



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:22 AM BST

PDB ID : 1NSB
Title : THE 2.2 ANGSTROMS RESOLUTION CRYSTAL STRUCTURE OF INFLUENZA B NEURAMINIDASE AND ITS COMPLEX WITH SIALIC ACID
Authors : Burmeister, W.P.; Ruigrok, R.W.H.; Cusack, S.
Deposited on : 1991-08-08
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.13.1

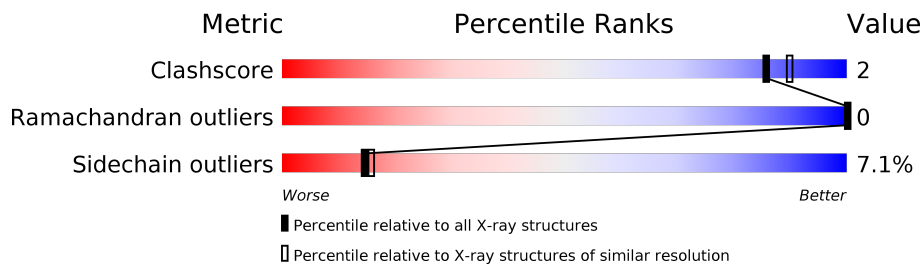
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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	
1	B	390	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8858 atoms, of which 2309 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
			Total	C	H	N	O	S			
1	A	390	Total 3734	C 1899	H 698	N 533	O 575	S 29	5	0	0
1	B	390	Total 3735	C 1899	H 699	N 533	O 575	S 29	5	0	0

- Molecule 2 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	H	N	O		
2	A	1	Total 27	C 8	H 13	N 1	O 5	0	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

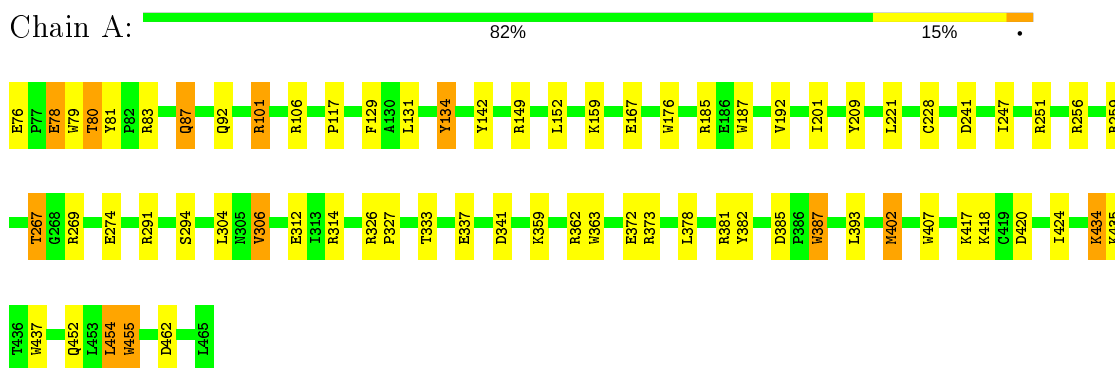
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	225	Total H O 673 448 225	0	0
4	B	221	Total H O 659 438 221	0	0

3 Residue-property plots [i](#)

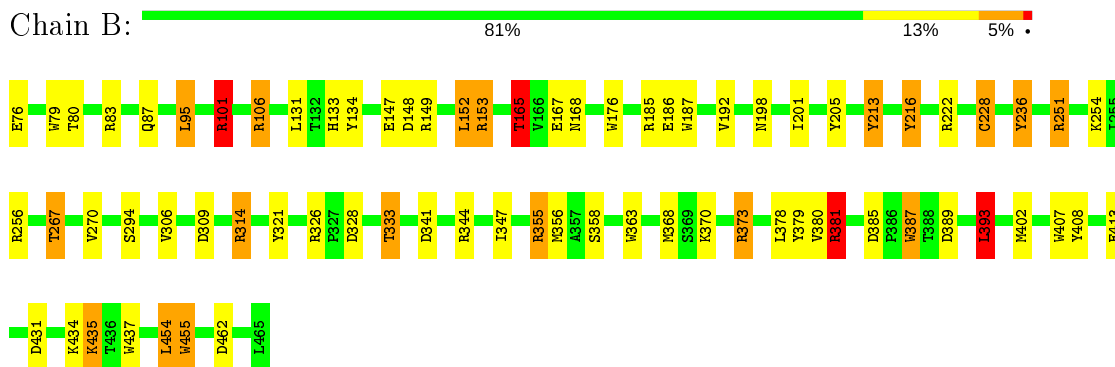
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: NEURAMINIDASE



4 Data and refinement statistics

Xtrriage (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)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8858	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: CA, NAG

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	0.98	2/3109 (0.1%)	1.68	70/4197 (1.7%)
1	B	0.99	1/3109 (0.0%)	1.84	79/4197 (1.9%)
All	All	0.98	3/6218 (0.0%)	1.76	149/8394 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLU	CG-CD	5.50	1.60	1.51
1	B	106	ARG	CZ-NH1	5.09	1.39	1.33
1	A	418	LYS	CD-CE	5.04	1.63	1.51

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ARG	NE-CZ-NH2	-27.85	106.38	120.30
1	B	355	ARG	NE-CZ-NH1	27.11	133.85	120.30
1	B	153	ARG	NE-CZ-NH2	-17.14	111.73	120.30
1	A	101	ARG	NE-CZ-NH2	-16.15	112.23	120.30
1	B	101	ARG	NE-CZ-NH2	-15.58	112.51	120.30
1	B	153	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	A	101	ARG	NE-CZ-NH1	13.74	127.17	120.30
1	B	251	ARG	NE-CZ-NH2	-12.08	114.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	B	101	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	B	381	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	187	TRP	CD1-CG-CD2	9.07	113.56	106.30
1	B	356	MET	CG-SD-CE	-8.93	85.91	100.20
1	A	291	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	A	185	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	251	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	B	79	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	B	165	THR	N-CA-CB	-8.44	94.27	110.30
1	B	83	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	437	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	B	270	VAL	N-CA-CB	-8.25	93.36	111.50
1	B	185	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	455	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	A	256	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	437	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	142	TYR	CB-CG-CD2	-7.74	116.36	121.00
1	A	79	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	381	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	79	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	A	462	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	187	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	B	368	MET	CG-SD-CE	-7.52	88.17	100.20
1	B	363	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	B	79	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	176	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	259	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	437	TRP	CE2-CD2-CG	-7.36	101.42	107.30
1	A	251	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	187	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	A	79	TRP	CB-CG-CD1	-7.19	117.66	127.00
1	A	363	TRP	CD1-CG-CD2	7.18	112.05	106.30
1	A	269	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	402	MET	CA-CB-CG	-7.14	101.15	113.30
1	B	187	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	362	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	267	THR	N-CA-CB	-7.12	96.78	110.30
1	A	79	TRP	CG-CD2-CE3	7.07	140.26	133.90
1	B	95	LEU	CA-CB-CG	7.07	131.55	115.30
1	B	402	MET	CG-SD-CE	-7.04	88.94	100.20
1	B	79	TRP	CB-CG-CD1	-7.03	117.86	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	455	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	455	TRP	CD1-CG-CD2	6.93	111.84	106.30
1	B	431	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	341	ASP	N-CA-CB	-6.88	98.21	110.60
1	B	455	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	B	176	TRP	CD1-CG-CD2	6.84	111.77	106.30
1	A	387	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	A	256	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	385	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	149	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	314	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	B	83	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	387	TRP	CE2-CD2-CG	-6.53	102.08	107.30
1	B	355	ARG	CG-CD-NE	-6.52	98.11	111.80
1	A	455	TRP	CG-CD2-CE3	6.46	139.72	133.90
1	A	420	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	80	THR	N-CA-CB	-6.44	98.06	110.30
1	B	256	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	387	TRP	CD1-CG-CD2	6.31	111.35	106.30
1	B	101	ARG	CB-CG-CD	-6.29	95.25	111.60
1	A	176	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	A	78	GLU	CA-CB-CG	6.25	127.15	113.40
1	B	434	LYS	CA-CB-CG	6.22	127.09	113.40
1	B	454	LEU	CA-CB-CG	6.20	129.57	115.30
1	A	407	TRP	CD1-CG-CD2	6.14	111.21	106.30
1	A	326	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	363	TRP	CE2-CD2-CG	-6.09	102.42	107.30
1	B	437	TRP	CE2-CD2-CG	-6.09	102.43	107.30
1	A	382	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	B	462	ASP	CB-CG-OD1	6.01	123.70	118.30
1	B	216	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	435	LYS	CB-CG-CD	5.95	127.08	111.60
1	B	408	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	187	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	A	363	TRP	CE2-CD2-CG	-5.90	102.58	107.30
1	B	434	LYS	N-CA-CB	-5.89	100.00	110.60
1	A	407	TRP	CE2-CD2-CG	-5.88	102.60	107.30
1	B	355	ARG	CD-NE-CZ	5.88	131.82	123.60
1	B	294	SER	N-CA-CB	-5.83	101.75	110.50
1	B	270	VAL	CB-CA-C	5.80	122.41	111.40
1	A	187	TRP	CB-CG-CD1	-5.77	119.50	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	176	TRP	CB-CG-CD1	-5.74	119.55	127.00
1	B	387	TRP	CE2-CD2-CG	-5.73	102.71	107.30
1	B	407	TRP	CD1-CG-CD2	5.70	110.86	106.30
1	A	259	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	402	MET	CG-SD-CE	-5.63	91.19	100.20
1	B	176	TRP	CE2-CD2-CG	-5.63	102.80	107.30
1	B	147	GLU	CA-CB-CG	5.61	125.75	113.40
1	B	148	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	407	TRP	CE2-CD2-CG	-5.59	102.82	107.30
1	A	363	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	B	167	GLU	CA-CB-CG	-5.56	101.16	113.40
1	A	437	TRP	CB-CG-CD1	-5.56	119.78	127.00
1	A	159	LYS	CG-CD-CE	-5.55	95.24	111.90
1	A	274	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	101	ARG	CB-CG-CD	-5.52	97.25	111.60
1	A	187	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	B	79	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	B	222	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	165	THR	OG1-CB-CG2	5.46	122.56	110.00
1	B	87	GLN	CG-CD-NE2	-5.43	103.66	116.70
1	A	79	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	B	413	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	A	385	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	373	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	149	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	187	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	B	326	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	424	ILE	CA-CB-CG1	-5.35	100.83	111.00
1	A	209	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	B	79	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	A	341	ASP	N-CA-CB	-5.31	101.05	110.60
1	B	309	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	147	GLU	CB-CA-C	-5.26	99.89	110.40
1	B	185	ARG	CG-CD-NE	-5.25	100.78	111.80
1	A	247	ILE	CA-CB-CG1	-5.22	101.08	111.00
1	A	381	ARG	CB-CG-CD	-5.22	98.03	111.60
1	A	306	VAL	N-CA-CB	-5.21	100.05	111.50
1	B	228	CYS	CA-CB-SG	5.20	123.37	114.00
1	B	213	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	B	152	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	333	THR	N-CA-CB	-5.18	100.45	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	373	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	A	176	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	A	455	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	A	437	TRP	CG-CD2-CE3	5.14	138.52	133.90
1	A	291	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	437	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	B	370	LYS	CG-CD-CE	-5.11	96.56	111.90
1	B	236	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	B	393	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	176	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	81	TYR	CB-CG-CD1	-5.02	117.98	121.00
1	A	381	ARG	CD-NE-CZ	-5.02	116.57	123.60
1	B	328	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	241	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	TYR	Sidechain
1	B	321	TYR	Sidechain
1	B	355	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3036	698	2923	15	0
1	B	3036	699	2923	13	0
2	A	14	13	13	0	0
2	B	14	13	13	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	225	448	0	4	0
4	B	221	438	0	2	0
All	All	6549	2309	5872	26	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 (26) 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:372:GLU:HG2	4:A:1804:HOH:O	1.82	0.78
1:A:192:VAL:HG22	1:A:201:ILE:HD13	1.69	0.73
1:B:192:VAL:HG22	1:B:201:ILE:HD13	1.75	0.67
1:B:165:THR:HG22	1:B:168:ASN:H	1.62	0.65
1:B:435:LYS:HE3	4:B:1944:HOH:O	2.01	0.60
1:A:434:LYS:HE3	1:A:434:LYS:H	1.71	0.55
1:A:92:GLN:HE22	1:A:454:LEU:H	1.55	0.55
1:A:337:GLU:HG2	4:A:1929:HOH:O	2.08	0.53
1:A:201:ILE:HG12	1:A:221:LEU:HD21	1.92	0.51
1:B:379:TYR:HB3	1:B:393:LEU:HB3	1.95	0.47
1:B:236:TYR:OH	1:B:254:LYS:HE3	2.15	0.47
1:A:134:TYR:O	1:B:101:ARG:HD3	2.17	0.45
1:B:216:TYR:CZ	1:B:251:ARG:HD3	2.52	0.45
1:B:380:VAL:HG22	1:B:381:ARG:N	2.32	0.44
1:A:314:ARG:HB2	1:A:387:TRP:CD1	2.53	0.43
1:B:347:ILE:HD12	1:B:373:ARG:HG2	2.00	0.43
1:A:167:GLU:OE2	1:B:165:THR:HG21	2.19	0.43
1:A:87:GLN:HG3	4:A:1725:HOH:O	2.19	0.42
1:A:106:ARG:NH2	4:A:1850:HOH:O	2.52	0.42
1:B:186:GLU:HB3	1:B:205:TYR:CZ	2.54	0.42
1:A:267:THR:HG22	1:A:312:GLU:HG3	2.03	0.41
1:A:117:PRO:HA	1:A:129:PHE:O	2.20	0.41
1:B:133:HIS:HE1	4:B:1525:HOH:O	2.03	0.41
1:A:76:GLU:N	1:A:76:GLU:OE1	2.53	0.41
1:B:314:ARG:HB2	1:B:387:TRP:CD1	2.56	0.41
1:A:434:LYS:H	1:A:434:LYS:CE	2.33	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	388/390 (100%)	376 (97%)	12 (3%)	0	100	100
1	B	388/390 (100%)	375 (97%)	13 (3%)	0	100	100
All	All	776/780 (100%)	751 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	301 (93%)	23 (7%)	14	16
1	B	324/324 (100%)	301 (93%)	23 (7%)	14	16
All	All	648/648 (100%)	602 (93%)	46 (7%)	14	16

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	80	THR
1	A	87	GLN
1	A	101	ARG
1	A	131	LEU
1	A	134	TYR
1	A	152	LEU
1	A	228	CYS
1	A	267	THR
1	A	294	SER
1	A	304	LEU
1	A	306	VAL
1	A	327	PRO
1	A	333	THR
1	A	359	LYS

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Mol	Chain	Res	Type
1	A	378	LEU
1	A	393	LEU
1	A	402	MET
1	A	417	LYS
1	A	434	LYS
1	A	452	GLN
1	A	454	LEU
1	A	455	TRP
1	B	76	GLU
1	B	80	THR
1	B	95	LEU
1	B	101	ARG
1	B	106	ARG
1	B	131	LEU
1	B	134	TYR
1	B	152	LEU
1	B	153	ARG
1	B	165	THR
1	B	198	ASN
1	B	228	CYS
1	B	267	THR
1	B	306	VAL
1	B	333	THR
1	B	344	ARG
1	B	358	SER
1	B	378	LEU
1	B	381	ARG
1	B	393	LEU
1	B	435	LYS
1	B	454	LEU
1	B	455	TRP

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

Mol	Chain	Res	Type
1	A	92	GLN
1	A	133	HIS
1	A	168	ASN
1	A	339	ASN
1	B	108	ASN
1	B	133	HIS
1	B	168	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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	B	1	1	14,14,15	1.29	1 (7%)	17,19,21	2.10	5 (29%)
2	NAG	A	1	1	14,14,15	0.95	1 (7%)	17,19,21	1.86	4 (23%)

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	-	0/6/23/26	0/1/1/1
2	NAG	A	1	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	-3.58	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	C1-C2	-2.15	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C8-C7-N2	5.39	125.23	116.10
2	A	1	NAG	C1-C2-N2	-4.10	103.49	110.49
2	B	1	NAG	C1-C2-N2	-3.67	104.21	110.49
2	B	1	NAG	O7-C7-N2	-3.38	115.75	121.95
2	A	1	NAG	C2-N2-C7	3.25	127.53	122.90
2	A	1	NAG	C1-O5-C5	3.07	116.34	112.19
2	B	1	NAG	C6-C5-C4	-2.56	107.01	113.00
2	B	1	NAG	C1-O5-C5	2.40	115.44	112.19
2	A	1	NAG	C3-C4-C5	-2.31	106.11	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.