



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 22, 2019 – 03:45 PM EST

PDB ID : 6N4D
Title : The crystal structure of neuraminidase from A/canine/IL/11613/2015 (H3N2) influenza virus.
Authors : Yang, H.; Stevens, J.
Deposited on : 2018-11-19
Resolution : 1.80 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-20031633
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-20031633

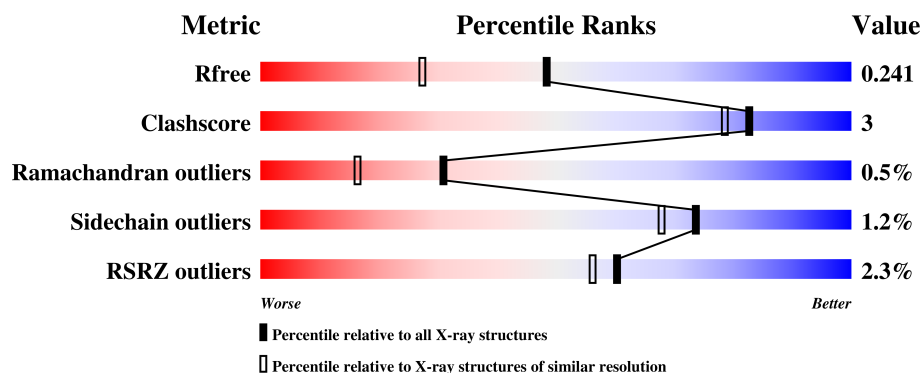
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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	397	<div> <div>2%</div> <div>90%</div> <div>8% ..</div> </div>
1	B	397	<div> <div>4%</div> <div>92%</div> <div>6% ..</div> </div>
1	C	397	<div> <div>2%</div> <div>92%</div> <div>6% ..</div> </div>
1	D	397	<div> <div>%</div> <div>90%</div> <div>7% ..</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
3	NAG	D	502	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12810 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	388	Total	C	N	O	S	0	1	0
			3017	1862	545	586	24			
1	B	388	Total	C	N	O	S	0	1	0
			3017	1862	545	586	24			
1	C	388	Total	C	N	O	S	0	1	0
			3017	1862	545	586	24			
1	D	388	Total	C	N	O	S	0	1	0
			3017	1862	545	586	24			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLY	-	expression tag	UNP A0A0H3YBU9
A	74	SER	-	expression tag	UNP A0A0H3YBU9
A	75	GLY	-	expression tag	UNP A0A0H3YBU9
A	76	ASP	-	expression tag	UNP A0A0H3YBU9
A	77	SER	-	expression tag	UNP A0A0H3YBU9
A	78	GLY	-	expression tag	UNP A0A0H3YBU9
A	79	SER	-	expression tag	UNP A0A0H3YBU9
A	80	PRO	-	expression tag	UNP A0A0H3YBU9
A	81	GLY	-	expression tag	UNP A0A0H3YBU9
B	73	GLY	-	expression tag	UNP A0A0H3YBU9
B	74	SER	-	expression tag	UNP A0A0H3YBU9
B	75	GLY	-	expression tag	UNP A0A0H3YBU9
B	76	ASP	-	expression tag	UNP A0A0H3YBU9
B	77	SER	-	expression tag	UNP A0A0H3YBU9
B	78	GLY	-	expression tag	UNP A0A0H3YBU9
B	79	SER	-	expression tag	UNP A0A0H3YBU9
B	80	PRO	-	expression tag	UNP A0A0H3YBU9
B	81	GLY	-	expression tag	UNP A0A0H3YBU9
C	73	GLY	-	expression tag	UNP A0A0H3YBU9
C	74	SER	-	expression tag	UNP A0A0H3YBU9
C	75	GLY	-	expression tag	UNP A0A0H3YBU9

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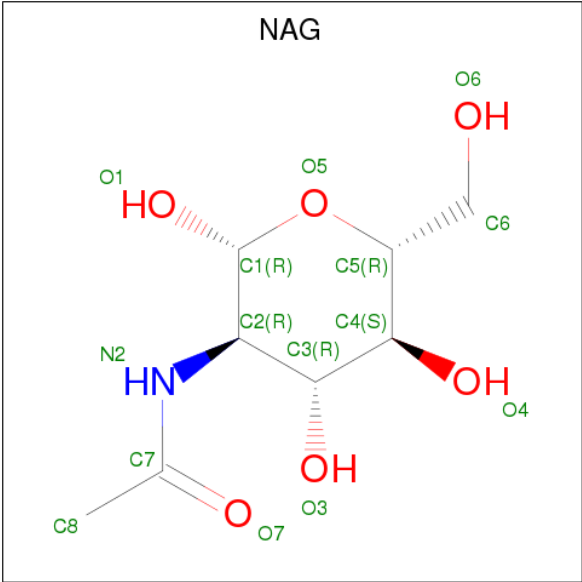
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Chain	Residue	Modelled	Actual	Comment	Reference
C	76	ASP	-	expression tag	UNP A0A0H3YBU9
C	77	SER	-	expression tag	UNP A0A0H3YBU9
C	78	GLY	-	expression tag	UNP A0A0H3YBU9
C	79	SER	-	expression tag	UNP A0A0H3YBU9
C	80	PRO	-	expression tag	UNP A0A0H3YBU9
C	81	GLY	-	expression tag	UNP A0A0H3YBU9
D	73	GLY	-	expression tag	UNP A0A0H3YBU9
D	74	SER	-	expression tag	UNP A0A0H3YBU9
D	75	GLY	-	expression tag	UNP A0A0H3YBU9
D	76	ASP	-	expression tag	UNP A0A0H3YBU9
D	77	SER	-	expression tag	UNP A0A0H3YBU9
D	78	GLY	-	expression tag	UNP A0A0H3YBU9
D	79	SER	-	expression tag	UNP A0A0H3YBU9
D	80	PRO	-	expression tag	UNP A0A0H3YBU9
D	81	GLY	-	expression tag	UNP A0A0H3YBU9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



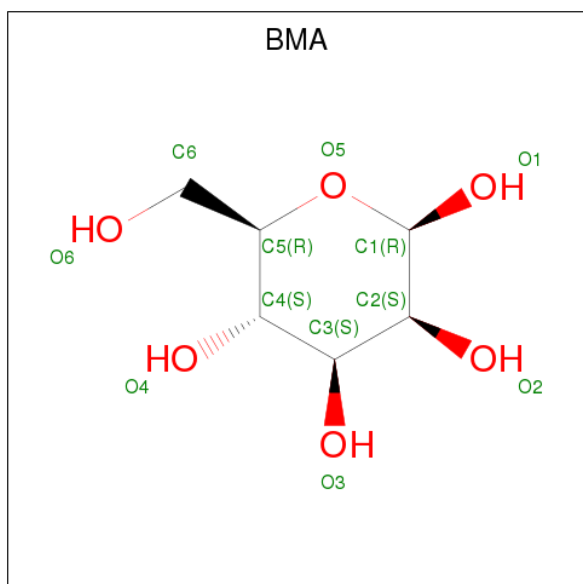
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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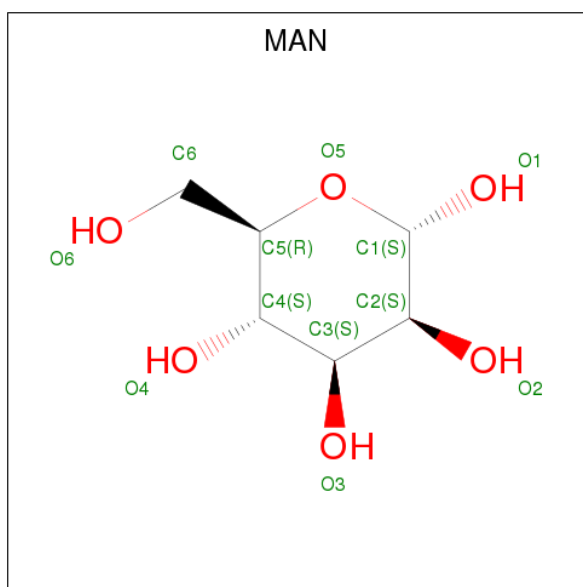
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

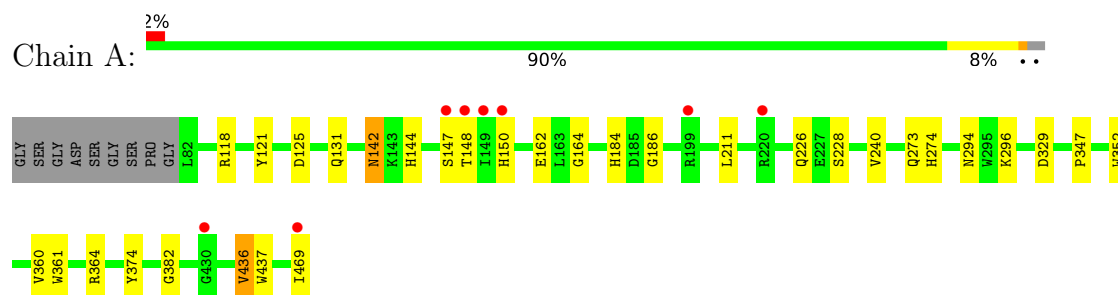
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total 97	O 97	0	0
6	B	40	Total 40	O 40	0	0
6	C	48	Total 48	O 48	0	0
6	D	97	Total 97	O 97	0	0

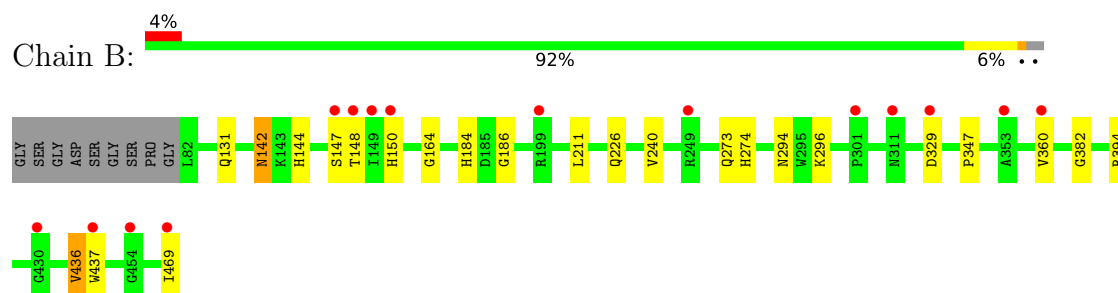
3 Residue-property plots [i](#)

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.

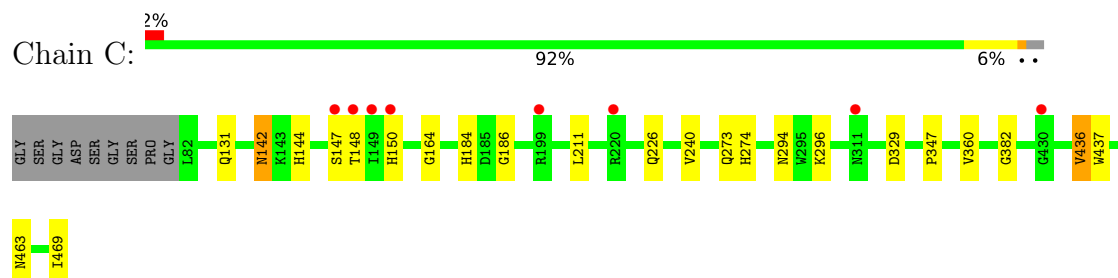
• Molecule 1: Neuraminidase



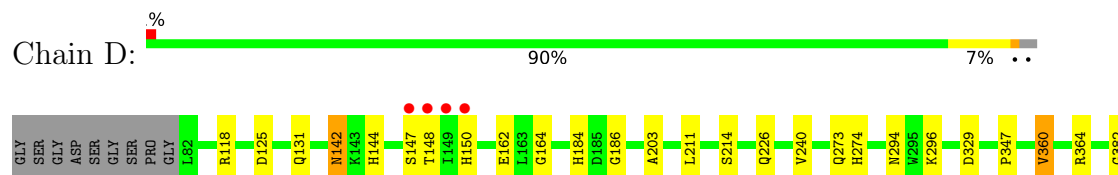
• Molecule 1: Neuraminidase

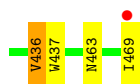


• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.45Å 110.56Å 126.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 1.80 35.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.43-1.80) 99.4 (35.39-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.210 , 0.238 0.216 , 0.241	Depositor DCC
R_{free} test set	7193 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 16.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.467 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12810	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2179e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.99	2/3089 (0.1%)	0.92	4/4195 (0.1%)
1	B	0.82	0/3089	0.86	2/4195 (0.0%)
1	C	0.80	0/3089	0.86	1/4195 (0.0%)
1	D	0.99	1/3089 (0.0%)	0.91	5/4195 (0.1%)
All	All	0.90	3/12356 (0.0%)	0.89	12/16780 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162	GLU	CD-OE1	-5.95	1.19	1.25
1	A	162	GLU	CD-OE1	-5.12	1.20	1.25
1	A	361	TRP	CE3-CZ3	5.01	1.47	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	VAL	N-CA-C	6.46	128.44	111.00
1	D	436	VAL	N-CA-C	6.46	128.44	111.00
1	B	436	VAL	N-CA-C	6.21	127.76	111.00
1	C	436	VAL	N-CA-C	6.09	127.46	111.00
1	D	125	ASP	CB-CG-OD1	5.78	123.50	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3017	0	2837	18	0
1	B	3017	0	2837	15	0
1	C	3017	0	2837	15	0
1	D	3017	0	2837	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	70	0	62	1	0
3	B	70	0	62	0	0
3	C	70	0	62	0	0
3	D	70	0	62	0	0
4	A	11	0	8	0	0
4	B	11	0	8	1	0
4	C	11	0	8	1	0
4	D	11	0	8	0	0
5	A	33	0	29	0	0
5	B	33	0	29	1	0
5	C	33	0	29	1	0
5	D	33	0	29	0	0
6	A	97	0	0	0	0
6	B	40	0	0	0	0
6	C	48	0	0	0	0
6	D	97	0	0	0	0
All	All	12810	0	11744	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 66 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:D:226:GLN:HE21	1:D:240:VAL:H	1.34	0.75
1:A:226:GLN:HE21	1:A:240:VAL:H	1.35	0.73
1:A:144:HIS:HE2	1:D:463:ASN:H	1.38	0.72
1:B:144:HIS:HE2	1:C:463:ASN:H	1.40	0.70
1:C:226:GLN:HE21	1:C:240:VAL:H	1.40	0.69

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	387/397 (98%)	366 (95%)	19 (5%)	2 (0%)	31	16
1	B	387/397 (98%)	366 (95%)	19 (5%)	2 (0%)	31	16
1	C	387/397 (98%)	366 (95%)	19 (5%)	2 (0%)	31	16
1	D	387/397 (98%)	366 (95%)	19 (5%)	2 (0%)	31	16
All	All	1548/1588 (98%)	1464 (95%)	76 (5%)	8 (0%)	31	16

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	PRO
1	B	347	PRO
1	C	347	PRO
1	D	347	PRO
1	A	437	TRP

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	339/343 (99%)	335 (99%)	4 (1%)	74	68
1	B	339/343 (99%)	335 (99%)	4 (1%)	74	68
1	C	339/343 (99%)	335 (99%)	4 (1%)	74	68
1	D	339/343 (99%)	335 (99%)	4 (1%)	74	68
All	All	1356/1372 (99%)	1340 (99%)	16 (1%)	74	68

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	329	ASP
1	C	142	ASN
1	D	142	ASN
1	B	211	LEU
1	D	148	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	393	ASN
1	C	142	ASN
1	D	356	ASN
1	B	419	ASN
1	C	104	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

32 non-standard protein/DNA/RNA residues 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$
3	NAG	A	502	1,3	14,14,15	0.70	0	17,19,21	2.32	5 (29%)
3	NAG	A	503	3	14,14,15	0.59	0	17,19,21	1.27	2 (11%)
3	NAG	A	504	1	14,14,15	0.67	0	17,19,21	1.27	1 (5%)
3	NAG	A	505	1,3	14,14,15	1.10	1 (7%)	17,19,21	1.61	4 (23%)
3	NAG	A	506	3,4	14,14,15	1.21	2 (14%)	17,19,21	1.98	4 (23%)
5	MAN	A	508	5,4	11,11,12	1.38	1 (9%)	15,15,17	1.36	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	509	5	11,11,12	1.34	1 (9%)	15,15,17	1.86	3 (20%)
5	MAN	A	510	4	11,11,12	0.88	0	15,15,17	2.13	5 (33%)
3	NAG	B	502	1,3	14,14,15	0.96	1 (7%)	17,19,21	0.77	0
3	NAG	B	503	3	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
3	NAG	B	504	1	14,14,15	0.50	0	17,19,21	1.28	2 (11%)
3	NAG	B	505	1,3	14,14,15	0.72	0	17,19,21	1.55	3 (17%)
3	NAG	B	506	3,4	14,14,15	0.93	1 (7%)	17,19,21	1.70	5 (29%)
5	MAN	B	508	5,4	11,11,12	0.81	0	15,15,17	1.54	3 (20%)
5	MAN	B	509	5	11,11,12	0.74	0	15,15,17	2.27	7 (46%)
5	MAN	B	510	4	11,11,12	0.95	0	15,15,17	1.65	3 (20%)
3	NAG	C	502	1,3	14,14,15	1.02	1 (7%)	17,19,21	0.81	0
3	NAG	C	503	3	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
3	NAG	C	504	1	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
3	NAG	C	505	1,3	14,14,15	0.67	0	17,19,21	1.51	3 (17%)
3	NAG	C	506	3,4	14,14,15	1.01	1 (7%)	17,19,21	2.02	7 (41%)
5	MAN	C	508	5,4	11,11,12	0.83	0	15,15,17	1.64	2 (13%)
5	MAN	C	509	5	11,11,12	0.64	0	15,15,17	2.49	6 (40%)
5	MAN	C	510	4	11,11,12	1.21	1 (9%)	15,15,17	1.98	4 (26%)
3	NAG	D	502	1,3	14,14,15	0.65	0	17,19,21	2.72	5 (29%)
3	NAG	D	503	3	14,14,15	0.58	0	17,19,21	1.30	1 (5%)
3	NAG	D	504	1	14,14,15	0.65	0	17,19,21	1.46	3 (17%)
3	NAG	D	505	1,3	14,14,15	1.10	2 (14%)	17,19,21	1.42	4 (23%)
3	NAG	D	506	3,4	14,14,15	1.11	2 (14%)	17,19,21	1.96	4 (23%)
5	MAN	D	508	5,4	11,11,12	1.51	2 (18%)	15,15,17	1.62	5 (33%)
5	MAN	D	509	5	11,11,12	1.17	1 (9%)	15,15,17	1.77	3 (20%)
5	MAN	D	510	4	11,11,12	0.82	0	15,15,17	1.93	3 (20%)

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	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	503	3	-	0/6/23/26	0/1/1/1
3	NAG	A	504	1	-	0/6/23/26	0/1/1/1
3	NAG	A	505	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	506	3,4	-	0/6/23/26	0/1/1/1
5	MAN	A	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	509	5	-	0/2/19/22	0/1/1/1
5	MAN	A	510	4	-	0/2/19/22	0/1/1/1
3	NAG	B	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	503	3	-	0/6/23/26	0/1/1/1
3	NAG	B	504	1	-	0/6/23/26	0/1/1/1
3	NAG	B	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	506	3,4	-	0/6/23/26	0/1/1/1
5	MAN	B	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	509	5	-	0/2/19/22	0/1/1/1
5	MAN	B	510	4	-	0/2/19/22	0/1/1/1
3	NAG	C	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	503	3	-	0/6/23/26	0/1/1/1
3	NAG	C	504	1	-	0/6/23/26	0/1/1/1
3	NAG	C	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	506	3,4	-	0/6/23/26	0/1/1/1
5	MAN	C	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	C	509	5	-	0/2/19/22	0/1/1/1
5	MAN	C	510	4	-	0/2/19/22	0/1/1/1
3	NAG	D	502	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	503	3	-	0/6/23/26	0/1/1/1
3	NAG	D	504	1	-	0/6/23/26	0/1/1/1
3	NAG	D	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	506	3,4	-	0/6/23/26	0/1/1/1
5	MAN	D	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	D	509	5	-	0/2/19/22	0/1/1/1
5	MAN	D	510	4	-	0/2/19/22	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	508	MAN	O5-C1	-3.73	1.37	1.43
5	A	508	MAN	O5-C1	-3.59	1.37	1.43
5	A	509	MAN	O5-C1	-3.45	1.38	1.43
3	C	502	NAG	O5-C1	-3.38	1.38	1.43
3	A	506	NAG	O5-C1	-2.97	1.38	1.43

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	506	NAG	O5-C1-C2	-5.91	103.37	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	NAG	O5-C1-C2	-5.60	103.79	111.52
3	D	503	NAG	C1-C2-N2	-4.07	103.53	110.49
5	A	509	MAN	C2-C3-C4	-3.81	104.26	110.87
3	A	502	NAG	O4-C4-C3	-3.73	101.63	110.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	502	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0
3	A	503	NAG	1	0
5	B	510	MAN	1	0
5	C	510	MAN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	502	1,3	14,14,15	0.70	0	17,19,21	2.32	5 (29%)
3	NAG	A	503	3	14,14,15	0.59	0	17,19,21	1.27	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	504	1	14,14,15	0.67	0	17,19,21	1.27	1 (5%)
3	NAG	A	505	1,3	14,14,15	1.10	1 (7%)	17,19,21	1.61	4 (23%)
3	NAG	A	506	3,4	14,14,15	1.21	2 (14%)	17,19,21	1.98	4 (23%)
4	BMA	A	507	3,5	11,11,12	0.93	1 (9%)	15,15,17	1.13	1 (6%)
5	MAN	A	508	5,4	11,11,12	1.38	1 (9%)	15,15,17	1.36	3 (20%)
5	MAN	A	509	5	11,11,12	1.34	1 (9%)	15,15,17	1.86	3 (20%)
5	MAN	A	510	4	11,11,12	0.88	0	15,15,17	2.13	5 (33%)
3	NAG	B	502	1,3	14,14,15	0.96	1 (7%)	17,19,21	0.77	0
3	NAG	B	503	3	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
3	NAG	B	504	1	14,14,15	0.50	0	17,19,21	1.28	2 (11%)
3	NAG	B	505	1,3	14,14,15	0.72	0	17,19,21	1.55	3 (17%)
3	NAG	B	506	3,4	14,14,15	0.93	1 (7%)	17,19,21	1.70	5 (29%)
4	BMA	B	507	3,5	11,11,12	0.66	0	15,15,17	1.54	2 (13%)
5	MAN	B	508	5,4	11,11,12	0.81	0	15,15,17	1.54	3 (20%)
5	MAN	B	509	5	11,11,12	0.74	0	15,15,17	2.27	7 (46%)
5	MAN	B	510	4	11,11,12	0.95	0	15,15,17	1.65	3 (20%)
3	NAG	C	502	1,3	14,14,15	1.02	1 (7%)	17,19,21	0.81	0
3	NAG	C	503	3	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
3	NAG	C	504	1	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
3	NAG	C	505	1,3	14,14,15	0.67	0	17,19,21	1.51	3 (17%)
3	NAG	C	506	3,4	14,14,15	1.01	1 (7%)	17,19,21	2.02	7 (41%)
4	BMA	C	507	3,5	11,11,12	0.45	0	15,15,17	1.43	3 (20%)
5	MAN	C	508	5,4	11,11,12	0.83	0	15,15,17	1.64	2 (13%)
5	MAN	C	509	5	11,11,12	0.64	0	15,15,17	2.49	6 (40%)
5	MAN	C	510	4	11,11,12	1.21	1 (9%)	15,15,17	1.98	4 (26%)
3	NAG	D	502	1,3	14,14,15	0.65	0	17,19,21	2.72	5 (29%)
3	NAG	D	503	3	14,14,15	0.58	0	17,19,21	1.30	1 (5%)
3	NAG	D	504	1	14,14,15	0.65	0	17,19,21	1.46	3 (17%)
3	NAG	D	505	1,3	14,14,15	1.10	2 (14%)	17,19,21	1.42	4 (23%)
3	NAG	D	506	3,4	14,14,15	1.11	2 (14%)	17,19,21	1.96	4 (23%)
4	BMA	D	507	3,5	11,11,12	1.22	2 (18%)	15,15,17	1.29	1 (6%)
5	MAN	D	508	5,4	11,11,12	1.51	2 (18%)	15,15,17	1.62	5 (33%)
5	MAN	D	509	5	11,11,12	1.17	1 (9%)	15,15,17	1.77	3 (20%)
5	MAN	D	510	4	11,11,12	0.82	0	15,15,17	1.93	3 (20%)

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	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	503	3	-	0/6/23/26	0/1/1/1
3	NAG	A	504	1	-	0/6/23/26	0/1/1/1
3	NAG	A	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	506	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	507	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	509	5	-	0/2/19/22	0/1/1/1
5	MAN	A	510	4	-	0/2/19/22	0/1/1/1
3	NAG	B	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	503	3	-	0/6/23/26	0/1/1/1
3	NAG	B	504	1	-	0/6/23/26	0/1/1/1
3	NAG	B	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	506	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	507	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	509	5	-	0/2/19/22	0/1/1/1
5	MAN	B	510	4	-	0/2/19/22	0/1/1/1
3	NAG	C	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	503	3	-	0/6/23/26	0/1/1/1
3	NAG	C	504	1	-	0/6/23/26	0/1/1/1
3	NAG	C	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	506	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	507	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	C	509	5	-	0/2/19/22	0/1/1/1
5	MAN	C	510	4	-	0/2/19/22	0/1/1/1
3	NAG	D	502	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	503	3	-	0/6/23/26	0/1/1/1
3	NAG	D	504	1	-	0/6/23/26	0/1/1/1
3	NAG	D	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	506	3,4	-	0/6/23/26	0/1/1/1
4	BMA	D	507	3,5	-	0/2/19/22	0/1/1/1
5	MAN	D	508	5,4	-	0/2/19/22	0/1/1/1
5	MAN	D	509	5	-	0/2/19/22	0/1/1/1
5	MAN	D	510	4	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	508	MAN	O5-C1	-3.73	1.37	1.43
5	A	508	MAN	O5-C1	-3.59	1.37	1.43
5	A	509	MAN	O5-C1	-3.45	1.38	1.43
3	C	502	NAG	O5-C1	-3.38	1.38	1.43
3	A	506	NAG	O5-C1	-2.97	1.38	1.43

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	506	NAG	O5-C1-C2	-5.91	103.37	111.52
3	A	506	NAG	O5-C1-C2	-5.60	103.79	111.52
4	D	507	BMA	C1-C2-C3	-4.25	104.28	109.66
3	D	503	NAG	C1-C2-N2	-4.07	103.53	110.49
5	A	509	MAN	C2-C3-C4	-3.81	104.26	110.87

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	502	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0
3	A	503	NAG	1	0
4	B	507	BMA	1	0
5	B	510	MAN	1	0
4	C	507	BMA	1	0
5	C	510	MAN	1	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	388/397 (97%)	0.01	8 (2%) 63 59	15, 23, 37, 91	0
1	B	388/397 (97%)	0.33	15 (3%) 39 34	21, 29, 43, 124	0
1	C	388/397 (97%)	0.15	8 (2%) 63 59	21, 29, 43, 118	0
1	D	388/397 (97%)	-0.01	5 (1%) 77 74	15, 23, 36, 88	0
All	All	1552/1588 (97%)	0.12	36 (2%) 60 56	15, 27, 40, 124	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	ILE	22.4
1	C	149	ILE	14.5
1	A	149	ILE	11.6
1	D	149	ILE	8.9
1	B	150	HIS	6.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
5	MAN	B	510	11/12	0.53	0.34	50,57,62,64	0
3	NAG	B	504	14/15	0.54	0.29	63,70,76,83	0
3	NAG	C	504	14/15	0.56	0.32	59,68,74,83	0
3	NAG	A	503	14/15	0.64	0.31	57,64,69,73	0
5	MAN	C	510	11/12	0.70	0.25	47,52,58,59	0
3	NAG	D	504	14/15	0.72	0.20	57,62,65,67	0
5	MAN	B	509	11/12	0.73	0.25	49,51,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	503	14/15	0.74	0.28	53,65,70,75	0
3	NAG	B	503	14/15	0.74	0.24	43,67,75,80	0
3	NAG	A	504	14/15	0.74	0.15	56,61,62,63	0
5	MAN	C	509	11/12	0.75	0.22	49,53,56,61	0
3	NAG	C	502	14/15	0.76	0.19	43,48,55,58	0
3	NAG	D	502	14/15	0.79	0.19	43,48,56,59	0
3	NAG	A	502	14/15	0.80	0.16	44,51,59,62	0
5	MAN	D	509	11/12	0.81	0.15	40,49,54,55	0
3	NAG	C	503	14/15	0.81	0.21	46,63,67,71	0
5	MAN	D	510	11/12	0.82	0.19	41,45,50,52	0
5	MAN	A	510	11/12	0.84	0.17	40,43,49,50	0
3	NAG	B	502	14/15	0.85	0.15	43,48,55,60	0
5	MAN	A	509	11/12	0.88	0.13	40,46,52,56	0
5	MAN	B	508	11/12	0.89	0.12	32,34,38,42	0
3	NAG	C	505	14/15	0.89	0.12	26,33,41,42	0
3	NAG	C	506	14/15	0.90	0.12	26,30,34,35	0
3	NAG	D	505	14/15	0.91	0.14	21,24,38,40	0
3	NAG	B	505	14/15	0.91	0.11	26,33,40,41	0
5	MAN	C	508	11/12	0.91	0.12	31,32,35,40	0
3	NAG	B	506	14/15	0.93	0.10	27,30,32,34	0
5	MAN	D	508	11/12	0.94	0.10	27,29,33,36	0
3	NAG	D	506	14/15	0.95	0.08	22,23,24,24	0
5	MAN	A	508	11/12	0.95	0.10	28,29,32,36	0
3	NAG	A	506	14/15	0.95	0.10	21,22,23,24	0
3	NAG	A	505	14/15	0.96	0.10	22,24,37,42	0

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
5	MAN	B	510	11/12	0.53	0.34	50,57,62,64	0
3	NAG	B	504	14/15	0.54	0.29	63,70,76,83	0
3	NAG	C	504	14/15	0.56	0.32	59,68,74,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	503	14/15	0.64	0.31	57,64,69,73	0
5	MAN	C	510	11/12	0.70	0.25	47,52,58,59	0
3	NAG	D	504	14/15	0.72	0.20	57,62,65,67	0
5	MAN	B	509	11/12	0.73	0.25	49,51,55,58	0
3	NAG	D	503	14/15	0.74	0.28	53,65,70,75	0
3	NAG	B	503	14/15	0.74	0.24	43,67,75,80	0
3	NAG	A	504	14/15	0.74	0.15	56,61,62,63	0
5	MAN	C	509	11/12	0.75	0.22	49,53,56,61	0
3	NAG	C	502	14/15	0.76	0.19	43,48,55,58	0
3	NAG	D	502	14/15	0.79	0.19	43,48,56,59	0
3	NAG	A	502	14/15	0.80	0.16	44,51,59,62	0
5	MAN	D	509	11/12	0.81	0.15	40,49,54,55	0
3	NAG	C	503	14/15	0.81	0.21	46,63,67,71	0
5	MAN	D	510	11/12	0.82	0.19	41,45,50,52	0
5	MAN	A	510	11/12	0.84	0.17	40,43,49,50	0
3	NAG	B	502	14/15	0.85	0.15	43,48,55,60	0
5	MAN	A	509	11/12	0.88	0.13	40,46,52,56	0
5	MAN	B	508	11/12	0.89	0.12	32,34,38,42	0
3	NAG	C	505	14/15	0.89	0.12	26,33,41,42	0
3	NAG	C	506	14/15	0.90	0.12	26,30,34,35	0
5	MAN	C	508	11/12	0.91	0.12	31,32,35,40	0
3	NAG	D	505	14/15	0.91	0.14	21,24,38,40	0
4	BMA	B	507	11/12	0.91	0.09	27,30,37,40	0
3	NAG	B	505	14/15	0.91	0.11	26,33,40,41	0
4	BMA	D	507	11/12	0.92	0.12	22,25,30,33	0
4	BMA	C	507	11/12	0.92	0.13	26,31,37,37	0
3	NAG	B	506	14/15	0.93	0.10	27,30,32,34	0
5	MAN	D	508	11/12	0.94	0.10	27,29,33,36	0
3	NAG	D	506	14/15	0.95	0.08	22,23,24,24	0
3	NAG	A	506	14/15	0.95	0.10	21,22,23,24	0
5	MAN	A	508	11/12	0.95	0.10	28,29,32,36	0
3	NAG	A	505	14/15	0.96	0.10	22,24,37,42	0
4	BMA	A	507	11/12	0.96	0.08	21,25,28,31	0
2	CA	D	501	1/1	0.99	0.05	24,24,24,24	0
2	CA	A	501	1/1	0.99	0.04	24,24,24,24	0
2	CA	B	501	1/1	0.99	0.07	26,26,26,26	0
2	CA	C	501	1/1	1.00	0.06	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.