



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:35 PM GMT

PDB ID : 1NN2
Title : THREE-DIMENSIONAL STRUCTURE OF THE NEURAMINIDASE OF INFLUENZA VIRUS A(SLASH)TOKYO(SLASH)3(SLASH)67AT 2.2 ANGSTROMS RESOLUTION
Authors : Varghese, J.N.; Colman, P.M.
Deposited on : 1991-03-28
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

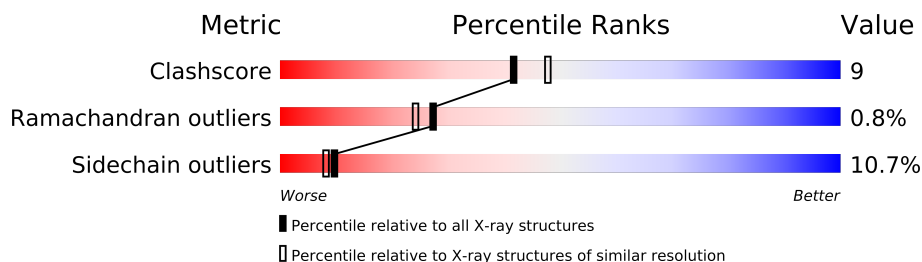
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	388	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4429 atoms, of which 1100 are hydrogens and 0 are deuterium.

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	388	Total	C	H	N	O	S	0	0	0
			3746	1866	724	545	588	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	H	N	O	28	0
			55	16	27	2	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	7	Total	C	H	N	O	S	69	0
			174	50	82	4	37	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

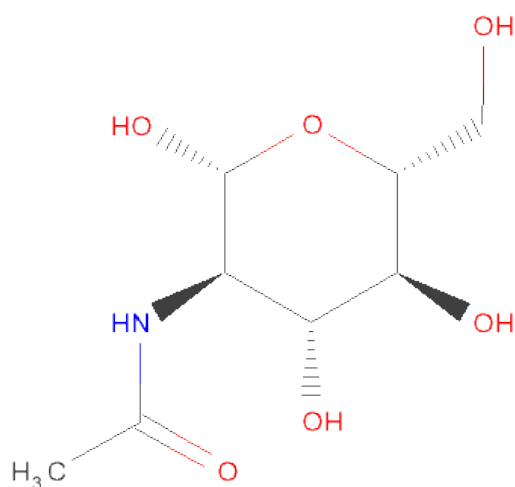
- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	6	Total	C	H	N	O	0	0
			139	40	67	2	30		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is water.

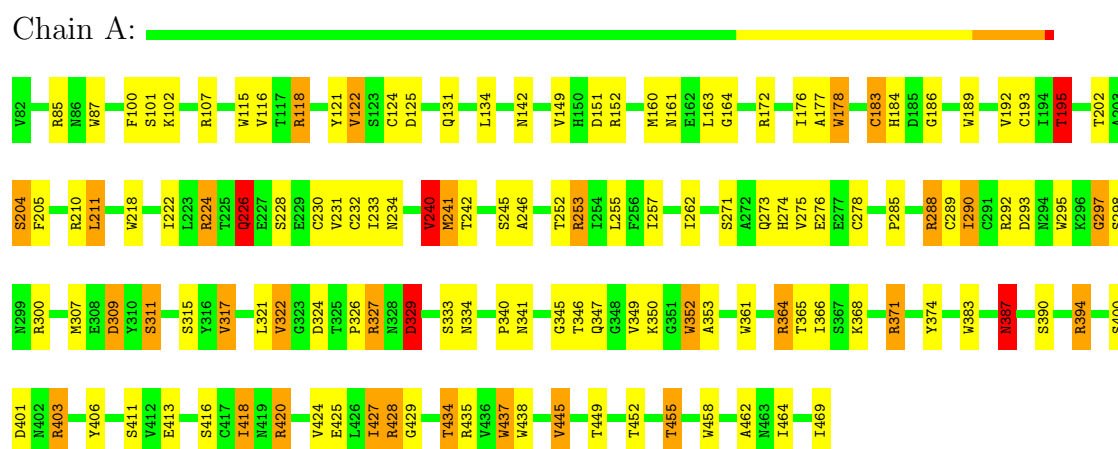
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	86	Total	H	O	0	0
			258	172	86		

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 ($RSRZ > 2$). 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.

Note EDS failed to run properly.

• Molecule 1: NEURAMINIDASE



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.60Å 139.60Å 191.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.585	Xtriage
Estimated twinning fraction	0.043 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.047 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 30245 reflections	Xtriage
Total number of atoms	4429	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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: BMA, NAG, CA, NGK, FUL, 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	0.99	3/3092 (0.1%)	1.91	104/4194 (2.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	VAL	CA-CB	5.83	1.67	1.54
1	A	122	VAL	CA-CB	5.56	1.66	1.54
1	A	231	VAL	CA-CB	5.20	1.65	1.54

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	A	124	CYS	N-CA-CB	-12.16	88.71	110.60
1	A	300	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	361	TRP	CD1-CG-CD2	10.44	114.66	106.30
1	A	224	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	A	224	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	253	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	300	ARG	NE-CZ-NH2	-9.47	115.57	120.30
1	A	160	MET	CG-SD-CE	9.39	115.23	100.20
1	A	241	MET	CG-SD-CE	-9.34	85.26	100.20
1	A	297	GLY	CA-C-N	-9.26	96.83	117.20
1	A	383	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	A	428	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	A	437	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	A	327	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	A	172	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	189	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	A	403	ARG	NE-CZ-NH1	8.16	124.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	A	107	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	178	TRP	CE2-CD2-CG	-8.01	100.90	107.30
1	A	371	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	364	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	455	THR	N-CA-CB	-7.90	95.29	110.30
1	A	361	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	293	ASP	CA-C-N	-7.84	99.96	117.20
1	A	371	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	420	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	383	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	A	115	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	87	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	A	152	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	189	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	A	178	TRP	CB-CG-CD1	-7.48	117.27	127.00
1	A	437	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	A	178	TRP	CG-CD2-CE3	7.34	140.51	133.90
1	A	124	CYS	CB-CA-C	7.33	125.06	110.40
1	A	87	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	438	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	A	434	THR	N-CA-CB	-7.22	96.58	110.30
1	A	292	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	438	TRP	CD1-CG-CD2	7.13	112.01	106.30
1	A	458	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	A	361	TRP	CG-CD1-NE1	-7.09	103.01	110.10
1	A	295	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	A	297	GLY	O-C-N	6.94	133.80	122.70
1	A	218	TRP	CD1-CG-CD2	6.93	111.84	106.30
1	A	210	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	218	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	172	ARG	CG-CD-NE	-6.85	97.42	111.80
1	A	115	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	A	226	GLN	CA-CB-CG	6.58	127.86	113.40
1	A	458	TRP	CD1-CG-CD2	6.56	111.55	106.30
1	A	253	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	352	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	A	352	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	A	406	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	A	394	ARG	CG-CD-NE	-6.19	98.80	111.80
1	A	347	GLN	CA-C-N	-6.17	103.85	116.20
1	A	295	TRP	CE2-CD2-CG	-6.15	102.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	383	TRP	CG-CD2-CE3	6.04	139.33	133.90
1	A	107	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	210	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	383	TRP	CB-CG-CD1	-5.95	119.26	127.00
1	A	383	TRP	CG-CD1-NE1	-5.94	104.16	110.10
1	A	288	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	290	ILE	N-CA-C	-5.92	95.03	111.00
1	A	438	TRP	CB-CG-CD1	-5.90	119.33	127.00
1	A	121	TYR	CA-CB-CG	5.88	124.57	113.40
1	A	317	VAL	CG1-CB-CG2	-5.86	101.53	110.90
1	A	403	ARG	CB-CG-CD	-5.85	96.38	111.60
1	A	87	TRP	CB-CG-CD1	-5.71	119.57	127.00
1	A	435	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	195	THR	OG1-CB-CG2	5.62	122.94	110.00
1	A	183	CYS	CA-CB-SG	5.56	124.01	114.00
1	A	230	CYS	O-C-N	-5.55	113.81	122.70
1	A	435	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	458	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	A	329	ASP	CA-CB-CG	5.49	125.49	113.40
1	A	87	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	295	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	A	458	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	276	GLU	N-CA-CB	-5.40	100.89	110.60
1	A	276	GLU	CA-CB-CG	5.33	125.13	113.40
1	A	437	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	118	ARG	CB-CG-CD	5.31	125.41	111.60
1	A	121	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	192	VAL	N-CA-C	-5.29	96.72	111.00
1	A	178	TRP	CA-CB-CG	5.28	123.73	113.70
1	A	118	ARG	CA-CB-CG	-5.28	101.79	113.40
1	A	364	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	416	SER	N-CA-CB	-5.23	102.66	110.50
1	A	230	CYS	CA-C-N	5.22	128.68	117.20
1	A	293	ASP	CA-C-O	5.18	130.98	120.10
1	A	309	ASP	CB-CA-C	-5.13	100.13	110.40
1	A	211	LEU	N-CA-C	-5.13	97.15	111.00
1	A	438	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	A	210	ARG	CA-CB-CG	5.10	124.62	113.40
1	A	116	VAL	CG1-CB-CG2	-5.07	102.78	110.90
1	A	292	ARG	CA-CB-CG	5.05	124.52	113.40
1	A	387	ASN	N-CA-C	5.04	124.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	THR	CA-C-N	-5.03	106.13	117.20
1	A	449	THR	CA-CB-CG2	5.01	119.42	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	724	2135	52	0
2	A	28	27	0	0	0
3	A	92	82	0	0	0
4	A	72	67	0	0	0
5	A	28	28	0	4	0
6	A	1	0	0	0	0
7	A	86	172	0	3	0
All	All	3329	1100	2135	53	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:ILE:HG22	1:A:234:ASN:ND2	2.03	0.74
1:A:322:VAL:HG12	1:A:327:ARG:HG3	1.71	0.72
1:A:101:SER:HB3	1:A:445:VAL:HG13	1.77	0.67
1:A:226:GLN:HG3	1:A:278:CYS:O	1.95	0.67
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.76	0.66
1:A:317:VAL:HG23	7:A:551:HOH:O	1.96	0.65
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.79	0.65
1:A:273:GLN:HG3	1:A:340:PRO:HG3	1.79	0.64
1:A:233:ILE:HG22	1:A:234:ASN:HD22	1.63	0.64
1:A:242:THR:HG21	1:A:275:VAL:O	1.99	0.61
1:A:234:ASN:ND2	5:A:485(A):NAG:C1	2.65	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:309:ASP:HB2	1:A:311:SER:OG	2.02	0.59
1:A:329:ASP:O	1:A:333:SER:HB3	2.01	0.59
1:A:334:ASN:HA	1:A:387:ASN:ND2	2.19	0.58
1:A:102:LYS:HZ1	7:A:561:HOH:H2	1.54	0.55
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.73	0.54
1:A:176:ILE:HG22	1:A:195:THR:HG21	1.90	0.53
1:A:245:SER:O	1:A:274:HIS:HE1	1.91	0.53
5:A:485(A):NAG:C1	5:A:485(A):NAG:O7	2.58	0.53
1:A:298:SER:HB2	1:A:341:ASN:HD21	1.75	0.51
1:A:326:PRO:HA	1:A:368:LYS:O	2.09	0.51
1:A:85:ARG:HD3	7:A:572:HOH:H2	1.74	0.51
1:A:365:THR:HG21	1:A:371:ARG:HA	1.92	0.51
1:A:307:MET:HB2	5:A:485(A):NAG:H81	1.93	0.51
1:A:349:VAL:CG2	1:A:371:ARG:HE	2.25	0.50
1:A:349:VAL:HG23	1:A:371:ARG:NE	2.27	0.50
1:A:184:HIS:CD2	1:A:186:GLY:H	2.29	0.50
1:A:285:PRO:HB2	5:A:485(A):NAG:H83	1.96	0.48
1:A:428:ARG:NH2	1:A:462:ALA:O	2.47	0.48
1:A:437:TRP:HD1	1:A:469:ILE:HG22	1.79	0.47
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.76	0.47
1:A:403:ARG:NH2	1:A:429:GLY:O	2.48	0.47
1:A:204:SER:HB3	1:A:211:LEU:HD11	1.97	0.46
1:A:131:GLN:HE22	1:A:163:LEU:HD12	1.80	0.46
1:A:131:GLN:NE2	1:A:164:GLY:H	2.14	0.46
1:A:242:THR:HG22	1:A:252:THR:HG23	1.98	0.46
1:A:183:CYS:SG	1:A:232:CYS:SG	3.14	0.45
1:A:349:VAL:HG23	1:A:371:ARG:HE	1.82	0.45
1:A:240:VAL:HG21	1:A:278:CYS:SG	2.57	0.45
1:A:425:GLU:HG2	1:A:427:ILE:HG22	1.99	0.45
1:A:298:SER:O	1:A:322:VAL:HG13	2.19	0.43
1:A:418:ILE:HD11	1:A:420:ARG:NH1	2.34	0.43
1:A:100:PHE:HB3	1:A:445:VAL:HG22	2.00	0.42
1:A:228:SER:HB3	1:A:350:LYS:CE	2.47	0.42
1:A:278:CYS:HB3	1:A:289:CYS:HB3	2.01	0.42
1:A:246:ALA:O	1:A:274:HIS:NE2	2.53	0.42
1:A:205:PHE:CE1	1:A:262:ILE:HD11	2.55	0.42
1:A:352:TRP:NE1	1:A:374:TYR:OH	2.53	0.42
1:A:241:MET:HE3	1:A:255:LEU:HG	2.01	0.41
1:A:290:ILE:HG12	1:A:353:ALA:HB3	2.02	0.41
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.50	0.41
1:A:366:ILE:HG21	1:A:400:SER:HB3	2.03	0.41
1:A:297:GLY:O	1:A:345:GLY:O	2.39	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	386/388 (100%)	353 (92%)	30 (8%)	3 (1%)	27 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	222	ILE
1	A	322	VAL

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	338/338 (100%)	302 (89%)	36 (11%)	10 8

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	122	VAL
1	A	125	ASP
1	A	134	LEU
1	A	142	ASN
1	A	149	VAL
1	A	151	ASP
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	178	TRP
1	A	195	THR
1	A	202	THR
1	A	204	SER
1	A	224	ARG
1	A	226	GLN
1	A	240	VAL
1	A	253	ARG
1	A	257	ILE
1	A	271	SER
1	A	288	ARG
1	A	311	SER
1	A	315	SER
1	A	324	ASP
1	A	364	ARG
1	A	387	ASN
1	A	390	SER
1	A	394	ARG
1	A	401	ASP
1	A	413	GLU
1	A	418	ILE
1	A	424	VAL
1	A	427	ILE
1	A	434	THR
1	A	445	VAL
1	A	452	THR
1	A	455	THR
1	A	464	ILE

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

Mol	Chain	Res	Type
1	A	131	GLN
1	A	142	ASN
1	A	161	ASN
1	A	200	ASN
1	A	226	GLN
1	A	234	ASN
1	A	274	HIS
1	A	334	ASN
1	A	387	ASN
1	A	419	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

15 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	470(A)	1,2	12,14,15	0.75	0	15,19,21	1.52	2 (13%)
2	NAG	A	471(B)	2	12,14,15	0.72	0	15,19,21	1.30	2 (13%)
3	NAG	A	472(A)	1,3	12,14,15	0.73	0	15,19,21	1.80	6 (40%)
3	NAG	A	473(B)	3	12,14,15	1.06	1 (8%)	15,19,21	1.21	1 (6%)
3	BMA	A	474(C)	3	10,11,12	1.02	0	11,15,17	1.30	2 (18%)
3	MAN	A	475(D)	3	10,11,12	0.88	0	11,15,17	1.07	1 (9%)
3	NAG	A	476(E)	3	12,14,15	1.07	2 (16%)	15,19,21	1.54	2 (13%)
3	NGK	A	477(F)	3	16,18,19	2.86	1 (6%)	22,26,28	1.95	5 (22%)
3	FUL	A	478(I)	3	9,10,11	3.35	3 (33%)	10,14,16	5.76	6 (60%)
4	NAG	A	479(A)	1,4	12,14,15	0.99	1 (8%)	15,19,21	1.17	2 (13%)
4	NAG	A	480(B)	4	12,14,15	0.89	0	15,19,21	2.13	5 (33%)
4	BMA	A	481(C)	4	10,11,12	0.70	0	11,15,17	1.28	2 (18%)
4	MAN	A	482(D)	4	10,11,12	0.64	0	11,15,17	1.34	1 (9%)
4	MAN	A	483(E)	4	10,11,12	0.57	0	11,15,17	0.95	0
4	MAN	A	484(F)	4	10,11,12	0.67	0	11,15,17	0.73	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	470(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	471(B)	2	-	0/6/23/26	0/1/1/1
3	NAG	A	472(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	473(B)	3	-	0/6/23/26	0/1/1/1
3	BMA	A	474(C)	3	-	0/2/19/22	0/1/1/1
3	MAN	A	475(D)	3	-	0/2/19/22	0/1/1/1
3	NAG	A	476(E)	3	-	0/6/23/26	0/1/1/1
3	NGK	A	477(F)	3	-	0/11/28/31	0/1/1/1
3	FUL	A	478(I)	3	-	0/0/17/20	0/1/1/1
4	NAG	A	479(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	480(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	A	481(C)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	482(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	483(E)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	484(F)	4	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	477(F)	NGK	O4-S	-11.09	1.42	1.60
3	A	478(I)	FUL	C4-C5	8.21	1.70	1.52
3	A	478(I)	FUL	C4-C3	4.74	1.65	1.52
3	A	478(I)	FUL	C6-C5	2.39	1.57	1.51
3	A	476(E)	NAG	C4-C5	2.38	1.58	1.53
3	A	476(E)	NAG	O4-C4	2.27	1.48	1.43
3	A	473(B)	NAG	C4-C5	2.12	1.57	1.53
4	A	479(A)	NAG	O4-C4	2.04	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	478(I)	FUL	C6-C5-C4	11.68	132.03	113.06
3	A	478(I)	FUL	O3-C3-C2	11.34	130.67	109.94
3	A	477(F)	NGK	C8-C7-N	5.65	127.16	116.11
4	A	480(B)	NAG	C3-C2-N2	-4.59	104.78	111.76
3	A	478(I)	FUL	C3-C4-C5	4.42	117.21	109.84
2	A	470(A)	NAG	C3-C2-N2	-4.26	105.27	111.76
3	A	478(I)	FUL	O2-C2-C3	-4.20	101.12	110.18
4	A	480(B)	NAG	O5-C5-C4	-4.06	105.50	110.65
3	A	478(I)	FUL	O4-C4-C3	3.83	118.95	110.35
4	A	480(B)	NAG	O5-C5-C6	3.68	110.84	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	477(F)	NGK	O7-C7-N	-3.62	114.34	121.90
3	A	476(E)	NAG	C3-C4-C5	-3.48	103.98	110.20
3	A	472(A)	NAG	C8-C7-N2	3.34	122.64	116.11
3	A	478(I)	FUL	C4-C3-C2	-3.34	106.02	110.50
3	A	476(E)	NAG	O4-C4-C5	3.17	117.63	109.28
2	A	471(B)	NAG	O5-C5-C4	-3.01	106.83	110.65
4	A	481(C)	BMA	O5-C5-C6	2.91	110.04	106.98
2	A	471(B)	NAG	C6-C5-C4	2.80	119.77	113.00
2	A	470(A)	NAG	O5-C5-C4	-2.79	107.11	110.65
3	A	477(F)	NGK	C4-O4-S	2.67	122.73	118.37
3	A	472(A)	NAG	C3-C2-N2	-2.57	107.85	111.76
3	A	474(C)	BMA	C4-C3-C2	-2.48	107.18	110.50
3	A	474(C)	BMA	C3-C4-C5	2.40	114.50	110.20
3	A	472(A)	NAG	O5-C5-C6	2.39	109.48	106.98
4	A	482(D)	MAN	C3-C4-C5	-2.21	106.25	110.20
4	A	479(A)	NAG	C8-C7-N2	2.21	120.42	116.11
4	A	481(C)	BMA	O5-C5-C4	-2.20	107.86	110.65
4	A	479(A)	NAG	O7-C7-C8	-2.19	117.78	122.04
3	A	472(A)	NAG	O4-C4-C3	-2.16	105.51	110.35
3	A	472(A)	NAG	O7-C7-N2	-2.16	117.40	121.90
4	A	480(B)	NAG	O4-C4-C3	-2.14	105.55	110.35
3	A	472(A)	NAG	C4-C3-C2	-2.12	106.13	111.32
3	A	477(F)	NGK	O4-S-O3S	2.08	114.16	105.54
3	A	475(D)	MAN	C3-C4-C5	2.08	113.92	110.20
3	A	473(B)	NAG	C8-C7-N2	2.07	120.16	116.11
3	A	477(F)	NGK	C4-C3-C2	-2.05	106.11	110.83
4	A	480(B)	NAG	C8-C7-N2	2.04	120.10	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	$\# Z > 2$
5	NAG	A	485(A)	-	12,14,15	0.92	1 (8%)	15,19,21	1.40	4 (26%)
5	NAG	A	486(B)	-	12,14,15	0.56	0	15,19,21	0.98	1 (6%)

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
5	NAG	A	485(A)	-	-	0/6/23/26	0/1/1/1
5	NAG	A	486(B)	-	-	0/6/23/26	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	485(A)	NAG	O5-C5	-2.39	1.41	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	485(A)	NAG	O5-C5-C4	-2.68	107.25	110.65
5	A	485(A)	NAG	C6-C5-C4	2.62	119.32	113.00
5	A	485(A)	NAG	C8-C7-N2	2.43	120.87	116.11
5	A	486(B)	NAG	O3-C3-C2	2.41	114.16	109.09
5	A	485(A)	NAG	O7-C7-C8	-2.07	118.00	122.04

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	486(B)	NAG	C1-C2-C3-C4-C5-O5

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.