wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 11:47 AM EST

PDB ID	:	6BE6
Title	:	ADAM10 Extracellular Domain
Authors	:	Seegar, T.C.M.
Deposited on	:	2017-10-24
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

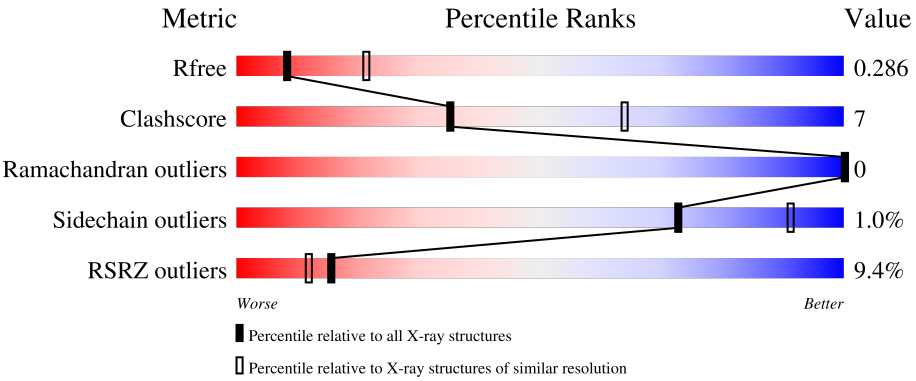
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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 >=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 <=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	449	6% 79% 17% .
1	B	449	11% 78% 18% .
1	C	449	11% 79% 17% .
1	D	449	8% 82% 14% .
2	E	5	80% 20%

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Mol	Chain	Length	Quality of chain
3	F	7	71% 29%
4	G	5	20% 80%
5	H	8	12% 25% 62%

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
8	SO4	C	704	-	-	X	-
8	SO4	D	704	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13995 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 Disintegrin and metalloproteinase domain-containing protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3311	2033	585	653	40			
1	B	431	Total	C	N	O	S	0	0	0
			3310	2033	585	652	40			
1	C	433	Total	C	N	O	S	0	0	0
			3324	2040	587	657	40			
1	D	433	Total	C	N	O	S	0	0	0
			3325	2040	587	658	40			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLN	ASN	conflict	UNP O14672
A	439	GLN	ASN	conflict	UNP O14672
A	551	GLN	ASN	conflict	UNP O14672
A	655	GLY	-	expression tag	UNP O14672
A	656	GLY	-	expression tag	UNP O14672
A	657	HIS	-	expression tag	UNP O14672
A	658	HIS	-	expression tag	UNP O14672
A	659	HIS	-	expression tag	UNP O14672
A	660	HIS	-	expression tag	UNP O14672
A	661	HIS	-	expression tag	UNP O14672
A	662	HIS	-	expression tag	UNP O14672
B	267	GLN	ASN	conflict	UNP O14672
B	439	GLN	ASN	conflict	UNP O14672
B	551	GLN	ASN	conflict	UNP O14672
B	655	GLY	-	expression tag	UNP O14672
B	656	GLY	-	expression tag	UNP O14672
B	657	HIS	-	expression tag	UNP O14672
B	658	HIS	-	expression tag	UNP O14672
B	659	HIS	-	expression tag	UNP O14672
B	660	HIS	-	expression tag	UNP O14672

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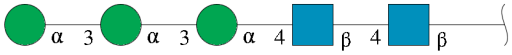
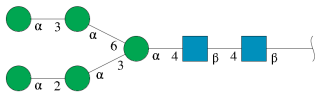
Chain	Residue	Modelled	Actual	Comment	Reference
B	661	HIS	-	expression tag	UNP O14672
B	662	HIS	-	expression tag	UNP O14672
C	267	GLN	ASN	conflict	UNP O14672
C	439	GLN	ASN	conflict	UNP O14672
C	551	GLN	ASN	conflict	UNP O14672
C	655	GLY	-	expression tag	UNP O14672
C	656	GLY	-	expression tag	UNP O14672
C	657	HIS	-	expression tag	UNP O14672
C	658	HIS	-	expression tag	UNP O14672
C	659	HIS	-	expression tag	UNP O14672
C	660	HIS	-	expression tag	UNP O14672
C	661	HIS	-	expression tag	UNP O14672
C	662	HIS	-	expression tag	UNP O14672
D	267	GLN	ASN	conflict	UNP O14672
D	439	GLN	ASN	conflict	UNP O14672
D	551	GLN	ASN	conflict	UNP O14672
D	655	GLY	-	expression tag	UNP O14672
D	656	GLY	-	expression tag	UNP O14672
D	657	HIS	-	expression tag	UNP O14672
D	658	HIS	-	expression tag	UNP O14672
D	659	HIS	-	expression tag	UNP O14672
D	660	HIS	-	expression tag	UNP O14672
D	661	HIS	-	expression tag	UNP O14672
D	662	HIS	-	expression tag	UNP O14672

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



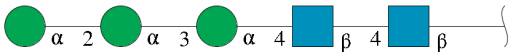
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	5	61	34	2	25	0	0	0

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



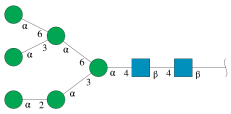
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	7	Total C N O 83 46 2 35	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-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	G	5	Total C N O 61 34 2 25	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-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
5	H	8	Total C N O 94 52 2 40	0	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0
6	C	1	Total Zn 1 1	0	0

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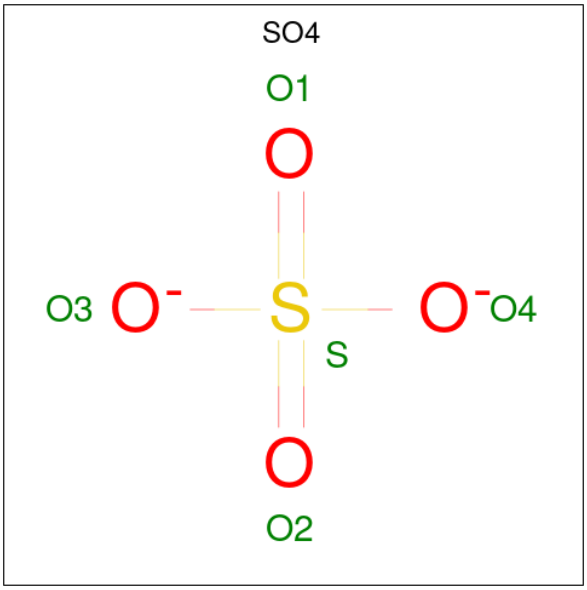
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Zn 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

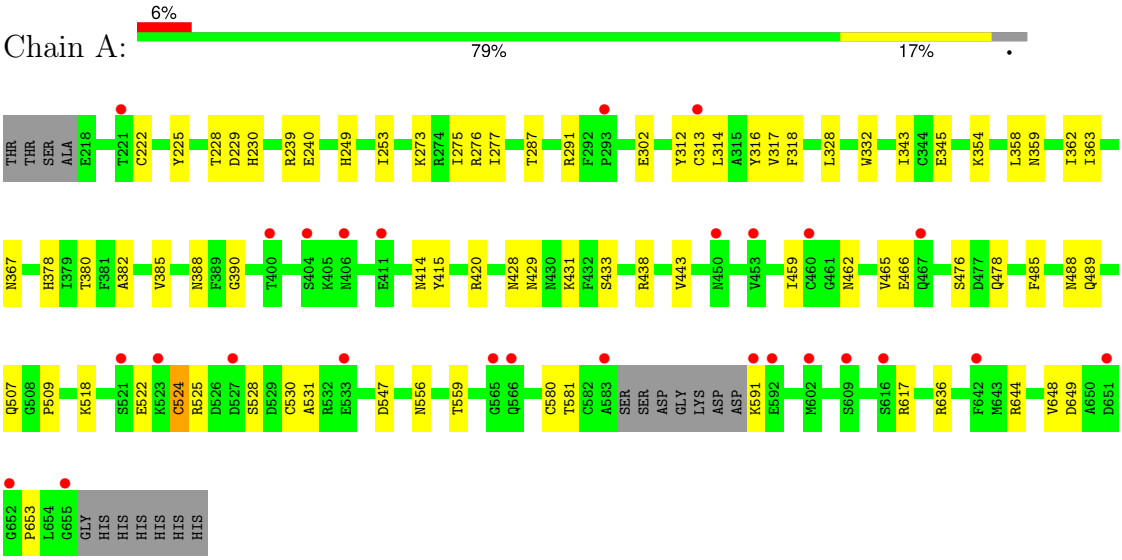
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	100	Total O 100 100	0	0
9	B	90	Total O 90 90	0	0
9	C	87	Total O 87 87	0	0
9	D	106	Total O 106 106	0	0

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.

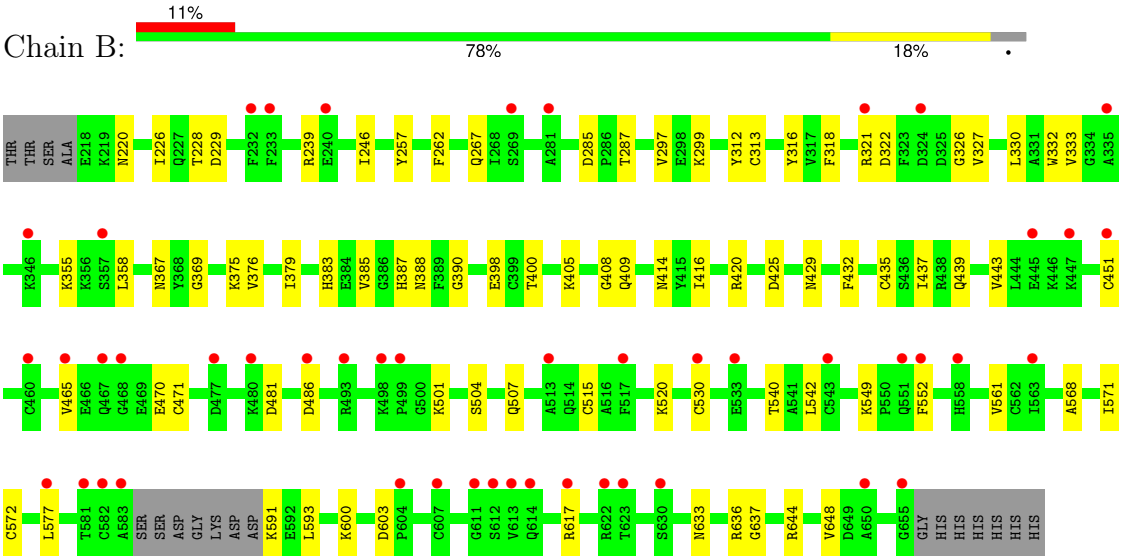
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10

Chain A:



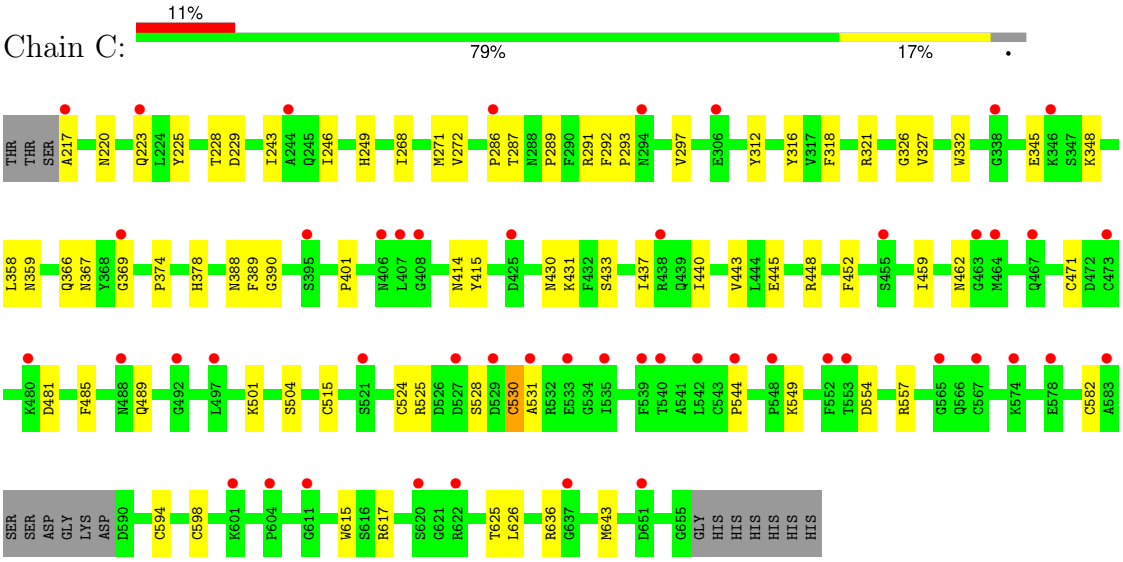
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10

Chain B:



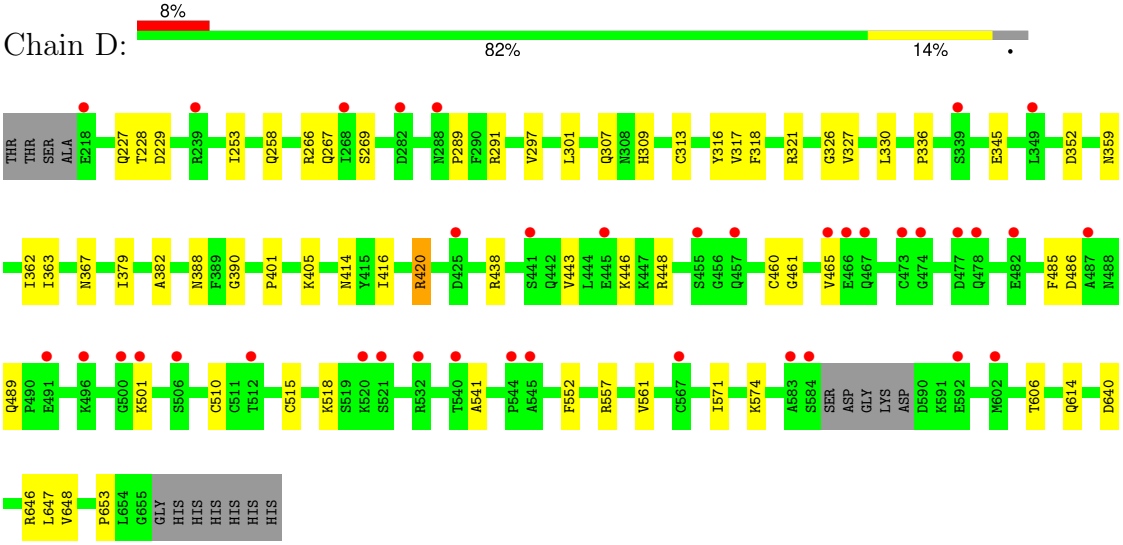
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10

Chain C:



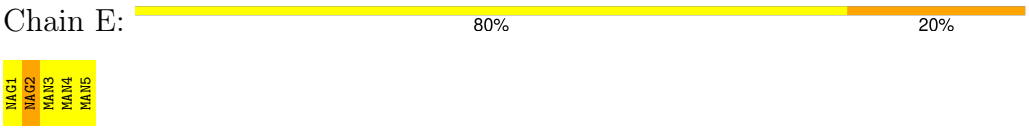
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10

Chain D:



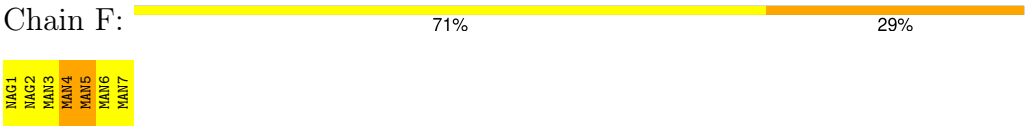
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



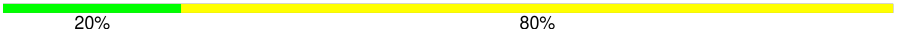
• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.42Å 188.78Å 86.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 2.80 47.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (47.48-2.80) 82.1 (47.48-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.87 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.236 , 0.284 0.236 , 0.286	Depositor DCC
R_{free} test set	2655 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	13995	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, ZN, MAN, SO4

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	0.25	0/3377	0.43	0/4549
1	B	0.26	0/3376	0.43	0/4547
1	C	0.25	0/3390	0.42	0/4567
1	D	0.25	0/3391	0.43	0/4568
All	All	0.25	0/13534	0.43	0/18231

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

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	3311	0	3125	45	1
1	B	3310	0	3123	53	0
1	C	3324	0	3134	49	0
1	D	3325	0	3134	46	0
2	E	61	0	52	5	0
3	F	83	0	70	4	0
4	G	61	0	52	2	0
5	H	94	0	79	4	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	5	0	0	0	0
8	B	10	0	0	1	0
8	C	10	0	0	3	1
8	D	10	0	0	2	0
9	A	100	0	0	2	0
9	B	90	0	0	4	0
9	C	87	0	0	7	0
9	D	106	0	0	6	0
All	All	13995	0	12769	193	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 7.

The worst 5 of 193 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:431:LYS:HE3	9:C:835:HOH:O	1.73	0.89
1:C:229:ASP:OD2	1:C:321:ARG:NH2	2.12	0.81
1:A:302:GLU:OE2	1:A:354:LYS:NZ	2.13	0.78
1:A:390:GLY:HA3	1:A:443:VAL:HG21	1.68	0.75
1:B:400:THR:OG1	1:B:414:ASN:ND2	2.21	0.74

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:617:ARG:NH2	8:C:704:SO4:O2[1_556]	1.30	0.90

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	427/449 (95%)	406 (95%)	21 (5%)	0	100	100
1	B	427/449 (95%)	399 (93%)	28 (7%)	0	100	100
1	C	429/449 (96%)	399 (93%)	30 (7%)	0	100	100
1	D	429/449 (96%)	400 (93%)	29 (7%)	0	100	100
All	All	1712/1796 (95%)	1604 (94%)	108 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	A	373/388 (96%)	368 (99%)	5 (1%)	65	88
1	B	373/388 (96%)	370 (99%)	3 (1%)	79	93
1	C	374/388 (96%)	369 (99%)	5 (1%)	65	88
1	D	375/388 (97%)	373 (100%)	2 (0%)	86	95
All	All	1495/1552 (96%)	1480 (99%)	15 (1%)	73	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	617	ARG
1	D	313	CYS
1	C	223	GLN

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Mol	Chain	Res	Type
1	D	420	ARG
1	C	530	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	367	ASN
1	D	614	GLN
1	D	388	ASN
1	D	478	GLN
1	B	439	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

25 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	$\#\|Z\|>2$
2	NAG	E	1	1,2	14,14,15	0.43	0	17,19,21	0.45	0
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	1.45	2 (11%)
2	MAN	E	3	2	11,11,12	0.72	0	15,15,17	0.88	2 (13%)
2	MAN	E	4	2	11,11,12	0.77	0	15,15,17	1.69	2 (13%)
2	MAN	E	5	2	11,11,12	0.86	0	15,15,17	0.85	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.26	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.45	0
3	MAN	F	3	3	11,11,12	0.77	0	15,15,17	1.24	2 (13%)
3	MAN	F	4	3	11,11,12	0.56	0	15,15,17	0.98	1 (6%)
3	MAN	F	5	3	11,11,12	0.94	1 (9%)	15,15,17	0.90	1 (6%)
3	MAN	F	6	3	11,11,12	1.01	0	15,15,17	1.17	1 (6%)
3	MAN	F	7	3	11,11,12	0.94	1 (9%)	15,15,17	1.34	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.30	0	17,19,21	0.45	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.47	0
4	MAN	G	3	4	11,11,12	0.73	0	15,15,17	1.18	1 (6%)
4	MAN	G	4	4	11,11,12	0.79	1 (9%)	15,15,17	1.15	1 (6%)
4	MAN	G	5	4	11,11,12	0.75	0	15,15,17	0.87	1 (6%)
5	NAG	H	1	1,5	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	H	2	5	14,14,15	0.21	0	17,19,21	0.45	0
5	MAN	H	3	5	11,11,12	0.86	0	15,15,17	1.06	2 (13%)
5	MAN	H	4	5	11,11,12	0.74	0	15,15,17	1.23	2 (13%)
5	MAN	H	5	5	11,11,12	1.37	2 (18%)	15,15,17	1.62	4 (26%)
5	MAN	H	6	5	11,11,12	1.10	1 (9%)	15,15,17	1.21	3 (20%)
5	MAN	H	7	5	11,11,12	0.79	0	15,15,17	0.96	2 (13%)
5	MAN	H	8	5	11,11,12	0.68	0	15,15,17	1.05	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	6/6/23/26	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	1/1/1/1
2	MAN	E	4	2	-	1/2/19/22	1/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	2/2/19/22	1/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	1/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	MAN	G	3	4	-	0/2/19/22	1/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	MAN	H	3	5	-	0/2/19/22	1/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	1/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	2/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	5	MAN	C1-C2	3.55	1.60	1.52
5	H	6	MAN	C1-C2	2.94	1.59	1.52
5	H	5	MAN	C2-C3	2.58	1.56	1.52
4	G	4	MAN	C1-C2	2.20	1.57	1.52
3	F	7	MAN	C1-C2	2.20	1.57	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	MAN	C1-O5-C5	4.87	118.71	112.19
2	E	2	NAG	C2-N2-C7	4.67	129.16	122.90
3	F	3	MAN	C1-O5-C5	3.57	116.96	112.19
4	G	3	MAN	C1-O5-C5	3.48	116.85	112.19
3	F	7	MAN	C1-O5-C5	3.31	116.62	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	4	MAN	O5-C5-C6-O6

5 of 6 ring outliers are listed below:

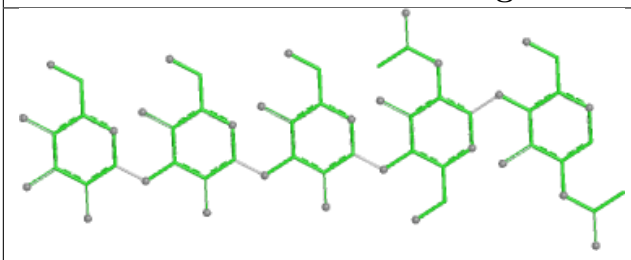
Mol	Chain	Res	Type	Atoms
3	F	3	MAN	C1-C2-C3-C4-C5-O5
2	E	4	MAN	C1-C2-C3-C4-C5-O5
3	F	6	MAN	C1-C2-C3-C4-C5-O5
2	E	3	MAN	C1-C2-C3-C4-C5-O5
4	G	3	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 15 short contacts:

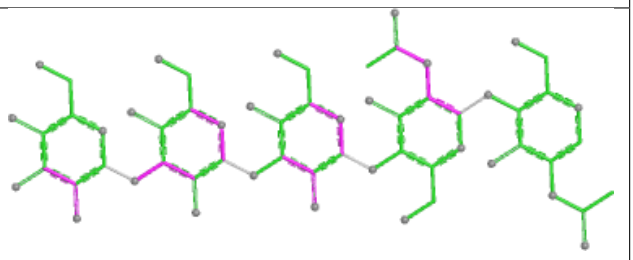
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
2	E	2	NAG	4	0
5	H	8	MAN	1	0
4	G	2	NAG	2	0
3	F	2	NAG	1	0
5	H	4	MAN	1	0
3	F	4	MAN	1	0
3	F	5	MAN	2	0
3	F	1	NAG	2	0
5	H	7	MAN	1	0
2	E	1	NAG	2	0
5	H	5	MAN	1	0
5	H	6	MAN	2	0

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

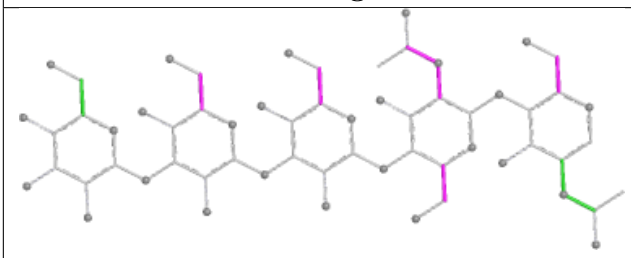
Oligosaccharide Chain E



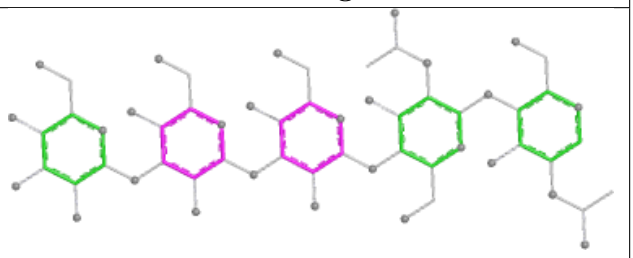
Bond lengths



Bond angles

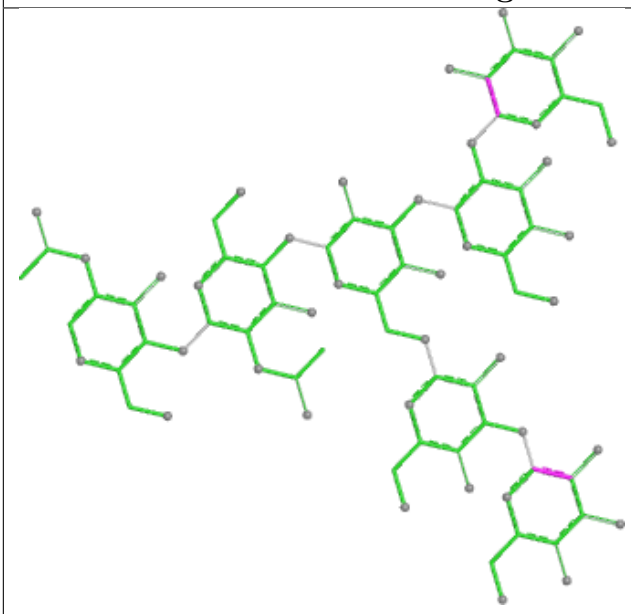


Torsions

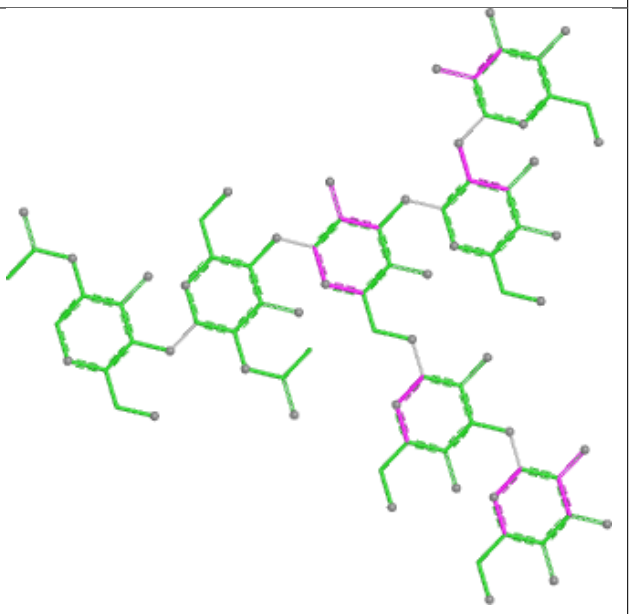


Rings

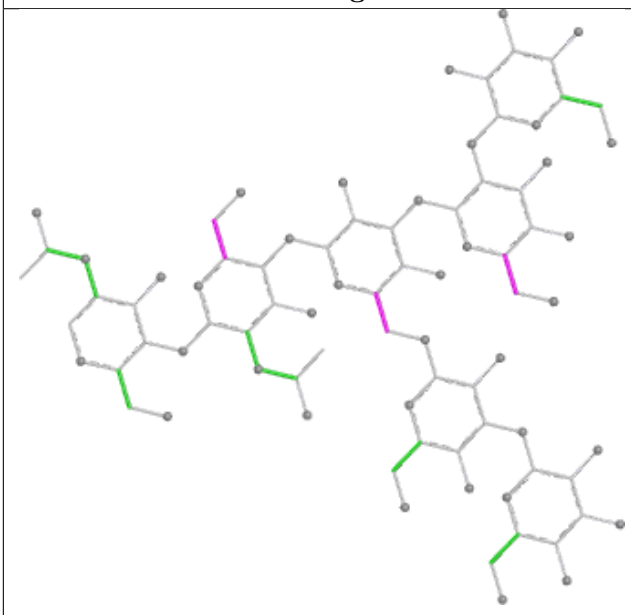
Oligosaccharide Chain F



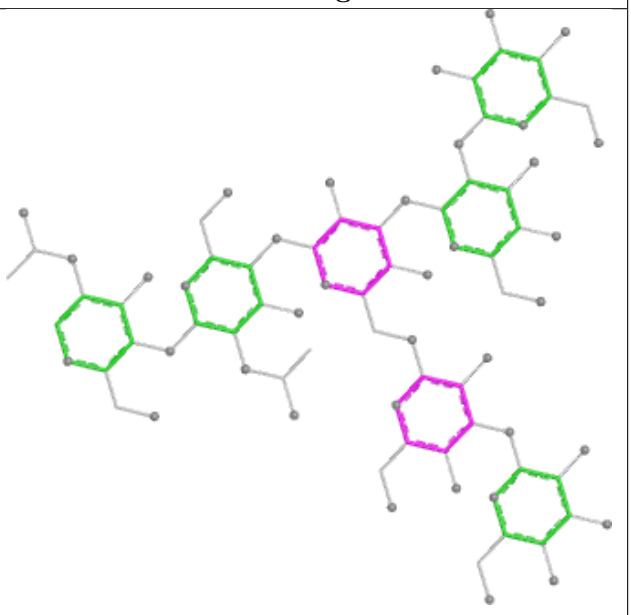
Bond lengths



Bond angles

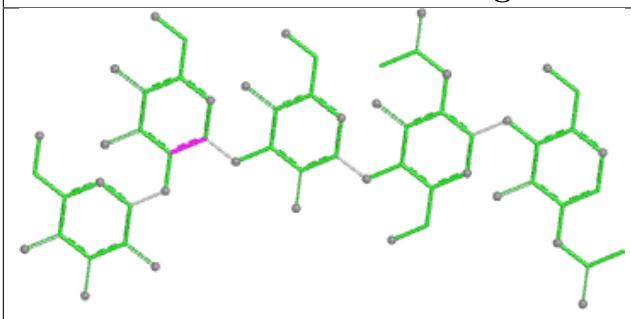


Torsions

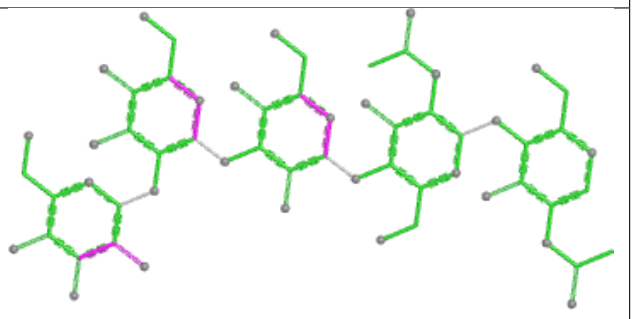


Rings

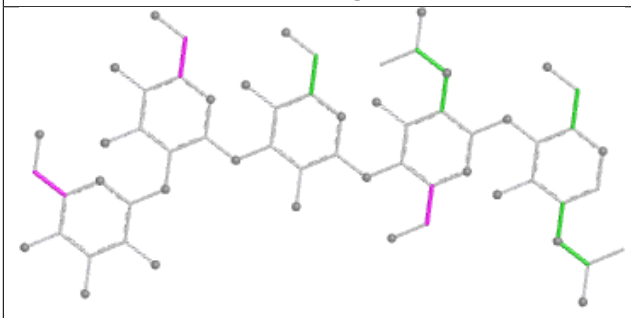
Oligosaccharide Chain G



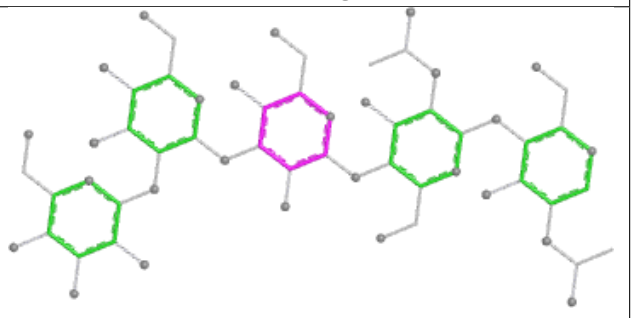
Bond lengths



Bond angles

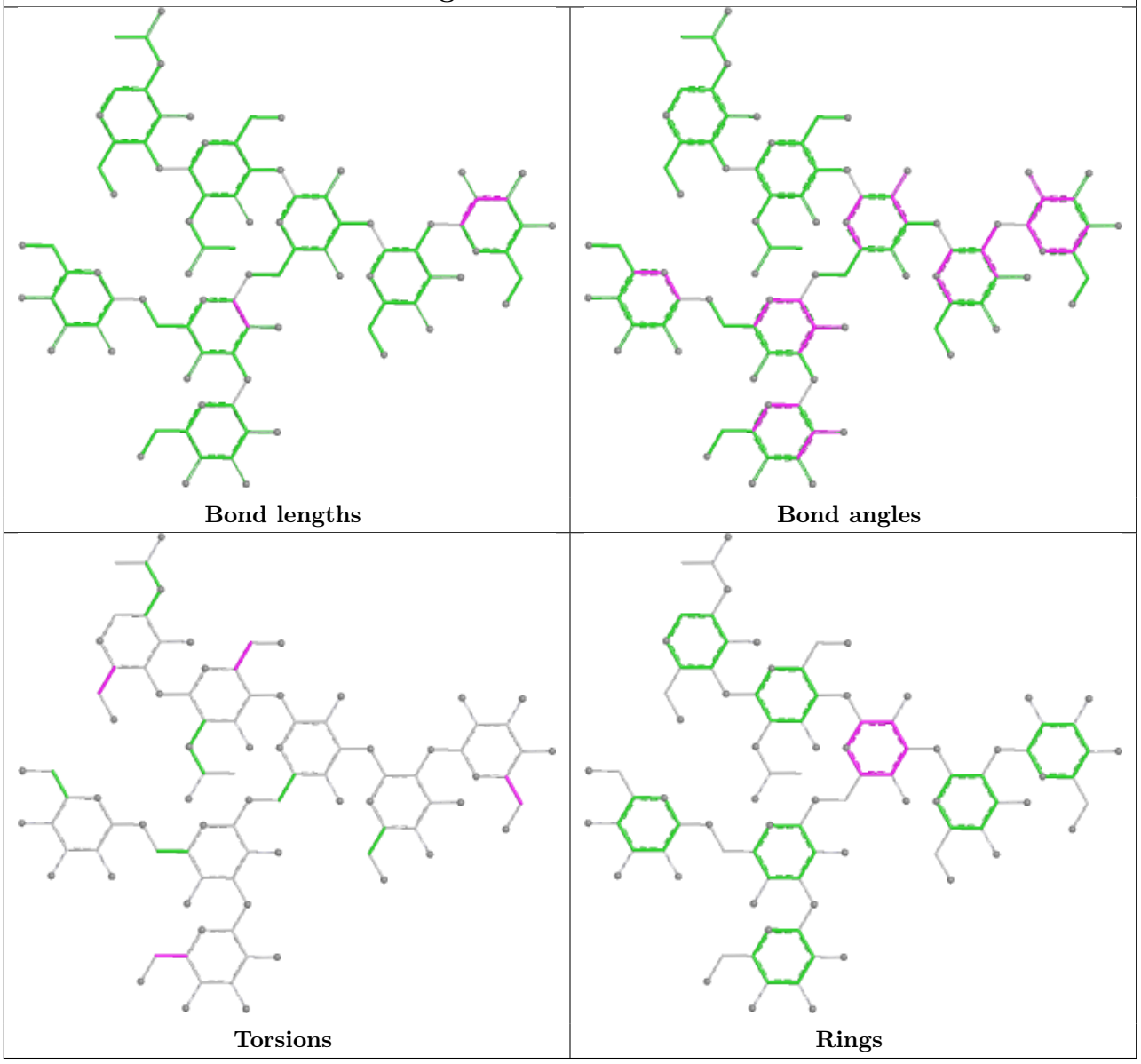


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	SO4	B	703	-	4,4,4	0.24	0	6,6,6	0.06	0
8	SO4	B	704	-	4,4,4	0.22	0	6,6,6	0.07	0
8	SO4	A	703	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	C	703	-	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	C	704	-	4,4,4	0.23	0	6,6,6	0.09	0
8	SO4	D	703	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	D	704	-	4,4,4	0.24	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	704	SO4	1	0
8	C	703	SO4	1	0
8	C	704	SO4	2	1
8	D	704	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	431/449 (95%)	0.69	27 (6%)	27	21	15, 39, 72, 102	0
1	B	431/449 (95%)	0.95	48 (11%)	12	9	17, 47, 78, 106	0
1	C	433/449 (96%)	0.90	49 (11%)	11	9	14, 47, 82, 104	0
1	D	433/449 (96%)	0.85	38 (8%)	17	13	19, 46, 91, 108	0
All	All	1728/1796 (96%)	0.85	162 (9%)	15	12	14, 45, 82, 108	0

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	425	ASP	5.8
1	D	583	ALA	4.7
1	A	602	MET	4.2
1	C	527	ASP	4.2
1	D	584	SER	4.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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^{th} 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
5	MAN	H	8	11/12	0.55	0.18	61,78,104,106	0
5	MAN	H	5	11/12	0.57	0.18	50,85,98,104	0

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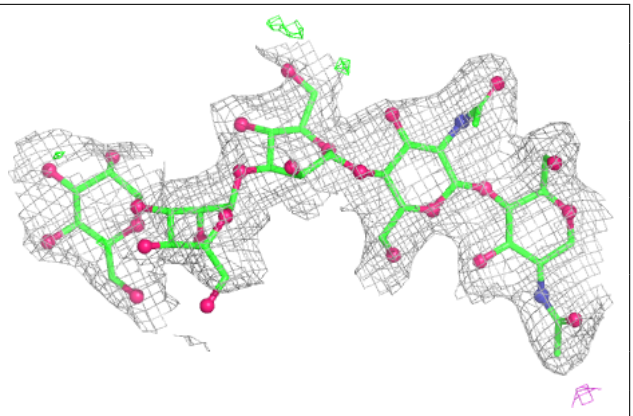
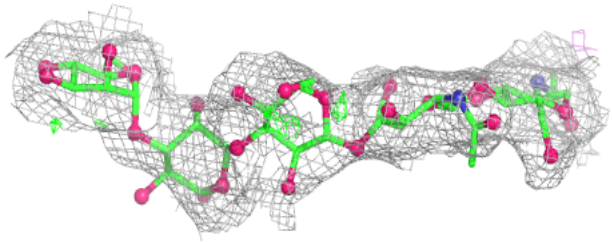
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	F	5	11/12	0.60	0.16	52,70,81,83	0
3	MAN	F	6	11/12	0.62	0.19	74,80,99,101	0
3	MAN	F	7	11/12	0.68	0.20	53,80,95,104	0
5	MAN	H	7	11/12	0.70	0.19	65,76,82,84	0
5	MAN	H	6	11/12	0.70	0.19	66,77,87,92	0
2	MAN	E	5	11/12	0.71	0.15	52,71,81,82	0
2	MAN	E	4	11/12	0.75	0.20	57,71,92,119	0
4	MAN	G	5	11/12	0.75	0.18	35,49,69,72	0
2	MAN	E	3	11/12	0.76	0.14	34,49,65,70	0
4	MAN	G	4	11/12	0.77	0.14	54,60,66,67	0
3	MAN	F	4	11/12	0.78	0.16	48,62,86,96	0
5	MAN	H	4	11/12	0.78	0.14	53,73,78,89	0
5	MAN	H	3	11/12	0.82	0.15	53,65,85,87	0
3	NAG	F	2	14/15	0.85	0.17	25,42,54,60	0
3	MAN	F	3	11/12	0.85	0.15	32,52,71,71	0
4	NAG	G	2	14/15	0.86	0.13	29,42,53,57	0
4	MAN	G	3	11/12	0.86	0.10	28,42,56,58	0
2	NAG	E	2	14/15	0.89	0.11	29,38,54,55	0
5	NAG	H	2	14/15	0.89	0.13	33,49,68,78	0
3	NAG	F	1	14/15	0.89	0.15	26,34,55,71	0
4	NAG	G	1	14/15	0.89	0.13	27,44,55,58	0
5	NAG	H	1	14/15	0.90	0.10	25,32,38,43	0
2	NAG	E	1	14/15	0.90	0.11	14,29,45,55	0

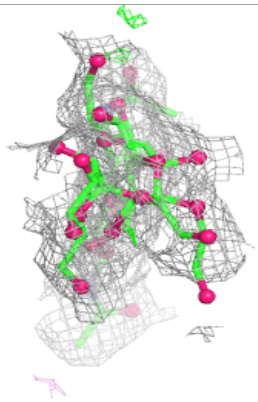
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

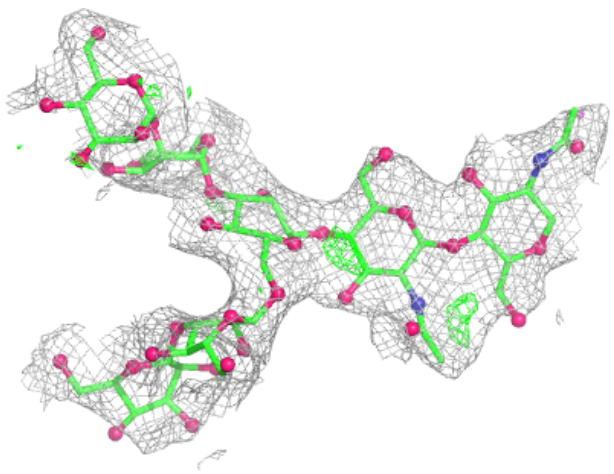


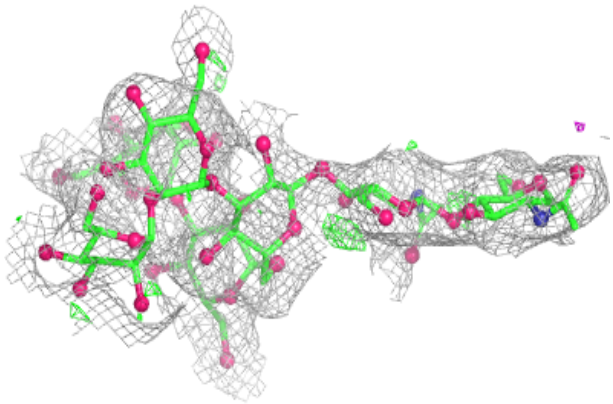


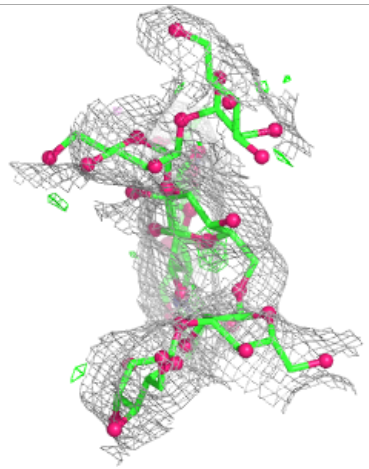


Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

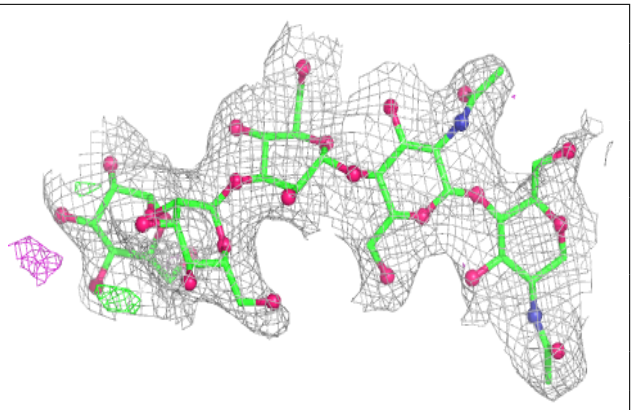


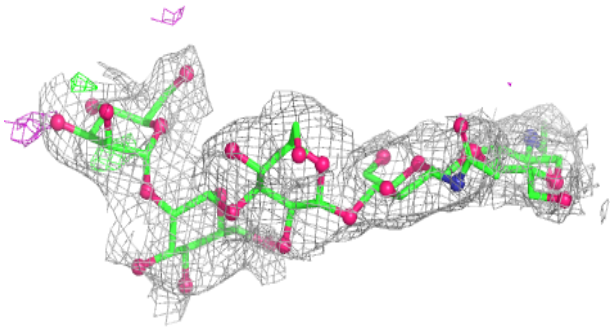




Electron density around Chain G:

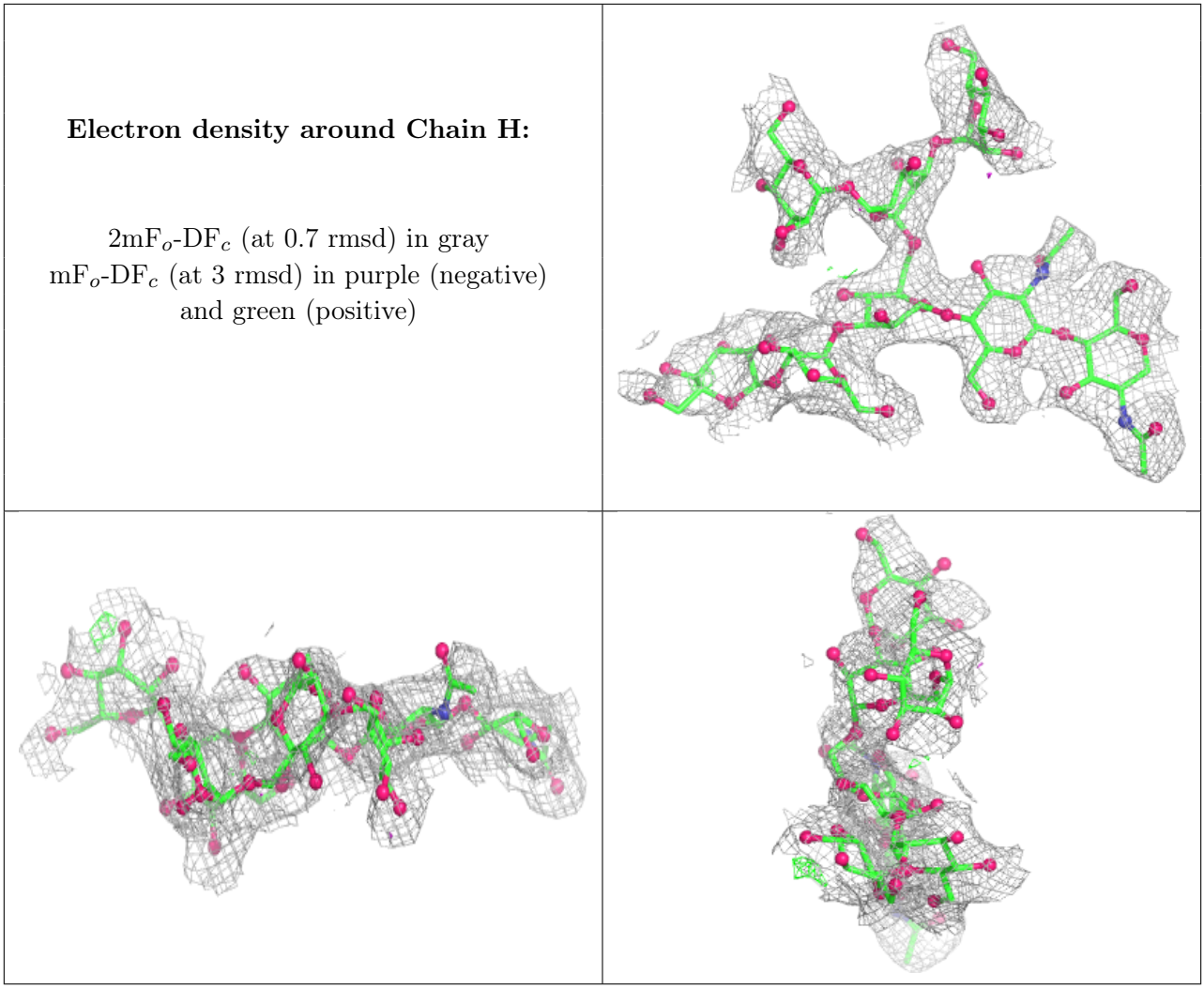
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around Chain H:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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, 95^{th} 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
8	SO4	C	703	5/5	0.47	0.14	106,109,123,124	0
8	SO4	C	704	5/5	0.75	0.19	72,89,99,110	0
8	SO4	D	704	5/5	0.79	0.17	51,84,101,102	0
8	SO4	B	704	5/5	0.82	0.20	50,77,100,118	0
8	SO4	A	703	5/5	0.84	0.12	72,78,81,81	0
7	CA	B	702	1/1	0.92	0.10	40,40,40,40	0
8	SO4	B	703	5/5	0.92	0.07	44,46,52,66	0
8	SO4	D	703	5/5	0.93	0.09	37,45,56,68	0
7	CA	C	702	1/1	0.96	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	D	702	1/1	0.97	0.06	38,38,38,38	0
6	ZN	A	701	1/1	0.97	0.04	22,22,22,22	0
7	CA	A	702	1/1	0.98	0.04	35,35,35,35	0
6	ZN	D	701	1/1	0.99	0.04	30,30,30,30	0
6	ZN	B	701	1/1	0.99	0.02	20,20,20,20	0
6	ZN	C	701	1/1	0.99	0.03	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.