



# Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2016 – 12:01 PM EDT

PDB ID : 5HUK  
Title : The crystal structure of neuraminidase from A/Northern pintail/Washington  
/40964/2014 influenza virus  
Authors : Yang, H.; Carney, P.J.; Guo, Z.; Chang, J.C.; Stevens, J.  
Deposited on : 2016-01-27  
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

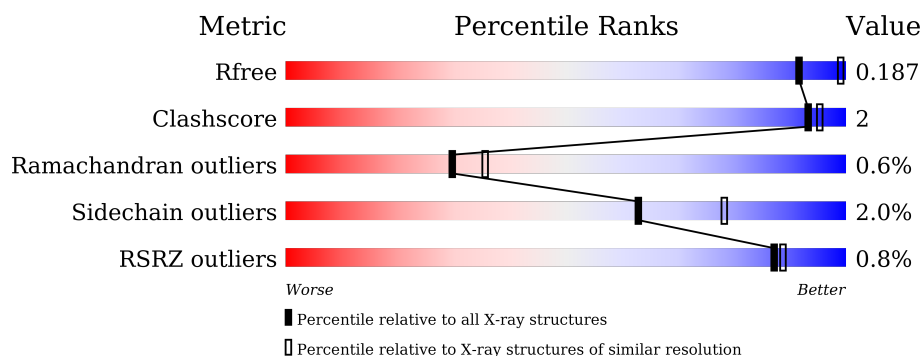
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	402	<div> <div>87%</div> <div>8%</div> <div>..</div> </div>
1	B	402	<div> <div>88%</div> <div>7%</div> <div>...</div> </div>
1	C	402	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	402	<div> <div>89%</div> <div>7%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	C	501	-	-	-	X
3	NAG	A	505	X	-	-	-
3	NAG	B	505	-	-	-	X
5	MAN	A	511	X	-	-	-
5	MAN	A	512	-	-	-	X
5	MAN	B	510	X	-	-	-
5	MAN	C	510	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12935 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
			3007	1854	540	589	24			
1	B	388	Total	C	N	O	S	0	1	0
			3007	1854	540	589	24			
1	C	388	Total	C	N	O	S	0	1	0
			3007	1854	540	589	24			
1	D	388	Total	C	N	O	S	0	1	0
			3007	1854	540	589	24			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	-	expression tag	UNP A0A0C4WXC5
A	69	LEU	-	expression tag	UNP A0A0C4WXC5
A	70	VAL	-	expression tag	UNP A0A0C4WXC5
A	71	PRO	-	expression tag	UNP A0A0C4WXC5
A	72	ARG	-	expression tag	UNP A0A0C4WXC5
A	73	GLY	-	expression tag	UNP A0A0C4WXC5
A	74	SER	-	expression tag	UNP A0A0C4WXC5
A	75	GLY	-	expression tag	UNP A0A0C4WXC5
A	76	ASP	-	expression tag	UNP A0A0C4WXC5
A	77	SER	-	expression tag	UNP A0A0C4WXC5
A	78	GLY	-	expression tag	UNP A0A0C4WXC5
A	79	SER	-	expression tag	UNP A0A0C4WXC5
A	80	PRO	-	expression tag	UNP A0A0C4WXC5
A	81	GLY	-	expression tag	UNP A0A0C4WXC5
A	82	ALA	-	expression tag	UNP A0A0C4WXC5
B	68	SER	-	expression tag	UNP A0A0C4WXC5
B	69	LEU	-	expression tag	UNP A0A0C4WXC5
B	70	VAL	-	expression tag	UNP A0A0C4WXC5
B	71	PRO	-	expression tag	UNP A0A0C4WXC5
B	72	ARG	-	expression tag	UNP A0A0C4WXC5
B	73	GLY	-	expression tag	UNP A0A0C4WXC5

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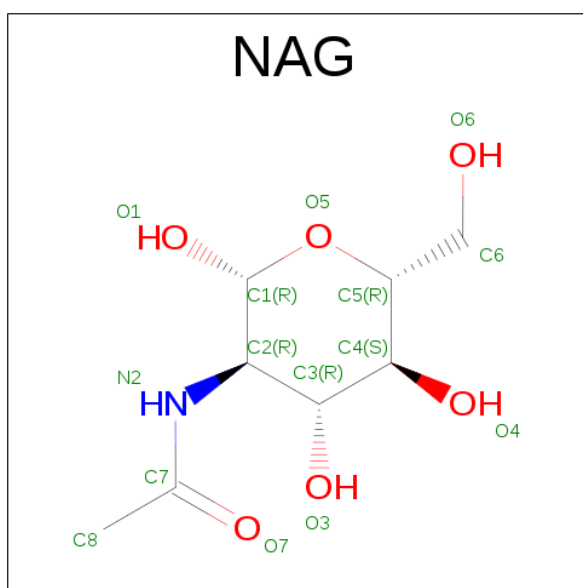
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Chain	Residue	Modelled	Actual	Comment	Reference
B	74	SER	-	expression tag	UNP A0A0C4WXC5
B	75	GLY	-	expression tag	UNP A0A0C4WXC5
B	76	ASP	-	expression tag	UNP A0A0C4WXC5
B	77	SER	-	expression tag	UNP A0A0C4WXC5
B	78	GLY	-	expression tag	UNP A0A0C4WXC5
B	79	SER	-	expression tag	UNP A0A0C4WXC5
B	80	PRO	-	expression tag	UNP A0A0C4WXC5
B	81	GLY	-	expression tag	UNP A0A0C4WXC5
B	82	ALA	-	expression tag	UNP A0A0C4WXC5
C	68	SER	-	expression tag	UNP A0A0C4WXC5
C	69	LEU	-	expression tag	UNP A0A0C4WXC5
C	70	VAL	-	expression tag	UNP A0A0C4WXC5
C	71	PRO	-	expression tag	UNP A0A0C4WXC5
C	72	ARG	-	expression tag	UNP A0A0C4WXC5
C	73	GLY	-	expression tag	UNP A0A0C4WXC5
C	74	SER	-	expression tag	UNP A0A0C4WXC5
C	75	GLY	-	expression tag	UNP A0A0C4WXC5
C	76	ASP	-	expression tag	UNP A0A0C4WXC5
C	77	SER	-	expression tag	UNP A0A0C4WXC5
C	78	GLY	-	expression tag	UNP A0A0C4WXC5
C	79	SER	-	expression tag	UNP A0A0C4WXC5
C	80	PRO	-	expression tag	UNP A0A0C4WXC5
C	81	GLY	-	expression tag	UNP A0A0C4WXC5
C	82	ALA	-	expression tag	UNP A0A0C4WXC5
D	68	SER	-	expression tag	UNP A0A0C4WXC5
D	69	LEU	-	expression tag	UNP A0A0C4WXC5
D	70	VAL	-	expression tag	UNP A0A0C4WXC5
D	71	PRO	-	expression tag	UNP A0A0C4WXC5
D	72	ARG	-	expression tag	UNP A0A0C4WXC5
D	73	GLY	-	expression tag	UNP A0A0C4WXC5
D	74	SER	-	expression tag	UNP A0A0C4WXC5
D	75	GLY	-	expression tag	UNP A0A0C4WXC5
D	76	ASP	-	expression tag	UNP A0A0C4WXC5
D	77	SER	-	expression tag	UNP A0A0C4WXC5
D	78	GLY	-	expression tag	UNP A0A0C4WXC5
D	79	SER	-	expression tag	UNP A0A0C4WXC5
D	80	PRO	-	expression tag	UNP A0A0C4WXC5
D	81	GLY	-	expression tag	UNP A0A0C4WXC5
D	82	ALA	-	expression tag	UNP A0A0C4WXC5

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

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

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



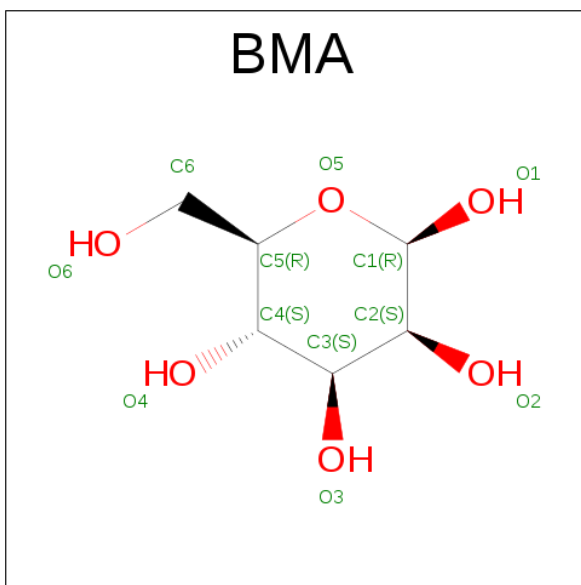
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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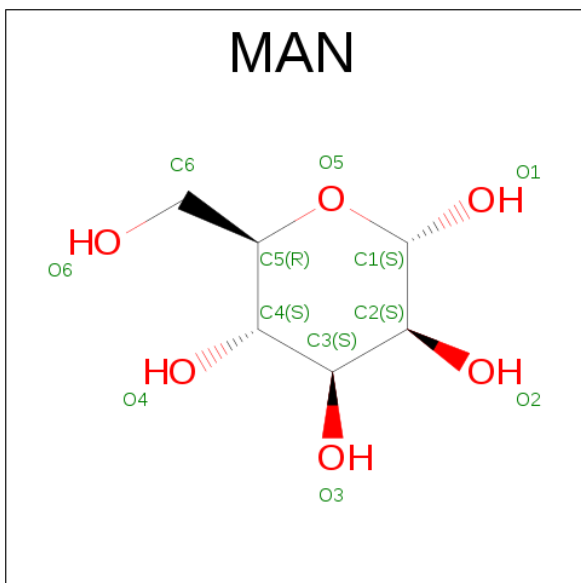
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	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<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	D	1	Total C O 11 6 5	0	0
5	D	1	Total C O 11 6 5	0	0
5	D	1	Total C O 11 6 5	0	0
5	D	1	Total C O 11 6 5	0	0

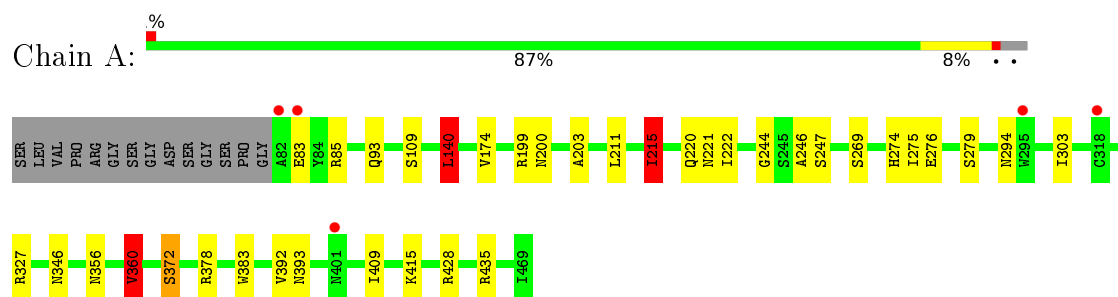
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	98	Total O 98 98	0	0
6	B	94	Total O 94 94	0	0
6	C	106	Total O 106 106	0	0
6	D	91	Total O 91 91	0	0

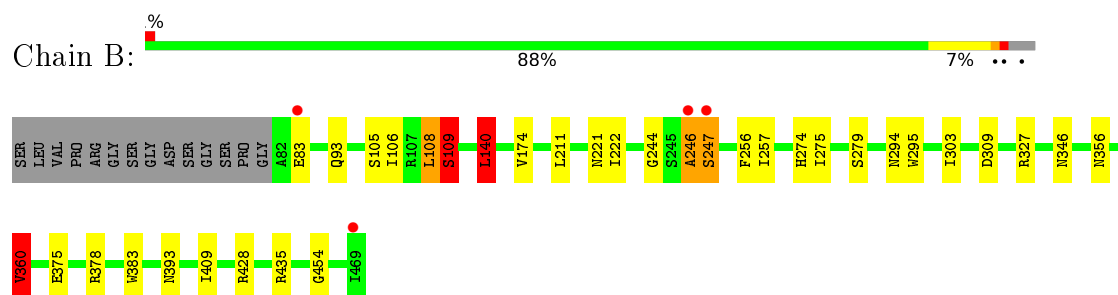
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

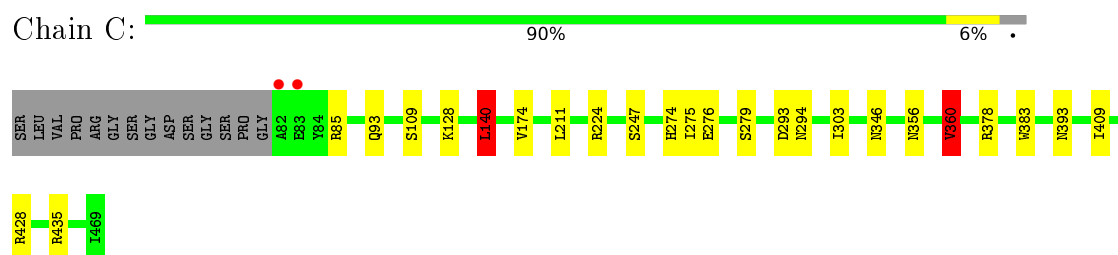
#### • Molecule 1: Neuraminidase



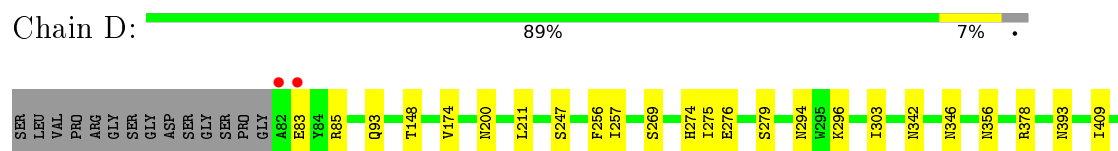
#### • Molecule 1: Neuraminidase



#### • Molecule 1: Neuraminidase



#### • Molecule 1: Neuraminidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.22Å 122.79Å 176.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 42.20 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.45) 98.3 (42.20-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.157 , 0.185 0.163 , 0.187	Depositor DCC
$R_{free}$ test set	4621 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.88	2/3080 (0.1%)	0.94	11/4184 (0.3%)
1	B	0.89	2/3080 (0.1%)	0.98	12/4184 (0.3%)
1	C	0.86	0/3080	0.98	11/4184 (0.3%)
1	D	0.88	2/3080 (0.1%)	0.94	10/4184 (0.2%)
All	All	0.88	6/12320 (0.0%)	0.96	44/16736 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	SER	CB-OG	-6.30	1.34	1.42
1	B	375	GLU	CG-CD	5.80	1.60	1.51
1	A	372	SER	CB-OG	-5.68	1.34	1.42
1	D	269	SER	CB-OG	-5.20	1.35	1.42
1	D	274	HIS	C-O	5.14	1.33	1.23
1	B	109	SER	N-CA	5.09	1.56	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	SER	N-CA-CB	13.36	130.53	110.50
1	C	294	ASN	N-CA-CB	-12.68	87.78	110.60
1	D	438	TRP	N-CA-C	10.46	139.25	111.00
1	B	108	LEU	N-CA-C	-9.02	86.66	111.00
1	B	360	VAL	CB-CA-C	-8.72	94.83	111.40
1	A	360	VAL	CB-CA-C	-8.60	95.05	111.40
1	C	360	VAL	CB-CA-C	-7.98	96.24	111.40
1	C	435	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	D	435	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	215	ILE	CB-CA-C	-6.65	98.31	111.60
1	C	274	HIS	N-CA-C	-6.56	93.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	224	ARG	NE-CZ-NH2	6.43	123.51	120.30
1	B	294	ASN	N-CA-CB	-6.28	99.30	110.60
1	A	428	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	274	HIS	N-CA-C	-6.21	94.23	111.00
1	D	85	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	428	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	D	438	TRP	CB-CA-C	-6.14	98.11	110.40
1	A	85	ARG	CB-CA-C	-6.12	98.15	110.40
1	C	85	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	140	LEU	CA-CB-CG	6.04	129.18	115.30
1	D	420	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	D	420	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	294	ASN	N-CA-CB	-5.92	99.94	110.60
1	D	85	ARG	CB-CA-C	-5.83	98.73	110.40
1	A	140	LEU	CA-CB-CG	5.81	128.66	115.30
1	C	293	ASP	C-N-CA	5.78	136.16	121.70
1	B	140	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	435	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	274	HIS	N-CA-C	-5.73	95.52	111.00
1	B	428	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	140	LEU	CB-CG-CD1	5.66	120.62	111.00
1	A	327	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	85	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	428	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	309	ASP	CB-CA-C	-5.47	99.45	110.40
1	D	439	THR	N-CA-C	5.45	125.72	111.00
1	C	85	ARG	CB-CA-C	-5.45	99.50	110.40
1	B	327	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	346	ASN	N-CA-CB	-5.32	101.03	110.60
1	B	435	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	294	ASN	N-CA-CB	-5.23	101.19	110.60
1	A	269	SER	N-CA-CB	-5.08	102.88	110.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3007	0	2814	12	0
1	B	3007	0	2814	18	0
1	C	3007	0	2814	8	0
1	D	3007	0	2814	9	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	84	0	74	0	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	0	0
4	C	11	0	8	1	0
4	D	11	0	8	0	0
5	A	44	0	38	0	0
5	B	44	0	38	1	0
5	C	44	0	38	0	0
5	D	44	0	38	0	0
6	A	98	0	0	0	0
6	B	94	0	0	0	0
6	C	106	0	0	0	0
6	D	91	0	0	0	0
All	All	12935	0	11700	46	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 2.

All (46) 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:148:THR:OG1	1:D:438:TRP:O	1.83	0.94
1:B:246:ALA:O	1:B:247:SER:OG	1.83	0.94
1:A:275:ILE:HD12	1:A:303:ILE:HD11	1.48	0.93
1:D:275:ILE:HD12	1:D:303:ILE:HD11	1.51	0.93
1:C:275:ILE:HD12	1:C:303:ILE:HD11	1.50	0.92
1:B:275:ILE:HD12	1:B:303:ILE:HD11	1.53	0.89
1:B:105:SER:O	1:B:108:LEU:O	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:SER:HB2	1:B:295:TRP:CE3	2.22	0.74
1:A:392:VAL:HG23	4:C:507:BMA:H61	1.82	0.61
1:C:360:VAL:HG13	1:C:383:TRP:HE3	1.67	0.59
1:B:247:SER:CB	1:B:295:TRP:CE3	2.86	0.58
1:A:199:ARG:HD2	1:A:220:GLN:O	2.04	0.57
1:B:246:ALA:O	1:B:247:SER:CB	2.53	0.56
1:A:360:VAL:HG13	1:A:383:TRP:HE3	1.72	0.54
1:A:109:SER:HB3	1:A:140:LEU:HG	1.90	0.53
1:B:93:GLN:HE22	1:B:356:ASN:HD21	1.57	0.53
1:C:93:GLN:HE22	1:C:356:ASN:HD21	1.56	0.53
1:A:93:GLN:HE22	1:A:356:ASN:HD21	1.57	0.53
1:D:93:GLN:HE22	1:D:356:ASN:HD21	1.56	0.53
1:B:360:VAL:HG13	1:B:383:TRP:HE3	1.73	0.52
1:A:378:ARG:NH2	1:A:393:ASN:OD1	2.44	0.51
1:A:203:ALA:HB3	1:A:215:ILE:HG13	1.93	0.51
1:D:378:ARG:NH2	1:D:393:ASN:OD1	2.44	0.50
1:C:378:ARG:NH2	1:C:393:ASN:OD1	2.44	0.50
1:C:360:VAL:HG13	1:C:383:TRP:CE3	2.45	0.50
1:B:378:ARG:NH2	1:B:393:ASN:OD1	2.45	0.49
1:C:279:SER:HB3	1:C:409:ILE:HG22	1.94	0.49
1:A:360:VAL:HG13	1:A:383:TRP:CE3	2.47	0.48
1:A:279:SER:HB3	1:A:409:ILE:HG22	1.95	0.48
1:B:360:VAL:HG13	1:B:383:TRP:CE3	2.48	0.47
5:B:510:MAN:H2	5:B:511:MAN:H2	1.95	0.47
1:A:221:ASN:HB3	1:A:244:GLY:HA2	1.97	0.47
1:B:221:ASN:HB3	1:B:244:GLY:HA2	1.95	0.47
1:D:279:SER:HB3	1:D:409:ILE:HG22	1.98	0.46
1:B:247:SER:HB2	1:B:295:TRP:CD2	2.52	0.45
1:C:109:SER:HB3	1:C:140:LEU:HG	1.99	0.45
1:B:279:SER:HB3	1:B:409:ILE:HG22	1.99	0.44
1:B:109:SER:HB3	1:B:140:LEU:HG	2.01	0.43
1:B:106:ILE:C	1:B:108:LEU:O	2.57	0.43
1:A:200:ASN:O	1:D:454:GLY:HA3	2.18	0.42
1:B:454:GLY:HA3	1:D:200:ASN:O	2.19	0.42
1:B:140:LEU:C	1:B:140:LEU:CD1	2.87	0.42
1:C:128:LYS:HE3	1:C:128:LYS:HB3	1.84	0.42
1:B:256:PHE:C	1:B:257:ILE:HG13	2.40	0.41
1:D:256:PHE:C	1:D:257:ILE:HG13	2.41	0.40
1:D:296:LYS:O	1:D:342:ASN:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/402 (96%)	372 (96%)	13 (3%)	2 (0%)	34	41
1	B	387/402 (96%)	372 (96%)	11 (3%)	4 (1%)	19	21
1	C	387/402 (96%)	375 (97%)	11 (3%)	1 (0%)	46	57
1	D	387/402 (96%)	373 (96%)	12 (3%)	2 (0%)	34	41
All	All	1548/1608 (96%)	1492 (96%)	47 (3%)	9 (1%)	30	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	247	SER
1	D	439	THR
1	B	109	SER
1	B	246	ALA
1	D	247	SER
1	A	246	ALA
1	C	247	SER
1	A	222	ILE
1	B	222	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	336/345 (97%)	325 (97%)	11 (3%)	45	61
1	B	336/345 (97%)	331 (98%)	5 (2%)	72	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	336/345 (97%)	330 (98%)	6 (2%)	66	81
1	D	336/345 (97%)	331 (98%)	5 (2%)	72	84
All	All	1344/1380 (97%)	1317 (98%)	27 (2%)	63	78

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	140	LEU
1	A	174	VAL
1	A	211	LEU
1	A	215	ILE
1	A	247	SER
1	A	276	GLU
1	A	346	ASN
1	A	360	VAL
1	A	372	SER
1	A	415	LYS
1	B	83	GLU
1	B	140	LEU
1	B	174	VAL
1	B	211	LEU
1	B	360	VAL
1	C	140	LEU
1	C	174	VAL
1	C	211	LEU
1	C	276	GLU
1	C	346	ASN
1	C	360	VAL
1	D	83	GLU
1	D	174	VAL
1	D	211	LEU
1	D	276	GLU
1	D	346	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	B	274	HIS

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Mol	Chain	Res	Type
1	B	356	ASN
1	C	356	ASN
1	C	432	GLN
1	D	356	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 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	0.51	0	15,19,21	1.47	2 (13%)
3	NAG	A	503	3	14,14,15	0.63	0	15,19,21	1.11	0
3	NAG	A	504	1,3	14,14,15	0.72	0	15,19,21	1.92	2 (13%)
3	NAG	A	505	3	14,14,15	0.95	1 (7%)	15,19,21	2.08	3 (20%)
3	NAG	A	506	1,3	14,14,15	1.17	2 (14%)	15,19,21	1.46	3 (20%)
3	NAG	A	507	3,4	14,14,15	1.23	1 (7%)	15,19,21	1.45	2 (13%)
4	BMA	A	508	3,5	11,11,12	0.73	0	15,15,17	1.44	2 (13%)
5	MAN	A	509	5,4	11,11,12	1.03	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
5	MAN	A	510	5	11,11,12	1.00	1 (9%)	15,15,17	1.81	7 (46%)
5	MAN	A	511	5,4	11,11,12	1.15	1 (9%)	15,15,17	4.54	11 (73%)
5	MAN	A	512	5	11,11,12	0.95	1 (9%)	15,15,17	2.52	4 (26%)
3	NAG	B	502	1,3	14,14,15	0.69	0	15,19,21	1.36	1 (6%)
3	NAG	B	503	3	14,14,15	0.78	0	15,19,21	1.86	4 (26%)
3	NAG	B	504	1	14,14,15	1.10	1 (7%)	15,19,21	2.28	5 (33%)
3	NAG	B	505	1,3	14,14,15	1.32	2 (14%)	15,19,21	1.88	4 (26%)
3	NAG	B	506	3,4	14,14,15	0.84	0	15,19,21	1.68	2 (13%)
4	BMA	B	507	3,5	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
5	MAN	B	508	5,4	11,11,12	0.96	0	15,15,17	1.23	3 (20%)
5	MAN	B	509	5	11,11,12	0.80	0	15,15,17	1.53	3 (20%)
5	MAN	B	510	5,4	11,11,12	0.96	0	15,15,17	2.32	8 (53%)
5	MAN	B	511	5	11,11,12	0.90	0	15,15,17	1.96	3 (20%)
3	NAG	C	502	1,3	14,14,15	0.84	1 (7%)	15,19,21	1.76	4 (26%)
3	NAG	C	503	3	14,14,15	1.12	2 (14%)	15,19,21	1.99	6 (40%)
3	NAG	C	504	1	14,14,15	0.82	1 (7%)	15,19,21	1.55	4 (26%)
3	NAG	C	505	1,3	14,14,15	1.18	2 (14%)	15,19,21	1.36	4 (26%)
3	NAG	C	506	3,4	14,14,15	1.18	1 (7%)	15,19,21	1.46	4 (26%)
4	BMA	C	507	3,5	11,11,12	0.93	1 (9%)	15,15,17	1.41	3 (20%)
5	MAN	C	508	5,4	11,11,12	0.87	0	15,15,17	2.56	5 (33%)
5	MAN	C	509	5	11,11,12	0.99	0	15,15,17	3.35	6 (40%)
5	MAN	C	510	5,4	11,11,12	1.05	0	15,15,17	3.98	9 (60%)
5	MAN	C	511	5	11,11,12	0.66	0	15,15,17	2.26	6 (40%)
3	NAG	D	502	1,3	14,14,15	0.70	0	15,19,21	1.62	3 (20%)
3	NAG	D	503	3	14,14,15	0.69	0	15,19,21	1.19	1 (6%)
3	NAG	D	504	1	14,14,15	0.86	0	15,19,21	3.41	7 (46%)
3	NAG	D	505	1,3	14,14,15	1.11	0	15,19,21	1.22	1 (6%)
3	NAG	D	506	3,4	14,14,15	0.97	1 (7%)	15,19,21	2.13	6 (40%)
4	BMA	D	507	3,5	11,11,12	0.98	1 (9%)	15,15,17	1.87	3 (20%)
5	MAN	D	508	5,4	11,11,12	0.78	0	15,15,17	2.32	6 (40%)
5	MAN	D	509	5	11,11,12	1.00	0	15,15,17	2.85	8 (53%)
5	MAN	D	510	5,4	11,11,12	0.95	0	15,15,17	2.80	8 (53%)
5	MAN	D	511	5	11,11,12	0.89	0	15,15,17	2.17	5 (33%)

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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	505	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	506	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	507	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	508	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	509	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	510	5	-	0/2/19/22	0/1/1/1
5	MAN	A	511	5,4	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	A	512	5	-	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	5,4	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	511	5	-	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	5,4	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	C	511	5	-	0/2/19/22	0/1/1/1
3	NAG	D	502	1,3	-	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	5,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	D	511	5	-	0/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	NAG	O5-C1	-4.02	1.37	1.43
3	C	506	NAG	O5-C1	-2.85	1.39	1.43
3	A	506	NAG	O5-C1	-2.60	1.39	1.43
3	A	506	NAG	C2-N2	-2.56	1.41	1.46
3	D	506	NAG	O5-C1	-2.53	1.39	1.43
3	C	505	NAG	O5-C1	-2.48	1.39	1.43
5	A	510	MAN	O3-C3	-2.44	1.37	1.43
5	A	509	MAN	O5-C1	-2.40	1.39	1.43
3	C	502	NAG	O5-C1	-2.39	1.39	1.43
3	B	505	NAG	O5-C1	-2.21	1.40	1.43
4	C	507	BMA	O5-C1	-2.17	1.40	1.43
4	D	507	BMA	O5-C1	-2.05	1.40	1.43
3	C	503	NAG	C3-C2	2.07	1.57	1.52
5	A	512	MAN	C4-C5	2.14	1.57	1.53
3	C	504	NAG	C1-C2	2.29	1.55	1.52
5	A	511	MAN	C4-C3	2.61	1.59	1.52
3	A	505	NAG	C1-C2	2.72	1.56	1.52
3	C	505	NAG	C1-C2	2.73	1.56	1.52
3	B	504	NAG	C1-C2	2.92	1.56	1.52
3	C	503	NAG	C1-C2	3.13	1.56	1.52
3	B	505	NAG	C1-C2	4.02	1.58	1.52

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	511	MAN	C1-C2-C3	-12.67	94.20	109.55
5	C	510	MAN	C1-C2-C3	-7.37	100.62	109.55
5	A	512	MAN	O5-C1-C2	-6.74	100.11	110.89
5	C	510	MAN	O5-C5-C4	-6.34	99.63	110.13
5	C	509	MAN	O4-C4-C3	-5.94	96.96	110.36
5	D	511	MAN	O5-C1-C2	-5.50	102.10	110.89
5	B	510	MAN	C1-C2-C3	-5.26	103.18	109.55
5	A	511	MAN	C1-O5-C5	-5.24	104.44	112.14
5	C	511	MAN	O5-C1-C2	-5.10	102.73	110.89
5	C	510	MAN	C1-O5-C5	-4.79	105.09	112.14
3	D	504	NAG	O7-C7-C8	-4.41	113.95	122.07
3	A	505	NAG	C3-C4-C5	-4.26	102.63	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	510	MAN	O5-C5-C4	-4.23	103.13	110.13
3	D	506	NAG	O4-C4-C3	-4.18	100.93	110.36
5	C	511	MAN	O3-C3-C2	-4.11	102.48	110.01
3	C	503	NAG	O5-C5-C4	-3.64	104.11	110.13
3	D	504	NAG	C4-C3-C2	-3.62	105.73	111.34
3	B	503	NAG	O5-C5-C4	-3.58	104.21	110.13
3	C	502	NAG	C3-C4-C5	-3.51	103.97	110.23
5	A	512	MAN	C1-O5-C5	-3.49	107.01	112.14
3	B	503	NAG	O7-C7-C8	-3.44	115.74	122.07
4	D	507	BMA	O4-C4-C3	-3.44	102.61	110.36
5	A	511	MAN	O4-C4-C5	-3.41	100.24	109.23
3	D	506	NAG	O6-C6-C5	-3.38	100.02	111.30
5	C	508	MAN	C3-C4-C5	-3.32	104.31	110.23
4	A	508	BMA	O6-C6-C5	-3.31	100.25	111.30
3	D	502	NAG	C3-C4-C5	-3.28	104.38	110.23
3	B	504	NAG	O5-C5-C4	-3.26	104.73	110.13
3	A	504	NAG	O3-C3-C2	-3.12	102.69	109.37
5	D	508	MAN	O6-C6-C5	-3.11	100.93	111.30
5	D	509	MAN	O4-C4-C3	-3.04	103.50	110.36
3	A	507	NAG	O4-C4-C3	-3.00	103.59	110.36
3	A	506	NAG	O5-C5-C4	-2.99	105.18	110.13
3	A	506	NAG	O4-C4-C3	-2.92	103.77	110.36
4	A	508	BMA	C1-C2-C3	-2.90	106.04	109.55
3	A	505	NAG	C2-N2-C7	-2.81	119.45	123.11
3	D	506	NAG	C1-O5-C5	-2.79	108.03	112.14
4	D	507	BMA	O3-C3-C4	-2.77	104.12	110.36
5	D	508	MAN	O2-C2-C3	-2.75	104.65	110.19
3	D	506	NAG	C3-C4-C5	-2.73	105.37	110.23
5	C	511	MAN	C1-C2-C3	-2.59	106.42	109.55
3	A	502	NAG	O7-C7-C8	-2.55	117.38	122.07
5	B	510	MAN	C1-O5-C5	-2.53	108.42	112.14
3	C	506	NAG	O4-C4-C3	-2.52	104.68	110.36
3	C	505	NAG	O7-C7-C8	-2.51	117.45	122.07
3	D	504	NAG	O3-C3-C4	-2.47	104.80	110.36
5	A	512	MAN	O4-C4-C3	-2.45	104.83	110.36
3	C	503	NAG	C1-O5-C5	-2.41	108.60	112.14
3	C	502	NAG	O4-C4-C3	-2.38	104.99	110.36
5	C	508	MAN	O3-C3-C4	-2.37	105.01	110.36
5	C	508	MAN	O6-C6-C5	-2.35	103.47	111.30
3	C	504	NAG	O7-C7-C8	-2.34	117.76	122.07
3	A	506	NAG	C2-N2-C7	-2.34	120.07	123.11
5	D	511	MAN	O4-C4-C3	-2.33	105.11	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	510	MAN	O4-C4-C5	-2.33	103.09	109.23
5	B	509	MAN	C1-C2-C3	-2.29	106.77	109.55
3	B	505	NAG	O3-C3-C4	-2.26	105.27	110.36
5	A	510	MAN	C1-C2-C3	-2.24	106.84	109.55
3	C	505	NAG	C4-C3-C2	-2.23	107.88	111.34
4	C	507	BMA	O6-C6-C5	-2.21	103.93	111.30
5	D	508	MAN	C3-C4-C5	-2.21	106.29	110.23
5	A	511	MAN	O5-C5-C4	-2.19	106.50	110.13
3	D	502	NAG	O7-C7-C8	-2.18	118.06	122.07
3	C	504	NAG	O5-C5-C4	-2.12	106.63	110.13
3	D	506	NAG	C2-N2-C7	-2.10	120.37	123.11
3	C	506	NAG	C6-C5-C4	-2.08	107.78	112.99
5	A	510	MAN	O4-C4-C5	-2.06	103.81	109.23
4	B	507	BMA	O6-C6-C5	-2.05	104.46	111.30
3	C	506	NAG	O6-C6-C5	-2.02	104.56	111.30
5	D	510	MAN	O4-C4-C3	-2.01	105.82	110.36
5	A	510	MAN	C6-C5-C4	-2.01	107.95	112.99
4	C	507	BMA	O3-C3-C4	-2.01	105.83	110.36
3	C	505	NAG	C1-O5-C5	2.00	115.09	112.14
3	B	503	NAG	O5-C5-C6	2.01	111.65	107.34
3	C	506	NAG	O3-C3-C2	2.02	113.70	109.37
5	C	511	MAN	O5-C5-C4	2.03	113.49	110.13
5	A	510	MAN	O2-C2-C1	2.06	113.36	109.23
5	D	508	MAN	O5-C5-C4	2.07	113.56	110.13
3	A	502	NAG	C4-C3-C2	2.07	114.56	111.34
5	A	510	MAN	O2-C2-C3	2.08	114.37	110.19
5	B	508	MAN	C6-C5-C4	2.08	118.20	112.99
4	B	507	BMA	O5-C5-C4	2.10	113.62	110.13
5	D	511	MAN	O2-C2-C1	2.11	113.46	109.23
5	B	510	MAN	C6-C5-C4	2.12	118.31	112.99
3	C	502	NAG	C4-C3-C2	2.18	114.72	111.34
3	D	503	NAG	O3-C3-C2	2.19	114.05	109.37
5	D	510	MAN	O3-C3-C4	2.19	115.29	110.36
3	D	505	NAG	O3-C3-C4	2.19	115.30	110.36
3	C	503	NAG	C4-C3-C2	2.23	114.80	111.34
5	B	508	MAN	O4-C4-C5	2.27	115.22	109.23
3	B	504	NAG	C2-N2-C7	2.28	126.07	123.11
5	B	511	MAN	C3-C4-C5	2.29	114.32	110.23
5	D	511	MAN	C2-C3-C4	2.32	115.10	111.05
5	C	511	MAN	C3-C4-C5	2.38	114.47	110.23
5	B	510	MAN	O5-C5-C6	2.42	112.53	107.34
3	C	503	NAG	O4-C4-C5	2.42	115.61	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	NAG	O3-C3-C2	2.46	114.64	109.37
5	B	508	MAN	C1-O5-C5	2.53	115.87	112.14
3	C	504	NAG	O4-C4-C5	2.60	116.08	109.23
3	C	504	NAG	O5-C5-C6	2.62	112.95	107.34
3	D	504	NAG	O7-C7-N2	2.63	127.20	121.84
3	B	502	NAG	C3-C4-C5	2.64	114.94	110.23
3	C	505	NAG	O5-C5-C4	2.68	114.57	110.13
5	C	510	MAN	O3-C3-C4	2.73	116.50	110.36
5	D	509	MAN	O6-C6-C5	2.75	120.49	111.30
5	C	511	MAN	C1-O5-C5	2.76	116.19	112.14
5	B	510	MAN	O2-C2-C3	2.76	115.75	110.19
5	A	510	MAN	C1-O5-C5	2.78	116.23	112.14
3	D	506	NAG	O3-C3-C2	2.81	115.39	109.37
5	A	509	MAN	C1-O5-C5	2.81	116.28	112.14
5	B	510	MAN	O3-C3-C4	2.84	116.77	110.36
5	B	509	MAN	O2-C2-C3	2.88	115.98	110.19
3	C	502	NAG	O4-C4-C5	2.93	116.93	109.23
5	C	510	MAN	C3-C4-C5	2.93	115.44	110.23
3	A	507	NAG	O3-C3-C2	2.93	115.64	109.37
5	A	511	MAN	O3-C3-C4	2.93	116.97	110.36
3	C	503	NAG	O5-C5-C6	2.97	113.71	107.34
5	D	509	MAN	O5-C5-C4	2.98	115.06	110.13
3	D	504	NAG	O5-C5-C6	2.98	113.72	107.34
5	B	509	MAN	O2-C2-C1	3.02	115.28	109.23
5	B	510	MAN	C3-C4-C5	3.04	115.65	110.23
5	C	510	MAN	O2-C2-C3	3.07	116.38	110.19
3	B	504	NAG	C1-O5-C5	3.16	116.79	112.14
5	A	511	MAN	O2-C2-C1	3.19	115.62	109.23
3	D	502	NAG	O4-C4-C5	3.25	117.78	109.23
5	A	510	MAN	O5-C5-C4	3.26	115.53	110.13
5	A	511	MAN	C6-C5-C4	3.27	121.19	112.99
5	D	510	MAN	O6-C6-C5	3.29	122.28	111.30
5	D	510	MAN	O5-C1-C2	3.32	116.20	110.89
3	B	503	NAG	C2-N2-C7	3.36	127.47	123.11
4	C	507	BMA	O3-C3-C2	3.38	116.21	110.01
5	D	510	MAN	O5-C5-C6	3.39	114.60	107.34
5	D	510	MAN	O3-C3-C2	3.43	116.29	110.01
5	D	509	MAN	O5-C5-C6	3.50	114.84	107.34
3	B	505	NAG	O5-C5-C4	3.52	115.96	110.13
3	B	505	NAG	C1-O5-C5	3.56	117.37	112.14
5	A	511	MAN	O5-C5-C6	3.59	115.02	107.34
3	B	506	NAG	O3-C3-C2	3.59	117.06	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	509	MAN	C3-C4-C5	3.65	116.73	110.23
4	D	507	BMA	O3-C3-C2	3.67	116.73	110.01
5	C	509	MAN	C3-C4-C5	3.71	116.84	110.23
5	B	511	MAN	C1-C2-C3	3.73	114.07	109.55
3	B	505	NAG	O4-C4-C5	3.74	119.08	109.23
3	B	504	NAG	C4-C3-C2	3.75	117.16	111.34
5	D	511	MAN	C3-C4-C5	3.76	116.93	110.23
5	D	509	MAN	C1-O5-C5	3.89	117.85	112.14
5	A	511	MAN	O6-C6-C5	3.90	124.34	111.30
5	C	508	MAN	C1-C2-C3	3.95	114.34	109.55
5	C	510	MAN	O6-C6-C5	4.03	124.75	111.30
5	A	512	MAN	C3-C4-C5	4.03	117.42	110.23
3	A	505	NAG	C1-O5-C5	4.08	118.14	112.14
5	A	511	MAN	O3-C3-C2	4.10	117.52	110.01
5	D	508	MAN	C1-C2-C3	4.27	114.73	109.55
5	D	509	MAN	O2-C2-C1	4.35	117.95	109.23
3	B	506	NAG	C1-O5-C5	4.42	118.64	112.14
5	C	509	MAN	O2-C2-C1	4.66	118.57	109.23
5	C	509	MAN	O5-C5-C4	4.67	117.88	110.13
5	C	509	MAN	C1-O5-C5	4.71	119.06	112.14
3	B	504	NAG	O5-C5-C6	4.96	117.97	107.34
5	C	510	MAN	O3-C3-C2	5.07	119.30	110.01
5	A	511	MAN	C3-C4-C5	5.18	119.47	110.23
3	D	504	NAG	O3-C3-C2	5.43	121.00	109.37
5	D	508	MAN	C1-O5-C5	5.48	120.19	112.14
5	B	511	MAN	C1-O5-C5	5.55	120.31	112.14
5	D	510	MAN	C1-O5-C5	5.67	120.47	112.14
5	D	509	MAN	O5-C1-C2	5.70	120.01	110.89
3	A	504	NAG	C1-O5-C5	6.05	121.03	112.14
5	C	509	MAN	O5-C1-C2	6.85	121.84	110.89
5	C	510	MAN	O5-C5-C6	6.85	122.00	107.34
5	C	508	MAN	C1-O5-C5	7.07	122.53	112.14
3	D	504	NAG	C1-O5-C5	9.03	125.41	112.14

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	511	MAN	C1
3	A	505	NAG	C1
5	B	510	MAN	C1
5	C	510	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	510	MAN	1	0
5	B	511	MAN	1	0
4	C	507	BMA	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 ⓘ

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	388/402 (96%)	-0.38	5 (1%) 79 81	32, 43, 62, 112	0
1	B	388/402 (96%)	-0.41	4 (1%) 84 86	31, 42, 63, 120	0
1	C	388/402 (96%)	-0.52	2 (0%) 91 92	33, 42, 61, 99	0
1	D	388/402 (96%)	-0.43	2 (0%) 91 92	32, 43, 61, 106	0
All	All	1552/1608 (96%)	-0.43	13 (0%) 87 89	31, 43, 62, 120	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	ALA	6.2
1	D	82	ALA	5.4
1	A	82	ALA	4.6
1	B	83	GLU	3.3
1	A	83	GLU	3.1
1	B	246	ALA	3.0
1	A	295	TRP	2.9
1	C	83	GLU	2.8
1	A	318	CYS	2.7
1	D	83	GLU	2.7
1	B	247	SER	2.3
1	B	469	ILE	2.1
1	A	401	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	A	512	11/12	0.81	0.24	3.71	85,100,109,110	0
3	NAG	B	505	14/15	0.95	0.18	2.43	42,52,56,64	0
2	CA	C	501	1/1	0.97	0.17	2.16	84,84,84,84	0
2	CA	A	501	1/1	0.93	0.22	1.36	82,82,82,82	0
3	NAG	C	505	14/15	0.98	0.12	0.26	37,42,46,50	0
3	NAG	D	505	14/15	0.98	0.11	-0.07	37,39,44,45	0
3	NAG	A	506	14/15	0.97	0.11	-0.25	40,47,59,63	0
3	NAG	D	506	14/15	0.98	0.10	-0.50	38,44,49,53	0
2	CA	D	501	1/1	0.95	0.09	-0.53	63,63,63,63	0
2	CA	B	501	1/1	0.97	0.08	-1.07	78,78,78,78	0
5	MAN	B	509	11/12	0.74	0.36	-	96,105,111,112	0
3	NAG	C	506	14/15	0.98	0.10	-	40,45,51,51	0
3	NAG	A	503	14/15	0.78	0.44	-	105,119,126,127	0
3	NAG	B	503	14/15	0.84	0.46	-	101,114,121,124	0
3	NAG	A	507	14/15	0.98	0.12	-	37,43,50,54	0
3	NAG	C	504	14/15	0.81	0.32	-	72,94,106,106	0
3	NAG	B	506	14/15	0.90	0.25	-	53,70,80,82	0
3	NAG	D	503	14/15	0.71	0.55	-	85,115,129,130	0
5	MAN	C	508	11/12	0.96	0.10	-	55,63,76,87	0
3	NAG	D	502	14/15	0.93	0.40	-	61,69,77,90	0
5	MAN	C	509	11/12	0.79	0.19	-	75,82,93,103	0
5	MAN	A	510	11/12	0.91	0.20	-	65,69,80,82	0
3	NAG	A	505	14/15	0.83	0.28	-	85,93,99,99	0
5	MAN	D	510	11/12	0.78	0.17	-	63,74,89,109	0
5	MAN	C	511	11/12	0.68	0.25	-	97,116,126,135	0
5	MAN	B	511	11/12	0.42	0.25	-	75,101,128,140	0
5	MAN	B	510	11/12	0.64	0.35	-	96,115,120,130	0
5	MAN	D	511	11/12	0.72	0.27	-	87,107,117,126	0
4	BMA	C	507	11/12	0.98	0.08	-	49,53,57,68	0
5	MAN	A	509	11/12	0.98	0.14	-	47,49,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	B	507	11/12	0.90	0.33	-	74,84,92,97	0
3	NAG	A	502	14/15	0.84	0.39	-	70,89,102,115	0
3	NAG	D	504	14/15	0.71	0.33	-	74,93,112,113	0
5	MAN	D	508	11/12	0.97	0.12	-	46,56,66,74	0
5	MAN	D	509	11/12	0.89	0.14	-	72,81,88,93	0
4	BMA	A	508	11/12	0.97	0.18	-	41,48,52,59	0
3	NAG	B	502	14/15	0.95	0.32	-	66,80,97,110	0
3	NAG	A	504	14/15	0.89	0.29	-	69,81,95,101	0
5	MAN	C	510	11/12	0.84	0.16	-	64,75,113,119	0
3	NAG	C	503	14/15	0.74	0.41	-	78,115,129,130	0
4	BMA	D	507	11/12	0.97	0.09	-	42,51,57,61	0
5	MAN	A	511	11/12	0.94	0.15	-	58,64,79,79	0
5	MAN	B	508	11/12	0.91	0.28	-	72,82,91,99	0
3	NAG	C	502	14/15	0.90	0.30	-	60,75,83,104	0
3	NAG	B	504	14/15	0.64	0.34	-	89,121,139,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.