



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 1USR / pdb\_00001usr  
Title : Newcastle disease virus hemagglutinin-neuraminidase: Evidence for a second sialic acid binding site and implications for fusion  
Authors : Zaitsev, V.; Von Itzstein, M.; Groves, D.; Kiefel, M.; Takimoto, T.; Portner, A.; Taylor, G.  
Deposited on : 2003-11-28  
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](mailto: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>.

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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

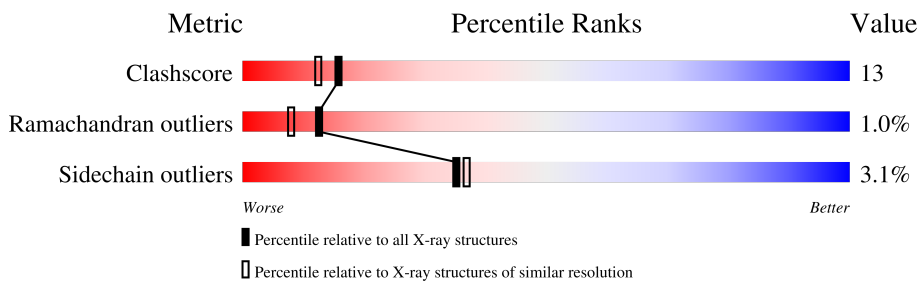
# 1 Overall quality at a glance

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  $\geq 3$ , 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	454	76% (green), 20% (yellow), 4% (orange), 0% (red), 0% (grey)
1	B	454	74% (green), 21% (yellow), 5% (orange), 0% (red), 0% (grey)
2	C	2	100% (yellow)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NDG	A	1573	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7943 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.

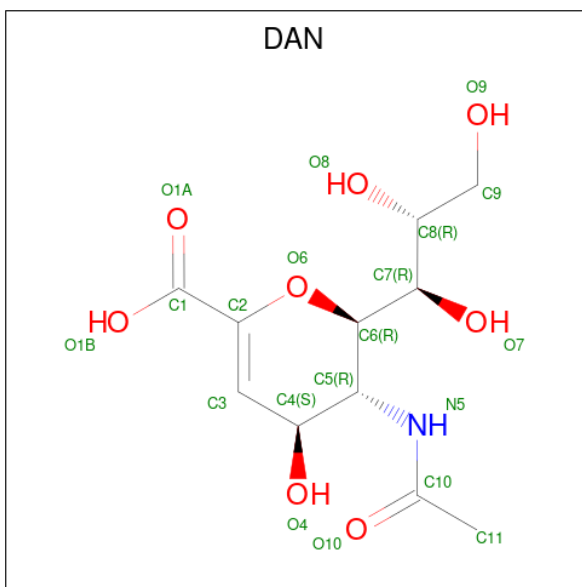
- Molecule 1 is a protein called HEMAGGLUTININ-NEURAMINIDASE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	Total	C	N	O	S	0	0	1
			3450	2174	589	668	19			
1	B	447	Total	C	N	O	S	0	0	1
			3446	2172	588	667	19			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-methyl 6-thio-beta-D-galactopyranoside.

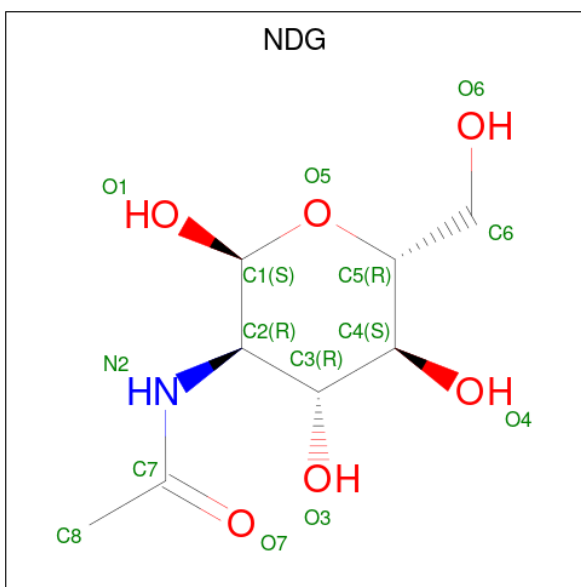
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	2	Total	C	N	O	S	0	0	0
			33	18	1	13	1			

- Molecule 3 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (CCD ID: DAN) (formula: C<sub>11</sub>H<sub>17</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	11	1	8		
3	B	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 4 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (CCD ID: NDG) (formula:  $C_8H_{15}NO_6$ ).

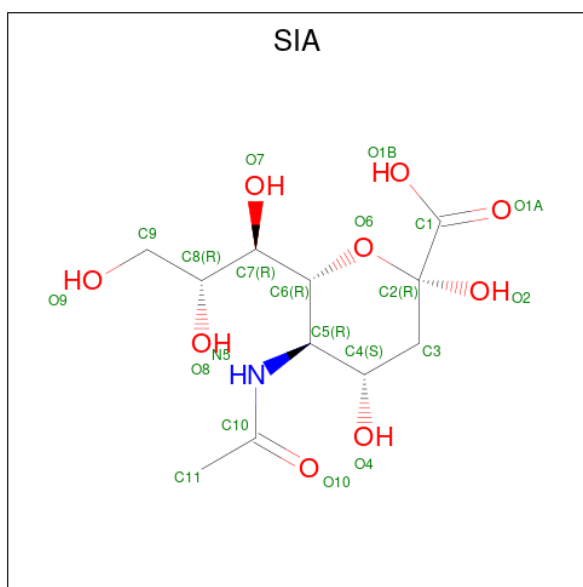


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	21	11	1	9	0	0

- Molecule 7 is water.

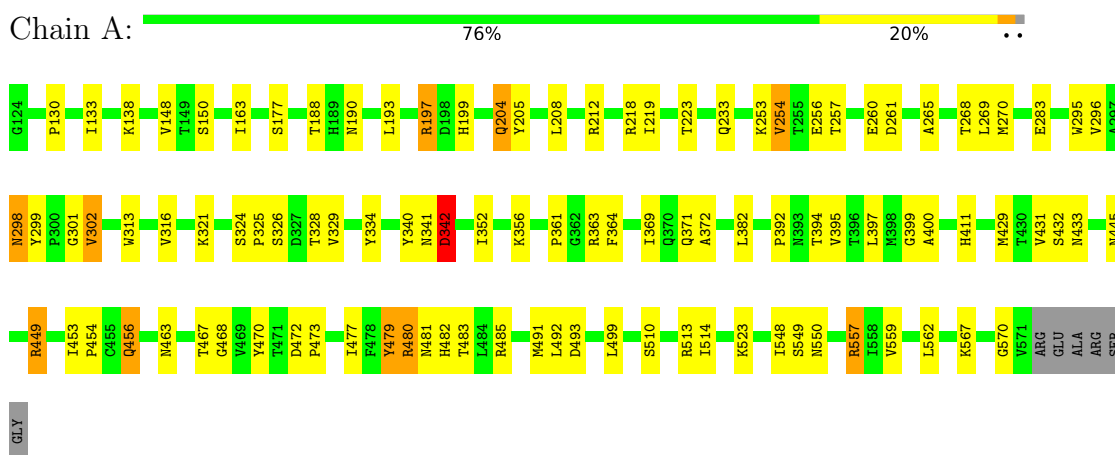
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	456	456	456	0	0
7	B	465	465	465	0	0

### 3 Residue-property plots [i](#)

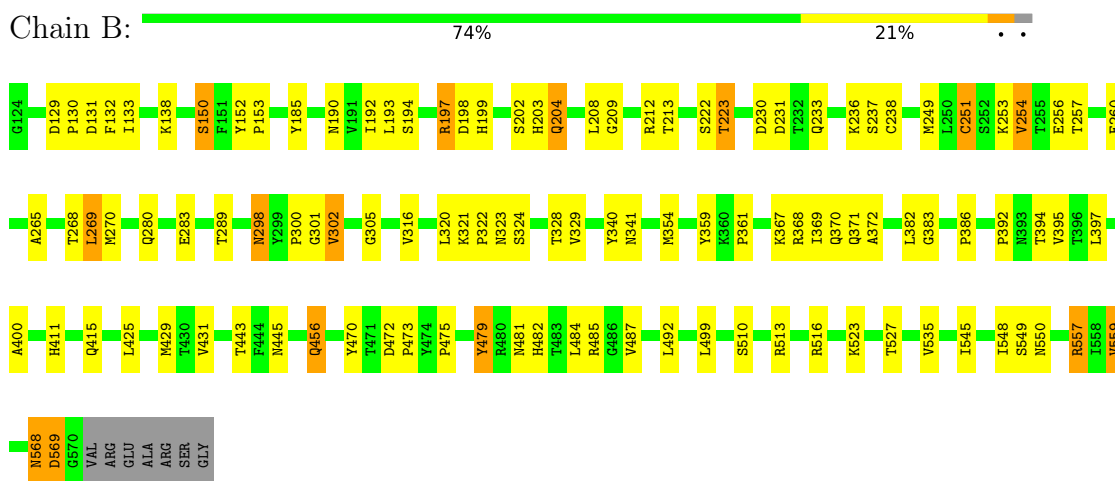
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: HEMAGGLUTININ-NEURAMINIDASE GLYCOPROTEIN



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-methyl 6-thio-beta-D-galactopyranoside



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.48Å 99.26Å 64.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.5 (12.00-2.00)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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: NDG, SIA, CA, WIA, DAN

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	0.39	1/3535 (0.0%)	0.95	15/4809 (0.3%)
1	B	0.41	1/3531 (0.0%)	0.97	15/4804 (0.3%)
All	All	0.40	2/7066 (0.0%)	0.96	30/9613 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	GLY	C-N	-5.61	1.25	1.33
1	B	569	ASP	C-N	-5.50	1.25	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	GLN	OE1-CD-NE2	-11.07	111.53	122.60
1	A	204	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	B	559	VAL	N-CA-C	8.12	116.75	107.89
1	A	559	VAL	N-CA-C	7.48	116.04	107.89
1	B	394	THR	N-CA-C	-7.27	104.41	113.28
1	B	150	SER	N-CA-C	-7.27	104.38	113.18
1	B	193	LEU	N-CA-C	7.10	118.67	111.07
1	A	150	SER	N-CA-C	-7.07	104.63	113.18
1	B	204	GLN	CG-CD-NE2	6.94	126.81	116.40
1	A	394	THR	N-CA-C	-6.93	104.57	113.16
1	A	204	GLN	CG-CD-NE2	6.77	126.55	116.40
1	A	163	ILE	N-CA-C	6.21	114.81	107.73
1	A	193	LEU	N-CA-C	6.09	117.58	111.07
1	B	254	VAL	N-CA-C	6.07	117.33	108.53
1	B	479	TYR	N-CA-C	-5.92	102.90	110.53
1	A	510	SER	N-CA-C	5.89	117.17	108.86
1	A	514	ILE	N-CA-C	5.80	117.53	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	SER	N-CA-C	5.63	117.80	109.69
1	A	479	TYR	N-CA-C	-5.60	103.31	110.53
1	A	472	ASP	N-CA-C	5.57	118.75	110.39
1	A	254	VAL	N-CA-C	5.52	117.28	108.89
1	B	513	ARG	N-CA-C	-5.36	103.07	110.35
1	A	265	ALA	N-CA-C	5.29	117.05	111.28
1	B	305	GLY	N-CA-C	-5.27	104.25	112.58
1	B	445	ASN	N-CA-C	5.26	118.48	111.75
1	B	265	ALA	N-CA-C	5.13	117.53	111.33
1	A	513	ARG	N-CA-C	-5.09	103.43	110.35
1	B	370	GLN	N-CA-C	5.08	117.77	109.59
1	B	472	ASP	N-CA-C	5.07	117.99	110.39
1	A	445	ASN	N-CA-C	5.06	118.23	111.75

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	3450	0	3345	84	0
1	B	3446	0	3343	95	0
2	C	33	0	27	0	0
3	A	20	0	16	0	0
3	B	20	0	16	0	0
4	A	15	0	12	8	0
4	B	15	0	12	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	21	0	18	0	0
7	A	456	0	0	13	0
7	B	465	0	0	15	0
All	All	7943	0	6789	182	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 13.

All (182) 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:481:ASN:HD21	4:A:1573:NDG:C1	1.73	1.01
1:A:190:ASN:HD22	1:A:204:GLN:HE21	1.11	0.95
1:B:238:CYS:HG	1:B:251:CYS:HG	1.11	0.91
1:B:301:GLY:O	1:B:302:VAL:HG22	1.74	0.88
1:A:550:ASN:HB2	1:A:557:ARG:HG2	1.55	0.87
1:B:197:ARG:NE	1:B:197:ARG:H	1.72	0.87
1:A:223:THR:HG21	7:A:2045:HOH:O	1.76	0.85
1:A:456:GLN:NE2	1:A:456:GLN:H	1.75	0.84
1:A:301:GLY:O	1:A:302:VAL:HG22	1.78	0.83
1:A:361:PRO:HD2	1:A:369:ILE:HD13	1.60	0.82
1:A:197:ARG:HD3	1:A:197:ARG:H	1.44	0.82
1:B:223:THR:HG21	7:B:2042:HOH:O	1.78	0.81
1:B:456:GLN:NE2	1:B:456:GLN:H	1.78	0.81
1:B:481:ASN:HD21	4:B:1571:NDG:C1	1.93	0.81
1:B:283:GLU:HA	1:B:382:LEU:HD13	1.65	0.79
1:A:483:THR:HB	4:A:1573:NDG:O1	1.83	0.77
1:A:481:ASN:ND2	4:A:1573:NDG:C1	2.48	0.77
1:B:481:ASN:ND2	4:B:1571:NDG:C1	2.48	0.76
1:A:283:GLU:HA	1:A:382:LEU:HD13	1.66	0.75
1:B:316:VAL:HG13	1:B:372:ALA:HB3	1.71	0.73
1:B:197:ARG:H	1:B:197:ARG:HE	1.35	0.72
1:A:371:GLN:HE22	1:A:400:ALA:H	1.36	0.71
1:B:185:TYR:OH	1:B:223:THR:HG22	1.90	0.71
1:B:289:THR:HG22	7:B:2198:HOH:O	1.90	0.71
1:B:289:THR:HG23	7:B:2196:HOH:O	1.90	0.71
1:A:321:LYS:HG2	7:A:2134:HOH:O	1.90	0.71
1:B:238:CYS:SG	1:B:251:CYS:HB3	2.32	0.70
1:B:361:PRO:HD2	1:B:369:ILE:HD13	1.73	0.70
1:A:190:ASN:HD22	1:A:204:GLN:NE2	1.87	0.69
1:B:190:ASN:HD22	1:B:204:GLN:HE21	1.40	0.69
1:A:269:LEU:HD23	1:A:270:MET:N	2.07	0.69
1:A:268:THR:H	1:A:298:ASN:HD21	1.42	0.68
1:A:456:GLN:H	1:A:456:GLN:HE21	1.40	0.68
1:B:550:ASN:HB2	1:B:557:ARG:HG2	1.76	0.68
1:A:371:GLN:NE2	1:A:400:ALA:H	1.91	0.67
1:A:392:PRO:O	1:A:395:VAL:HG12	1.94	0.67
1:A:316:VAL:HG13	1:A:372:ALA:HB3	1.77	0.66
1:A:548:ILE:O	1:A:557:ARG:HG3	1.95	0.66
4:A:1573:NDG:C7	7:A:2448:HOH:O	2.44	0.66
1:B:484:LEU:HD13	7:B:2203:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:O	1:B:535:VAL:HG22	1.96	0.65
1:B:268:THR:H	1:B:298:ASN:HD21	1.44	0.65
1:B:475:PRO:HB3	7:B:2203:HOH:O	1.96	0.65
1:B:371:GLN:HE21	1:B:415:GLN:HE21	1.45	0.65
1:A:148:VAL:HG13	1:A:477:ILE:HD12	1.79	0.64
1:B:548:ILE:O	1:B:557:ARG:HG3	1.98	0.64
1:B:238:CYS:HG	1:B:251:CYS:CB	2.11	0.62
1:B:371:GLN:NE2	1:B:415:GLN:HE21	1.96	0.62
1:A:550:ASN:CB	1:A:557:ARG:HG2	2.27	0.62
1:A:480:ARG:HG2	1:A:480:ARG:NH1	2.15	0.61
1:B:320:LEU:HB2	7:B:2233:HOH:O	2.00	0.61
1:B:268:THR:H	1:B:298:ASN:ND2	1.99	0.60
1:A:480:ARG:HG2	1:A:480:ARG:HH11	1.67	0.60
1:B:231:ASP:HB2	7:B:2136:HOH:O	2.01	0.60
1:A:257:THR:OG1	1:A:260:GLU:HG3	2.02	0.59
1:B:249:MET:HG2	1:B:251:CYS:SG	2.41	0.59
1:A:479:TYR:CE1	4:A:1573:NDG:H6C2	2.37	0.59
1:A:479:TYR:CE2	1:A:485:ARG:HG2	2.38	0.58
1:B:369:ILE:N	1:B:369:ILE:HD12	2.18	0.58
1:A:268:THR:H	1:A:298:ASN:ND2	2.00	0.58
1:A:369:ILE:HD12	1:A:369:ILE:N	2.19	0.58
1:B:324:SER:O	1:B:328:THR:HG23	2.05	0.57
1:B:238:CYS:SG	1:B:251:CYS:CB	2.93	0.57
1:A:233:GLN:CD	1:A:253:LYS:HZ3	2.12	0.57
1:A:328:THR:HG22	7:A:2210:HOH:O	2.05	0.57
1:B:209:GLY:HA3	1:B:223:THR:HA	1.87	0.57
1:B:197:ARG:CZ	1:B:197:ARG:HB2	2.36	0.56
1:A:197:ARG:HD3	1:A:197:ARG:N	2.18	0.55
1:A:296:VAL:CG1	1:A:321:LYS:HG3	2.35	0.55
1:B:233:GLN:NE2	1:B:253:LYS:HZ2	2.05	0.55
1:A:301:GLY:O	1:A:302:VAL:CG2	2.54	0.55
1:B:233:GLN:HE22	1:B:253:LYS:HZ2	1.55	0.55
1:A:371:GLN:HE21	1:A:399:GLY:HA2	1.71	0.54
1:B:233:GLN:NE2	1:B:253:LYS:NZ	2.54	0.54
1:A:199:HIS:HE1	1:A:254:VAL:HG21	1.73	0.54
1:A:483:THR:CB	4:A:1573:NDG:O1	2.53	0.54
1:B:257:THR:OG1	1:B:260:GLU:HG3	2.06	0.54
1:B:354:MET:HA	1:B:354:MET:HE2	1.88	0.54
1:A:233:GLN:NE2	1:A:253:LYS:HZ3	2.06	0.54
1:B:367:LYS:HE3	7:B:2293:HOH:O	2.07	0.54
1:A:325:PRO:O	1:A:329:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:HD11	1:A:562:LEU:HD21	1.91	0.53
1:A:479:TYR:CD1	1:A:485:ARG:HD2	2.44	0.53
1:A:453:ILE:HG23	1:A:454:PRO:HA	1.91	0.52
1:A:296:VAL:HG12	1:A:321:LYS:HG3	1.91	0.52
1:A:299:TYR:O	1:A:316:VAL:HG23	2.10	0.52
1:B:269:LEU:HD23	1:B:270:MET:H	1.74	0.52
1:B:479:TYR:CE2	1:B:485:ARG:HG2	2.45	0.52
1:B:411:HIS:HB2	1:B:429:MET:O	2.10	0.51
1:B:233:GLN:HE22	1:B:253:LYS:NZ	2.07	0.51
1:A:197:ARG:H	1:A:197:ARG:CD	2.12	0.51
1:B:320:LEU:HD12	7:B:2233:HOH:O	2.11	0.51
1:A:363:ARG:HD2	7:A:2350:HOH:O	2.10	0.51
1:B:456:GLN:H	1:B:456:GLN:HE21	1.58	0.51
4:A:1573:NDG:H4	7:A:2450:HOH:O	2.11	0.51
1:B:203:HIS:HB3	1:B:230:ASP:OD1	2.11	0.51
1:B:268:THR:N	1:B:298:ASN:HD21	2.09	0.51
1:A:256:GLU:OE2	1:A:261:ASP:HA	2.11	0.50
1:B:527:THR:HA	1:B:545:ILE:O	2.11	0.50
1:B:208:LEU:HD23	1:B:208:LEU:C	2.37	0.49
1:A:567:LYS:HE3	7:A:2024:HOH:O	2.13	0.49
1:B:192:ILE:HG21	1:B:198:ASP:HB3	1.94	0.49
1:B:199:HIS:CE1	1:B:254:VAL:HG21	2.47	0.49
1:B:253:LYS:NZ	1:B:283:GLU:OE2	2.46	0.49
1:A:411:HIS:HB2	1:A:429:MET:O	2.12	0.49
1:A:392:PRO:HG2	1:A:395:VAL:HG12	1.96	0.48
1:B:481:ASN:CG	4:B:1571:NDG:C1	2.87	0.48
1:B:550:ASN:CB	1:B:557:ARG:HG2	2.43	0.47
1:A:233:GLN:NE2	1:A:253:LYS:NZ	2.63	0.47
1:B:499:LEU:HD23	1:B:523:LYS:HA	1.97	0.47
1:A:326:SER:O	1:A:329:VAL:HG22	2.15	0.46
7:A:2044:HOH:O	1:B:203:HIS:HE1	1.98	0.46
1:A:432:SER:O	1:A:433:ASN:HB2	2.14	0.46
1:B:383:GLY:O	1:B:386:PRO:HD3	2.15	0.46
1:B:470:TYR:C	1:B:470:TYR:CD1	2.94	0.46
1:B:371:GLN:HE22	1:B:400:ALA:H	1.63	0.46
1:A:456:GLN:HE21	1:A:456:GLN:N	2.10	0.46
1:A:479:TYR:CD2	1:A:485:ARG:HG2	2.50	0.46
1:B:359:TYR:O	1:B:368:ARG:HA	2.16	0.46
1:B:367:LYS:O	1:B:369:ILE:HD12	2.15	0.46
1:B:425:LEU:HD23	1:B:443:THR:HG22	1.97	0.46
1:B:197:ARG:NE	1:B:197:ARG:N	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:SER:O	1:A:557:ARG:HD2	2.17	0.45
1:B:516:ARG:HG2	1:B:516:ARG:HH11	1.81	0.45
1:A:361:PRO:CD	1:A:369:ILE:HD13	2.39	0.45
1:B:202:SER:OG	1:B:236:LYS:HE3	2.17	0.45
1:B:237:SER:O	1:B:300:PRO:HB2	2.15	0.45
1:A:334:TYR:CD1	1:A:356:LYS:HE3	2.52	0.45
1:A:295:TRP:O	1:A:321:LYS:HE2	2.17	0.45
1:B:392:PRO:O	1:B:395:VAL:HG12	2.16	0.45
1:B:371:GLN:NE2	1:B:400:ALA:H	2.15	0.44
1:B:484:LEU:HD22	7:B:2203:HOH:O	2.17	0.44
1:A:449:ARG:O	1:A:449:ARG:NE	2.51	0.44
1:A:499:LEU:HD23	1:A:523:LYS:HA	1.99	0.44
1:B:197:ARG:H	1:B:197:ARG:CD	2.29	0.44
1:B:199:HIS:HE1	1:B:254:VAL:HG21	1.82	0.44
1:B:198:ASP:OD1	1:B:199:HIS:N	2.51	0.44
1:B:535:VAL:HG21	7:B:2007:HOH:O	2.16	0.44
1:B:368:ARG:HB3	7:B:2233:HOH:O	2.18	0.43
1:B:475:PRO:HA	1:B:487:VAL:HG12	1.99	0.43
1:B:479:TYR:CD1	1:B:485:ARG:HD2	2.53	0.43
1:A:253:LYS:HD2	1:A:269:LEU:HD22	2.01	0.43
1:A:177:SER:HB3	1:A:188:THR:HG22	2.01	0.43
1:A:233:GLN:HE22	1:A:253:LYS:NZ	2.16	0.43
1:B:481:ASN:O	1:B:482:HIS:HB2	2.18	0.43
1:A:324:SER:O	1:A:328:THR:HG23	2.18	0.43
1:A:470:TYR:C	1:A:470:TYR:CD1	2.96	0.43
1:B:321:LYS:HG2	7:B:2142:HOH:O	2.18	0.43
1:A:208:LEU:C	1:A:208:LEU:HD23	2.44	0.42
1:B:212:ARG:HG3	1:B:222:SER:HB2	2.00	0.42
1:A:341:ASN:O	1:A:342:ASP:C	2.62	0.42
1:B:130:PRO:HA	1:B:133:ILE:HG12	2.00	0.42
1:B:249:MET:HE3	1:B:251:CYS:SG	2.59	0.42
1:B:392:PRO:HG2	1:B:395:VAL:HG12	2.01	0.42
1:A:218:ARG:HD3	7:A:2042:HOH:O	2.18	0.42
1:A:334:TYR:CZ	1:A:352:ILE:HG23	2.55	0.42
1:A:130:PRO:HA	1:A:133:ILE:HG12	2.02	0.42
1:A:313:TRP:CH2	1:A:431:VAL:HG23	2.55	0.42
1:A:454:PRO:HA	1:A:456:GLN:HE22	1.83	0.42
1:B:138:LYS:HD3	1:B:138:LYS:HA	1.92	0.42
1:B:132:PHE:CE2	1:B:213:THR:HG23	2.55	0.41
1:B:523:LYS:HB3	1:B:549:SER:HB3	2.02	0.41
1:A:138:LYS:HE3	7:A:2014:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:HA	1:A:205:TYR:O	2.21	0.41
1:B:559:VAL:O	1:B:559:VAL:HG23	2.20	0.41
1:B:129:ASP:OD2	1:B:212:ARG:HB3	2.21	0.41
4:A:1573:NDG:H3	7:A:2447:HOH:O	2.21	0.41
1:B:329:VAL:HG13	7:B:2236:HOH:O	2.19	0.41
1:A:467:THR:OG1	1:A:468:GLY:N	2.54	0.41
1:B:322:PRO:O	1:B:323:ASN:HB2	2.19	0.41
1:A:453:ILE:HA	1:A:456:GLN:NE2	2.36	0.41
1:A:364:PHE:HB2	7:A:2260:HOH:O	2.20	0.41
1:A:481:ASN:O	1:A:482:HIS:HB2	2.20	0.41
1:B:369:ILE:HD11	7:B:2282:HOH:O	2.20	0.41
1:B:152:TYR:HB2	1:B:153:PRO:HD2	2.03	0.40
1:A:369:ILE:N	1:A:369:ILE:CD1	2.83	0.40
1:A:431:VAL:HG12	7:A:2314:HOH:O	2.21	0.40
1:A:491:MET:HE2	1:A:493:ASP:HA	2.03	0.40
1:B:150:SER:HA	1:B:568:ASN:ND2	2.36	0.40
1:B:194:SER:OG	1:B:198:ASP:HB2	2.21	0.40
1:B:369:ILE:N	1:B:369:ILE:CD1	2.83	0.40
1:A:199:HIS:O	1:A:199:HIS:ND1	2.54	0.40

There are no symmetry-related clashes.

## 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	446/454 (98%)	420 (94%)	22 (5%)	4 (1%)	14	9
1	B	445/454 (98%)	414 (93%)	26 (6%)	5 (1%)	11	7
All	All	891/908 (98%)	834 (94%)	48 (5%)	9 (1%)	12	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	568	ASN
1	B	569	ASP
1	B	340	TYR
1	A	342	ASP
1	A	340	TYR
1	B	473	PRO
1	A	473	PRO
1	B	302	VAL
1	A	302	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	387/392 (99%)	376 (97%)	11 (3%)	38	41
1	B	387/392 (99%)	374 (97%)	13 (3%)	32	33
All	All	774/784 (99%)	750 (97%)	24 (3%)	35	37

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ARG
1	A	212	ARG
1	A	298	ASN
1	A	342	ASP
1	A	397	LEU
1	A	449	ARG
1	A	456	GLN
1	A	463	ASN
1	A	480	ARG
1	A	492	LEU
1	A	557	ARG
1	B	197	ARG
1	B	223	THR
1	B	251	CYS
1	B	256	GLU

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Mol	Chain	Res	Type
1	B	269	LEU
1	B	280	GLN
1	B	298	ASN
1	B	341	ASN
1	B	397	LEU
1	B	431	VAL
1	B	456	GLN
1	B	492	LEU
1	B	557	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	203	HIS
1	A	204	GLN
1	A	233	GLN
1	A	282	HIS
1	A	298	ASN
1	A	371	GLN
1	A	433	ASN
1	A	456	GLN
1	A	463	ASN
1	A	496	GLN
1	B	190	ASN
1	B	203	HIS
1	B	204	GLN
1	B	233	GLN
1	B	282	HIS
1	B	298	ASN
1	B	348	GLN
1	B	371	GLN
1	B	456	GLN
1	B	481	ASN
1	B	496	GLN
1	B	568	ASN

### 5.3.3 RNA

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](#)

2 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	WIA	C	1	2	13,13,13	3.73	4 (30%)	17,18,18	1.60	2 (11%)
2	SIA	C	2	2	20,20,21	5.11	13 (65%)	21,28,31	2.78	11 (52%)

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	WIA	C	1	2	-	0/4/24/24	0/1/1/1
2	SIA	C	2	2	-	1/18/34/38	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	SIA	O8-C8	-15.94	1.09	1.43
2	C	1	WIA	C6-S6	-12.29	1.56	1.81
2	C	2	SIA	C11-C10	-11.48	1.26	1.50
2	C	2	SIA	C5-N5	-5.34	1.37	1.45
2	C	2	SIA	O1A-C1	-5.06	1.07	1.22
2	C	2	SIA	C8-C7	3.63	1.59	1.53
2	C	2	SIA	O6-C6	3.45	1.49	1.44
2	C	2	SIA	C6-C5	3.19	1.58	1.53
2	C	2	SIA	C2-C1	3.18	1.56	1.52
2	C	2	SIA	C7-C6	-2.82	1.49	1.52
2	C	1	WIA	O1-C1	2.73	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	SIA	C3-C2	2.56	1.56	1.52
2	C	2	SIA	C4-C5	2.42	1.55	1.53
2	C	1	WIA	C4-C5	2.27	1.57	1.53
2	C	2	SIA	O6-C2	2.21	1.47	1.43
2	C	1	WIA	O5-C1	2.09	1.47	1.41
2	C	2	SIA	C9-C8	2.03	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	WIA	O1-C1-C2	5.46	114.44	108.14
2	C	2	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	C	2	SIA	C9-C8-C7	-4.97	102.05	112.17
2	C	2	SIA	O7-C7-C8	4.39	118.91	108.93
2	C	2	SIA	O10-C10-C11	-4.22	114.53	122.05
2	C	2	SIA	C8-C7-C6	-4.16	105.23	113.05
2	C	2	SIA	O1B-C1-C2	3.57	122.00	112.71
2	C	2	SIA	O10-C10-N5	3.01	127.31	121.98
2	C	2	SIA	O8-C8-C9	3.00	115.85	109.03
2	C	2	SIA	O7-C7-C6	-2.95	103.06	109.44
2	C	1	WIA	O5-C5-C6	2.32	110.38	106.49
2	C	2	SIA	C6-C5-N5	2.17	114.37	110.91
2	C	2	SIA	C5-N5-C10	2.16	128.15	123.11

There are no chirality outliers.

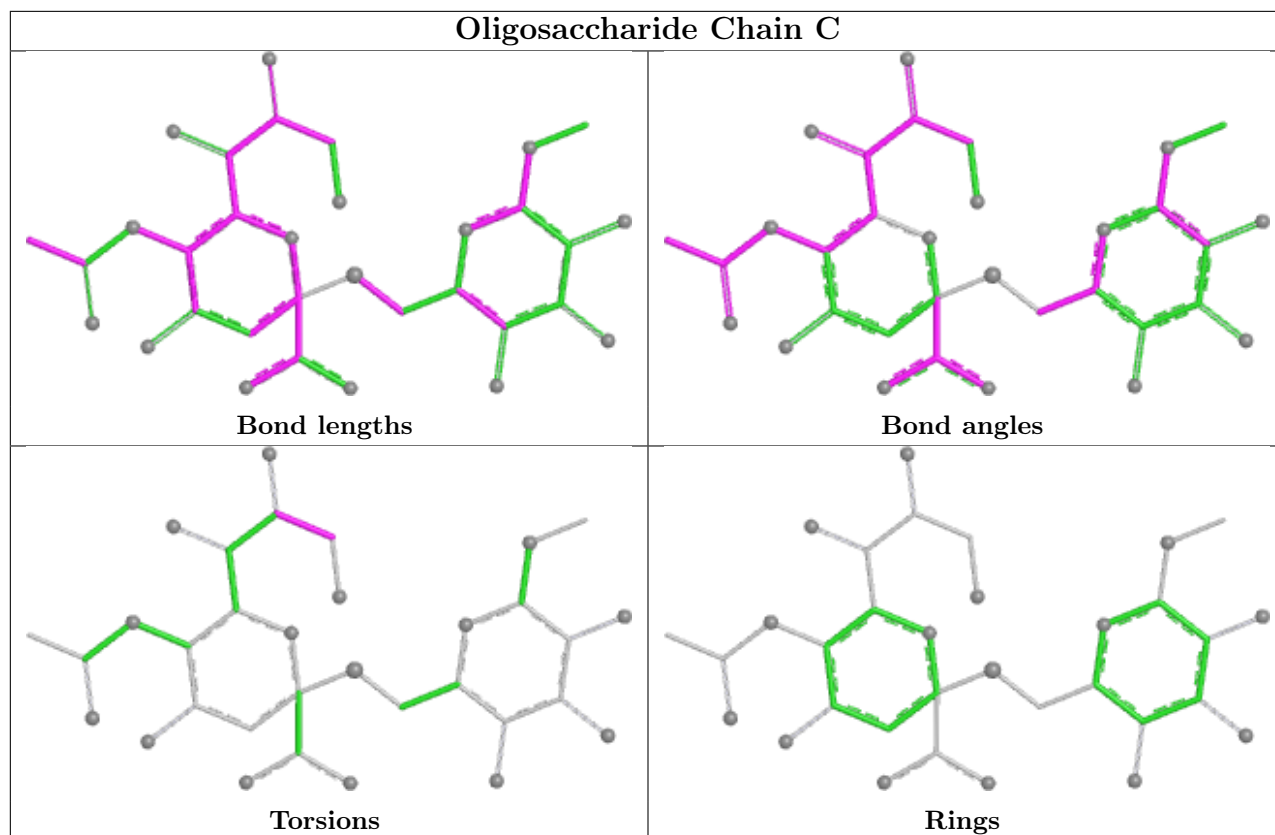
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	SIA	O8-C8-C9-O9

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	NDG	A	1573	-	15,15,15	0.52	0	21,21,21	0.71	1 (4%)
4	NDG	B	1571	-	15,15,15	0.47	0	21,21,21	0.69	0
3	DAN	A	1572	-	20,20,20	2.01	6 (30%)	24,28,28	2.18	7 (29%)
6	SIA	B	1572	-	21,21,21	0.84	0	24,31,31	1.02	2 (8%)
3	DAN	B	1570	-	20,20,20	1.62	4 (20%)	24,28,28	1.89	5 (20%)

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	NDG	A	1573	-	-	2/6/26/26	0/1/1/1
4	NDG	B	1571	-	-	1/6/26/26	0/1/1/1
3	DAN	A	1572	-	-	1/18/34/34	0/1/1/1
6	SIA	B	1572	-	-	1/20/38/38	0/1/1/1
3	DAN	B	1570	-	-	0/18/34/34	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1572	DAN	C2-C1	-6.41	1.34	1.48
3	B	1570	DAN	C3-C2	3.96	1.40	1.33
3	B	1570	DAN	C2-C1	-3.45	1.41	1.48
3	A	1572	DAN	O8-C8	3.15	1.49	1.43
3	A	1572	DAN	O6-C6	-2.92	1.41	1.46
3	A	1572	DAN	O1B-C1	-2.35	1.24	1.30
3	B	1570	DAN	O1B-C1	-2.23	1.24	1.30
3	B	1570	DAN	O8-C8	2.16	1.47	1.43
3	A	1572	DAN	O4-C4	-2.08	1.39	1.43
3	A	1572	DAN	C3-C2	2.02	1.36	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1570	DAN	O1A-C1-C2	5.81	134.80	120.57
3	A	1572	DAN	C4-C3-C2	-4.88	113.19	121.45
3	A	1572	DAN	O1B-C1-C2	4.46	124.16	114.06
3	A	1572	DAN	C3-C2-C1	-4.26	114.33	123.56
3	B	1570	DAN	O4-C4-C3	-4.03	100.15	109.27
3	A	1572	DAN	C8-C7-C6	-3.13	107.17	113.05
3	A	1572	DAN	O6-C2-C3	3.00	127.97	124.62
6	B	1572	SIA	O1A-C1-C2	-2.91	118.99	123.85
3	B	1570	DAN	O1B-C1-C2	-2.84	107.62	114.06
3	B	1570	DAN	O1B-C1-O1A	-2.73	117.39	123.90
3	A	1572	DAN	O6-C2-C1	2.37	116.74	112.02
3	A	1572	DAN	O1A-C1-C2	-2.33	114.85	120.57
4	A	1573	NDG	C1-C2-C3	-2.21	107.54	110.54
6	B	1572	SIA	C8-C7-C6	-2.10	109.10	113.05
3	B	1570	DAN	C4-C3-C2	-2.03	118.02	121.45

There are no chirality outliers.

All (5) torsion outliers are listed below:

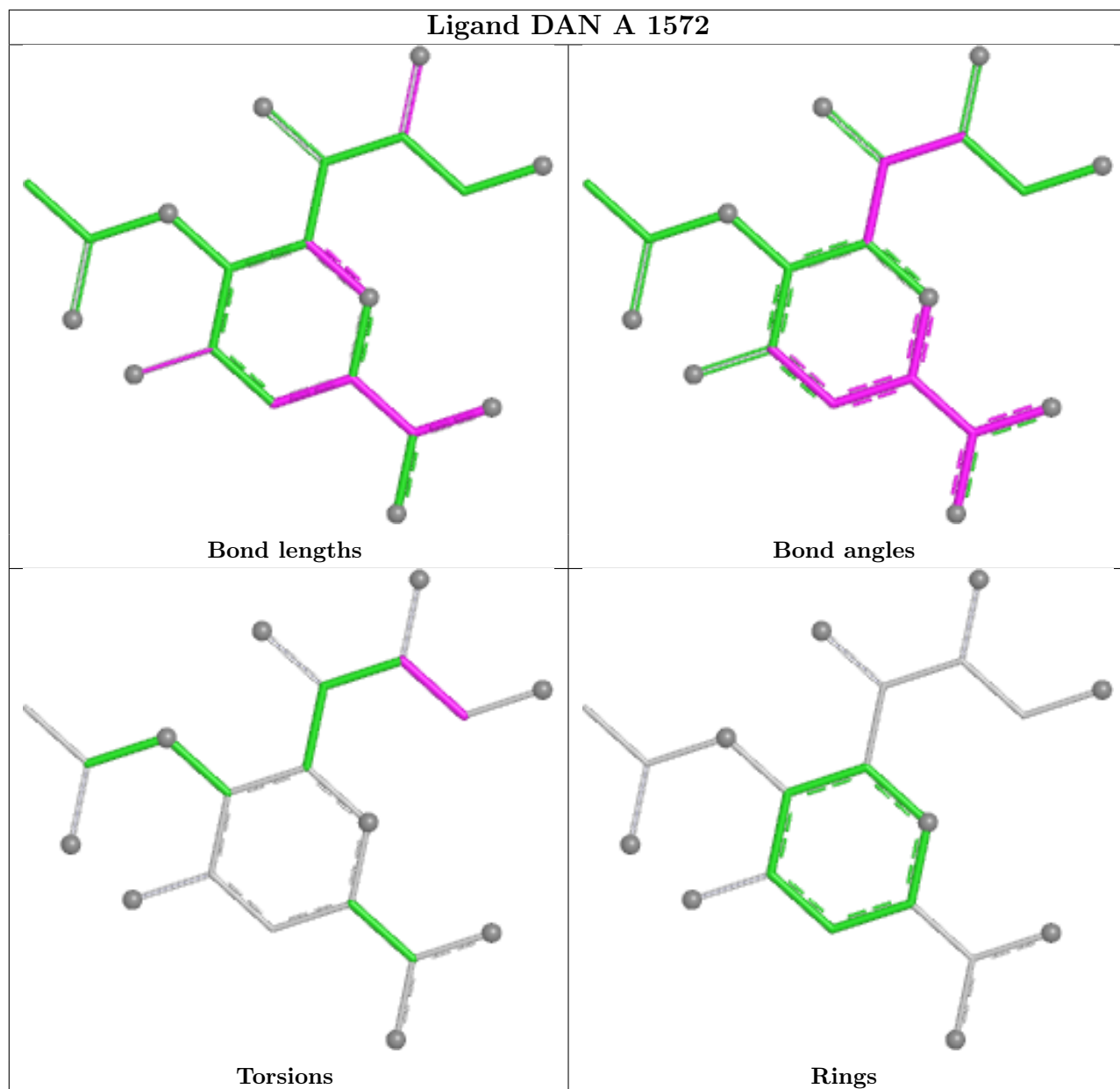
Mol	Chain	Res	Type	Atoms
4	A	1573	NDG	C4-C5-C6-O6
4	A	1573	NDG	O5-C5-C6-O6
4	B	1571	NDG	O5-C5-C6-O6
3	A	1572	DAN	O8-C8-C9-O9
6	B	1572	SIA	O1B-C1-C2-C3

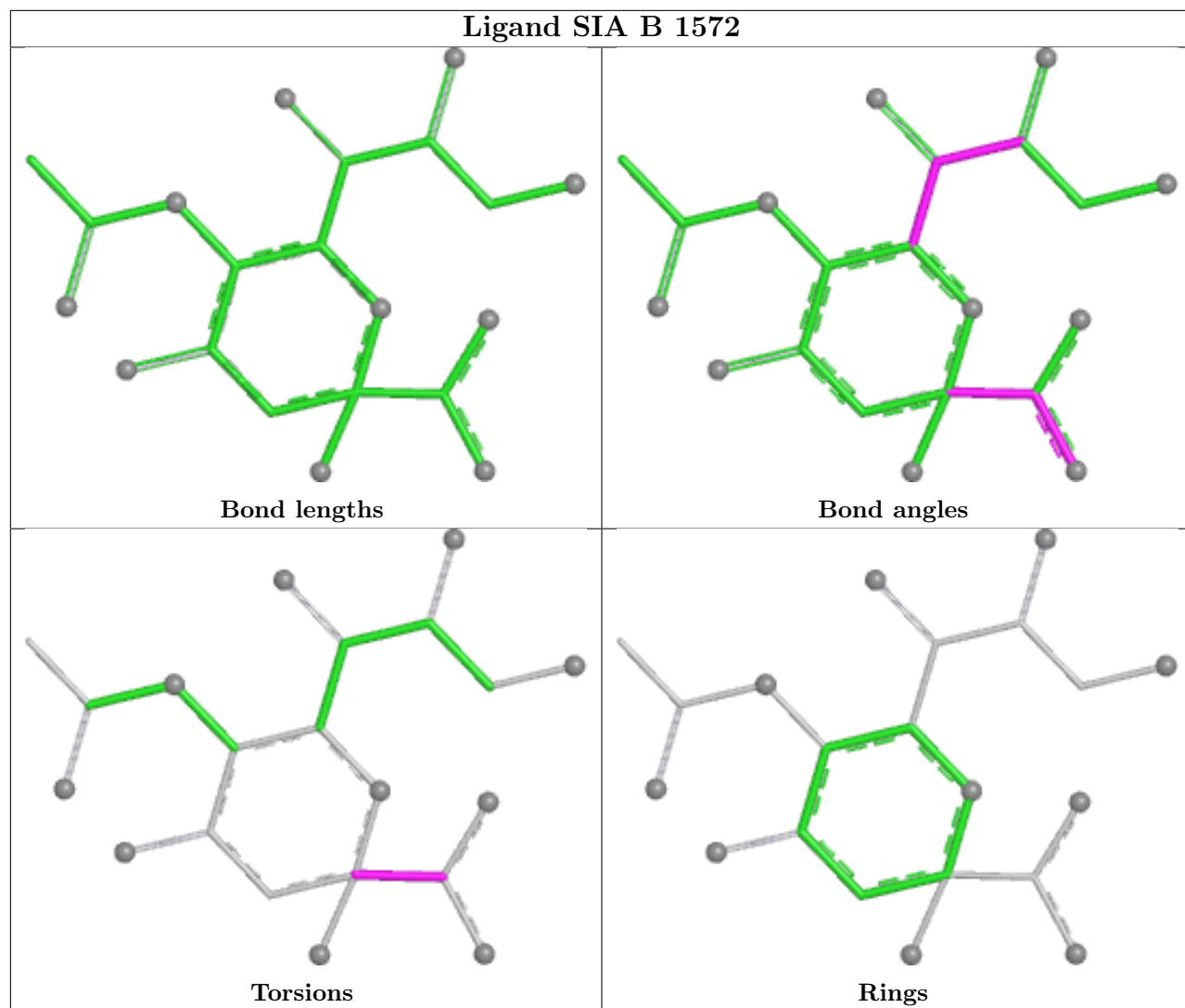
There are no ring outliers.

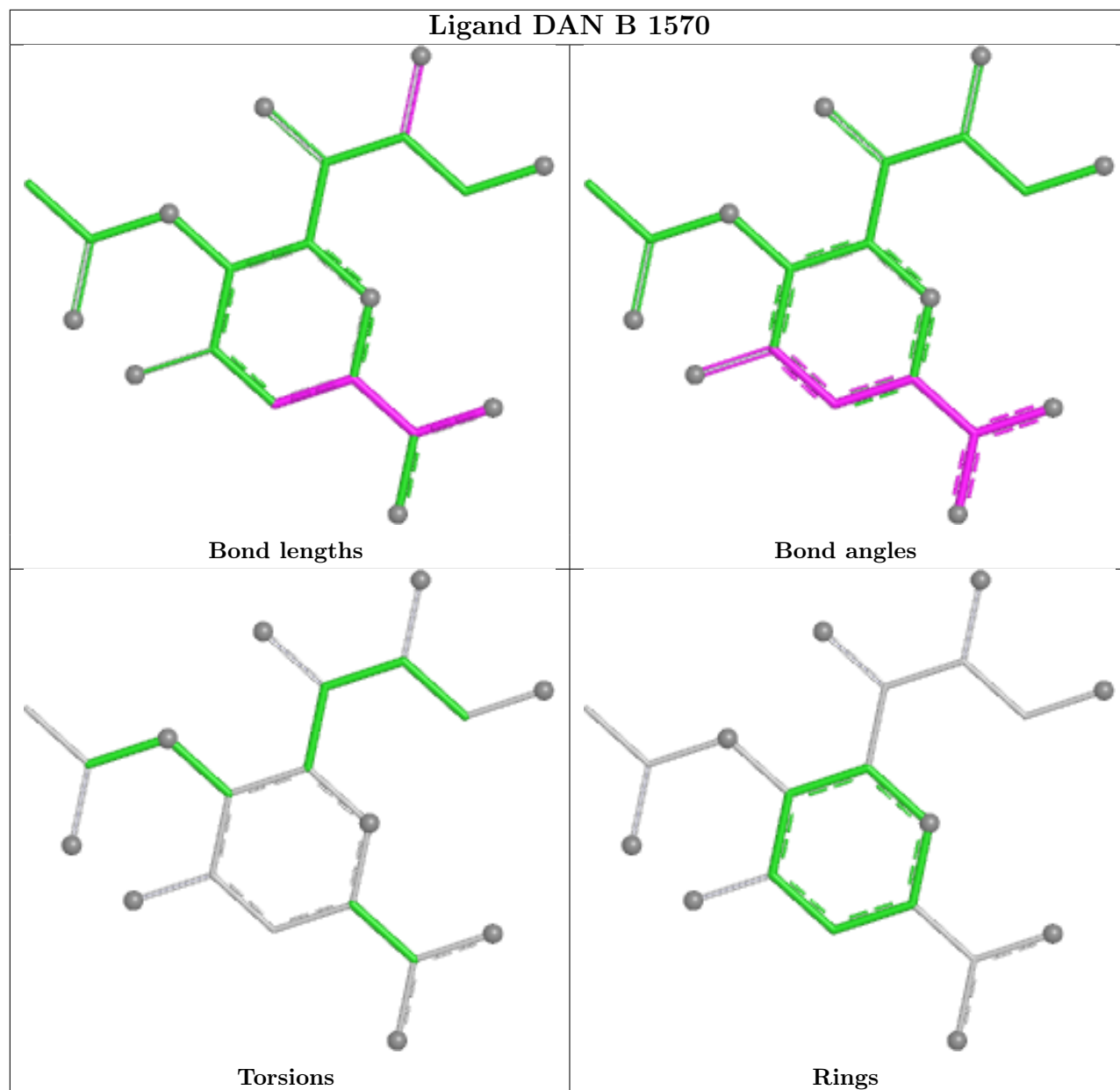
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1573	NDG	8	0
4	B	1571	NDG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.