



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:25 AM UTC

PDB ID : 1NSB / pdb_00001nsb
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 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
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

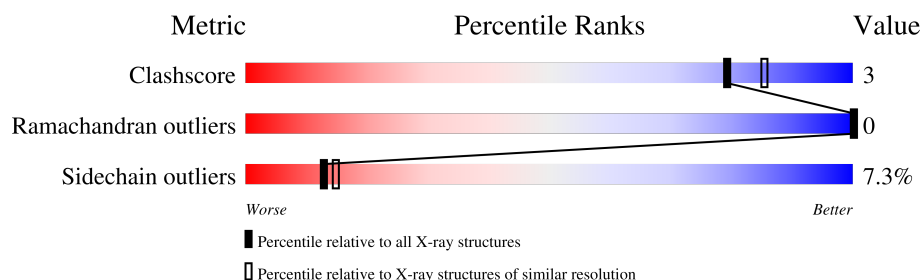
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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	 79% 17% . .
1	B	390	 76% 20% . .

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
1	A	390	Total	C	H	N	O	S	5	0	0
			3734	1899	698	533	575	29			
1	B	390	Total	C	H	N	O	S	5	0	0
			3735	1899	699	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
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

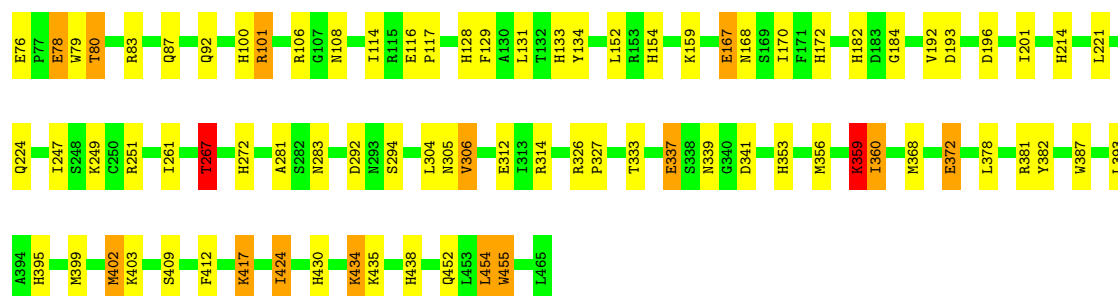
3 Residue-property plots

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.

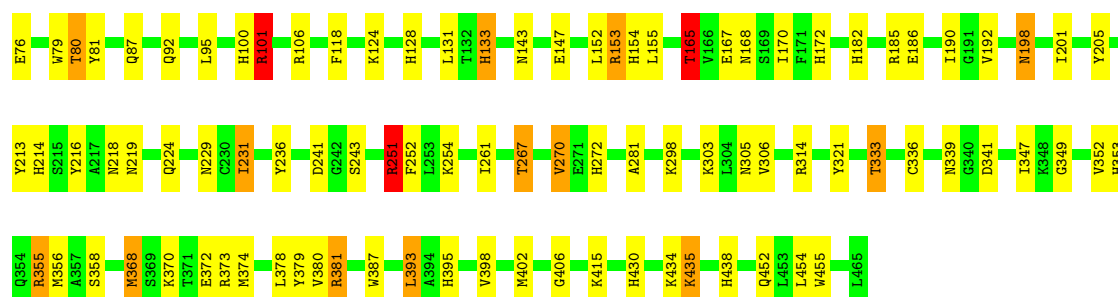
• Molecule 1: NEURAMINIDASE

Chain A:  79% 17% . .



• Molecule 1: NEURAMINIDASE

Chain B:  76% 20% . .



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	88.90 Å 88.90 Å 222.80 Å 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.	Xtriage
Total number of atoms	8858	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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

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	1.21	17/3109 (0.5%)	1.79	66/4197 (1.6%)
1	B	1.24	17/3109 (0.5%)	1.91	77/4197 (1.8%)
All	All	1.22	34/6218 (0.5%)	1.85	143/8394 (1.7%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	HIS	CD2-NE2	-7.85	1.29	1.37
1	A	100	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	182	HIS	CD2-NE2	-6.96	1.30	1.37
1	A	353	HIS	CD2-NE2	-6.89	1.30	1.37
1	A	133	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	133	HIS	CD2-NE2	-6.52	1.30	1.37
1	B	272	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	430	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	430	HIS	CG-ND1	-6.08	1.31	1.38
1	A	395	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	353	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	360	ILE	CA-CB	5.92	1.61	1.54
1	A	128	HIS	CD2-NE2	-5.85	1.31	1.37
1	B	231	ILE	CA-CB	5.83	1.61	1.54
1	A	214	HIS	CD2-NE2	-5.83	1.31	1.37
1	B	100	HIS	CD2-NE2	-5.75	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	272	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	172	HIS	CD2-NE2	-5.68	1.31	1.37
1	B	430	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	214	HIS	CG-ND1	-5.57	1.32	1.38
1	B	154	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	170	ILE	CB-CG1	-5.48	1.42	1.53
1	B	128	HIS	CD2-NE2	-5.36	1.31	1.37
1	B	272	HIS	CG-ND1	-5.29	1.32	1.38
1	A	272	HIS	CG-ND1	-5.23	1.32	1.38
1	A	438	HIS	CD2-NE2	-5.23	1.32	1.37
1	B	430	HIS	CG-ND1	-5.16	1.32	1.38
1	B	155	LEU	CA-CB	5.15	1.60	1.53
1	B	352	VAL	CA-CB	5.15	1.62	1.55
1	A	172	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	167	GLU	CA-CB	-5.07	1.45	1.53
1	A	251	ARG	NE-CZ	5.05	1.38	1.33
1	B	372	GLU	CA-CB	-5.03	1.45	1.53

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	VAL	N-CA-CB	-14.46	93.36	112.16
1	B	355	ARG	NE-CZ-NH2	-14.25	106.38	119.20
1	B	355	ARG	NE-CZ-NH1	12.36	133.85	121.50
1	B	224	GLN	N-CA-C	11.50	123.89	111.36
1	B	165	THR	N-CA-CB	-11.19	94.27	111.05
1	B	267	THR	N-CA-CB	-8.90	96.78	111.20
1	B	270	VAL	CB-CA-C	8.82	122.41	111.65
1	B	87	GLN	CG-CD-NE2	-8.49	103.66	116.40
1	B	341	ASP	CA-CB-CG	8.40	121.00	112.60
1	B	153	ARG	NE-CZ-NH2	-8.30	111.73	119.20
1	B	224	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	A	80	THR	N-CA-CB	-8.10	98.06	109.97
1	A	305	ASN	OD1-CG-ND2	-8.03	114.57	122.60
1	B	198	ASN	CA-CB-CG	-7.95	104.65	112.60
1	B	341	ASP	N-CA-CB	-7.92	98.21	110.56
1	B	133	HIS	CB-CG-CD2	-7.85	120.99	131.20
1	A	224	GLN	N-CA-C	7.81	119.87	111.36
1	A	101	ARG	NE-CZ-NH2	-7.75	112.23	119.20
1	B	101	ARG	NE-CZ-NH2	-7.43	112.51	119.20
1	A	224	GLN	OE1-CD-NE2	-7.41	115.19	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	A	108	ASN	CB-CG-ND2	7.22	127.23	116.40
1	B	333	THR	CA-CB-OG1	-7.10	98.96	109.60
1	A	159	LYS	CG-CD-CE	-6.98	95.24	111.30
1	B	101	ARG	CB-CG-CD	-6.98	95.25	111.30
1	A	193	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	108	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	A	435	LYS	CB-CG-CD	6.86	127.08	111.30
1	B	219	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	B	356	MET	CG-SD-CE	-6.82	85.91	100.90
1	B	252	PHE	CA-CB-CG	-6.80	107.00	113.80
1	B	165	THR	OG1-CB-CG2	6.63	122.56	109.30
1	B	333	THR	N-CA-CB	-6.58	100.45	110.45
1	A	281	ALA	N-CA-C	-6.55	104.32	112.90
1	A	78	GLU	CA-CB-CG	6.53	127.15	114.10
1	B	434	LYS	CA-CB-CG	6.49	127.09	114.10
1	A	402	MET	CA-CB-CG	-6.47	101.15	114.10
1	B	167	GLU	CA-CB-CG	-6.47	101.16	114.10
1	B	370	LYS	CG-CD-CE	-6.41	96.56	111.30
1	B	143	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	A	79	TRP	CG-CD2-CE3	6.36	140.26	133.90
1	A	167	GLU	N-CA-C	6.34	118.28	111.36
1	B	305	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	B	355	ARG	CG-CD-NE	-6.32	98.11	112.00
1	B	182	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	A	368	MET	N-CA-C	-6.27	104.52	111.36
1	B	243	SER	CA-C-O	6.20	128.01	121.19
1	A	79	TRP	CB-CG-CD1	-6.16	117.66	126.90
1	A	154	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	B	241	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	78	GLU	CB-CG-CD	6.12	123.01	112.60
1	A	261	ILE	N-CA-C	-6.12	107.03	112.90
1	A	101	ARG	CB-CG-CD	-6.11	97.25	111.30
1	A	341	ASP	N-CA-CB	-6.10	101.05	110.56
1	A	326	ARG	CA-C-N	6.09	126.06	120.21
1	A	326	ARG	C-N-CA	6.09	126.06	120.21
1	B	80	THR	N-CA-CB	-6.08	101.03	109.97
1	B	153	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	B	434	LYS	N-CA-CB	-6.07	100.00	110.32
1	B	438	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	B	79	TRP	CB-CG-CD1	-6.03	117.86	126.90
1	A	372	GLU	CB-CG-CD	5.98	122.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	THR	OG1-CB-CG2	5.95	121.20	109.30
1	A	154	HIS	CB-CG-ND1	5.93	131.59	122.70
1	A	267	THR	N-CA-CB	-5.91	101.62	111.20
1	A	339	ASN	CB-CG-ND2	5.89	125.23	116.40
1	B	154	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	A	395	HIS	CB-CG-CD2	-5.86	123.59	131.20
1	A	395	HIS	CB-CG-ND1	5.86	131.48	122.70
1	A	283	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	168	ASN	CA-CB-CG	5.82	118.42	112.60
1	B	147	GLU	CA-CB-CG	5.82	125.75	114.10
1	A	455	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	B	349	GLY	CA-C-N	5.80	125.49	119.92
1	B	349	GLY	C-N-CA	5.80	125.49	119.92
1	B	368	MET	CG-SD-CE	-5.79	88.17	100.90
1	B	170	ILE	CB-CA-C	-5.78	102.21	110.83
1	A	399	MET	N-CA-C	-5.78	105.33	112.90
1	A	381	ARG	CB-CG-CD	-5.77	98.03	111.30
1	B	218	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	116	GLU	O-C-N	-5.76	118.88	121.53
1	B	100	HIS	CA-CB-CG	-5.72	108.08	113.80
1	B	452	GLN	CG-CD-NE2	-5.71	107.84	116.40
1	B	128	HIS	CA-CB-CG	5.68	119.48	113.80
1	A	167	GLU	CA-CB-CG	-5.68	102.74	114.10
1	B	133	HIS	CB-CG-ND1	5.68	131.22	122.70
1	A	172	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	A	101	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	B	229	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	133	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	B	303	LYS	N-CA-C	-5.65	99.20	108.41
1	B	165	THR	CB-CA-C	5.64	120.83	110.24
1	A	424	ILE	CA-CB-CG1	-5.63	100.83	110.40
1	B	395	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	381	ARG	CD-NE-CZ	-5.59	116.57	124.40
1	A	283	ASN	O-C-N	-5.58	114.76	122.46
1	A	182	HIS	CB-CG-CD2	-5.57	123.97	131.20
1	B	81	TYR	O-C-N	-5.56	117.93	121.88
1	B	261	ILE	N-CA-C	-5.53	107.40	113.43
1	B	92	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	292	ASP	N-CA-C	-5.50	98.25	107.99
1	B	251	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	247	ILE	CA-CB-CG1	-5.49	101.08	110.40
1	A	83	ARG	NE-CZ-NH2	-5.47	114.28	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ILE	CA-C-O	-5.47	116.22	121.63
1	B	143	ASN	CB-CG-ND2	5.43	124.55	116.40
1	B	402	MET	CG-SD-CE	-5.43	88.94	100.90
1	A	80	THR	CB-CA-C	5.43	118.93	109.65
1	B	224	GLN	CG-CD-NE2	5.40	124.50	116.40
1	B	214	HIS	CA-CB-CG	-5.37	108.43	113.80
1	A	251	ARG	CB-CG-CD	5.37	123.65	111.30
1	A	412	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	196	ASP	N-CA-C	5.36	117.81	111.33
1	B	118	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	409	SER	CA-CB-OG	5.34	121.79	111.10
1	B	124	LYS	CG-CD-CE	-5.34	99.03	111.30
1	B	172	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	100	HIS	CA-CB-CG	-5.33	108.47	113.80
1	B	355	ARG	CD-NE-CZ	5.30	131.82	124.40
1	A	438	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	B	406	GLY	N-CA-C	-5.28	100.67	113.18
1	B	415	LYS	CG-CD-CE	5.27	123.43	111.30
1	A	337	GLU	N-CA-C	5.27	119.56	113.18
1	B	218	ASN	CA-CB-CG	-5.25	107.35	112.60
1	B	198	ASN	CA-C-O	-5.25	116.79	121.67
1	A	306	VAL	N-CA-CB	-5.24	100.05	111.05
1	A	184	GLY	N-CA-C	-5.22	107.68	113.79
1	A	170	ILE	N-CA-C	-5.17	100.93	108.17
1	A	249	LYS	CA-CB-CG	-5.15	103.80	114.10
1	A	100	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	A	101	ARG	N-CA-C	-5.14	106.84	113.01
1	B	281	ALA	N-CA-C	-5.13	106.87	113.23
1	B	80	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	185	ARG	CG-CD-NE	-5.10	100.78	112.00
1	B	339	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	417	LYS	CG-CD-CE	5.08	122.98	111.30
1	B	80	THR	CA-CB-CG2	5.08	119.13	110.50
1	B	395	HIS	CB-CG-ND1	5.07	130.30	122.70
1	B	368	MET	N-CA-C	-5.07	105.46	111.69
1	A	359	LYS	CB-CG-CD	-5.05	99.69	111.30
1	B	353	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	B	87	GLN	CB-CG-CD	5.04	121.17	112.60
1	A	79	TRP	CE2-CD2-CG	-5.02	101.18	107.20

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	17	0
1	B	3036	699	2923	17	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	32	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 3.

All (32) 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:B:373:ARG:O	1:B:374:MET:HE2	2.07	0.54
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:A:356:MET:HE1	1:A:382:TYR:CE1	2.48	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:298:LYS:NZ	1:B:336:CYS:O	2.47	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:356:MET:HE3	1:A:359:LYS:HG3	2.02	0.41
1:B:368:MET:HE1	1:B:398:VAL:HG13	2.03	0.41
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:B:368:MET:HE3	1:B:368:MET:HB2	1.78	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

5.3.1 Protein backbone

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 ⓘ

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%)	13	16
1	B	324/324 (100%)	300 (93%)	24 (7%)	13	14
All	All	648/648 (100%)	601 (93%)	47 (7%)	13	15

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	80	THR
1	A	101	ARG
1	A	131	LEU
1	A	152	LEU
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
1	A	360	ILE
1	A	378	LEU
1	A	393	LEU
1	A	402	MET
1	A	403	LYS
1	A	417	LYS
1	A	424	ILE
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

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Mol	Chain	Res	Type
1	B	106	ARG
1	B	131	LEU
1	B	152	LEU
1	B	153	ARG
1	B	165	THR
1	B	190	ILE
1	B	198	ASN
1	B	231	ILE
1	B	251	ARG
1	B	267	THR
1	B	270	VAL
1	B	306	VAL
1	B	333	THR
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	133	HIS
1	A	168	ASN
1	A	229	ASN
1	A	339	ASN
1	B	108	ASN
1	B	133	HIS
1	B	168	ASN
1	B	198	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	1	1	14,14,15	0.98	1 (7%)	17,19,21	1.91	4 (23%)
2	NAG	B	1	1	14,14,15	1.36	1 (7%)	17,19,21	2.16	5 (29%)

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	1	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1	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)
2	B	1	NAG	C1-C2	-3.93	1.47	1.52
2	A	1	NAG	C1-C2	-2.36	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	5.50	125.23	116.12
2	A	1	NAG	C1-C2-N2	-4.41	103.49	110.43
2	B	1	NAG	C1-C2-N2	-3.95	104.21	110.43
2	B	1	NAG	O7-C7-N2	-3.53	115.75	121.98
2	A	1	NAG	C2-N2-C7	3.46	127.53	122.90
2	A	1	NAG	C1-O5-C5	3.10	116.34	112.19
2	B	1	NAG	C6-C5-C4	-2.45	107.01	113.02
2	B	1	NAG	C1-O5-C5	2.43	115.44	112.19
2	A	1	NAG	C3-C4-C5	-2.27	106.11	110.23

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.