



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:29 AM BST

PDB ID : 4KVN
Title : Crystal structure of Fab 39.29 in complex with Influenza Hemagglutinin A/Perth/16/2009 (H3N2)
Authors : Fong, R.; Swem, L.R.; Lupardus, P.J.
Deposited on : 2013-05-22
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

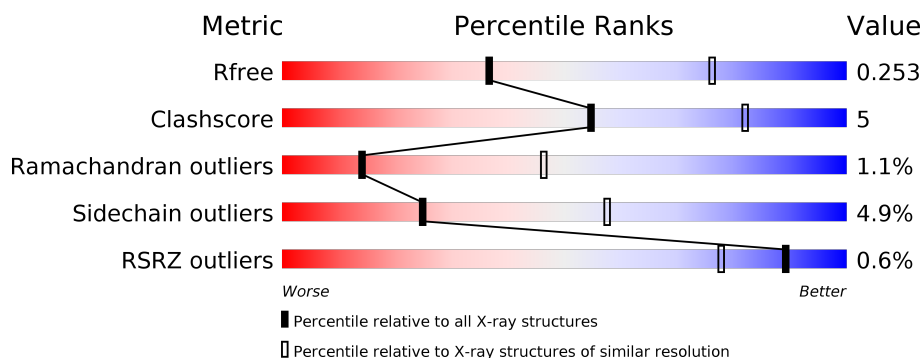
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	505	
2	H	227	
3	L	215	
4	B	3	
4	C	3	
5	D	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7147 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	A	470	Total	C	N	O	S	23	0	0
			3711	2314	665	714	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ALA	-	expression tag	UNP C6KNH7
A	24	GLY	-	expression tag	UNP C6KNH7
A	521	SER	-	expression tag	UNP C6KNH7
A	522	GLY	-	expression tag	UNP C6KNH7
A	523	ARG	-	expression tag	UNP C6KNH7
A	524	LEU	-	expression tag	UNP C6KNH7
A	525	VAL	-	expression tag	UNP C6KNH7
A	526	PRO	-	expression tag	UNP C6KNH7
A	527	ARG	-	expression tag	UNP C6KNH7

- Molecule 2 is a protein called Human IgG Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	14	0	0
			1605	1024	266	310	5			

- Molecule 3 is a protein called Human IgG Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	7	0	0
			1635	1027	282	322	4			

- Molecule 4 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.



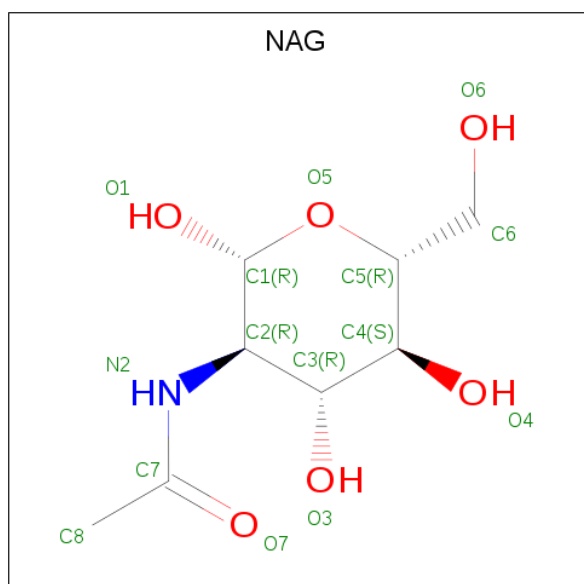
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



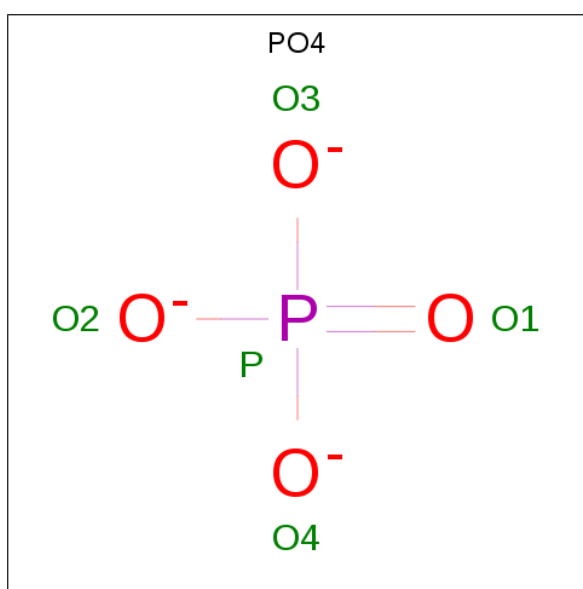
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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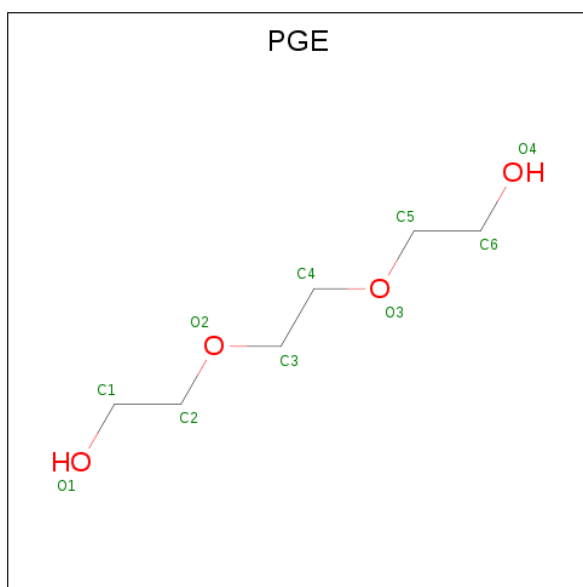
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			10	6	4		

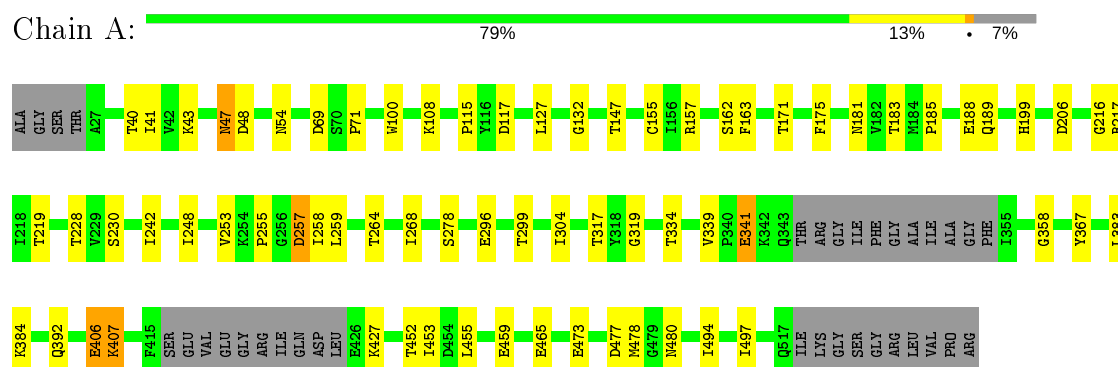
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	O	0	0
			4	4		
9	L	1	Total	O	0	0
			1	1		

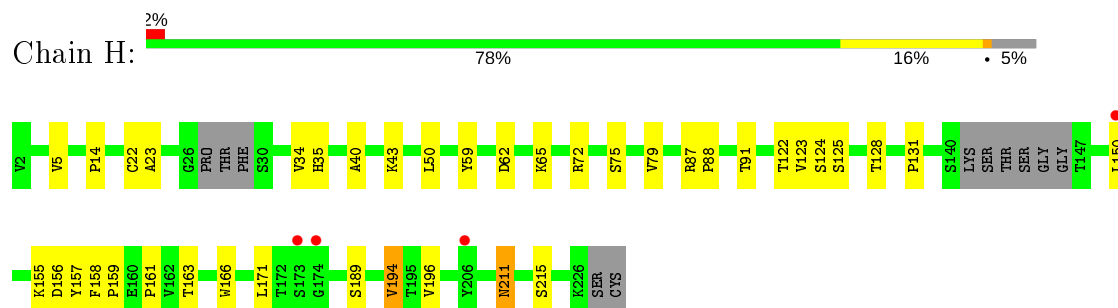
3 Residue-property plots [i](#)

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.

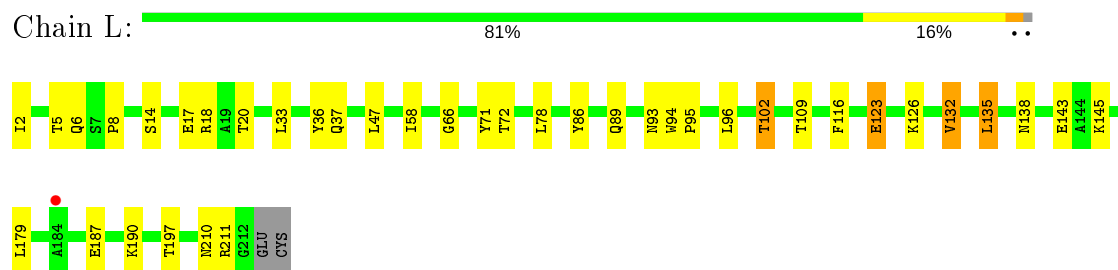
- Molecule 1: Hemagglutinin



- Molecule 2: Human IgG Heavy Chain



- Molecule 3: Human IgG Light Chain



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

Chain B:  33% 67%

HA01
HA02
BO03

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

Chain C:  33% 67%

HA01
HA02
BO03

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

HA01
HA02

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	204.37Å 204.37Å 204.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.63 – 3.10 64.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.63-3.10) 100.0 (64.63-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.202 , 0.248 0.214 , 0.253	Depositor DCC
R_{free} test set	1316 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: PO4, BMA, PGE, 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	0.45	1/3787 (0.0%)	0.71	2/5126 (0.0%)
2	H	0.47	0/1650	0.69	0/2262
3	L	0.42	0/1674	0.66	0/2279
All	All	0.45	1/7111 (0.0%)	0.70	2/9667 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	PRO	N-CD	-5.04	1.40	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	GLU	C-N-CA	7.99	141.68	121.70
1	A	407	LYS	N-CA-C	-5.88	95.14	111.00

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	3711	0	3587	30	1
2	H	1605	0	1539	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1635	0	1597	16	0
4	B	39	0	34	1	0
4	C	39	0	34	1	0
5	D	28	0	25	3	0
6	A	70	0	65	0	0
7	L	5	0	0	0	1
8	L	10	0	14	0	0
9	A	4	0	0	0	0
9	L	1	0	0	0	0
All	All	7147	0	6895	72	1

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 5.

All (72) 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:384:LYS:HA	3:L:94:TRP:HB2	1.57	0.84
3:L:132:VAL:HG23	3:L:179:LEU:HB3	1.69	0.73
2:H:14:PRO:HD2	2:H:125:SER:HB3	1.69	0.73
2:H:128:THR:HG22	2:H:215:SER:HB2	1.78	0.64
1:A:115:PRO:HG2	1:A:242:ILE:HB	1.82	0.61
2:H:34:VAL:HG11	2:H:79:VAL:HG21	1.84	0.59
2:H:35:HIS:CE1	2:H:50:LEU:CD2	2.86	0.59
2:H:124:SER:HG	2:H:158:PHE:HZ	1.51	0.58
2:H:35:HIS:CE1	2:H:50:LEU:HD22	2.40	0.57
1:A:217:ARG:NH1	1:A:230:SER:HB2	2.20	0.56
1:A:181:ASN:HB2	5:D:1:NAG:H83	1.89	0.54
3:L:145:LYS:HB3	3:L:197:THR:HB	1.90	0.54
1:A:339:VAL:O	1:A:358:GLY:HA3	2.08	0.53
3:L:123:GLU:HA	3:L:126:LYS:HE2	1.89	0.53
1:A:341:GLU:HG2	1:A:358:GLY:O	2.10	0.52
2:H:91:THR:HG23	2:H:122:THR:HA	1.91	0.52
2:H:128:THR:HG23	2:H:159:PRO:HD3	1.91	0.52
2:H:131:PRO:HB3	2:H:157:TYR:HB3	1.92	0.50
1:A:216:GLY:HA3	1:A:264:THR:OG1	2.11	0.50
2:H:62:ASP:HA	2:H:65:LYS:HD2	1.94	0.50
1:A:494:ILE:HA	1:A:497:ILE:HD12	1.95	0.49
1:A:54:ASN:HB3	1:A:334:THR:O	2.13	0.49
2:H:35:HIS:CE1	2:H:50:LEU:HD23	2.47	0.49
2:H:166:TRP:HB2	2:H:171:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1:NAG:H3	5:D:1:NAG:O7	2.13	0.48
2:H:171:LEU:HD11	2:H:194:VAL:HG11	1.96	0.48
1:A:253:VAL:HG21	1:A:259:LEU:HB2	1.96	0.48
1:A:199:HIS:HB2	1:A:268:ILE:HD11	1.95	0.47
2:H:72:ARG:HB3	2:H:79:VAL:HG12	1.95	0.47
3:L:47:LEU:HD23	3:L:58:ILE:HD12	1.97	0.47
2:H:171:LEU:HD12	2:H:171:LEU:O	2.15	0.46
1:A:189:GLN:HA	1:A:255:PRO:HB3	1.98	0.46
1:A:383:LEU:HB3	3:L:93:ASN:HB3	1.98	0.46
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.97	0.46
1:A:100:TRP:CE2	1:A:132:GLY:HA2	2.51	0.46
1:A:392:GLN:HB3	1:A:455:LEU:HD11	1.97	0.46
1:A:219:THR:HG23	1:A:228:THR:HG22	1.98	0.46
2:H:166:TRP:CB	2:H:171:LEU:HD11	2.46	0.46
1:A:185:PRO:HB3	1:A:258:ILE:HG12	1.98	0.46
2:H:87:ARG:HG2	2:H:88:PRO:HD2	1.97	0.45
1:A:253:VAL:HG13	1:A:257:ASP:HB3	1.98	0.45
3:L:14:SER:O	3:L:17:GLU:HB2	2.17	0.45
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.99	0.45
2:H:5:VAL:HG23	2:H:23:ALA:HB3	1.99	0.45
1:A:157:ARG:NH1	1:A:162:SER:OG	2.51	0.44
1:A:217:ARG:NH2	1:A:228:THR:OG1	2.50	0.44
1:A:185:PRO:HA	1:A:258:ILE:HA	1.99	0.44
2:H:88:PRO:HA	2:H:123:VAL:HB	2.00	0.44
3:L:94:TRP:HB3	3:L:95:PRO:HD3	1.99	0.44
4:C:1:NAG:H83	4:C:2:NAG:H82	2.00	0.43
3:L:8:PRO:O	3:L:102:THR:HB	2.19	0.43
1:A:188:GLU:O	1:A:189:GLN:HG2	2.19	0.43
3:L:6:GLN:HE21	3:L:102:THR:HG23	1.83	0.43
1:A:296:GLU:O	1:A:319:GLY:HA3	2.19	0.43
2:H:155:LYS:HA	2:H:189:SER:HB2	2.01	0.42
5:D:1:NAG:C3	5:D:1:NAG:O7	2.68	0.42
3:L:66:GLY:HA3	3:L:71:TYR:HA	2.02	0.42
3:L:33:LEU:HA	3:L:89:GLN:O	2.19	0.42
3:L:36:TYR:O	3:L:86:TYR:HA	2.20	0.41
1:A:147:THR:HB	1:A:171:THR:HB	2.02	0.41
1:A:217:ARG:HH11	1:A:230:SER:HB2	1.85	0.41
1:A:40:THR:OG1	4:B:1:NAG:H81	2.20	0.41
2:H:163:THR:HG23	2:H:211:ASN:HB2	2.01	0.41
1:A:43:LYS:HG2	1:A:48:ASP:O	2.20	0.41
2:H:50:LEU:HD11	2:H:59:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:HB3	1:A:407:LYS:H	1.54	0.41
1:A:162:SER:OG	1:A:163:PHE:N	2.49	0.41
2:H:22:CYS:HB3	2:H:79:VAL:HG23	2.03	0.41
3:L:116:PHE:HB2	3:L:135:LEU:HB3	2.03	0.41
2:H:171:LEU:CD1	2:H:194:VAL:HG11	2.52	0.40
3:L:190:LYS:HE2	3:L:210:ASN:HB3	2.04	0.40
1:A:299:THR:HG22	1:A:317:THR:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:OD1	7:L:301:PO4:O2[10_554]	1.81	0.39

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	464/505 (92%)	426 (92%)	32 (7%)	6 (1%)	12	42
2	H	210/227 (92%)	189 (90%)	19 (9%)	2 (1%)	15	49
3	L	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	52
All	All	885/947 (94%)	816 (92%)	59 (7%)	10 (1%)	14	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ASN
2	H	156	ASP
1	A	257	ASP
1	A	278	SER
1	A	427	LYS

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Mol	Chain	Res	Type
3	L	143	GLU
1	A	478	MET
3	L	138	ASN
1	A	477	ASP
2	H	161	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	A	409/438 (93%)	390 (95%)	19 (5%)	27	59
2	H	178/192 (93%)	173 (97%)	5 (3%)	43	73
3	L	183/185 (99%)	169 (92%)	14 (8%)	13	41
All	All	770/815 (94%)	732 (95%)	38 (5%)	25	57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	47	ASN
1	A	69	ASP
1	A	108	LYS
1	A	117	ASP
1	A	127	LEU
1	A	155	CYS
1	A	175	PHE
1	A	183	THR
1	A	206	ASP
1	A	248	ILE
1	A	304	ILE
1	A	341	GLU
1	A	367	TYR
1	A	452	THR
1	A	453	ILE
1	A	459	GLU

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Mol	Chain	Res	Type
1	A	465	GLU
1	A	473	GLU
2	H	75	SER
2	H	150	LEU
2	H	194	VAL
2	H	196	VAL
2	H	211	ASN
3	L	2	ILE
3	L	5	THR
3	L	18	ARG
3	L	20	THR
3	L	72	THR
3	L	78	LEU
3	L	96	LEU
3	L	102	THR
3	L	109	THR
3	L	123	GLU
3	L	132	VAL
3	L	135	LEU
3	L	187	GLU
3	L	211	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 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	B	1	1,4	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	B	2	4	14,14,15	0.29	0	17,19,21	1.04	1 (5%)
4	BMA	B	3	4	11,11,12	0.41	0	15,15,17	0.62	0
4	NAG	C	1	1,4	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
4	NAG	C	2	4	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
4	BMA	C	3	4	11,11,12	0.44	0	15,15,17	1.13	2 (13%)
5	NAG	D	1	1,5	14,14,15	0.38	0	17,19,21	1.23	2 (11%)
5	NAG	D	2	5	14,14,15	0.30	0	17,19,21	0.83	1 (5%)

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	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1	NAG	O5-C1-C2	-3.68	105.48	111.29
4	B	2	NAG	O5-C1-C2	-3.60	105.60	111.29
4	C	3	BMA	C1-O5-C5	2.90	116.12	112.19
4	C	3	BMA	C1-C2-C3	2.84	113.16	109.67
5	D	1	NAG	C2-N2-C7	2.52	126.49	122.90
4	C	1	NAG	C1-O5-C5	2.34	115.37	112.19
4	C	2	NAG	O5-C1-C2	-2.17	107.86	111.29
5	D	2	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

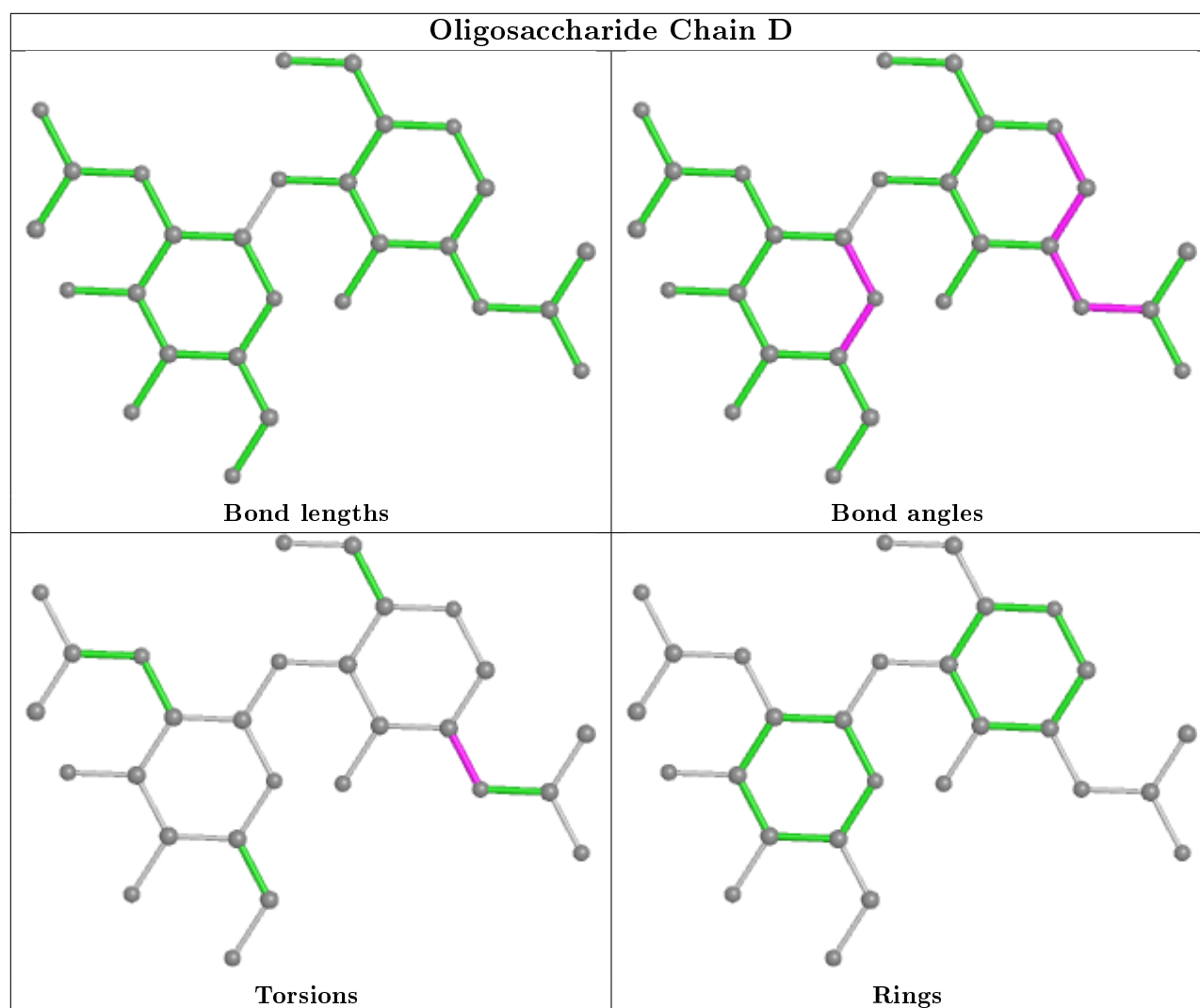
Mol	Chain	Res	Type	Atoms
5	D	1	NAG	C3-C2-N2-C7
4	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	NAG	1	0
5	D	1	NAG	3	0
4	B	1	NAG	1	0
4	C	2	NAG	1	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](#)

7 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	$\# Z > 2$
6	NAG	A	612	1	14,14,15	0.37	0	17,19,21	1.83	2 (11%)
6	NAG	A	606	1	14,14,15	0.31	0	17,19,21	0.79	1 (5%)
8	PGE	L	302	-	9,9,9	0.33	0	8,8,8	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	605	1	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
6	NAG	A	613	1	14,14,15	0.37	0	17,19,21	1.91	2 (11%)
6	NAG	A	604	1	14,14,15	0.31	0	17,19,21	0.70	0
7	PO4	L	301	-	4,4,4	1.91	0	6,6,6	0.58	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	A	612	1	-	2/6/23/26	0/1/1/1
6	NAG	A	606	1	-	0/6/23/26	0/1/1/1
8	PGE	L	302	-	-	1/7/7/7	-
6	NAG	A	605	1	-	0/6/23/26	0/1/1/1
6	NAG	A	613	1	-	1/6/23/26	0/1/1/1
6	NAG	A	604	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	613	NAG	C1-O5-C5	6.82	121.43	112.19
6	A	612	NAG	O5-C1-C2	5.59	120.11	111.29
6	A	612	NAG	C1-O5-C5	4.78	118.67	112.19
6	A	613	NAG	O5-C1-C2	3.27	116.46	111.29
6	A	606	NAG	O5-C1-C2	-2.51	107.33	111.29
6	A	605	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	612	NAG	O5-C5-C6-O6
6	A	613	NAG	C4-C5-C6-O6
8	L	302	PGE	C1-C2-O2-C3
6	A	612	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	301	PO4	0	1

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, 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	470/505 (93%)	-0.11	0	100 100	40, 70, 113, 157	5 (1%)
2	H	216/227 (95%)	0.04	4 (1%)	66 46	59, 94, 130, 152	4 (1%)
3	L	213/215 (99%)	-0.03	1 (0%)	91 81	52, 75, 118, 128	2 (0%)
All	All	899/947 (94%)	-0.05	5 (0%)	89 78	40, 75, 121, 157	11 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	206	TYR	2.8
3	L	184	ALA	2.8
2	H	150	LEU	2.6
2	H	174	GLY	2.2
2	H	173	SER	2.2

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.

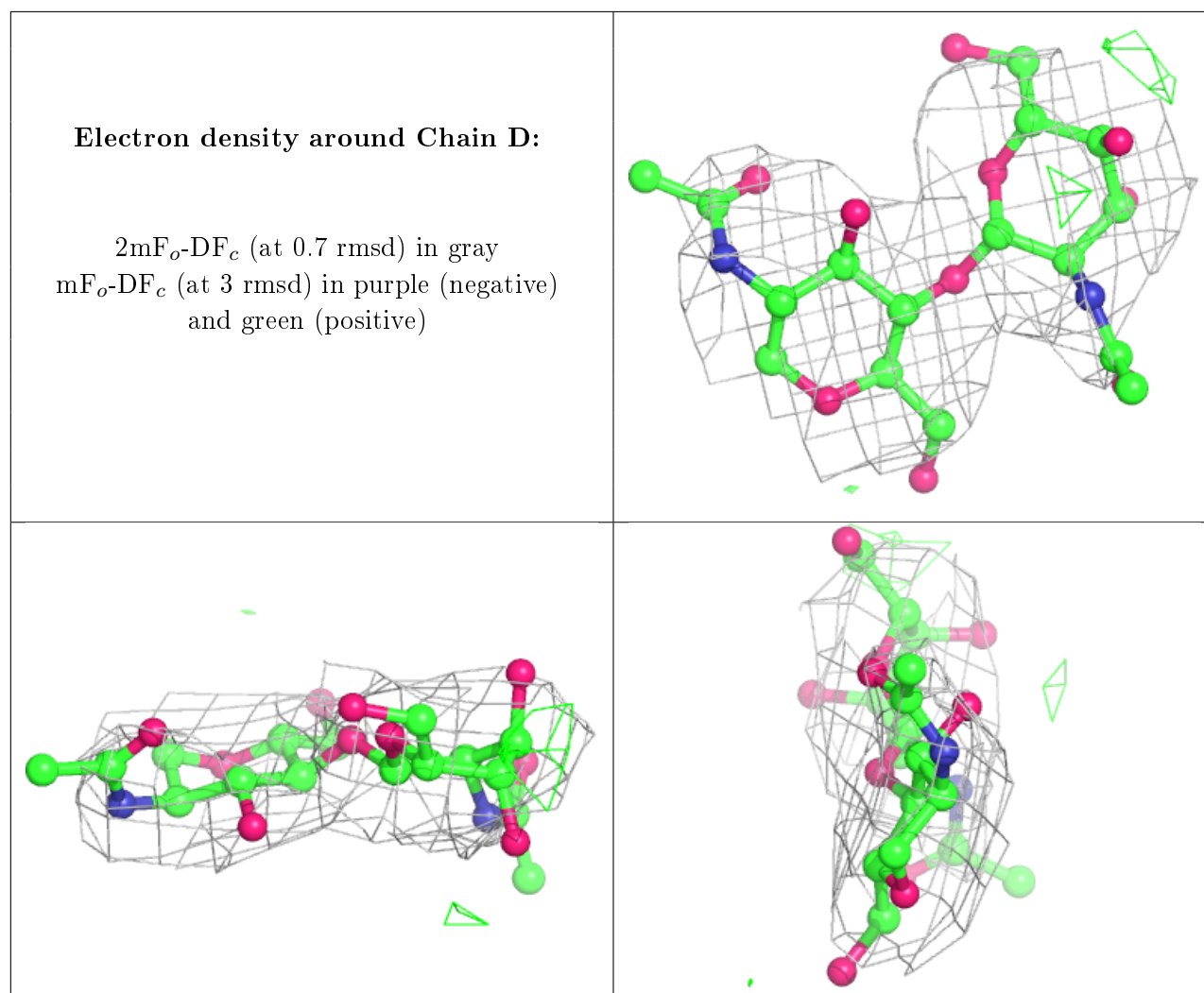
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	B	3	11/12	0.77	0.16	121,126,128,128	0
4	BMA	C	3	11/12	0.82	0.16	114,115,117,117	0
5	NAG	D	1	14/15	0.86	0.27	118,121,124,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	C	2	14/15	0.86	0.21	106,109,117,117	0
5	NAG	D	2	14/15	0.87	0.26	130,132,133,134	0
4	NAG	C	1	14/15	0.88	0.22	100,104,110,113	0
4	NAG	B	2	14/15	0.90	0.18	91,99,107,115	0
4	NAG	B	1	14/15	0.96	0.18	67,71,75,82	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 ⓘ

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
6	NAG	A	613	14/15	0.76	0.26	135,138,139,139	0
6	NAG	A	606	14/15	0.78	0.28	109,113,116,118	0
6	NAG	A	612	14/15	0.84	0.18	99,104,106,107	0
6	NAG	A	605	14/15	0.87	0.15	107,110,111,111	0
6	NAG	A	604	14/15	0.88	0.20	94,96,102,103	0
8	PGE	L	302	10/10	0.91	0.23	58,65,70,70	0
7	PO4	L	301	5/5	0.92	0.19	111,111,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.