Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 02:13 PM EDT

PDB ID	:	2BAT
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 (i) 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 (1)) were used in the production of this report:

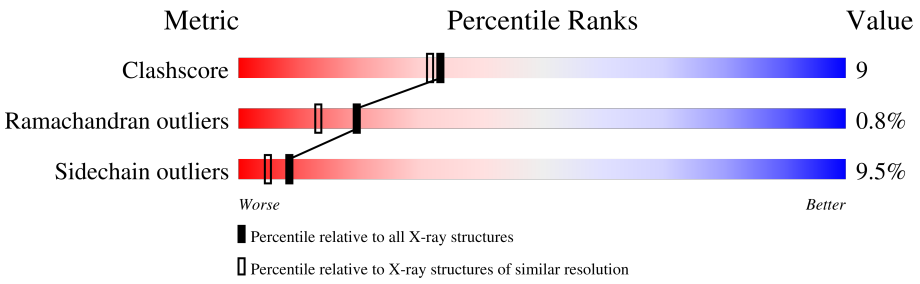
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	65% 27% 6% •
2	B	7	100%
3	C	6	33% 67%

2 Entry composition (i)

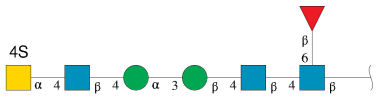
There are 7 unique types of molecules in this entry. The entry contains 3352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

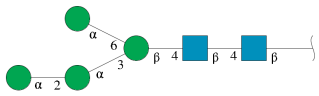
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3022	1866	546	587	23	0	0	0

- 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-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



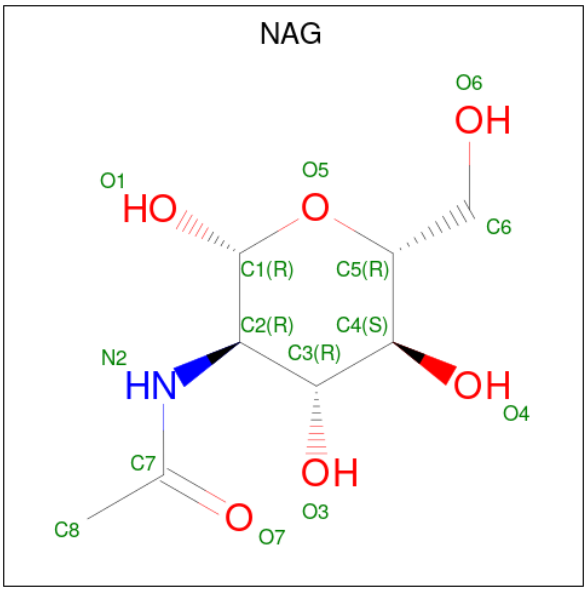
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	7	92	50	4	37	1	38	0	0

- 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.



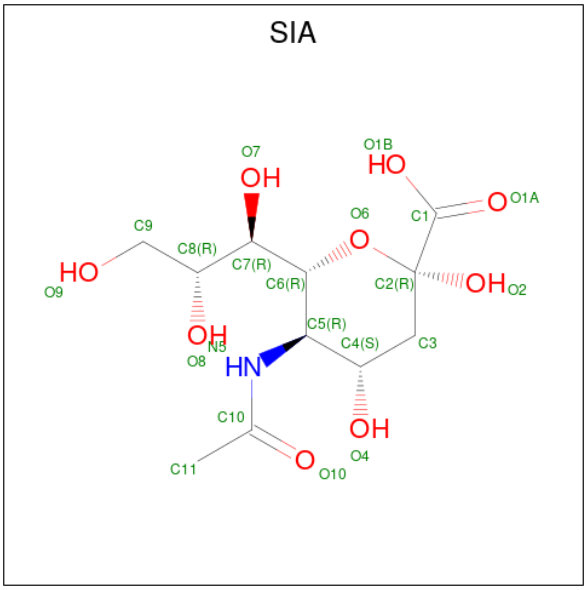
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	6	72	40	2	30	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is water.

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

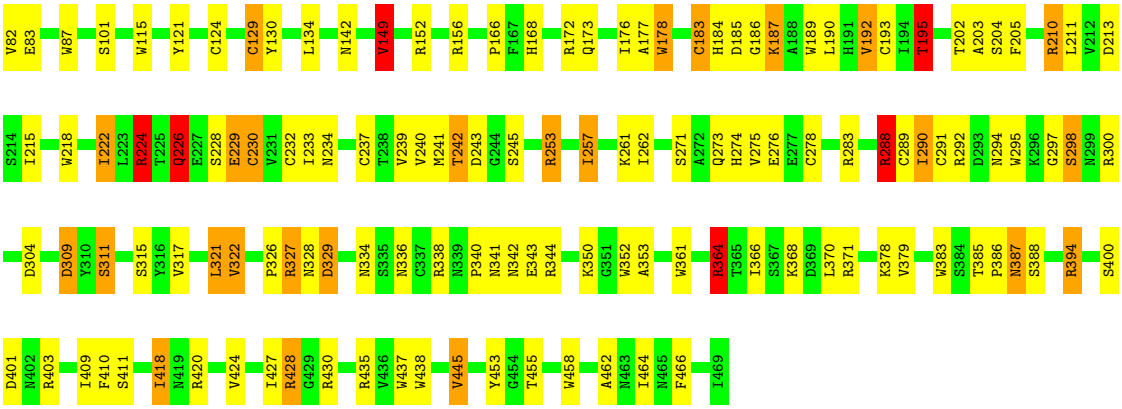
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: NEURAMINIDASE N2

Chain A: 65% 27% 6% •

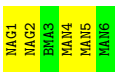


• Molecule 2: 2-acetamido-2-deoxy-4-O-sulfo-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

• 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

Chain C: 33% 67%



4 Data and refinement statistics (i)

Xtriage (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.	Xtriage
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, NAG, MAN, CA, BMA, SIA, 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	1.00	0/3092	1.89	101/4194 (2.4%)

There are no bond length outliers.

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	428	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	A	224	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	A	124	CYS	N-CA-CB	-11.22	90.40	110.60
1	A	428	ARG	NE-CZ-NH1	9.85	125.23	120.30
1	A	288	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	A	364	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	338	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	A	437	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	A	361	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	A	327	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	A	383	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	241	MET	CG-SD-CE	-8.49	86.62	100.20
1	A	352	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	A	458	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	178	TRP	CD1-CG-CD2	7.93	112.65	106.30
1	A	437	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	A	152	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	458	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	A	87	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	210	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	438	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	435	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	178	TRP	CB-CG-CD1	-7.50	117.25	127.00
1	A	438	TRP	CE2-CD2-CG	-7.47	101.32	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	TRP	CE2-CD2-CG	-7.41	101.38	107.30
1	A	172	ARG	CG-CD-NE	-7.26	96.56	111.80
1	A	130	TYR	CB-CG-CD1	-7.22	116.67	121.00
1	A	361	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	115	TRP	CD1-CG-CD2	7.16	112.03	106.30
1	A	218	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	A	87	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	A	364	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	292	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	189	TRP	CD1-CG-CD2	6.91	111.83	106.30
1	A	352	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	A	239	VAL	CG1-CB-CG2	-6.88	99.89	110.90
1	A	229	GLU	N-CA-CB	-6.80	98.36	110.60
1	A	383	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	A	218	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	A	121	TYR	CA-CB-CG	6.74	126.20	113.40
1	A	156	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	455	THR	N-CA-CB	-6.66	97.66	110.30
1	A	253	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	224	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	295	TRP	CD1-CG-CD2	6.54	111.53	106.30
1	A	178	TRP	CG-CD2-CE3	6.52	139.76	133.90
1	A	189	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	295	TRP	CE2-CD2-CG	-6.42	102.17	107.30
1	A	394	ARG	CG-CD-NE	-6.42	98.32	111.80
1	A	438	TRP	CB-CG-CD1	-6.31	118.79	127.00
1	A	115	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	A	297	GLY	CA-C-N	-6.28	103.38	117.20
1	A	124	CYS	CB-CA-C	6.26	122.92	110.40
1	A	378	LYS	CB-CG-CD	-6.23	95.40	111.60
1	A	435	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	361	TRP	CG-CD1-NE1	-6.13	103.97	110.10
1	A	309	ASP	CB-CA-C	-6.12	98.16	110.40
1	A	253	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	438	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	A	149	VAL	CB-CA-C	-6.00	100.00	111.40
1	A	195	THR	N-CA-CB	5.97	121.65	110.30
1	A	321	LEU	CA-C-N	5.96	130.30	117.20
1	A	437	TRP	CG-CD2-CE3	5.83	139.15	133.90
1	A	83	GLU	CA-CB-CG	5.82	126.21	113.40
1	A	87	TRP	CB-CG-CD1	-5.79	119.48	127.00
1	A	437	TRP	CG-CD1-NE1	-5.77	104.33	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	CYS	CA-CB-SG	5.74	124.34	114.00
1	A	172	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	458	TRP	CB-CG-CD1	-5.67	119.63	127.00
1	A	383	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	A	383	TRP	CB-CG-CD1	-5.61	119.71	127.00
1	A	290	ILE	N-CA-C	-5.60	95.88	111.00
1	A	437	TRP	CB-CG-CD1	-5.57	119.75	127.00
1	A	327	ARG	CA-CB-CG	5.56	125.63	113.40
1	A	371	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	210	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	466	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	A	300	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	226	GLN	CA-CB-CG	5.45	125.38	113.40
1	A	124	CYS	CA-CB-SG	5.45	123.80	114.00
1	A	243	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	178	TRP	CG-CD1-NE1	-5.42	104.67	110.10
1	A	195	THR	OG1-CB-CG2	5.40	122.43	110.00
1	A	192	VAL	N-CA-C	-5.36	96.53	111.00
1	A	271	SER	N-CA-C	5.34	125.41	111.00
1	A	327	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	453	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	230	CYS	O-C-N	-5.27	114.28	122.70
1	A	458	TRP	CG-CD2-CE3	5.26	138.63	133.90
1	A	292	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	329	ASP	CA-CB-CG	5.25	124.95	113.40
1	A	383	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	A	229	GLU	N-CA-C	5.17	124.97	111.00
1	A	344	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	430	ARG	O-C-N	-5.14	114.48	122.70
1	A	458	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	129	CYS	CA-CB-SG	5.08	123.14	114.00
1	A	283	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	178	TRP	CA-CB-CG	5.06	123.32	113.70
1	A	187	LYS	CA-C-N	5.04	128.30	117.20
1	A	173	GLN	CA-CB-CG	-5.02	102.36	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	53	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	53	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 (53) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	19 13

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%)	306 (90%)	32 (10%)	8 5

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	CYS
1	A	134	LEU
1	A	142	ASN
1	A	149	VAL
1	A	178	TRP
1	A	192	VAL
1	A	195	THR
1	A	202	THR
1	A	210	ARG
1	A	224	ARG
1	A	226	GLN
1	A	242	THR
1	A	253	ARG
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	464	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	131	GLN
1	A	142	ASN
1	A	161	ASN
1	A	168	HIS
1	A	184	HIS
1	A	226	GLN

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Mol	Chain	Res	Type
1	A	274	HIS
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	2,1	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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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	2,1	-	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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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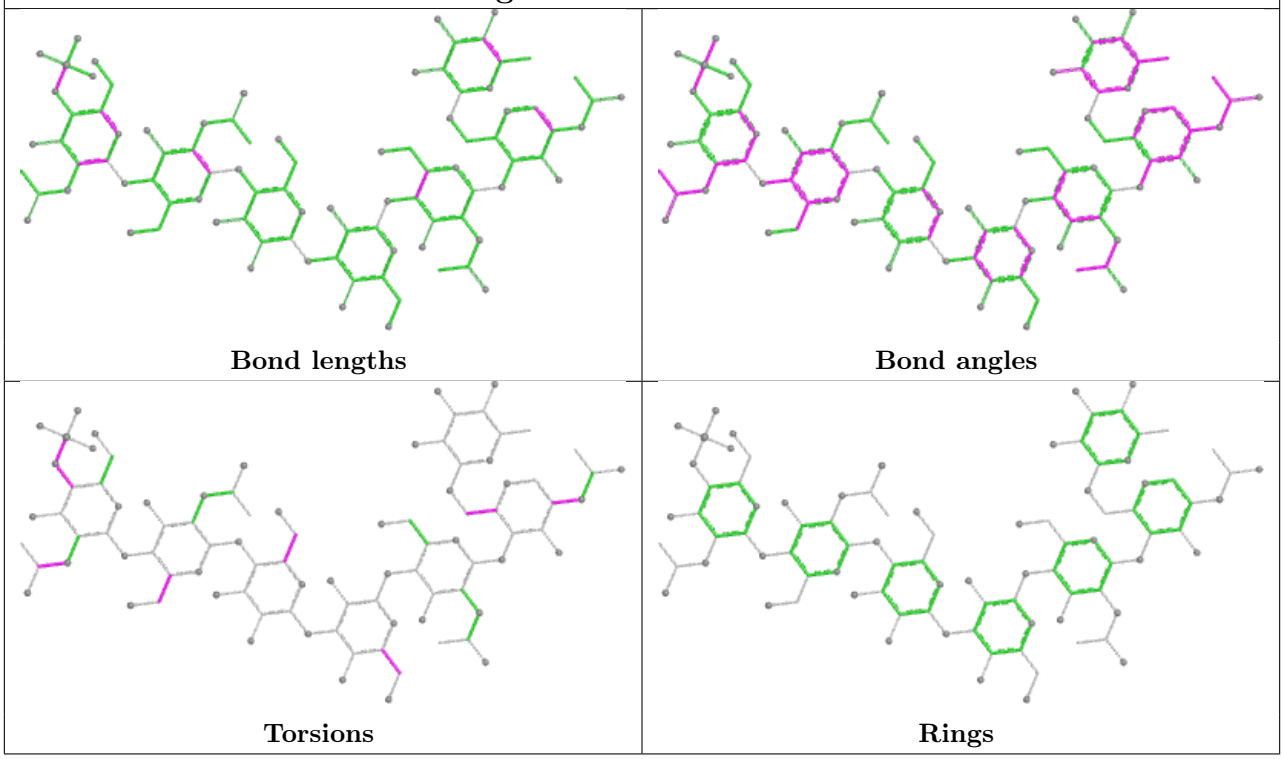
Mol	Chain	Res	Type	Atoms
2	B	5	NAG	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	6	NGK	C8-C7-N2-C2
2	B	6	NGK	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	5	NAG	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
2	B	6	NGK	C5-C4-O4-S
3	C	5	MAN	O5-C5-C6-O6
2	B	6	NGK	C4-O4-S-O2S
2	B	6	NGK	C4-O4-S-O3S

There are no ring outliers.

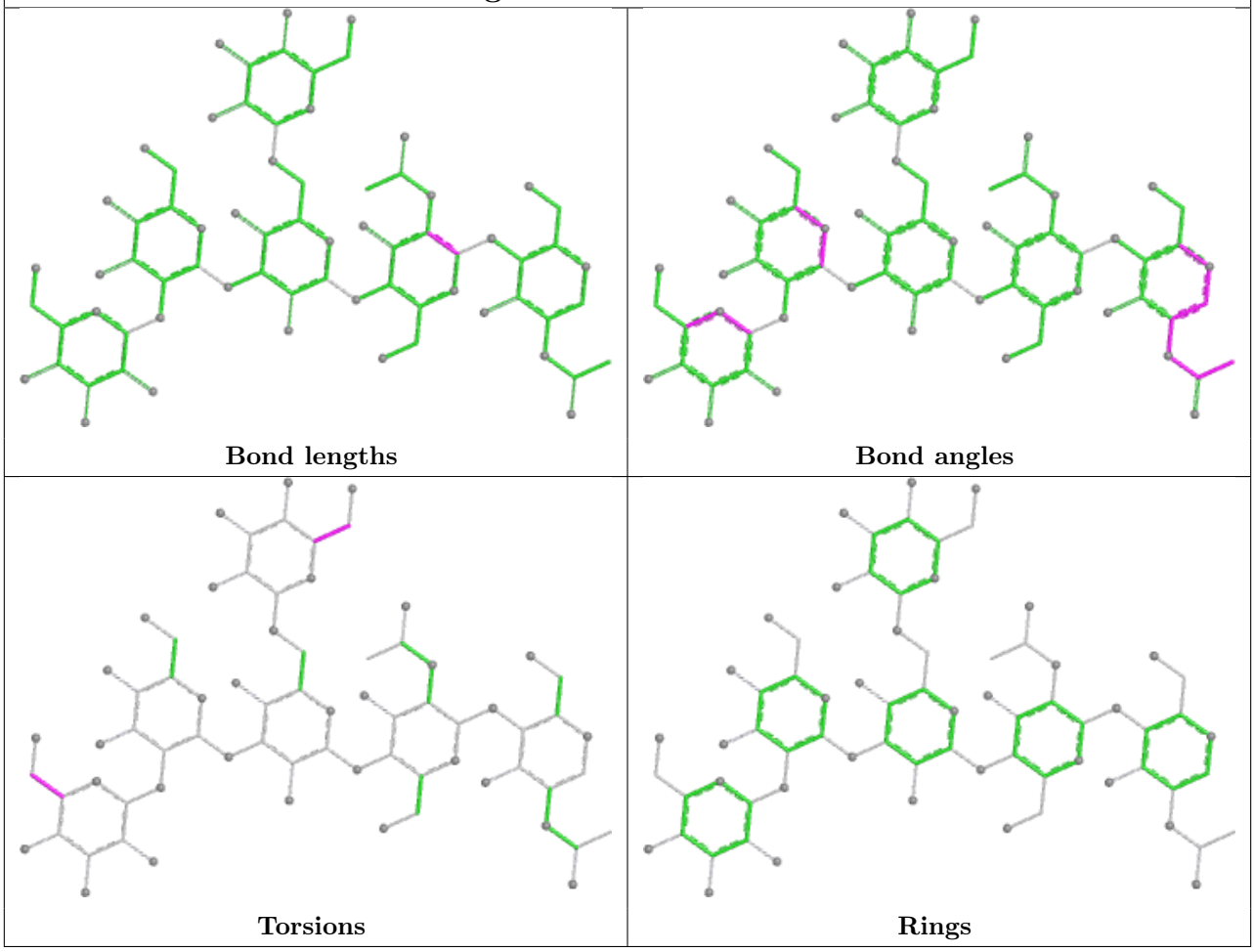
No monomer is involved in short contacts.

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

Oligosaccharide Chain B



Oligosaccharide Chain C



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	$\#\|Z\| > 2$
5	SIA	A	600	-	21,21,21	1.13	2 (9%)	24,31,31	1.34	3 (12%)
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%)

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	SIA	A	600	-	-	2/20/38/38	0/1/1/1
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

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(^{o})	Ideal(^{o})
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

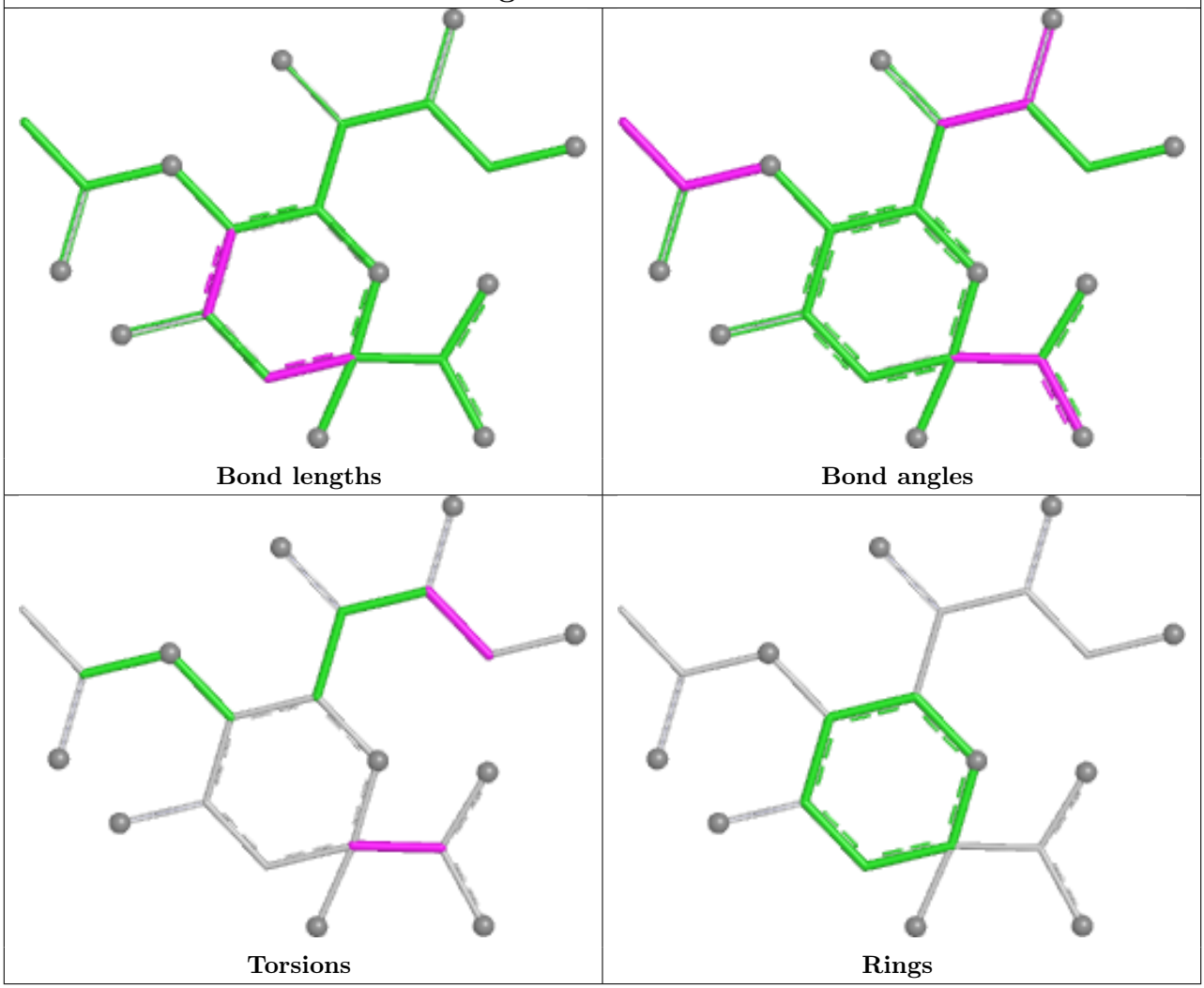
There are no ring outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SIA A 600



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.