



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 02:19 PM EDT

PDB ID : 4JZJ  
Title : Crystal Structure of Receptor-Fab Complex  
Authors : Broughton, S.E.; Parker, M.W.  
Deposited on : 2013-04-03  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

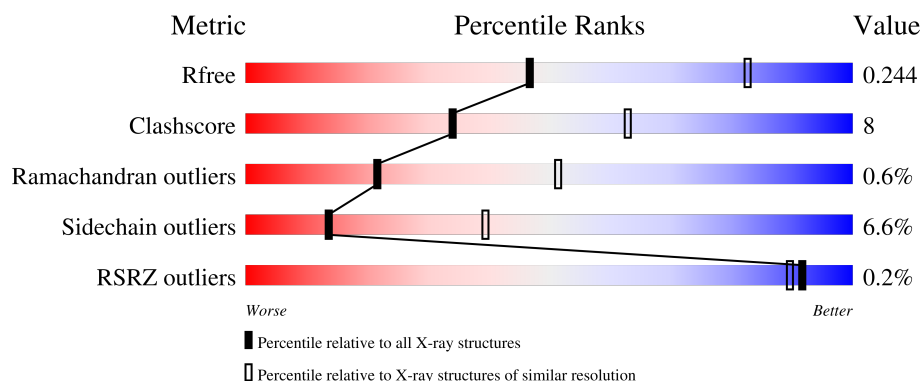
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	C	287	
1	D	287	
2	A	221	
2	H	221	
3	B	220	

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Mol	Chain	Length	Quality of chain
3	L	220	
4	E	7	
5	F	5	
6	G	3	

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
5	NAG	F	1	-	-	X	-
5	NAG	F	2	-	-	X	-
5	FUL	F	4	-	-	X	-
6	NAG	G	1	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10972 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 Interleukin-3 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	250	Total	C	N	O	S	0	0	0
			2024	1283	359	369	13			
1	D	251	Total	C	N	O	S	0	0	0
			2035	1293	359	370	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	144	LYS	ASN	SEE REMARK 999	UNP P26951
C	?	-	ARG	deletion	UNP P26951
C	298	VAL	ALA	engineered mutation	UNP P26951
D	144	LYS	ASN	SEE REMARK 999	UNP P26951
D	?	-	ARG	deletion	UNP P26951
D	298	VAL	ALA	engineered mutation	UNP P26951

- Molecule 2 is a protein called Fab Heavy Chain.

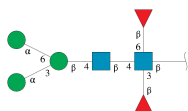
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	214	Total	C	N	O	S	0	0	0
			1628	1041	267	311	9			
2	H	215	Total	C	N	O	S	0	0	0
			1634	1044	268	313	9			

- Molecule 3 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	219	Total	C	N	O	S	0	0	0
			1699	1062	282	350	5			
3	L	219	Total	C	N	O	S	0	0	0
			1699	1062	282	350	5			

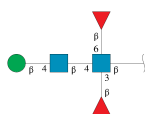
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)][beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



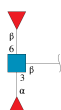
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	7	Total	C	N	O	0	0	0
			81	46	2	33			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)][beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



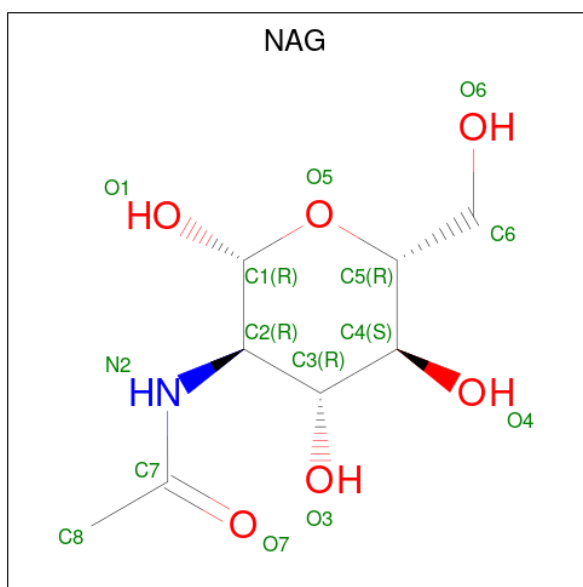
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	5	Total	C	N	O	0	0	0
			59	34	2	23			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



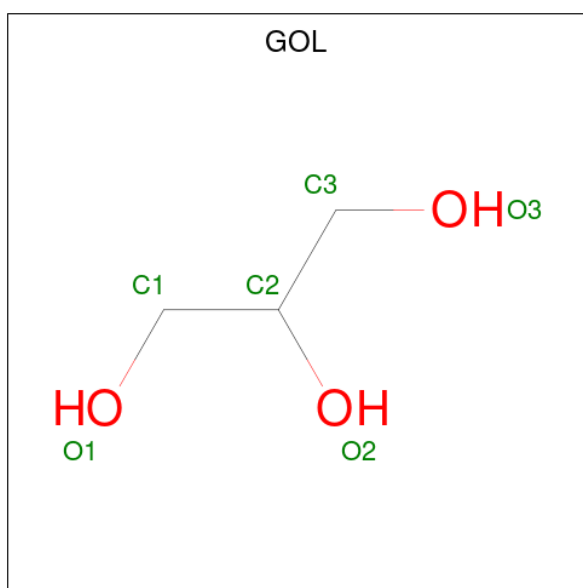
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	3	Total	C	N	O	0	0	0
			34	20	1	13			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

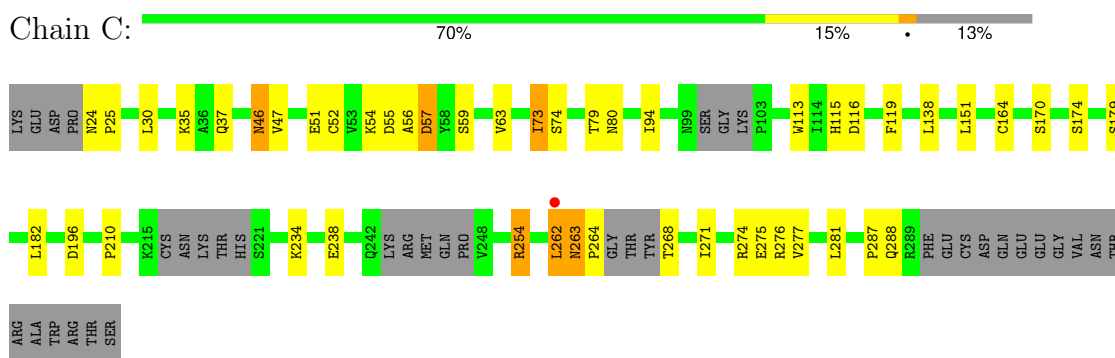
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	9	Total 9	O 9	0	0
9	D	7	Total 7	O 7	0	0
9	A	2	Total 2	O 2	0	0
9	B	6	Total 6	O 6	0	0
9	H	12	Total 12	O 12	0	0
9	L	3	Total 3	O 3	0	0

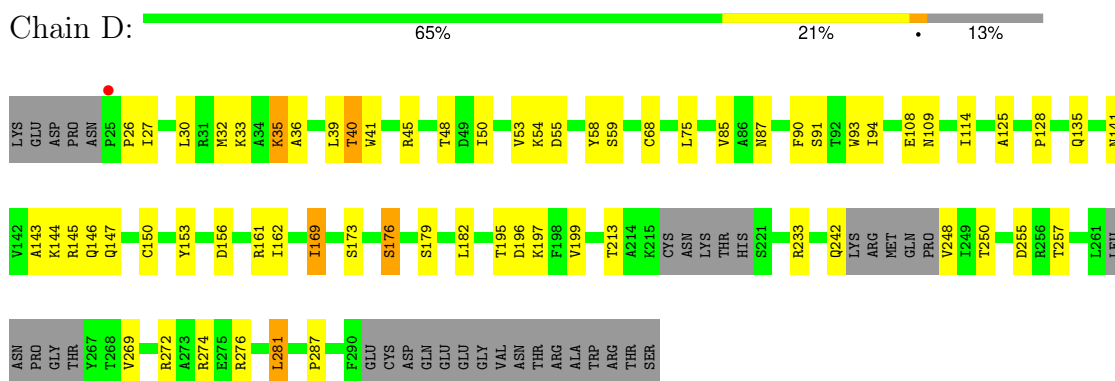
### 3 Residue-property plots

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.

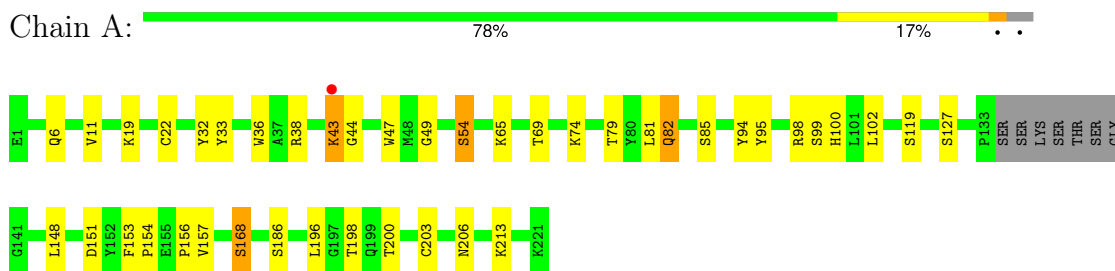
- Molecule 1: Interleukin-3 receptor subunit alpha



- Molecule 1: Interleukin-3 receptor subunit alpha




- Molecule 2: Fab Heavy Chain



- Molecule 2: Fab Heavy Chain



Chain H:  84% 13% •




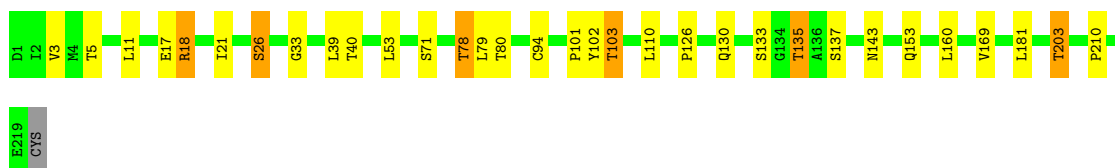
- Molecule 3: Fab Light Chain

Chain B:  90% 8% •



- Molecule 3: Fab Light Chain

Chain L:  85% 12% •



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)][beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  43% 57%

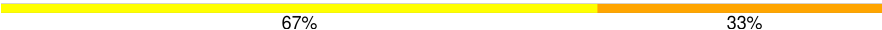


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)][beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  40% 60%



- Molecule 6: alpha-L-fucopyranose-(1-3)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.30Å 120.65Å 92.97Å 90.00° 97.45° 90.00°	Depositor
Resolution (Å)	49.67 – 2.80 49.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.67-2.80) 99.1 (49.67-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.81Å)	Xtriage
Refinement program	PHENIX dev_1218	Depositor
R, $R_{free}$	0.185 , 0.244 0.192 , 0.244	Depositor DCC
$R_{free}$ test set	2381 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: FUC, FUL, NAG, GOL, BMA, 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	C	0.60	1/2074 (0.0%)	0.72	1/2814 (0.0%)
1	D	0.51	0/2087	0.70	1/2830 (0.0%)
2	A	0.48	0/1671	0.63	0/2270
2	H	0.56	0/1677	0.68	1/2278 (0.0%)
3	B	0.52	0/1737	0.65	0/2362
3	L	0.58	0/1737	0.65	0/2362
All	All	0.54	1/10983 (0.0%)	0.68	3/14916 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	THR	C-N	5.69	1.47	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	281	LEU	CA-CB-CG	7.03	131.47	115.30
1	C	151	LEU	CA-CB-CG	5.75	128.52	115.30
2	H	185	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2024	0	1958	28	0
1	D	2035	0	1968	39	0
2	A	1628	0	1608	19	0
2	H	1634	0	1613	12	0
3	B	1699	0	1630	10	0
3	L	1699	0	1630	18	0
4	E	81	0	70	9	0
5	F	59	0	51	33	0
6	G	34	0	31	10	0
7	C	14	0	13	2	0
7	D	14	0	13	2	0
8	D	6	0	8	1	0
8	H	6	0	8	1	0
9	A	2	0	0	1	0
9	B	6	0	0	0	0
9	C	9	0	0	0	0
9	D	7	0	0	0	0
9	H	12	0	0	3	0
9	L	3	0	0	0	0
All	All	10972	0	10601	159	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 8.

The worst 5 of 159 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:C:46:ASN:HD22	7:C:408:NAG:C1	0.99	1.57
5:F:1:NAG:H62	5:F:2:NAG:C7	1.36	1.51
1:D:109:ASN:HD21	6:G:1:NAG:C1	1.22	1.48
5:F:1:NAG:C6	5:F:2:NAG:C7	2.27	1.11
1:C:80:ASN:CG	4:E:1:NAG:C1	2.23	1.06

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	C	240/287 (84%)	222 (92%)	15 (6%)	3 (1%)	10	32
1	D	243/287 (85%)	220 (90%)	20 (8%)	3 (1%)	11	34
2	A	210/221 (95%)	197 (94%)	12 (6%)	1 (0%)	25	56
2	H	211/221 (96%)	201 (95%)	9 (4%)	1 (0%)	25	56
3	B	217/220 (99%)	205 (94%)	12 (6%)	0	100	100
3	L	217/220 (99%)	212 (98%)	5 (2%)	0	100	100
All	All	1338/1456 (92%)	1257 (94%)	73 (6%)	8 (1%)	22	51

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	254	ARG
1	D	35	LYS
1	D	48	THR
1	D	287	PRO
2	H	220	PRO

### 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	C	223/256 (87%)	210 (94%)	13 (6%)	17	45
1	D	223/256 (87%)	203 (91%)	20 (9%)	8	25
2	A	181/187 (97%)	166 (92%)	15 (8%)	9	28
2	H	182/187 (97%)	171 (94%)	11 (6%)	16	44
3	B	194/195 (100%)	185 (95%)	9 (5%)	23	55
3	L	194/195 (100%)	183 (94%)	11 (6%)	17	46
All	All	1197/1276 (94%)	1118 (93%)	79 (7%)	14	39

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	7	SER
3	L	53	LEU
2	H	45	LEU
2	H	122	SER
3	L	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	178	GLN
3	L	27	GLN
3	L	144	ASN
3	L	35	GLN
3	L	143	ASN

### 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 ⓘ

15 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	E	1	4,1	14,14,15	1.18	1 (7%)	17,19,21	2.17	7 (41%)
4	NAG	E	2	4	14,14,15	0.77	0	17,19,21	1.27	2 (11%)
4	BMA	E	3	4	11,11,12	0.66	0	15,15,17	1.04	1 (6%)
4	MAN	E	4	4	11,11,12	0.66	0	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	E	5	4	11,11,12	0.59	0	15,15,17	1.36	2 (13%)
4	FUL	E	6	4	10,10,11	0.81	0	14,14,16	2.64	5 (35%)
4	FUL	E	7	4	10,10,11	0.59	0	14,14,16	1.86	4 (28%)
5	NAG	F	1	1,5	14,14,15	0.94	0	17,19,21	5.92	11 (64%)
5	NAG	F	2	5	14,14,15	1.88	6 (42%)	17,19,21	3.26	8 (47%)
5	BMA	F	3	5	11,11,12	0.74	0	15,15,17	1.53	2 (13%)
5	FUL	F	4	5	10,10,11	0.48	0	14,14,16	0.95	2 (14%)
5	FUL	F	5	5	10,10,11	0.30	0	14,14,16	0.58	0
6	NAG	G	1	6,1	14,14,15	0.46	0	17,19,21	1.57	4 (23%)
6	FUC	G	2	6	10,10,11	0.76	0	14,14,16	1.12	1 (7%)
6	FUL	G	3	6	10,10,11	0.81	0	14,14,16	1.86	2 (14%)

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	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	FUL	E	6	4	-	-	0/1/1/1
4	FUL	E	7	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	FUL	F	4	5	-	-	0/1/1/1
5	FUL	F	5	5	-	-	0/1/1/1
6	NAG	G	1	6,1	-	2/6/23/26	0/1/1/1
6	FUC	G	2	6	-	-	0/1/1/1
6	FUL	G	3	6	-	-	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	NAG	C2-N2	-3.36	1.40	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	NAG	C3-C2	-2.91	1.46	1.52
5	F	2	NAG	C1-C2	-2.51	1.48	1.52
5	F	2	NAG	O5-C1	-2.30	1.39	1.43
4	E	1	NAG	C1-C2	-2.27	1.49	1.52

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C4-C3-C2	-15.03	88.99	111.02
5	F	1	NAG	C3-C4-C5	-10.05	92.01	110.23
5	F	2	NAG	O4-C4-C3	-8.73	89.80	110.38
5	F	1	NAG	C1-C2-N2	8.00	123.05	110.43
4	E	6	FUL	C1-C2-C3	-7.86	98.20	109.64

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C1-C2-N2-C7
4	E	1	NAG	C8-C7-N2-C2
4	E	3	BMA	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6

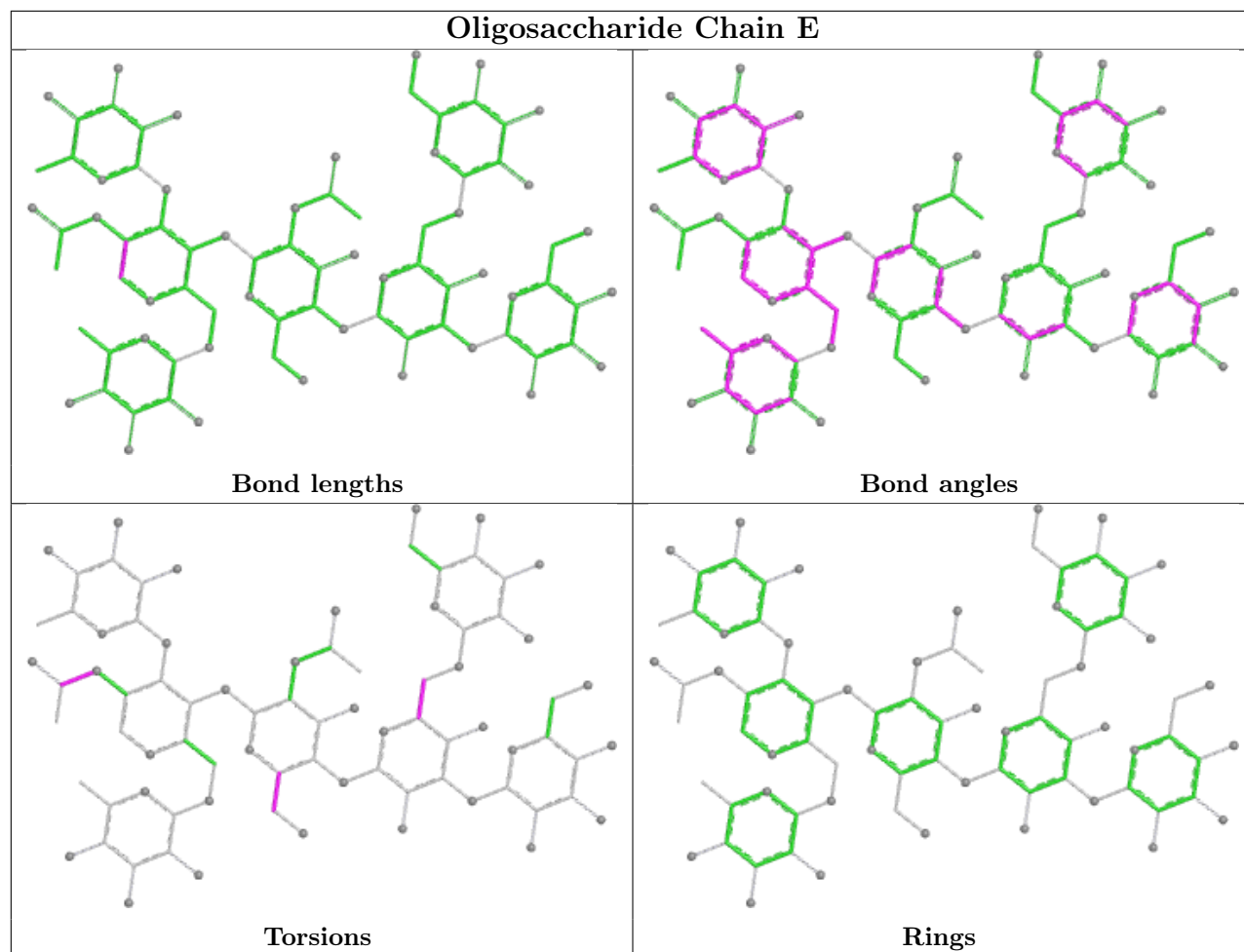
There are no ring outliers.

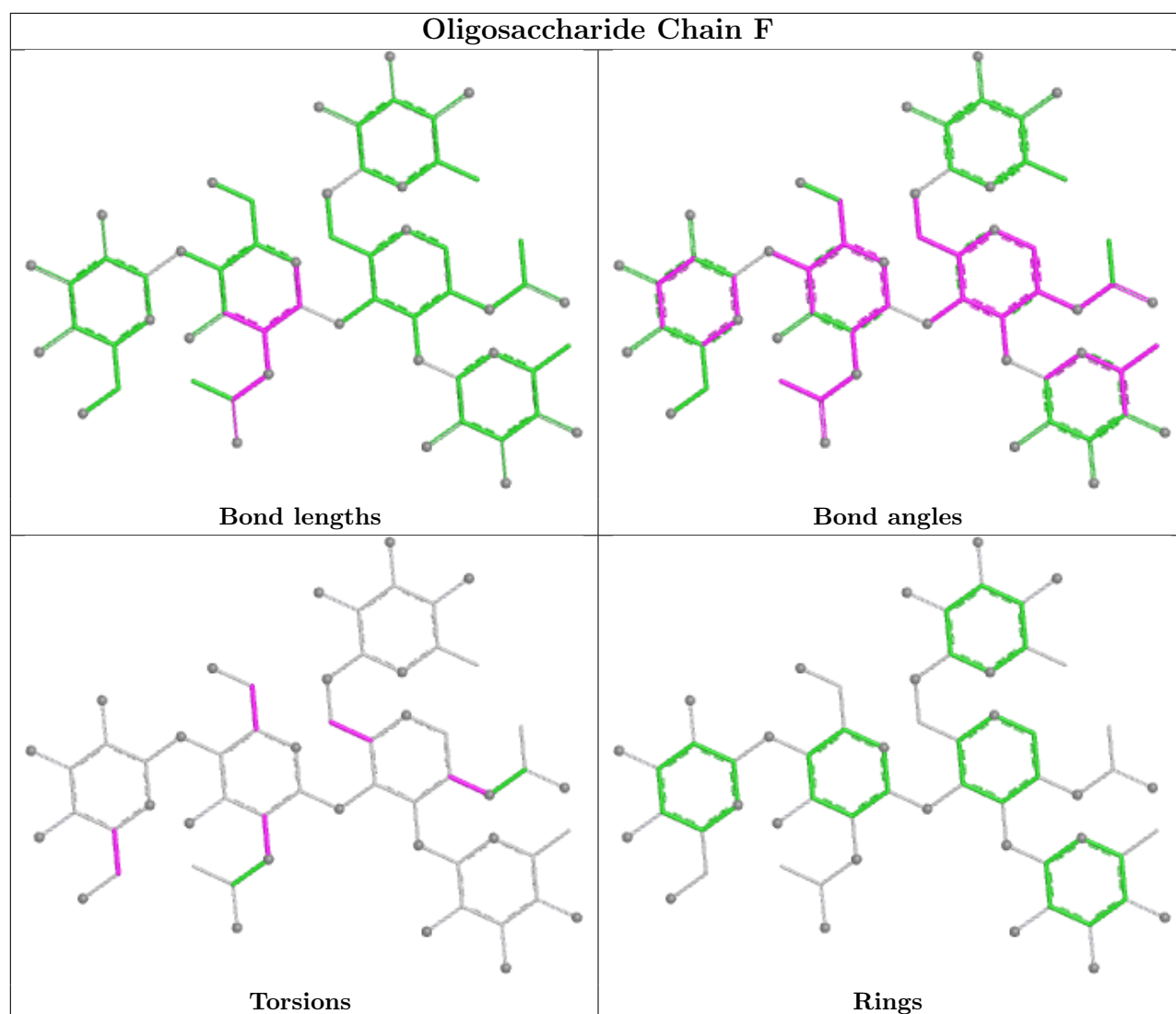
9 monomers are involved in 52 short contacts:

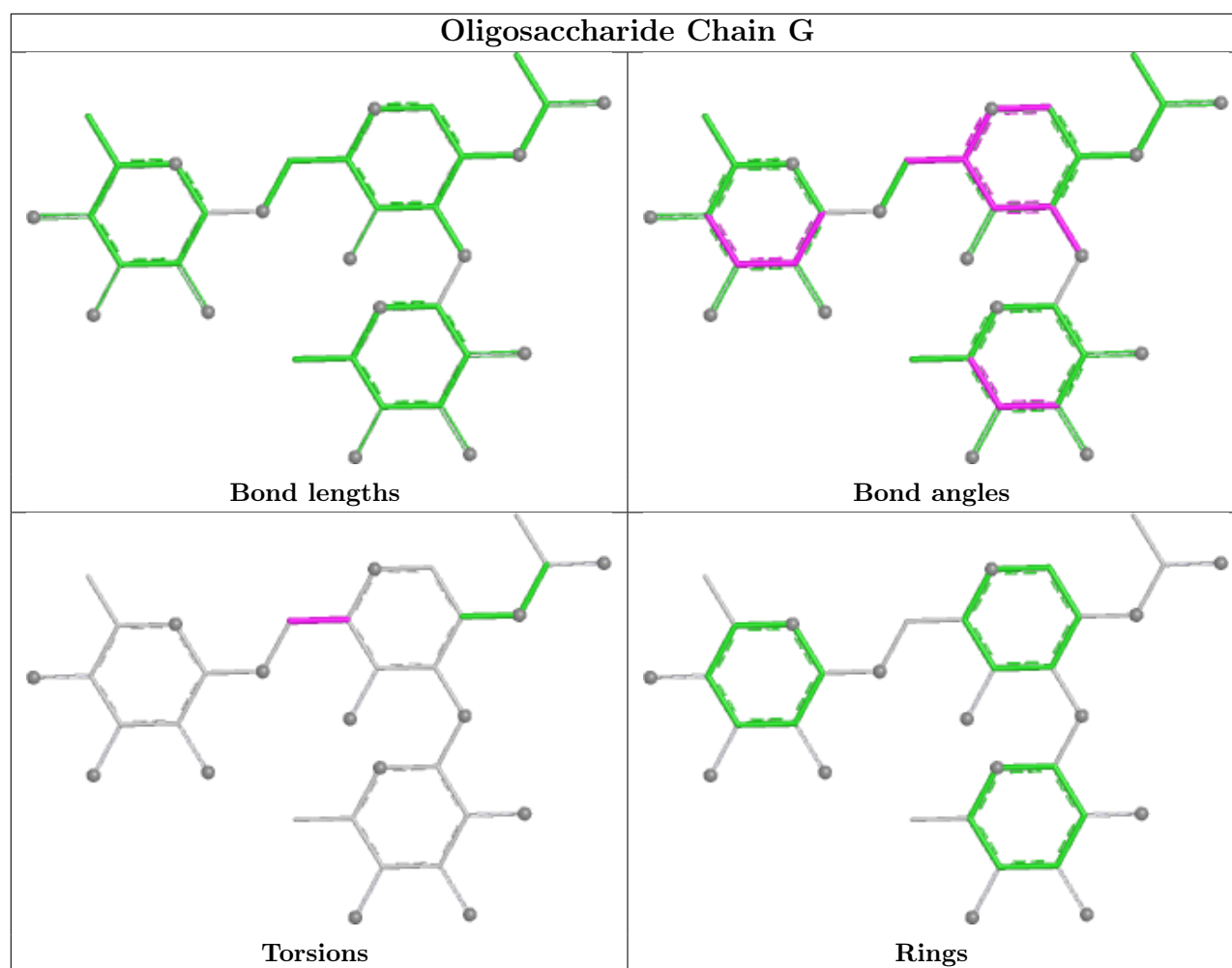
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	26	0
5	F	2	NAG	17	0
4	E	7	FUL	2	0
6	G	1	NAG	10	0
4	E	5	MAN	3	0
4	E	1	NAG	4	0
5	F	4	FUL	10	0
5	F	5	FUL	5	0
4	E	3	BMA	2	0

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	$\# Z  > 2$
7	NAG	D	409	-	14,14,15	0.68	0	17,19,21	1.68	2 (11%)
8	GOL	D	410	-	5,5,5	0.36	0	5,5,5	0.43	0
8	GOL	H	301	-	5,5,5	0.48	0	5,5,5	0.64	0
7	NAG	C	408	1	14,14,15	0.76	1 (7%)	17,19,21	1.73	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
7	NAG	D	409	-	-	2/6/23/26	0/1/1/1
8	GOL	D	410	-	-	4/4/4/4	-
8	GOL	H	301	-	-	4/4/4/4	-
7	NAG	C	408	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	408	NAG	C1-C2	2.37	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	409	NAG	O5-C1-C2	-5.57	102.68	111.29
7	C	408	NAG	O5-C1-C2	-3.66	105.63	111.29
7	C	408	NAG	C1-O5-C5	3.19	116.46	112.19
7	D	409	NAG	C3-C4-C5	2.75	115.22	110.23
7	C	408	NAG	C3-C4-C5	-2.74	105.27	110.23

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	410	GOL	O1-C1-C2-C3
8	H	301	GOL	O1-C1-C2-C3
8	H	301	GOL	C1-C2-C3-O3
7	D	409	NAG	C8-C7-N2-C2
7	D	409	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	409	NAG	2	0
8	D	410	GOL	1	0
8	H	301	GOL	1	0
7	C	408	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	250/287 (87%)	-0.72	1 (0%) 89 85	21, 38, 93, 116	0
1	D	251/287 (87%)	-0.55	1 (0%) 89 85	29, 57, 96, 113	0
2	A	214/221 (96%)	-0.80	1 (0%) 87 83	32, 50, 78, 94	0
2	H	215/221 (97%)	-0.88	0 100 100	22, 38, 59, 77	0
3	B	219/220 (99%)	-0.86	0 100 100	23, 45, 90, 102	0
3	L	219/220 (99%)	-0.96	0 100 100	22, 42, 67, 87	0
All	All	1368/1456 (93%)	-0.79	3 (0%) 92 89	21, 45, 87, 116	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	262	LEU	3.9
1	D	25	PRO	3.6
2	A	43	LYS	2.4

### 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](#)

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	GOL	D	410	6/6	0.65	0.17	83,83,83,83	0
8	GOL	H	301	6/6	0.73	0.18	47,47,47,47	0
7	NAG	C	408	14/15	0.79	0.14	105,120,134,135	0
7	NAG	D	409	14/15	0.83	0.10	81,81,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.