



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:01 AM GMT

PDB ID : 3NN9  
Title : REFINED ATOMIC STRUCTURES OF N9 SUBTYPE INFLUENZA VIRUS  
NEURAMINIDASE AND ESCAPE MUTANTS  
Authors : Tulip, W.R.; Varghese, J.N.; Baker, A.T.; Vandonkelaar, A.; Laver, W.G.;  
Webster, R.G.; Colman, P.M.  
Deposited on : 1991-03-28  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

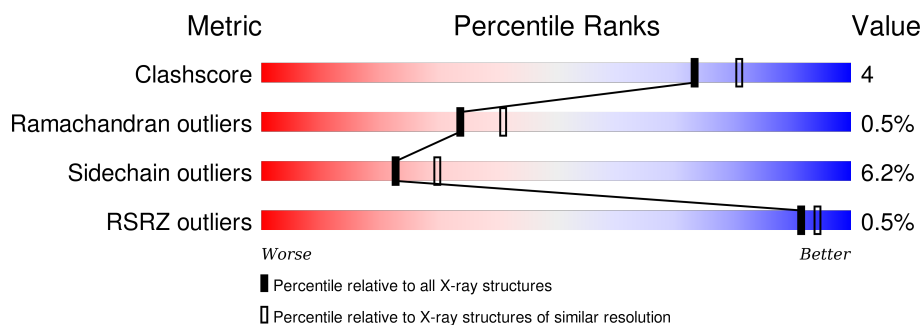
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	

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
2	BMA	A	471(C)	-	-	-	X
2	MAN	A	474(F)	-	-	-	X
4	CA	A	18	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3268 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NEURAMINIDASE N9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3067	1914	537	593	23	0	0	0

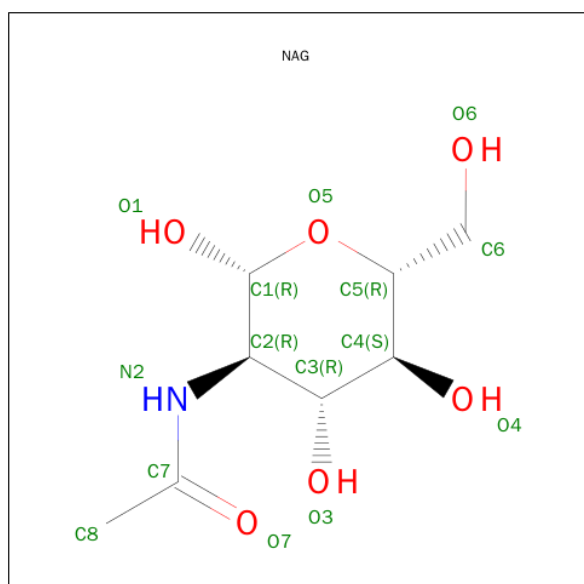
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	ASP	ASN	CONFLICT	UNP P03472

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	7	83	46	2	35	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

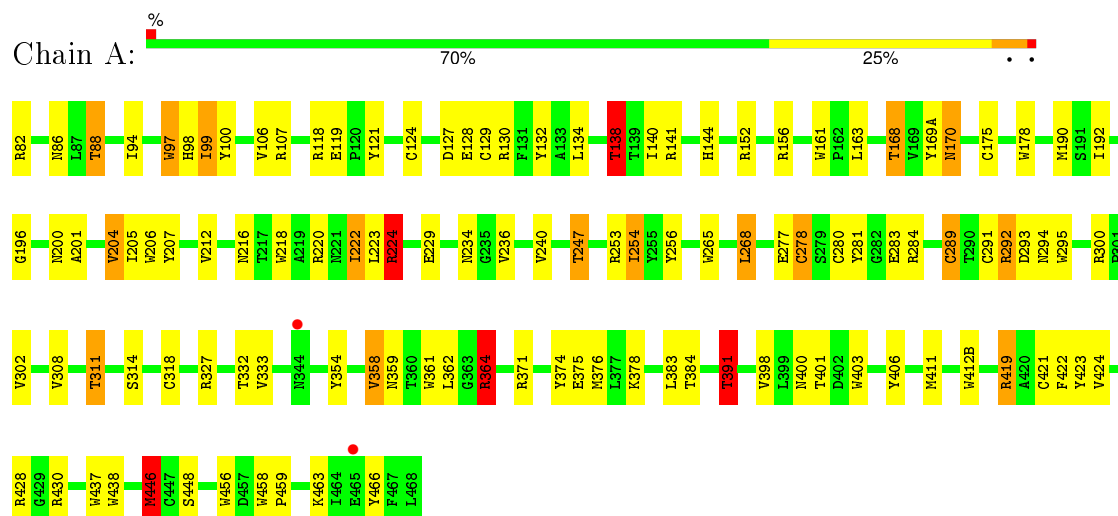
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

#### • Molecule 1: NEURAMINIDASE N9



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.10Å 185.10Å 185.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 6.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 69.9 (6.00-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.178 , (Not available) 0.191 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 15932 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, NAG, MAN

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	1.13	7/3150 (0.2%)	2.19	145/4290 (3.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	CYS	CB-SG	11.43	2.01	1.82
1	A	289	CYS	CB-SG	-10.13	1.65	1.82
1	A	175	CYS	CB-SG	6.65	1.93	1.82
1	A	278	CYS	CA-CB	-6.63	1.39	1.53
1	A	204	VAL	CA-CB	5.72	1.66	1.54
1	A	291	CYS	CB-SG	5.63	1.91	1.82
1	A	256	TYR	CB-CG	5.34	1.59	1.51

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ARG	NE-CZ-NH1	20.42	130.51	120.30
1	A	253	ARG	NE-CZ-NH1	18.34	129.47	120.30
1	A	406	TYR	CB-CG-CD2	-16.54	111.08	121.00
1	A	284	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	A	371	ARG	NE-CZ-NH1	13.36	126.98	120.30
1	A	220	ARG	NE-CZ-NH2	-12.55	114.03	120.30
1	A	206	TRP	CD1-CG-CD2	11.81	115.75	106.30
1	A	97	TRP	CD1-CG-CD2	11.63	115.61	106.30
1	A	403	TRP	CD1-CG-CD2	10.95	115.06	106.30
1	A	107	ARG	NE-CZ-NH2	-10.87	114.86	120.30
1	A	220	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	A	118	ARG	NE-CZ-NH1	10.63	125.62	120.30
1	A	403	TRP	CE2-CD2-CG	-10.59	98.83	107.30
1	A	456	TRP	CD1-CG-CD2	10.28	114.53	106.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	284	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	A	265	TRP	CG-CD2-CE3	9.76	142.68	133.90
1	A	206	TRP	CE2-CD2-CG	-9.54	99.67	107.30
1	A	437	TRP	CG-CD2-CE3	9.53	142.48	133.90
1	A	437	TRP	CE2-CD2-CG	-9.50	99.70	107.30
1	A	456	TRP	CE2-CD2-CG	-9.43	99.76	107.30
1	A	253	ARG	NH1-CZ-NH2	-9.42	109.04	119.40
1	A	438	TRP	CD1-CG-CD2	9.29	113.73	106.30
1	A	99	ILE	CB-CA-C	-9.23	93.14	111.60
1	A	265	TRP	CE2-CD2-CG	-9.20	99.94	107.30
1	A	97	TRP	CE2-CD2-CG	-9.15	99.98	107.30
1	A	406	TYR	CB-CG-CD1	9.13	126.48	121.00
1	A	178	TRP	CE2-CD2-CG	-8.74	100.31	107.30
1	A	178	TRP	CG-CD2-CE3	8.71	141.74	133.90
1	A	422	PHE	CB-CG-CD1	-8.69	114.72	120.80
1	A	437	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	A	374	TYR	CB-CG-CD1	-8.65	115.81	121.00
1	A	100	TYR	CB-CG-CD1	-8.48	115.91	121.00
1	A	178	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	A	438	TRP	CB-CG-CD1	-8.05	116.53	127.00
1	A	412(B)	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	A	265	TRP	CB-CG-CD1	-7.91	116.71	127.00
1	A	354	TYR	CB-CG-CD1	-7.88	116.27	121.00
1	A	456	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	A	236	VAL	CG1-CB-CG2	-7.85	98.34	110.90
1	A	265	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	A	293	ASP	CB-CG-OD1	7.76	125.28	118.30
1	A	419	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	295	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	A	207	TYR	CB-CG-CD1	-7.62	116.43	121.00
1	A	175	CYS	CA-CB-SG	7.48	127.47	114.00
1	A	437	TRP	NE1-CE2-CZ2	-7.42	122.24	130.40
1	A	421	CYS	CA-CB-SG	7.37	127.27	114.00
1	A	118	ARG	NH1-CZ-NH2	-7.36	111.31	119.40
1	A	265	TRP	NE1-CE2-CZ2	-7.25	122.43	130.40
1	A	97	TRP	CG-CD1-NE1	-7.20	102.90	110.10
1	A	292	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	438	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	A	190	MET	CG-SD-CE	7.13	111.61	100.20
1	A	218	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	A	456	TRP	CG-CD1-NE1	-7.00	103.10	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	300	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	A	121	TYR	CG-CD1-CE1	-6.95	115.74	121.30
1	A	458	TRP	CD1-CG-CD2	6.86	111.78	106.30
1	A	403	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	A	218	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	A	152	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	364	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	206	TRP	CB-CG-CD1	-6.73	118.25	127.00
1	A	206	TRP	CG-CD1-NE1	-6.67	103.43	110.10
1	A	446	MET	CG-SD-CE	-6.66	89.54	100.20
1	A	224	ARG	CA-CB-CG	6.61	127.94	113.40
1	A	358	VAL	N-CA-CB	-6.60	96.98	111.50
1	A	438	TRP	CG-CD2-CE3	6.50	139.75	133.90
1	A	106	VAL	CG1-CB-CG2	-6.43	100.61	110.90
1	A	311	THR	CA-CB-CG2	-6.42	103.42	112.40
1	A	295	TRP	CG-CD1-NE1	-6.39	103.71	110.10
1	A	280	CYS	CA-CB-SG	6.37	125.46	114.00
1	A	437	TRP	CG-CD1-NE1	-6.32	103.78	110.10
1	A	223	LEU	CA-CB-CG	6.29	129.76	115.30
1	A	100	TYR	CB-CG-CD2	6.27	124.76	121.00
1	A	359	ASN	CB-CG-ND2	6.24	131.67	116.70
1	A	212	VAL	CG1-CB-CG2	-6.21	100.97	110.90
1	A	424	VAL	CG1-CB-CG2	-6.21	100.97	110.90
1	A	438	TRP	CG-CD1-NE1	-6.14	103.96	110.10
1	A	446	MET	CA-CB-CG	6.14	123.74	113.30
1	A	138	THR	N-CA-CB	6.12	121.92	110.30
1	A	295	TRP	CE2-CD2-CG	-6.05	102.46	107.30
1	A	88	THR	N-CA-CB	-6.03	98.85	110.30
1	A	403	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	A	374	TYR	CG-CD1-CE1	-5.99	116.50	121.30
1	A	411	MET	CG-SD-CE	5.99	109.79	100.20
1	A	412(B)	TRP	CD1-CG-CD2	5.96	111.06	106.30
1	A	268	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	371	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
1	A	127	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	161	TRP	CA-CB-CG	5.87	124.85	113.70
1	A	430	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	428	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	A	419	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
1	A	132	TYR	CB-CG-CD1	5.72	124.43	121.00
1	A	295	TRP	CG-CD2-CE3	5.72	139.05	133.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
1	A	156	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	99	ILE	N-CA-CB	5.66	123.82	110.80
1	A	403	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	A	265	TRP	NE1-CE2-CD2	5.63	112.93	107.30
1	A	412(B)	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	A	463	LYS	CG-CD-CE	-5.62	95.06	111.90
1	A	374	TYR	CB-CG-CD2	5.60	124.36	121.00
1	A	163	LEU	CA-C-N	-5.57	104.94	117.20
1	A	178	TRP	CB-CG-CD1	-5.57	119.76	127.00
1	A	376	MET	CG-SD-CE	-5.53	91.36	100.20
1	A	206	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	88	THR	CA-CB-CG2	5.48	120.08	112.40
1	A	391	THR	CA-CB-CG2	5.45	120.03	112.40
1	A	437	TRP	NE1-CE2-CD2	5.44	112.74	107.30
1	A	132	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	423	TYR	CB-CG-CD1	5.43	124.26	121.00
1	A	398	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	A	138	THR	CB-CA-C	-5.41	96.98	111.60
1	A	178	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	A	391	THR	CA-CB-OG1	-5.36	97.75	109.00
1	A	459	PRO	CA-C-N	5.35	128.97	117.20
1	A	169(A)	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	277	GLU	N-CA-C	5.31	125.34	111.00
1	A	220	ARG	N-CA-C	5.28	125.25	111.00
1	A	224	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	229	GLU	CA-CB-CG	5.26	124.96	113.40
1	A	419	ARG	CB-CG-CD	-5.23	97.99	111.60
1	A	119	GLU	CA-CB-CG	5.23	124.91	113.40
1	A	333	VAL	N-CA-C	-5.20	96.97	111.00
1	A	362	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	A	361	TRP	CE2-CD2-CG	-5.18	103.15	107.30
1	A	308	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	A	281	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	216	ASN	OD1-CG-ND2	-5.13	110.10	121.90
1	A	358	VAL	CB-CA-C	5.13	121.15	111.40
1	A	121	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	361	TRP	CD1-CG-CD2	5.07	110.35	106.30
1	A	97	TRP	CG-CD2-CE3	5.05	138.44	133.90
1	A	293	ASP	CA-C-N	5.04	128.29	117.20
1	A	332	THR	OG1-CB-CG2	-5.04	98.42	110.00
1	A	333	VAL	CA-CB-CG1	-5.04	103.35	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	TRP	CB-CG-CD1	-5.01	120.48	127.00
1	A	247	THR	N-CA-CB	-5.01	100.78	110.30
1	A	212	VAL	N-CA-CB	-5.01	100.48	111.50
1	A	254	ILE	CG1-CB-CG2	-5.01	100.38	111.40
1	A	97	TRP	CB-CG-CD2	-5.00	120.09	126.60

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	3067	0	2891	25	0
2	A	83	0	70	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	89	0	0	2	0
All	All	3268	0	2987	25	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 4.

All (25) 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:278:CYS:SG	1:A:278:CYS:CB	2.01	1.46
1:A:466:TYR:OH	5:A:484:HOH:O	1.97	0.81
1:A:98:HIS:CE1	1:A:419:ARG:HH21	2.15	0.65
1:A:292:ARG:HH21	1:A:294:ASN:ND2	1.97	0.63
1:A:378:LYS:HD3	1:A:391:THR:HG22	1.81	0.62
1:A:168:THR:HG22	1:A:170:ASN:H	1.69	0.57
1:A:94:ILE:HG23	1:A:448:SER:HB2	1.88	0.55
1:A:138:THR:HG23	1:A:144:HIS:HB2	1.89	0.53
1:A:318:CYS:SG	1:A:383:LEU:O	2.67	0.53
1:A:138:THR:CG2	1:A:144:HIS:HB2	2.42	0.50

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:CYS:HA	1:A:129:CYS:HA	1.94	0.50
1:A:128:GLU:OE2	1:A:130:ARG:HD2	2.12	0.49
1:A:364:ARG:HD2	1:A:375:GLU:OE2	2.14	0.47
1:A:140:ILE:HD11	5:A:496:HOH:O	2.15	0.47
1:A:192:ILE:HG12	1:A:205:ILE:HG13	1.96	0.47
1:A:168:THR:H	1:A:170:ASN:ND2	2.14	0.46
1:A:222:ILE:O	1:A:224:ARG:HG3	2.16	0.44
1:A:86:ASN:OD1	1:A:234:ASN:HB2	2.17	0.44
1:A:97:TRP:HB3	1:A:446:MET:HG2	1.99	0.44
1:A:168:THR:HB	1:A:170:ASN:ND2	2.34	0.42
1:A:302:VAL:O	1:A:314:SER:HA	2.20	0.42
1:A:278:CYS:HB3	1:A:289:CYS:HB3	2.02	0.41
1:A:98:HIS:HE1	1:A:419:ARG:HH21	1.66	0.41
1:A:240:VAL:HG22	1:A:254:ILE:HG13	2.04	0.40
1:A:196:GLY:HA3	1:A:201:ALA:HA	2.02	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	386/388 (100%)	362 (94%)	22 (6%)	2 (0%)	34	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ILE
1	A	200	ASN

### 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	341/341 (100%)	320 (94%)	21 (6%)	23	30

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	88	THR
1	A	99	ILE
1	A	134	LEU
1	A	138	THR
1	A	141	ARG
1	A	168	THR
1	A	170	ASN
1	A	204	VAL
1	A	224	ARG
1	A	247	THR
1	A	268	LEU
1	A	283	GLU
1	A	311	THR
1	A	358	VAL
1	A	364	ARG
1	A	384	THR
1	A	391	THR
1	A	400	ASN
1	A	401	THR
1	A	446	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	98	HIS
1	A	150	HIS
1	A	170	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	233	HIS
1	A	294	ASN
1	A	346	ASN
1	A	400	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 ⓘ

7 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	469(A)	1,2	14,14,15	0.95	0	15,19,21	2.36	4 (26%)
2	NAG	A	470(B)	2	14,14,15	0.90	0	15,19,21	1.81	3 (20%)
2	BMA	A	471(C)	2	11,11,12	1.00	1 (9%)	14,15,17	1.64	4 (28%)
2	MAN	A	472(D)	2	11,11,12	0.77	0	14,15,17	1.86	5 (35%)
2	MAN	A	473(E)	2	11,11,12	1.13	1 (9%)	14,15,17	0.88	0
2	MAN	A	474(F)	2	11,11,12	0.84	0	14,15,17	2.35	3 (21%)
2	MAN	A	475(G)	2	11,11,12	0.65	0	14,15,17	1.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	469(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	470(B)	2	-	0/6/23/26	0/1/1/1
2	BMA	A	471(C)	2	-	0/2/19/22	0/1/1/1
2	MAN	A	472(D)	2	-	0/2/19/22	0/1/1/1
2	MAN	A	473(E)	2	-	0/2/19/22	0/1/1/1
2	MAN	A	474(F)	2	-	0/2/19/22	0/1/1/1
2	MAN	A	475(G)	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	471(C)	BMA	C2-C3	-2.18	1.49	1.52
2	A	473(E)	MAN	O5-C1	2.34	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	474(F)	MAN	O3-C3-C2	-3.61	103.48	110.00
2	A	472(D)	MAN	C2-C3-C4	-3.30	105.43	111.04
2	A	474(F)	MAN	C3-C4-C5	-3.20	104.62	110.20
2	A	472(D)	MAN	O2-C2-C1	-2.64	103.92	109.21
2	A	470(B)	NAG	O7-C7-N2	-2.55	116.66	121.86
2	A	471(C)	BMA	O4-C4-C3	-2.55	104.61	110.34
2	A	471(C)	BMA	O3-C3-C2	-2.51	105.47	110.00
2	A	470(B)	NAG	C4-C3-C2	-2.26	107.71	111.23
2	A	469(A)	NAG	C8-C7-N2	-2.19	111.92	116.11
2	A	472(D)	MAN	O5-C1-C2	2.14	114.34	110.86
2	A	471(C)	BMA	C6-C5-C4	2.82	119.96	113.02
2	A	472(D)	MAN	O3-C3-C2	2.98	115.39	110.00
2	A	471(C)	BMA	O2-C2-C1	3.07	115.36	109.21
2	A	469(A)	NAG	O7-C7-N2	3.17	128.32	121.86
2	A	469(A)	NAG	C1-O5-C5	3.30	116.44	112.25
2	A	472(D)	MAN	C1-O5-C5	3.35	116.50	112.25
2	A	470(B)	NAG	C8-C7-N2	4.48	124.68	116.11
2	A	474(F)	MAN	C1-O5-C5	5.89	119.72	112.25
2	A	469(A)	NAG	C2-N2-C7	7.04	132.08	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
3	NAG	A	476(A)	1	14,14,15	1.12	1 (7%)	15,19,21	1.54	5 (33%)
3	NAG	A	477(A)	1	14,14,15	0.92	0	15,19,21	1.64	4 (26%)

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
3	NAG	A	476(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	A	477(A)	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	476(A)	NAG	C4-C5	2.61	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	477(A)	NAG	C4-C3-C2	-2.53	107.30	111.23
3	A	476(A)	NAG	C3-C4-C5	-2.44	105.94	110.20
3	A	476(A)	NAG	O4-C4-C3	-2.11	105.58	110.34
3	A	477(A)	NAG	C1-O5-C5	2.09	114.90	112.25
3	A	476(A)	NAG	O4-C4-C5	2.22	115.13	109.24
3	A	476(A)	NAG	C6-C5-C4	2.26	118.58	113.02
3	A	477(A)	NAG	C2-N2-C7	2.50	126.25	123.04
3	A	476(A)	NAG	O3-C3-C2	2.73	114.52	109.11
3	A	477(A)	NAG	O3-C3-C2	3.07	115.19	109.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	388/388 (100%)	-0.80	2 (0%) 91 94	3, 12, 23, 41	10 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	GLU	2.6
1	A	344	ASN	2.5

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	A	474(F)	11/12	0.95	0.11	2.15	25,26,29,30	0
2	BMA	A	471(C)	11/12	0.94	0.13	2.03	18,22,27,31	0
2	NAG	A	469(A)	14/15	0.95	0.11	1.12	17,18,23,26	0
2	MAN	A	475(G)	11/12	0.80	0.28	-	37,40,46,48	0
2	MAN	A	472(D)	11/12	0.94	0.12	-	20,21,24,26	0
2	NAG	A	470(B)	14/15	0.93	0.13	-	16,18,23,23	0
2	MAN	A	473(E)	11/12	0.94	0.12	-	19,21,23,24	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	A	18	1/1	0.98	0.21	9.40	2,2,2,2	0
3	NAG	A	476(A)	14/15	0.87	0.21	-	36,41,45,45	0
3	NAG	A	477(A)	14/15	0.90	0.18	-	29,34,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.