



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:04 AM BST

PDB ID : 1KTW  
Title : IOTA-CARRAGEENASE COMPLEXED TO IOTA-CARRAGEENAN FRAGMENTS  
Authors : Michel, G.; Kahn, R.; Dideberg, O.  
Deposited on : 2002-01-18  
Resolution : 2.00 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](mailto: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.

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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 : 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

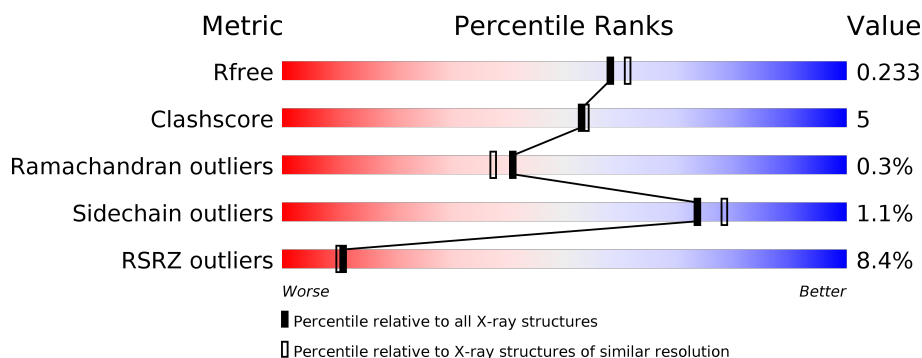
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	B	464	<div> <div>11%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>••</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	4	<div> <div>50%</div> <div>25%</div> <div>25%</div> </div>

## 2 Entry composition [i](#)

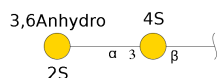
There are 7 unique types of molecules in this entry. The entry contains 7837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IOTA-CARRAGEENASE.

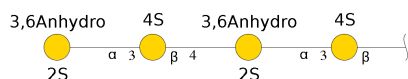
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	16	0	0
			3605	2259	639	692	15			
1	B	457	Total	C	N	O	S	37	0	0
			3605	2259	639	692	15			

- Molecule 2 is an oligosaccharide called 3,6-anhydro-2-O-sulfo- $\alpha$ -D-galactopyranose-(1-3)-4-O-sulfo- $\beta$ -D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	S	0	0	0
			30	12	16	2			

- Molecule 3 is an oligosaccharide called 3,6-anhydro-2-O-sulfo- $\alpha$ -D-galactopyranose-(1-3)-4-O-sulfo- $\beta$ -D-galactopyranose-(1-4)-3,6-anhydro-2-O-sulfo- $\alpha$ -D-galactopyranose-(1-3)-4-O-sulfo- $\beta$ -D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	O	S	0	0	0
			59	24	31	4			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total Ca 5 5	0	0
4	A	5	Total Ca 5 5	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Na 2 2	0	0
5	A	2	Total Na 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

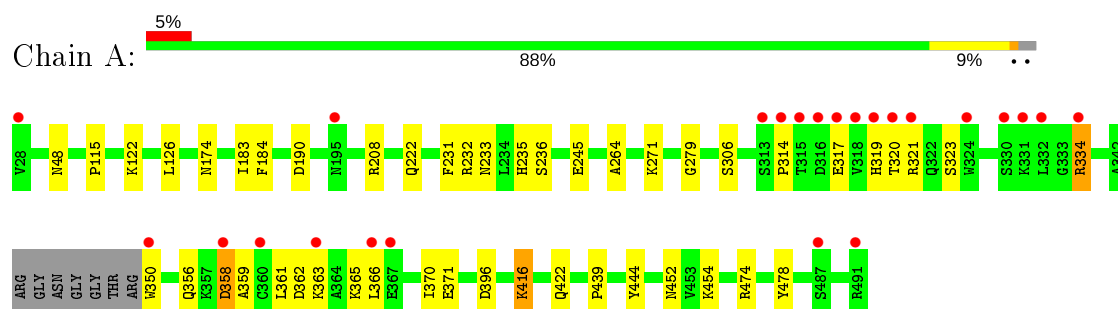
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	289	Total O 289 289	0	0
7	B	233	Total O 233 233	0	0

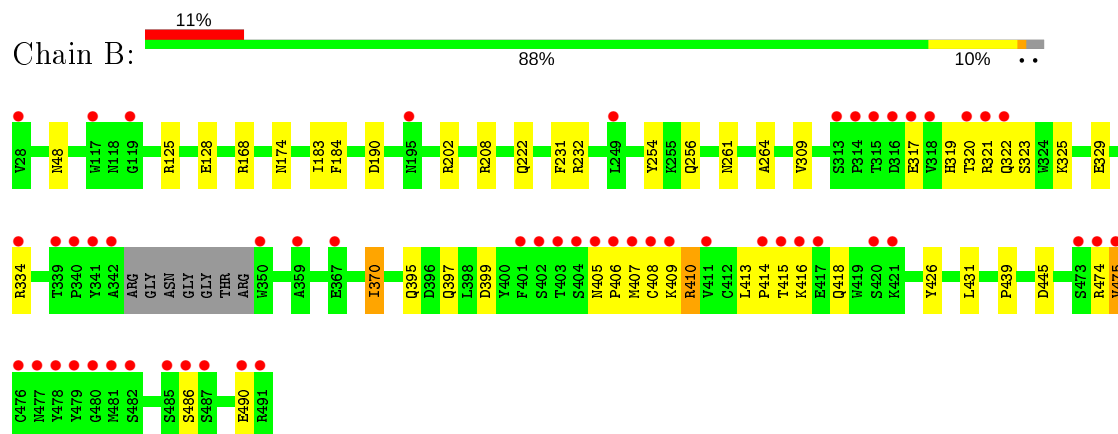
### 3 Residue-property plots

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: IOTA-CARRAGEENASE



- Molecule 1: IOTA-CARRAGEENASE



- Molecule 2: 3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose



- Molecule 3: 3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose-(1-4)-3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.73Å 122.31Å 91.94Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	23.17 – 2.00 23.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (23.17-2.00) 97.2 (23.17-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 1.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.203 , 0.238 0.197 , 0.233	Depositor DCC
$R_{free}$ test set	3986 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 83.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, G4S, DGS, CL

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	0.54	0/3678	0.69	0/4970
1	B	0.48	0/3678	0.67	0/4970
All	All	0.51	0/7356	0.68	0/9940

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	3605	0	3500	37	0
1	B	3605	0	3500	37	0
2	C	30	0	18	3	0
3	D	59	0	32	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	1	0
7	A	289	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	233	0	0	2	0
All	All	7837	0	7050	77	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 5.

All (77) 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:B:405:ASN:HD21	1:B:409:LYS:H	1.01	0.95
1:B:320:THR:HG22	1:B:321:ARG:N	1.97	0.80
1:B:405:ASN:ND2	1:B:409:LYS:H	1.83	0.73
1:B:320:THR:CG2	1:B:321:ARG:H	2.03	0.71
1:A:334:ARG:CD	1:A:334:ARG:H	2.03	0.71
1:A:320:THR:H	1:A:323:SER:HB3	1.56	0.70
2:C:2:DGS:H3	2:C:2:DGS:O8	1.91	0.70
1:B:405:ASN:HD21	1:B:409:LYS:N	1.82	0.69
1:B:320:THR:CG2	1:B:321:ARG:N	2.56	0.68
1:B:415:THR:OG1	1:B:418:GLN:HG3	1.94	0.68
1:A:334:ARG:H	1:A:334:ARG:HD3	1.58	0.67
1:B:261:ASN:HB3	7:B:738:HOH:O	1.94	0.67
1:B:320:THR:HG22	1:B:321:ARG:H	1.59	0.67
1:A:334:ARG:N	1:A:334:ARG:HD3	2.12	0.65
1:A:416:LYS:H	1:A:416:LYS:CE	2.09	0.65
1:B:416:LYS:HD3	1:B:416:LYS:H	1.63	0.64
1:B:254:TYR:O	1:B:256:GLN:HG3	1.99	0.63
1:B:125:ARG:HD3	1:B:128:GLU:OE2	1.99	0.61
1:B:320:THR:H	1:B:323:SER:HB3	1.65	0.60
1:A:115:PRO:HB3	1:A:126:LEU:HD21	1.84	0.60
1:B:399:ASP:OD1	1:B:474:ARG:HA	2.02	0.59
1:B:416:LYS:H	1:B:416:LYS:CD	2.16	0.58
1:B:416:LYS:HD3	1:B:416:LYS:N	2.20	0.57
1:B:409:LYS:O	1:B:410:ARG:HB2	2.06	0.56
1:A:365:LYS:CD	1:A:371:GLU:HG2	2.36	0.56
3:D:2:DGS:O8	3:D:2:DGS:H3	2.07	0.55
1:A:314:PRO:HG2	1:A:317:GLU:HB3	1.87	0.55
1:A:321:ARG:NH1	1:A:350:TRP:HZ3	2.05	0.55
1:A:365:LYS:HE2	1:A:371:GLU:HG2	1.89	0.54
1:B:183:ILE:O	1:B:184:PHE:HB2	2.07	0.53
1:A:365:LYS:CE	1:A:371:GLU:HG2	2.38	0.53
1:B:413:LEU:HD12	1:B:414:PRO:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:HD3	1:A:422:GLN:NE2	2.25	0.51
1:A:416:LYS:H	1:A:416:LYS:CD	2.22	0.51
1:A:334:ARG:CD	1:A:334:ARG:N	2.72	0.50
1:B:168:ARG:NE	1:B:202:ARG:HD3	2.26	0.50
1:A:416:LYS:HE2	1:A:416:LYS:H	1.75	0.50
1:B:329:GLU:OE1	1:B:334:ARG:HA	2.12	0.49
1:A:231:PHE:O	1:A:264:ALA:HA	2.13	0.49
1:B:395:GLN:NE2	1:B:426:TYR:OH	2.37	0.49
1:A:271:LYS:HE2	7:A:818:HOH:O	2.12	0.48
1:A:365:LYS:HD3	1:A:371:GLU:HG2	1.96	0.48
1:A:361:LEU:O	1:A:365:LYS:HG3	2.13	0.48
1:B:486:SER:HB3	1:B:490:GLU:OE2	2.13	0.48
1:A:416:LYS:HD3	1:A:416:LYS:N	2.29	0.48
1:A:365:LYS:NZ	1:A:444:TYR:HE2	2.13	0.47
1:A:362:ASP:O	1:A:366:LEU:HG	2.14	0.47
2:C:2:DGS:C3	2:C:2:DGS:O8	2.62	0.47
1:A:416:LYS:N	1:A:416:LYS:CD	2.78	0.46
1:A:317:GLU:CD	1:A:319:HIS:HE2	2.19	0.46
1:B:317:GLU:HB3	1:B:319:HIS:CD2	2.50	0.46
1:B:168:ARG:CZ	1:B:202:ARG:HD3	2.45	0.46
1:B:309:VAL:HG13	1:B:370:ILE:HG21	1.98	0.46
1:A:356:GLN:O	1:A:356:GLN:HG3	2.15	0.45
1:B:174:ASN:HA	1:B:208:ARG:O	2.15	0.45
1:A:174:ASN:HA	1:A:208:ARG:O	2.16	0.45
1:A:306:SER:HB2	1:A:439:PRO:HD3	1.98	0.45
1:B:320:THR:HG22	1:B:322:GLN:H	1.82	0.45
1:A:122:LYS:HA	2:C:2:DGS:O7	2.17	0.45
1:B:325:LYS:HE2	1:B:329:GLU:OE2	2.17	0.44
1:A:365:LYS:HG2	1:A:370:ILE:O	2.17	0.44
1:A:232:ARG:HG2	1:A:233:ASN:ND2	2.33	0.44
1:B:222:GLN:NE2	6:B:531:CL:CL	2.88	0.43
1:B:231:PHE:O	1:B:264:ALA:HA	2.19	0.43
1:A:183:ILE:O	1:A:184:PHE:HB2	2.17	0.43
1:B:397:GLN:HB3	1:B:431:LEU:CD1	2.49	0.43
1:A:222:GLN:NE2	6:A:530:CL:CL	2.89	0.43
1:B:406:PRO:O	1:B:475:VAL:HB	2.18	0.42
1:A:474:ARG:HH21	1:A:478:TYR:H	1.66	0.42
1:A:359:ALA:O	1:A:363:LYS:HG3	2.20	0.42
1:A:245:GLU:HA	1:A:279:GLY:O	2.20	0.42
1:B:232:ARG:HD2	7:B:615:HOH:O	2.19	0.42
1:A:235:HIS:HD2	1:A:236:SER:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASN:OD1	1:A:454:LYS:HE2	2.20	0.41
1:B:407:MET:O	1:B:408:CYS:C	2.59	0.41
1:B:439:PRO:O	1:B:445:ASP:HB2	2.20	0.40
1:B:409:LYS:O	1:B:410:ARG:CB	2.69	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	453/464 (98%)	429 (95%)	23 (5%)	1 (0%)	47	44
1	B	453/464 (98%)	418 (92%)	33 (7%)	2 (0%)	34	30
All	All	906/928 (98%)	847 (94%)	56 (6%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ASP
1	B	410	ARG
1	B	475	VAL

### 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	395/399 (99%)	389 (98%)	6 (2%)	65	69
1	B	395/399 (99%)	392 (99%)	3 (1%)	81	86
All	All	790/798 (99%)	781 (99%)	9 (1%)	73	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	190	ASP
1	A	334	ARG
1	A	358	ASP
1	A	396	ASP
1	A	416	LYS
1	B	48	ASN
1	B	190	ASP
1	B	370	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	222	GLN
1	A	422	GLN
1	B	60	ASN
1	B	195	ASN
1	B	222	GLN
1	B	235	HIS
1	B	395	GLN
1	B	405	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 ⓘ

6 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	G4S	C	1	2	16,16,16	0.56	0	19,24,24	0.51	0
2	DGS	C	2	2	15,15,16	1.03	1 (6%)	18,23,25	1.82	4 (22%)
3	G4S	D	1	3	16,16,16	0.48	0	19,24,24	0.59	0
3	DGS	D	2	3	15,15,16	0.89	0	18,23,25	1.96	2 (11%)
3	G4S	D	3	3	15,15,16	0.74	0	17,22,24	0.68	0
3	DGS	D	4	3	15,15,16	0.88	0	18,23,25	2.66	4 (22%)

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	G4S	C	1	2	-	1/7/27/27	0/1/1/1
2	DGS	C	2	2	-	2/5/27/30	0/3/2/2
3	G4S	D	1	3	-	1/7/27/27	0/1/1/1
3	DGS	D	2	3	-	2/5/27/30	0/3/2/2
3	G4S	D	3	3	-	1/7/24/27	0/1/1/1
3	DGS	D	4	3	-	2/5/27/30	0/3/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	DGS	C1-C2	2.50	1.55	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	DGS	O2-C2-C3	9.63	117.31	106.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	DGS	O2-C2-C3	6.48	113.82	106.65
2	C	2	DGS	O2-C2-C3	4.74	111.89	106.65
2	C	2	DGS	C1-O5-C5	3.14	116.44	112.19
3	D	2	DGS	O5-C5-C6	-2.78	109.20	113.33
2	C	2	DGS	C4-C3-C2	-2.67	107.35	113.84
3	D	4	DGS	O5-C5-C6	-2.46	109.68	113.33
3	D	4	DGS	C1-O5-C5	2.36	115.39	112.19
3	D	4	DGS	O9-S-O8	-2.35	102.79	112.22
2	C	2	DGS	O5-C5-C6	-2.25	109.99	113.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	DGS	C1-C2-O2-S
3	D	4	DGS	C3-C2-O2-S
2	C	2	DGS	C1-C2-O2-S
2	C	2	DGS	C3-C2-O2-S
3	D	2	DGS	C1-C2-O2-S
3	D	2	DGS	C3-C2-O2-S
2	C	1	G4S	O5-C5-C6-O6
3	D	3	G4S	O5-C5-C6-O6
3	D	1	G4S	O5-C5-C6-O6

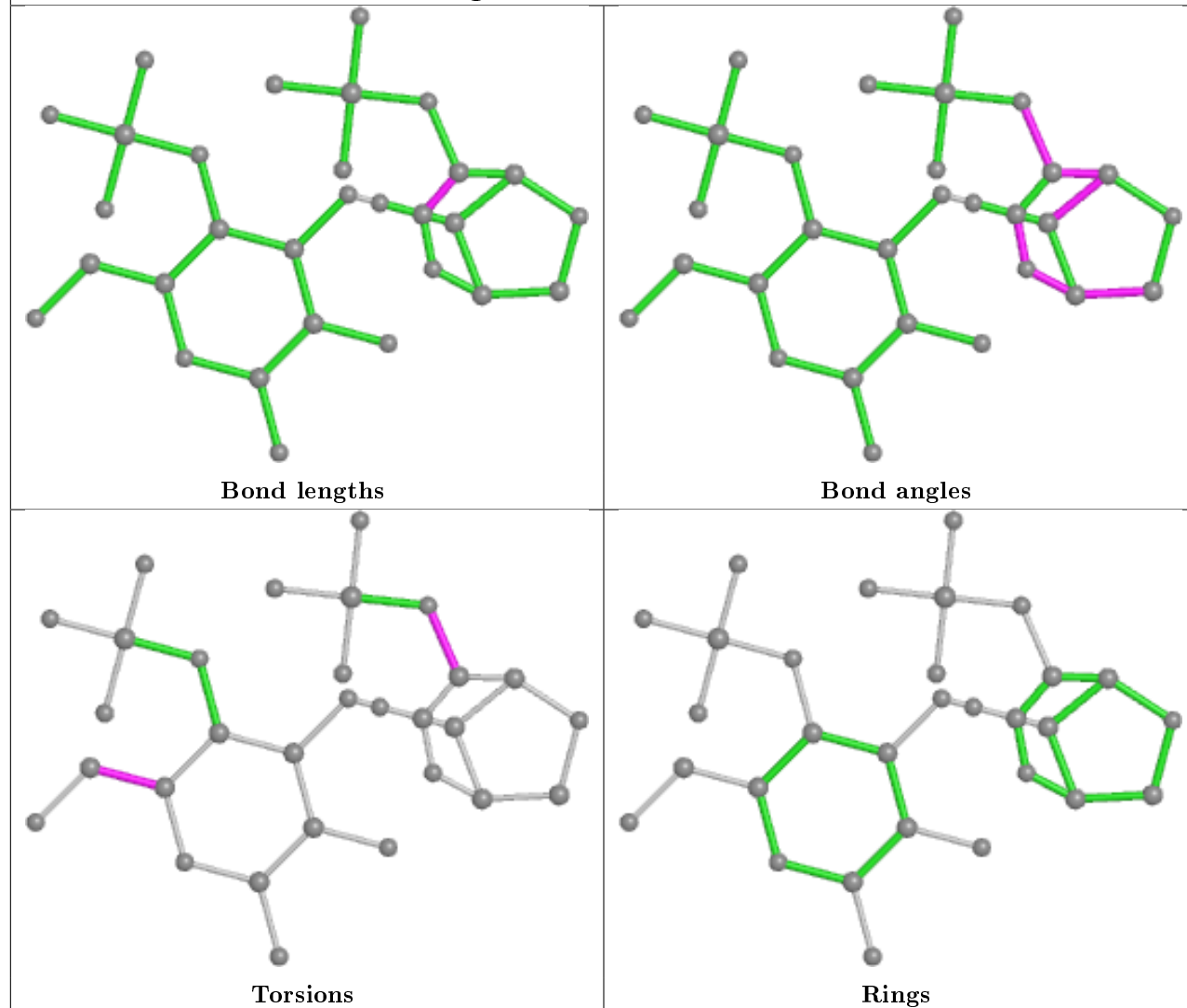
There are no ring outliers.

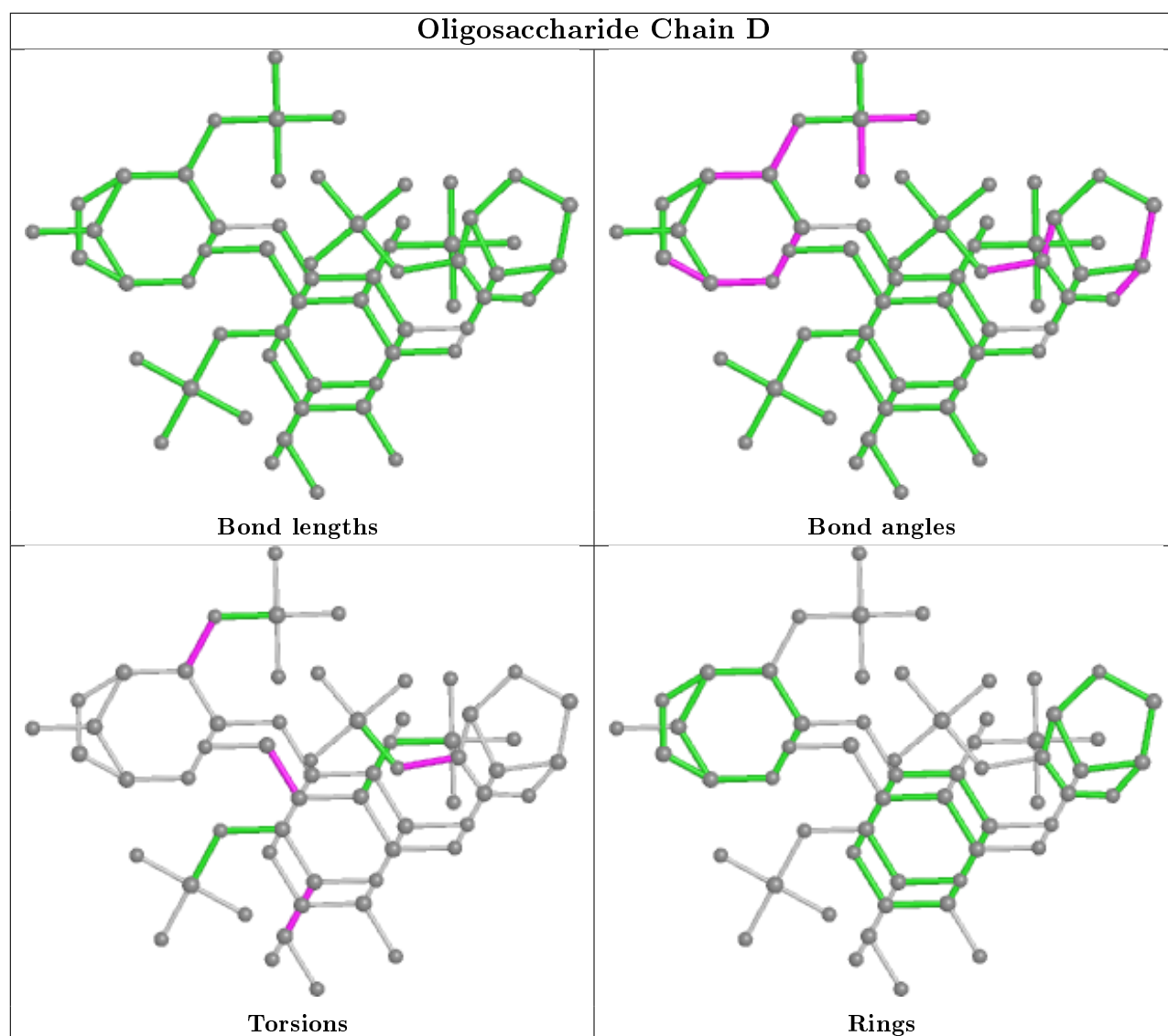
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	DGS	3	0
3	D	2	DGS	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.

## Oligosaccharide Chain C





## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	457/464 (98%)	-0.06	24 (5%) 26 25	7, 16, 51, 61	7 (1%)
1	B	457/464 (98%)	0.32	53 (11%) 4 4	8, 19, 57, 71	12 (2%)
All	All	914/928 (98%)	0.13	77 (8%) 11 10	7, 17, 55, 71	19 (2%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	MET	8.5
1	B	316	ASP	7.3
1	B	476	CYS	7.2
1	A	315	THR	7.0
1	B	318	VAL	6.5
1	B	315	THR	5.6
1	B	350	TRP	5.6
1	B	490	GLU	5.5
1	B	475	VAL	5.5
1	B	314	PRO	5.3
1	B	477	ASN	5.1
1	B	480	GLY	5.0
1	B	402	SER	4.8
1	A	316	ASP	4.8
1	B	408	CYS	4.5
1	B	473	SER	4.3
1	B	342	ALA	4.2
1	B	479	TYR	4.0
1	B	341	TYR	3.9
1	B	486	SER	3.9
1	A	360	CYS	3.9
1	B	409	LYS	3.8
1	B	482	SER	3.8
1	B	474	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	350	TRP	3.7
1	B	487	SER	3.6
1	B	406	PRO	3.6
1	A	317	GLU	3.5
1	B	478	TYR	3.5
1	A	318	VAL	3.5
1	A	314	PRO	3.4
1	B	401	PHE	3.4
1	A	366	LEU	3.4
1	B	317	GLU	3.4
1	A	334	ARG	3.3
1	B	420	SER	3.2
1	B	334	ARG	3.2
1	B	416	LYS	3.1
1	A	320	THR	3.1
1	B	313	SER	3.0
1	A	367	GLU	3.0
1	A	330	SER	3.0
1	A	363	LYS	2.9
1	A	358	ASP	2.8
1	B	481	MET	2.8
1	B	411	VAL	2.8
1	B	421	LYS	2.7
1	A	324	TRP	2.6
1	B	405	ASN	2.5
1	A	487	SER	2.5
1	B	491	ARG	2.4
1	B	414	PRO	2.4
1	B	340	PRO	2.4
1	B	321	ARG	2.4
1	B	485	SER	2.4
1	B	249	LEU	2.3
1	B	367	GLU	2.3
1	B	320	THR	2.3
1	B	403	THR	2.3
1	B	417	GLU	2.3
1	B	339	THR	2.3
1	A	321	ARG	2.3
1	A	319	HIS	2.2
1	A	332	LEU	2.2
1	A	28	VAL	2.2
1	B	404	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLN	2.1
1	A	313	SER	2.1
1	A	331	LYS	2.1
1	B	117	TRP	2.1
1	A	195	ASN	2.1
1	B	28	VAL	2.1
1	B	195	ASN	2.0
1	A	491	ARG	2.0
1	B	119	GLY	2.0
1	B	359	ALA	2.0
1	B	415	THR	2.0

## 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 ⓘ

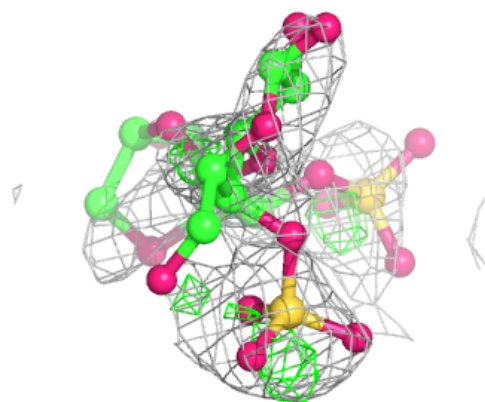
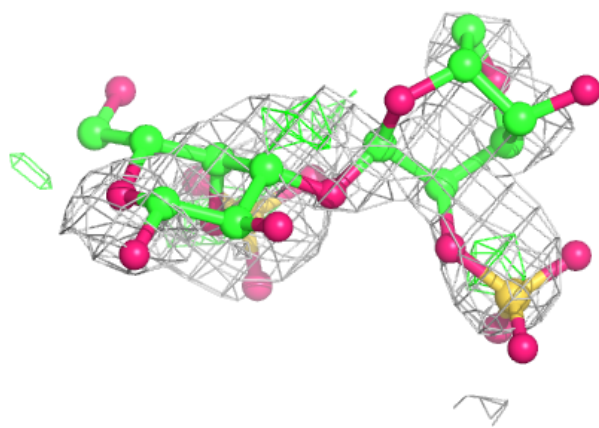
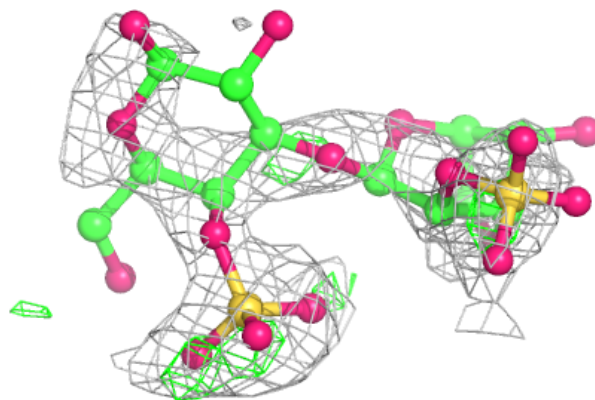
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

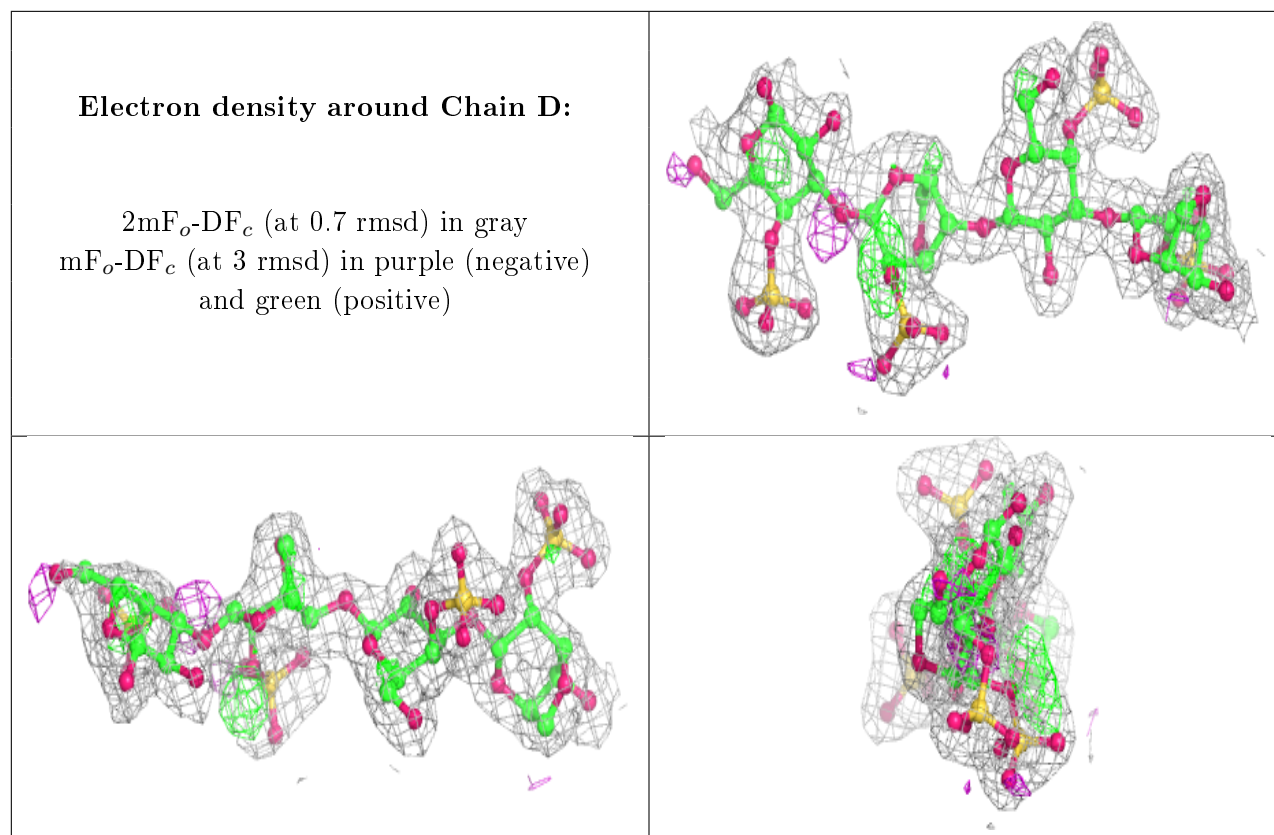
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DGS	C	2	14/15	0.63	0.40	69,70,70,70	14
2	G4S	C	1	16/16	0.71	0.39	66,67,68,69	16
3	G4S	D	1	16/16	0.86	0.21	47,52,54,56	0
3	DGS	D	2	14/15	0.86	0.18	27,37,50,50	0
3	DGS	D	4	14/15	0.95	0.11	17,21,21,22	0
3	G4S	D	3	15/16	0.97	0.08	17,20,24,26	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 ⓘ

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( $\text{\AA}^2$ )	Q<0.9
4	CA	B	10	1/1	0.95	0.06	27,27,27,27	0
4	CA	A	9	1/1	0.97	0.05	22,22,22,22	0
5	NA	B	14	1/1	0.98	0.07	19,19,19,19	0
5	NA	A	13	1/1	0.98	0.11	14,14,14,14	0
4	CA	A	496	1/1	0.99	0.04	14,14,14,14	0
4	CA	A	5	1/1	0.99	0.04	15,15,15,15	0
4	CA	B	4	1/1	0.99	0.03	17,17,17,17	0
6	CL	B	531	1/1	0.99	0.16	37,37,37,37	0
5	NA	B	12	1/1	0.99	0.06	19,19,19,19	0
4	CA	A	3	1/1	0.99	0.03	15,15,15,15	0
4	CA	B	2	1/1	0.99	0.04	16,16,16,16	0
5	NA	A	11	1/1	0.99	0.12	13,13,13,13	0
4	CA	B	8	1/1	0.99	0.06	24,24,24,24	0
4	CA	B	6	1/1	0.99	0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	A	530	1/1	0.99	0.06	30,30,30,30	0
4	CA	A	7	1/1	1.00	0.04	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.