



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:42 AM UTC

PDB ID : 3FVC / pdb_00003fvc
Title : Crystal structure of a trimeric variant of the Epstein-Barr virus glycoprotein B
Authors : Backovic, M.
Deposited on : 2009-01-15
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

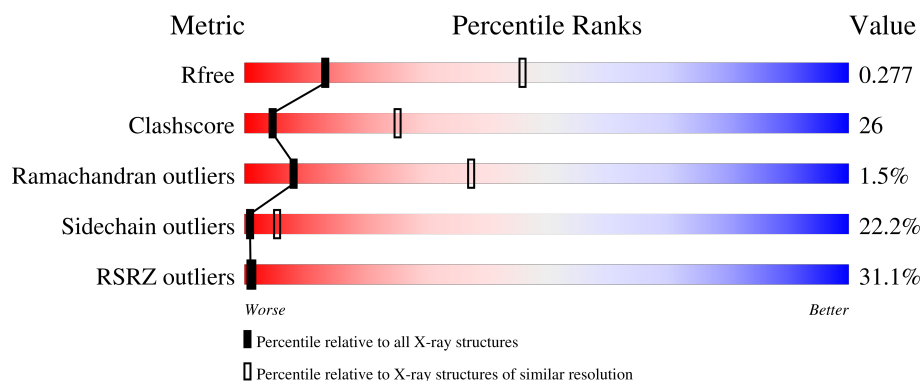
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	663	26% 41% 32% 10% 16%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4552 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.

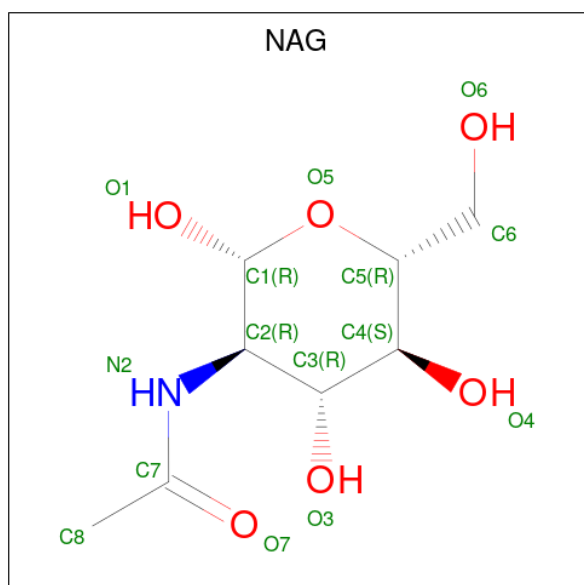
- Molecule 1 is a protein called Glycoprotein GP110.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4501	2833	775	872	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	HIS	TRP	engineered mutation	UNP P03188
A	113	ARG	TYR	engineered mutation	UNP P03188
A	193	ARG	TRP	engineered mutation	UNP P03188
A	194	VAL	LEU	engineered mutation	UNP P03188
A	195	GLU	ILE	engineered mutation	UNP P03188
A	196	ALA	TRP	engineered mutation	UNP P03188

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.80Å 106.80Å 210.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.61 – 3.20 26.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (26.61-3.20) 98.2 (26.61-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.17Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.283 0.238 , 0.277	Depositor DCC
R_{free} test set	2155 reflections (9.25%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	4552	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.96	3/4590 (0.1%)	1.20	31/6209 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	ASN	CA-C	-5.25	1.46	1.52
1	A	332	VAL	CA-CB	5.24	1.61	1.54
1	A	668	ALA	CA-CB	-5.16	1.45	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	CYS	CA-C-N	10.20	130.37	119.05
1	A	295	CYS	C-N-CA	10.20	130.37	119.05
1	A	138	ILE	N-CA-C	-7.88	105.81	113.53
1	A	176	ASN	N-CA-C	6.75	121.09	112.86
1	A	554	ARG	CA-C-N	6.54	128.02	119.84
1	A	554	ARG	C-N-CA	6.54	128.02	119.84
1	A	44	THR	N-CA-C	6.50	119.04	108.26
1	A	233	SER	N-CA-C	6.38	117.74	109.64
1	A	529	VAL	CA-C-N	6.09	126.41	119.83
1	A	529	VAL	C-N-CA	6.09	126.41	119.83
1	A	295	CYS	N-CA-C	6.05	120.31	107.91
1	A	76	ASN	N-CA-C	5.99	118.18	108.41
1	A	250	SER	N-CA-C	-5.87	106.16	113.38
1	A	259	ILE	CB-CA-C	-5.74	102.89	110.98
1	A	138	ILE	N-CA-CB	-5.68	104.46	112.12
1	A	132	THR	N-CA-C	-5.59	104.59	111.75
1	A	132	THR	CA-C-N	-5.59	112.59	122.26
1	A	132	THR	C-N-CA	-5.59	112.59	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	CA-C-N	5.56	125.56	119.89
1	A	169	LYS	C-N-CA	5.56	125.56	119.89
1	A	233	SER	CA-C-N	-5.49	114.16	119.87
1	A	233	SER	C-N-CA	-5.49	114.16	119.87
1	A	281	THR	N-CA-C	-5.48	105.96	113.30
1	A	670	ASN	N-CA-C	5.44	116.89	111.07
1	A	162	VAL	CB-CA-C	-5.38	103.85	111.38
1	A	147	MET	N-CA-C	5.25	116.27	108.60
1	A	238	GLY	CA-C-N	-5.17	118.74	126.86
1	A	238	GLY	C-N-CA	-5.17	118.74	126.86
1	A	143	ASN	N-CA-C	-5.13	107.18	112.93
1	A	540	LYS	N-CA-C	5.11	116.93	111.36
1	A	172	GLY	N-CA-C	-5.09	104.85	112.89

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	4501	0	4362	232	0
2	A	42	0	39	2	0
3	A	9	0	0	0	0
All	All	4552	0	4401	232	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 26.

All (232) 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:A:623:GLN:HG3	1:A:625:PHE:CE1	1.71	1.25
1:A:660:ILE:C	1:A:660:ILE:HD12	1.67	1.17
1:A:361:ARG:HH11	1:A:361:ARG:HG2	0.98	1.08
1:A:533:GLN:HE21	1:A:533:GLN:CA	1.69	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLN:HA	1:A:533:GLN:NE2	1.64	1.04
1:A:554:ARG:HB2	1:A:571:GLN:HE21	1.24	0.99
1:A:361:ARG:HG2	1:A:361:ARG:NH1	1.76	0.96
1:A:533:GLN:HE21	1:A:533:GLN:HA	0.80	0.96
1:A:538:LEU:HA	1:A:557:VAL:HG12	1.47	0.93
1:A:592:SER:OG	1:A:607:ASP:HA	1.72	0.90
1:A:238:GLY:O	1:A:239:LYS:HB2	1.73	0.87
1:A:259:ILE:HD11	1:A:274:ARG:NE	1.90	0.85
1:A:323:THR:O	1:A:323:THR:HG23	1.76	0.85
1:A:602:ILE:HD12	1:A:619:ILE:HD12	1.58	0.85
1:A:623:GLN:CG	1:A:625:PHE:CE1	2.58	0.84
1:A:81:LEU:HD12	1:A:383:LEU:HD11	1.59	0.84
1:A:361:ARG:HH11	1:A:361:ARG:CG	1.87	0.83
1:A:632:LEU:HD23	1:A:632:LEU:H	1.42	0.83
1:A:554:ARG:HB2	1:A:571:GLN:NE2	1.94	0.83
1:A:259:ILE:HD11	1:A:274:ARG:CZ	2.09	0.82
1:A:232:MET:HE2	1:A:244:PHE:CD2	2.14	0.82
1:A:660:ILE:HD12	1:A:660:ILE:O	1.79	0.82
1:A:542:MET:HB2	1:A:608:TYR:HB3	1.63	0.81
1:A:47:PRO:O	1:A:49:ARG:HG3	1.81	0.80
1:A:605:TYR:CD2	1:A:610:HIS:HA	2.17	0.80
1:A:106:ILE:HD11	1:A:187:LEU:HD11	1.62	0.80
1:A:71:PHE:HD2	1:A:71:PHE:C	1.91	0.78
1:A:184:GLN:OE1	1:A:184:GLN:HA	1.81	0.78
1:A:672:ALA:HB1	1:A:675:ARG:NH1	1.99	0.77
1:A:71:PHE:C	1:A:71:PHE:CD2	2.62	0.76
1:A:374:THR:HG22	1:A:376:GLY:H	1.49	0.76
1:A:237:ASP:OD1	1:A:237:ASP:N	2.17	0.76
1:A:184:GLN:OE1	1:A:184:GLN:CA	2.34	0.75
1:A:592:SER:HG	1:A:607:ASP:HA	1.48	0.75
1:A:330:THR:HG21	1:A:372:PHE:HD2	1.50	0.74
1:A:188:TYR:CE2	1:A:201:ARG:HD2	2.24	0.72
1:A:334:ILE:HB	1:A:370:THR:HB	1.70	0.72
1:A:574:THR:O	1:A:575:ASP:HB2	1.89	0.70
1:A:660:ILE:C	1:A:660:ILE:CD1	2.48	0.70
1:A:160:ASP:OD1	1:A:202:THR:HB	1.92	0.70
1:A:295:CYS:SG	1:A:296:PRO:HD2	2.32	0.70
1:A:168:LEU:CD2	1:A:183:SER:HB3	2.22	0.69
1:A:348:ASN:HD22	1:A:348:ASN:C	2.00	0.69
1:A:369:ILE:HD13	1:A:383:LEU:HB3	1.75	0.69
1:A:192:GLY:HA3	1:A:199:ARG:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:GLN:HG3	1:A:625:PHE:HE1	1.51	0.68
1:A:672:ALA:HB1	1:A:675:ARG:HH11	1.57	0.68
1:A:554:ARG:CB	1:A:571:GLN:HE21	2.05	0.68
1:A:81:LEU:HG	1:A:385:LEU:HD11	1.75	0.68
1:A:61:ARG:HG3	1:A:62:PHE:N	2.09	0.67
1:A:605:TYR:CE2	1:A:610:HIS:HB2	2.29	0.67
1:A:330:THR:HG21	1:A:372:PHE:CD2	2.28	0.67
1:A:323:THR:O	1:A:323:THR:CG2	2.43	0.66
1:A:647:ASP:OD2	1:A:647:ASP:N	2.24	0.66
1:A:101:LYS:HD3	1:A:145:VAL:HG22	1.77	0.66
1:A:632:LEU:H	1:A:632:LEU:CD2	2.08	0.66
1:A:374:THR:CG2	1:A:376:GLY:H	2.09	0.65
1:A:383:LEU:O	1:A:383:LEU:HD13	1.97	0.65
1:A:601:GLU:HB3	1:A:615:GLU:HA	1.79	0.65
1:A:593:GLN:O	1:A:594:TYR:HD2	1.80	0.64
1:A:232:MET:HE2	1:A:244:PHE:HD2	1.63	0.63
1:A:168:LEU:HD23	1:A:183:SER:HB3	1.78	0.63
1:A:232:MET:HE1	1:A:244:PHE:HE2	1.64	0.63
1:A:348:ASN:C	1:A:348:ASN:ND2	2.57	0.62
1:A:232:MET:HE2	1:A:244:PHE:CE2	2.34	0.62
1:A:46:PHE:N	1:A:46:PHE:CD2	2.68	0.62
1:A:112:HIS:HB2	1:A:195:GLU:OE2	2.00	0.61
1:A:128:ASP:O	1:A:132:THR:HG23	2.00	0.61
1:A:559:PHE:HE2	1:A:561:PHE:CE2	2.18	0.61
1:A:232:MET:CE	1:A:244:PHE:CE2	2.83	0.61
1:A:509:ILE:HG13	1:A:510:TYR:N	2.15	0.61
1:A:168:LEU:HD12	1:A:208:ILE:HD12	1.82	0.61
1:A:542:MET:HE3	1:A:552:TYR:O	2.00	0.61
1:A:81:LEU:HD12	1:A:383:LEU:CD1	2.31	0.61
1:A:124:LYS:O	1:A:281:THR:HA	2.00	0.61
1:A:626:ILE:HD12	1:A:626:ILE:H	1.66	0.61
1:A:448:LYS:HD2	1:A:449:SER:H	1.66	0.60
1:A:101:LYS:HD3	1:A:145:VAL:CG2	2.32	0.60
1:A:273:ARG:CZ	1:A:288:LEU:HD23	2.31	0.60
1:A:374:THR:HG22	1:A:376:GLY:N	2.15	0.60
1:A:671:ILE:HA	1:A:674:LEU:HD22	1.83	0.59
1:A:138:ILE:O	1:A:139:TYR:HB2	2.02	0.59
1:A:168:LEU:HD12	1:A:208:ILE:CD1	2.33	0.59
1:A:50:VAL:O	1:A:50:VAL:HG13	2.02	0.58
1:A:99:TYR:C	1:A:100:THR:HG22	2.28	0.58
1:A:325:SER:OG	1:A:462:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:HZ	1:A:599:GLY:H	1.52	0.58
1:A:67:GLN:O	1:A:69:PRO:HD3	2.04	0.58
1:A:542:MET:CB	1:A:608:TYR:HB3	2.34	0.58
1:A:626:ILE:HD12	1:A:626:ILE:N	2.19	0.57
1:A:559:PHE:HE2	1:A:561:PHE:CZ	2.22	0.57
1:A:656:ASP:O	1:A:657:LEU:C	2.43	0.57
1:A:678:LEU:O	1:A:679:ASP:C	2.47	0.57
1:A:645:SER:O	1:A:649:GLN:HG2	2.04	0.57
1:A:486:GLU:O	1:A:490:GLN:HG2	2.05	0.57
1:A:600:ASN:C	1:A:601:GLU:HG3	2.30	0.56
1:A:605:TYR:CE2	1:A:610:HIS:HA	2.39	0.56
1:A:658:GLU:HG3	1:A:662:ARG:HD3	1.86	0.56
1:A:55:SER:O	1:A:56:HIS:C	2.48	0.56
1:A:465:TYR:CD1	1:A:465:TYR:C	2.84	0.56
1:A:660:ILE:HD12	1:A:661:PHE:N	2.18	0.56
1:A:259:ILE:CD1	1:A:274:ARG:CZ	2.82	0.55
1:A:313:LYS:O	1:A:331:THR:CG2	2.55	0.55
1:A:672:ALA:CB	1:A:675:ARG:HH11	2.19	0.55
1:A:57:GLY:O	1:A:58:ASP:OD1	2.26	0.54
1:A:354:LYS:HD3	1:A:354:LYS:N	2.23	0.53
1:A:46:PHE:H	1:A:46:PHE:HD2	1.56	0.53
1:A:80:GLY:HA2	1:A:385:LEU:HD12	1.89	0.53
1:A:560:SER:OG	1:A:561:PHE:N	2.42	0.53
1:A:188:TYR:CD2	1:A:201:ARG:HB3	2.44	0.53
1:A:343:ILE:O	1:A:344:GLU:C	2.52	0.52
1:A:331:THR:O	1:A:332:VAL:HB	2.10	0.52
1:A:347:VAL:HG12	1:A:348:ASN:N	2.25	0.52
1:A:348:ASN:HD22	1:A:349:LYS:N	2.08	0.52
1:A:533:GLN:CA	1:A:533:GLN:NE2	2.44	0.52
1:A:623:GLN:HG3	1:A:625:PHE:CZ	2.36	0.51
1:A:380:LEU:HD12	1:A:380:LEU:N	2.26	0.51
1:A:361:ARG:NH1	1:A:361:ARG:CG	2.54	0.51
1:A:144:ALA:CB	2:A:1:NAG:H82	2.41	0.51
1:A:380:LEU:N	1:A:380:LEU:CD1	2.74	0.51
1:A:334:ILE:HG22	1:A:372:PHE:CZ	2.46	0.51
1:A:554:ARG:NH1	1:A:572:LEU:O	2.43	0.50
1:A:593:GLN:NE2	1:A:595:TYR:OH	2.43	0.50
1:A:152:LEU:N	1:A:152:LEU:HD23	2.27	0.50
1:A:247:ARG:HB2	1:A:250:SER:OG	2.11	0.50
1:A:672:ALA:HA	1:A:675:ARG:HD3	1.94	0.50
1:A:542:MET:HB2	1:A:608:TYR:CB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:CE2	1:A:561:PHE:CE2	3.00	0.50
1:A:237:ASP:OD1	1:A:240:ASN:HB2	2.11	0.49
1:A:215:SER:HB2	1:A:222:PHE:HB3	1.94	0.49
1:A:249:ASP:N	1:A:249:ASP:OD1	2.44	0.49
1:A:478:ASP:OD1	1:A:478:ASP:N	2.43	0.49
1:A:295:CYS:SG	1:A:296:PRO:CD	3.00	0.49
1:A:531:VAL:HG12	1:A:561:PHE:CE1	2.47	0.49
1:A:80:GLY:HA3	1:A:382:TRP:CH2	2.48	0.49
1:A:351:MET:SD	1:A:383:LEU:HD12	2.53	0.49
1:A:63:SER:O	1:A:64:SER:C	2.56	0.48
1:A:71:PHE:CZ	1:A:477:GLY:HA2	2.48	0.48
1:A:62:PHE:O	1:A:63:SER:C	2.55	0.48
1:A:129:SER:O	1:A:130:TYR:C	2.55	0.48
1:A:617:ASP:OD1	1:A:617:ASP:N	2.47	0.48
1:A:144:ALA:HB3	2:A:1:NAG:H82	1.95	0.48
1:A:183:SER:HG	1:A:206:CYS:H	1.61	0.48
1:A:232:MET:CE	1:A:244:PHE:HE2	2.22	0.48
1:A:450:LEU:HD12	1:A:450:LEU:H	1.79	0.48
1:A:529:VAL:HG13	1:A:529:VAL:O	2.14	0.48
1:A:656:ASP:O	1:A:660:ILE:HG23	2.12	0.48
1:A:605:TYR:CZ	1:A:610:HIS:HB2	2.49	0.47
1:A:650:ARG:C	1:A:652:SER:H	2.21	0.47
1:A:505:VAL:O	1:A:509:ILE:HG23	2.14	0.47
1:A:129:SER:HA	1:A:132:THR:HG23	1.96	0.47
1:A:372:PHE:HB2	1:A:380:LEU:HB2	1.95	0.47
1:A:60:PHE:CD1	1:A:60:PHE:N	2.81	0.47
1:A:379:LEU:HB2	1:A:450:LEU:HD23	1.96	0.47
1:A:505:VAL:O	1:A:509:ILE:CG2	2.63	0.47
1:A:575:ASP:O	1:A:576:ASN:HB2	2.14	0.47
1:A:238:GLY:O	1:A:239:LYS:CB	2.49	0.47
1:A:497:LEU:HD23	1:A:497:LEU:HA	1.77	0.47
1:A:181:TYR:O	1:A:207:LEU:HD23	2.16	0.46
1:A:259:ILE:HD12	1:A:259:ILE:HG21	1.71	0.46
1:A:328:THR:OG1	1:A:330:THR:HG23	2.16	0.46
1:A:461:ILE:C	1:A:463:PHE:N	2.74	0.45
1:A:448:LYS:HD2	1:A:449:SER:N	2.32	0.45
1:A:221:PHE:C	1:A:221:PHE:CD2	2.95	0.45
1:A:313:LYS:O	1:A:331:THR:HG22	2.15	0.45
1:A:355:TYR:CD1	1:A:355:TYR:C	2.92	0.45
1:A:657:LEU:HA	1:A:657:LEU:HD22	1.64	0.45
1:A:150:ASP:C	1:A:152:LEU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:MET:HE3	1:A:246:GLU:HG3	1.99	0.45
1:A:108:ILE:O	1:A:108:ILE:HG23	2.17	0.45
1:A:138:ILE:HD13	1:A:138:ILE:HG21	1.66	0.45
1:A:143:ASN:HB2	1:A:158:ASP:HB2	1.98	0.45
1:A:318:VAL:HG11	1:A:470:ARG:HH12	1.82	0.45
1:A:510:TYR:HD2	1:A:514:VAL:HG11	1.82	0.45
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.72	0.44
1:A:259:ILE:HD11	1:A:274:ARG:CD	2.46	0.44
1:A:141:CYS:O	1:A:166:VAL:HG22	2.17	0.44
1:A:66:ILE:CG1	1:A:488:LYS:HA	2.47	0.44
1:A:71:PHE:CE1	1:A:480:ALA:HB2	2.53	0.44
1:A:313:LYS:O	1:A:331:THR:HG23	2.18	0.44
1:A:574:THR:O	1:A:575:ASP:CB	2.62	0.44
1:A:184:GLN:OE1	1:A:184:GLN:C	2.60	0.43
1:A:518:ARG:HE	1:A:518:ARG:HB3	1.66	0.43
1:A:509:ILE:HD12	1:A:509:ILE:O	2.18	0.43
1:A:257:TYR:CD2	1:A:274:ARG:HD3	2.53	0.43
1:A:306:THR:HG22	1:A:319:THR:HB	2.00	0.43
1:A:550:MET:HE2	1:A:550:MET:HB3	1.91	0.43
1:A:498:THR:HG22	1:A:505:VAL:HG11	2.01	0.43
1:A:554:ARG:HA	1:A:555:PRO:HD3	1.91	0.43
1:A:604:VAL:O	1:A:605:TYR:HD2	2.01	0.43
1:A:193:ARG:H	1:A:193:ARG:HG2	1.69	0.43
1:A:321:GLU:C	1:A:323:THR:H	2.26	0.43
1:A:140:GLN:HA	1:A:166:VAL:O	2.19	0.43
1:A:605:TYR:CE2	1:A:610:HIS:CB	2.98	0.43
1:A:184:GLN:N	1:A:205:ASN:OD1	2.40	0.43
1:A:494:LEU:O	1:A:498:THR:HG23	2.19	0.43
1:A:542:MET:HE2	1:A:608:TYR:CD2	2.53	0.43
1:A:49:ARG:HD3	1:A:513:ALA:HB1	1.99	0.42
1:A:664:TYR:CD2	1:A:664:TYR:C	2.97	0.42
1:A:259:ILE:HG23	1:A:259:ILE:HD13	1.76	0.42
1:A:63:SER:C	1:A:65:ASP:N	2.74	0.42
1:A:283:THR:HG22	1:A:284:LEU:N	2.33	0.42
1:A:303:PHE:HB3	1:A:306:THR:CG2	2.49	0.42
1:A:576:ASN:HD21	1:A:598:SER:HA	1.83	0.42
1:A:108:ILE:HD13	1:A:108:ILE:C	2.45	0.42
1:A:174:LEU:O	1:A:175:ALA:C	2.62	0.42
1:A:265:ARG:HE	1:A:265:ARG:HB2	1.31	0.42
1:A:217:SER:HA	1:A:219:PHE:N	2.35	0.42
1:A:650:ARG:C	1:A:652:SER:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:O	1:A:355:TYR:C	2.63	0.42
1:A:58:ASP:O	1:A:525:VAL:N	2.52	0.42
1:A:104:THR:HB	1:A:203:THR:HG23	2.02	0.42
1:A:457:ALA:O	1:A:458:THR:C	2.61	0.42
1:A:542:MET:HE2	1:A:608:TYR:HD2	1.85	0.41
1:A:539:ARG:HD3	1:A:556:LEU:CB	2.49	0.41
1:A:71:PHE:HZ	1:A:476:LEU:O	2.03	0.41
1:A:576:ASN:HD21	1:A:598:SER:CA	2.33	0.41
1:A:602:ILE:HG22	1:A:603:HIS:N	2.36	0.41
1:A:358:VAL:O	1:A:358:VAL:HG13	2.20	0.41
1:A:295:CYS:HA	1:A:296:PRO:HD3	1.69	0.41
1:A:366:GLN:OE1	1:A:384:PRO:HD3	2.20	0.41
1:A:85:PHE:O	1:A:378:LEU:HD12	2.21	0.41
1:A:159:ARG:O	1:A:160:ASP:C	2.63	0.41
1:A:360:ASP:OD2	1:A:360:ASP:N	2.53	0.41
1:A:461:ILE:O	1:A:462:GLN:C	2.63	0.41
1:A:650:ARG:O	1:A:652:SER:N	2.54	0.41
1:A:201:ARG:HH11	1:A:201:ARG:HD3	1.68	0.40
1:A:324:SER:HB2	1:A:459:VAL:HG23	2.02	0.40
1:A:299:HIS:CG	1:A:346:GLN:HE22	2.40	0.40
1:A:63:SER:O	1:A:65:ASP:N	2.55	0.40
1:A:66:ILE:HG12	1:A:488:LYS:HA	2.04	0.40
1:A:85:PHE:CD1	1:A:299:HIS:HA	2.56	0.40

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	547/663 (82%)	479 (88%)	60 (11%)	8 (2%)	8 37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	VAL
1	A	341	LYS
1	A	651	ALA
1	A	48	PHE
1	A	534	ALA
1	A	503	THR
1	A	358	VAL
1	A	57	GLY

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	500/585 (86%)	389 (78%)	111 (22%)	1 5

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	46	PHE
1	A	49	ARG
1	A	51	CYS
1	A	59	LEU
1	A	64	SER
1	A	66	ILE
1	A	71	PHE
1	A	76	ASN
1	A	78	THR
1	A	84	VAL
1	A	86	LYS
1	A	87	ASP
1	A	88	ASN
1	A	96	VAL
1	A	99	TYR
1	A	100	THR
1	A	105	ASN
1	A	107	LEU

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Mol	Chain	Res	Type
1	A	108	ILE
1	A	138	ILE
1	A	148	THR
1	A	152	LEU
1	A	153	THR
1	A	155	VAL
1	A	157	VAL
1	A	176	ASN
1	A	178	VAL
1	A	179	ARG
1	A	184	GLN
1	A	187	LEU
1	A	199	ARG
1	A	200	THR
1	A	202	THR
1	A	203	THR
1	A	207	LEU
1	A	223	VAL
1	A	229	THR
1	A	232	MET
1	A	241	LYS
1	A	242	GLU
1	A	243	THR
1	A	247	ARG
1	A	253	VAL
1	A	255	THR
1	A	259	ILE
1	A	267	THR
1	A	279	LYS
1	A	284	LEU
1	A	297	LEU
1	A	302	THR
1	A	304	ASP
1	A	309	THR
1	A	318	VAL
1	A	319	THR
1	A	323	THR
1	A	327	VAL
1	A	334	ILE
1	A	342	CYS
1	A	347	VAL
1	A	348	ASN

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Mol	Chain	Res	Type
1	A	354	LYS
1	A	358	VAL
1	A	360	ASP
1	A	361	ARG
1	A	364	LYS
1	A	373	ILE
1	A	374	THR
1	A	378	LEU
1	A	383	LEU
1	A	386	THR
1	A	448	LYS
1	A	450	LEU
1	A	453	LEU
1	A	472	ILE
1	A	475	MET
1	A	478	ASP
1	A	479	LEU
1	A	481	ARG
1	A	488	LYS
1	A	489	ARG
1	A	509	ILE
1	A	510	TYR
1	A	512	LYS
1	A	523	ILE
1	A	531	VAL
1	A	533	GLN
1	A	540	LYS
1	A	550	MET
1	A	554	ARG
1	A	557	VAL
1	A	567	THR
1	A	569	GLU
1	A	574	THR
1	A	591	THR
1	A	601	GLU
1	A	614	ILE
1	A	617	ASP
1	A	625	PHE
1	A	632	LEU
1	A	643	LEU
1	A	647	ASP
1	A	650	ARG

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Mol	Chain	Res	Type
1	A	652	SER
1	A	657	LEU
1	A	660	ILE
1	A	663	GLU
1	A	670	ASN
1	A	671	ILE
1	A	674	LEU
1	A	678	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	134	GLN
1	A	140	GLN
1	A	228	GLN
1	A	252	HIS
1	A	256	ASN
1	A	329	ASN
1	A	346	GLN
1	A	348	ASN
1	A	533	GLN
1	A	571	GLN
1	A	576	ASN
1	A	593	GLN
1	A	669	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1	1	14,14,15	0.87	0	17,19,21	2.39	5 (29%)
2	NAG	A	687	1	14,14,15	0.83	1 (7%)	17,19,21	1.34	1 (5%)
2	NAG	A	686	1	14,14,15	0.97	1 (7%)	17,19,21	1.67	3 (17%)

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	1	1	-	0/6/23/26	0/1/1/1
2	NAG	A	687	1	-	2/6/23/26	0/1/1/1
2	NAG	A	686	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	686	NAG	C8-C7	2.37	1.55	1.50
2	A	687	NAG	C1-C2	2.19	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C1-O5-C5	6.57	121.00	112.19
2	A	687	NAG	C1-O5-C5	4.14	117.73	112.19
2	A	686	NAG	O5-C5-C6	4.07	115.59	107.66
2	A	1	NAG	O5-C1-C2	-3.78	105.44	111.29
2	A	1	NAG	C2-N2-C7	3.35	127.39	122.90
2	A	686	NAG	C4-C3-C2	-3.30	106.18	111.02
2	A	686	NAG	C1-C2-N2	3.09	115.30	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C1-C2-N2	-2.60	106.33	110.43
2	A	1	NAG	O4-C4-C5	2.59	115.69	109.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	687	NAG	O5-C5-C6-O6
2	A	687	NAG	C4-C5-C6-O6
2	A	686	NAG	C8-C7-N2-C2
2	A	686	NAG	C4-C5-C6-O6
2	A	686	NAG	O5-C5-C6-O6
2	A	686	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	2	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, 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	559/663 (84%)	1.66	174 (31%) ⓘ ⓘ	57, 77, 100, 108	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	565	THR	8.2
1	A	566	LYS	7.8
1	A	331	THR	7.1
1	A	332	VAL	6.1
1	A	552	TYR	5.9
1	A	53	LEU	5.7
1	A	550	MET	5.6
1	A	52	GLU	5.4
1	A	590	ALA	5.1
1	A	592	SER	5.1
1	A	68	CYS	4.8
1	A	334	ILE	4.8
1	A	65	ASP	4.7
1	A	551	CYS	4.7
1	A	561	PHE	4.6
1	A	575	ASP	4.4
1	A	42	GLN	4.4
1	A	141	CYS	4.4
1	A	555	PRO	4.2
1	A	267	THR	4.1
1	A	113	ARG	4.1
1	A	191	PRO	4.1
1	A	109	TYR	4.0
1	A	510	TYR	4.0
1	A	616	LEU	4.0
1	A	119	ASN	3.9
1	A	336	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	594	TYR	3.8
1	A	200	THR	3.8
1	A	66	ILE	3.8
1	A	106	ILE	3.8
1	A	620	ALA	3.8
1	A	615	GLU	3.8
1	A	603	HIS	3.8
1	A	199	ARG	3.8
1	A	579	PHE	3.8
1	A	118	THR	3.7
1	A	330	THR	3.7
1	A	554	ARG	3.7
1	A	122	GLU	3.6
1	A	335	GLU	3.6
1	A	591	THR	3.6
1	A	114	ALA	3.6
1	A	516	ALA	3.6
1	A	198	TYR	3.6
1	A	572	LEU	3.6
1	A	57	GLY	3.5
1	A	609	HIS	3.5
1	A	625	PHE	3.5
1	A	624	THR	3.5
1	A	189	ASP	3.5
1	A	578	ILE	3.5
1	A	190	ALA	3.4
1	A	158	ASP	3.4
1	A	304	ASP	3.4
1	A	536	VAL	3.4
1	A	128	ASP	3.4
1	A	514	VAL	3.4
1	A	203	THR	3.4
1	A	513	ALA	3.3
1	A	569	GLU	3.3
1	A	130	TYR	3.3
1	A	107	LEU	3.3
1	A	105	ASN	3.3
1	A	116	SER	3.2
1	A	614	ILE	3.2
1	A	188	TYR	3.2
1	A	538	LEU	3.1
1	A	202	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	596	PHE	3.1
1	A	577	GLU	3.1
1	A	146	LYS	3.0
1	A	535	THR	3.0
1	A	117	VAL	2.9
1	A	43	GLN	2.9
1	A	44	THR	2.9
1	A	543	ARG	2.9
1	A	54	SER	2.9
1	A	162	VAL	2.9
1	A	192	GLY	2.9
1	A	160	ASP	2.9
1	A	622	LEU	2.9
1	A	194	VAL	2.9
1	A	201	ARG	2.9
1	A	568	TYR	2.9
1	A	388	ARG	2.8
1	A	484	CYS	2.8
1	A	390	LEU	2.8
1	A	521	ASP	2.8
1	A	197	THR	2.8
1	A	560	SER	2.7
1	A	204	VAL	2.7
1	A	470	ARG	2.7
1	A	70	SER	2.7
1	A	313	LYS	2.7
1	A	357	ALA	2.7
1	A	597	GLN	2.7
1	A	389	SER	2.6
1	A	112	HIS	2.6
1	A	108	ILE	2.6
1	A	314	SER	2.6
1	A	466	ASP	2.6
1	A	103	VAL	2.6
1	A	142	TYR	2.6
1	A	55	SER	2.6
1	A	102	ILE	2.5
1	A	56	HIS	2.5
1	A	206	CYS	2.5
1	A	553	SER	2.5
1	A	278	ASP	2.5
1	A	630	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	51	CYS	2.5
1	A	623	GLN	2.5
1	A	163	ASN	2.5
1	A	272	GLU	2.5
1	A	637	ASP	2.5
1	A	63	SER	2.5
1	A	67	GLN	2.5
1	A	606	ASN	2.5
1	A	679	ASP	2.5
1	A	121	HIS	2.5
1	A	627	SER	2.5
1	A	605	TYR	2.5
1	A	183	SER	2.4
1	A	310	GLU	2.4
1	A	104	THR	2.4
1	A	115	ASP	2.4
1	A	607	ASP	2.4
1	A	520	GLY	2.4
1	A	164	ILE	2.4
1	A	143	ASN	2.4
1	A	475	MET	2.4
1	A	60	PHE	2.4
1	A	321	GLU	2.4
1	A	76	ASN	2.3
1	A	196	ALA	2.3
1	A	339	ALA	2.3
1	A	342	CYS	2.3
1	A	167	ASN	2.3
1	A	501	ASN	2.3
1	A	320	ASP	2.3
1	A	79	GLU	2.3
1	A	496	GLU	2.3
1	A	47	PRO	2.3
1	A	368	ALA	2.3
1	A	138	ILE	2.2
1	A	537	THR	2.2
1	A	621	THR	2.2
1	A	266	GLY	2.2
1	A	312	GLY	2.2
1	A	46	PHE	2.2
1	A	311	THR	2.2
1	A	75	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	111	GLY	2.2
1	A	134	GLN	2.2
1	A	602	ILE	2.2
1	A	528	CYS	2.2
1	A	58	ASP	2.2
1	A	159	ARG	2.2
1	A	526	SER	2.2
1	A	541	SER	2.2
1	A	205	ASN	2.2
1	A	534	ALA	2.1
1	A	611	PHE	2.1
1	A	327	VAL	2.1
1	A	207	LEU	2.1
1	A	120	ARG	2.1
1	A	268	ASN	2.1
1	A	154	ARG	2.0
1	A	176	ASN	2.0
1	A	515	ALA	2.0
1	A	613	THR	2.0
1	A	367	GLU	2.0
1	A	187	LEU	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NAG	A	687	14/15	0.10	0.27	102,106,107,107	0
2	NAG	A	686	14/15	0.49	0.22	99,102,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	1	14/15	0.74	0.17	68,69,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.