



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:27 AM UTC

PDB ID : 9HJ9 / pdb_00009hj9
Title : H1-H3 chimeric hemagglutinin
Authors : Seraj, N.; Harshbarger, W.; Mallett, C.P.; Vassilev, V.
Deposited on : 2024-11-28
Resolution : 2.06 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

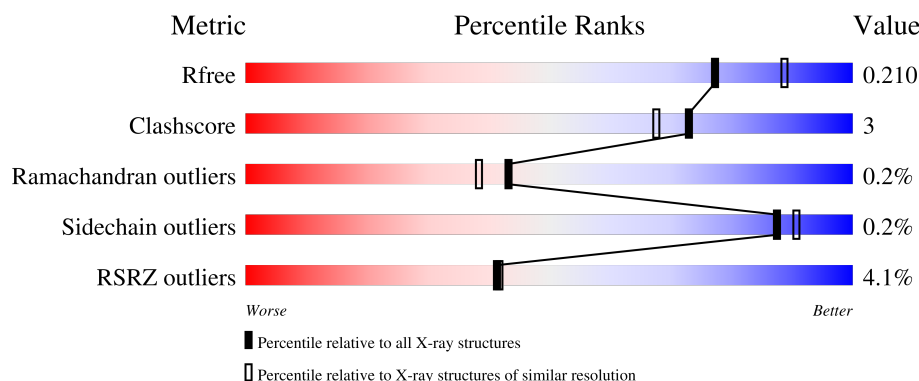
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	B	227	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>7%</div> </div> </div>
2	C	237	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
3	D	222	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>.</div> <div>.</div> </div> </div>
4	A	2	<div> <div>50%</div> <div>50%</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
9	GOL	D	302	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5637 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	212	Total	C	N	O	S	0	1	0
			1674	1069	285	316	4			

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	132	GLN	-	expression tag	UNP A7Y8A2
B	133	ASN	-	expression tag	UNP A7Y8A2
B	134	GLY	-	expression tag	UNP A7Y8A2
B	135	GLY	-	expression tag	UNP A7Y8A2
B	136	SER	-	expression tag	UNP A7Y8A2
B	137	ASN	-	expression tag	UNP A7Y8A2
B	138	SER	-	expression tag	UNP A7Y8A2
B	139	CYS	-	expression tag	UNP A7Y8A2
B	140	SER	-	expression tag	UNP A7Y8A2
B	141	HIS	-	expression tag	UNP A7Y8A2
B	142	ASN	-	expression tag	UNP A7Y8A2
B	143	GLY	-	expression tag	UNP A7Y8A2
B	144	GLU	-	expression tag	UNP A7Y8A2
B	145	SER	-	expression tag	UNP A7Y8A2
B	146	SER	-	expression tag	UNP A7Y8A2
B	147	PHE	-	expression tag	UNP A7Y8A2
B	148	TYR	-	expression tag	UNP A7Y8A2
B	149	LYS	-	expression tag	UNP A7Y8A2
B	150	ASN	-	expression tag	UNP A7Y8A2
B	151	LEU	-	expression tag	UNP A7Y8A2
B	152	LEU	-	expression tag	UNP A7Y8A2
B	153	TRP	-	expression tag	UNP A7Y8A2
B	154	LEU	-	expression tag	UNP A7Y8A2
B	155	THR	-	expression tag	UNP A7Y8A2
B	156	LYS	-	expression tag	UNP A7Y8A2
B	157	SER	-	expression tag	UNP A7Y8A2
B	158	GLY	-	expression tag	UNP A7Y8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	159	SER	-	expression tag	UNP A7Y8A2
B	160	LEU	-	expression tag	UNP A7Y8A2
B	161	TYR	-	expression tag	UNP A7Y8A2
B	162	PRO	-	expression tag	UNP A7Y8A2
B	163	ASN	-	expression tag	UNP A7Y8A2
B	164	LEU	-	expression tag	UNP A7Y8A2
B	165	SER	-	expression tag	UNP A7Y8A2
B	166	LYS	-	expression tag	UNP A7Y8A2
B	167	SER	-	expression tag	UNP A7Y8A2
B	168	TYR	-	expression tag	UNP A7Y8A2
B	169	ALA	-	expression tag	UNP A7Y8A2
B	170	ASN	-	expression tag	UNP A7Y8A2
B	171	ASN	-	expression tag	UNP A7Y8A2
B	172	LYS	-	expression tag	UNP A7Y8A2
B	173	GLU	-	expression tag	UNP A7Y8A2
B	174	LYS	-	expression tag	UNP A7Y8A2
B	175	GLU	-	expression tag	UNP A7Y8A2
B	176	VAL	-	expression tag	UNP A7Y8A2
B	177	LEU	-	expression tag	UNP A7Y8A2
B	178	VAL	-	expression tag	UNP A7Y8A2
B	179	LEU	-	expression tag	UNP A7Y8A2
B	180	TRP	-	expression tag	UNP A7Y8A2
B	181	GLY	-	expression tag	UNP A7Y8A2
B	182	VAL	-	expression tag	UNP A7Y8A2
B	183	HIS	-	expression tag	UNP A7Y8A2
B	184	HIS	-	expression tag	UNP A7Y8A2
B	185	PRO	-	expression tag	UNP A7Y8A2
B	186	PRO	-	expression tag	UNP A7Y8A2
B	187	THR	-	expression tag	UNP A7Y8A2
B	188	ILE	-	expression tag	UNP A7Y8A2
B	189	GLN	-	expression tag	UNP A7Y8A2
B	190	GLU	-	expression tag	UNP A7Y8A2
B	191	GLN	-	expression tag	UNP A7Y8A2
B	192	THR	-	expression tag	UNP A7Y8A2
B	193	SER	-	expression tag	UNP A7Y8A2
B	194	LEU	-	expression tag	UNP A7Y8A2
B	195	TYR	-	expression tag	UNP A7Y8A2
B	196	VAL	-	expression tag	UNP A7Y8A2
B	197	LYS	-	expression tag	UNP A7Y8A2
B	198	GLU	-	expression tag	UNP A7Y8A2
B	199	ASN	-	expression tag	UNP A7Y8A2
B	200	ALA	-	expression tag	UNP A7Y8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	201	TYR	-	expression tag	UNP A7Y8A2
B	202	VAL	-	expression tag	UNP A7Y8A2
B	203	SER	-	expression tag	UNP A7Y8A2
B	204	VAL	-	expression tag	UNP A7Y8A2
B	205	VAL	-	expression tag	UNP A7Y8A2
B	206	SER	-	expression tag	UNP A7Y8A2
B	207	SER	-	expression tag	UNP A7Y8A2
B	208	HIS	-	expression tag	UNP A7Y8A2
B	209	TYR	-	expression tag	UNP A7Y8A2
B	210	SER	-	expression tag	UNP A7Y8A2
B	211	ARG	-	expression tag	UNP A7Y8A2
B	212	LYS	-	expression tag	UNP A7Y8A2
B	213	PHE	-	expression tag	UNP A7Y8A2
B	214	THR	-	expression tag	UNP A7Y8A2
B	215	PRO	-	expression tag	UNP A7Y8A2
B	216	GLU	-	expression tag	UNP A7Y8A2
B	217	ILE	-	expression tag	UNP A7Y8A2
B	218	ALA	-	expression tag	UNP A7Y8A2
B	219	LYS	-	expression tag	UNP A7Y8A2
B	220	ARG	-	expression tag	UNP A7Y8A2
B	221	PRO	-	expression tag	UNP A7Y8A2
B	222	LYS	-	expression tag	UNP A7Y8A2
B	223	VAL	-	expression tag	UNP A7Y8A2
B	224	ARG	-	expression tag	UNP A7Y8A2
B	225	ASP	-	expression tag	UNP A7Y8A2
B	226	GLN	-	expression tag	UNP A7Y8A2
B	227	GLU	-	expression tag	UNP A7Y8A2
B	228	GLY	-	expression tag	UNP A7Y8A2
B	229	ARG	-	expression tag	UNP A7Y8A2
B	230	ILE	-	expression tag	UNP A7Y8A2
B	231	ASN	-	expression tag	UNP A7Y8A2
B	232	TYR	-	expression tag	UNP A7Y8A2
B	233	TYR	-	expression tag	UNP A7Y8A2
B	234	TRP	-	expression tag	UNP A7Y8A2
B	235	THR	-	expression tag	UNP A7Y8A2
B	236	LEU	-	expression tag	UNP A7Y8A2
B	237	LEU	-	expression tag	UNP A7Y8A2
B	238	GLU	-	expression tag	UNP A7Y8A2
B	239	PRO	-	expression tag	UNP A7Y8A2
B	240	GLY	-	expression tag	UNP A7Y8A2
B	241	ASP	-	expression tag	UNP A7Y8A2
B	242	THR	-	expression tag	UNP A7Y8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	243	ILE	-	expression tag	UNP A7Y8A2
B	244	ILE	-	expression tag	UNP A7Y8A2
B	245	PHE	-	expression tag	UNP A7Y8A2
B	246	GLU	-	expression tag	UNP A7Y8A2
B	247	ALA	-	expression tag	UNP A7Y8A2
B	248	ASN	-	expression tag	UNP A7Y8A2
B	249	GLY	-	expression tag	UNP A7Y8A2
B	250	ASN	-	expression tag	UNP A7Y8A2
B	251	LEU	-	expression tag	UNP A7Y8A2
B	252	ILE	-	expression tag	UNP A7Y8A2
B	253	ALA	-	expression tag	UNP A7Y8A2
B	254	PRO	-	expression tag	UNP A7Y8A2
B	255	ARG	-	expression tag	UNP A7Y8A2
B	256	TYR	-	expression tag	UNP A7Y8A2
B	257	ALA	-	expression tag	UNP A7Y8A2
B	258	PHE	-	expression tag	UNP A7Y8A2
B	259	ALA	-	expression tag	UNP A7Y8A2
B	260	LEU	-	expression tag	UNP A7Y8A2
B	261	SER	-	expression tag	UNP A7Y8A2
B	262	ARG	-	expression tag	UNP A7Y8A2
B	263	GLY	-	expression tag	UNP A7Y8A2
B	264	SER	-	expression tag	UNP A7Y8A2
B	265	GLY	-	expression tag	UNP A7Y8A2
B	266	LEU	-	expression tag	UNP A7Y8A2
B	267	VAL	-	expression tag	UNP A7Y8A2
B	268	PRO	-	expression tag	UNP A7Y8A2
B	269	ARG	-	expression tag	UNP A7Y8A2
B	270	GLY	-	expression tag	UNP A7Y8A2
B	271	SER	-	expression tag	UNP A7Y8A2
B	272	GLY	-	expression tag	UNP A7Y8A2
B	273	HIS	-	expression tag	UNP A7Y8A2
B	274	HIS	-	expression tag	UNP A7Y8A2
B	275	HIS	-	expression tag	UNP A7Y8A2
B	276	HIS	-	expression tag	UNP A7Y8A2
B	277	HIS	-	expression tag	UNP A7Y8A2
B	278	HIS	-	expression tag	UNP A7Y8A2

- Molecule 2 is a protein called FluA-20 fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	227	Total	C	N	O	S	0	4	0
			1701	1073	274	347	7			

- Molecule 3 is a protein called FluA-20 fab light chain.

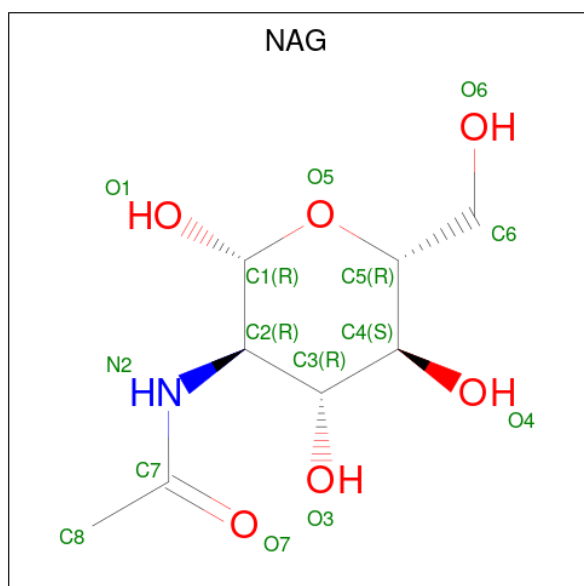
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	1	0
			1629	1024	271	329	5			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

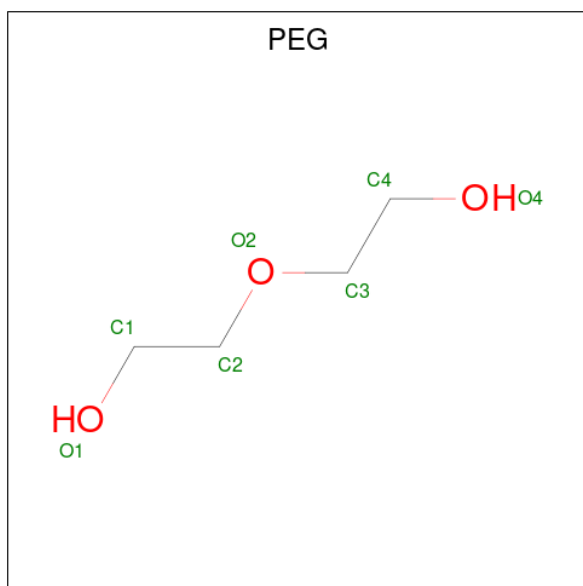


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

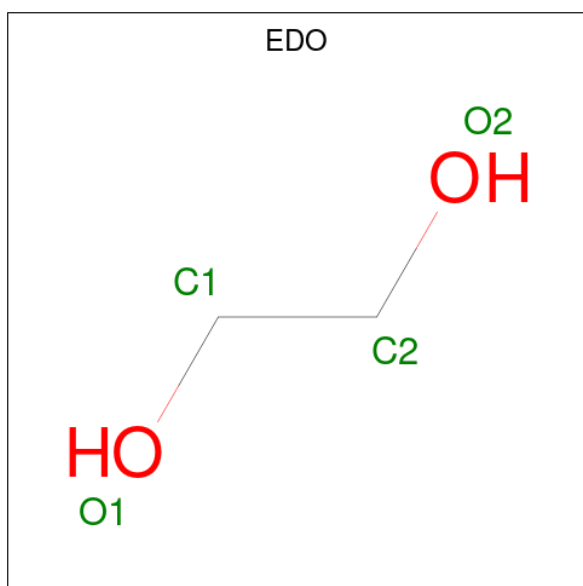
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



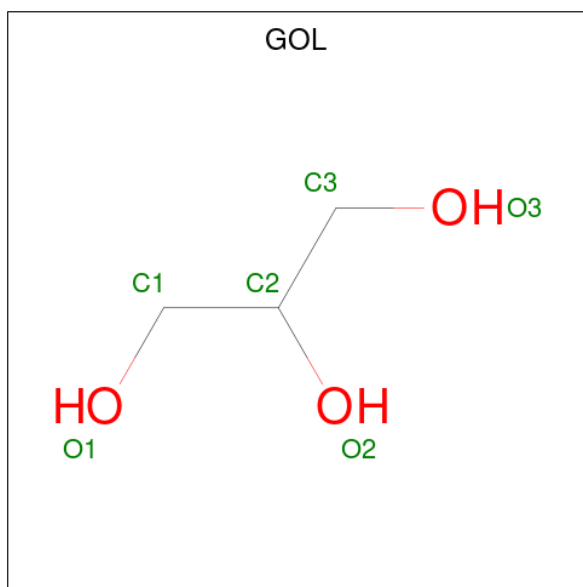
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	159	Total	O	0	0
			159	159		
10	C	208	Total	O	0	0
			208	208		
10	D	202	Total	O	0	0
			202	202		

3 Residue-property plots [i](#)


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

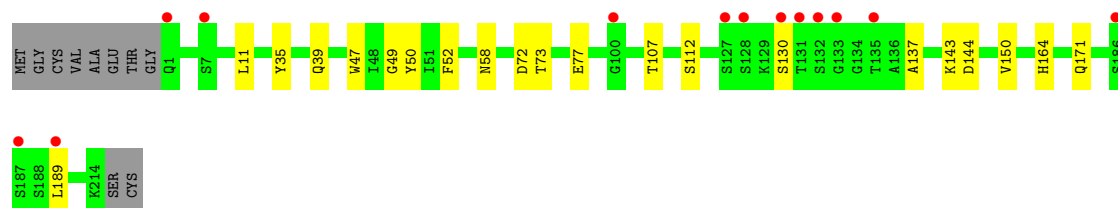
- Molecule 1: Hemagglutinin

Chain B: 



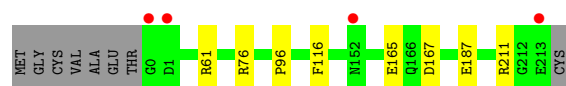
- Molecule 2: FluA-20 fab heavy chain

Chain C: 



- Molecule 3: FluA-20 fab light chain

Chain D: 



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.64Å 93.47Å 86.43Å 90.00° 93.48° 90.00°	Depositor
Resolution (Å)	44.82 – 2.06 44.82 – 2.06	Depositor EDS
% Data completeness (in resolution range)	72.9 (44.82-2.06) 92.0 (44.82-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.168 , 0.210 0.168 , 0.210	Depositor DCC
R_{free} test set	1993 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5637	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, NA, PEG, EDO

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	B	0.13	0/1728	0.34	0/2356
2	C	0.17	0/1756	0.40	0/2404
3	D	0.16	0/1669	0.38	0/2271
All	All	0.15	0/5153	0.37	0/7031

There are no bond length outliers.

There are no bond angle outliers.

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	B	1674	0	1572	6	0
2	C	1701	0	1645	19	0
3	D	1629	0	1559	10	0
4	A	28	0	25	0	0
5	B	14	0	13	0	0
6	B	1	0	0	0	0
7	C	7	0	10	1	0
8	C	4	0	6	0	0
8	D	4	0	6	0	0
9	D	6	0	8	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	159	0	0	1	0
10	C	208	0	0	2	0
10	D	202	0	0	0	0
All	All	5637	0	4844	32	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.

All (32) 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)
2:C:143:LYS:NZ	2:C:171:GLN:OE1	2.30	0.65
2:C:164:HIS:ND1	9:D:302:GOL:H2	2.13	0.64
3:D:167:ASP:OD2	9:D:302:GOL:O2	2.21	0.59
2:C:39:GLN:NE2	10:C:402:HOH:O	2.26	0.57
3:D:167:ASP:HB2	9:D:302:GOL:H12	1.88	0.56
3:D:165:GLU:O	9:D:302:GOL:H11	2.09	0.53
2:C:164:HIS:CE1	9:D:302:GOL:H2	2.43	0.52
2:C:47:TRP:CH2	2:C:49:GLY:HA2	2.47	0.50
1:B:163:ASN:ND2	10:B:406:HOH:O	2.43	0.49
2:C:47:TRP:CD2	3:D:96:PRO:HD2	2.48	0.49
2:C:130:SER:HA	3:D:116:PHE:HD2	1.77	0.48
2:C:47:TRP:CE3	3:D:96:PRO:HD2	2.49	0.47
2:C:73:THR:HG23	10:C:457:HOH:O	2.13	0.47
1:B:97:GLY:HA3	1:B:230:ILE:O	2.15	0.46
2:C:11:LEU:HD22	2:C:112:SER:HB3	1.97	0.46
3:D:167:ASP:CA	9:D:302:GOL:H12	2.47	0.45
2:C:130:SER:OG	2:C:130:SER:O	2.35	0.44
2:C:72:ASP:HB3	2:C:77[B]:GLU:HG2	1.99	0.43
2:C:107:THR:HA	7:C:301:PEG:H12	1.99	0.43
1:B:65:ILE:HD12	1:B:65:ILE:HA	1.90	0.43
2:C:130:SER:OG	2:C:137:ALA:O	2.27	0.43
2:C:72:ASP:HB3	2:C:77[B]:GLU:CG	2.49	0.43
2:C:189:LEU:HD23	2:C:189:LEU:HA	1.87	0.42
3:D:61:ARG:HB2	3:D:76:ARG:O	2.19	0.41
1:B:201:TYR:HB2	1:B:212:LYS:HE3	2.02	0.41
2:C:50:TYR:CE2	2:C:58:ASN:HB3	2.55	0.41
2:C:143:LYS:HG2	2:C:144:ASP:CG	2.45	0.41
1:B:69:PRO:HB2	1:B:141:HIS:HB2	2.01	0.41
3:D:167:ASP:CB	9:D:302:GOL:H12	2.50	0.41
1:B:52:ALA:HA	1:B:53:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:GLU:O	3:D:211:ARG:NH2	2.54	0.40
2:C:35:TYR:HB3	2:C:52:PHE:CZ	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	B	211/227 (93%)	206 (98%)	4 (2%)	1 (0%)	24	17
2	C	229/237 (97%)	223 (97%)	6 (3%)	0	100	100
3	D	213/222 (96%)	206 (97%)	7 (3%)	0	100	100
All	All	653/686 (95%)	635 (97%)	17 (3%)	1 (0%)	43	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	TYR

5.3.2 Protein sidechains [i](#)

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	B	180/200 (90%)	180 (100%)	0	100	100
2	C	198/204 (97%)	197 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	182/195 (93%)	182 (100%)	0	100	100
All	All	560/599 (94%)	559 (100%)	1 (0%)	87	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	HIS
1	B	226	GLN
2	C	192	GLN
3	D	152	ASN
3	D	160	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 ⓘ

2 monosaccharides 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	$\# Z > 2$
4	NAG	A	1	4,1	14,14,15	0.26	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2	4	14,14,15	0.22	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	C1-O5-C5	2.17	115.10	112.19

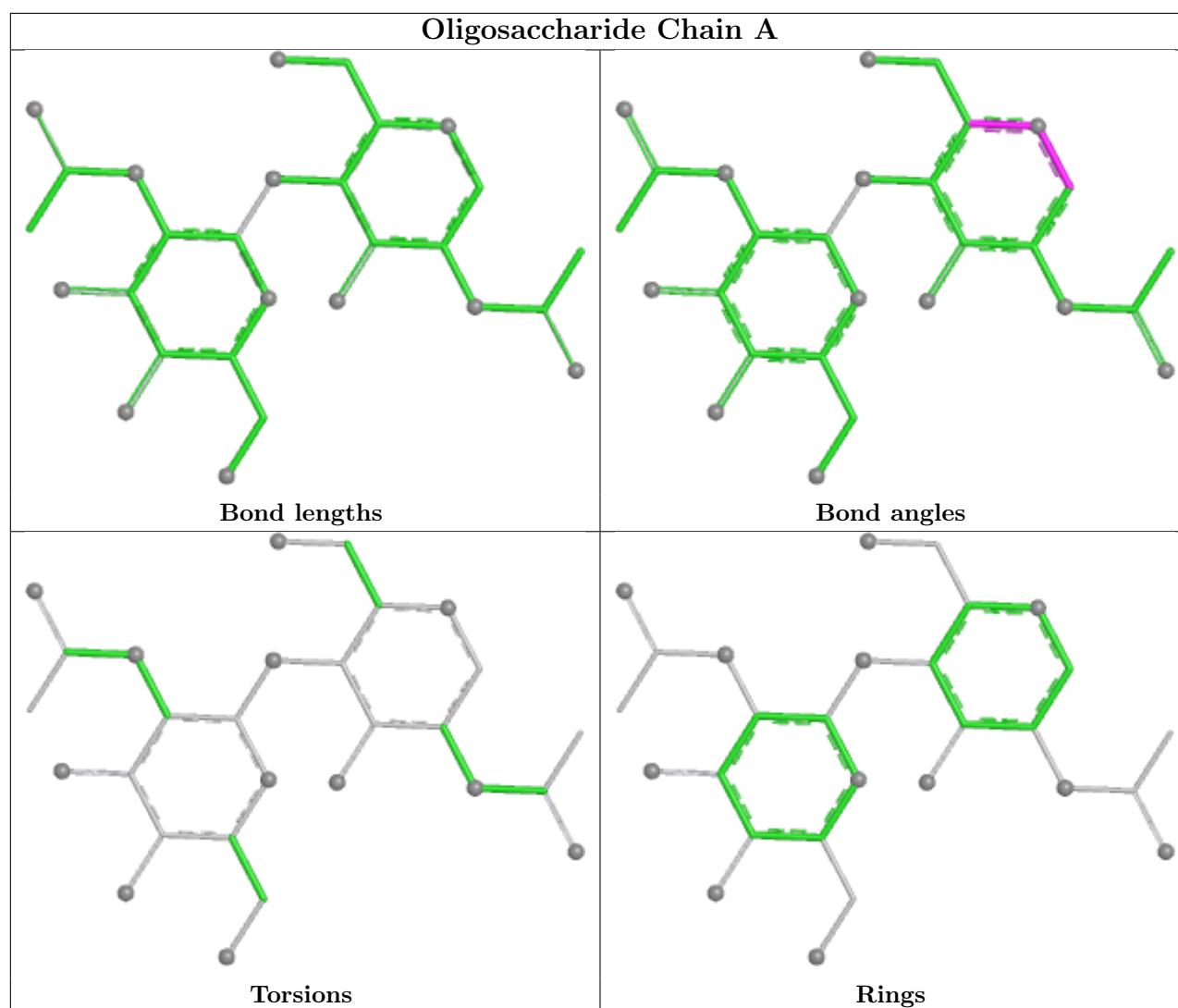
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
8	EDO	D	301	-	3,3,3	0.49	0	2,2,2	0.26	0
7	PEG	C	301	-	6,6,6	0.20	0	5,5,5	0.14	0
8	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	301	1	14,14,15	0.37	0	17,19,21	0.56	0
9	GOL	D	302	-	5,5,5	1.00	0	5,5,5	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	D	301	-	-	1/1/1/1	-
7	PEG	C	301	-	-	3/4/4/4	-
8	EDO	C	302	-	-	0/1/1/1	-
5	NAG	B	301	1	-	0/6/23/26	0/1/1/1
9	GOL	D	302	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	302	GOL	O1-C1-C2-C3
9	D	302	GOL	C1-C2-C3-O3
7	C	301	PEG	C1-C2-O2-C3
9	D	302	GOL	O1-C1-C2-O2
9	D	302	GOL	O2-C2-C3-O3
7	C	301	PEG	C4-C3-O2-C2
7	C	301	PEG	O2-C3-C4-O4
8	D	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	301	PEG	1	0
9	D	302	GOL	7	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	B	212/227 (93%)	0.07	10 (4%) 36 36	18, 34, 56, 81	1 (0%)
2	C	227/237 (95%)	-0.08	13 (5%) 29 29	14, 27, 60, 79	4 (1%)
3	D	214/222 (96%)	-0.21	4 (1%) 66 68	16, 27, 55, 73	1 (0%)
All	All	653/686 (95%)	-0.07	27 (4%) 41 42	14, 29, 57, 81	6 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	ILE	4.9
2	C	132	SER	4.4
2	C	133	GLY	4.0
3	D	0	GLY	3.6
2	C	131	THR	3.5
2	C	130	SER	3.4
1	B	135	GLY	3.4
2	C	128	SER	3.3
3	D	213	GLU	2.9
1	B	134	GLY	2.9
1	B	133	ASN	2.7
3	D	152	ASN	2.7
3	D	1	ASP	2.6
2	C	135	THR	2.6
1	B	74	LEU	2.6
1	B	240	GLY	2.5
2	C	1	GLN	2.5
1	B	132	GLN	2.4
1	B	263	GLY	2.4
2	C	189	LEU	2.3
2	C	127	SER	2.3
1	B	73	LEU	2.2
2	C	7	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	187	SER	2.1
1	B	171	ASN	2.1
2	C	100	GLY	2.1
2	C	186	SER	2.1

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

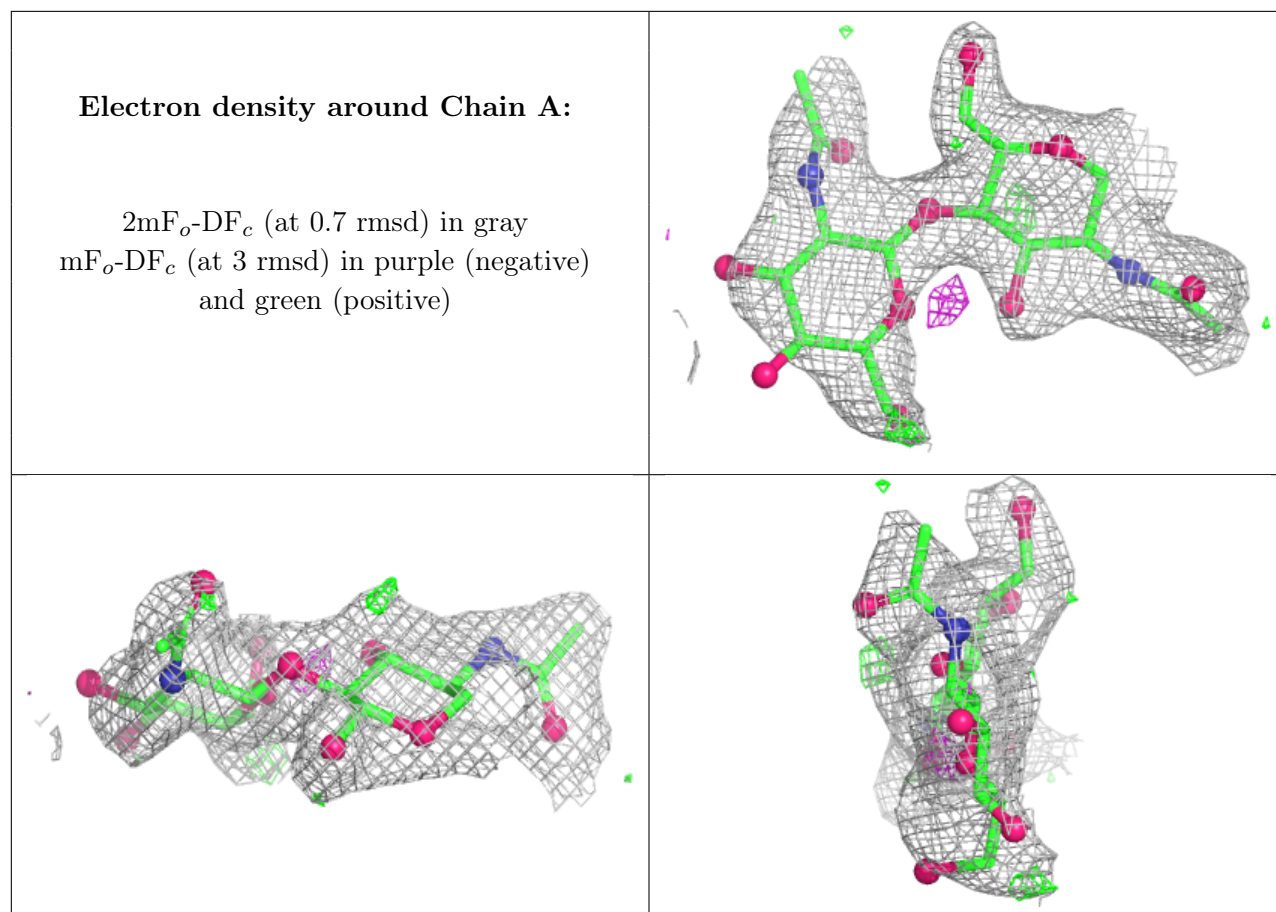
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
4	NAG	A	1	14/15	-	-	28,43,62,65	0
4	NAG	A	2	14/15	-	-	66,72,86,91	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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	NAG	B	301	14/15	0.68	0.14	54,70,84,91	0
9	GOL	D	302	6/6	0.86	0.19	25,32,38,40	0
7	PEG	C	301	7/7	0.89	0.13	26,40,54,58	0
8	EDO	C	302	4/4	0.93	0.10	30,31,37,38	0
8	EDO	D	301	4/4	0.97	0.06	17,29,29,34	0
6	NA	B	302	1/1	0.99	0.06	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.