



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 AM UTC

PDB ID : 2FUQ / pdb_00002fuq
Title : Crystal Structure of Heparinase II
Authors : Shaya, D.; Cygler, M.
Deposited on : 2006-01-27
Resolution : 2.15 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 : 4-5-2 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

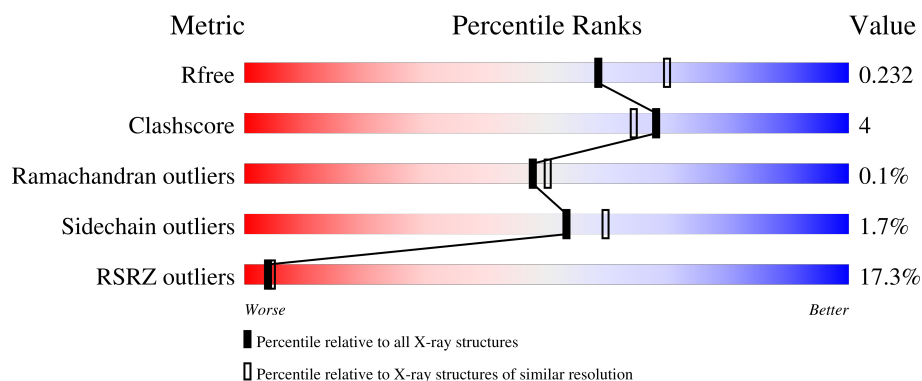
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	747	14% 92% 8%
1	B	747	21% 89% 10%
2	C	4	25% 75%
2	D	4	25% 75%

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
2	XYS	D	3	X	-	-	-
5	FMT	A	943	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12987 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.

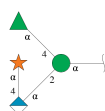
- Molecule 1 is a protein called heparinase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5978	3850	1008	1097	23			
1	B	747	Total	C	N	O	S	0	0	0
			5978	3850	1008	1097	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	PCA	-	modified residue	GB 924923
A	758	ALA	PRO	engineered mutation	GB 924923
B	26	PCA	-	modified residue	GB 924923
B	758	ALA	PRO	engineered mutation	GB 924923

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			41	23	18			
2	D	4	Total	C	O	0	0	0
			41	23	18			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

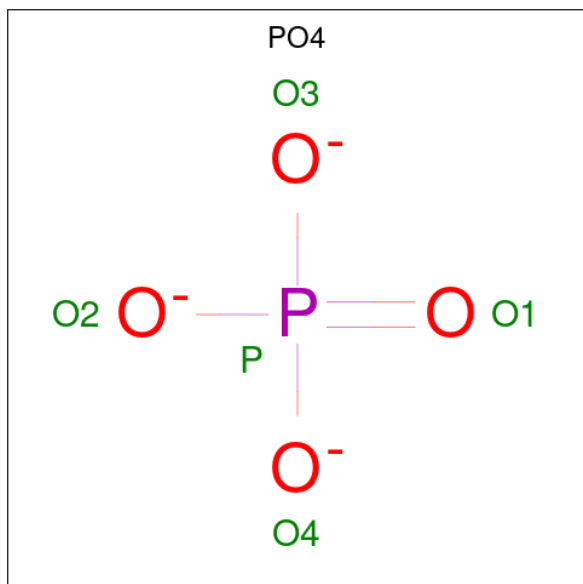
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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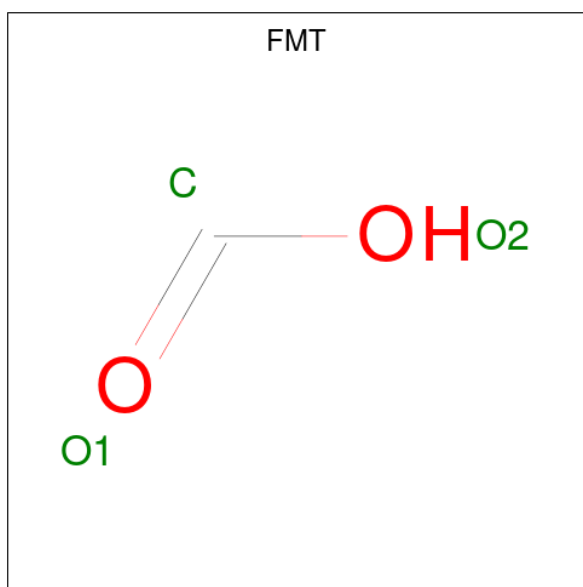
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

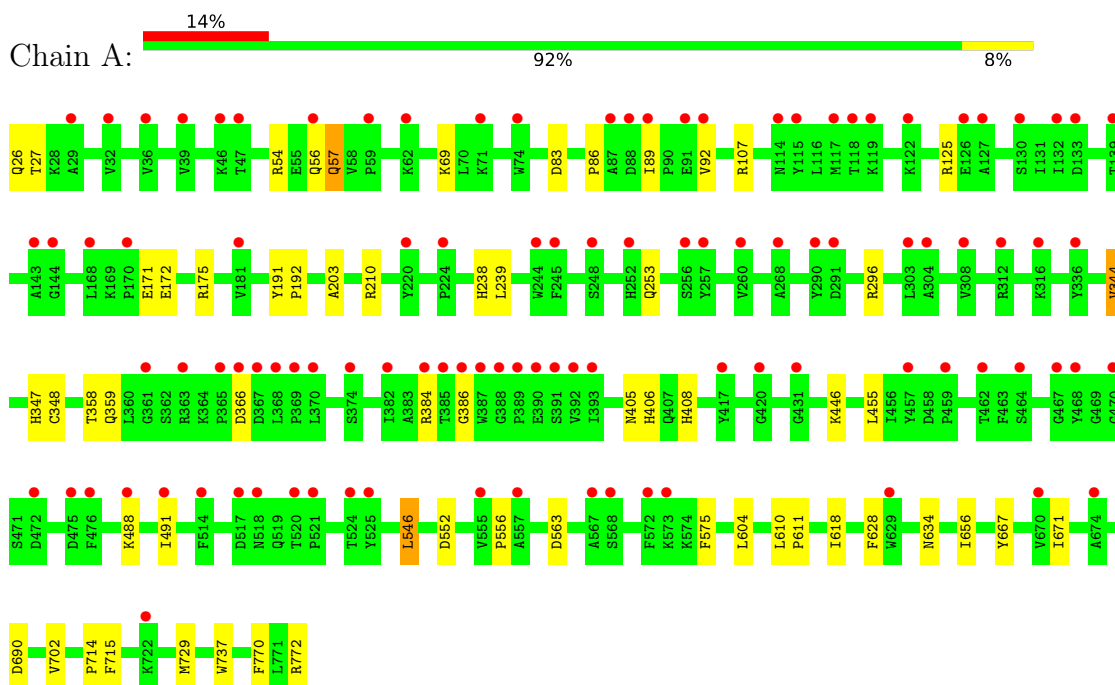
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	461	Total	O	0	0
			461	461		
6	B	467	Total	O	0	0
			467	467		

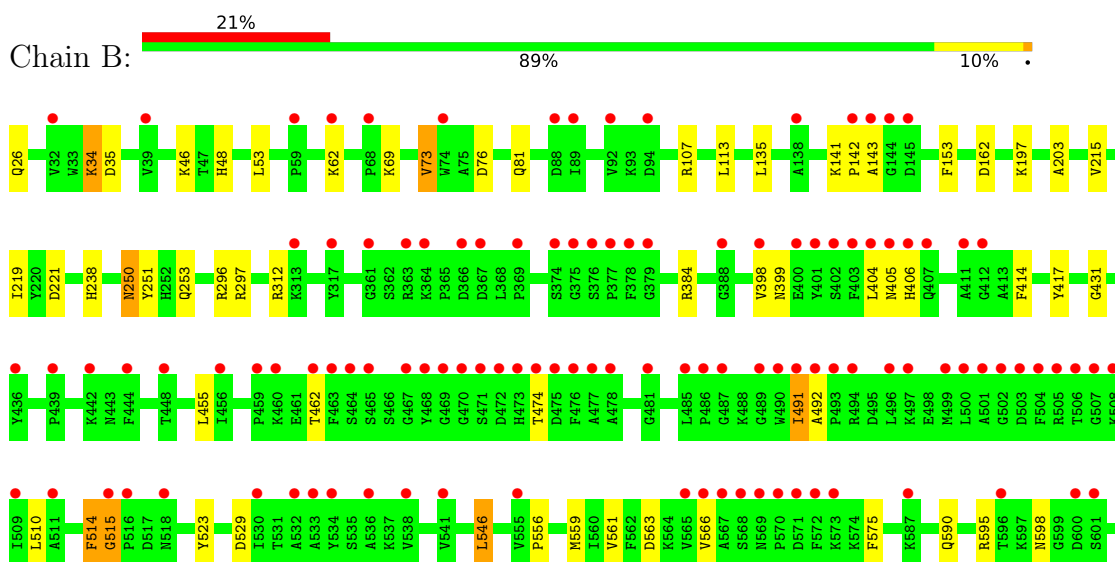
3 Residue-property plots [i](#)

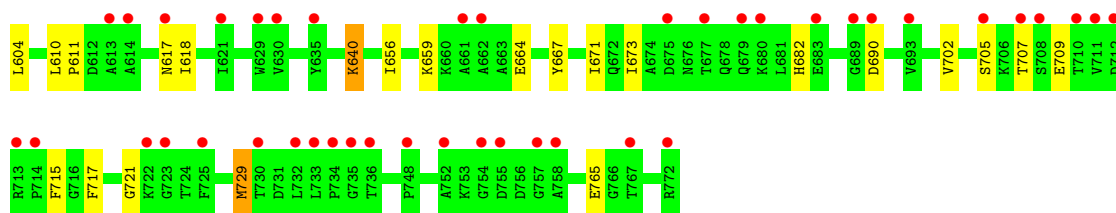
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: heparinase II protein



- Molecule 1: heparinase II protein





- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-mannopyranose

Chain C: 25% 75%



- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-mannopyranose

Chain D: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.05Å 119.34Å 200.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.60 – 2.15 102.58 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (102.60-2.15) 98.7 (102.58-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.235 0.195 , 0.232	Depositor DCC
R_{free} test set	6824 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	1.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6404e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MAN, ZN, PCA, XYS, GCU, RAM, FMT, PO4

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	0.62	6/6133 (0.1%)	0.76	1/8303 (0.0%)
1	B	0.52	0/6133	0.78	2/8303 (0.0%)
All	All	0.57	6/12266 (0.0%)	0.77	3/16606 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	ARG	CZ-NH1	20.60	1.61	1.32
1	A	175	ARG	CZ-NH1	8.54	1.44	1.32
1	A	172	GLU	CD-OE2	8.16	1.40	1.25
1	A	125	ARG	NE-CZ	8.15	1.42	1.33
1	A	175	ARG	CD-NE	5.51	1.53	1.46
1	A	175	ARG	CZ-NH2	5.30	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	PHE	CA-C-N	5.70	130.81	121.87
1	B	514	PHE	C-N-CA	5.70	130.81	121.87
1	A	366	ASP	N-CA-C	5.16	117.65	111.71

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	5978	0	5889	29	0
1	B	5978	0	5889	56	0
2	C	41	0	30	0	0
2	D	41	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	6	0	3	0	0
5	B	3	0	1	0	0
6	A	461	0	0	0	0
6	B	467	0	0	4	0
All	All	12987	0	11842	85	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 4.

All (85) 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:640:LYS:H	1:B:640:LYS:HE3	0.96	1.08
1:B:640:LYS:HE3	1:B:640:LYS:N	1.81	0.95
1:B:559:MET:HE3	1:B:561:VAL:CG2	2.02	0.89
1:B:640:LYS:H	1:B:640:LYS:CE	1.87	0.83
1:B:62:LYS:HD2	1:B:62:LYS:H	1.44	0.80
1:B:250:ASN:HD22	1:B:251:TYR:H	1.32	0.77
1:A:628:PHE:H	1:A:634:ASN:HD21	1.31	0.77
1:B:707:THR:HG23	1:B:709:GLU:H	1.52	0.74
1:B:431:GLY:HA2	1:B:640:LYS:HE2	1.71	0.72
1:B:491:ILE:HD13	1:B:492:ALA:H	1.54	0.71
1:A:253:GLN:HE22	1:A:406:HIS:H	1.38	0.70
1:B:253:GLN:HE22	1:B:406:HIS:H	1.40	0.70
1:A:210:ARG:HH12	1:A:347:HIS:CD2	2.11	0.69
1:B:515:GLY:HA2	1:B:523:TYR:CE2	2.30	0.67
1:B:253:GLN:HE22	1:B:405:ASN:HB3	1.60	0.67
1:B:62:LYS:HD2	1:B:62:LYS:N	2.12	0.64
1:B:595:ARG:HH12	1:B:598:ASN:HD22	1.47	0.63
1:B:297:ARG:HD3	1:B:417:TYR:CE1	2.36	0.61
1:B:455:LEU:HB2	1:B:575:PHE:HB2	1.82	0.61
1:A:210:ARG:HH12	1:A:347:HIS:HD2	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:O	1:A:384:ARG:NH2	2.31	0.60
1:B:566:VAL:HG22	1:B:664:GLU:HG3	1.83	0.60
1:B:717:PHE:HE1	1:B:729:MET:HE1	1.65	0.60
1:B:559:MET:HE3	1:B:561:VAL:HG23	1.81	0.59
1:B:546:LEU:HD22	1:B:702:VAL:HG21	1.87	0.57
1:A:83:ASP:OD1	1:A:107:ARG:NH2	2.38	0.56
1:A:54:ARG:H	1:A:57:GLN:HE21	1.52	0.56
1:B:48:HIS:HD2	1:B:162:ASP:OD1	1.89	0.56
1:A:455:LEU:HB2	1:A:575:PHE:HB2	1.88	0.55
1:A:610:LEU:HA	1:A:611:PRO:C	2.33	0.54
1:B:69:LYS:HE3	1:B:69:LYS:H	1.73	0.54
1:B:143:ALA:HB1	6:B:1403:HOH:O	2.06	0.54
1:B:296:ARG:O	1:B:384:ARG:NH2	2.40	0.54
1:B:682:HIS:HE1	6:B:994:HOH:O	1.91	0.53
1:B:203:ALA:O	1:B:238:HIS:HE1	1.92	0.53
1:B:610:LEU:HA	1:B:611:PRO:C	2.34	0.53
1:B:690:ASP:O	1:B:715:PHE:HB2	2.10	0.52
1:A:344:VAL:HG13	1:A:348:CYS:HB2	1.93	0.51
1:B:515:GLY:HA2	1:B:523:TYR:CD2	2.46	0.51
1:B:414:PHE:CD1	1:B:559:MET:HE1	2.46	0.50
1:B:414:PHE:CG	1:B:559:MET:HE1	2.47	0.50
1:A:203:ALA:O	1:A:238:HIS:HE1	1.95	0.50
1:B:197:LYS:HE3	1:B:491:ILE:HD12	1.94	0.50
1:B:398:VAL:O	1:B:399:ASN:HB2	2.13	0.49
1:A:618:ILE:HG12	1:A:656:ILE:HG12	1.94	0.49
1:A:253:GLN:HE22	1:A:405:ASN:HB3	1.77	0.49
1:A:191:TYR:HA	1:A:192:PRO:C	2.37	0.48
1:B:604:LEU:HG	1:B:671:ILE:HG23	1.94	0.48
1:A:690:ASP:O	1:A:715:PHE:HB2	2.14	0.47
1:A:27:THR:HG21	1:A:56:GLN:NE2	2.29	0.47
1:A:54:ARG:H	1:A:57:GLN:NE2	2.12	0.47
1:B:81:GLN:HE21	1:B:107:ARG:HA	1.80	0.47
1:B:729:MET:HE3	1:B:729:MET:HB3	1.58	0.46
1:B:510:LEU:HD11	1:B:529:ASP:HB2	1.96	0.46
1:B:253:GLN:NE2	1:B:406:HIS:H	2.10	0.46
1:B:81:GLN:NE2	6:B:1299:HOH:O	2.50	0.45
1:B:618:ILE:HG12	1:B:656:ILE:HG12	1.98	0.45
1:B:491:ILE:HD13	1:B:492:ALA:N	2.26	0.44
1:B:617:ASN:ND2	1:B:659:LYS:HG2	2.32	0.44
1:B:556:PRO:HD2	1:B:673:ILE:O	2.18	0.44
1:A:563:ASP:HB2	1:A:667:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:PRO:HA	1:A:770:PHE:O	2.18	0.44
1:B:312:ARG:HD3	6:B:1187:HOH:O	2.18	0.44
1:B:721:GLY:O	1:B:765:GLU:HB3	2.17	0.43
1:A:69:LYS:HD2	1:A:358:THR:HB	2.00	0.43
1:A:604:LEU:HG	1:A:671:ILE:HG23	2.00	0.43
1:A:737:TRP:CE2	1:A:772:ARG:HD3	2.53	0.43
1:A:552:ASP:O	1:A:556:PRO:HA	2.18	0.43
1:A:488:LYS:O	1:A:491:ILE:HD12	2.18	0.43
1:A:628:PHE:H	1:A:634:ASN:ND2	2.07	0.43
1:A:546:LEU:HD22	1:A:702:VAL:HG21	1.99	0.42
1:B:135:LEU:HA	1:B:153:PHE:CE2	2.53	0.42
1:B:705:SER:OG	1:B:707:THR:HG22	2.19	0.42
1:B:717:PHE:CE1	1:B:729:MET:HE1	2.49	0.42
1:A:384:ARG:HD3	1:A:386:GLY:O	2.19	0.42
1:B:563:ASP:HB2	1:B:667:TYR:HB2	2.02	0.42
1:B:48:HIS:HE1	1:B:221:ASP:OD1	2.03	0.42
1:A:408:HIS:CD2	1:A:446:LYS:HG2	2.55	0.41
1:A:86:PRO:HA	1:A:89:ILE:HD12	2.03	0.41
1:B:141:LYS:HA	1:B:142:PRO:HD3	1.92	0.41
1:B:431:GLY:CA	1:B:640:LYS:HE2	2.45	0.41
1:B:73:VAL:O	1:B:76:ASP:HB2	2.20	0.40
1:B:215:VAL:O	1:B:219:ILE:HG12	2.21	0.40
1:B:514:PHE:O	1:B:515:GLY:O	2.39	0.40
1:B:34:LYS:HD2	1:B:35:ASP:N	2.37	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	745/747 (100%)	711 (95%)	34 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	745/747 (100%)	713 (96%)	30 (4%)	2 (0%)	36	34
All	All	1490/1494 (100%)	1424 (96%)	64 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	515	GLY
1	B	474	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	632/632 (100%)	624 (99%)	8 (1%)	61	68
1	B	632/632 (100%)	619 (98%)	13 (2%)	47	52
All	All	1264/1264 (100%)	1243 (98%)	21 (2%)	53	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	92	VAL
1	A	171	GLU
1	A	239	LEU
1	A	344	VAL
1	A	359	GLN
1	A	546	LEU
1	A	729	MET
1	B	34	LYS
1	B	46	LYS
1	B	53	LEU
1	B	73	VAL
1	B	113	LEU
1	B	250	ASN

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Mol	Chain	Res	Type
1	B	404	LEU
1	B	462	THR
1	B	491	ILE
1	B	546	LEU
1	B	590	GLN
1	B	640	LYS
1	B	729	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	56	GLN
1	A	57	GLN
1	A	66	ASN
1	A	81	GLN
1	A	238	HIS
1	A	252	HIS
1	A	253	GLN
1	A	347	HIS
1	A	437	ASN
1	A	441	ASN
1	A	473	HIS
1	A	634	ASN
1	A	678	GLN
1	B	48	HIS
1	B	66	ASN
1	B	81	GLN
1	B	238	HIS
1	B	250	ASN
1	B	253	GLN
1	B	259	ASN
1	B	335	ASN
1	B	359	GLN
1	B	598	ASN
1	B	682	HIS
1	B	738	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	B	26	1	7,8,9	1.90	1 (14%)	9,10,12	2.15	5 (55%)
1	PCA	A	26	1	7,8,9	1.95	1 (14%)	9,10,12	2.18	5 (55%)

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
1	PCA	B	26	1	-	0/0/11/13	0/1/1/1
1	PCA	A	26	1	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	PCA	CD-N	4.95	1.46	1.34
1	B	26	PCA	CD-N	4.87	1.46	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PCA	CA-N-CD	-2.98	103.37	113.58
1	B	26	PCA	CB-CA-N	2.94	111.34	103.24
1	B	26	PCA	CA-N-CD	-2.94	103.52	113.58
1	A	26	PCA	CB-CA-C	-2.88	108.70	112.66
1	A	26	PCA	OE-CD-CG	-2.78	121.76	126.72
1	A	26	PCA	CB-CA-N	2.75	110.80	103.24
1	B	26	PCA	OE-CD-CG	-2.73	121.85	126.72
1	B	26	PCA	CB-CA-C	-2.58	109.12	112.66
1	B	26	PCA	CG-CD-N	2.46	114.40	108.39
1	A	26	PCA	CG-CD-N	2.38	114.21	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	MAN	C	1	1,2	11,11,12	1.80	2 (18%)	15,15,17	2.39	2 (13%)
2	GCU	C	2	2	12,12,13	1.32	1 (8%)	14,17,19	2.09	3 (21%)
2	XYS	C	3	2	8,8,10	1.29	1 (12%)	8,10,14	1.50	1 (12%)
2	RAM	C	4	2	10,10,11	0.65	0	14,14,16	0.92	0
2	MAN	D	1	1,2	11,11,12	1.79	2 (18%)	15,15,17	2.60	4 (26%)
2	GCU	D	2	2	12,12,13	1.35	1 (8%)	14,17,19	1.72	1 (7%)
2	XYS	D	3	2	8,8,10	1.49	1 (12%)	8,10,14	1.62	1 (12%)
2	RAM	D	4	2	10,10,11	0.57	0	14,14,16	0.68	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
2	MAN	C	1	1,2	-	0/2/19/22	0/1/1/1
2	GCU	C	2	2	-	0/4/21/24	0/1/1/1
2	XYS	C	3	2	-	-	0/1/1/1
2	RAM	C	4	2	-	-	0/1/1/1
2	MAN	D	1	1,2	-	0/2/19/22	0/1/1/1
2	GCU	D	2	2	-	0/4/21/24	0/1/1/1
2	XYS	D	3	2	1/1/2/4	-	0/1/1/1
2	RAM	D	4	2	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	MAN	O2-C2	-4.28	1.34	1.43
2	D	1	MAN	O2-C2	-4.19	1.34	1.43
2	D	1	MAN	O4-C4	-3.87	1.33	1.43
2	D	2	GCU	O4-C4	-3.85	1.33	1.43
2	C	1	MAN	O4-C4	-3.82	1.33	1.43
2	C	2	GCU	O4-C4	-3.72	1.33	1.43
2	D	3	XYS	O5-C1	-3.69	1.36	1.43
2	C	3	XYS	O5-C1	-3.13	1.37	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MAN	O2-C2-C3	7.86	126.44	110.15
2	C	1	MAN	O2-C2-C3	7.43	125.54	110.15
2	D	2	GCU	O4-C4-C5	6.02	123.51	109.76
2	C	2	GCU	O4-C4-C5	5.81	123.03	109.76
2	C	1	MAN	O4-C4-C5	4.49	120.37	109.32
2	C	2	GCU	O4-C4-C3	4.38	120.70	110.38
2	D	1	MAN	O4-C4-C3	-4.22	100.43	110.38
2	C	3	XYS	C5-O5-C1	4.14	115.79	110.02
2	D	3	XYS	C4-C3-C2	3.64	114.03	111.12
2	D	1	MAN	O2-C2-C1	-3.19	101.92	109.22
2	D	1	MAN	C1-O5-C5	3.05	116.27	112.19
2	C	2	GCU	C1-C2-C3	2.01	112.57	109.64

All (1) chirality outliers are listed below:

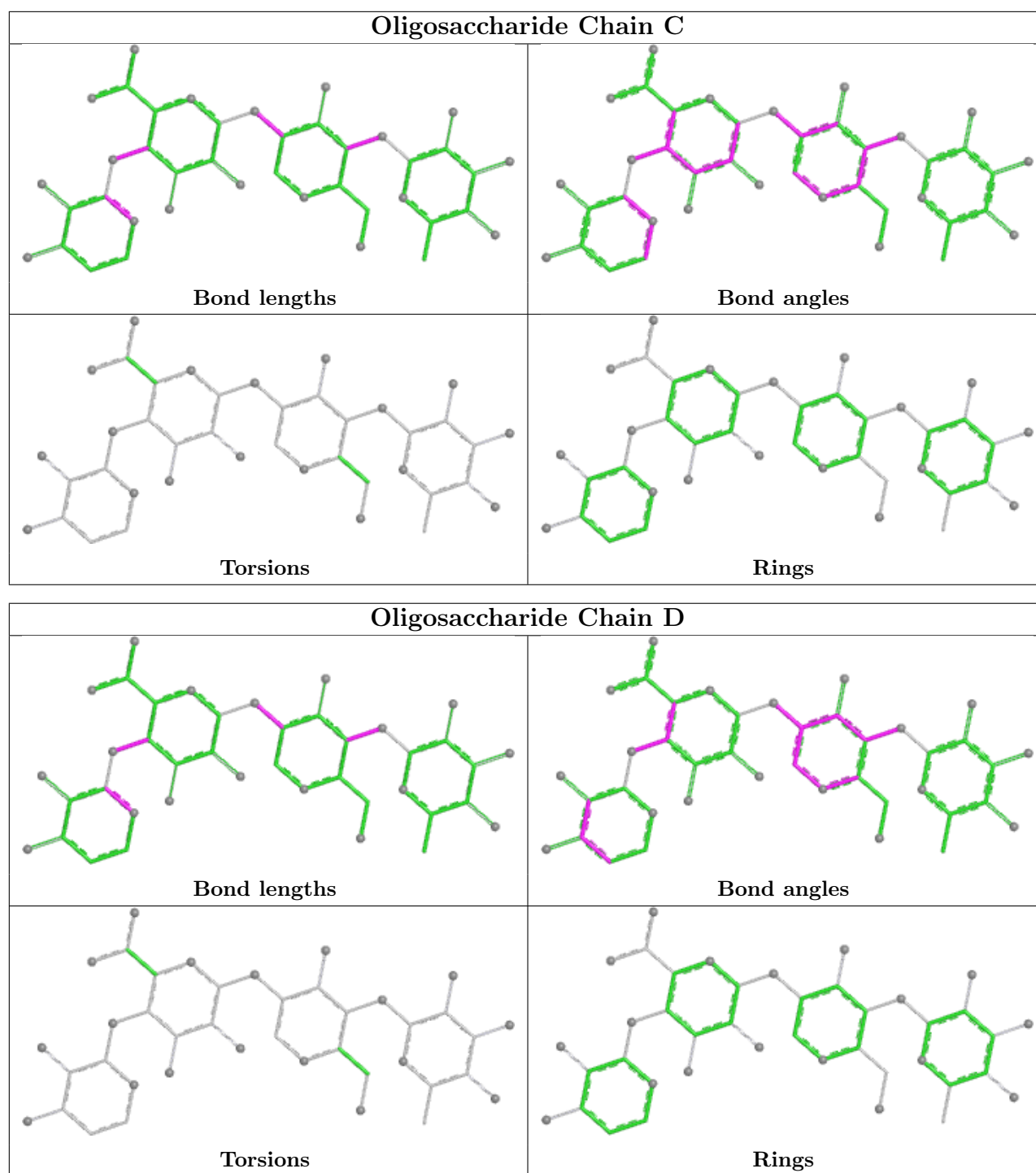
Mol	Chain	Res	Type	Atom
2	D	3	XYS	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
5	FMT	A	943	-	2,2,2	5.75	2 (100%)	1,1,1	3.11	1 (100%)
4	PO4	A	944	-	4,4,4	1.01	0	6,6,6	0.49	0
5	FMT	B	942	-	2,2,2	0.76	0	1,1,1	0.27	0
5	FMT	A	941	-	2,2,2	0.76	0	1,1,1	0.28	0
4	PO4	B	945	-	4,4,4	0.92	0	6,6,6	0.61	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	943	FMT	O2-C	5.90	1.58	1.28
5	A	943	FMT	O1-C	5.60	1.53	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	943	FMT	O2-C-O1	-3.11	93.29	126.59

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 [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	746/747 (99%)	1.07	103 (13%) 6 7	24, 29, 35, 46	0
1	B	746/747 (99%)	1.29	155 (20%) 2 3	24, 28, 36, 51	0
All	All	1492/1494 (99%)	1.18	258 (17%) 4 4	24, 29, 36, 51	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	GLY	8.6
1	B	515	GLY	5.9
1	B	471	SER	5.8
1	B	143	ALA	5.6
1	B	476	PHE	5.2
1	B	474	THR	5.1
1	B	491	ILE	4.9
1	B	472	ASP	4.9
1	B	489	GLY	4.7
1	B	504	PHE	4.3
1	B	735	GLY	4.2
1	B	477	ALA	4.1
1	B	462	THR	4.1
1	B	317	TYR	4.0
1	B	502	GLY	4.0
1	B	496	LEU	4.0
1	B	733	LEU	3.9
1	B	533	ALA	3.9
1	B	567	ALA	3.9
1	B	754	GLY	3.8
1	B	473	HIS	3.8
1	A	92	VAL	3.8
1	B	499	MET	3.8
1	B	755	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	493	PRO	3.7
1	B	573	LYS	3.7
1	B	722	LYS	3.6
1	B	707	THR	3.6
1	B	142	PRO	3.6
1	B	144	GLY	3.6
1	B	690	ASP	3.5
1	B	518	ASN	3.5
1	A	386	GLY	3.5
1	B	490	TRP	3.5
1	A	567	ALA	3.5
1	A	361	GLY	3.4
1	B	475	ASP	3.4
1	B	401	TYR	3.4
1	B	568	SER	3.4
1	A	308	VAL	3.4
1	A	524	THR	3.4
1	A	629	TRP	3.4
1	B	570	PRO	3.4
1	A	32	VAL	3.3
1	B	464	SER	3.3
1	B	680	LYS	3.3
1	B	714	PRO	3.3
1	B	94	ASP	3.3
1	B	571	ASP	3.2
1	B	485	LEU	3.1
1	B	361	GLY	3.1
1	B	494	ARG	3.1
1	B	752	ALA	3.1
1	B	468	TYR	3.1
1	A	470	GLY	3.1
1	B	572	PHE	3.1
1	B	92	VAL	3.1
1	A	132	ILE	3.1
1	B	569	ASN	3.0
1	B	555	VAL	3.0
1	B	757	GLY	3.0
1	B	736	THR	3.0
1	B	403	PHE	3.0
1	B	478	ALA	3.0
1	B	630	VAL	3.0
1	B	711	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	379	GLY	3.0
1	A	520	THR	3.0
1	B	313	LYS	3.0
1	B	772	ARG	2.9
1	A	674	ALA	2.9
1	A	555	VAL	2.9
1	A	476	PHE	2.9
1	A	365	PRO	2.9
1	B	74	TRP	2.9
1	A	46	LYS	2.9
1	B	492	ALA	2.9
1	B	506	THR	2.9
1	B	661	ALA	2.9
1	A	59	PRO	2.8
1	B	376	SER	2.8
1	B	710	THR	2.8
1	A	170	PRO	2.8
1	A	514	PHE	2.8
1	B	675	ASP	2.8
1	B	532	ALA	2.8
1	B	536	ALA	2.8
1	B	683	GLU	2.8
1	A	71	LYS	2.8
1	A	518	ASN	2.8
1	B	601	SER	2.8
1	B	511	ALA	2.8
1	B	635	TYR	2.8
1	B	500	LEU	2.8
1	B	509	ILE	2.8
1	B	629	TRP	2.8
1	B	708	SER	2.7
1	B	375	GLY	2.7
1	B	436	TYR	2.7
1	A	91	GLU	2.7
1	B	505	ARG	2.7
1	A	304	ALA	2.7
1	B	679	GLN	2.7
1	B	439	PRO	2.7
1	A	420	GLY	2.7
1	B	469	GLY	2.7
1	A	74	TRP	2.7
1	B	378	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	486	PRO	2.6
1	B	534	TYR	2.6
1	B	507	GLY	2.6
1	B	723	GLY	2.6
1	B	662	ALA	2.6
1	B	68	PRO	2.6
1	B	497	LYS	2.6
1	A	363	ARG	2.6
1	A	568	SER	2.6
1	B	444	PHE	2.6
1	B	487	GLY	2.6
1	A	303	LEU	2.6
1	A	119	LYS	2.5
1	A	369	PRO	2.5
1	A	459	PRO	2.5
1	A	89	ILE	2.5
1	B	364	LYS	2.5
1	B	713	ARG	2.5
1	B	88	ASP	2.5
1	B	730	THR	2.5
1	A	391	SER	2.5
1	B	613	ALA	2.5
1	B	541	VAL	2.5
1	B	617	ASN	2.5
1	B	614	ALA	2.5
1	A	488	LYS	2.5
1	A	114	ASN	2.5
1	A	387	TRP	2.5
1	A	139	THR	2.4
1	A	521	PRO	2.4
1	B	412	GLY	2.4
1	A	392	VAL	2.4
1	B	565	VAL	2.4
1	B	621	ILE	2.4
1	A	220	TYR	2.4
1	B	705	SER	2.4
1	A	224	PRO	2.4
1	A	312	ARG	2.4
1	A	431	GLY	2.4
1	B	388	GLY	2.4
1	A	56	GLN	2.4
1	B	600	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	566	VAL	2.4
1	A	256	SER	2.4
1	B	442	LYS	2.4
1	A	252	HIS	2.4
1	A	370	LEU	2.4
1	A	388	GLY	2.4
1	B	463	PHE	2.4
1	A	384	ARG	2.4
1	A	670	VAL	2.4
1	A	468	TYR	2.3
1	A	168	LEU	2.3
1	A	573	LYS	2.3
1	B	693	VAL	2.3
1	B	369	PRO	2.3
1	B	596	THR	2.3
1	A	143	ALA	2.3
1	A	268	ALA	2.3
1	A	417	TYR	2.3
1	B	411	ALA	2.3
1	A	144	GLY	2.3
1	A	260	VAL	2.3
1	B	538	VAL	2.3
1	B	677	THR	2.3
1	B	501	ALA	2.3
1	A	244	TRP	2.3
1	B	481	GLY	2.3
1	B	732	LEU	2.3
1	B	407	GLN	2.3
1	A	47	THR	2.3
1	A	367	ASP	2.3
1	B	689	GLY	2.3
1	A	457	TYR	2.3
1	A	464	SER	2.2
1	A	393	ILE	2.2
1	B	405	ASN	2.2
1	B	587	LYS	2.2
1	A	467	GLY	2.2
1	A	390	GLU	2.2
1	A	374	SER	2.2
1	B	725	PHE	2.2
1	A	389	PRO	2.2
1	A	722	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	377	PRO	2.2
1	B	508	LYS	2.2
1	B	516	PRO	2.2
1	B	734	PRO	2.2
1	B	366	ASP	2.2
1	B	138	ALA	2.2
1	B	400	GLU	2.2
1	B	758	ALA	2.2
1	A	115	TYR	2.2
1	B	374	SER	2.2
1	B	402	SER	2.2
1	A	382	ILE	2.2
1	A	572	PHE	2.2
1	B	59	PRO	2.2
1	B	367	ASP	2.2
1	B	530	ILE	2.2
1	B	39	VAL	2.2
1	B	406	HIS	2.2
1	A	248	SER	2.2
1	B	363	ARG	2.2
1	A	525	TYR	2.2
1	A	62	LYS	2.2
1	A	117	MET	2.2
1	A	472	ASP	2.2
1	B	767	THR	2.2
1	B	398	VAL	2.1
1	A	557	ALA	2.1
1	B	404	LEU	2.1
1	B	465	SER	2.1
1	B	460	LYS	2.1
1	A	336	TYR	2.1
1	A	118	THR	2.1
1	A	245	PHE	2.1
1	B	89	ILE	2.1
1	B	456	ILE	2.1
1	A	36	VAL	2.1
1	A	181	VAL	2.1
1	A	87	ALA	2.1
1	A	122	LYS	2.1
1	A	130	SER	2.1
1	A	88	ASP	2.1
1	B	503	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	257	TYR	2.1
1	A	462	THR	2.1
1	A	368	LEU	2.1
1	A	366	ASP	2.1
1	A	475	ASP	2.1
1	A	517	ASP	2.1
1	A	385	THR	2.1
1	B	467	GLY	2.1
1	A	39	VAL	2.1
1	B	32	VAL	2.1
1	A	29	ALA	2.1
1	A	291	ASP	2.0
1	B	145	ASP	2.0
1	A	316	LYS	2.0
1	A	491	ILE	2.0
1	A	126	GLU	2.0
1	A	127	ALA	2.0
1	A	133	ASP	2.0
1	B	712	ASP	2.0
1	B	62	LYS	2.0
1	B	448	THR	2.0
1	B	459	PRO	2.0
1	B	748	PRO	2.0
1	A	290	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	A	26	8/9	0.91	0.10	31,31,31,32	0
1	PCA	B	26	8/9	0.92	0.10	30,31,31,31	0

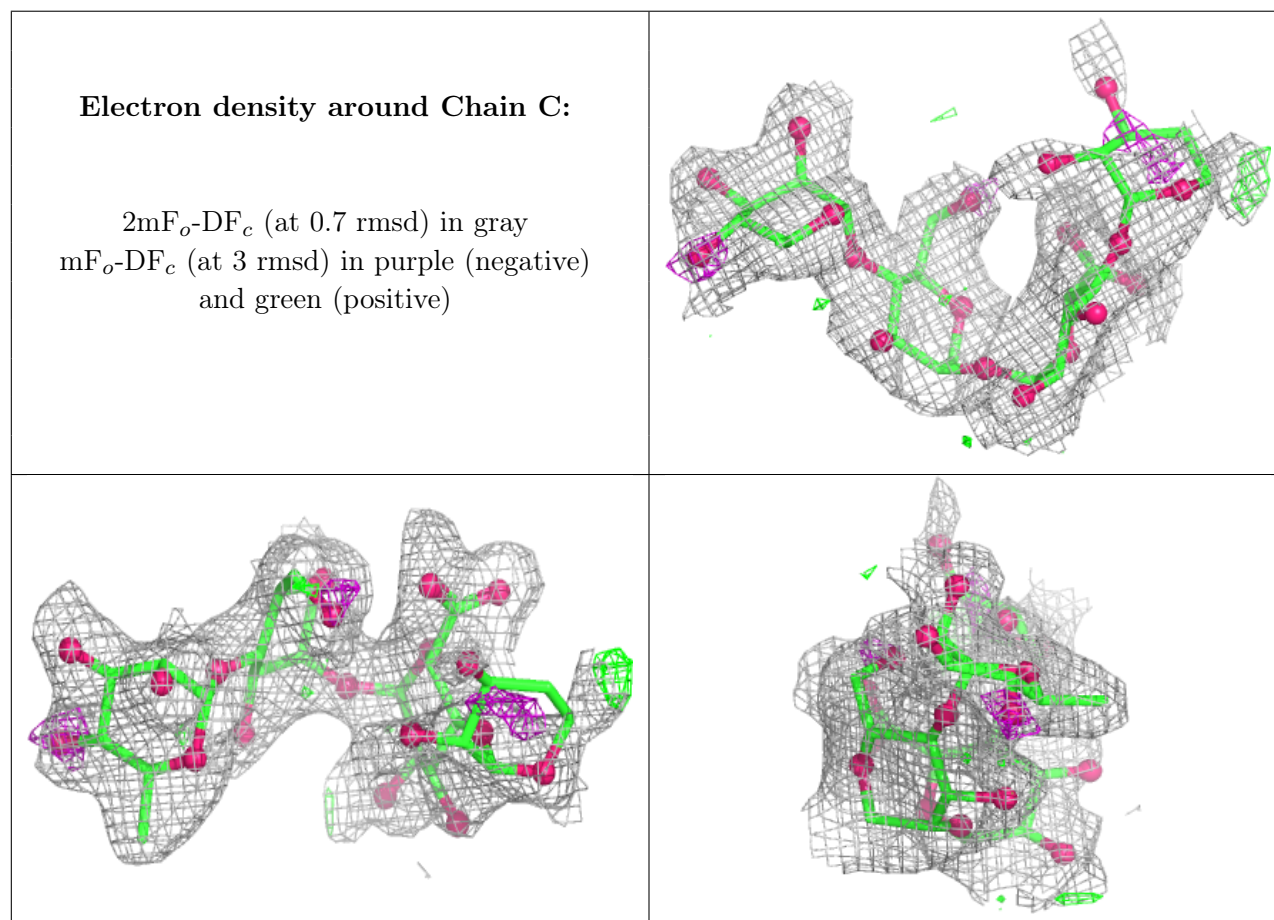
6.3 Carbohydrates [i](#)

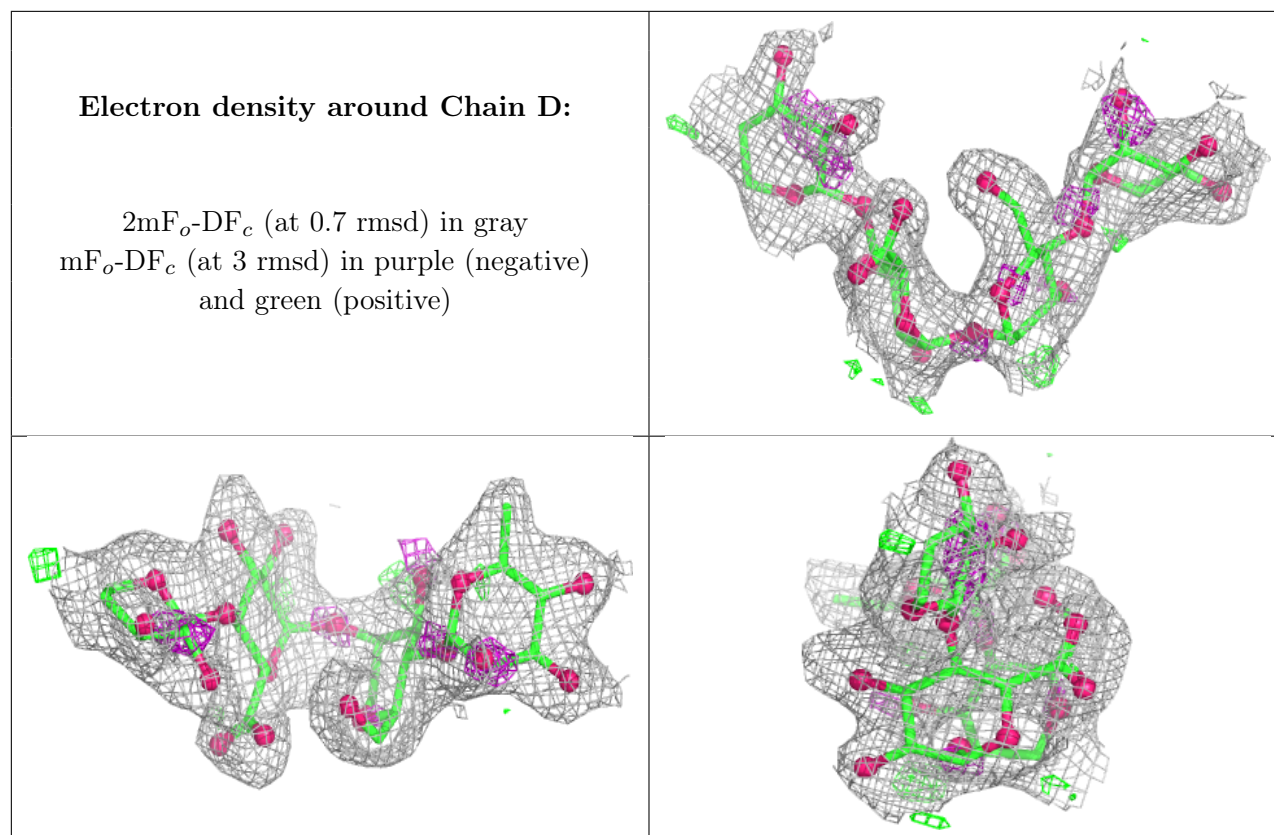
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XYS	C	3	8/10	0.40	0.19	68,69,69,69	0
2	XYS	D	3	8/10	0.45	0.20	56,57,57,58	0
2	GCU	C	2	12/13	0.66	0.14	56,58,60,65	0
2	RAM	D	4	10/11	0.82	0.13	34,36,37,37	0
2	MAN	C	1	11/12	0.84	0.12	36,38,41,52	0
2	RAM	C	4	10/11	0.84	0.12	37,39,39,40	0
2	MAN	D	1	11/12	0.86	0.11	32,34,37,43	0
2	GCU	D	2	12/13	0.86	0.10	45,46,48,53	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](#)

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($\text{\AA}^2$)	Q<0.9
5	FMT	A	943	3/3	0.42	0.32	118,118,118,118	0
4	PO4	B	945	5/5	0.86	0.18	51,51,51,52	0
4	PO4	A	944	5/5	0.92	0.17	39,40,41,41	0
5	FMT	B	942	3/3	0.93	0.10	28,28,28,28	0
5	FMT	A	941	3/3	0.96	0.13	26,26,26,26	0
3	ZN	B	2	1/1	0.99	0.11	29,29,29,29	0
3	ZN	A	1	1/1	1.00	0.10	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.