



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 03:34 am GMT

PDB ID : 4BSE
Title : Human H7N9 Influenza Virus Haemagglutinin in Complex with Human Receptor Analogue LSTc
Authors : Xiong, X.; Haire, L.F.; Martin, S.R.; Wharton, S.A.; Daniels, R.S.; Bennett, M.S.; McCauley, J.W.; Collins, P.J.; Walker, P.A.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2013-06-10
Resolution : 2.55 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

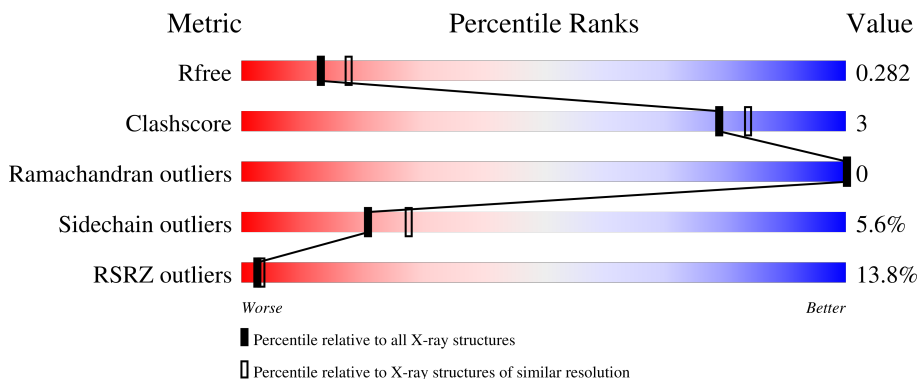
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



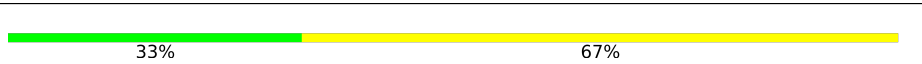
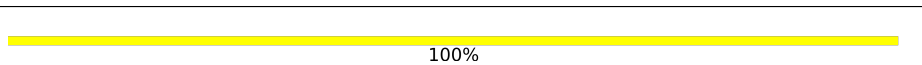
The reported resolution of this entry is 2.55 Å.

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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	
2	B	177	
3	C	3	
4	D	2	

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
3	NAG	C	1	-	-	-	X
5	NAG	A	1319	-	-	-	X
6	SO4	A	1324	-	-	-	X
6	SO4	A	1325	-	-	-	X
6	SO4	A	1331	-	-	-	X
6	SO4	B	1176	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4069 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 HAEMAGGLUTININ HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2413	1498	437	463	15	0	0	1

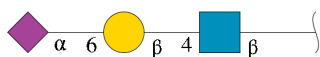
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LEU	ILE	SEE REMARK 999	UNP M4YV75

- Molecule 2 is a protein called HAEMAGGLUTININ HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	170	1379	851	241	280	7	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	46	25	2	19	0	0	0

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

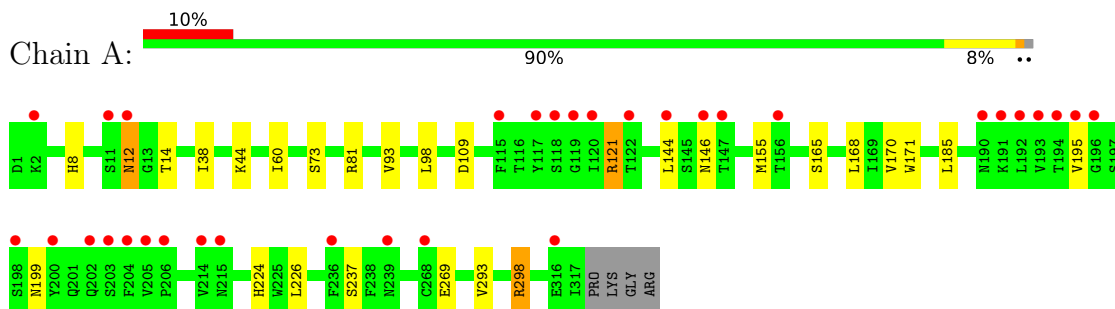
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	62	Total	O	0	0
			62	62		
7	B	24	Total	O	0	0
			24	24		

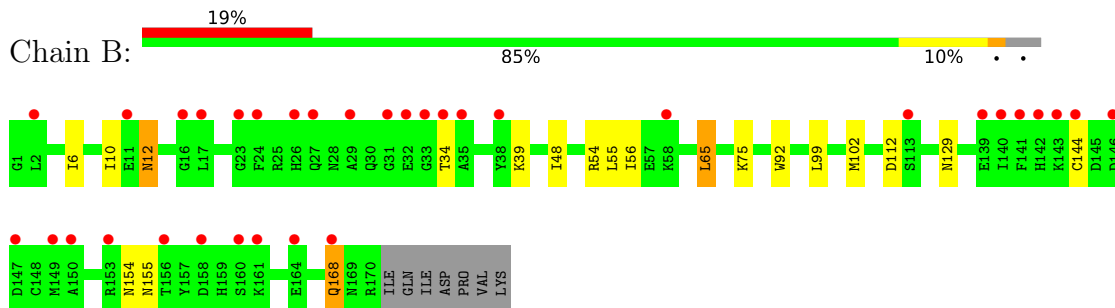
3 Residue-property plots [i](#)

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: HAEMAGGLUTININ HA1



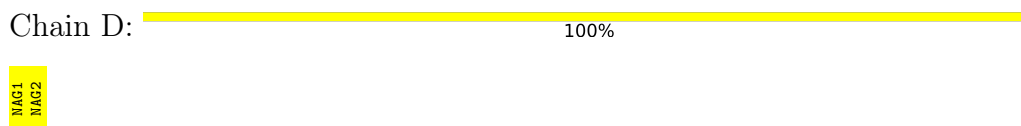
- Molecule 2: HAEMAGGLUTININ HA2



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	115.89Å 115.89Å 296.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.58 – 2.55 41.55 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.58-2.55) 99.9 (41.55-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.233 , 0.279 0.236 , 0.282	Depositor DCC
R_{free} test set	1292 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.019 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.010 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, SIA, GAL

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	0.38	0/2459	0.62	0/3324
2	B	0.33	0/1403	0.55	0/1890
All	All	0.36	0/3862	0.59	0/5214

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	2413	0	2371	13	0
2	B	1379	0	1280	11	0
3	C	46	0	40	0	0
4	D	28	0	25	2	0
5	A	42	0	39	1	0
6	A	55	0	0	1	0
6	B	20	0	0	0	0
7	A	62	0	0	1	0
7	B	24	0	0	2	0
All	All	4069	0	3755	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ASN:HD22	2:B:12:ASN:C	2.07	0.57
1:A:185:LEU:HA	7:A:2033:HOH:O	2.06	0.56
2:B:75:LYS:HE3	4:D:1:NAG:H81	1.87	0.55
1:A:44:LYS:HE2	1:A:269:GLU:HB2	1.91	0.53
7:B:2011:HOH:O	4:D:1:NAG:H83	2.10	0.51
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.93	0.50
1:A:12:ASN:ND2	5:A:1319:NAG:H83	2.26	0.50
2:B:154:ASN:HB3	7:B:2020:HOH:O	2.10	0.50
1:A:171:TRP:CZ2	1:A:195:VAL:HG21	2.48	0.49
1:A:293:VAL:HG11	2:B:65:LEU:HD13	1.96	0.48
1:A:60:ILE:HG21	1:A:170:VAL:HG21	1.95	0.48
1:A:298:ARG:HG2	2:B:92:TRP:CE2	2.51	0.45
2:B:168:GLN:HE21	2:B:168:GLN:HB3	1.64	0.45
1:A:121:ARG:NH1	1:A:146:ASN:O	2.51	0.44
1:A:298:ARG:HG2	2:B:92:TRP:CD2	2.52	0.44
1:A:98:LEU:HD11	1:A:168:LEU:HD21	2.02	0.42
1:A:93:VAL:HG21	1:A:224:HIS:CD2	2.55	0.41
1:A:165:SER:N	6:A:1328:SO4:O3	2.53	0.41
2:B:55:LEU:HD22	2:B:99:LEU:HD21	2.02	0.41
2:B:56:ILE:O	2:B:56:ILE:HG22	2.21	0.41
1:A:155:MET:O	1:A:237:SER:HA	2.21	0.40
2:B:10:ILE:N	2:B:10:ILE:HD12	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	315/321 (98%)	300 (95%)	15 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	168/177 (95%)	163 (97%)	5 (3%)	0	100	100
All	All	483/498 (97%)	463 (96%)	20 (4%)	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	265/269 (98%)	253 (96%)	12 (4%)	27	37
2	B	145/152 (95%)	134 (92%)	11 (8%)	13	17
All	All	410/421 (97%)	387 (94%)	23 (6%)	21	28

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	12	ASN
1	A	14	THR
1	A	38	ILE
1	A	73	SER
1	A	81	ARG
1	A	109	ASP
1	A	121	ARG
1	A	144	LEU
1	A	199	ASN
1	A	226	LEU
1	A	298	ARG
2	B	12	ASN
2	B	34	THR
2	B	39	LYS
2	B	48	ILE
2	B	54	ARG
2	B	65	LEU

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Mol	Chain	Res	Type
2	B	102	MET
2	B	129	ASN
2	B	144	CYS
2	B	155	ASN
2	B	168	GLN

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

Mol	Chain	Res	Type
1	A	199	ASN
1	A	224	HIS
2	B	12	ASN
2	B	62	GLN
2	B	168	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](#)

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
3	NAG	C	1	3	15,15,15	0.45	0	21,21,21	1.09	2 (9%)
3	GAL	C	2	3	11,11,12	0.36	0	15,15,17	0.82	0
3	SIA	C	3	3	20,20,21	0.59	0	24,28,31	1.26	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	1	2,4	14,14,15	0.53	0	17,19,21	0.89	0
4	NAG	D	2	4	14,14,15	0.56	0	17,19,21	0.96	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
3	NAG	C	1	3	-	2/6/26/26	0/1/1/1
3	GAL	C	2	3	-	1/2/19/22	0/1/1/1
3	SIA	C	3	3	-	2/18/34/38	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	SIA	C4-C5-N5	-3.25	103.93	110.38
4	D	2	NAG	C4-C3-C2	2.60	114.83	111.02
3	C	1	NAG	C1-C2-N2	-2.53	107.80	110.73
3	C	3	SIA	O6-C2-C1	2.47	112.55	107.70
3	C	3	SIA	C6-O6-C2	2.32	116.30	111.34
3	C	3	SIA	O1B-C1-C2	2.13	119.11	113.03
3	C	1	NAG	C8-C7-N2	2.11	119.67	116.10

There are no chirality outliers.

All (7) torsion outliers are listed below:

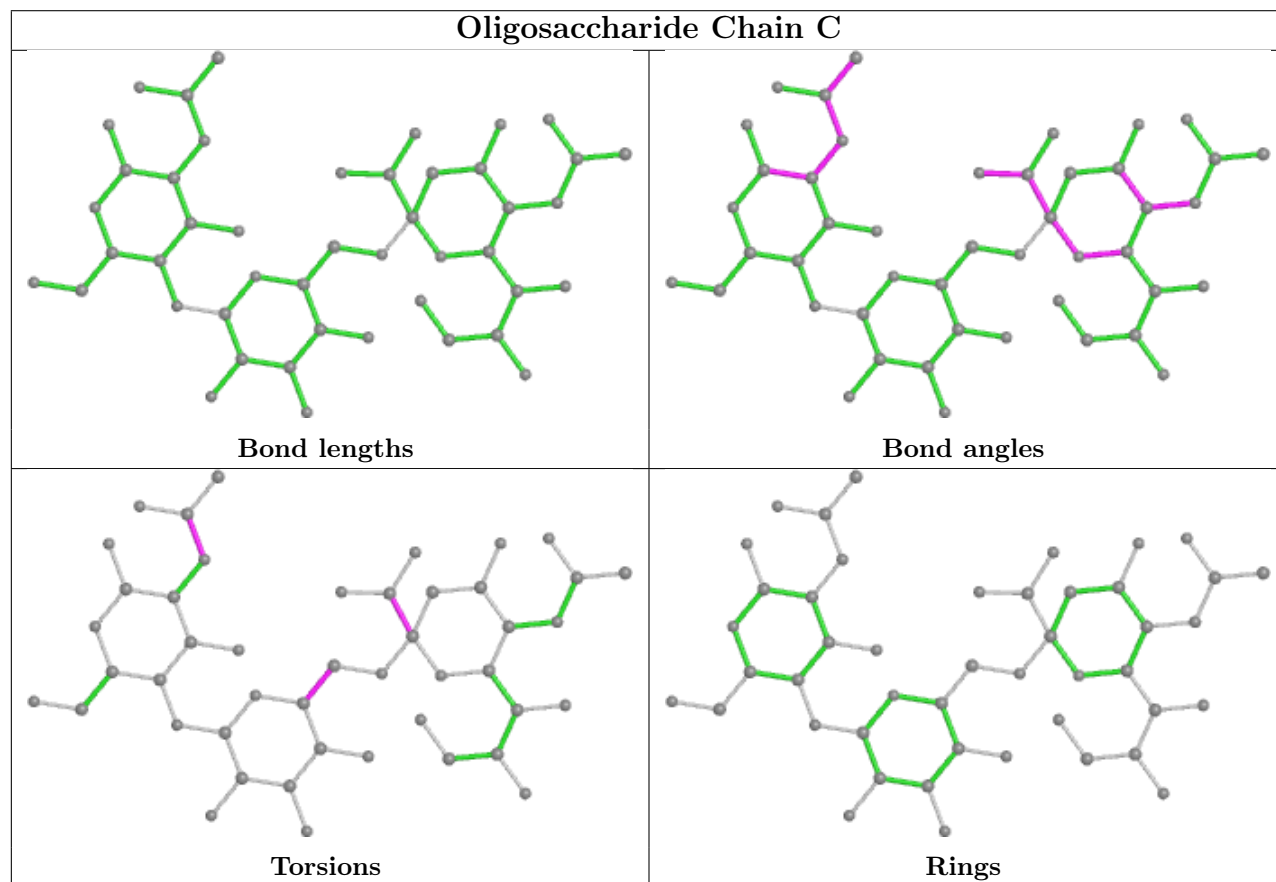
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	GAL	C4-C5-C6-O6
3	C	3	SIA	O1A-C1-C2-C3
3	C	3	SIA	O1B-C1-C2-C3

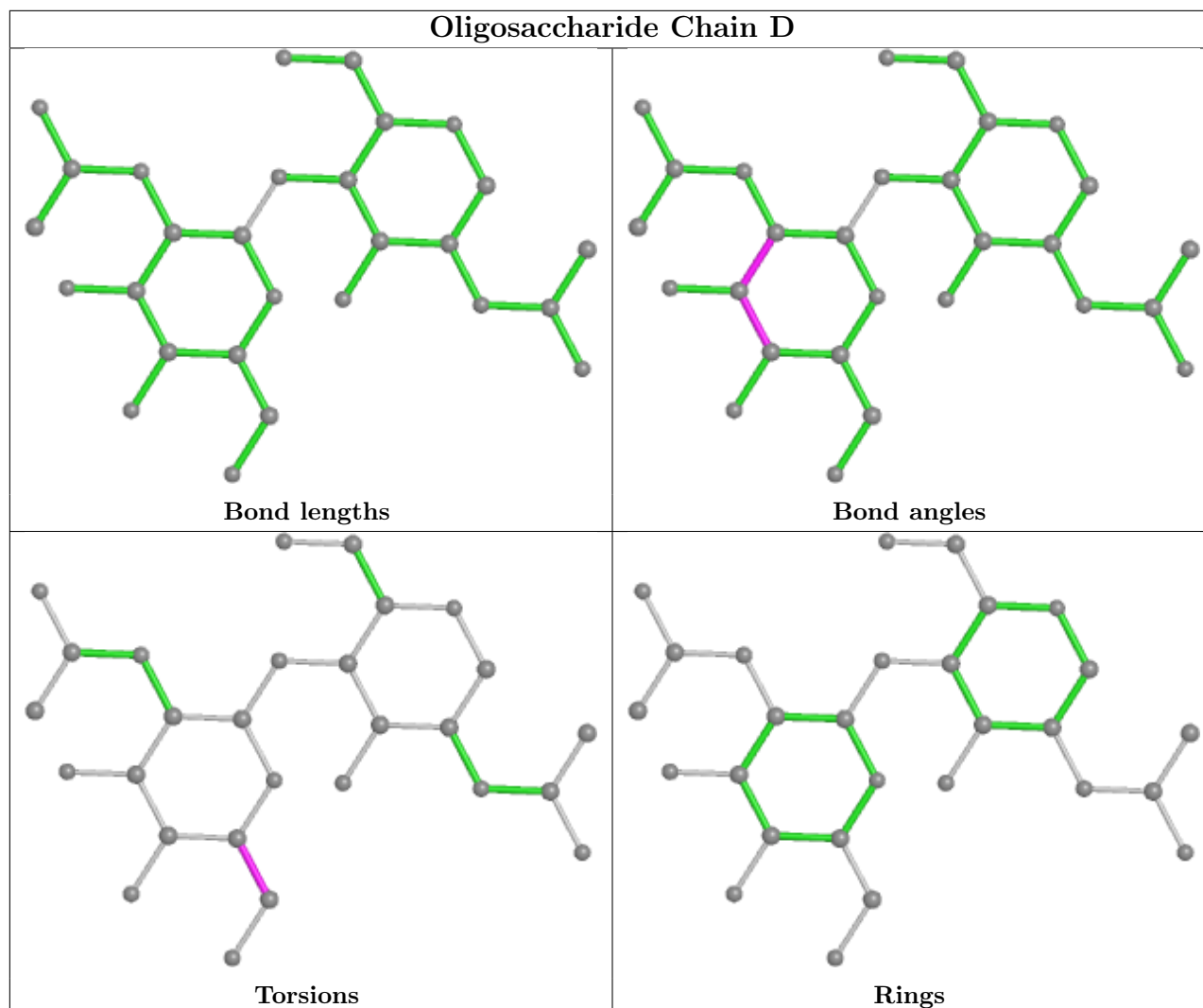
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	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](#)

18 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	SO4	B	1175	-	4,4,4	0.35	0	6,6,6	0.09	0
5	NAG	A	1319	1	14,14,15	0.51	0	17,19,21	1.50	4 (23%)
6	SO4	A	1331	-	4,4,4	0.34	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	B	1174	-	4,4,4	0.38	0	6,6,6	0.22	0
6	SO4	B	1173	-	4,4,4	0.36	0	6,6,6	0.25	0
6	SO4	B	1176	-	4,4,4	0.33	0	6,6,6	0.22	0
6	SO4	A	1328	-	4,4,4	0.37	0	6,6,6	0.23	0
6	SO4	A	1323	-	4,4,4	0.35	0	6,6,6	0.06	0
6	SO4	A	1333	-	4,4,4	0.44	0	6,6,6	0.18	0
5	NAG	A	1317	1	14,14,15	0.44	0	17,19,21	0.89	1 (5%)
6	SO4	A	1327	-	4,4,4	0.37	0	6,6,6	0.19	0
5	NAG	A	1318	1	14,14,15	0.46	0	17,19,21	1.18	1 (5%)
6	SO4	A	1329	-	4,4,4	0.35	0	6,6,6	0.18	0
6	SO4	A	1330	-	4,4,4	0.37	0	6,6,6	0.19	0
6	SO4	A	1332	-	4,4,4	0.35	0	6,6,6	0.09	0
6	SO4	A	1325	-	4,4,4	0.34	0	6,6,6	0.07	0
6	SO4	A	1324	-	4,4,4	0.36	0	6,6,6	0.15	0
6	SO4	A	1326	-	4,4,4	0.35	0	6,6,6	0.07	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	NAG	A	1317	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1319	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1318	1	-	2/6/23/26	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(°)
5	A	1319	NAG	C8-C7-N2	3.31	121.71	116.10
5	A	1318	NAG	C1-O5-C5	3.08	116.36	112.19
5	A	1319	NAG	C1-O5-C5	2.92	116.15	112.19
5	A	1319	NAG	O7-C7-C8	-2.65	117.14	122.06
5	A	1319	NAG	C2-N2-C7	2.58	126.58	122.90
5	A	1317	NAG	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1318	NAG	C4-C5-C6-O6
5	A	1317	NAG	C4-C5-C6-O6
5	A	1319	NAG	C8-C7-N2-C2
5	A	1319	NAG	O7-C7-N2-C2
5	A	1318	NAG	O5-C5-C6-O6
5	A	1317	NAG	O5-C5-C6-O6
5	A	1319	NAG	O5-C5-C6-O6
5	A	1319	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1319	NAG	1	0
6	A	1328	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/321 (98%)	0.55	33 (10%) 6 8	27, 53, 103, 131	0
2	B	170/177 (96%)	1.09	34 (20%) 1 1	23, 78, 128, 136	0
All	All	487/498 (97%)	0.73	67 (13%) 2 3	23, 60, 118, 136	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	27	GLN	5.8
2	B	143	LYS	5.6
1	A	190	ASN	5.1
2	B	141	PHE	4.5
2	B	31	GLY	4.5
1	A	196	GLY	4.3
1	A	118	SER	3.9
1	A	12	ASN	3.9
2	B	139	GLU	3.6
2	B	34	THR	3.6
1	A	117	TYR	3.6
2	B	16	GLY	3.5
1	A	146	ASN	3.4
2	B	161	LYS	3.4
2	B	26	HIS	3.3
2	B	140	ILE	3.3
2	B	32	GLU	3.3
2	B	23	GLY	3.2
2	B	2	LEU	3.2
1	A	200	TYR	3.1
2	B	160	SER	3.1
2	B	168	GLN	3.1
1	A	316	GLU	3.1
1	A	147	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	ILE	3.0
2	B	144	CYS	3.0
1	A	119	GLY	2.9
2	B	164	GLU	2.9
2	B	33	GLY	2.9
1	A	11	SER	2.9
1	A	195	VAL	2.9
2	B	149	MET	2.9
2	B	158	ASP	2.8
1	A	144	LEU	2.7
2	B	35	ALA	2.7
1	A	203	SER	2.7
2	B	58	LYS	2.7
2	B	153	ARG	2.7
2	B	11	GLU	2.6
2	B	142	HIS	2.6
1	A	156	THR	2.6
1	A	204	PHE	2.6
2	B	113	SER	2.6
2	B	147	ASP	2.6
1	A	215	ASN	2.5
2	B	146	ASP	2.5
2	B	24	PHE	2.5
1	A	206	PRO	2.5
1	A	192	LEU	2.4
2	B	17	LEU	2.4
1	A	193	VAL	2.4
1	A	202	GLN	2.4
2	B	38	TYR	2.4
1	A	194	THR	2.4
1	A	198	SER	2.4
1	A	214	VAL	2.3
1	A	268	CYS	2.3
2	B	29	ALA	2.3
1	A	236	PHE	2.3
1	A	122	THR	2.3
1	A	205	VAL	2.2
2	B	156	THR	2.2
1	A	239	ASN	2.2
1	A	191	LYS	2.1
1	A	115	PHE	2.1
2	B	150	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	LYS	2.1

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

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

6.3 Carbohydrates [\(i\)](#)

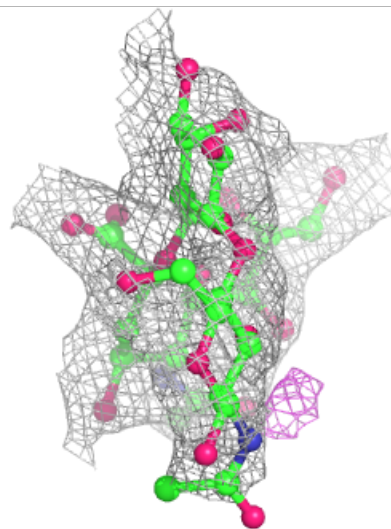
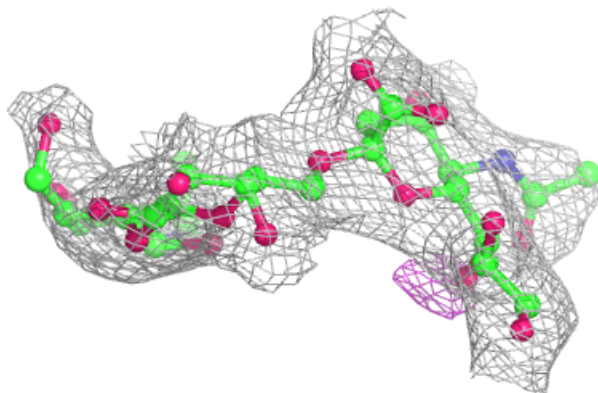
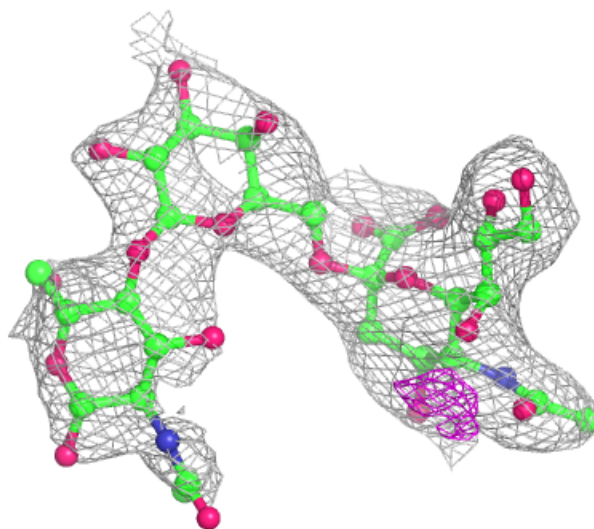
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

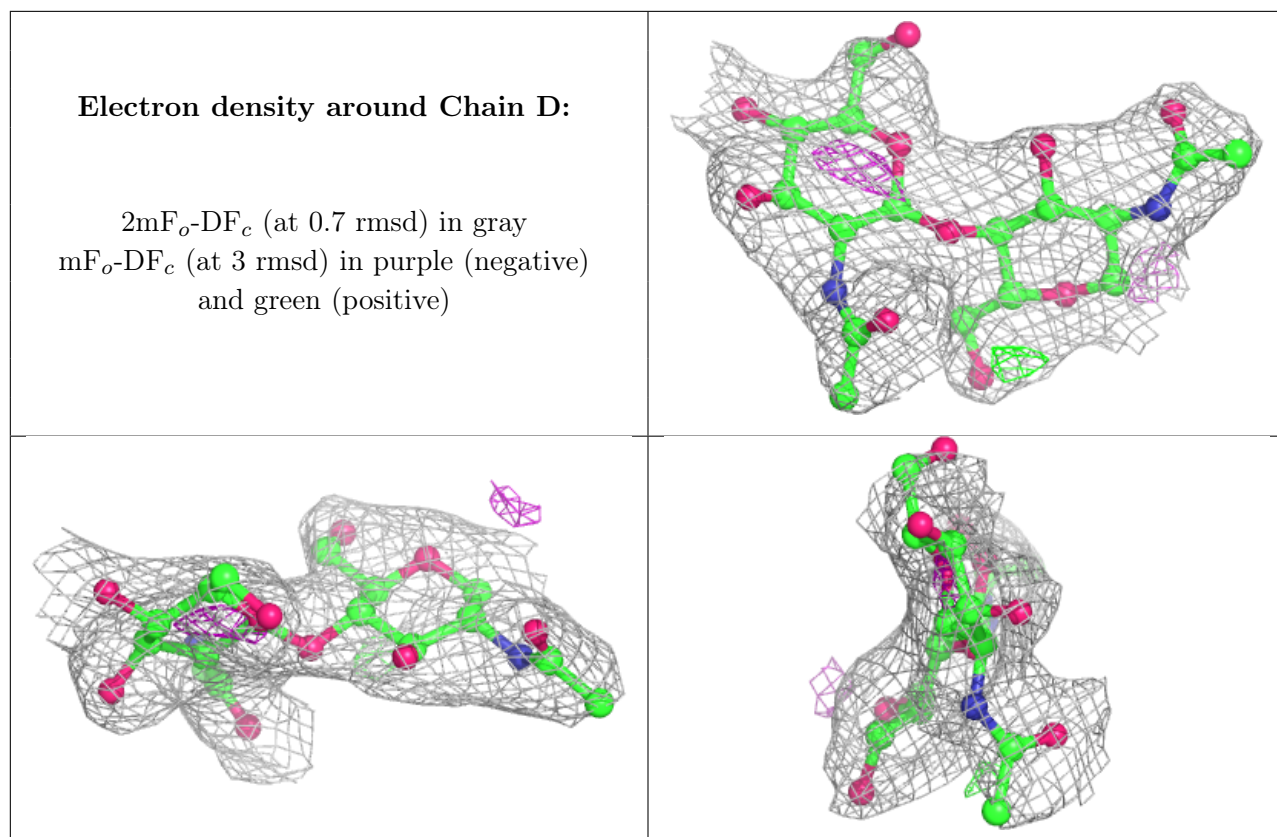
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	15/15	0.78	0.48	100,108,110,111	0
4	NAG	D	2	14/15	0.81	0.26	64,73,78,80	0
3	GAL	C	2	11/12	0.86	0.27	72,92,99,101	0
3	SIA	C	3	20/21	0.91	0.21	55,61,65,66	0
4	NAG	D	1	14/15	0.92	0.12	47,58,62,68	0

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 C:

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





6.4 Ligands [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
6	SO4	A	1324	5/5	0.59	0.45	104,106,112,113	0
6	SO4	B	1176	5/5	0.59	0.49	89,92,95,106	3
6	SO4	A	1325	5/5	0.63	0.49	134,138,139,140	0
5	NAG	A	1319	14/15	0.68	0.62	86,95,99,99	0
5	NAG	A	1317	14/15	0.70	0.34	67,75,81,85	0
6	SO4	A	1331	5/5	0.79	0.51	104,109,109,110	0
6	SO4	B	1175	5/5	0.81	0.27	112,113,115,120	0
6	SO4	A	1328	5/5	0.84	0.18	76,82,84,85	0
5	NAG	A	1318	14/15	0.85	0.45	67,81,87,89	0
6	SO4	A	1326	5/5	0.85	0.47	105,106,108,110	0
6	SO4	A	1323	5/5	0.86	0.40	112,113,116,117	0
6	SO4	A	1332	5/5	0.86	0.48	98,99,101,102	0
6	SO4	B	1174	5/5	0.88	0.23	84,86,88,89	0
6	SO4	A	1329	5/5	0.88	0.33	99,100,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	B	1173	5/5	0.88	0.22	81,82,91,95	0
6	SO4	A	1327	5/5	0.89	0.24	80,80,88,91	0
6	SO4	A	1330	5/5	0.90	0.20	70,76,77,78	0
6	SO4	A	1333	5/5	0.91	0.17	66,69,76,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.