



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2021 – 11:19 AM EDT

PDB ID : 3K38
Title : Crystal Structure of B/Perth Neuraminidase D197E mutant
Authors : Oakley, A.J.; McKimm-Breschkin, J.L.
Deposited on : 2009-10-02
Resolution : 2.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

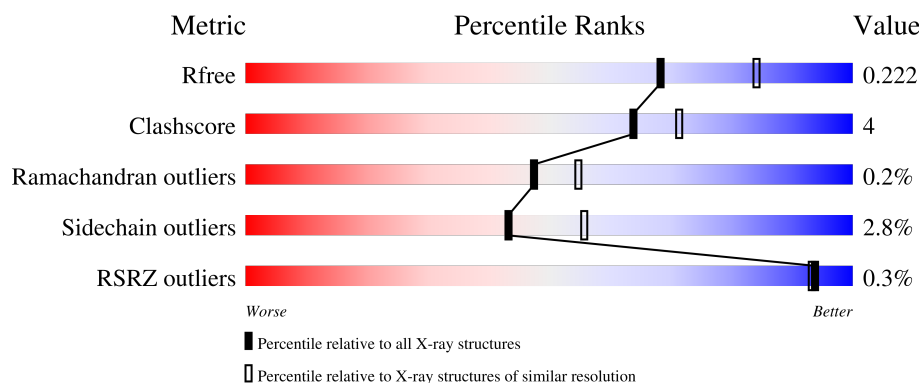
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 $\leq 5\%$. 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	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 88% 9% .. </div> </div>
1	B	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 10% .. </div> </div>
1	C	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 10% .. </div> </div>
1	D	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 9% .. </div> </div>
1	E	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 86% 11% .. </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	397	<div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	G	397	<div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	H	397	<div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	I	397	<div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	J	397	<div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	K	397	<div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	L	397	<div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	M	397	<div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	N	397	<div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	O	397	<div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	P	397	<div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 50572 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.

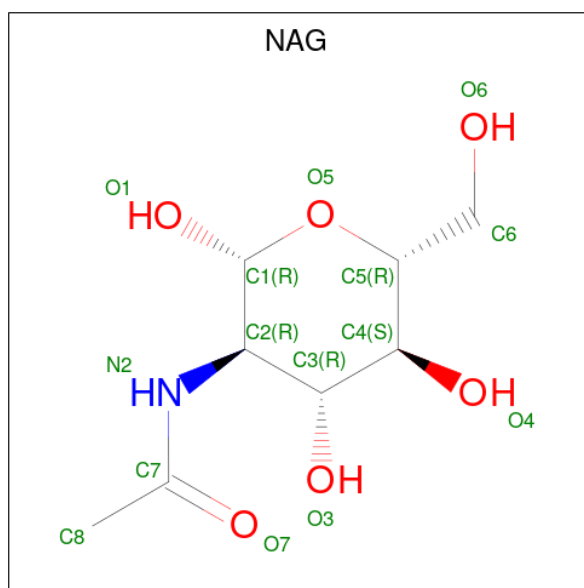
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	B	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	C	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	D	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	E	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	F	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	G	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	H	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	I	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	J	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	K	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	L	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	M	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	N	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	O	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			
1	P	389	Total	C	N	O	S	12	8	0
			3058	1921	529	579	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLU	ASP	engineered mutation	UNP Q3S340
B	197	GLU	ASP	engineered mutation	UNP Q3S340
C	197	GLU	ASP	engineered mutation	UNP Q3S340
D	197	GLU	ASP	engineered mutation	UNP Q3S340
E	197	GLU	ASP	engineered mutation	UNP Q3S340
F	197	GLU	ASP	engineered mutation	UNP Q3S340
G	197	GLU	ASP	engineered mutation	UNP Q3S340
H	197	GLU	ASP	engineered mutation	UNP Q3S340
I	197	GLU	ASP	engineered mutation	UNP Q3S340
J	197	GLU	ASP	engineered mutation	UNP Q3S340
K	197	GLU	ASP	engineered mutation	UNP Q3S340
L	197	GLU	ASP	engineered mutation	UNP Q3S340
M	197	GLU	ASP	engineered mutation	UNP Q3S340
N	197	GLU	ASP	engineered mutation	UNP Q3S340
O	197	GLU	ASP	engineered mutation	UNP Q3S340
P	197	GLU	ASP	engineered mutation	UNP Q3S340

- 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
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	N	1	Total	C	N	O	0	0
			14	8	1	5		
2	O	1	Total	C	N	O	0	0
			14	8	1	5		
2	P	1	Total	C	N	O	0	0
			14	8	1	5		

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

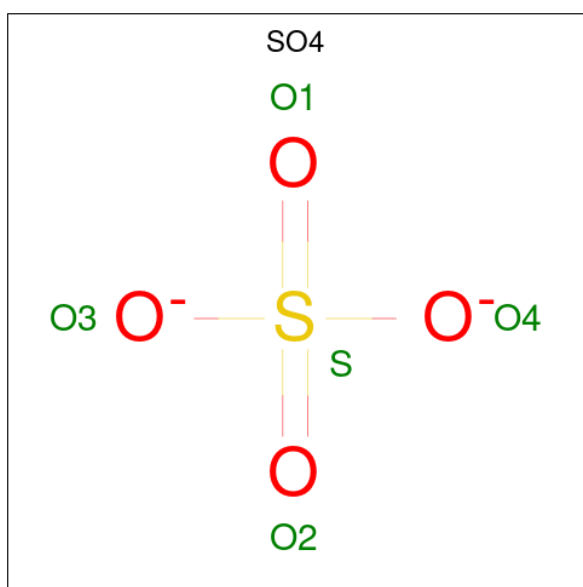
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	I	1	Total 1	Ca 1	0	0
3	J	1	Total 1	Ca 1	0	0
3	K	1	Total 1	Ca 1	0	0
3	L	1	Total 1	Ca 1	0	0
3	M	1	Total 1	Ca 1	0	0
3	N	1	Total 1	Ca 1	0	0
3	O	1	Total 1	Ca 1	0	0
3	P	1	Total 1	Ca 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	O	1	Total O S 5 4 1	0	0
4	P	1	Total O S 5 4 1	0	0

- Molecule 5 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Y 2 2	0	0
5	B	1	Total Y 1 1	0	0
5	C	1	Total Y 1 1	0	0
5	D	1	Total Y 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total 2	Y 2	0	0
5	F	1	Total 1	Y 1	0	0
5	G	1	Total 1	Y 1	0	0
5	H	1	Total 1	Y 1	0	0
5	I	2	Total 2	Y 2	0	0
5	J	1	Total 1	Y 1	0	0
5	K	1	Total 1	Y 1	0	0
5	L	1	Total 1	Y 1	0	0
5	M	1	Total 1	Y 1	0	0
5	N	2	Total 2	Y 2	0	0
5	O	1	Total 1	Y 1	0	0
5	P	1	Total 1	Y 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total 99	O 99	0	0
6	B	100	Total 100	O 100	0	0
6	C	96	Total 96	O 96	0	0
6	D	91	Total 91	O 91	0	0
6	E	77	Total 77	O 77	0	0
6	F	72	Total 72	O 72	0	0
6	G	69	Total 69	O 69	0	0

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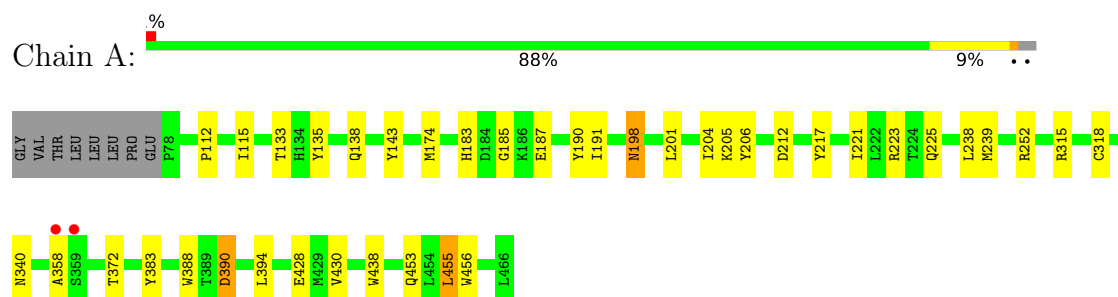
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	67	Total 67	O 67	0	0
6	I	84	Total 84	O 84	0	0
6	J	86	Total 86	O 86	0	0
6	K	106	Total 106	O 106	0	0
6	L	85	Total 85	O 85	0	0
6	M	78	Total 78	O 78	0	0
6	N	62	Total 62	O 62	0	0
6	O	67	Total 67	O 67	0	0
6	P	65	Total 65	O 65	0	0

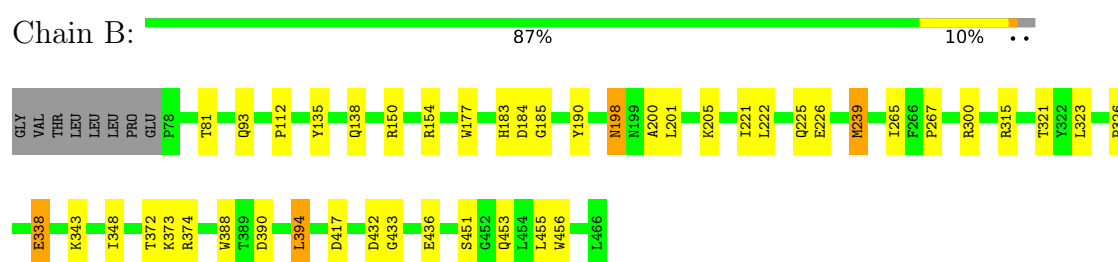
3 Residue-property plots [i](#)

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 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.

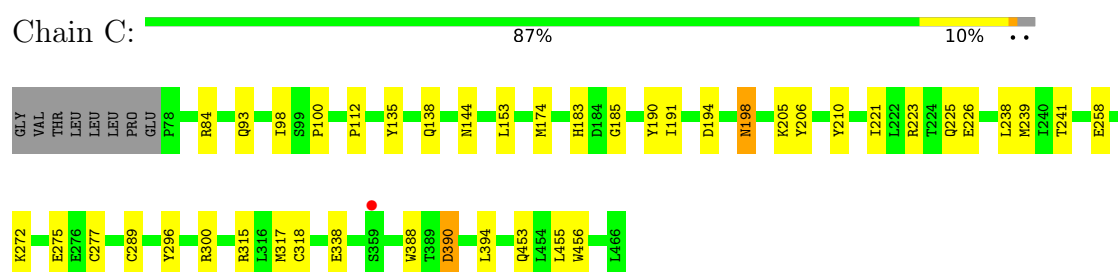
- Molecule 1: Neuraminidase



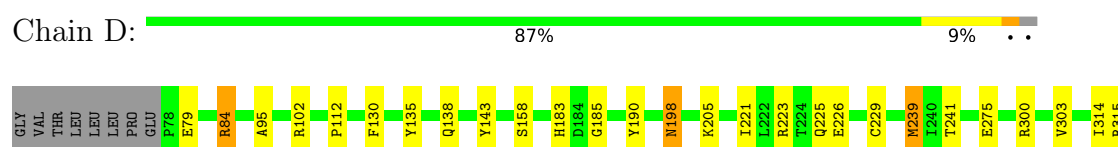
- Molecule 1: Neuraminidase

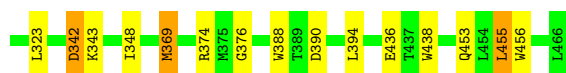


- Molecule 1: Neuraminidase



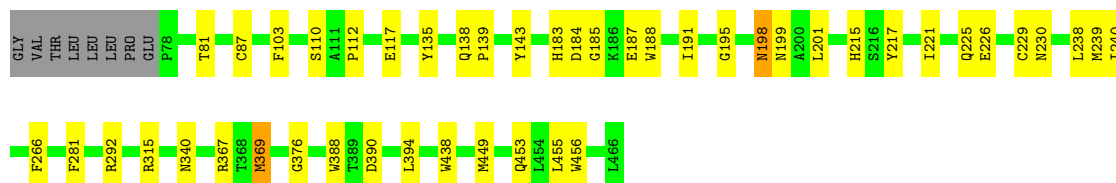
- Molecule 1: Neuraminidase





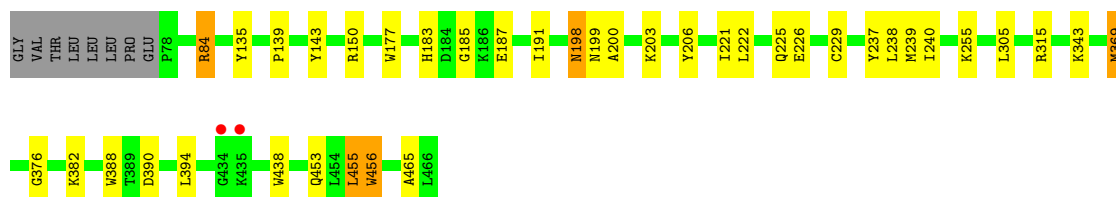
• Molecule 1: Neuraminidase

Chain E: 86% 11% ..



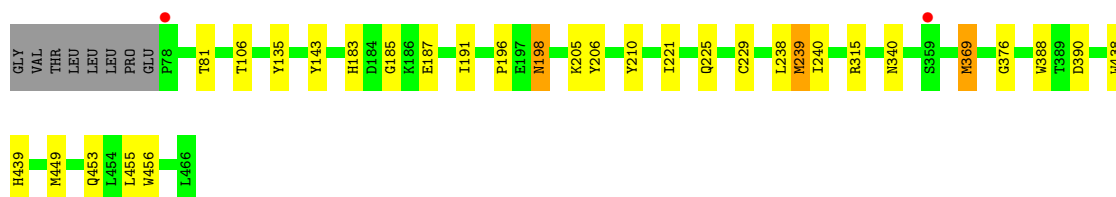
• Molecule 1: Neuraminidase

Chain F: 88% 9% ..



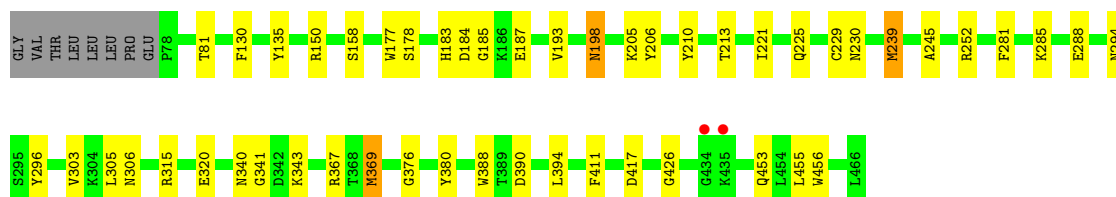
• Molecule 1: Neuraminidase

Chain G: 90% 7% ..



• Molecule 1: Neuraminidase

Chain H: 85% 12% ..



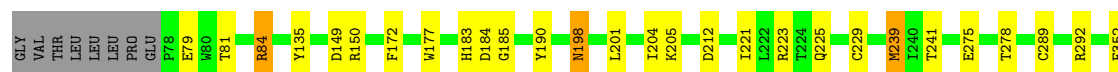
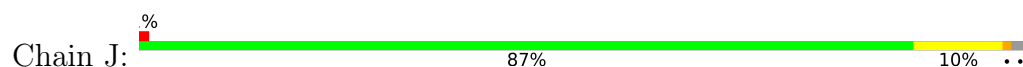
• Molecule 1: Neuraminidase

Chain I: 85% 12% ..

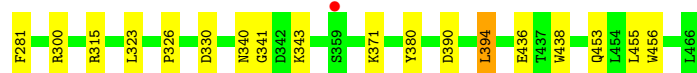
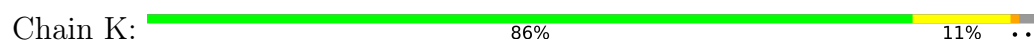




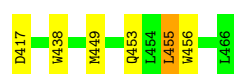
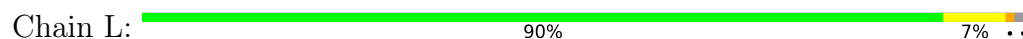
● Molecule 1: Neuraminidase



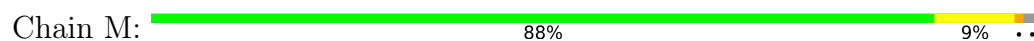
● Molecule 1: Neuraminidase



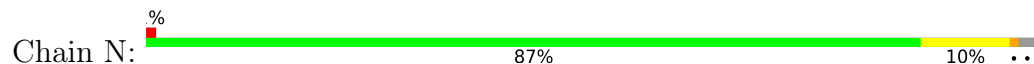
● Molecule 1: Neuraminidase

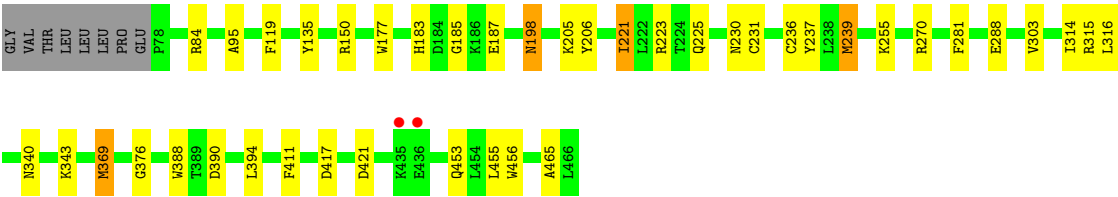


● Molecule 1: Neuraminidase

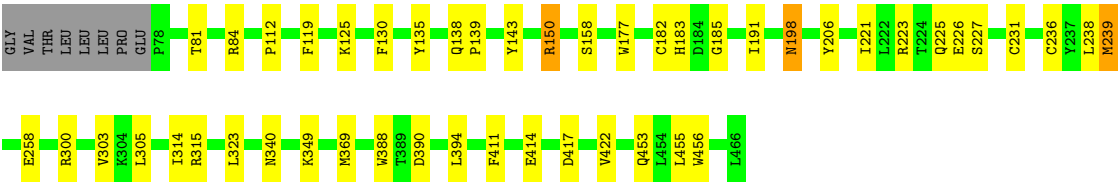
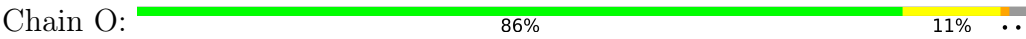


● Molecule 1: Neuraminidase

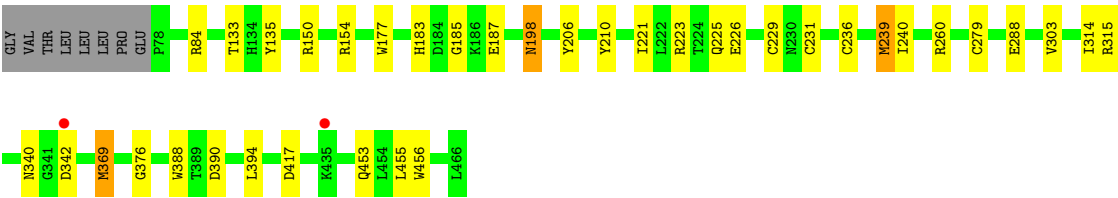
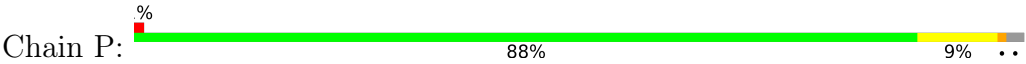




• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	111.16Å 123.68Å 123.79Å 90.04° 90.19° 90.19°	Depositor
Resolution (Å)	61.78 – 2.19 30.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.2 (61.78-2.19) 93.4 (30.81-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.220 0.213 , 0.222	Depositor DCC
R_{free} test set	15932 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 5.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.218 for h,l,-k 0.218 for h,-l,k 0.467 for h,-k,-l 0.458 for -h,k,-l 0.457 for -h,-k,l 0.217 for -h,l,k 0.218 for -h,-l,-k	Xtriage
Reported twinning fraction	0.415 for H, K, L 0.049 for -H, -L, -K 0.137 for -H, K, -L 0.096 for -h,-k,l 0.226 for h,-k,-l 0.076 for -H, L, K	Depositor
Outliers	0 of 316771 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	50572	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 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG, SO4, YT3, CA

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	0.83	3/3149 (0.1%)	0.78	4/4249 (0.1%)
1	B	0.84	2/3149 (0.1%)	0.80	3/4249 (0.1%)
1	C	0.84	2/3149 (0.1%)	0.79	4/4249 (0.1%)
1	D	0.82	2/3149 (0.1%)	0.79	5/4249 (0.1%)
1	E	0.81	2/3149 (0.1%)	0.84	6/4249 (0.1%)
1	F	0.83	2/3149 (0.1%)	0.76	1/4249 (0.0%)
1	G	0.80	0/3149	0.78	2/4249 (0.0%)
1	H	0.83	3/3149 (0.1%)	0.78	5/4249 (0.1%)
1	I	0.86	3/3149 (0.1%)	0.81	4/4249 (0.1%)
1	J	0.84	3/3149 (0.1%)	0.79	6/4249 (0.1%)
1	K	0.91	2/3149 (0.1%)	0.83	6/4249 (0.1%)
1	L	0.85	3/3149 (0.1%)	0.79	3/4249 (0.1%)
1	M	0.85	3/3149 (0.1%)	0.82	6/4249 (0.1%)
1	N	0.84	3/3149 (0.1%)	0.79	5/4249 (0.1%)
1	O	0.84	3/3149 (0.1%)	0.78	4/4249 (0.1%)
1	P	0.83	3/3149 (0.1%)	0.77	4/4249 (0.1%)
All	All	0.84	39/50384 (0.1%)	0.79	68/67984 (0.1%)

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	A	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	N	0	1
1	O	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
All	All	0	8

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	453[A]	GLN	CB-CG	-15.08	1.11	1.52
1	K	453[B]	GLN	CB-CG	-15.08	1.11	1.52
1	L	453[A]	GLN	CB-CG	-11.09	1.22	1.52
1	L	453[B]	GLN	CB-CG	-11.09	1.22	1.52
1	N	453[A]	GLN	CB-CG	-10.44	1.24	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	453[A]	GLN	CA-CB-CG	13.80	143.76	113.40
1	E	453[B]	GLN	CA-CB-CG	13.80	143.76	113.40
1	M	453[A]	GLN	CA-CB-CG	12.00	139.81	113.40
1	M	453[B]	GLN	CA-CB-CG	12.00	139.81	113.40
1	K	453[A]	GLN	CA-CB-CG	11.97	139.73	113.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	ASN	Peptide
1	E	340	ASN	Peptide
1	G	340	ASN	Peptide
1	H	340	ASN	Peptide
1	I	340	ASN	Peptide

5.2 Too-close contacts [i](#)

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	3058	0	2976	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3058	0	2976	62	0
1	C	3058	0	2976	25	0
1	D	3058	0	2976	25	2
1	E	3058	0	2976	27	0
1	F	3058	0	2976	28	0
1	G	3058	0	2976	22	0
1	H	3058	0	2976	25	0
1	I	3058	0	2976	61	0
1	J	3058	0	2976	30	0
1	K	3058	0	2976	27	2
1	L	3058	0	2976	20	0
1	M	3058	0	2976	22	0
1	N	3058	0	2976	30	0
1	O	3058	0	2976	23	0
1	P	3058	0	2976	21	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	0	0
2	K	14	0	13	0	0
2	L	14	0	13	0	0
2	M	14	0	13	1	0
2	N	14	0	13	0	0
2	O	14	0	13	0	0
2	P	14	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
4	K	5	0	0	0	0
4	L	5	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	O	5	0	0	0	0
4	P	5	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	2	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
6	A	99	0	0	1	0
6	B	100	0	0	1	0
6	C	96	0	0	1	0
6	D	91	0	0	3	0
6	E	77	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	72	0	0	3	0
6	G	69	0	0	4	0
6	H	67	0	0	2	0
6	I	84	0	0	1	0
6	J	86	0	0	7	0
6	K	106	0	0	4	0
6	L	85	0	0	0	0
6	M	78	0	0	2	0
6	N	62	0	0	2	0
6	O	67	0	0	0	0
6	P	65	0	0	2	0
All	All	50572	0	47824	405	2

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.

The worst 5 of 405 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:G:81[B]:THR:CG2	6:G:580:HOH:O	1.64	1.30
1:G:81[B]:THR:HG23	6:G:580:HOH:O	1.21	1.17
1:B:436:GLU:O	1:I:343:LYS:NZ	1.90	1.05
1:I:225:GLN:HE21	1:I:239:MET:H	1.05	1.00
1:J:225:GLN:HE21	1:J:239:MET:H	1.08	1.00

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:LYS:NZ	1:K:436:GLU:O[1_545]	1.90	0.30
1:D:436:GLU:O	1:K:343:LYS:NZ[1_545]	2.06	0.14

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	395/397 (100%)	378 (96%)	16 (4%)	1 (0%)	41	46
1	B	395/397 (100%)	382 (97%)	12 (3%)	1 (0%)	41	46
1	C	395/397 (100%)	377 (95%)	18 (5%)	0	100	100
1	D	395/397 (100%)	379 (96%)	16 (4%)	0	100	100
1	E	395/397 (100%)	379 (96%)	14 (4%)	2 (0%)	29	31
1	F	395/397 (100%)	379 (96%)	14 (4%)	2 (0%)	29	31
1	G	395/397 (100%)	377 (95%)	17 (4%)	1 (0%)	41	46
1	H	395/397 (100%)	379 (96%)	15 (4%)	1 (0%)	41	46
1	I	395/397 (100%)	383 (97%)	12 (3%)	0	100	100
1	J	395/397 (100%)	377 (95%)	17 (4%)	1 (0%)	41	46
1	K	395/397 (100%)	378 (96%)	17 (4%)	0	100	100
1	L	395/397 (100%)	381 (96%)	13 (3%)	1 (0%)	41	46
1	M	395/397 (100%)	380 (96%)	14 (4%)	1 (0%)	41	46
1	N	395/397 (100%)	379 (96%)	15 (4%)	1 (0%)	41	46
1	O	395/397 (100%)	379 (96%)	16 (4%)	0	100	100
1	P	395/397 (100%)	378 (96%)	17 (4%)	0	100	100
All	All	6320/6352 (100%)	6065 (96%)	243 (4%)	12 (0%)	47	55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	199	ASN
1	F	199	ASN
1	A	358	ALA
1	J	358	ALA
1	B	221	ILE

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	330/329 (100%)	324 (98%)	6 (2%)	59	72
1	B	330/329 (100%)	320 (97%)	10 (3%)	41	53
1	C	330/329 (100%)	322 (98%)	8 (2%)	49	62
1	D	330/329 (100%)	321 (97%)	9 (3%)	44	57
1	E	330/329 (100%)	322 (98%)	8 (2%)	49	62
1	F	330/329 (100%)	320 (97%)	10 (3%)	41	53
1	G	330/329 (100%)	322 (98%)	8 (2%)	49	62
1	H	330/329 (100%)	319 (97%)	11 (3%)	38	49
1	I	330/329 (100%)	321 (97%)	9 (3%)	44	57
1	J	330/329 (100%)	321 (97%)	9 (3%)	44	57
1	K	330/329 (100%)	321 (97%)	9 (3%)	44	57
1	L	330/329 (100%)	321 (97%)	9 (3%)	44	57
1	M	330/329 (100%)	321 (97%)	9 (3%)	44	57
1	N	330/329 (100%)	322 (98%)	8 (2%)	49	62
1	O	330/329 (100%)	319 (97%)	11 (3%)	38	49
1	P	330/329 (100%)	320 (97%)	10 (3%)	41	53
All	All	5280/5264 (100%)	5136 (97%)	144 (3%)	43	57

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	135	TYR
1	P	456	TRP
1	N	390	ASP
1	O	390	ASP
1	F	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	225	GLN
1	O	225	GLN
1	J	198	ASN
1	O	198	ASN
1	P	225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 68 ligands modelled in this entry, 36 are monoatomic - leaving 32 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	C	900	1	14,14,15	0.57	0	17,19,21	1.64	2 (11%)
4	SO4	D	1001	5	4,4,4	0.44	0	6,6,6	0.70	0
4	SO4	B	1001	5	4,4,4	0.41	0	6,6,6	0.75	0
4	SO4	L	1001	5	4,4,4	0.43	0	6,6,6	0.78	0
4	SO4	C	1001	5	4,4,4	0.32	0	6,6,6	0.67	0
4	SO4	G	1001	5	4,4,4	0.29	0	6,6,6	0.63	0
2	NAG	M	900	1	14,14,15	0.65	0	17,19,21	1.56	3 (17%)
2	NAG	P	900	1	14,14,15	0.63	0	17,19,21	1.87	4 (23%)
2	NAG	D	900	1	14,14,15	0.52	0	17,19,21	1.77	3 (17%)
4	SO4	E	1001	5	4,4,4	0.35	0	6,6,6	0.67	0
4	SO4	A	1001	5	4,4,4	0.27	0	6,6,6	0.52	0
4	SO4	N	1001	5	4,4,4	0.19	0	6,6,6	0.49	0
4	SO4	M	1001	5	4,4,4	0.29	0	6,6,6	0.72	0
2	NAG	O	900	1	14,14,15	0.66	0	17,19,21	1.44	2 (11%)
2	NAG	B	900	1	14,14,15	0.54	0	17,19,21	1.89	3 (17%)
2	NAG	L	900	1	14,14,15	0.72	0	17,19,21	2.16	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	K	1001	5	4,4,4	0.62	0	6,6,6	0.72	0
2	NAG	J	900	1	14,14,15	0.57	0	17,19,21	1.86	3 (17%)
2	NAG	G	900	1	14,14,15	0.59	0	17,19,21	1.53	3 (17%)
4	SO4	I	1001	5	4,4,4	0.35	0	6,6,6	0.43	0
4	SO4	P	1001	5	4,4,4	0.30	0	6,6,6	0.63	0
4	SO4	H	1001	5	4,4,4	0.29	0	6,6,6	0.49	0
2	NAG	E	900	1	14,14,15	0.55	0	17,19,21	2.03	2 (11%)
4	SO4	O	1001	5	4,4,4	0.31	0	6,6,6	0.42	0
2	NAG	I	900	1	14,14,15	0.66	0	17,19,21	1.50	4 (23%)
2	NAG	F	900	1	14,14,15	0.75	0	17,19,21	1.51	2 (11%)
2	NAG	H	900	1	14,14,15	0.68	0	17,19,21	1.68	2 (11%)
4	SO4	J	1001	5	4,4,4	0.62	0	6,6,6	0.68	0
2	NAG	K	900	1	14,14,15	0.90	1 (7%)	17,19,21	2.17	6 (35%)
4	SO4	F	1001	5	4,4,4	0.24	0	6,6,6	0.63	0
2	NAG	A	900	1	14,14,15	0.77	0	17,19,21	2.03	2 (11%)
2	NAG	N	900	1	14,14,15	0.90	1 (7%)	17,19,21	1.83	2 (11%)

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	C	900	1	-	2/6/23/26	0/1/1/1
2	NAG	H	900	1	-	1/6/23/26	0/1/1/1
2	NAG	N	900	1	-	2/6/23/26	0/1/1/1
2	NAG	B	900	1	-	2/6/23/26	0/1/1/1
2	NAG	K	900	1	-	2/6/23/26	0/1/1/1
2	NAG	E	900	1	-	2/6/23/26	0/1/1/1
2	NAG	L	900	1	-	2/6/23/26	0/1/1/1
2	NAG	O	900	1	-	2/6/23/26	0/1/1/1
2	NAG	I	900	1	-	1/6/23/26	0/1/1/1
2	NAG	A	900	1	-	2/6/23/26	0/1/1/1
2	NAG	M	900	1	-	2/6/23/26	0/1/1/1
2	NAG	P	900	1	-	2/6/23/26	0/1/1/1
2	NAG	J	900	1	-	2/6/23/26	0/1/1/1
2	NAG	D	900	1	-	1/6/23/26	0/1/1/1
2	NAG	G	900	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	900	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	K	900	NAG	C1-C2	2.33	1.55	1.52
2	N	900	NAG	C1-C2	2.23	1.55	1.52

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	900	NAG	C1-C2-N2	-6.10	100.07	110.49
2	A	900	NAG	C1-C2-N2	-6.00	100.24	110.49
2	E	900	NAG	C1-O5-C5	5.55	119.71	112.19
2	K	900	NAG	C1-C2-N2	-5.54	101.03	110.49
2	H	900	NAG	C1-O5-C5	5.49	119.62	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	900	NAG	O5-C5-C6-O6
2	M	900	NAG	O5-C5-C6-O6
2	G	900	NAG	O5-C5-C6-O6
2	J	900	NAG	O5-C5-C6-O6
2	L	900	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	900	NAG	1	0

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	389/397 (97%)	-0.30	2 (0%) 91 90	15, 21, 27, 31	3 (0%)
1	B	389/397 (97%)	-0.29	0 100 100	16, 21, 26, 32	3 (0%)
1	C	389/397 (97%)	-0.27	1 (0%) 94 93	16, 21, 28, 34	3 (0%)
1	D	389/397 (97%)	-0.30	0 100 100	16, 21, 26, 31	3 (0%)
1	E	389/397 (97%)	-0.24	0 100 100	17, 22, 28, 32	3 (0%)
1	F	389/397 (97%)	-0.22	2 (0%) 91 90	17, 22, 29, 34	3 (0%)
1	G	389/397 (97%)	-0.25	2 (0%) 91 90	16, 22, 28, 33	3 (0%)
1	H	389/397 (97%)	-0.20	2 (0%) 91 90	16, 22, 29, 34	3 (0%)
1	I	389/397 (97%)	-0.31	1 (0%) 94 93	15, 20, 25, 31	3 (0%)
1	J	389/397 (97%)	-0.26	2 (0%) 91 90	15, 21, 29, 34	3 (0%)
1	K	389/397 (97%)	-0.29	1 (0%) 94 93	16, 20, 26, 30	3 (0%)
1	L	389/397 (97%)	-0.26	1 (0%) 94 93	16, 22, 28, 34	3 (0%)
1	M	389/397 (97%)	-0.26	0 100 100	16, 21, 27, 31	3 (0%)
1	N	389/397 (97%)	-0.21	2 (0%) 91 90	17, 23, 30, 35	3 (0%)
1	O	389/397 (97%)	-0.26	0 100 100	16, 22, 28, 32	3 (0%)
1	P	389/397 (97%)	-0.23	2 (0%) 91 90	17, 23, 30, 35	3 (0%)
All	All	6224/6352 (97%)	-0.26	18 (0%) 94 93	15, 21, 28, 35	48 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	359	SER	3.7
1	F	434	GLY	3.4
1	F	435	LYS	3.2
1	P	435	LYS	2.9
1	A	359	SER	2.9

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](#)

There are no monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	NAG	E	900	14/15	0.83	0.19	17,18,21,21	0
2	NAG	O	900	14/15	0.83	0.20	16,18,19,21	0
2	NAG	L	900	14/15	0.84	0.21	14,18,19,21	0
2	NAG	N	900	14/15	0.84	0.24	17,18,19,19	0
2	NAG	D	900	14/15	0.84	0.23	17,18,20,21	0
2	NAG	K	900	14/15	0.85	0.25	17,19,21,22	0
2	NAG	F	900	14/15	0.85	0.24	17,19,19,20	0
2	NAG	C	900	14/15	0.86	0.20	15,18,19,20	0
2	NAG	H	900	14/15	0.86	0.26	17,19,20,23	0
2	NAG	P	900	14/15	0.86	0.20	18,18,19,21	0
2	NAG	G	900	14/15	0.87	0.17	16,18,20,23	0
2	NAG	M	900	14/15	0.88	0.19	16,18,19,22	0
2	NAG	J	900	14/15	0.88	0.19	16,18,19,22	0
2	NAG	A	900	14/15	0.88	0.16	14,18,19,22	0
2	NAG	I	900	14/15	0.88	0.23	17,18,20,20	0
2	NAG	B	900	14/15	0.89	0.22	16,18,19,19	0
3	CA	O	1000	1/1	0.92	0.16	24,24,24,24	0
3	CA	N	1000	1/1	0.93	0.18	23,23,23,23	0
3	CA	J	1000	1/1	0.94	0.11	23,23,23,23	0
3	CA	F	1000	1/1	0.94	0.10	20,20,20,20	0
3	CA	I	1000	1/1	0.94	0.12	24,24,24,24	0
3	CA	M	1000	1/1	0.95	0.16	24,24,24,24	0
3	CA	H	1000	1/1	0.95	0.14	23,23,23,23	0
3	CA	K	1000	1/1	0.95	0.14	23,23,23,23	0
3	CA	C	1000	1/1	0.96	0.22	24,24,24,24	0
3	CA	E	1000	1/1	0.97	0.14	22,22,22,22	0
3	CA	G	1000	1/1	0.97	0.12	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	L	1000	1/1	0.97	0.11	22,22,22,22	0
3	CA	P	1000	1/1	0.97	0.12	21,21,21,21	0
3	CA	A	1000	1/1	0.98	0.13	19,19,19,19	0
3	CA	D	1000	1/1	0.98	0.10	21,21,21,21	0
4	SO4	B	1001	5/5	0.98	0.10	12,15,17,18	0
4	SO4	D	1001	5/5	0.98	0.10	14,15,16,19	0
4	SO4	E	1001	5/5	0.98	0.08	14,14,15,16	0
4	SO4	F	1001	5/5	0.98	0.12	13,15,16,17	0
4	SO4	H	1001	5/5	0.98	0.10	13,14,15,16	0
4	SO4	J	1001	5/5	0.98	0.08	14,14,16,16	0
4	SO4	K	1001	5/5	0.98	0.08	11,15,16,18	0
4	SO4	L	1001	5/5	0.98	0.10	13,14,17,18	0
4	SO4	M	1001	5/5	0.98	0.11	14,15,15,16	0
4	SO4	P	1001	5/5	0.98	0.15	15,16,17,17	0
5	YT3	A	1	1/1	0.98	0.03	18,18,18,18	0
5	YT3	E	2	1/1	0.98	0.03	21,21,21,21	0
4	SO4	G	1001	5/5	0.99	0.08	13,14,15,15	0
4	SO4	A	1001	5/5	0.99	0.06	14,14,14,15	0
4	SO4	N	1001	5/5	0.99	0.09	15,15,17,18	0
4	SO4	O	1001	5/5	0.99	0.12	14,16,17,18	0
4	SO4	I	1001	5/5	0.99	0.06	12,16,18,18	0
5	YT3	A	1002	1/1	0.99	0.02	13,13,13,13	1
3	CA	B	1000	1/1	0.99	0.09	22,22,22,22	0
5	YT3	C	1002	1/1	0.99	0.04	15,15,15,15	1
5	YT3	D	1002	1/1	0.99	0.02	14,14,14,14	1
4	SO4	C	1001	5/5	0.99	0.09	15,15,16,16	0
5	YT3	E	1002	1/1	0.99	0.03	15,15,15,15	1
5	YT3	G	1002	1/1	0.99	0.03	15,15,15,15	1
5	YT3	H	1002	1/1	0.99	0.03	16,16,16,16	1
5	YT3	I	3	1/1	0.99	0.02	19,19,19,19	0
5	YT3	I	1002	1/1	0.99	0.02	15,15,15,15	1
5	YT3	J	1002	1/1	0.99	0.03	15,15,15,15	1
5	YT3	K	1002	1/1	0.99	0.02	15,15,15,15	1
5	YT3	L	1002	1/1	0.99	0.02	15,15,15,15	1
5	YT3	N	4	1/1	0.99	0.03	20,20,20,20	0
5	YT3	N	1002	1/1	0.99	0.03	16,16,16,16	1
5	YT3	O	1002	1/1	0.99	0.02	14,14,14,14	1
5	YT3	P	1002	1/1	0.99	0.03	17,17,17,17	1
5	YT3	B	1002	1/1	1.00	0.01	15,15,15,15	1
5	YT3	M	1002	1/1	1.00	0.02	17,17,17,17	1
5	YT3	F	1002	1/1	1.00	0.02	16,16,16,16	1

6.5 Other polymers [i](#)

There are no such residues in this entry.