



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2018 – 01:19 AM EDT

PDB ID : 6HG5
Title : Influenza A virus N6 neuraminidase complex with Oseltamivir (Duck/England/56).
Authors : Salinger, M.T.; Hobbs, J.R.; Murray, J.W.; Laver, W.G.; Kuhn, P.; Garman, E.F.
Deposited on : 2018-08-22
Resolution : 1.60 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

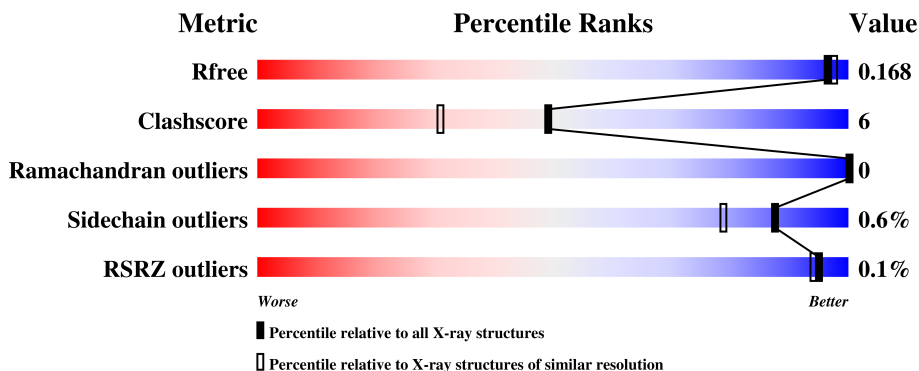
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	111664	2957 (1.60-1.60)
Clashscore	122126	3202 (1.60-1.60)
Ramachandran outliers	120053	3117 (1.60-1.60)
Sidechain outliers	120020	3116 (1.60-1.60)
RSRZ outliers	108989	2883 (1.60-1.60)

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. 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	389	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	B	389	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	389	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	D	389	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>

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
8	CO2	D	514	-	-	X	-

2 Entry composition [i](#)

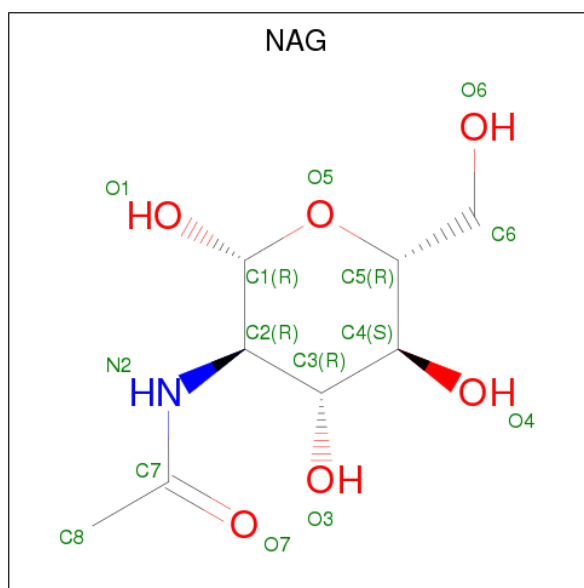
There are 9 unique types of molecules in this entry. The entry contains 15100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	22	0
			3189	1980	570	605	34			
1	B	389	Total	C	N	O	S	0	23	0
			3195	1988	568	606	33			
1	C	389	Total	C	N	O	S	0	19	0
			3135	1956	556	593	30			
1	D	389	Total	C	N	O	S	0	18	0
			3148	1961	561	594	32			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



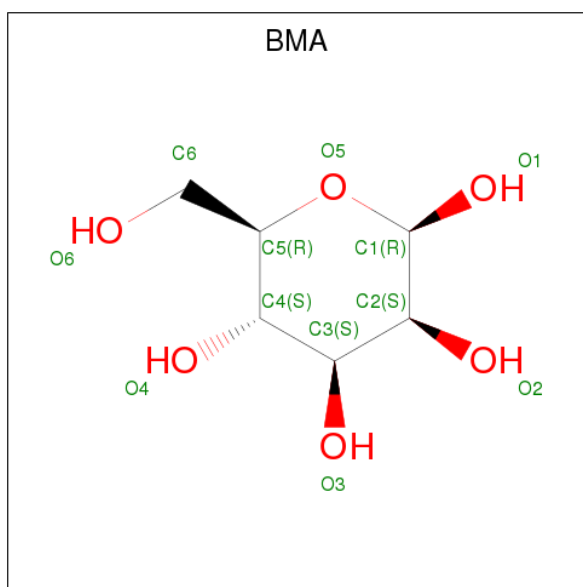
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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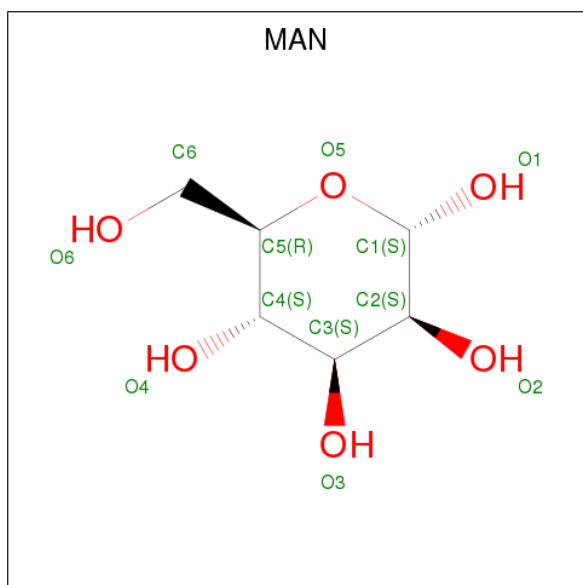
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



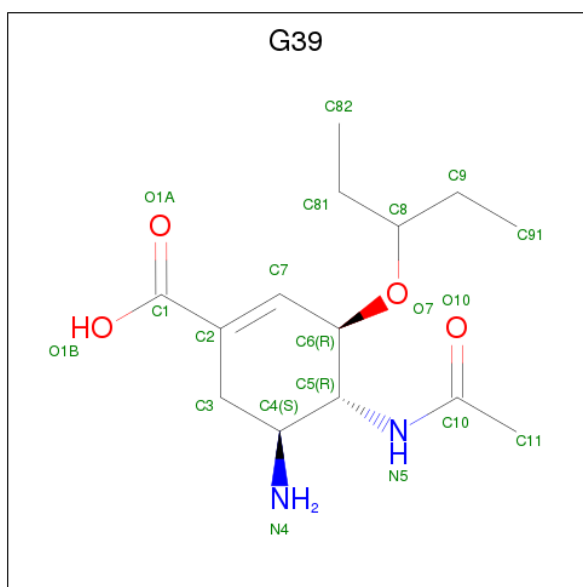
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



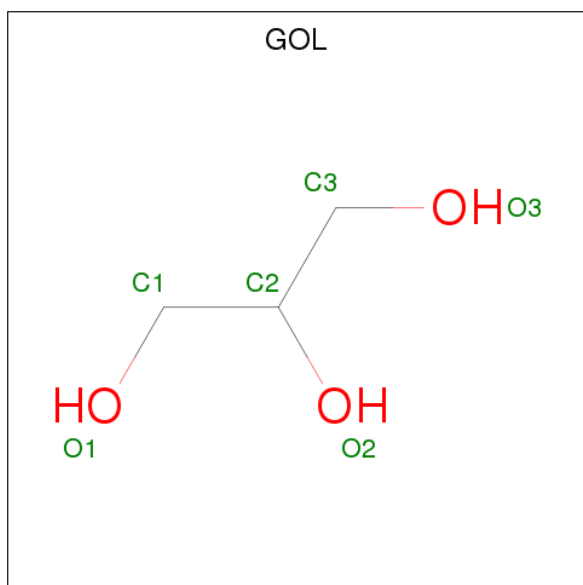
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (three-letter code: G39) (formula: C₁₄H₂₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	14	2	4		
5	B	1	Total	C	N	O	0	0
			20	14	2	4		
5	C	1	Total	C	N	O	0	0
			20	14	2	4		
5	D	1	Total	C	N	O	0	0
			20	14	2	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

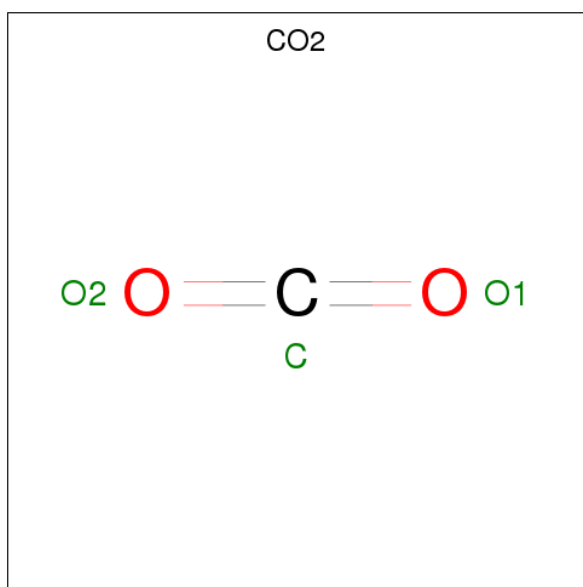


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			3	1	2		

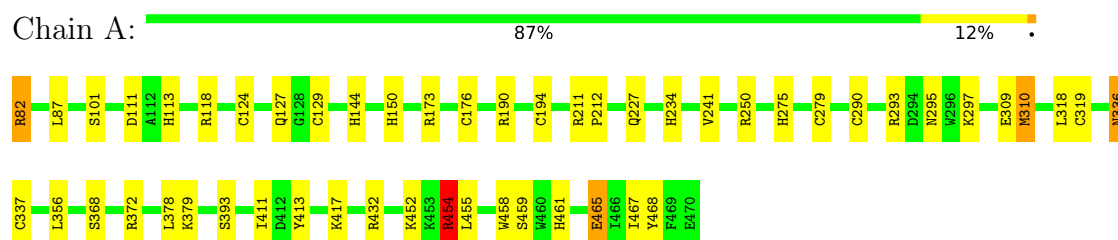
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	454	Total	O	0	0
			454	454		
9	B	466	Total	O	0	0
			466	466		
9	C	463	Total	O	0	0
			463	463		
9	D	444	Total	O	0	1
			445	445		

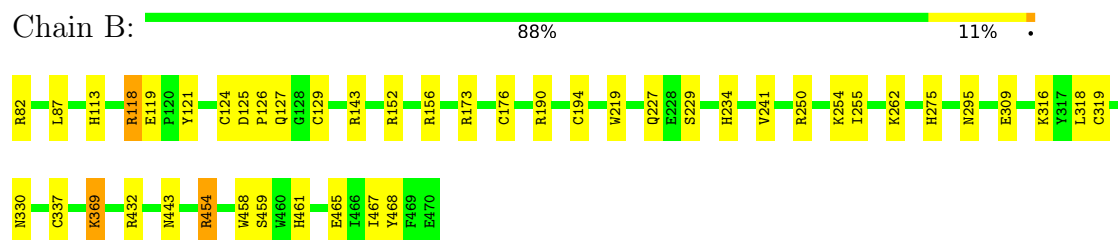
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

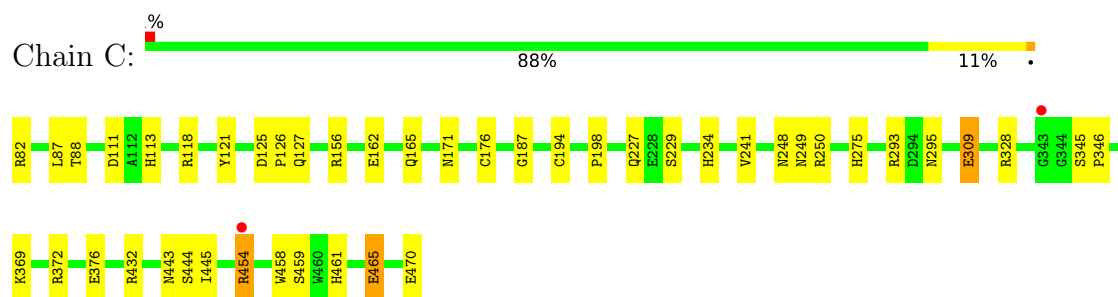
• Molecule 1: Neuraminidase



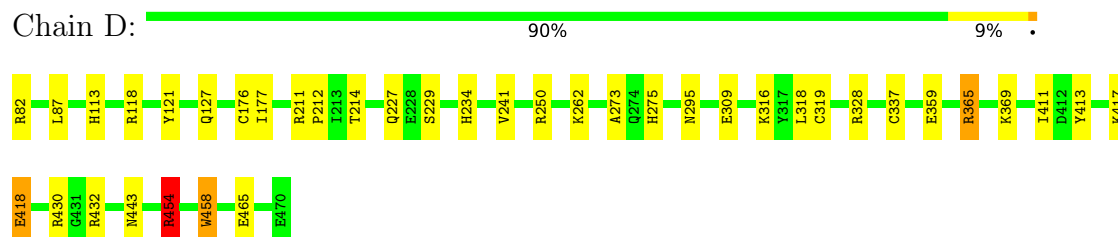
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.21Å 75.18Å 106.39Å 90.00° 90.52° 90.00°	Depositor
Resolution (Å)	61.47 – 1.60 61.40 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (61.47-1.60) 97.8 (61.40-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.133 , 0.158 0.146 , 0.168	Depositor DCC
R_{free} test set	10772 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	9.0	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,k,-h 0.013 for h,-k,-l 0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15100	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CO2, NAG, G39, CA, BMA, 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	0.86	4/3266 (0.1%)	1.00	12/4427 (0.3%)
1	B	0.90	4/3275 (0.1%)	1.01	10/4437 (0.2%)
1	C	0.92	6/3231 (0.2%)	1.02	10/4381 (0.2%)
1	D	0.93	6/3234 (0.2%)	1.02	7/4383 (0.2%)
All	All	0.91	20/13006 (0.2%)	1.01	39/17628 (0.2%)

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	3
1	B	0	2
1	C	0	2
1	D	0	4
All	All	0	11

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369[A]	LYS	C-O	-8.68	1.06	1.23
1	B	369[B]	LYS	C-O	-8.68	1.06	1.23
1	B	369[C]	LYS	C-O	-8.68	1.06	1.23
1	C	162	GLU	CD-OE1	7.44	1.33	1.25
1	B	119	GLU	CD-OE1	6.49	1.32	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	D	250	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	C	156	ARG	NE-CZ-NH2	8.57	124.58	120.30
1	C	156	ARG	NE-CZ-NH1	-8.27	116.17	120.30
1	B	152	ARG	NE-CZ-NH2	-8.16	116.22	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	ARG	Sidechain
1	A	454	ARG	Sidechain
1	A	82[A]	ARG	Sidechain
1	B	432	ARG	Sidechain
1	B	454	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	3189	0	3046	51	0
1	B	3195	0	3065	33	0
1	C	3135	0	3034	47	0
1	D	3148	0	3024	33	0
2	A	70	0	62	0	0
2	B	56	0	49	4	0
2	C	70	0	62	2	0
2	D	70	0	62	1	0
3	A	11	0	8	0	0
3	B	11	0	8	0	0
3	C	11	0	9	0	0
3	D	11	0	9	0	0
4	A	44	0	38	0	0
4	B	44	0	38	2	0
4	C	33	0	28	0	0
4	D	33	0	28	0	0
5	A	20	0	23	0	0
5	B	20	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	20	0	23	0	0
5	D	20	0	23	0	0
6	A	6	0	8	0	0
6	B	24	0	32	3	0
6	C	12	0	16	0	0
6	D	12	0	16	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	D	3	0	0	4	0
9	A	454	0	0	9	0
9	B	466	0	0	12	0
9	C	463	0	0	18	0
9	D	445	0	0	7	0
All	All	15100	0	12734	167	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 6.

The worst 5 of 167 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:B:319:CYS:SG	1:B:337[B]:CYS:HB3	1.77	1.23
9:A:748:HOH:O	1:C:454[A]:ARG:HD2	1.38	1.18
1:D:82:ARG:NH2	1:D:127:GLN:HE22	1.44	1.13
1:C:369[B]:LYS:HD3	9:C:814:HOH:O	1.47	1.12
1:D:319:CYS:SG	1:D:337[C]:CYS:HB3	1.93	1.08

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	409/389 (105%)	393 (96%)	16 (4%)	0	100	100
1	B	412/389 (106%)	401 (97%)	11 (3%)	0	100	100
1	C	406/389 (104%)	391 (96%)	15 (4%)	0	100	100
1	D	405/389 (104%)	391 (96%)	14 (4%)	0	100	100
All	All	1632/1556 (105%)	1576 (97%)	56 (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	354/331 (107%)	349 (99%)	5 (1%)	69	50
1	B	356/331 (108%)	354 (99%)	2 (1%)	87	79
1	C	350/331 (106%)	349 (100%)	1 (0%)	93	88
1	D	349/331 (105%)	345 (99%)	4 (1%)	76	60
All	All	1409/1324 (106%)	1397 (99%)	12 (1%)	87	68

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458[A]	TRP
1	B	458[B]	TRP
1	D	454	ARG
1	A	458[B]	TRP
1	D	418	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	402	ASN
1	C	165	GLN
1	D	275	HIS

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Mol	Chain	Res	Type
1	B	416	ASN
1	B	443	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 55 ligands modelled in this entry, 4 are monoatomic - leaving 51 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	501	1	14,14,15	1.27	1 (7%)	17,19,21	1.42	2 (11%)
2	NAG	A	502	1,2	14,14,15	1.13	0	17,19,21	1.21	1 (5%)
2	NAG	A	503	2	14,14,15	0.77	0	17,19,21	1.91	4 (23%)
2	NAG	A	504	1,2	14,14,15	1.65	1 (7%)	17,19,21	2.68	4 (23%)
2	NAG	A	505	3,2	14,14,15	0.66	0	17,19,21	1.76	5 (29%)
3	BMA	A	506	2,4	11,11,12	1.07	0	15,15,17	1.55	2 (13%)
4	MAN	A	507	3	11,11,12	2.02	3 (27%)	15,15,17	1.70	4 (26%)
4	MAN	A	508	3,4	11,11,12	2.07	3 (27%)	15,15,17	1.24	2 (13%)
4	MAN	A	509	4	11,11,12	1.42	3 (27%)	15,15,17	2.37	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	510	4	11,11,12	0.91	0	15,15,17	1.49	3 (20%)
5	G39	A	511	-	15,20,20	0.50	0	14,27,27	1.02	1 (7%)
6	GOL	A	512	-	5,5,5	0.54	0	5,5,5	1.08	0
2	NAG	B	501	1,2	14,14,15	1.32	2 (14%)	17,19,21	1.18	1 (5%)
2	NAG	B	502	2	14,14,15	0.94	0	17,19,21	1.54	4 (23%)
2	NAG	B	503	1,2	14,14,15	1.45	3 (21%)	17,19,21	3.03	7 (41%)
2	NAG	B	504	3,2	14,14,15	1.66	3 (21%)	17,19,21	2.11	7 (41%)
3	BMA	B	505	2,4	11,11,12	0.81	0	15,15,17	1.73	4 (26%)
4	MAN	B	506	3,4	11,11,12	1.82	2 (18%)	15,15,17	2.04	4 (26%)
4	MAN	B	507	4	11,11,12	2.72	3 (27%)	15,15,17	2.14	7 (46%)
4	MAN	B	508	4	11,11,12	1.04	1 (9%)	15,15,17	1.41	3 (20%)
4	MAN	B	509	3	11,11,12	1.14	1 (9%)	15,15,17	2.44	4 (26%)
5	G39	B	510	-	15,20,20	0.46	0	14,27,27	0.80	0
6	GOL	B	511	-	5,5,5	0.48	0	5,5,5	1.02	1 (20%)
6	GOL	B	512	-	5,5,5	0.82	0	5,5,5	1.01	0
6	GOL	B	513	-	5,5,5	0.61	0	5,5,5	0.67	0
6	GOL	B	514	-	5,5,5	0.30	0	5,5,5	0.63	0
2	NAG	C	501	1	14,14,15	1.29	3 (21%)	17,19,21	2.01	4 (23%)
2	NAG	C	502	1,2	14,14,15	1.37	3 (21%)	17,19,21	1.74	3 (17%)
2	NAG	C	503	2	14,14,15	1.35	2 (14%)	17,19,21	1.77	5 (29%)
2	NAG	C	504	1,2	14,14,15	1.15	1 (7%)	17,19,21	2.47	6 (35%)
2	NAG	C	505	3,2	14,14,15	1.70	3 (21%)	17,19,21	1.68	5 (29%)
3	BMA	C	506	2,4	11,11,12	0.87	0	15,15,17	2.17	6 (40%)
4	MAN	C	507	3,4	11,11,12	1.26	1 (9%)	15,15,17	1.36	1 (6%)
4	MAN	C	508	4	11,11,12	1.21	0	15,15,17	1.70	4 (26%)
4	MAN	C	509	4	11,11,12	1.49	2 (18%)	15,15,17	2.55	6 (40%)
5	G39	C	510	-	15,20,20	0.54	0	14,27,27	0.92	0
6	GOL	C	511	-	5,5,5	0.46	0	5,5,5	0.80	0
6	GOL	C	512	-	5,5,5	0.35	0	5,5,5	0.90	0
2	NAG	D	501	1	14,14,15	1.98	4 (28%)	17,19,21	1.83	6 (35%)
2	NAG	D	502	1,2	14,14,15	1.38	3 (21%)	17,19,21	1.41	2 (11%)
2	NAG	D	503	2	14,14,15	1.14	0	17,19,21	1.91	6 (35%)
2	NAG	D	504	1,2	14,14,15	1.35	2 (14%)	17,19,21	3.50	8 (47%)
2	NAG	D	505	3,2	14,14,15	1.40	4 (28%)	17,19,21	1.43	4 (23%)
3	BMA	D	506	2,4	11,11,12	1.29	1 (9%)	15,15,17	2.54	5 (33%)
4	MAN	D	507	3,4	11,11,12	1.11	1 (9%)	15,15,17	1.18	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	D	508	4	11,11,12	1.15	1 (9%)	15,15,17	2.21	4 (26%)
4	MAN	D	509	4	11,11,12	1.96	5 (45%)	15,15,17	2.11	6 (40%)
5	G39	D	510	-	15,20,20	0.63	0	14,27,27	0.93	0
6	GOL	D	511	-	5,5,5	0.65	0	5,5,5	1.50	1 (20%)
6	GOL	D	512	-	5,5,5	0.62	0	5,5,5	0.54	0
8	CO2	D	514	-	2,2,2	0.37	0	1,1,1	0.54	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	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	503	2	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	505	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	506	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	507	3	-	0/2/19/22	0/1/1/1
4	MAN	A	508	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	509	4	-	0/2/19/22	0/1/1/1
4	MAN	A	510	4	-	0/2/19/22	0/1/1/1
5	G39	A	511	-	-	0/12/32/32	0/1/1/1
6	GOL	A	512	-	-	0/4/4/4	0/0/0/0
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	504	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	505	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	506	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	507	4	-	0/2/19/22	0/1/1/1
4	MAN	B	508	4	-	0/2/19/22	0/1/1/1
4	MAN	B	509	3	-	0/2/19/22	0/1/1/1
5	G39	B	510	-	-	0/12/32/32	0/1/1/1
6	GOL	B	511	-	-	0/4/4/4	0/0/0/0
6	GOL	B	512	-	-	0/4/4/4	0/0/0/0
6	GOL	B	513	-	-	0/4/4/4	0/0/0/0
6	GOL	B	514	-	-	0/4/4/4	0/0/0/0
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	502	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	503	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	505	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	506	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	507	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	508	4	-	0/2/19/22	0/1/1/1
4	MAN	C	509	4	-	0/2/19/22	0/1/1/1
5	G39	C	510	-	-	0/12/32/32	0/1/1/1
6	GOL	C	511	-	-	0/4/4/4	0/0/0/0
6	GOL	C	512	-	-	0/4/4/4	0/0/0/0
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	502	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	503	2	-	0/6/23/26	0/1/1/1
2	NAG	D	504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	505	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	506	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	507	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	508	4	-	0/2/19/22	0/1/1/1
4	MAN	D	509	4	-	0/2/19/22	0/1/1/1
5	G39	D	510	-	-	0/12/32/32	0/1/1/1
6	GOL	D	511	-	-	0/4/4/4	0/0/0/0
6	GOL	D	512	-	-	0/4/4/4	0/0/0/0
8	CO2	D	514	-	-	0/0/0/0	0/0/0/0

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	508	MAN	O5-C1	-4.97	1.35	1.43
4	B	506	MAN	O5-C1	-4.37	1.36	1.43
2	C	502	NAG	O5-C1	-3.10	1.38	1.43
2	B	501	NAG	O5-C1	-2.82	1.39	1.43
3	D	506	BMA	C1-C2	-2.65	1.46	1.52

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	NAG	O5-C1-C2	-11.24	96.00	111.52
2	A	504	NAG	O5-C1-C2	-9.09	98.98	111.52
2	B	503	NAG	O5-C1-C2	-7.45	101.24	111.52
2	C	504	NAG	O5-C1-C2	-6.67	102.32	111.52
3	D	506	BMA	O5-C5-C6	-6.42	96.98	107.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	NAG	4	0
2	B	504	NAG	1	0
4	B	509	MAN	2	0
6	B	513	GOL	1	0
6	B	514	GOL	2	0
2	C	501	NAG	2	0
2	D	501	NAG	1	0
6	D	511	GOL	1	0
8	D	514	CO2	4	0

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 [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, 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	389/389 (100%)	-0.56	0 100 100	5, 10, 18, 28	0
1	B	389/389 (100%)	-0.57	0 100 100	5, 9, 16, 30	0
1	C	389/389 (100%)	-0.51	2 (0%) 90 90	5, 9, 16, 27	0
1	D	389/389 (100%)	-0.58	0 100 100	5, 10, 16, 25	1 (0%)
All	All	1556/1556 (100%)	-0.55	2 (0%) 95 94	5, 9, 17, 30	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	GLY	2.3
1	C	454[A]	ARG	2.1

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 carbohydrates 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
6	GOL	B	512	6/6	0.48	0.24	40,42,46,48	0
2	NAG	D	501	14/15	0.49	0.28	36,41,45,46	0
6	GOL	B	513	6/6	0.53	0.17	43,44,45,46	0
4	MAN	B	509	11/12	0.66	0.30	38,45,47,51	0
4	MAN	D	509	11/12	0.68	0.23	33,34,38,41	0
2	NAG	C	503	14/15	0.73	0.21	34,39,41,44	0
4	MAN	C	509	11/12	0.73	0.23	34,35,39,41	0
4	MAN	C	508	11/12	0.76	0.19	32,36,38,39	0
2	NAG	D	503	14/15	0.76	0.22	33,39,49,54	0
3	BMA	D	506	11/12	0.77	0.18	26,28,30,31	0
2	NAG	A	504	14/15	0.78	0.23	22,26,33,34	0
2	NAG	B	503	14/15	0.78	0.20	23,27,36,37	0
2	NAG	A	503	14/15	0.79	0.28	36,43,50,52	0
4	MAN	A	509	11/12	0.80	0.16	24,25,29,30	0
4	MAN	D	508	11/12	0.81	0.24	34,37,39,42	0
3	BMA	C	506	11/12	0.81	0.16	27,30,32,33	0
2	NAG	B	502	14/15	0.83	0.22	33,39,49,50	0
4	MAN	B	507	11/12	0.84	0.15	25,26,29,32	0
4	MAN	A	507	11/12	0.84	0.14	25,27,29,29	0
4	MAN	D	507	11/12	0.85	0.16	29,31,32,33	0
4	MAN	B	508	11/12	0.85	0.16	21,24,25,27	0
2	NAG	C	501	14/15	0.85	0.20	28,34,41,44	0
6	GOL	B	514	6/6	0.86	0.20	33,36,38,39	0
8	CO2	D	514	3/3	0.86	0.15	26,26,29,31	3
2	NAG	A	505	14/15	0.86	0.14	18,20,22,23	0
2	NAG	C	504	14/15	0.87	0.12	20,23,29,29	0
2	NAG	C	505	14/15	0.87	0.12	20,22,25,27	0
4	MAN	C	507	11/12	0.87	0.20	30,33,35,35	0
6	GOL	D	512	6/6	0.88	0.16	17,20,20,21	0
6	GOL	D	511	6/6	0.88	0.15	23,25,28,40	0
2	NAG	D	505	14/15	0.89	0.13	19,21,25,27	0
6	GOL	C	511	6/6	0.90	0.11	17,20,22,23	0
2	NAG	D	504	14/15	0.90	0.14	19,21,25,26	0
2	NAG	B	504	14/15	0.91	0.14	19,20,23,26	0
2	NAG	A	501	14/15	0.91	0.11	20,22,27,29	0
4	MAN	A	508	11/12	0.92	0.11	19,20,22,23	0
4	MAN	B	506	11/12	0.92	0.10	22,23,24,25	0
6	GOL	B	511	6/6	0.92	0.11	16,17,18,19	0
4	MAN	A	510	11/12	0.93	0.11	19,20,21,22	0
2	NAG	B	501	14/15	0.93	0.10	15,17,22,27	0
2	NAG	A	502	14/15	0.93	0.08	16,17,24,29	0
3	BMA	A	506	11/12	0.94	0.11	19,20,21,23	0
3	BMA	B	505	11/12	0.94	0.08	22,23,26,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	C	512	6/6	0.96	0.07	17,19,19,19	0
5	G39	B	510	20/20	0.96	0.08	7,8,15,15	0
5	G39	D	510	20/20	0.96	0.07	8,9,14,14	0
5	G39	A	511	20/20	0.96	0.08	8,9,14,15	0
5	G39	C	510	20/20	0.96	0.08	6,7,13,14	0
2	NAG	D	502	14/15	0.96	0.08	14,16,21,26	0
2	NAG	C	502	14/15	0.96	0.07	16,17,25,29	0
6	GOL	A	512	6/6	0.97	0.07	16,17,17,18	0
7	CA	D	513	1/1	0.99	0.05	18,18,18,18	0
7	CA	B	515	1/1	0.99	0.08	16,16,16,16	0
7	CA	A	513	1/1	1.00	0.05	17,17,17,17	0
7	CA	C	513	1/1	1.00	0.06	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.