1	A	116	VAL	N-CA-C	-5.68	100.40	108.58
1	A	422	PHE	CA-CB-CG	5.66	119.46	113.80
1	A	443	ILE	CB-CG1-CD1	-5.65	101.94	113.80
1	A	226	GLN	CA-CB-CG	5.64	125.38	114.10
1	A	275	VAL	O-C-N	-5.64	117.22	123.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	VAL	N-CA-C	-5.63	99.39	107.78
1	A	180	SER	N-CA-C	5.62	116.49	108.74
1	A	442	SER	O-C-N	-5.61	115.33	122.78
1	A	159	LEU	CA-C-O	-5.59	114.69	121.28
1	A	142	ASN	CB-CG-ND2	5.57	124.75	116.40
1	A	195	THR	CB-CA-C	-5.54	98.30	110.67
1	A	83	GLU	N-CA-CB	-5.54	102.05	111.69
1	A	299	ASN	N-CA-C	-5.53	103.08	110.55
1	A	309	ASP	N-CA-CB	5.52	118.77	110.65
1	A	354	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	287	VAL	N-CA-C	-5.50	100.31	108.45
1	A	296	LYS	N-CA-C	5.45	119.91	112.88
1	A	442	SER	CA-CB-OG	5.45	121.99	111.10
1	A	91	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	293	ASP	N-CA-C	-5.43	98.37	107.99
1	A	438	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	438	TRP	CB-CG-CD1	-5.40	118.79	126.90
1	A	161	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	329	ASP	N-CA-C	-5.38	99.33	110.80
1	A	418	ILE	CB-CG1-CD1	-5.35	102.57	113.80
1	A	341	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	302	VAL	N-CA-C	-5.33	100.44	108.12
1	A	254	ILE	N-CA-C	-5.30	100.75	108.17
1	A	97	PHE	CA-CB-CG	-5.28	108.53	113.80
1	A	296	LYS	CB-CG-CD	-5.27	99.19	111.30
1	A	428	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	A	277	GLU	N-CA-C	5.27	122.02	110.80
1	A	437	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	A	457	SER	N-CA-C	-5.25	99.03	108.48
1	A	274	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	437	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	194	ILE	N-CA-CB	-5.19	104.89	111.64
1	A	330	ASP	N-CA-C	5.19	118.71	112.38
1	A	104	ASN	N-CA-C	5.17	118.73	111.90
1	A	327	ARG	N-CA-CB	-5.14	103.44	111.56
1	A	178	TRP	CA-CB-CG	5.12	123.32	113.60
1	A	153	ILE	N-CA-C	-5.08	103.27	109.01
1	A	458	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	A	220	GLN	CG-CD-NE2	5.06	124.00	116.40
1	A	124	CYS	N-CA-C	5.04	116.62	108.26
1	A	203	ALA	CA-C-O	-5.04	114.97	120.36
1	A	402	ASN	CA-CB-CG	-5.03	107.57	112.60

There are no chirality outliers.

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	3022	0	2854	54	1
2	B	92	0	70	0	0
3	C	72	0	61	0	0
4	A	28	0	26	0	0
5	A	21	0	18	0	0
6	A	1	0	0	0	0
7	A	116	0	0	5	6
All	All	3352	0	3029	54	6

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 9.

All (54) 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:A:226:GLN:HG3	1:A:278:CYS:O	1.88	0.74
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.72	0.72
1:A:242:THR:HG21	1:A:275:VAL:O	1.92	0.69
1:A:322:VAL:HG12	1:A:327:ARG:HG3	1.75	0.69
1:A:184:HIS:HD2	1:A:186:GLY:H	1.41	0.69
1:A:184:HIS:CD2	1:A:186:GLY:H	2.11	0.68
1:A:101:SER:HB3	1:A:445:VAL:HG13	1.77	0.66
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.61	0.65
1:A:328:ASN:ND2	1:A:343:GLU:HG2	2.11	0.65
1:A:190:LEU:HD11	1:A:257:ILE:HD11	1.81	0.61
1:A:317:VAL:HG23	7:A:666:HOH:O	2.00	0.61
1:A:230:CYS:HA	7:A:695(X):HOH:O	2.03	0.58
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.86	0.56
1:A:183:CYS:SG	1:A:232:CYS:SG	3.05	0.54
1:A:317:VAL:HA	7:A:694(X):HOH:O	2.07	0.54
1:A:327:ARG:CZ	1:A:364:ARG:HD3	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:NH2	1:A:462:ALA:O	2.43	0.52
1:A:418:ILE:HD11	1:A:420:ARG:NH1	2.25	0.52
1:A:241:MET:HE3	1:A:255:LEU:HG	1.92	0.51
1:A:226:GLN:HE22	1:A:240:VAL:HG22	1.75	0.51
1:A:82:VAL:HG12	1:A:187:LYS:HG2	1.92	0.50
1:A:288:ARG:HD3	1:A:304:ASP:OD1	2.11	0.50
1:A:309:ASP:HB2	1:A:311:SER:OG	2.11	0.50
1:A:240:VAL:HG21	1:A:278:CYS:SG	2.52	0.50
1:A:298:SER:HB2	1:A:341:ASN:HD21	1.78	0.47
1:A:274:HIS:HD2	1:A:294:ASN:H	1.63	0.46
1:A:176:ILE:HG22	1:A:195:THR:HG21	1.98	0.45
1:A:276:GLU:O	1:A:291:CYS:HB3	2.16	0.45
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.98	0.45
1:A:203:ALA:HB3	1:A:215:ILE:HG22	1.99	0.45
1:A:228:SER:HB3	1:A:350:LYS:CE	2.45	0.45
1:A:149:VAL:HG22	7:A:617:HOH:O	2.16	0.45
1:A:321:LEU:HD12	1:A:379:VAL:HG22	1.98	0.45
1:A:232:CYS:HA	1:A:237:CYS:HA	2.00	0.44
1:A:327:ARG:NH2	1:A:364:ARG:HD3	2.33	0.44
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.48	0.44
1:A:213:ASP:OD2	1:A:261:LYS:HD3	2.17	0.43
1:A:273:GLN:HG3	1:A:340:PRO:HG3	2.00	0.43
1:A:166:PRO:O	1:A:168:HIS:HD2	2.02	0.42
1:A:326:PRO:HA	1:A:368:LYS:O	2.19	0.42
1:A:101:SER:HB3	1:A:445:VAL:CG1	2.48	0.42
1:A:366:ILE:HG21	1:A:400:SER:HB3	2.01	0.42
1:A:190:LEU:CD1	1:A:257:ILE:HD11	2.50	0.41
1:A:205:PHE:CE1	1:A:262:ILE:HD11	2.55	0.41
1:A:226:GLN:NE2	1:A:240:VAL:HG22	2.34	0.41
1:A:290:ILE:HG12	1:A:353:ALA:HB3	2.01	0.41
1:A:385:THR:HA	1:A:386:PRO:HD2	1.79	0.41
1:A:222:ILE:O	1:A:224:ARG:HG3	2.21	0.41
1:A:233:ILE:HG22	1:A:234:ASN:OD1	2.20	0.41
1:A:176:ILE:HG22	1:A:195:THR:CG2	2.51	0.41
1:A:185:ASP:N	7:A:703(X):HOH:O	2.54	0.41
1:A:204:SER:HB3	1:A:211:LEU:HD11	2.03	0.41
1:A:229:GLU:OE1	1:A:410:PHE:HA	2.19	0.41
1:A:245:SER:O	1:A:274:HIS:HE1	2.04	0.40

All (6) 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)
7:A:701(X):HOH:O	7:A:702(X):HOH:O[16_665]	1.56	0.64
7:A:707(X):HOH:O	7:A:708(X):HOH:O[16_665]	1.71	0.49
7:A:698(X):HOH:O	7:A:707(X):HOH:O[16_665]	1.75	0.45
7:A:697(X):HOH:O	7:A:698(X):HOH:O[16_665]	1.78	0.42
1:A:336:ASN:O	7:A:697(X):HOH:O[16_665]	2.00	0.20
7:A:698(X):HOH:O	7:A:698(X):HOH:O[16_665]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	386/388 (100%)	354 (92%)	29 (8%)	3 (1%)	16 11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	222	ILE
1	A	322	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	338/338 (100%)	299 (88%)	39 (12%)	5 3

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	129	CYS
1	A	134	LEU
1	A	142	ASN
1	A	148	THR
1	A	149	VAL
1	A	165	VAL
1	A	192	VAL
1	A	195	THR
1	A	202	THR
1	A	210	ARG
1	A	211	LEU
1	A	224	ARG
1	A	226	GLN
1	A	231	VAL
1	A	240	VAL
1	A	242	THR
1	A	253	ARG
1	A	255	LEU
1	A	257	ILE
1	A	288	ARG
1	A	298	SER
1	A	311	SER
1	A	315	SER
1	A	342	ASN
1	A	364	ARG
1	A	370	LEU
1	A	387	ASN
1	A	388	SER
1	A	394	ARG
1	A	401	ASP
1	A	403	ARG
1	A	409	ILE
1	A	418	ILE
1	A	424	VAL
1	A	427	ILE
1	A	445	VAL
1	A	455	THR
1	A	464	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	142	ASN
1	A	161	ASN
1	A	168	HIS
1	A	226	GLN
1	A	274	HIS
1	A	328	ASN
1	A	334	ASN
1	A	356	ASN
1	A	387	ASN
1	A	393	ASN
1	A	419	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

13 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	B	1	1,2	14,14,15	1.11	1 (7%)	17,19,21	3.04	7 (41%)
2	NAG	B	2	2	14,14,15	0.98	1 (7%)	17,19,21	1.24	3 (17%)
2	BMA	B	3	2	11,11,12	0.94	0	15,15,17	1.34	2 (13%)
2	MAN	B	4	2	11,11,12	0.84	0	15,15,17	0.94	1 (6%)
2	NAG	B	5	2	14,14,15	1.25	1 (7%)	17,19,21	2.71	6 (35%)
2	NGK	B	6	2	18,18,19	1.96	3 (16%)	21,26,28	2.36	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUL	B	7	2	10,10,11	1.27	1 (10%)	14,14,16	1.89	5 (35%)
3	NAG	C	1	3,1	14,14,15	0.63	0	17,19,21	1.49	4 (23%)
3	NAG	C	2	3	14,14,15	1.23	1 (7%)	17,19,21	1.11	0
3	BMA	C	3	3	11,11,12	0.57	0	15,15,17	0.78	0
3	MAN	C	4	3	11,11,12	0.56	0	15,15,17	1.22	1 (6%)
3	MAN	C	5	3	11,11,12	0.45	0	15,15,17	0.94	1 (6%)
3	MAN	C	6	3	11,11,12	0.74	0	15,15,17	0.97	0

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	B	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
2	NAG	B	5	2	-	2/6/23/26	0/1/1/1
2	NGK	B	6	2	-	6/11/28/31	0/1/1/1
2	FUL	B	7	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	1/2/19/22	0/1/1/1
3	MAN	C	6	3	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	NGK	O4-S	-5.18	1.41	1.57
2	B	6	NGK	C1-C2	5.16	1.59	1.52
3	C	2	NAG	C1-C2	-3.93	1.47	1.52
2	B	1	NAG	C1-C2	3.16	1.56	1.52
2	B	5	NAG	C1-C2	2.91	1.56	1.52
2	B	2	NAG	C4-C5	2.56	1.58	1.53
2	B	6	NGK	O5-C5	2.41	1.48	1.43
2	B	7	FUL	C4-C5	2.19	1.57	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-C2-N2	9.72	125.75	110.43
2	B	5	NAG	C1-O5-C5	8.51	123.59	112.19
2	B	6	NGK	C8-C7-N2	5.80	125.74	116.12
2	B	6	NGK	C1-O5-C5	5.36	119.37	112.19
2	B	1	NAG	C1-O5-C5	4.43	118.12	112.19
2	B	6	NGK	O7-C7-N2	-4.11	114.72	121.98
2	B	5	NAG	C4-C3-C2	-3.98	105.19	111.02
2	B	7	FUL	C3-C4-C5	3.89	115.72	109.81
2	B	3	BMA	C1-O5-C5	3.55	116.94	112.19
2	B	6	NGK	O2S-S-O4	3.49	114.40	106.37
2	B	1	NAG	C2-N2-C7	3.49	127.58	122.90
2	B	5	NAG	O5-C1-C2	3.46	116.65	111.29
2	B	1	NAG	C8-C7-N2	2.92	120.96	116.12
2	B	7	FUL	C6-C5-C4	2.88	118.35	113.08
3	C	1	NAG	O5-C1-C2	-2.74	107.05	111.29
3	C	1	NAG	C1-O5-C5	2.74	115.86	112.19
2	B	5	NAG	C3-C4-C5	-2.62	105.48	110.23
3	C	1	NAG	C8-C7-N2	2.61	120.45	116.12
2	B	7	FUL	O5-C1-C2	-2.57	104.66	110.79
3	C	4	MAN	C1-O5-C5	2.55	115.61	112.19
2	B	4	MAN	C1-O5-C5	2.52	115.56	112.19
3	C	1	NAG	C1-C2-N2	2.52	114.40	110.43
2	B	5	NAG	C6-C5-C4	2.40	118.91	113.02
3	C	5	MAN	C1-O5-C5	2.32	115.30	112.19
2	B	1	NAG	O7-C7-N2	-2.31	117.90	121.98
2	B	3	BMA	C2-C3-C4	-2.30	106.81	110.86
2	B	7	FUL	O2-C2-C1	2.30	114.49	109.22
2	B	6	NGK	C1-C2-N2	2.25	113.98	110.43
2	B	5	NAG	O4-C4-C5	2.17	114.66	109.32
2	B	2	NAG	C3-C4-C5	-2.10	106.42	110.23
2	B	1	NAG	O4-C4-C3	-2.10	105.43	110.38
2	B	2	NAG	C4-C3-C2	-2.09	107.95	111.02
2	B	2	NAG	C8-C7-N2	2.09	119.58	116.12
2	B	6	NGK	C2-N2-C7	2.06	125.65	122.90
2	B	1	NAG	C4-C3-C2	-2.04	108.03	111.02
2	B	7	FUL	C1-O5-C5	2.02	117.73	112.97

There are no chirality outliers.

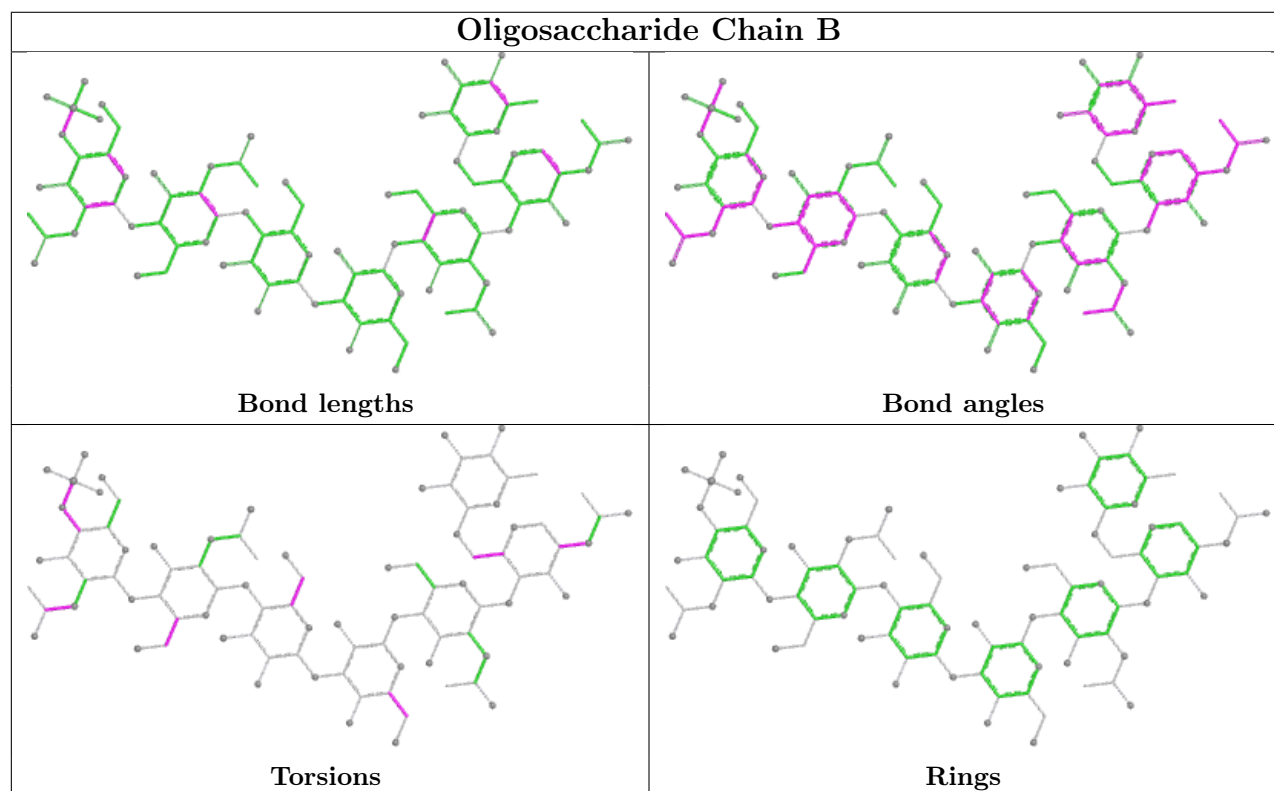
All (16) torsion outliers are listed below:

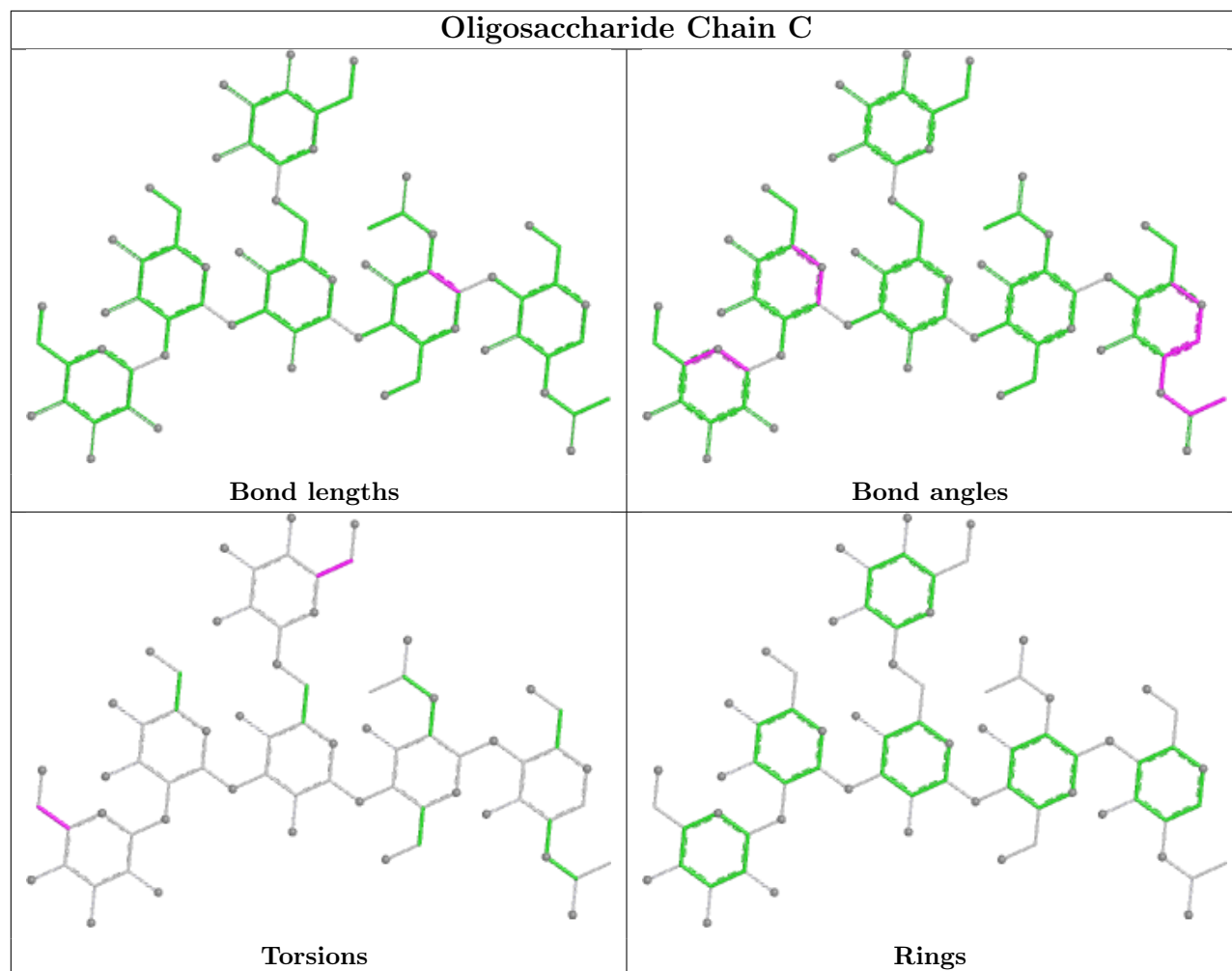
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C1-C2-N2-C7
2	B	6	NGK	C3-C4-O4-S
2	B	3	BMA	O5-C5-C6-O6
2	B	5	NAG	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	6	NGK	C8-C7-N2-C2
2	B	6	NGK	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	5	NAG	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
2	B	6	NGK	C5-C4-O4-S
3	C	5	MAN	O5-C5-C6-O6
2	B	6	NGK	C4-O4-S-O2S
2	B	6	NGK	C4-O4-S-O3S

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	NAG	A	470(A)	1	14,14,15	0.55	0	17,19,21	1.08	1 (5%)
4	NAG	A	484(A)	1	14,14,15	0.60	0	17,19,21	1.30	2 (11%)
5	SIA	A	600	-	21,21,21	1.13	2 (9%)	24,31,31	1.34	3 (12%)

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	NAG	A	470(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	A	484(A)	1	-	0/6/23/26	0/1/1/1
5	SIA	A	600	-	-	2/20/38/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	SIA	C3-C2	2.64	1.55	1.51
5	A	600	SIA	C4-C5	-2.11	1.51	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	484(A)	NAG	C1-O5-C5	2.95	116.14	112.19
5	A	600	SIA	O1A-C1-C2	-2.84	119.12	123.85
4	A	470(A)	NAG	C1-O5-C5	2.58	115.64	112.19
5	A	600	SIA	C11-C10-N5	-2.48	112.00	116.12
5	A	600	SIA	O8-C8-C7	-2.29	103.88	109.25
4	A	484(A)	NAG	C8-C7-N2	2.25	119.85	116.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

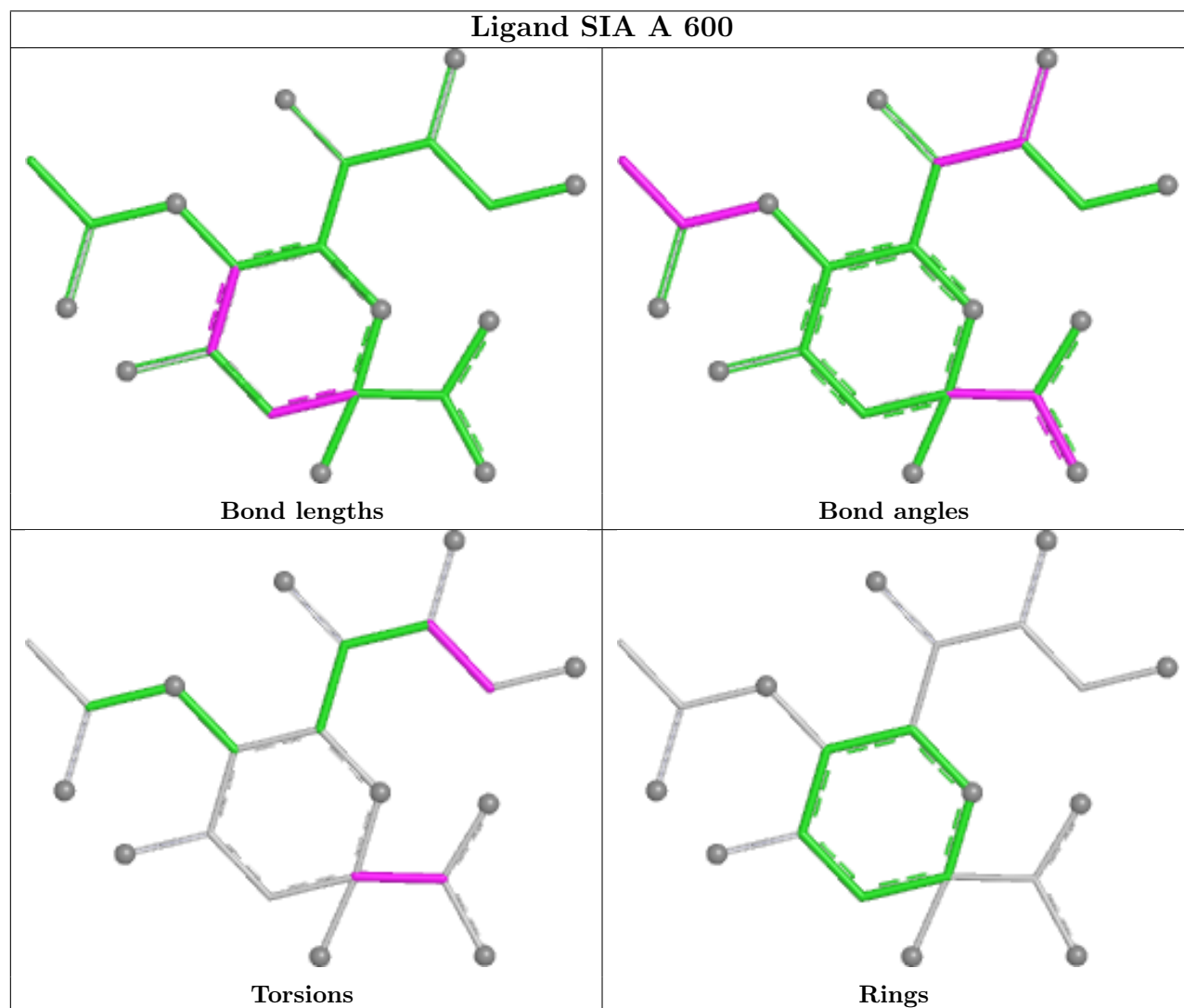
Mol	Chain	Res	Type	Atoms
5	A	600	SIA	O8-C8-C9-O9
5	A	600	SIA	O1B-C1-C2-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.