



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:00 PM UTC

PDB ID : 7PGM / pdb\_00007pgm  
Title : HHIP-C in complex with heparin  
Authors : Griffiths, S.C.; Schwab, R.A.; El Omari, K.; Bishop, B.; Iverson, E.J.; Malinuskas, T.; Dubey, R.; Qian, M.; Covey, D.F.; Gilbert, R.J.C.; Rohatgi, R.; Siebold, C.  
Deposited on : 2021-08-14  
Resolution : 2.70 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

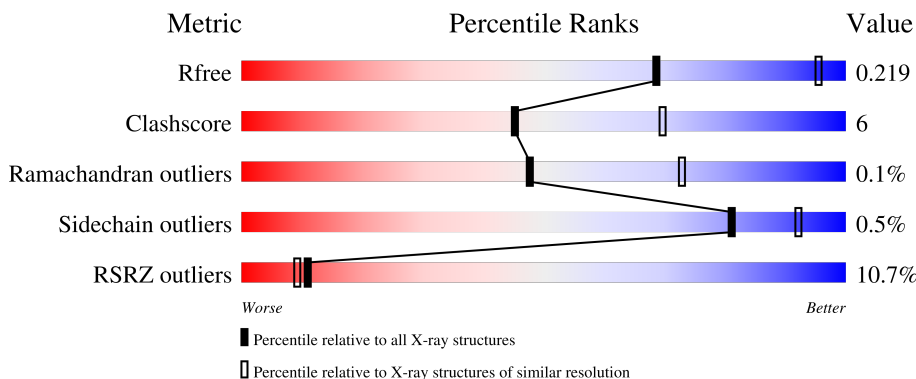
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	470	 9% 81% 14% 5%
1	B	470	 11% 80% 10% 9%
1	C	470	 9% 80% 11% 9%
2	D	8	 25% 75%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 10309 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 Hedgehog-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3484	2186	614	656	28	0	0	0
1	B	427	3335	2095	594	619	27	0	0	0
1	C	429	3349	2105	591	626	27	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

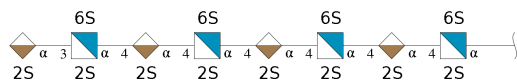
Chain	Residue	Modelled	Actual	Comment	Reference
A	210	GLU	-	expression tag	UNP Q96QV1
A	211	THR	-	expression tag	UNP Q96QV1
A	212	GLY	-	expression tag	UNP Q96QV1
A	671	GLY	-	expression tag	UNP Q96QV1
A	672	THR	-	expression tag	UNP Q96QV1
A	673	LYS	-	expression tag	UNP Q96QV1
A	674	HIS	-	expression tag	UNP Q96QV1
A	675	HIS	-	expression tag	UNP Q96QV1
A	676	HIS	-	expression tag	UNP Q96QV1
A	677	HIS	-	expression tag	UNP Q96QV1
A	678	HIS	-	expression tag	UNP Q96QV1
A	679	HIS	-	expression tag	UNP Q96QV1
B	210	GLU	-	expression tag	UNP Q96QV1
B	211	THR	-	expression tag	UNP Q96QV1
B	212	GLY	-	expression tag	UNP Q96QV1
B	671	GLY	-	expression tag	UNP Q96QV1
B	672	THR	-	expression tag	UNP Q96QV1
B	673	LYS	-	expression tag	UNP Q96QV1
B	674	HIS	-	expression tag	UNP Q96QV1
B	675	HIS	-	expression tag	UNP Q96QV1
B	676	HIS	-	expression tag	UNP Q96QV1
B	677	HIS	-	expression tag	UNP Q96QV1
B	678	HIS	-	expression tag	UNP Q96QV1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	679	HIS	-	expression tag	UNP Q96QV1
C	210	GLU	-	expression tag	UNP Q96QV1
C	211	THR	-	expression tag	UNP Q96QV1
C	212	GLY	-	expression tag	UNP Q96QV1
C	671	GLY	-	expression tag	UNP Q96QV1
C	672	THR	-	expression tag	UNP Q96QV1
C	673	LYS	-	expression tag	UNP Q96QV1
C	674	HIS	-	expression tag	UNP Q96QV1
C	675	HIS	-	expression tag	UNP Q96QV1
C	676	HIS	-	expression tag	UNP Q96QV1
C	677	HIS	-	expression tag	UNP Q96QV1
C	678	HIS	-	expression tag	UNP Q96QV1
C	679	HIS	-	expression tag	UNP Q96QV1

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-3)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.

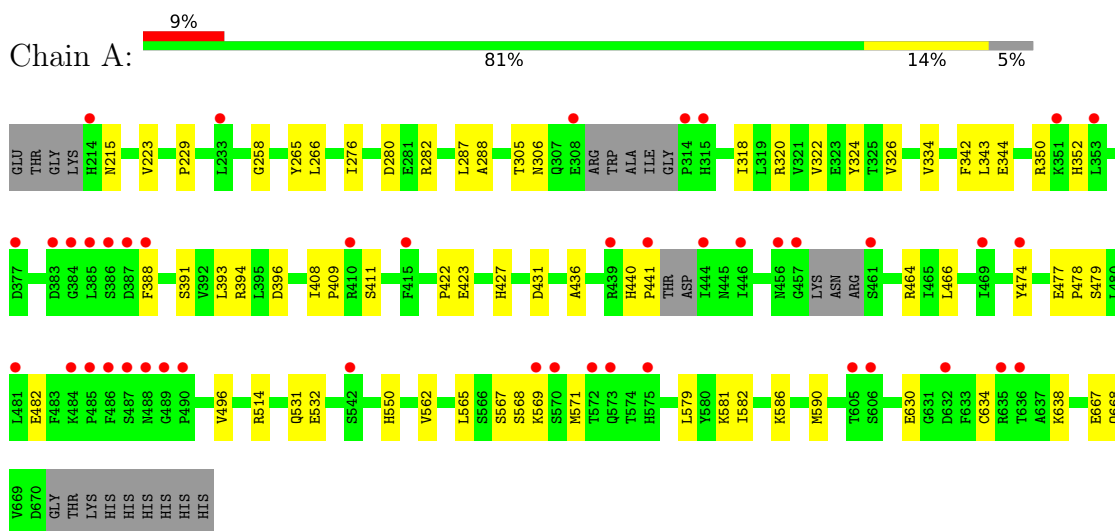


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				S
2	D	8	141	48	4	77	12	0	0	0

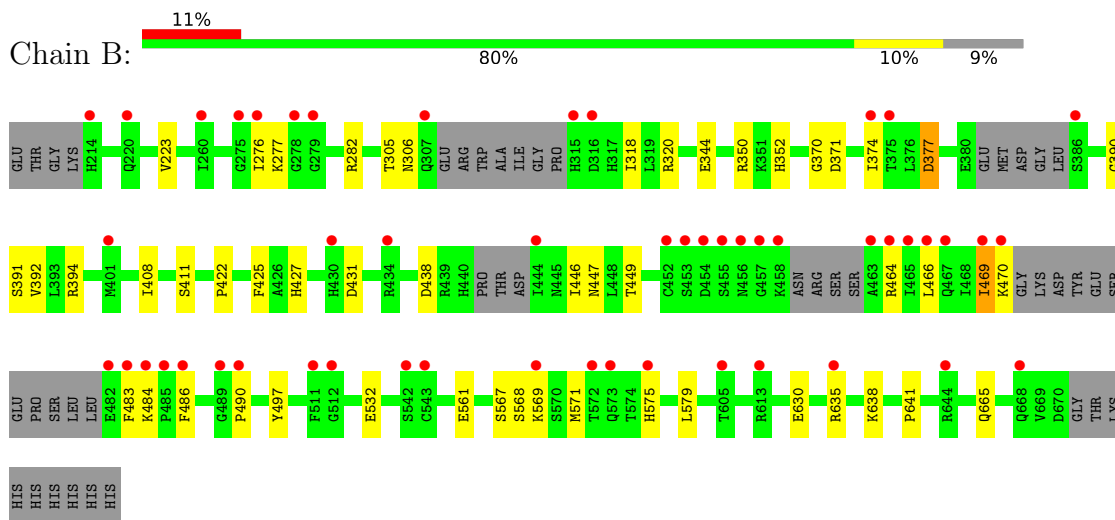
### 3 Residue-property plots [i](#)

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.

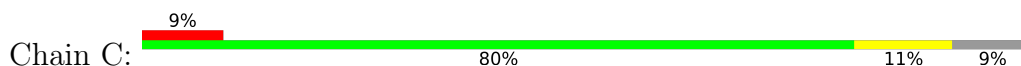
- Molecule 1: Hedgehog-interacting protein

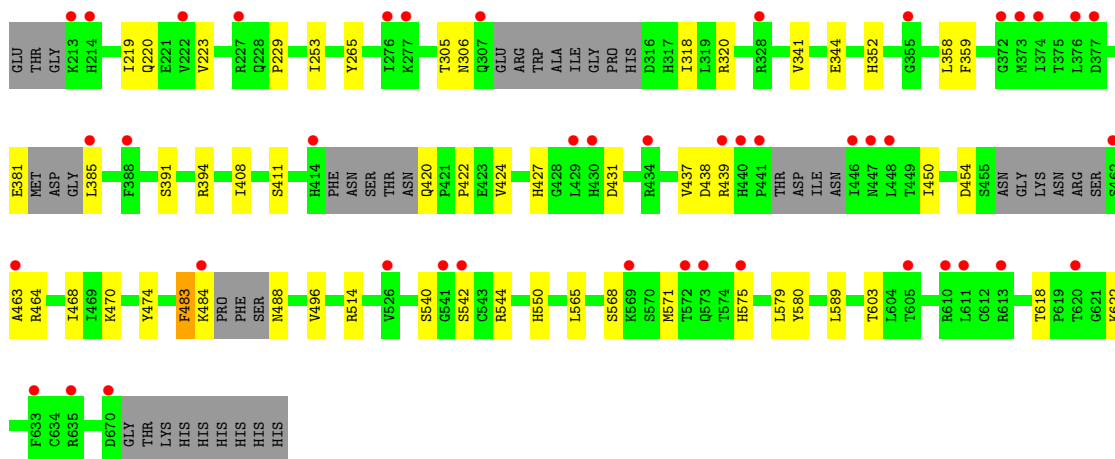


- Molecule 1: Hedgehog-interacting protein



- Molecule 1: Hedgehog-interacting protein





- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-3)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain D: 25% 75%

SGN1  
IDS2  
SGN3  
IDS4  
SGN5  
IDS6  
SGN7  
IDS8

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.64Å 105.25Å 148.43Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	84.86 – 2.70 84.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (84.86-2.70) 99.3 (84.86-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (dev_2645: ???)	Depositor
R, $R_{free}$	0.216 , 0.240 (Not available) , 0.219	Depositor DCC
$R_{free}$ test set	3679 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.3	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10309	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SGN, IDS

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	0.22	0/3563	0.47	0/4812
1	B	0.22	0/3408	0.50	0/4598
1	C	0.20	0/3420	0.45	0/4612
All	All	0.21	0/10391	0.47	0/14022

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 [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	3484	0	3384	49	0
1	B	3335	0	3251	36	0
1	C	3349	0	3272	35	0
2	D	141	0	52	8	0
All	All	10309	0	9959	120	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 6.

All (120) 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:318:ILE:HD11	1:A:344:GLU:HB3	1.51	0.90
1:C:394:ARG:HH12	1:C:411:SER:HB2	1.38	0.86
1:B:318:ILE:HD11	1:B:344:GLU:HB3	1.57	0.85
1:C:318:ILE:HD11	1:C:344:GLU:HB3	1.59	0.82
1:B:447:ASN:HB2	1:B:470:LYS:HG3	1.65	0.78
1:B:569:LYS:NZ	2:D:3:SGN:S2	2.60	0.75
1:C:358:LEU:HD13	1:C:437:VAL:HG11	1.69	0.74
1:A:320:ARG:NH1	1:A:344:GLU:OE1	2.24	0.70
1:A:394:ARG:HH12	1:A:411:SER:HB2	1.57	0.70
1:B:575:HIS:ND1	1:B:575:HIS:O	2.25	0.69
1:B:484:LYS:HE2	1:B:532:GLU:HB2	1.75	0.67
1:A:282:ARG:HD2	1:A:350:ARG:HG2	1.75	0.67
1:B:568:SER:H	1:B:571:MET:HB2	1.60	0.67
1:B:394:ARG:HH12	1:B:411:SER:HB2	1.59	0.67
1:A:276:ILE:HG22	1:B:635:ARG:HH22	1.59	0.67
1:A:514:ARG:HG2	1:A:550:HIS:HB3	1.77	0.65
1:A:408:ILE:HD11	1:A:423:GLU:HG3	1.77	0.65
1:B:408:ILE:HG12	1:B:422:PRO:HB2	1.79	0.65
1:B:569:LYS:NZ	2:D:3:SGN:O4S	2.30	0.64
1:C:575:HIS:O	1:C:575:HIS:ND1	2.29	0.64
1:A:265:TYR:O	1:A:334:VAL:HG12	1.98	0.64
1:A:569:LYS:HD2	1:A:569:LYS:H	1.63	0.64
1:C:229:PRO:HB2	1:C:565:LEU:HD22	1.81	0.62
1:A:391:SER:HA	1:A:427:HIS:HA	1.83	0.60
1:C:568:SER:H	1:C:571:MET:HB2	1.66	0.59
1:B:370:GLY:O	1:B:390:GLY:N	2.35	0.59
1:A:568:SER:H	1:A:571:MET:HB2	1.67	0.58
1:C:391:SER:HA	1:C:427:HIS:HA	1.87	0.57
1:B:394:ARG:NH1	1:B:411:SER:HB2	2.19	0.57
1:A:229:PRO:HB2	1:A:565:LEU:HD22	1.85	0.56
1:C:394:ARG:NH1	1:C:411:SER:HB2	2.14	0.56
2:D:7:SGN:O4	2:D:8:IDS:O2S	2.23	0.56
1:A:280:ASP:OD1	1:A:282:ARG:HD3	2.06	0.56
1:C:420:GLN:HG2	1:C:424:VAL:HG11	1.89	0.55
1:C:359:PHE:O	1:C:439:ARG:NH2	2.36	0.55
1:B:276:ILE:HG13	1:B:277:LYS:H	1.72	0.55
1:A:320:ARG:HG3	1:A:344:GLU:HG2	1.89	0.54
1:C:408:ILE:HG12	1:C:422:PRO:HB2	1.90	0.54
1:C:438:ASP:HA	1:C:496:VAL:HG21	1.89	0.54
1:B:446:ILE:HD11	1:B:469:ILE:HG12	1.88	0.53
1:B:464:ARG:NH1	1:B:466:LEU:HD21	2.24	0.53
1:A:266:LEU:HD13	1:A:334:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:HIS:CG	1:B:431:ASP:HB2	2.44	0.53
1:A:326:VAL:HA	1:A:334:VAL:HA	1.91	0.52
1:C:223:VAL:HG12	1:C:579:LEU:HB3	1.90	0.52
1:A:324:TYR:HB3	1:A:334:VAL:HG21	1.91	0.51
1:A:581:LYS:HD3	1:C:542:SER:OG	2.09	0.51
1:C:306:ASN:OD1	1:C:306:ASN:N	2.42	0.51
1:A:408:ILE:HG13	1:A:422:PRO:HB2	1.93	0.51
1:C:468:ILE:HA	1:C:474:TYR:OH	2.10	0.51
1:B:276:ILE:HG13	1:B:277:LYS:N	2.26	0.51
1:B:377:ASP:OD1	1:B:377:ASP:N	2.28	0.51
1:A:215:ASN:OD1	1:A:586:LYS:HE3	2.10	0.50
1:A:306:ASN:N	1:A:306:ASN:OD1	2.44	0.50
2:D:6:IDS:O6B	2:D:6:IDS:O4	2.30	0.50
1:B:484:LYS:HE2	1:B:532:GLU:CB	2.42	0.50
1:C:437:VAL:HG12	1:C:450:ILE:HG12	1.94	0.49
1:A:394:ARG:NH1	1:A:411:SER:HB2	2.24	0.49
1:A:630:GLU:HB3	1:A:638:LYS:HD2	1.93	0.49
1:C:463:ALA:HB3	1:C:483:PHE:HD2	1.78	0.49
1:A:305:THR:HG21	1:A:320:ARG:HH21	1.77	0.49
1:C:305:THR:HG23	1:C:318:ILE:HG23	1.95	0.49
1:A:223:VAL:HG22	1:A:579:LEU:HB3	1.95	0.49
1:A:396:ASP:HB2	1:A:409:PRO:HG3	1.94	0.48
1:A:464:ARG:NH2	1:A:466:LEU:HD21	2.27	0.48
1:B:306:ASN:N	1:B:306:ASN:OD1	2.46	0.48
1:C:381:GLU:HG3	1:C:385:LEU:HD12	1.95	0.48
1:C:484:LYS:NZ	1:C:488:ASN:HB2	2.28	0.47
1:B:223:VAL:HG22	1:B:579:LEU:HB3	1.96	0.47
1:A:320:ARG:HD2	1:A:322:VAL:CG2	2.44	0.47
1:C:463:ALA:HB3	1:C:483:PHE:CD2	2.49	0.47
1:A:590:MET:HB2	1:C:540:SER:HB3	1.96	0.47
1:C:320:ARG:HD3	1:C:341:VAL:HG12	1.96	0.47
1:A:440:HIS:N	1:A:441:PRO:HD3	2.31	0.46
1:A:352:HIS:CG	1:A:431:ASP:HB2	2.51	0.46
1:B:371:ASP:O	1:B:374:ILE:HG12	2.16	0.46
1:C:305:THR:HG21	1:C:320:ARG:NH1	2.31	0.46
1:C:253:ILE:HG13	1:C:265:TYR:HB2	1.97	0.46
1:C:514:ARG:HG2	1:C:550:HIS:HB3	1.98	0.45
1:B:391:SER:HA	1:B:427:HIS:HA	1.98	0.45
1:A:342:PHE:C	1:A:343:LEU:HD12	2.42	0.45
1:C:411:SER:O	1:C:470:LYS:HD2	2.16	0.45
2:D:2:IDS:H4	2:D:3:SGN:N2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:GLU:HB3	1:B:638:LYS:HD2	1.99	0.44
1:B:282:ARG:HH21	1:B:282:ARG:HG3	1.82	0.44
1:B:484:LYS:HD3	1:B:486:PHE:CD2	2.53	0.44
1:C:320:ARG:NH2	1:C:344:GLU:OE1	2.51	0.44
1:B:438:ASP:HB3	1:B:449:THR:HB	2.01	0.43
1:A:479:SER:OG	1:A:482:GLU:OE1	2.35	0.43
1:A:567:SER:HA	1:A:571:MET:HE2	2.00	0.43
1:B:350:ARG:NH2	2:D:6:IDS:O6A	2.46	0.43
1:A:388:PHE:O	1:A:391:SER:OG	2.34	0.43
1:C:219:ILE:CG2	1:C:580:TYR:HB3	2.49	0.43
1:A:477:GLU:OE1	1:A:478:PRO:HD2	2.19	0.42
2:D:7:SGN:H3	2:D:8:IDS:H2	1.84	0.42
1:A:320:ARG:HD2	1:A:322:VAL:HG22	2.01	0.42
1:A:667:GLU:HG2	1:A:668:GLN:HG3	2.00	0.42
1:A:388:PHE:HB3	1:A:393:LEU:HD11	2.02	0.42
1:A:436:ALA:HB1	1:A:496:VAL:HG23	2.02	0.42
1:A:630:GLU:O	1:A:634:CYS:HA	2.20	0.42
1:A:474:TYR:HA	1:A:477:GLU:HB2	2.01	0.41
1:B:305:THR:HG21	1:B:320:ARG:NH1	2.36	0.41
1:A:305:THR:HG21	1:A:320:ARG:NH2	2.35	0.41
1:B:641:PRO:HG2	1:B:665:GLN:CD	2.46	0.41
1:C:454:ASP:O	1:C:464:ARG:HB3	2.21	0.41
1:A:280:ASP:OD2	1:A:282:ARG:NH2	2.54	0.41
1:A:287:LEU:HD23	1:A:288:ALA:N	2.35	0.41
1:B:392:VAL:HG23	1:B:425:PHE:HB3	2.02	0.41
1:A:531:GLN:HG2	1:A:532:GLU:N	2.36	0.41
1:B:567:SER:HA	1:B:571:MET:HE2	2.02	0.41
1:C:352:HIS:ND1	1:C:431:ASP:HB2	2.36	0.41
1:A:258:GLY:HA3	1:C:544:ARG:HE	1.85	0.41
1:B:277:LYS:NZ	2:D:5:SGN:H5	2.35	0.41
1:B:497:TYR:OH	1:B:561:GLU:OE1	2.39	0.41
1:C:589:LEU:HD23	1:C:589:LEU:HA	1.87	0.40
1:B:352:HIS:ND1	1:B:431:ASP:HB2	2.36	0.40
1:B:484:LYS:NZ	1:B:532:GLU:N	2.69	0.40
1:A:282:ARG:HD2	1:A:350:ARG:CG	2.46	0.40
1:A:562:VAL:HG23	1:A:582:ILE:HD12	2.04	0.40
1:C:618:THR:HG22	1:C:622:LYS:O	2.21	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	439/470 (93%)	430 (98%)	9 (2%)	0	100	100
1	B	415/470 (88%)	406 (98%)	8 (2%)	1 (0%)	43	68
1	C	415/470 (88%)	410 (99%)	5 (1%)	0	100	100
All	All	1269/1410 (90%)	1246 (98%)	22 (2%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	PRO

### 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	390/409 (95%)	390 (100%)	0	100	100
1	B	372/409 (91%)	369 (99%)	3 (1%)	73	88
1	C	374/409 (91%)	371 (99%)	3 (1%)	73	88
All	All	1136/1227 (93%)	1130 (100%)	6 (0%)	81	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	377	ASP
1	B	469	ILE

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Mol	Chain	Res	Type
1	B	483	PHE
1	C	220	GLN
1	C	483	PHE
1	C	603	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	273	GLN
1	A	427	HIS
1	A	515	ASN
1	A	517	ASN
1	B	349	HIS
1	B	430	HIS
1	B	599	GLN
1	B	614	ASN
1	C	273	GLN
1	C	599	GLN
1	C	602	GLN
1	C	614	ASN

### 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](#)

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
2	SGN	D	1	2	20,20,20	4.48	2 (10%)	25,31,31	1.40	4 (16%)
2	IDS	D	2	2	16,16,17	1.27	3 (18%)	16,24,26	1.24	2 (12%)
2	SGN	D	3	2	19,19,20	1.26	2 (10%)	23,29,31	1.77	5 (21%)
2	IDS	D	4	2	16,16,17	1.20	2 (12%)	16,24,26	1.03	1 (6%)
2	SGN	D	5	2	19,19,20	1.24	2 (10%)	23,29,31	1.47	3 (13%)
2	IDS	D	6	2	16,16,17	1.52	2 (12%)	16,24,26	1.17	2 (12%)
2	SGN	D	7	2	19,19,20	4.61	2 (10%)	23,29,31	2.02	7 (30%)
2	IDS	D	8	2	16,16,17	1.11	2 (12%)	16,24,26	0.96	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	SGN	D	1	2	-	6/11/31/31	0/1/1/1
2	IDS	D	2	2	-	0/9/26/29	0/1/1/1
2	SGN	D	3	2	-	3/11/28/31	0/1/1/1
2	IDS	D	4	2	-	3/9/26/29	0/1/1/1
2	SGN	D	5	2	-	4/11/28/31	0/1/1/1
2	IDS	D	6	2	-	0/9/26/29	0/1/1/1
2	SGN	D	7	2	-	6/11/28/31	0/1/1/1
2	IDS	D	8	2	-	2/9/26/29	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	SGN	O1S-S1	19.26	1.64	1.42
2	D	7	SGN	O1S-S1	19.20	1.63	1.42
2	D	6	IDS	O1S-S	4.32	1.64	1.45
2	D	1	SGN	O4S-S2	4.30	1.64	1.45
2	D	7	SGN	O4S-S2	4.29	1.64	1.45
2	D	3	SGN	O3S-S1	3.43	1.64	1.47
2	D	5	SGN	O3S-S1	3.39	1.63	1.47
2	D	4	IDS	O2-C2	-2.73	1.43	1.47
2	D	2	IDS	O2-C2	-2.68	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	IDS	O2-C2	-2.49	1.43	1.47
2	D	6	IDS	O2-C2	-2.39	1.43	1.47
2	D	2	IDS	C1-C2	2.27	1.55	1.51
2	D	3	SGN	O6S-S2	2.24	1.64	1.50
2	D	8	IDS	O3S-S	2.18	1.64	1.50
2	D	2	IDS	O3S-S	2.18	1.64	1.50
2	D	5	SGN	O6S-S2	2.18	1.64	1.50
2	D	4	IDS	O3S-S	2.10	1.63	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	SGN	O1S-S1-O2S	-5.29	108.59	120.36
2	D	7	SGN	O1S-S1-O2S	-5.09	109.03	120.36
2	D	3	SGN	O1S-S1-O2S	-4.85	109.57	120.36
2	D	1	SGN	O1S-S1-O2S	-4.81	109.65	120.36
2	D	7	SGN	O5-C1-C2	-4.58	104.20	111.29
2	D	3	SGN	O5-C1-C2	-4.48	104.35	111.29
2	D	5	SGN	O5-C1-C2	-3.04	106.59	111.29
2	D	4	IDS	O2-C2-C3	2.97	111.10	106.95
2	D	7	SGN	C4-C3-C2	-2.93	106.73	111.02
2	D	3	SGN	C1-C2-N2	2.91	114.82	110.22
2	D	7	SGN	C1-O5-C5	2.86	116.02	112.19
2	D	8	IDS	O2-C2-C3	2.86	110.94	106.95
2	D	2	IDS	O4-C4-C5	2.79	116.14	109.76
2	D	6	IDS	O4-C4-C3	2.59	116.49	110.38
2	D	2	IDS	O2-C2-C3	2.54	110.50	106.95
2	D	7	SGN	O6-C6-C5	2.53	112.07	107.57
2	D	7	SGN	C3-C2-N2	2.53	113.64	110.32
2	D	6	IDS	O2-C2-C3	2.36	110.25	106.95
2	D	1	SGN	O4-C4-C3	-2.35	104.84	110.38
2	D	7	SGN	O3-C3-C4	2.34	115.90	110.38
2	D	3	SGN	O6S-S2-O6	2.33	111.73	106.37
2	D	1	SGN	O6-C6-C5	2.12	111.34	107.57
2	D	1	SGN	O4-C4-C5	2.09	114.47	109.32
2	D	3	SGN	O4-C4-C3	-2.07	105.50	110.38
2	D	5	SGN	O6-C6-C5	-2.02	103.96	107.57

There are no chirality outliers.

All (24) torsion outliers are listed below:

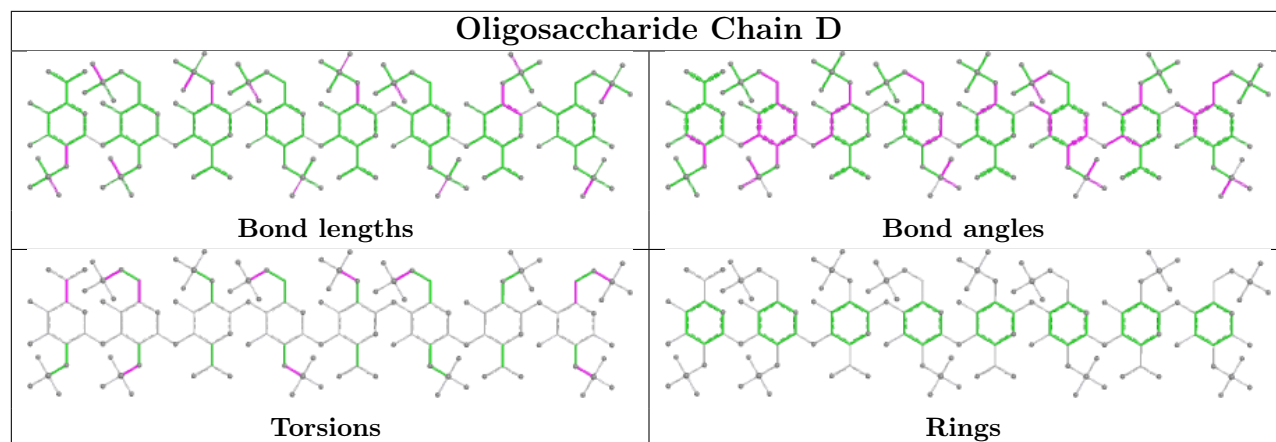
Mol	Chain	Res	Type	Atoms
2	D	1	SGN	C4-C5-C6-O6
2	D	1	SGN	O5-C5-C6-O6
2	D	1	SGN	C6-O6-S2-O6S
2	D	5	SGN	C6-O6-S2-O4S
2	D	7	SGN	C4-C5-C6-O6
2	D	8	IDS	C4-C5-C6-O6A
2	D	8	IDS	C4-C5-C6-O6B
2	D	5	SGN	C6-O6-S2-O5S
2	D	7	SGN	C6-O6-S2-O4S
2	D	5	SGN	C6-O6-S2-O6S
2	D	7	SGN	C6-O6-S2-O6S
2	D	1	SGN	C6-O6-S2-O4S
2	D	1	SGN	C6-O6-S2-O5S
2	D	3	SGN	C6-O6-S2-O5S
2	D	7	SGN	C6-O6-S2-O5S
2	D	3	SGN	C6-O6-S2-O4S
2	D	1	SGN	C2-N2-S1-O2S
2	D	7	SGN	O5-C5-C6-O6
2	D	4	IDS	C2-O2-S-O3S
2	D	3	SGN	C6-O6-S2-O6S
2	D	7	SGN	C2-N2-S1-O2S
2	D	4	IDS	C2-O2-S-O1S
2	D	4	IDS	C2-O2-S-O2S
2	D	5	SGN	C2-N2-S1-O2S

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	8	IDS	2	0
2	D	7	SGN	2	0
2	D	2	IDS	1	0
2	D	6	IDS	2	0
2	D	3	SGN	3	0
2	D	5	SGN	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](#)

There are no ligands in this entry.

## 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<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	447/470 (95%)	0.56	44 (9%) 13 11	48, 87, 168, 212	0
1	B	427/470 (90%)	0.52	51 (11%) 9 7	43, 79, 155, 202	0
1	C	429/470 (91%)	0.60	44 (10%) 12 10	53, 97, 166, 230	0
All	All	1303/1410 (92%)	0.56	139 (10%) 11 9	43, 88, 165, 230	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	PHE	7.7
1	C	372	GLY	6.0
1	A	486	PHE	5.9
1	B	466	LEU	5.9
1	B	465	ILE	5.7
1	A	314	PRO	5.7
1	B	490	PRO	5.7
1	B	444	ILE	5.5
1	C	373	MET	5.4
1	C	448	LEU	5.1
1	A	444	ILE	5.0
1	A	569	LYS	4.9
1	A	457	GLY	4.6
1	C	446	ILE	4.6
1	A	635	ARG	4.5
1	C	441	PRO	4.4
1	B	573	GLN	4.3
1	B	276	ILE	4.3
1	B	542	SER	4.2
1	B	464	ARG	4.1
1	B	575	HIS	3.9
1	B	485	PRO	3.9
1	C	385	LEU	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	605	THR	3.8
1	A	542	SER	3.8
1	C	277	LYS	3.8
1	A	308	GLU	3.7
1	A	488	ASN	3.7
1	A	485	PRO	3.6
1	B	470	LYS	3.6
1	A	572	THR	3.6
1	C	440	HIS	3.5
1	B	375	THR	3.5
1	B	386	SER	3.5
1	B	489	GLY	3.5
1	A	441	PRO	3.5
1	B	482	GLU	3.5
1	B	569	LYS	3.4
1	A	385	LEU	3.4
1	A	636	THR	3.3
1	A	214	HIS	3.3
1	A	315	HIS	3.3
1	A	573	GLN	3.3
1	A	474	TYR	3.3
1	B	458	LYS	3.3
1	C	214	HIS	3.2
1	B	278	GLY	3.2
1	A	386	SER	3.2
1	C	526	VAL	3.2
1	B	484	LYS	3.2
1	B	214	HIS	3.1
1	B	315	HIS	3.1
1	B	467	GLN	3.1
1	C	307	GLN	3.1
1	B	463	ALA	3.1
1	A	484	LYS	3.1
1	C	374	ILE	3.1
1	B	613	ARG	3.1
1	C	414	HIS	3.0
1	B	486	PHE	3.0
1	B	455	SER	3.0
1	C	633	PHE	3.0
1	B	668	GLN	2.9
1	A	489	GLY	2.9
1	B	453	SER	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	543	CYS	2.8
1	C	376	LEU	2.8
1	A	461	SER	2.8
1	C	670	ASP	2.8
1	C	276	ILE	2.8
1	C	569	LYS	2.7
1	B	469	ILE	2.7
1	C	484	LYS	2.7
1	A	605	THR	2.7
1	B	457	GLY	2.7
1	A	384	GLY	2.7
1	B	279	GLY	2.7
1	A	570	SER	2.7
1	B	635	ARG	2.6
1	A	446	ILE	2.6
1	C	377	ASP	2.6
1	A	456	ASN	2.6
1	B	454	ASP	2.6
1	A	481	LEU	2.6
1	C	611	LEU	2.6
1	C	328	ARG	2.6
1	C	463	ALA	2.6
1	B	452	CYS	2.5
1	C	213	LYS	2.5
1	B	572	THR	2.5
1	A	233	LEU	2.5
1	A	439	ARG	2.5
1	B	307	GLN	2.5
1	C	605	THR	2.4
1	B	260	ILE	2.3
1	A	383	ASP	2.3
1	B	374	ILE	2.3
1	B	401	MET	2.3
1	B	434	ARG	2.3
1	A	415	PHE	2.3
1	C	388	PHE	2.3
1	C	613	ARG	2.3
1	C	575	HIS	2.2
1	C	572	THR	2.2
1	C	227	ARG	2.2
1	C	573	GLN	2.2
1	C	355	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	542	SER	2.2
1	A	490	PRO	2.2
1	C	447	ASN	2.2
1	A	351	LYS	2.2
1	B	512	GLY	2.1
1	C	434	ARG	2.1
1	C	439	ARG	2.1
1	A	387	ASP	2.1
1	A	469	ILE	2.1
1	A	632	ASP	2.1
1	C	222	VAL	2.1
1	A	487	SER	2.1
1	B	644	ARG	2.1
1	C	610	ARG	2.1
1	B	456	ASN	2.1
1	A	575	HIS	2.1
1	B	511	PHE	2.1
1	C	429	LEU	2.1
1	A	377	ASP	2.0
1	A	606	SER	2.0
1	B	220	GLN	2.0
1	B	430	HIS	2.0
1	C	430	HIS	2.0
1	C	541	GLY	2.0
1	A	388	PHE	2.0
1	A	410	ARG	2.0
1	B	316	ASP	2.0
1	C	462	SER	2.0
1	C	620	THR	2.0
1	A	353	LEU	2.0
1	B	275	GLY	2.0
1	C	635	ARG	2.0

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

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

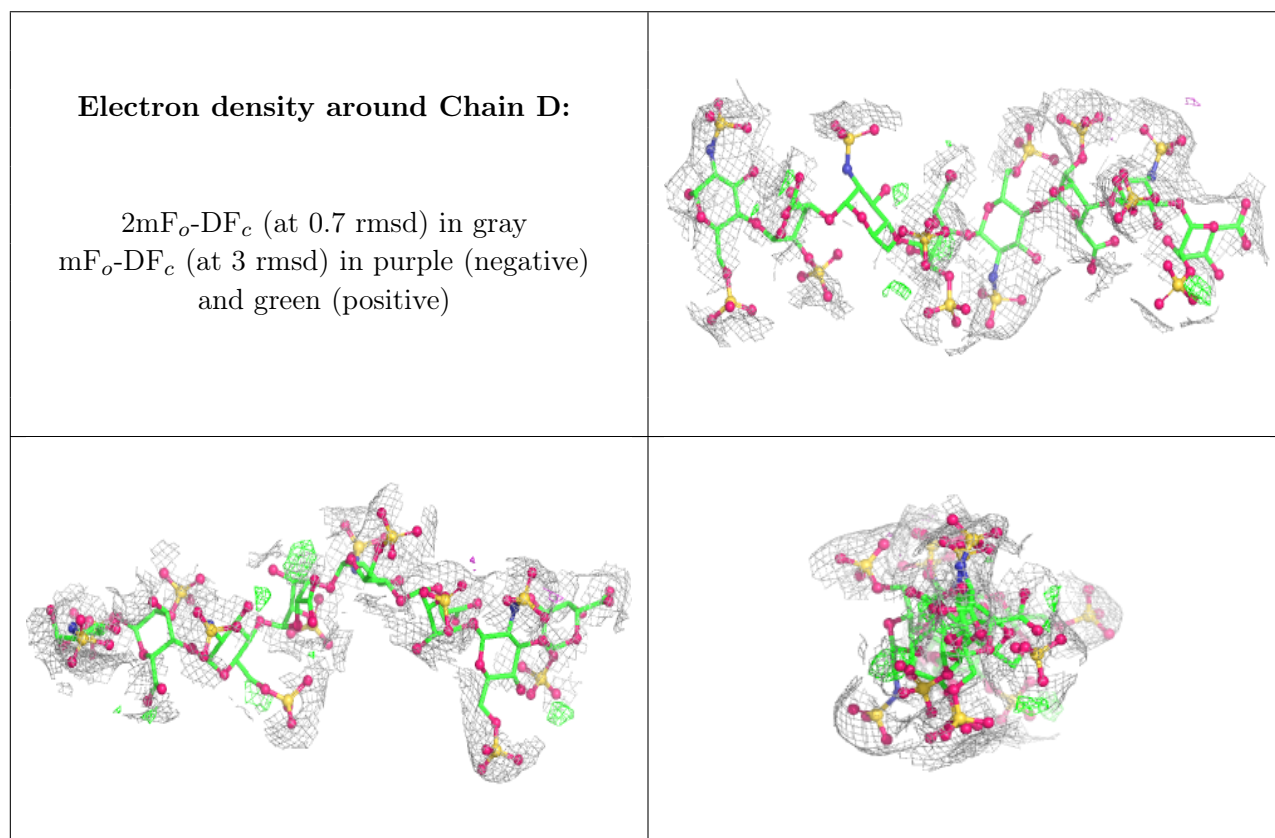
## 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SGN	D	1	20/20	0.60	0.11	216,225,229,230	0
2	SGN	D	7	19/20	0.61	0.13	176,193,198,199	0
2	IDS	D	8	16/17	0.65	0.11	192,203,206,208	0
2	IDS	D	2	16/17	0.67	0.10	211,225,230,230	0
2	SGN	D	3	19/20	0.68	0.10	178,196,208,208	0
2	SGN	D	5	19/20	0.73	0.11	142,164,186,187	0
2	IDS	D	6	16/17	0.82	0.11	154,164,168,171	0
2	IDS	D	4	16/17	0.83	0.10	152,173,184,184	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.