



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2025 – 12:30 PM EDT

PDB ID : 9NIG / pdb\_00009nig  
Title : PB TCR in complex with HLA-DR4 presenting citrullinated Tenascin C peptide  
Authors : Dao, H.T.; Loh, T.J.; Lim, J.J.; Rossjohn, J.  
Deposited on : 2025-02-26  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

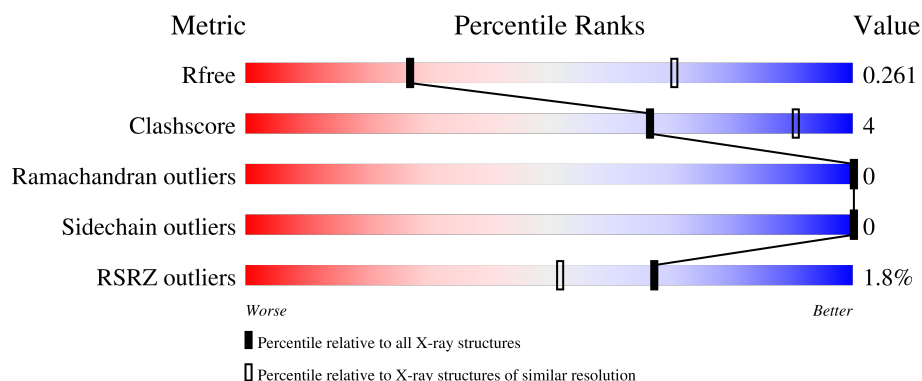
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (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  $\geq 3$ , 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	189	
1	C	189	
1	H	189	
2	B	190	
2	D	190	

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Mol	Chain	Length	Quality of chain
2	I	190	
3	E	208	
3	J	208	
3	M	208	
4	F	239	
4	K	239	
4	N	239	
5	G	14	
5	L	14	
5	P	14	
6	O	3	
7	V	2	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18764 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1397	906	226	260	5			
1	C	176	Total	C	N	O	S	0	0	0
			1302	837	217	243	5			
1	H	178	Total	C	N	O	S	0	0	0
			1367	890	220	252	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ILE	-	expression tag	UNP P01903
A	2	LYS	-	expression tag	UNP P01903
A	3	GLU	-	expression tag	UNP P01903
A	4	GLU	-	expression tag	UNP P01903
A	182	THR	-	expression tag	UNP P01903
A	183	SER	-	expression tag	UNP P01903
A	184	GLY	-	expression tag	UNP P01903
A	185	ASP	-	expression tag	UNP P01903
A	186	ASP	-	expression tag	UNP P01903
A	187	ASP	-	expression tag	UNP P01903
A	188	ASP	-	expression tag	UNP P01903
A	189	LYS	-	expression tag	UNP P01903
C	1	ILE	-	expression tag	UNP P01903
C	2	LYS	-	expression tag	UNP P01903
C	3	GLU	-	expression tag	UNP P01903
C	4	GLU	-	expression tag	UNP P01903
C	182	THR	-	expression tag	UNP P01903
C	183	SER	-	expression tag	UNP P01903
C	184	GLY	-	expression tag	UNP P01903
C	185	ASP	-	expression tag	UNP P01903
C	186	ASP	-	expression tag	UNP P01903
C	187	ASP	-	expression tag	UNP P01903
C	188	ASP	-	expression tag	UNP P01903

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Chain	Residue	Modelled	Actual	Comment	Reference
C	189	LYS	-	expression tag	UNP P01903
H	1	ILE	-	expression tag	UNP P01903
H	2	LYS	-	expression tag	UNP P01903
H	3	GLU	-	expression tag	UNP P01903
H	4	GLU	-	expression tag	UNP P01903
H	182	THR	-	expression tag	UNP P01903
H	183	SER	-	expression tag	UNP P01903
H	184	GLY	-	expression tag	UNP P01903
H	185	ASP	-	expression tag	UNP P01903
H	186	ASP	-	expression tag	UNP P01903
H	187	ASP	-	expression tag	UNP P01903
H	188	ASP	-	expression tag	UNP P01903
H	189	LYS	-	expression tag	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	0	0
			1512	958	269	280	5			
2	D	190	Total	C	N	O	S	0	0	0
			1489	945	262	277	5			
2	I	159	Total	C	N	O	S	0	0	0
			1203	754	217	227	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	THR	ARG	conflict	UNP A0A1V1IGJ9
D	191	THR	ARG	conflict	UNP A0A1V1IGJ9
I	191	THR	ARG	conflict	UNP A0A1V1IGJ9

- Molecule 3 is a protein called PB TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	193	Total	C	N	O	S	0	0	0
			1437	898	238	292	9			
3	E	203	Total	C	N	O	S	0	0	0
			1535	959	250	317	9			
3	J	202	Total	C	N	O	S	0	0	0
			1513	952	244	308	9			

- Molecule 4 is a protein called PB TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	238	Total	C	N	O	S	0	0	0
			1868	1187	325	349	7			
4	F	238	Total	C	N	O	S	0	0	0
			1862	1183	321	351	7			
4	K	238	Total	C	N	O	S	0	0	0
			1864	1187	325	345	7			

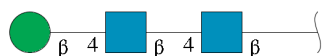
- Molecule 5 is a protein called Tenascin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	12	Total	C	N	O	0	0	0
			102	64	17	21			
5	G	11	Total	C	N	O	0	0	0
			98	62	16	20			
5	L	12	Total	C	N	O	0	0	0
			102	64	17	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1025	LYS	-	insertion	UNP P24821
P	1026	LYS	-	insertion	UNP P24821
G	1025	LYS	-	insertion	UNP P24821
G	1026	LYS	-	insertion	UNP P24821
L	1025	LYS	-	insertion	UNP P24821
L	1026	LYS	-	insertion	UNP P24821

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 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
7	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	C	O	0	0
			4	2	2		



### 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.

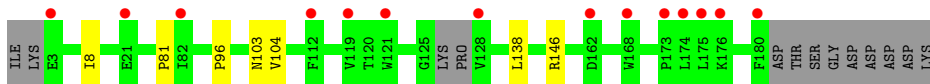
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A: 




- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain C: 




- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain H: 




- Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain B: 

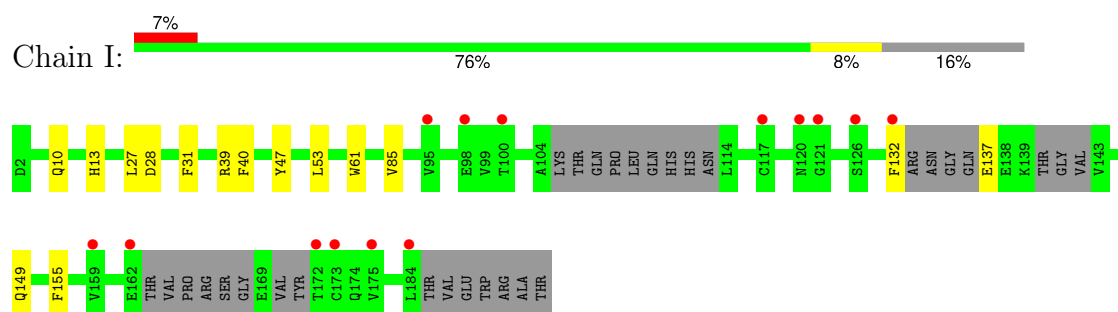


- Molecule 2: HLA class II histocompatibility antigen DR beta chain

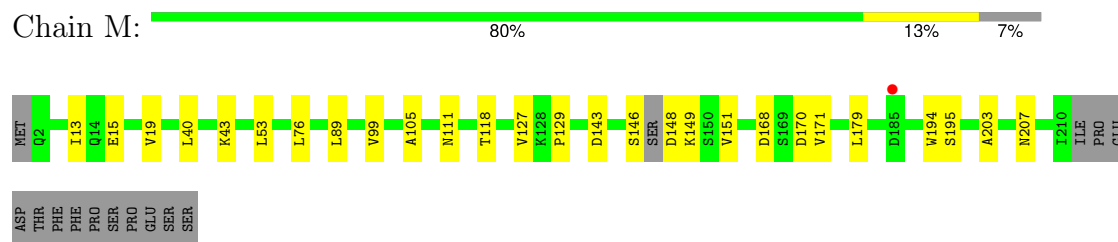
Chain D: 



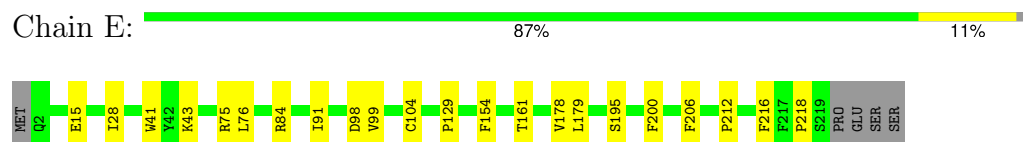
- Molecule 2: HLA class II histocompatibility antigen DR beta chain



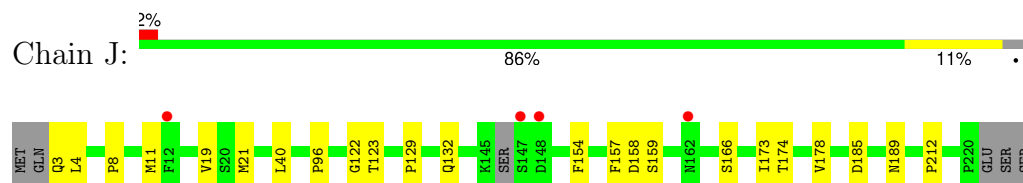
- Molecule 3: PB TCR alpha chain



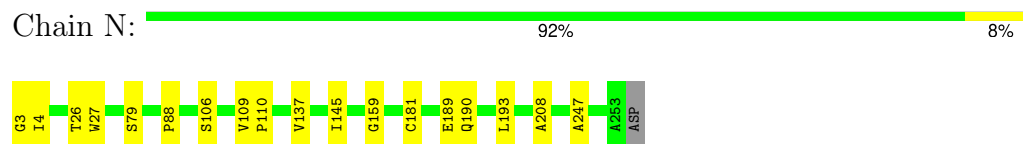
- Molecule 3: PB TCR alpha chain



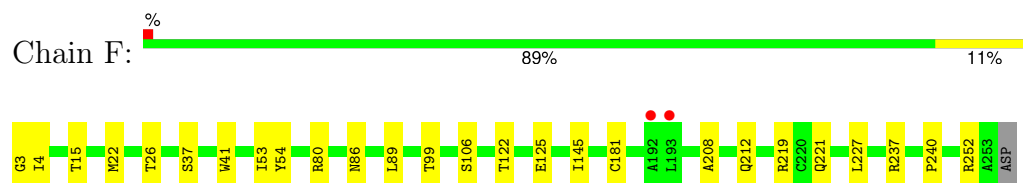
- Molecule 3: PB TCR alpha chain




- Molecule 4: PB TCR beta chain

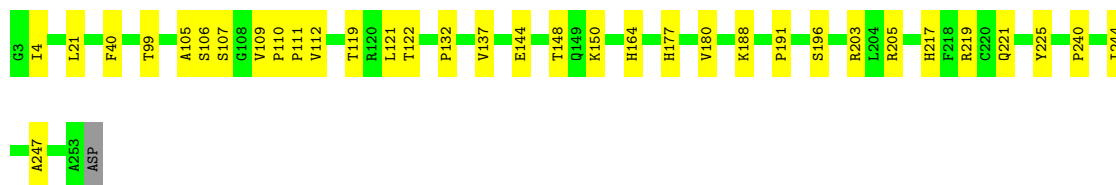


- Molecule 4: PB TCR beta chain



- Molecule 4: PB TCR beta chain

Chain K:  85% 14%



- Molecule 5: Tenascin

Chain P:  50% 21% 14% 14%



- Molecule 5: Tenascin

Chain G:  7% 50% 21% 7% 21%



- Molecule 5: Tenascin

Chain L:  50% 21% 7% 7% 14%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.93Å 88.67Å 126.07Å 81.47° 76.75° 65.45°	Depositor
Resolution (Å)	44.32 – 3.20 44.32 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.32-3.20) 98.9 (44.32-3.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.219 , 0.260 0.219 , 0.261	Depositor DCC
$R_{free}$ test set	2438 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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, 0.333 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: EDO, BMA, CIR, 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	0.15	0/1440	0.30	0/1975
1	C	0.13	0/1339	0.31	0/1843
1	H	0.19	1/1410 (0.1%)	0.30	0/1938
2	B	0.13	0/1556	0.32	0/2123
2	D	0.12	0/1531	0.30	0/2094
2	I	0.11	0/1229	0.29	0/1668
3	E	0.13	0/1567	0.31	0/2131
3	J	0.13	0/1545	0.34	1/2101 (0.0%)
3	M	0.14	0/1464	0.29	0/1990
4	F	0.13	0/1918	0.34	0/2623
4	K	0.14	0/1920	0.36	2/2624 (0.1%)
4	N	0.14	0/1924	0.36	2/2629 (0.1%)
5	G	0.10	0/76	0.25	0/101
5	L	0.10	0/80	0.26	0/106
5	P	0.15	0/80	0.28	0/106
All	All	0.14	1/19079 (0.0%)	0.32	5/26052 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	G	0	4
5	L	0	4
5	P	0	4
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	114	PRO	C-N	5.38	1.46	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	122	GLY	N-CA-C	6.22	117.86	111.95
4	N	109	VAL	CA-C-N	5.44	125.98	120.38
4	N	109	VAL	C-N-CA	5.44	125.98	120.38
4	K	109	VAL	CA-C-N	5.05	125.58	120.38
4	K	109	VAL	C-N-CA	5.05	125.58	120.38

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	1013	ASP	Mainchain
5	P	1013	ASP	Mainchain
5	P	1014	CIR	Mainchain
5	P	1015	TYR	Mainchain
5	P	1016	CIR	Mainchain

## 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	1397	0	1285	9	0
1	C	1302	0	1135	5	0
1	H	1367	0	1239	9	0
2	B	1512	0	1375	13	0
2	D	1489	0	1350	13	0
2	I	1203	0	1028	10	0
3	E	1535	0	1431	12	0
3	J	1513	0	1412	13	0
3	M	1437	0	1334	14	0
4	F	1862	0	1742	14	0
4	K	1864	0	1763	20	0
4	N	1868	0	1760	10	0
5	G	98	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	102	0	85	3	0
5	P	102	0	85	1	0
6	O	39	0	34	0	0
7	V	28	0	25	0	0
8	C	14	0	13	0	0
8	D	14	0	13	0	0
8	H	14	0	13	0	0
9	F	4	0	6	0	0
All	All	18764	0	17210	131	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 4.

The worst 5 of 131 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)
3:M:151:VAL:HG23	3:M:194:TRP:HB3	1.76	0.68
2:B:10:GLN:HB2	2:B:31:PHE:HB2	1.77	0.67
4:F:3:GLY:N	4:F:26:THR:HG1	1.96	0.64
4:F:99:THR:HG23	4:F:122:THR:HA	1.81	0.62
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.82	0.62

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	176/189 (93%)	171 (97%)	5 (3%)	0	100	100
1	C	172/189 (91%)	165 (96%)	7 (4%)	0	100	100
1	H	176/189 (93%)	170 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	187/190 (98%)	181 (97%)	6 (3%)	0	100	100
2	D	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
2	I	148/190 (78%)	145 (98%)	3 (2%)	0	100	100
3	E	201/208 (97%)	195 (97%)	6 (3%)	0	100	100
3	J	198/208 (95%)	189 (96%)	9 (4%)	0	100	100
3	M	189/208 (91%)	181 (96%)	8 (4%)	0	100	100
4	F	236/239 (99%)	229 (97%)	7 (3%)	0	100	100
4	K	236/239 (99%)	223 (94%)	13 (6%)	0	100	100
4	N	236/239 (99%)	227 (96%)	9 (4%)	0	100	100
5	G	7/14 (50%)	7 (100%)	0	0	100	100
5	L	8/14 (57%)	7 (88%)	1 (12%)	0	100	100
5	P	8/14 (57%)	8 (100%)	0	0	100	100
All	All	2366/2520 (94%)	2281 (96%)	85 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	147/173 (85%)	147 (100%)	0	100	100
1	C	127/173 (73%)	127 (100%)	0	100	100
1	H	140/173 (81%)	140 (100%)	0	100	100
2	B	156/172 (91%)	156 (100%)	0	100	100
2	D	152/172 (88%)	152 (100%)	0	100	100
2	I	114/172 (66%)	114 (100%)	0	100	100
3	E	173/184 (94%)	173 (100%)	0	100	100
3	J	168/184 (91%)	168 (100%)	0	100	100
3	M	157/184 (85%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	199/209 (95%)	199 (100%)	0	100	100
4	K	199/209 (95%)	199 (100%)	0	100	100
4	N	200/209 (96%)	200 (100%)	0	100	100
5	G	9/11 (82%)	9 (100%)	0	100	100
5	L	9/11 (82%)	9 (100%)	0	100	100
5	P	9/11 (82%)	9 (100%)	0	100	100
All	All	1959/2247 (87%)	1959 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	156	GLN
1	H	84	ASN
2	D	64	GLN
4	F	223	GLN
1	C	84	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CIR	G	1014	5	9,10,11	1.44	1 (11%)	6,11,13	0.33	0
5	CIR	P	1016	5	9,10,11	1.80	1 (11%)	6,11,13	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CIR	L	1014	5	9,10,11	1.66	1 (11%)	6,11,13	0.64	0
5	CIR	L	1016	5	9,10,11	1.84	1 (11%)	6,11,13	0.57	0
5	CIR	P	1014	5	9,10,11	1.63	1 (11%)	6,11,13	0.60	0
5	CIR	G	1016	5	9,10,11	1.83	1 (11%)	6,11,13	0.43	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
5	CIR	G	1014	5	-	0/8/9/11	-
5	CIR	P	1016	5	-	1/8/9/11	-
5	CIR	L	1014	5	-	1/8/9/11	-
5	CIR	L	1016	5	-	1/8/9/11	-
5	CIR	P	1014	5	-	3/8/9/11	-
5	CIR	G	1016	5	-	1/8/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1016	CIR	O-C	5.45	1.40	1.20
5	G	1016	CIR	O-C	5.41	1.40	1.20
5	P	1016	CIR	O-C	5.34	1.40	1.20
5	L	1014	CIR	O-C	4.90	1.38	1.20
5	P	1014	CIR	O-C	4.80	1.38	1.20

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	1014	CIR	C4-C3-CA-C
5	G	1016	CIR	C3-C4-C5-N6
5	P	1014	CIR	O7-C7-N6-C5
5	P	1014	CIR	N8-C7-N6-C5
5	P	1016	CIR	C3-C4-C5-N6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1014	CIR	1	0

## 5.5 Carbohydrates [i](#)

5 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
6	NAG	O	1	2,6	14,14,15	0.34	0	17,19,21	0.57	0
6	NAG	O	2	6	14,14,15	0.23	0	17,19,21	0.50	0
6	BMA	O	3	6	11,11,12	0.66	0	15,15,17	0.89	0
7	NAG	V	1	2,7	14,14,15	0.28	0	17,19,21	0.45	0
7	NAG	V	2	7	14,14,15	0.37	0	17,19,21	0.41	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
6	NAG	O	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
7	NAG	V	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	V	1	NAG	O5-C5-C6-O6

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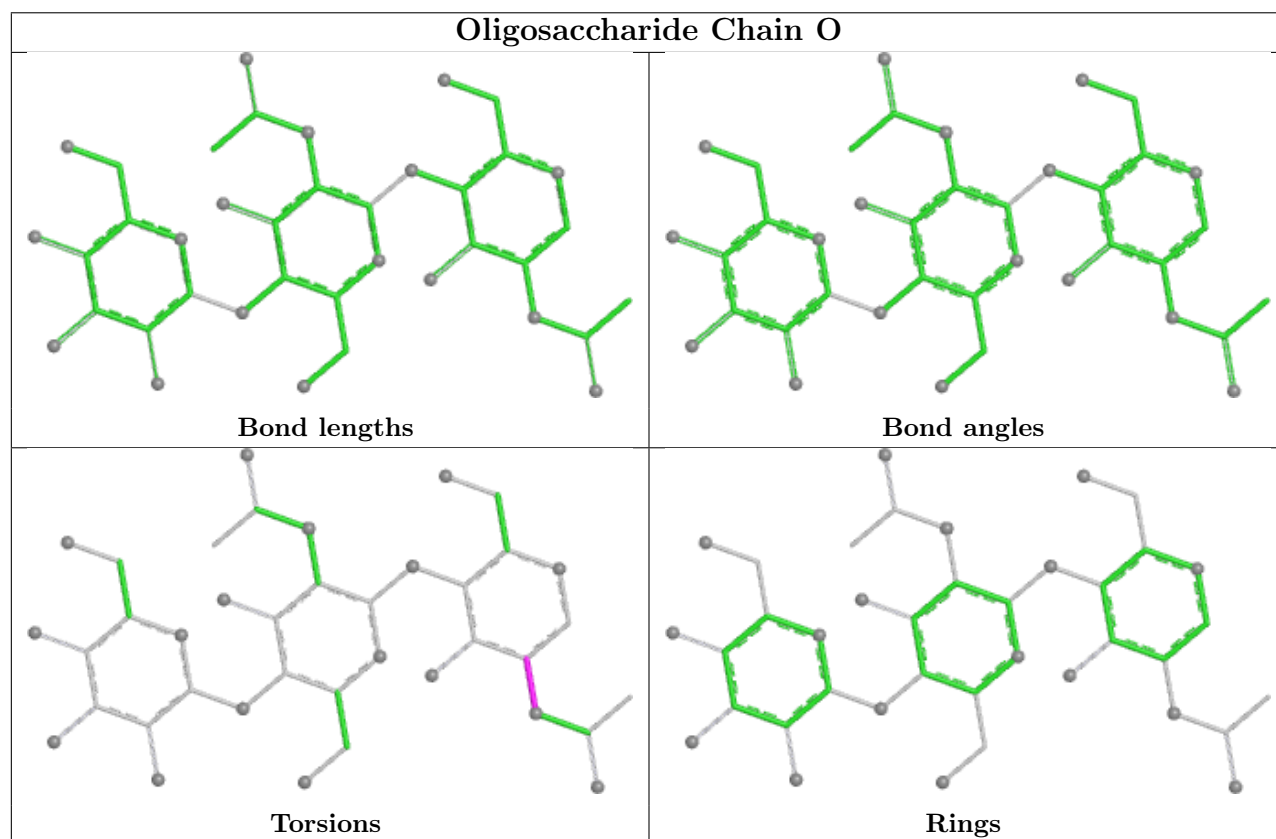
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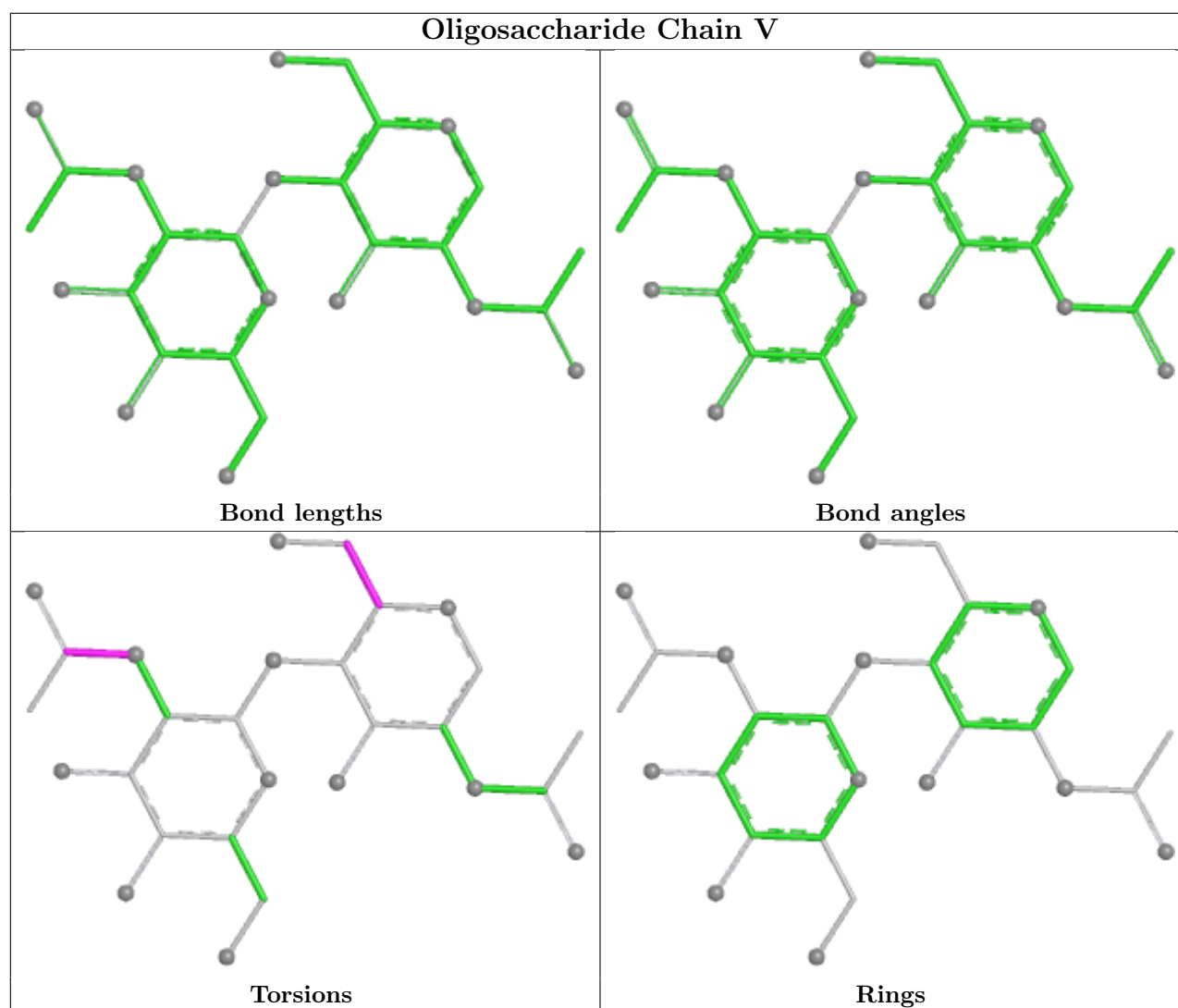
Mol	Chain	Res	Type	Atoms
7	V	1	NAG	C4-C5-C6-O6
7	V	2	NAG	C8-C7-N2-C2
7	V	2	NAG	O7-C7-N2-C2
6	O	1	NAG	C1-C2-N2-C7

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](#)

4 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	$\# Z  > 2$
8	NAG	H	201	1	14,14,15	0.32	0	17,19,21	0.44	0
8	NAG	C	201	1	14,14,15	0.23	0	17,19,21	0.43	0
9	EDO	F	301	-	3,3,3	0.45	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	D	201	2	14,14,15	0.32	0	17,19,21	0.43	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	NAG	H	201	1	-	2/6/23/26	0/1/1/1
8	NAG	C	201	1	-	2/6/23/26	0/1/1/1
9	EDO	F	301	-	-	0/1/1/1	-
8	NAG	D	201	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	201	NAG	C8-C7-N2-C2
8	C	201	NAG	O7-C7-N2-C2
8	H	201	NAG	C8-C7-N2-C2
8	H	201	NAG	O7-C7-N2-C2
8	D	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	178/189 (94%)	-0.24	0 <span>100</span> <span>100</span>	31, 53, 84, 97	0
1	C	176/189 (93%)	0.62	14 (7%) <span>20</span> <span>14</span>	42, 78, 115, 133	0
1	H	178/189 (94%)	0.45	3 (1%) <span>69</span> <span>53</span>	51, 79, 106, 123	0
2	B	189/190 (99%)	-0.35	1 (0%) <span>87</span> <span>78</span>	33, 48, 70, 83	0
2	D	190/190 (100%)	0.01	3 (1%) <span>70</span> <span>55</span>	34, 56, 97, 114	0
2	I	159/190 (83%)	0.66	14 (8%) <span>17</span> <span>12</span>	52, 84, 131, 154	0
3	E	203/208 (97%)	-0.11	0 <span>100</span> <span>100</span>	33, 48, 73, 99	0
3	J	202/208 (97%)	0.14	4 (1%) <span>64</span> <span>49</span>	34, 56, 82, 96	0
3	M	193/208 (92%)	-0.11	1 (0%) <span>87</span> <span>78</span>	29, 50, 84, 96	0
4	F	238/239 (99%)	-0.20	2 (0%) <span>82</span> <span>70</span>	28, 49, 68, 120	0
4	K	238/239 (99%)	-0.08	0 <span>100</span> <span>100</span>	34, 52, 78, 88	0
4	N	238/239 (99%)	-0.38	0 <span>100</span> <span>100</span>	24, 42, 62, 71	0
5	G	9/14 (64%)	0.63	1 (11%) <span>12</span> <span>8</span>	41, 55, 77, 95	0
5	L	10/14 (71%)	0.70	0 <span>100</span> <span>100</span>	57, 61, 80, 83	0
5	P	10/14 (71%)	-0.14	0 <span>100</span> <span>100</span>	28, 36, 44, 61	0
All	All	2411/2520 (95%)	0.01	43 (1%) <span>67</span> <span>52</span>	24, 54, 100, 154	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	GLU	3.5
1	C	174	LEU	3.3
1	C	175	LEU	2.9
2	I	162	GLU	2.8
2	I	132	PHE	2.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	CIR	L	1014	11/12	0.80	0.15	52,63,80,81	0
5	CIR	P	1014	11/12	0.86	0.16	39,46,62,63	0
5	CIR	G	1014	11/12	0.89	0.13	42,48,56,56	0
5	CIR	L	1016	11/12	0.89	0.17	46,61,78,81	0
5	CIR	P	1016	11/12	0.90	0.12	34,39,43,43	0
5	CIR	G	1016	11/12	0.94	0.09	35,41,47,52	0

## 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	D	201	14/15	0.54	0.16	71,98,115,116	0
8	NAG	C	201	14/15	0.62	0.11	80,103,112,113	0
8	NAG	H	201	14/15	0.66	0.12	79,89,93,98	0
9	EDO	F	301	4/4	0.77	0.20	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.