



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:02 PM UTC

PDB ID : 1H4H / pdb_00001h4h
Title : Oligosaccharide-binding to family 11 xylanases: both covalent intermediate and mutant-product complexes display 2,5B conformations at the active-centre
Authors : Sabini, E.; Wilson, K.S.; Danielsen, S.; Schulein, M.; Davies, G.J.
Deposited on : 2001-05-11
Resolution : 1.90 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

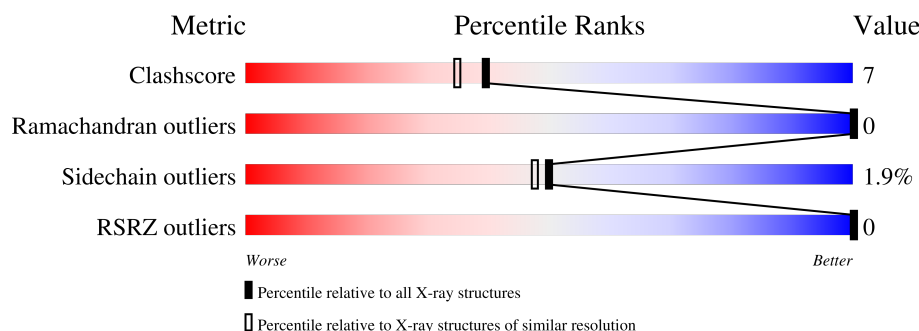
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	209	 67% 29% . .
1	B	209	 67% 30% .
1	C	209	 71% 26% . .
1	D	209	 67% 29% .
2	E	3	 67% 33%
2	F	3	 100%

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Mol	Chain	Length	Quality of chain
2	G	3	 100%
2	H	3	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7172 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.

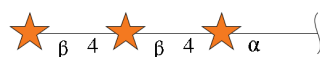
- Molecule 1 is a protein called XYLANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	2	0
			1640	1032	289	313	6			
1	B	209	Total	C	N	O	S	0	1	0
			1652	1040	290	316	6			
1	C	207	Total	C	N	O	S	0	1	0
			1636	1030	288	312	6			
1	D	208	Total	C	N	O	S	0	1	0
			1643	1034	289	314	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLU	modified residue	PDB 1H4H
B	1	PCA	GLU	modified residue	PDB 1H4H
C	1	PCA	GLU	modified residue	PDB 1H4H
D	1	PCA	GLU	modified residue	PDB 1H4H
A	94	ALA	GLU	engineered mutation	PDB 1H4H
B	94	ALA	GLU	engineered mutation	PDB 1H4H
C	94	ALA	GLU	engineered mutation	PDB 1H4H
D	94	ALA	GLU	engineered mutation	PDB 1H4H

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			28	15	13			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	3	Total	C	O	0	0	0
			28	15	13			
2	G	3	Total	C	O	0	0	0
			28	15	13			
2	H	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 3 is water.

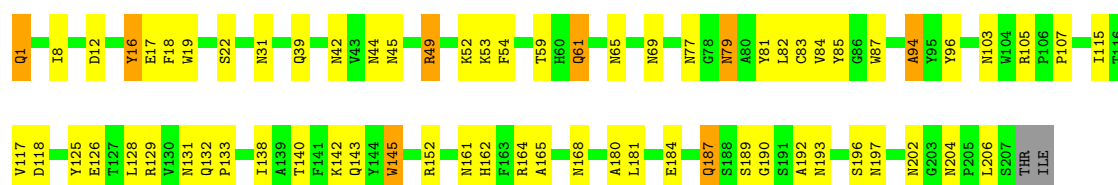
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	142	Total	O	0	0
			142	142		
3	C	106	Total	O	0	0
			106	106		
3	D	110	Total	O	0	0
			110	110		

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.

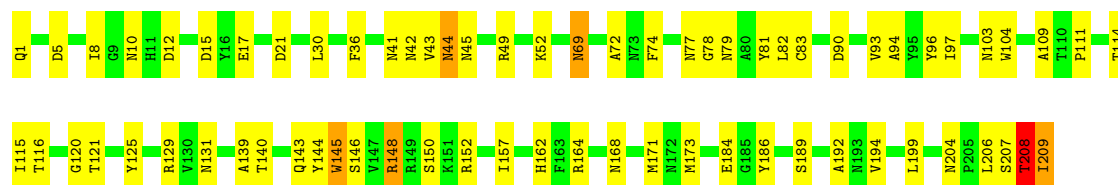
• Molecule 1: XYLANASE

Chain A: 



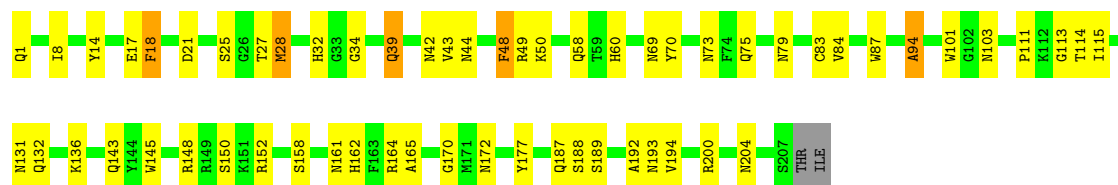
• Molecule 1: XYLANASE

Chain B: 



• Molecule 1: XYLANASE

Chain C: 



• Molecule 1: XYLANASE

Chain D: 





- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.34Å 78.89Å 76.27Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	77.5 (20.00-1.90) 77.2 (20.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.241 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.179 for h,-k,-l 0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7172	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, XYS, XYP

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	1.24	3/1687 (0.2%)	2.08	64/2294 (2.8%)
1	B	1.46	7/1694 (0.4%)	2.14	66/2303 (2.9%)
1	C	1.21	5/1678 (0.3%)	2.09	55/2282 (2.4%)
1	D	1.18	5/1685 (0.3%)	2.05	55/2292 (2.4%)
All	All	1.28	20/6744 (0.3%)	2.09	240/9171 (2.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	2
All	All	0	5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148[A]	ARG	NE-CZ	21.71	1.56	1.33
1	B	148[B]	ARG	NE-CZ	21.71	1.56	1.33
1	A	87	TRP	NE1-CE2	10.45	1.49	1.37
1	D	87	TRP	NE1-CE2	10.41	1.49	1.37
1	C	87	TRP	NE1-CE2	10.39	1.48	1.37
1	B	145	TRP	NE1-CE2	10.36	1.48	1.37
1	A	145	TRP	NE1-CE2	10.33	1.48	1.37
1	B	43	VAL	C-N	-8.70	1.20	1.33
1	C	145	TRP	NE1-CE2	8.05	1.46	1.37
1	D	1	PCA	C-N	7.12	1.43	1.33
1	C	113	GLY	N-CA	6.51	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	C-N	6.10	1.41	1.33
1	D	102	GLY	C-O	5.76	1.31	1.23
1	B	17	GLU	C-N	-5.75	1.25	1.33
1	D	185	GLY	CA-C	5.74	1.56	1.52
1	D	158	SER	CA-CB	5.70	1.60	1.52
1	B	1	PCA	C-N	5.70	1.41	1.33
1	B	116	THR	C-N	-5.52	1.28	1.33
1	C	60	HIS	ND1-CE1	5.42	1.38	1.32
1	A	1	PCA	C-N	5.40	1.41	1.33

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASN	OD1-CG-ND2	13.52	136.12	122.60
1	B	69	ASN	O-C-N	-12.91	108.50	123.22
1	B	49	ARG	CG-CD-NE	12.56	139.64	112.00
1	A	69	ASN	O-C-N	-11.63	109.75	123.13
1	D	1	PCA	O-C-N	-11.54	104.54	123.00
1	D	69	ASN	O-C-N	-11.23	110.02	123.27
1	C	79	ASN	CA-CB-CG	-11.17	101.43	112.60
1	B	208	THR	CA-C-N	10.86	141.25	121.70
1	B	208	THR	C-N-CA	10.86	141.25	121.70
1	B	8	ILE	CA-C-O	-10.20	109.97	120.27
1	A	131	ASN	CA-CB-CG	-10.16	102.44	112.60
1	A	79	ASN	OD1-CG-ND2	10.12	132.72	122.60
1	C	18	PHE	O-C-N	-9.97	112.01	123.27
1	A	18	PHE	CA-CB-CG	9.96	123.75	113.80
1	B	45	ASN	CA-CB-CG	9.84	122.44	112.60
1	B	148[A]	ARG	NE-CZ-NH2	-9.77	110.41	119.20
1	B	148[B]	ARG	NE-CZ-NH2	-9.77	110.41	119.20
1	D	18	PHE	O-C-N	-9.54	112.01	123.27
1	A	79	ASN	CA-CB-CG	9.33	121.93	112.60
1	B	49	ARG	CD-NE-CZ	9.22	137.31	124.40
1	A	1	PCA	O-C-N	-9.10	108.44	123.00
1	D	48	PHE	CA-CB-CG	9.04	122.84	113.80
1	A	84	VAL	N-CA-CB	8.69	123.07	111.25
1	C	69	ASN	N-CA-CB	-8.58	96.44	110.42
1	C	1	PCA	O-C-N	-8.54	109.34	123.00
1	B	74	PHE	CA-CB-CG	8.49	122.29	113.80
1	C	73	ASN	OD1-CG-ND2	-8.49	114.11	122.60
1	A	197	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	B	77	ASN	CA-CB-CG	-8.17	104.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148[A]	ARG	NE-CZ-NH1	8.07	129.57	121.50
1	B	148[B]	ARG	NE-CZ-NH1	8.07	129.57	121.50
1	B	131	ASN	CA-CB-CG	-8.06	104.54	112.60
1	A	184	GLU	CA-C-N	-7.89	115.14	122.80
1	A	184	GLU	C-N-CA	-7.89	115.14	122.80
1	A	94	ALA	CA-C-O	-7.74	112.21	120.80
1	C	32	HIS	CA-CB-CG	-7.71	106.09	113.80
1	A	1	PCA	CA-C-N	7.67	135.50	121.70
1	A	1	PCA	C-N-CA	7.67	135.50	121.70
1	A	31	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	D	2	ILE	CA-CB-CG1	-7.64	97.41	110.40
1	C	101	TRP	CG-CD2-CE3	-7.60	126.30	133.90
1	D	31	ASN	CA-CB-CG	-7.59	105.01	112.60
1	B	162	HIS	CA-CB-CG	-7.51	106.29	113.80
1	D	44	ASN	CA-CB-CG	-7.41	105.19	112.60
1	C	170	GLY	CA-C-O	-7.26	110.93	119.06
1	C	103	ASN	OD1-CG-ND2	7.26	129.86	122.60
1	C	83	CYS	CA-C-O	7.21	129.00	121.36
1	D	75	GLN	CA-C-N	7.13	127.11	119.76
1	D	75	GLN	C-N-CA	7.13	127.11	119.76
1	B	10	ASN	CA-C-N	7.05	132.94	123.00
1	B	10	ASN	C-N-CA	7.05	132.94	123.00
1	B	121	THR	O-C-N	7.02	131.52	123.31
1	C	39	GLN	N-CA-CB	-6.99	98.63	111.13
1	A	184	GLU	CA-C-O	-6.98	112.82	120.36
1	B	131	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	C	114	THR	CA-C-N	-6.92	113.33	122.94
1	C	114	THR	C-N-CA	-6.92	113.33	122.94
1	C	162	HIS	CA-C-O	-6.90	113.10	120.42
1	C	131	ASN	OD1-CG-ND2	-6.89	115.71	122.60
1	A	42	ASN	CA-CB-CG	-6.88	105.72	112.60
1	C	69	ASN	CA-C-O	-6.84	113.04	120.36
1	D	105	ARG	CA-C-N	6.84	127.42	120.38
1	D	105	ARG	C-N-CA	6.84	127.42	120.38
1	B	173	MET	CA-C-O	-6.81	113.46	121.16
1	D	79	ASN	OD1-CG-ND2	6.78	129.38	122.60
1	C	60	HIS	CA-CB-CG	6.78	120.58	113.80
1	C	161	ASN	CA-C-O	-6.77	113.37	120.55
1	B	83	CYS	CA-C-N	-6.73	114.45	122.93
1	B	83	CYS	C-N-CA	-6.73	114.45	122.93
1	D	68	ILE	CA-C-O	6.67	127.40	120.39
1	B	77	ASN	CA-C-N	6.67	131.09	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASN	C-N-CA	6.67	131.09	120.55
1	B	90	ASP	CB-CA-C	-6.65	97.07	110.17
1	C	8	ILE	CA-C-O	-6.62	113.21	120.43
1	D	168	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	B	5	ASP	N-CA-CB	6.56	121.93	111.56
1	D	36	PHE	CA-C-O	-6.55	113.90	121.10
1	A	12	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	58	GLN	CA-C-O	-6.53	113.79	120.71
1	B	10	ASN	CA-C-O	-6.52	113.32	120.30
1	C	132	GLN	CG-CD-NE2	6.51	126.17	116.40
1	C	25	SER	N-CA-CB	-6.47	100.85	111.66
1	D	5	ASP	O-C-N	-6.45	115.68	123.10
1	B	114	THR	O-C-N	6.40	130.91	123.17
1	B	121	THR	CA-CB-OG1	-6.40	100.00	109.60
1	D	60	HIS	CA-CB-CG	6.39	120.19	113.80
1	A	206	LEU	N-CA-C	6.37	118.52	110.24
1	D	103	ASN	N-CA-C	6.30	120.97	113.28
1	D	163	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	85	TYR	CA-C-N	-6.29	111.64	120.56
1	A	85	TYR	C-N-CA	-6.29	111.64	120.56
1	A	164	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	A	44	ASN	CA-CB-CG	-6.25	106.35	112.60
1	D	84	VAL	N-CA-C	-6.25	99.42	108.17
1	D	171	MET	CA-C-O	6.25	127.74	120.49
1	D	125	TYR	CA-C-O	-6.24	114.35	121.40
1	A	84	VAL	N-CA-C	-6.24	99.44	108.17
1	B	114	THR	CA-C-N	-6.23	113.71	122.75
1	B	114	THR	C-N-CA	-6.23	113.71	122.75
1	B	139	ALA	O-C-N	6.23	129.52	123.29
1	C	188	SER	CA-C-N	6.19	132.31	122.59
1	C	188	SER	C-N-CA	6.19	132.31	122.59
1	D	113	GLY	O-C-N	-6.16	118.00	123.92
1	C	42	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	C	101	TRP	CE2-CD2-CE3	6.16	124.95	118.80
1	B	1	PCA	O-C-N	-6.14	113.17	123.00
1	C	84	VAL	N-CA-C	-6.12	99.60	108.17
1	C	161	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	D	204	ASN	CB-CA-C	-6.08	102.91	109.85
1	C	94	ALA	CA-C-N	-6.08	113.04	122.59
1	C	94	ALA	C-N-CA	-6.08	113.04	122.59
1	B	1	PCA	CA-C-N	6.08	132.64	121.70
1	B	1	PCA	C-N-CA	6.08	132.64	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ASN	CA-CB-CG	-6.08	106.52	112.60
1	C	172	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	A	164	ARG	NE-CZ-NH1	-6.02	115.48	121.50
1	B	90	ASP	O-C-N	6.02	128.24	121.32
1	C	172	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	109	ALA	CA-C-O	-5.98	113.50	121.46
1	B	8	ILE	O-C-N	5.92	129.33	123.18
1	A	65	ASN	CA-C-O	-5.90	113.91	120.70
1	C	204	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	45	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	D	45	ASN	CB-CG-ND2	5.86	125.19	116.40
1	D	65	ASN	CA-C-N	-5.84	114.18	122.94
1	D	65	ASN	C-N-CA	-5.84	114.18	122.94
1	C	75	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	22	SER	CA-C-O	-5.81	114.79	121.47
1	C	27	THR	O-C-N	-5.77	116.56	123.31
1	B	90	ASP	CA-C-O	-5.77	112.26	120.16
1	C	158	SER	CA-C-O	5.74	129.35	122.41
1	D	72	ALA	CA-C-N	-5.73	115.40	122.84
1	D	72	ALA	C-N-CA	-5.73	115.40	122.84
1	A	61	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	B	15	ASP	CA-CB-CG	-5.71	106.89	112.60
1	D	95	TYR	CA-C-N	5.69	130.81	122.39
1	D	95	TYR	C-N-CA	5.69	130.81	122.39
1	D	1	PCA	CA-C-N	5.67	131.92	121.70
1	D	1	PCA	C-N-CA	5.67	131.92	121.70
1	C	189	SER	CA-C-N	-5.66	113.10	120.91
1	C	189	SER	C-N-CA	-5.66	113.10	120.91
1	A	180	ALA	N-CA-C	5.64	117.69	108.55
1	B	184	GLU	CA-C-N	-5.63	118.30	122.18
1	B	184	GLU	C-N-CA	-5.63	118.30	122.18
1	A	187	GLN	CA-C-O	-5.61	115.09	121.65
1	A	184	GLU	O-C-N	5.60	129.97	123.30
1	C	94	ALA	CA-C-O	-5.57	114.61	120.80
1	A	202	ASN	CA-C-O	-5.57	114.65	121.28
1	B	77	ASN	CB-CG-ND2	-5.55	108.07	116.40
1	D	171	MET	O-C-N	-5.55	116.19	123.02
1	D	148[A]	ARG	O-C-N	-5.54	116.06	122.87
1	D	148[B]	ARG	O-C-N	-5.54	116.06	122.87
1	B	10	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	B	111	PRO	CA-C-O	-5.53	115.03	121.34
1	C	158	SER	O-C-N	-5.52	115.10	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	LEU	O-C-N	-5.51	116.49	123.05
1	C	200	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	A	161	ASN	N-CA-CB	5.51	118.31	110.16
1	A	190	GLY	CA-C-O	-5.47	116.06	121.48
1	C	136	LYS	CA-C-O	-5.47	113.93	120.55
1	B	82	LEU	CA-C-O	-5.47	114.61	120.46
1	D	149	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	D	10	ASN	O-C-N	-5.46	116.80	123.30
1	B	204	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	138	ILE	CA-C-O	-5.45	114.36	120.95
1	D	44	ASN	N-CA-C	-5.44	103.23	111.56
1	D	96	TYR	O-C-N	-5.43	116.32	123.28
1	B	204	ASN	N-CA-C	5.43	117.29	109.04
1	C	111	PRO	N-CA-CB	5.42	108.14	103.31
1	B	36	PHE	CA-C-O	-5.40	115.16	121.10
1	D	102	GLY	N-CA-C	-5.37	100.46	113.18
1	D	103	ASN	CA-CB-CG	5.37	117.97	112.60
1	D	80	ALA	CB-CA-C	-5.34	100.84	110.03
1	C	48	PHE	CA-C-N	-5.34	111.06	121.91
1	C	48	PHE	C-N-CA	-5.34	111.06	121.91
1	B	42	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	B	78	GLY	O-C-N	-5.34	119.37	123.80
1	B	15	ASP	CA-C-O	-5.33	114.58	120.60
1	D	26	GLY	CA-C-O	5.33	126.04	121.19
1	A	81	TYR	CA-C-O	-5.33	114.53	120.66
1	A	192	ALA	O-C-N	5.32	129.48	123.42
1	A	79	ASN	CB-CG-OD1	-5.32	110.16	120.80
1	A	39	GLN	CG-CD-OE1	5.31	131.41	120.80
1	D	152	ARG	N-CA-CB	5.31	120.53	111.66
1	A	103	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	D	194	VAL	CA-C-O	-5.29	116.09	121.70
1	A	45	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	192	ALA	CA-C-N	-5.28	115.36	123.07
1	A	192	ALA	C-N-CA	-5.28	115.36	123.07
1	D	161	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	8	ILE	CA-C-O	-5.28	114.77	120.36
1	C	49	ARG	CD-NE-CZ	-5.28	117.02	124.40
1	A	16	TYR	CA-C-N	-5.27	112.72	121.89
1	A	16	TYR	C-N-CA	-5.27	112.72	121.89
1	C	152	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	189	SER	O-C-N	-5.26	115.42	122.94
1	B	44	ASN	CA-CB-CG	-5.24	107.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	SER	N-CA-CB	-5.24	102.02	110.71
1	A	83	CYS	N-CA-C	5.24	115.96	108.74
1	D	76	PRO	N-CA-CB	5.22	107.96	103.31
1	D	76	PRO	O-C-N	-5.21	116.73	123.03
1	A	187	GLN	O-C-N	5.20	128.82	122.58
1	B	189	SER	O-C-N	-5.20	116.14	123.11
1	A	42	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	C	70	TYR	N-CA-C	5.20	116.19	108.86
1	D	106	PRO	N-CA-CB	5.19	108.12	103.08
1	B	146	SER	CA-C-N	-5.19	115.61	122.98
1	B	146	SER	C-N-CA	-5.19	115.61	122.98
1	B	207	SER	CA-CB-OG	-5.19	100.73	111.10
1	C	17	GLU	CA-C-N	5.18	129.86	122.72
1	C	17	GLU	C-N-CA	5.18	129.86	122.72
1	D	79	ASN	CB-CG-OD1	-5.18	110.45	120.80
1	D	184	GLU	CA-CB-CG	-5.17	103.75	114.10
1	C	164	ARG	CD-NE-CZ	5.17	131.64	124.40
1	B	41	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	39	GLN	CG-CD-NE2	-5.16	108.66	116.40
1	C	177	TYR	N-CA-C	-5.14	107.56	113.88
1	A	54	PHE	CA-C-N	-5.12	114.94	122.83
1	A	54	PHE	C-N-CA	-5.12	114.94	122.83
1	B	30	LEU	CA-C-O	-5.12	114.82	120.60
1	D	49	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	A	19	TRP	CA-C-O	-5.11	114.00	120.28
1	A	49	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	A	152	ARG	N-CA-CB	5.09	120.99	111.52
1	B	96	TYR	CB-CG-CD2	-5.09	113.17	120.80
1	B	164	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	A	165	ALA	CA-C-O	-5.09	115.48	120.82
1	D	8	ILE	CA-C-O	-5.08	114.97	120.36
1	B	96	TYR	CB-CG-CD1	5.06	128.39	120.80
1	D	118	ASP	CB-CG-OD1	5.06	130.04	118.40
1	A	140	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	17	GLU	CA-C-O	-5.05	113.40	120.21
1	C	113	GLY	O-C-N	-5.04	119.08	123.92
1	B	93	VAL	CA-C-O	-5.04	115.21	120.76
1	A	162	HIS	CA-CB-CG	-5.04	108.76	113.80
1	B	152	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	C	73	ASN	N-CA-C	-5.02	100.32	108.41
1	A	197	ASN	CB-CG-ND2	5.02	123.93	116.40
1	C	84	VAL	N-CA-CB	5.01	118.06	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	TYR	CB-CG-CD2	-5.00	113.29	120.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PCA	Mainchain
1	B	208	THR	Peptide
1	B	97	ILE	Mainchain
1	D	1	PCA	Mainchain
1	D	120	GLY	Mainchain

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	1640	0	1552	20	0
1	B	1652	0	1566	32	0
1	C	1636	0	1548	18	0
1	D	1643	0	1555	18	0
2	E	28	0	9	2	0
2	F	28	0	9	0	0
2	G	28	0	9	0	0
2	H	28	0	9	0	0
3	A	131	0	0	5	0
3	B	142	0	0	8	0
3	C	106	0	0	8	0
3	D	110	0	0	6	0
All	All	7172	0	6257	87	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 7.

All (87) 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:148[A]:ARG:CZ	1:B:148[A]:ARG:NE	1.72	1.52
1:B:12:ASP:OD1	1:B:209:ILE:HA	1.72	0.89
1:A:181:LEU:HD21	3:A:2052:HOH:O	1.79	0.83
1:B:148[A]:ARG:HD3	1:B:150:SER:O	1.79	0.81
1:B:208:THR:HG22	1:B:209:ILE:HB	1.64	0.80
1:A:126:GLU:OE2	1:A:142:LYS:HE2	1.83	0.79
1:C:39:GLN:OE1	3:C:2028:HOH:O	2.03	0.76
1:A:143[B]:GLN:OE1	3:A:2091:HOH:O	2.04	0.75
1:C:148[A]:ARG:HD3	1:C:150:SER:O	1.87	0.74
1:B:12:ASP:OD1	1:B:208:THR:HG23	1.87	0.74
1:B:206:LEU:HD22	3:B:2044:HOH:O	1.91	0.70
1:B:199:LEU:O	1:B:206:LEU:HD12	1.92	0.70
1:C:194:VAL:HG13	3:C:2043:HOH:O	1.92	0.69
1:B:72:ALA:HB1	3:B:2060:HOH:O	1.91	0.69
1:B:194:VAL:HG13	3:B:2128:HOH:O	1.92	0.68
1:B:157:ILE:HD11	3:B:2072:HOH:O	1.93	0.67
1:B:208:THR:CG2	1:B:209:ILE:HD12	2.28	0.63
1:A:52:LYS:HD2	1:A:53:LYS:O	2.01	0.60
1:B:199:LEU:HB3	1:B:206:LEU:HD13	1.84	0.60
1:C:28:MET:HB2	1:C:48:PHE:CD2	2.38	0.59
1:C:192:ALA:CB	3:C:2097:HOH:O	2.51	0.58
1:D:148[A]:ARG:HD3	1:D:150:SER:O	2.03	0.58
1:B:192:ALA:HB1	3:B:2060:HOH:O	2.05	0.57
1:D:12:ASP:O	1:D:208:THR:HG22	2.05	0.56
1:B:208:THR:HG22	1:B:209:ILE:CB	2.34	0.56
1:C:28:MET:HB2	1:C:48:PHE:HD2	1.71	0.56
1:D:70:TYR:HD2	3:D:2043:HOH:O	1.88	0.56
1:D:157:ILE:HD11	3:D:2054:HOH:O	2.05	0.55
1:D:118:ASP:OD2	3:D:2064:HOH:O	2.18	0.54
1:B:81:TYR:OH	3:B:2065:HOH:O	1.84	0.54
1:D:34:GLY:HA2	1:D:50:LYS:HD3	1.89	0.54
1:B:209:ILE:HG22	3:B:2139:HOH:O	2.07	0.54
1:C:165:ALA:HB3	3:C:2079:HOH:O	2.08	0.53
1:A:49:ARG:HD3	3:A:2043:HOH:O	2.09	0.53
1:A:187:GLN:NE2	3:A:2114:HOH:O	2.41	0.52
1:B:12:ASP:OD1	1:B:209:ILE:CA	2.52	0.52
1:A:128:LEU:HD13	1:A:142:LYS:HD3	1.92	0.51
1:A:187:GLN:HG2	1:B:104:TRP:CE2	2.44	0.51
1:A:187:GLN:NE2	1:B:79:ASN:OD1	2.44	0.51
1:B:208:THR:CG2	1:B:209:ILE:N	2.74	0.50
1:C:115:ILE:HD12	1:C:165:ALA:HB2	1.93	0.50
1:D:132:GLN:HB3	1:D:133:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:O	1:C:187:GLN:HA	2.12	0.49
1:D:157:ILE:CD1	3:D:2054:HOH:O	2.60	0.49
1:A:125:TYR:HB2	1:A:145:TRP:HB2	1.95	0.49
1:B:209:ILE:HG23	1:B:209:ILE:O	2.12	0.49
1:B:79:ASN:HB3	1:B:186:TYR:O	2.13	0.48
1:D:201:ILE:O	1:D:202:ASN:HB2	2.12	0.48
1:C:21:ASP:OD1	1:C:44:ASN:HB3	2.14	0.48
1:A:193:ASN:ND2	3:A:2120:HOH:O	2.46	0.48
1:D:85:TYR:HD2	3:D:2033:HOH:O	1.96	0.48
1:C:194:VAL:HG23	3:C:2097:HOH:O	2.12	0.47
1:B:208:THR:CG2	1:B:209:ILE:CD1	2.92	0.47
1:C:192:ALA:HB3	3:C:2097:HOH:O	2.12	0.47
1:C:18:PHE:C	1:C:18:PHE:CD1	2.91	0.47
1:D:115:ILE:HD12	1:D:165:ALA:HB2	1.96	0.47
1:A:204:ASN:ND2	1:A:204:ASN:N	2.63	0.46
1:C:14:TYR:HB3	1:C:50:LYS:HG2	1.97	0.46
1:D:18:PHE:C	1:D:18:PHE:CD1	2.93	0.46
1:C:94:ALA:O	1:C:143:GLN:HA	2.16	0.46
1:B:94:ALA:O	1:B:143:GLN:HA	2.16	0.45
1:A:132:GLN:HB3	1:A:133:PRO:CD	2.48	0.44
1:A:117:VAL:HG22	1:A:118:ASP:N	2.32	0.44
1:B:120:GLY:HA3	1:B:148[A]:ARG:CZ	2.47	0.44
1:C:193:ASN:ND2	3:C:2098:HOH:O	2.50	0.44
1:A:105:ARG:HH11	1:A:105:ARG:HD3	1.61	0.43
1:A:132:GLN:HB3	1:A:133:PRO:HD2	2.00	0.43
1:B:52:LYS:HD3	1:B:206:LEU:HD21	2.00	0.42
1:B:144:TYR:CZ	1:B:171:MET:HB3	2.53	0.42
1:D:49:ARG:HH11	1:D:49:ARG:HD3	1.73	0.42
1:C:39:GLN:HG3	3:C:2096:HOH:O	2.19	0.42
1:A:129:ARG:HH21	2:E:1:XYS:H2	1.84	0.42
1:D:79:ASN:ND2	3:D:2049:HOH:O	2.51	0.42
1:B:21:ASP:OD1	1:B:44:ASN:HB2	2.19	0.42
1:A:16:TYR:CD1	1:A:16:TYR:C	2.97	0.42
2:E:1:XYS:H2	2:E:1:XYS:H51	1.56	0.42
1:B:79:ASN:ND2	3:B:2065:HOH:O	2.49	0.41
1:D:52:LYS:HD3	1:D:206:LEU:HD21	2.01	0.41
1:A:59:THR:HB	1:A:61:GLN:OE1	2.20	0.41
1:D:94:ALA:O	1:D:143:GLN:HA	2.21	0.41
1:D:28:MET:HE2	1:D:30:LEU:CD2	2.51	0.41
1:B:129:ARG:O	1:B:140:THR:HA	2.20	0.41
1:C:34:GLY:HA2	1:C:50:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TYR:HB2	1:B:145:TRP:HB2	2.02	0.40
1:B:206:LEU:HD12	1:B:206:LEU:H	1.86	0.40
1:D:83:CYS:O	1:D:181:LEU:HD22	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	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
1	B	208/209 (100%)	199 (96%)	9 (4%)	0	100	100
1	C	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
1	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
All	All	828/836 (99%)	794 (96%)	34 (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	175/175 (100%)	170 (97%)	5 (3%)	37	31
1	B	176/175 (101%)	171 (97%)	5 (3%)	38	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	174/175 (99%)	173 (99%)	1 (1%)	78	81
1	D	175/175 (100%)	173 (99%)	2 (1%)	65	67
All	All	700/700 (100%)	687 (98%)	13 (2%)	50	47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	79	ASN
1	A	107	PRO
1	A	115	ILE
1	A	168	ASN
1	B	69	ASN
1	B	115	ILE
1	B	168	ASN
1	B	208	THR
1	B	209	ILE
1	C	28	MET
1	D	103	ASN
1	D	206	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	65	ASN
1	A	168	ASN
1	A	187	GLN
1	A	193	ASN
1	A	204	ASN
1	B	39	GLN
1	B	42	ASN
1	B	193	ASN
1	C	31	ASN
1	C	42	ASN
1	C	77	ASN
1	C	143	GLN
1	C	193	ASN
1	D	31	ASN
1	D	58	GLN

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Mol	Chain	Res	Type
1	D	77	ASN
1	D	79	ASN
1	D	103	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	A	1	1	7,8,9	1.48	2 (28%)	9,10,12	2.48	3 (33%)
1	PCA	C	1	1	7,8,9	2.03	2 (28%)	9,10,12	3.68	8 (88%)
1	PCA	B	1	1	7,8,9	1.31	2 (28%)	9,10,12	1.72	1 (11%)
1	PCA	D	1	1	7,8,9	1.59	2 (28%)	9,10,12	2.17	3 (33%)

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	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CG-CD	3.41	1.59	1.50
1	D	1	PCA	O-C	3.03	1.31	1.20
1	C	1	PCA	O-C	2.85	1.30	1.20
1	B	1	PCA	CG-CD	2.63	1.57	1.50
1	A	1	PCA	CG-CD	2.26	1.56	1.50
1	D	1	PCA	CG-CD	2.10	1.56	1.50
1	B	1	PCA	O-C	2.08	1.27	1.20
1	A	1	PCA	OE-CD	2.08	1.27	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	OE-CD-CG	-6.96	114.30	126.72
1	A	1	PCA	CB-CA-C	-5.60	104.97	112.66
1	C	1	PCA	CB-CA-C	-5.41	105.24	112.66
1	D	1	PCA	OE-CD-CG	-4.50	118.70	126.72
1	C	1	PCA	O-C-CA	3.96	134.94	124.77
1	B	1	PCA	CB-CA-C	-3.53	107.81	112.66
1	A	1	PCA	CB-CA-N	2.98	111.44	103.24
1	C	1	PCA	CB-CA-N	2.68	110.62	103.24
1	C	1	PCA	CB-CG-CD	-2.63	100.34	104.41
1	D	1	PCA	CB-CG-CD	-2.54	100.48	104.41
1	C	1	PCA	CA-N-CD	-2.27	105.80	113.58
1	A	1	PCA	CA-N-CD	-2.26	105.86	113.58
1	C	1	PCA	OE-CD-N	-2.24	120.10	124.96
1	D	1	PCA	CB-CA-C	-2.15	109.71	112.66
1	C	1	PCA	CG-CB-CA	-2.02	96.46	104.33

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

12 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	XYS	E	1	2	10,10,10	1.26	1 (10%)	14,14,14	3.24	9 (64%)
2	XYP	E	2	2	9,9,10	1.07	0	10,12,14	2.02	3 (30%)
2	XYP	E	3	2	9,9,10	1.21	1 (11%)	10,12,14	2.64	5 (50%)
2	XYS	F	1	2	10,10,10	1.17	1 (10%)	14,14,14	3.56	10 (71%)
2	XYP	F	2	2	9,9,10	1.46	2 (22%)	10,12,14	1.96	3 (30%)
2	XYP	F	3	2	9,9,10	1.48	1 (11%)	10,12,14	1.96	5 (50%)
2	XYS	G	1	2	10,10,10	1.35	1 (10%)	14,14,14	3.37	9 (64%)
2	XYP	G	2	2	9,9,10	1.04	0	10,12,14	1.97	3 (30%)
2	XYP	G	3	2	9,9,10	1.37	0	10,12,14	2.35	2 (20%)
2	XYS	H	1	2	10,10,10	1.23	1 (10%)	14,14,14	2.73	8 (57%)
2	XYP	H	2	2	9,9,10	1.09	0	10,12,14	1.92	3 (30%)
2	XYP	H	3	2	9,9,10	1.30	0	10,12,14	2.41	5 (50%)

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	XYS	E	1	2	-	-	1/1/1/1
2	XYP	E	2	2	-	-	0/1/1/1
2	XYP	E	3	2	-	-	0/1/1/1
2	XYS	F	1	2	-	-	1/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1
2	XYP	F	3	2	-	-	0/1/1/1
2	XYS	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	XYP	G	3	2	-	-	0/1/1/1
2	XYS	H	1	2	-	-	0/1/1/1
2	XYP	H	2	2	-	-	0/1/1/1
2	XYP	H	3	2	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	XYS	O4-C4	-2.56	1.38	1.43
2	H	1	XYS	O4-C4	-2.53	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	XYP	C5-C4	2.51	1.58	1.52
2	E	3	XYP	O5-C1	-2.29	1.38	1.43
2	E	1	XYS	C5-C4	2.17	1.57	1.52
2	F	1	XYS	C5-C4	2.15	1.57	1.52
2	F	2	XYP	O4-C4	-2.09	1.39	1.43
2	F	3	XYP	O5-C5	2.08	1.46	1.43

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	XYS	O3-C3-C2	-6.56	94.92	110.38
2	E	3	XYP	C5-O5-C1	6.22	121.45	111.42
2	G	1	XYS	O3-C3-C2	-6.09	96.01	110.38
2	G	1	XYS	O3-C3-C4	-5.72	98.39	110.05
2	F	1	XYS	C5-C4-C3	-5.37	101.83	109.64
2	E	1	XYS	O3-C3-C2	-5.26	97.97	110.38
2	G	3	XYP	O3-C3-C2	-5.23	99.39	110.05
2	H	1	XYS	O3-C3-C2	-5.12	98.30	110.38
2	F	1	XYS	C5-O5-C1	4.97	122.78	112.46
2	E	1	XYS	C5-C4-C3	-4.96	102.42	109.64
2	F	1	XYS	O5-C1-C2	-4.50	96.81	109.94
2	E	1	XYS	O3-C3-C4	-4.37	101.14	110.05
2	G	3	XYP	C5-O5-C1	4.35	118.44	111.42
2	H	1	XYS	O4-C4-C5	-4.23	99.54	109.22
2	F	1	XYS	O1-C1-O5	4.21	120.71	109.91
2	G	1	XYS	C1-C2-C3	4.06	118.64	110.36
2	E	1	XYS	O5-C1-C2	-3.87	98.64	109.94
2	E	1	XYS	O1-C1-O5	3.86	119.80	109.91
2	F	2	XYP	O3-C3-C4	-3.83	102.25	110.05
2	F	1	XYS	O4-C4-C3	3.80	118.03	110.15
2	G	1	XYS	C5-O5-C1	3.77	120.28	112.46
2	H	3	XYP	C4-C3-C2	-3.76	106.46	110.92
2	H	1	XYS	O4-C4-C3	3.57	117.54	110.15
2	H	3	XYP	O3-C3-C4	-3.54	102.82	110.05
2	G	1	XYS	O2-C2-C3	-3.53	102.05	110.38
2	E	1	XYS	C1-C2-C3	-3.51	103.19	110.36
2	H	3	XYP	O2-C2-C3	-3.47	102.96	110.15
2	E	3	XYP	C4-C3-C2	-3.40	106.88	110.92
2	G	1	XYS	C4-C3-C2	3.40	116.83	110.86
2	E	2	XYP	C4-C3-C2	-3.37	106.91	110.92
2	G	2	XYP	O2-C2-C3	-3.36	103.18	110.15
2	E	2	XYP	O2-C2-C3	-3.35	103.22	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	XYP	C5-C4-C3	-3.28	104.86	109.64
2	G	1	XYS	O4-C4-C3	3.26	116.91	110.15
2	G	1	XYS	O2-C2-C1	-3.25	101.74	109.25
2	F	3	XYP	C4-C3-C2	-3.24	107.07	110.92
2	E	2	XYP	C5-O5-C1	3.22	116.62	111.42
2	F	2	XYP	C4-C3-C2	-3.17	107.16	110.92
2	H	2	XYP	C4-C3-C2	-3.12	107.21	110.92
2	G	2	XYP	C4-C3-C2	-3.11	107.22	110.92
2	H	2	XYP	O2-C2-C3	-3.09	103.75	110.15
2	E	1	XYS	O4-C4-C3	3.08	116.53	110.15
2	E	1	XYS	O1-C1-C2	-3.05	100.14	108.98
2	H	3	XYP	O3-C3-C2	-3.04	103.86	110.05
2	H	1	XYS	O2-C2-C3	-3.00	103.31	110.38
2	F	1	XYS	C1-C2-C3	-2.98	104.28	110.36
2	H	2	XYP	O3-C3-C4	-2.94	104.05	110.05
2	H	1	XYS	O3-C3-C4	-2.88	104.17	110.05
2	H	1	XYS	O1-C1-C2	-2.77	100.95	108.98
2	H	1	XYS	C5-C4-C3	-2.61	105.84	109.64
2	F	2	XYP	C5-C4-C3	-2.56	105.91	109.64
2	E	1	XYS	C4-C3-C2	-2.55	106.38	110.86
2	F	1	XYS	O5-C5-C4	-2.52	104.79	110.79
2	H	3	XYP	C5-O5-C1	2.49	115.43	111.42
2	G	2	XYP	O3-C3-C4	-2.47	105.02	110.05
2	F	1	XYS	O4-C4-C5	-2.46	103.58	109.22
2	G	1	XYS	C5-C4-C3	-2.39	106.16	109.64
2	F	3	XYP	C1-C2-C3	-2.37	106.20	109.64
2	E	3	XYP	C5-C4-C3	-2.31	106.28	109.64
2	E	3	XYP	C1-C2-C3	-2.23	106.39	109.64
2	F	1	XYS	O3-C3-C4	-2.16	105.65	110.05
2	F	3	XYP	O2-C2-C1	-2.14	104.33	109.22
2	E	3	XYP	O4-C4-C5	-2.11	104.40	109.22
2	H	1	XYS	C5-O5-C1	2.10	116.83	112.46
2	F	3	XYP	O3-C3-C4	-2.08	105.80	110.05

There are no chirality outliers.

There are no torsion outliers.

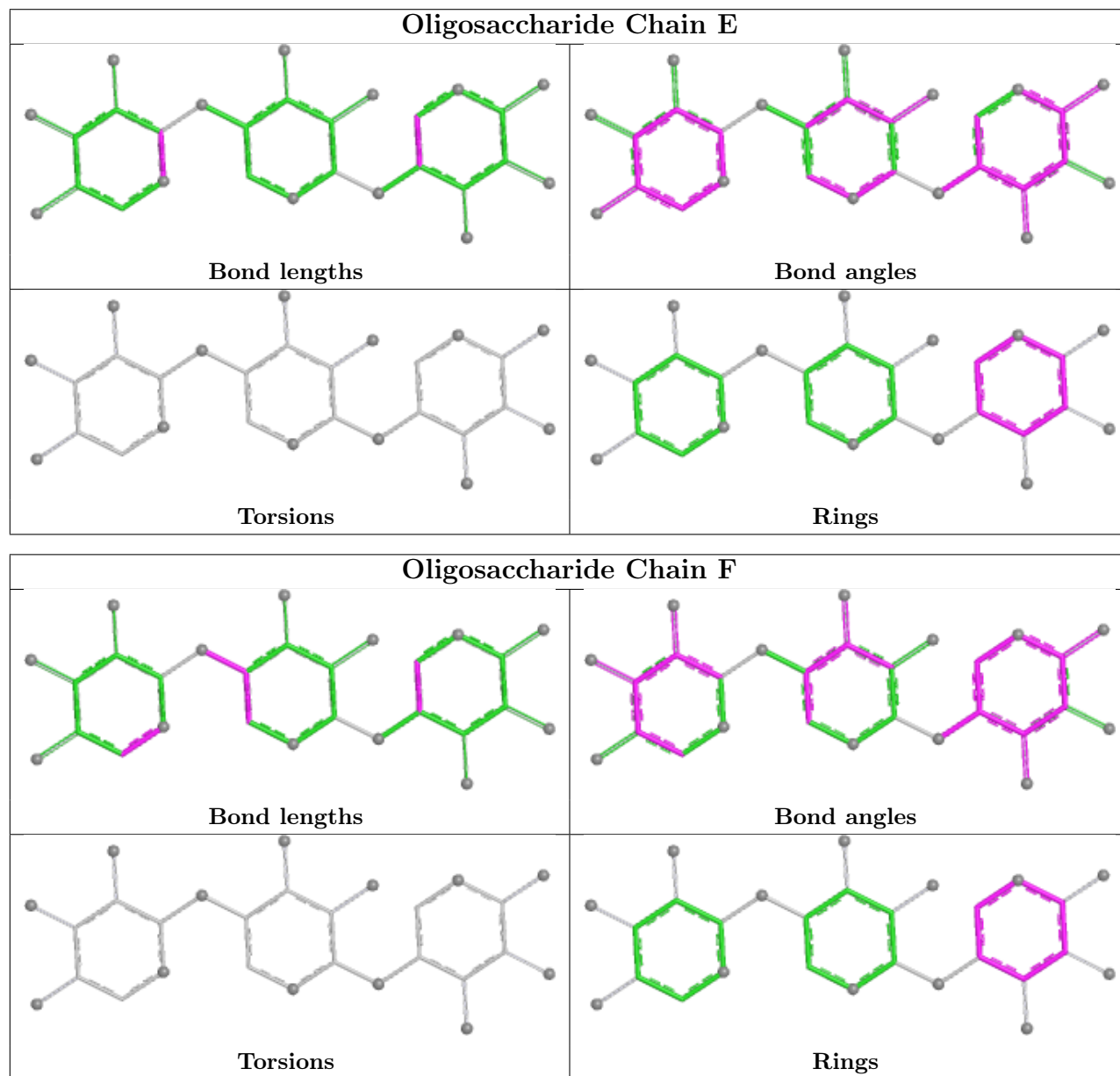
All (2) ring outliers are listed below:

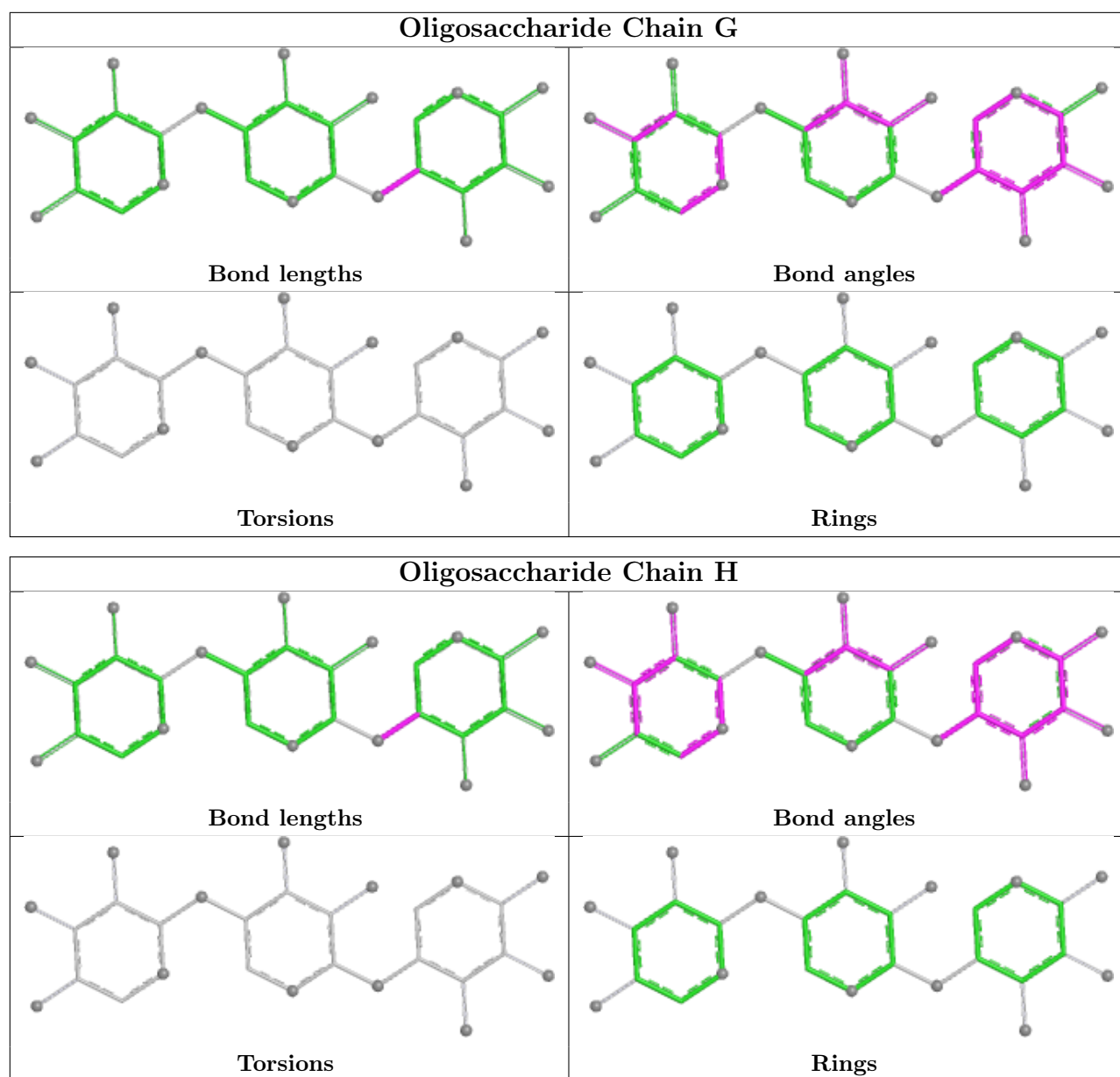
Mol	Chain	Res	Type	Atoms
2	F	1	XYS	C1-C2-C3-C4-C5-O5
2	E	1	XYS	C1-C2-C3-C4-C5-O5

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	XYS	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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	43:VAL	C	44:ASN	N	1.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	206/209 (98%)	-1.60	0 100 100	10, 21, 32, 52	2 (0%)
1	B	208/209 (99%)	-1.58	0 100 100	10, 21, 31, 44	1 (0%)
1	C	206/209 (98%)	-1.58	0 100 100	11, 23, 32, 51	1 (0%)
1	D	207/209 (99%)	-1.59	0 100 100	12, 23, 33, 60	1 (0%)
All	All	827/836 (98%)	-1.59	0 100 100	10, 22, 33, 60	5 (0%)

There are no RSRZ outliers to report.

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.

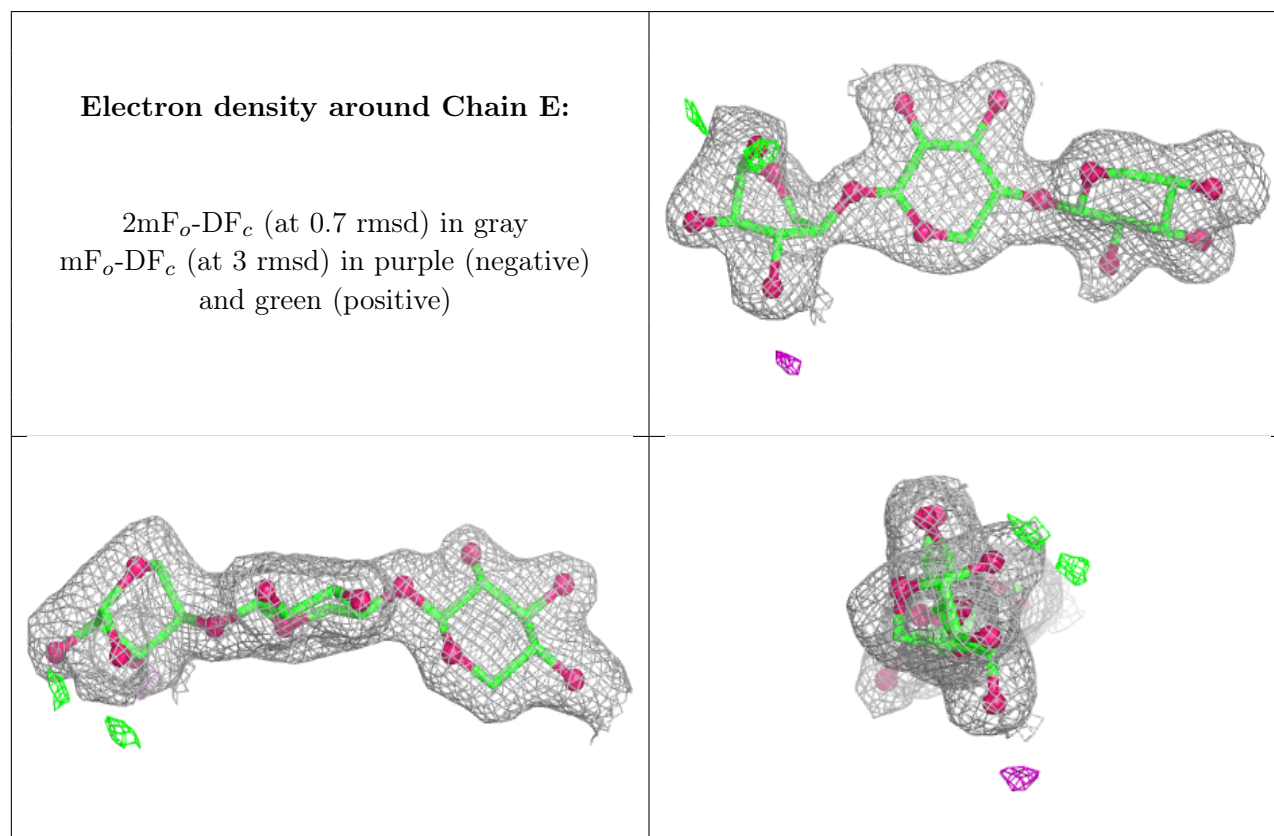
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	B	1	8/9	0.99	0.02	18,19,21,22	0
1	PCA	C	1	8/9	0.99	0.02	24,26,27,29	0
1	PCA	A	1	8/9	1.00	0.01	19,21,22,23	0
1	PCA	D	1	8/9	1.00	0.01	26,27,29,30	0

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.

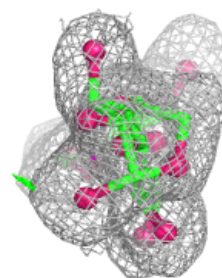
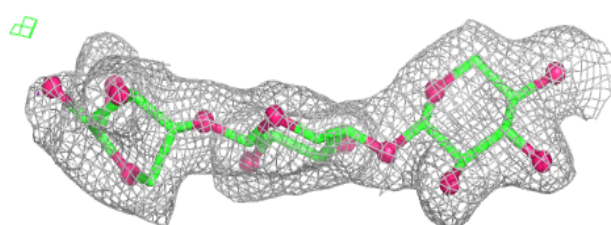
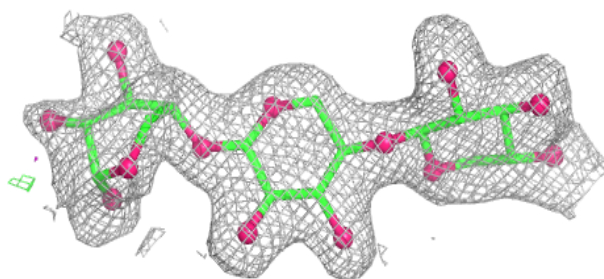
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XYS	E	1	10/10	0.99	0.03	24,26,33,38	0
2	XYP	E	3	9/10	0.99	0.03	27,31,37,40	0
2	XYS	F	1	10/10	0.99	0.03	21,29,34,39	0
2	XYP	F	3	9/10	0.99	0.02	21,28,32,33	0
2	XYS	G	1	10/10	0.99	0.03	26,36,41,42	0
2	XYP	G	2	9/10	0.99	0.02	20,22,23,24	0
2	XYP	G	3	9/10	0.99	0.02	25,28,29,31	0
2	XYS	H	1	10/10	0.99	0.03	23,33,38,38	0
2	XYP	H	3	9/10	0.99	0.02	27,30,33,34	0
2	XYP	E	2	9/10	1.00	0.01	17,20,23,23	0
2	XYP	H	2	9/10	1.00	0.01	18,21,23,23	0
2	XYP	F	2	9/10	1.00	0.02	16,19,21,22	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.

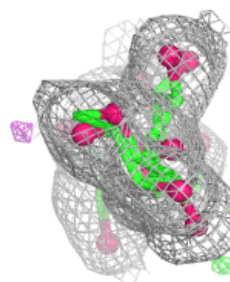
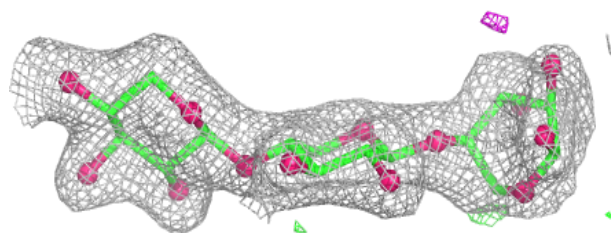
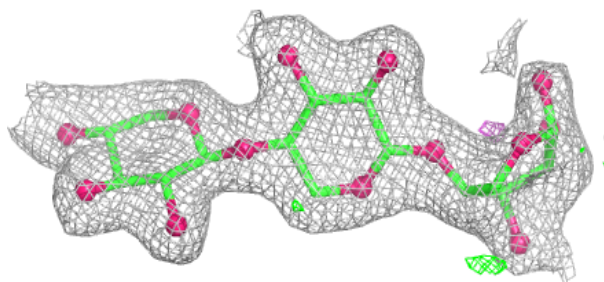


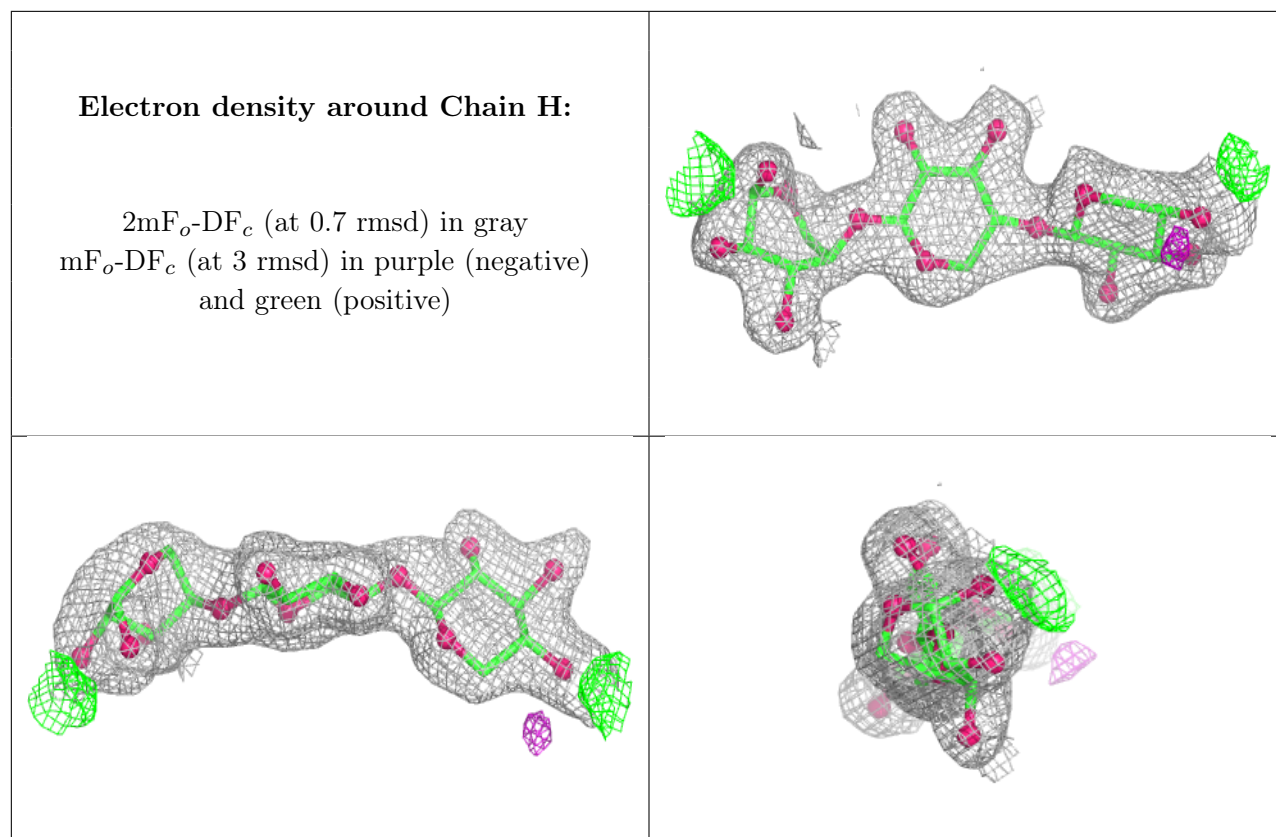
Electron density around Chain F:

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

**Electron density around Chain G:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.