



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:38 PM UTC

PDB ID : 1NSC / pdb_00001nsc
Title : INFLUENZA B VIRUS NEURAMINIDASE CAN SYNTHESIZE ITS OWN INHIBITOR
Authors : Burmeister, W.P.; Ruigrok, R.W.H.; Cusack, S.
Deposited on : 1993-05-24
Resolution : 1.70 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

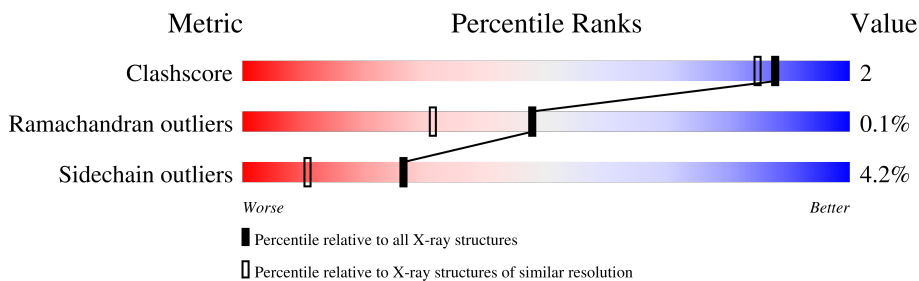
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	390	 86% 12% ..
1	B	390	 85% 14% .

2 Entry composition [i](#)

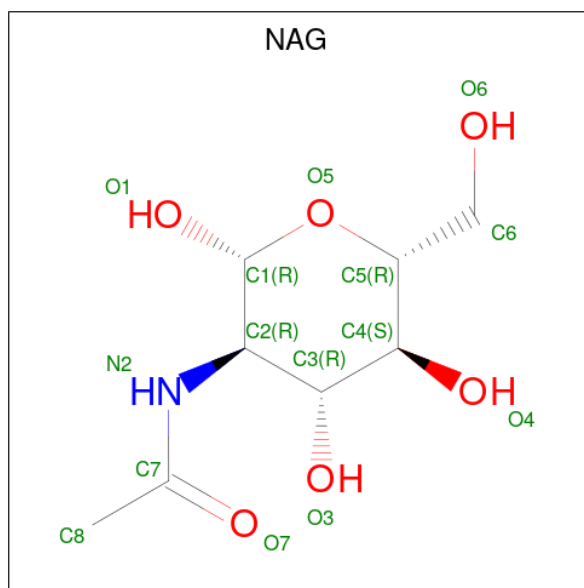
There are 5 unique types of molecules in this entry. The entry contains 9121 atoms, of which 2470 are hydrogens and 0 are deuteriums.

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.

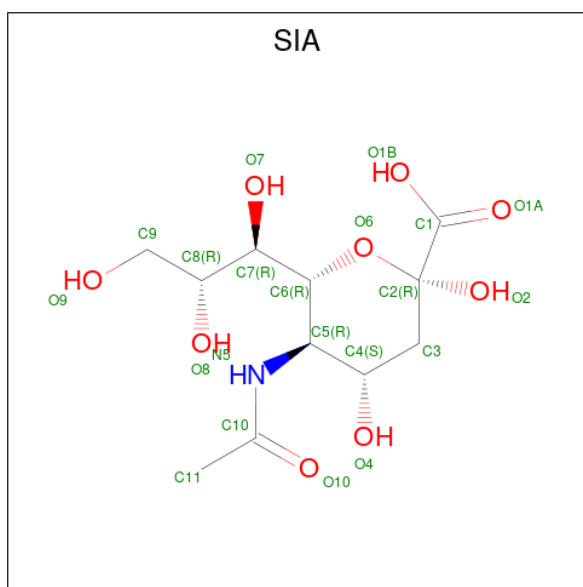
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	390	Total	C	H	N	O	S	5	0	0
			3737	1899	701	533	575	29			
1	B	390	Total	C	H	N	O	S	5	0	0
			3737	1899	701	533	575	29			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0
			39	11	18	1	9	
3	B	1	Total	C	H	N	O	0
			39	11	18	1	9	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

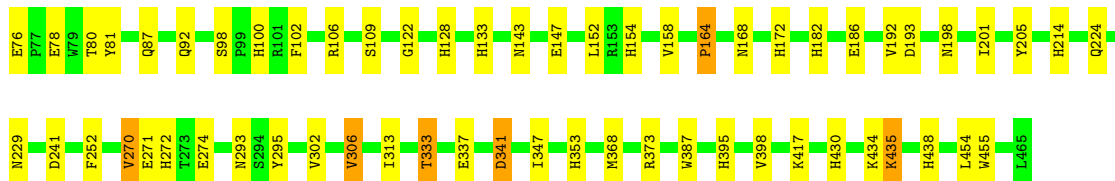
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	255	Total	H	O	0	0
			763	508	255		
5	B	251	Total	H	O	0	0
			747	496	251		

Note EDS was not executed.

Chain A: 86% 12% ..



Chain B: 85% 14% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.90Å 88.90Å 222.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9121	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: CA, NAG, SIA

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	13/3109 (0.4%)	1.56	33/4197 (0.8%)
1	B	1.01	13/3109 (0.4%)	1.57	36/4197 (0.9%)
All	All	1.01	26/6218 (0.4%)	1.57	69/8394 (0.8%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	395	HIS	CD2-NE2	-6.63	1.30	1.37
1	B	353	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	353	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	182	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	172	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	133	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	395	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	438	HIS	CD2-NE2	-6.20	1.31	1.37
1	B	214	HIS	CD2-NE2	-6.18	1.31	1.37
1	B	272	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	100	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	214	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	438	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	133	HIS	CD2-NE2	-5.91	1.31	1.37
1	B	100	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	430	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	430	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	272	HIS	CG-ND1	-5.53	1.32	1.38
1	B	272	HIS	CG-ND1	-5.53	1.32	1.38
1	A	172	HIS	CD2-NE2	-5.45	1.31	1.37
1	A	430	HIS	CG-ND1	-5.40	1.32	1.38
1	B	154	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	182	HIS	CG-ND1	-5.32	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	154	HIS	CD2-NE2	-5.13	1.32	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	VAL	N-CA-CB	-13.11	95.32	112.36
1	B	341	ASP	CA-CB-CG	12.11	124.71	112.60
1	A	402	MET	CA-CB-CG	-10.81	92.48	114.10
1	A	162	LYS	CA-C-N	-10.51	102.69	122.13
1	A	162	LYS	C-N-CA	-10.51	102.69	122.13
1	B	224	GLN	N-CA-C	9.13	121.31	111.36
1	B	270	VAL	CB-CA-C	9.07	120.91	110.93
1	A	224	GLN	N-CA-C	8.35	121.50	111.82
1	A	235	CYS	CA-C-N	-8.29	109.29	122.73
1	A	235	CYS	C-N-CA	-8.29	109.29	122.73
1	A	305	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	B	341	ASP	N-CA-CB	-7.37	99.22	110.42
1	B	241	ASP	CA-CB-CG	6.68	119.28	112.60
1	B	133	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	A	236	TYR	CA-C-O	-6.26	113.46	120.66
1	B	229	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	A	395	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	A	372	GLU	CB-CG-CD	6.14	123.04	112.60
1	A	100	HIS	CA-CB-CG	-6.13	107.67	113.80
1	A	162	LYS	CB-CA-C	-6.10	99.73	109.80
1	B	172	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	B	438	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	A	108	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	B	92	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	B	333	THR	N-CA-CB	-5.71	102.19	110.36
1	A	415	LYS	CG-CD-CE	5.71	124.43	111.30
1	A	154	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	B	271	GLU	N-CA-C	5.70	118.43	111.82
1	A	133	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	B	252	PHE	CA-CB-CG	-5.67	108.12	113.80
1	B	395	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	101	ARG	N-CA-C	-5.62	106.27	113.01
1	B	143	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	B	168	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	B	434	LYS	CA-CB-CG	5.56	125.22	114.10
1	A	87	GLN	CB-CG-CD	5.52	121.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	VAL	N-CA-CB	-5.51	100.79	110.77
1	B	434	LYS	N-CA-CB	-5.50	100.97	110.32
1	B	193	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	436	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	124	LYS	CG-CD-CE	-5.41	98.85	111.30
1	A	168	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	122	GLY	CA-C-N	5.39	125.03	119.05
1	B	122	GLY	C-N-CA	5.39	125.03	119.05
1	A	339	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	B	100	HIS	CA-CB-CG	-5.36	108.44	113.80
1	B	182	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	B	387	TRP	CG-CD1-NE1	-5.24	103.39	110.20
1	A	185	ARG	NE-CZ-NH2	-5.23	114.49	119.20
1	B	172	HIS	N-CA-C	5.21	118.10	111.69
1	B	81	TYR	O-C-N	-5.21	118.18	121.88
1	A	356	MET	CG-SD-CE	-5.19	89.47	100.90
1	A	87	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	334	GLY	CA-C-N	5.19	125.47	119.92
1	A	334	GLY	C-N-CA	5.19	125.47	119.92
1	B	353	HIS	CB-CG-CD2	-5.17	124.47	131.20
1	A	251	ARG	N-CA-C	-5.16	101.45	109.24
1	B	295	TYR	N-CA-C	5.13	120.53	113.97
1	A	79	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	B	306	VAL	CA-CB-CG2	-5.13	101.68	110.40
1	B	434	LYS	CB-CG-CD	-5.10	99.57	111.30
1	A	381	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	87	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	80	THR	N-CA-CB	-5.07	102.51	109.97
1	B	98	SER	CA-C-N	5.07	124.56	119.19
1	B	98	SER	C-N-CA	5.07	124.56	119.19
1	A	159	LYS	CG-CD-CE	-5.05	99.69	111.30
1	B	214	HIS	N-CA-C	5.01	117.94	110.52
1	B	164	PRO	N-CA-CB	5.00	106.05	102.65

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	3036	701	2923	11	0
1	B	3036	701	2923	14	0
2	A	14	14	13	0	0
2	B	14	14	13	0	0
3	A	21	18	18	0	0
3	B	21	18	18	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	255	508	0	1	0
5	B	251	496	0	3	0
All	All	6651	2470	5908	24	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 2.

All (24) 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:192:VAL:HG22	1:A:201:ILE:HD13	1.76	0.67
1:B:78:GLU:HB2	5:B:707:HOH:O	2.04	0.58
1:A:200:LEU:HG	1:B:454:LEU:HD12	1.89	0.54
1:B:192:VAL:HG22	1:B:201:ILE:HD13	1.89	0.54
1:A:368:MET:HE1	1:A:398:VAL:HG13	1.93	0.49
1:B:302:VAL:HG22	1:B:313:ILE:HG12	1.95	0.48
1:A:356:MET:HE1	1:A:382:TYR:CE1	2.50	0.46
1:B:368:MET:HE3	1:B:368:MET:HB2	1.65	0.46
1:B:368:MET:HE1	1:B:398:VAL:HG13	1.98	0.46
1:B:435:LYS:HE3	5:B:651:HOH:O	2.14	0.46
1:B:158:VAL:HG11	1:B:164:PRO:HA	1.97	0.45
1:A:368:MET:HB3	1:A:402:MET:HG3	1.99	0.44
1:A:106:ARG:HD2	5:A:499:HOH:O	2.18	0.44
1:B:186:GLU:HB3	1:B:205:TYR:CZ	2.53	0.44
1:A:76:GLU:N	1:A:76:GLU:OE1	2.52	0.43
1:A:87:GLN:O	1:A:87:GLN:HG2	2.18	0.43
1:A:186:GLU:HB3	1:A:205:TYR:CZ	2.54	0.42
1:A:353:HIS:HD2	1:A:360:ILE:HD11	1.84	0.42
1:B:274:GLU:OE2	1:B:293:ASN:HB2	2.19	0.42
1:B:102:PHE:O	1:B:109:SER:HB2	2.19	0.42
1:A:201:ILE:HB	1:A:213:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LYS:HB3	1:B:417:LYS:HE2	1.75	0.42
1:B:347:ILE:HD12	1:B:373:ARG:HG2	2.01	0.41
1:B:80:THR:HG21	5:B:674:HOH:O	2.19	0.41

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	388/390 (100%)	375 (97%)	12 (3%)	1 (0%)	36	22
1	B	388/390 (100%)	377 (97%)	11 (3%)	0	100	100
All	All	776/780 (100%)	752 (97%)	23 (3%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ILE

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	324/324 (100%)	309 (95%)	15 (5%)	24	9
1	B	324/324 (100%)	312 (96%)	12 (4%)	30	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	648/648 (100%)	621 (96%)	27 (4%)	26	11

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	87	GLN
1	A	106	ARG
1	A	200	LEU
1	A	228	CYS
1	A	267	THR
1	A	271	GLU
1	A	304	LEU
1	A	306	VAL
1	A	333	THR
1	A	360	ILE
1	A	378	LEU
1	A	402	MET
1	A	417	LYS
1	A	455	TRP
1	B	76	GLU
1	B	106	ARG
1	B	147	GLU
1	B	152	LEU
1	B	198	ASN
1	B	270	VAL
1	B	306	VAL
1	B	333	THR
1	B	337	GLU
1	B	341	ASP
1	B	435	LYS
1	B	455	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	168	ASN
1	A	339	ASN
1	B	108	ASN
1	B	133	HIS

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Mol	Chain	Res	Type
1	B	168	ASN
1	B	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
2	NAG	A	466	1	14,14,15	0.64	0	17,19,21	1.65	5 (29%)
3	SIA	B	467	-	21,21,21	1.06	1 (4%)	24,31,31	4.11	8 (33%)
2	NAG	B	466	1	14,14,15	0.63	0	17,19,21	1.70	4 (23%)
3	SIA	A	467	-	21,21,21	0.93	1 (4%)	24,31,31	4.28	9 (37%)

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	A	466	1	-	2/6/23/26	0/1/1/1
3	SIA	B	467	-	-	1/20/38/38	0/1/1/1
2	NAG	B	466	1	-	1/6/23/26	0/1/1/1
3	SIA	A	467	-	-	1/20/38/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	467	SIA	O2-C2	2.66	1.43	1.39
3	B	467	SIA	C4-C5	2.60	1.55	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	467	SIA	O2-C2-O6	-10.32	83.51	109.51
3	A	467	SIA	O2-C2-C1	-10.08	89.44	110.73
3	B	467	SIA	O2-C2-C1	-9.78	90.08	110.73
3	B	467	SIA	O2-C2-O6	-9.58	85.37	109.51
3	A	467	SIA	O2-C2-C3	8.41	122.18	109.44
3	B	467	SIA	C3-C2-C1	8.12	127.92	112.84
3	A	467	SIA	C3-C2-C1	7.67	127.08	112.84
3	B	467	SIA	O2-C2-C3	7.56	120.90	109.44
3	B	467	SIA	O1A-C1-C2	-7.36	111.57	123.85
3	A	467	SIA	O1A-C1-C2	-7.33	111.63	123.85
2	B	466	NAG	C1-O5-C5	4.18	117.79	112.19
2	A	466	NAG	C8-C7-N2	3.64	122.16	116.12
2	B	466	NAG	C8-C7-N2	3.61	122.11	116.12
2	A	466	NAG	C1-O5-C5	3.28	116.58	112.19
3	A	467	SIA	C5-N5-C10	3.25	130.73	123.11
3	B	467	SIA	C4-C5-N5	-3.15	104.24	110.44
3	A	467	SIA	C4-C5-N5	-2.87	104.78	110.44
3	A	467	SIA	O1B-C1-O1A	-2.73	115.11	123.86
3	B	467	SIA	O1B-C1-O1A	-2.51	115.83	123.86
3	B	467	SIA	C5-N5-C10	2.42	128.77	123.11
2	A	466	NAG	O7-C7-N2	-2.21	118.07	121.98
2	A	466	NAG	C1-C2-N2	-2.14	107.07	110.43
2	A	466	NAG	C2-N2-C7	2.12	125.73	122.90
3	A	467	SIA	O8-C8-C7	-2.09	104.35	109.25
2	B	466	NAG	C1-C2-N2	-2.09	107.14	110.43
2	B	466	NAG	C2-N2-C7	2.08	125.68	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

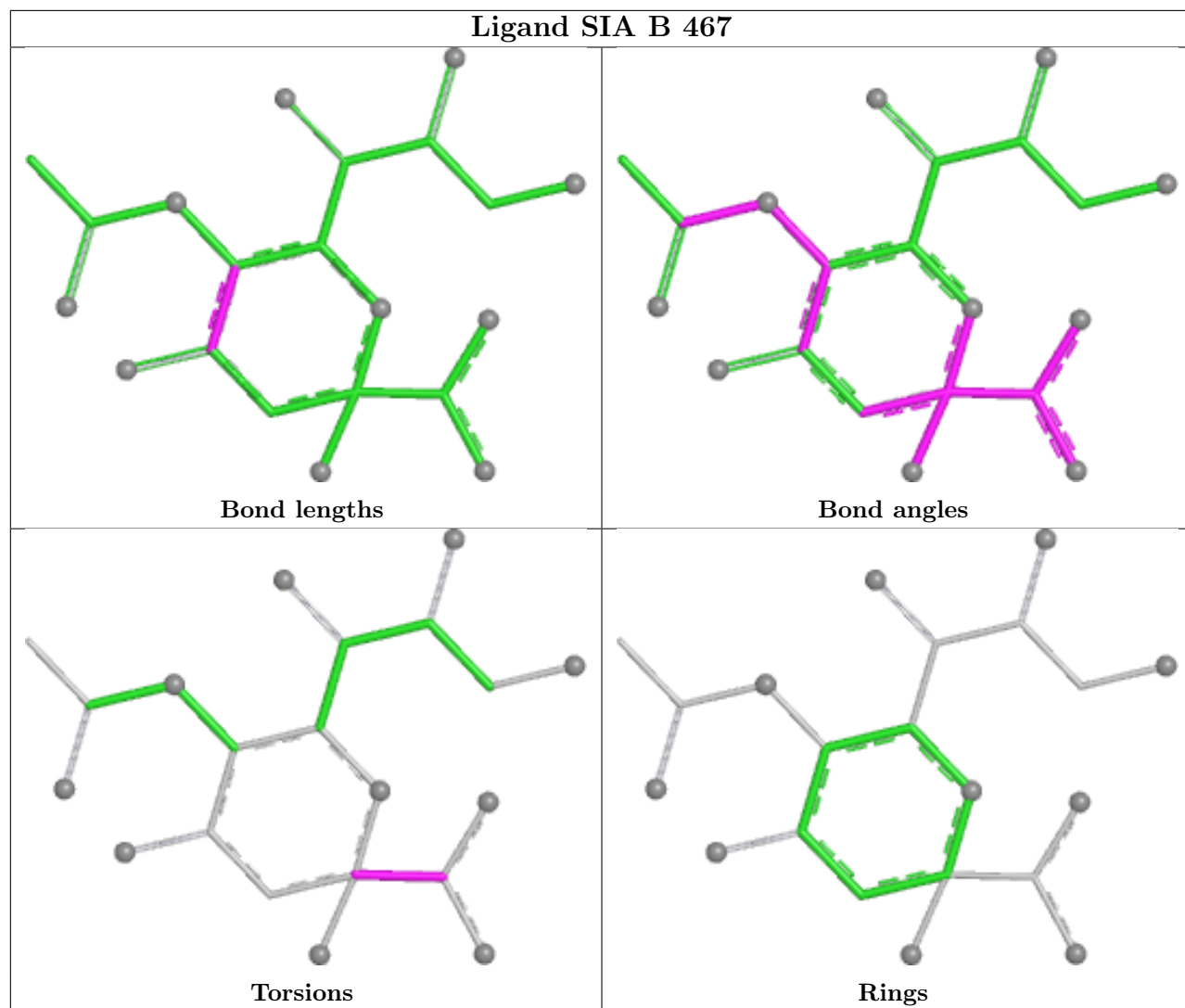
Mol	Chain	Res	Type	Atoms
2	A	466	NAG	O5-C5-C6-O6
2	A	466	NAG	C4-C5-C6-O6
2	B	466	NAG	O5-C5-C6-O6
3	A	467	SIA	O1B-C1-C2-O6
3	B	467	SIA	O1B-C1-C2-O6

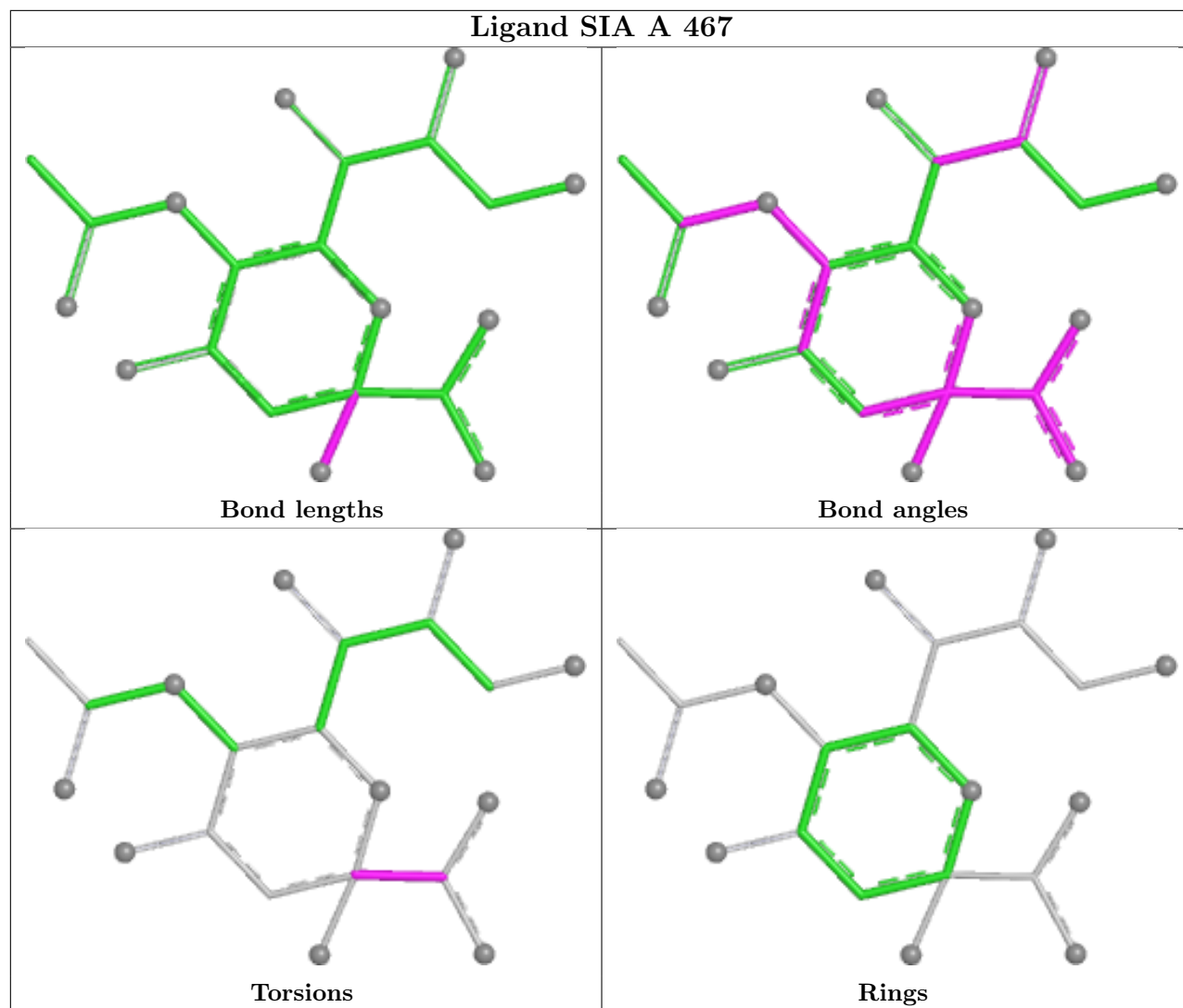
There are no ring outliers.

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.

Ligand SIA B 467





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.