



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:40 AM EDT

PDB ID : 2W9L / pdb_00002w9l
Title : CANINE ADENOVIRUS TYPE 2 FIBRE HEAD IN COMPLEX WITH CAR
DOMAIN D1 AND SIALIC ACID
Authors : Seiradake, E.; Henaff, D.; Wodrich, H.; Billet, O.; Perreau, M.; Hippert, C.;
Mennechet, F.; Schoehn, G.; Lortat-Jacob, H.; Dreja, H.; Ibanes, S.; Kalatzis,
V.; Wang, J.P.; Finberg, R.W.; Cusack, S.; Kremer, E.J.
Deposited on : 2009-01-26
Resolution : 2.91 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

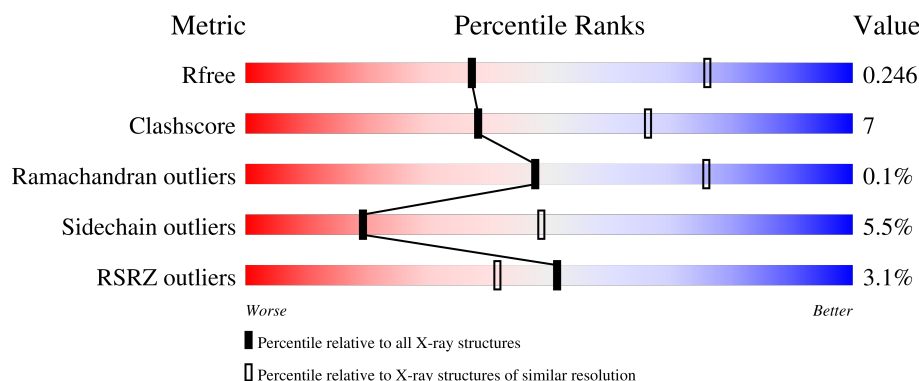
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

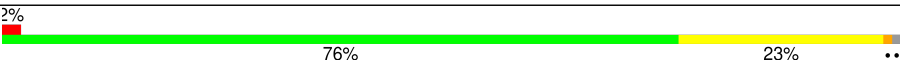
The reported resolution of this entry is 2.91 Å.

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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	124	
1	B	124	
1	G	124	
1	J	124	

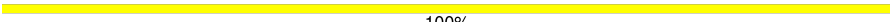
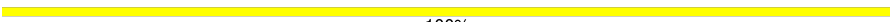
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Mol	Chain	Length	Quality of chain
1	K	124	
1	O	124	
1	P	124	
1	T	124	
1	V	124	
1	X	124	
1	Y	124	
1	Z	124	
2	C	197	
2	D	197	
2	E	197	
2	F	197	
2	H	197	
2	I	197	
2	L	197	
2	M	197	
2	N	197	
2	Q	197	
2	R	197	
2	S	197	
3	U	2	
3	W	2	
3	a	2	
3	c	2	
3	d	2	

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Mol	Chain	Length	Quality of chain
3	e	2	 100%
3	f	2	 100%
3	h	2	 100%
3	i	2	 50% 50%
3	j	2	 100%
4	b	2	 100%
4	g	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GAL	U	1	X	-	-	-
3	GAL	W	1	X	-	-	-
3	GAL	d	1	X	-	-	-
3	GAL	e	1	X	-	-	-
3	GAL	f	1	X	-	-	-
3	GAL	h	1	X	-	-	-
3	GAL	i	1	X	-	-	-
3	GAL	j	1	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28671 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 COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			914	581	147	183	3			
1	B	117	Total	C	N	O	S	0	0	0
			914	583	147	181	3			
1	G	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	J	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	K	123	Total	C	N	O	S	0	0	0
			963	615	156	189	3			
1	O	118	Total	C	N	O	S	0	0	0
			917	587	145	182	3			
1	P	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	T	119	Total	C	N	O	S	0	0	0
			928	591	149	185	3			
1	V	121	Total	C	N	O	S	0	0	0
			944	600	154	187	3			
1	X	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	Y	119	Total	C	N	O	S	0	0	0
			928	591	149	185	3			
1	Z	117	Total	C	N	O	S	0	0	0
			914	581	147	183	3			

- Molecule 2 is a protein called FIBRE PROTEIN.

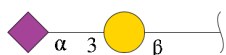
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	D	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	F	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	H	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	I	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	L	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	M	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	N	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	Q	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	R	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	S	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



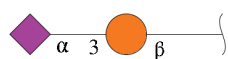
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	U	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	W	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	a	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	c	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	d	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	e	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	f	2	Total	C	N	O	0	0	0
			32	17	1	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	h	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	i	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	j	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-gulopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	b	2	Total	C	N	O	0	0	0
			32	17	1	14			
4	g	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	4	Total	O	0	0
			4	4		
5	C	5	Total	O	0	0
			5	5		
5	D	5	Total	O	0	0
			5	5		
5	E	4	Total	O	0	0
			4	4		
5	F	12	Total	O	0	0
			12	12		
5	G	9	Total	O	0	0
			9	9		
5	H	9	Total	O	0	0
			9	9		
5	I	10	Total	O	0	0
			10	10		
5	J	2	Total	O	0	0
			2	2		

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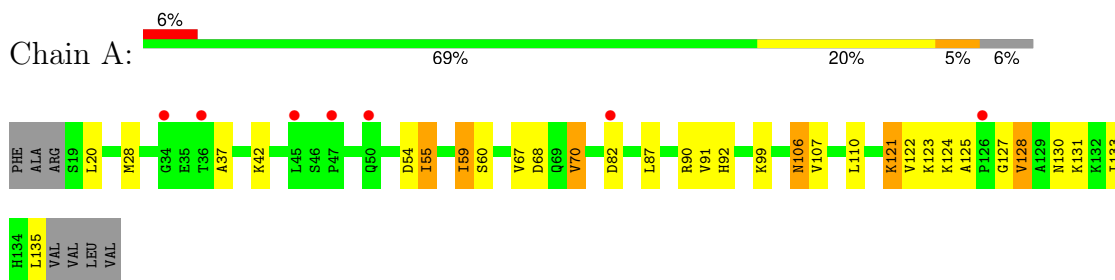
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	1	Total 1	O 1	0	0
5	L	11	Total 11	O 11	0	0
5	M	14	Total 14	O 14	0	0
5	N	17	Total 17	O 17	0	0
5	O	5	Total 5	O 5	0	0
5	P	1	Total 1	O 1	0	0
5	Q	13	Total 13	O 13	0	0
5	R	10	Total 10	O 10	0	0
5	S	7	Total 7	O 7	0	0
5	T	5	Total 5	O 5	0	0
5	V	1	Total 1	O 1	0	0
5	X	3	Total 3	O 3	0	0
5	Y	2	Total 2	O 2	0	0
5	Z	5	Total 5	O 5	0	0

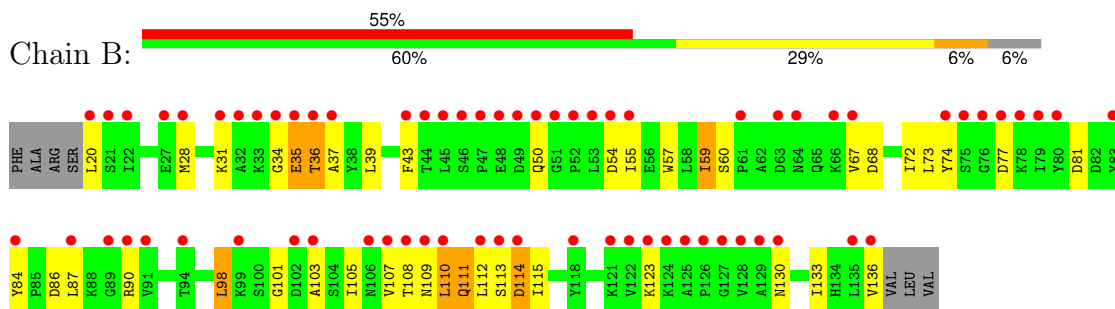
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

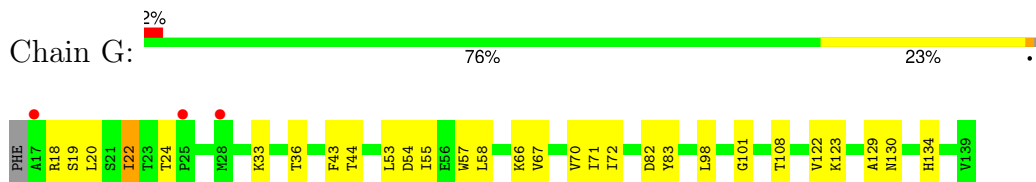
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



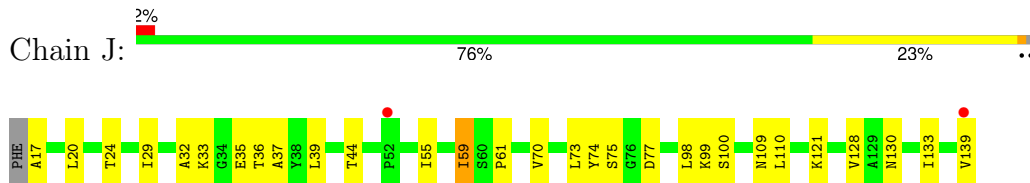
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

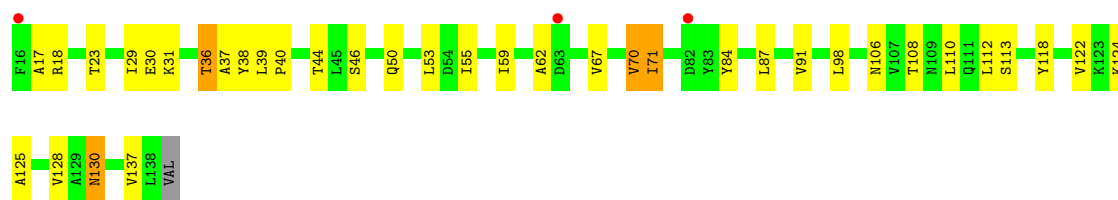


• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

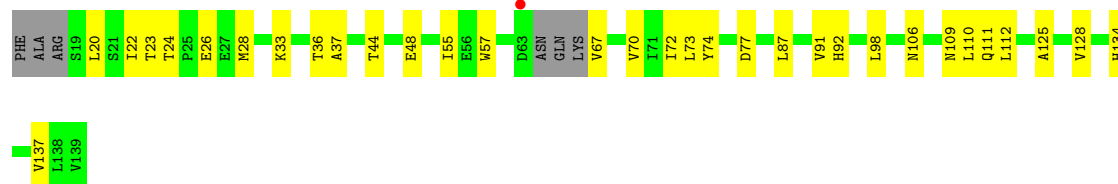


• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

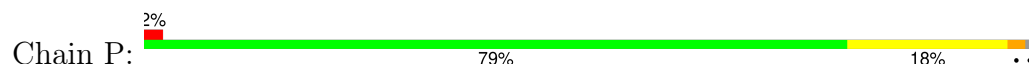




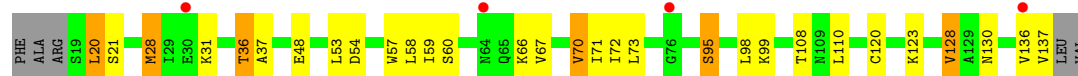
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



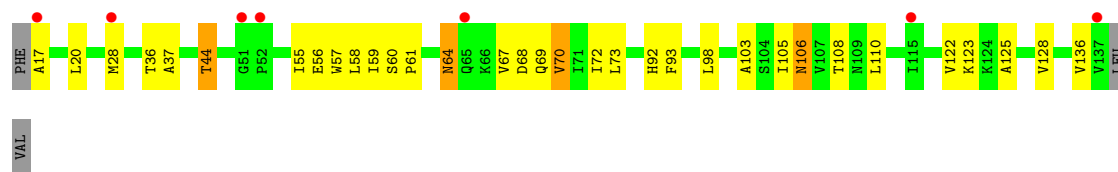
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



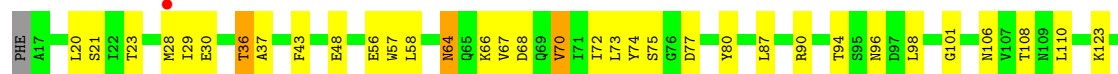
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

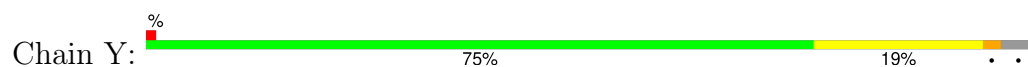


• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR





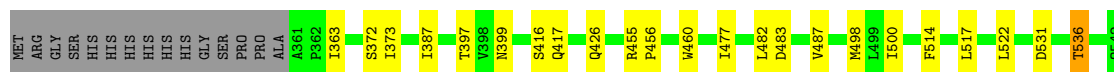
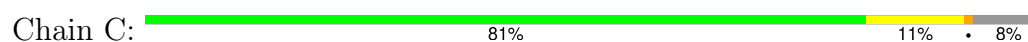
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



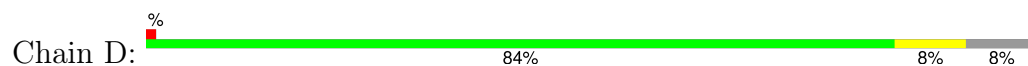
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



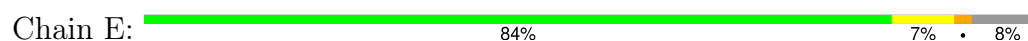
• Molecule 2: FIBRE PROTEIN



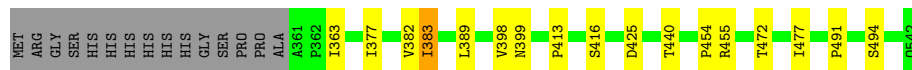
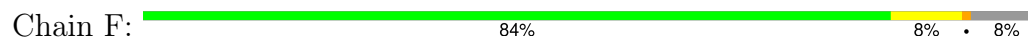
• Molecule 2: FIBRE PROTEIN



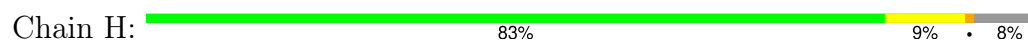
• Molecule 2: FIBRE PROTEIN

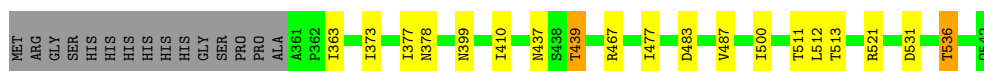


• Molecule 2: FIBRE PROTEIN

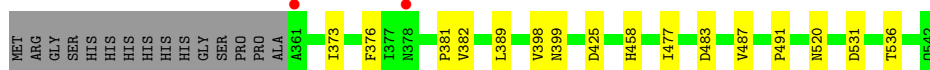
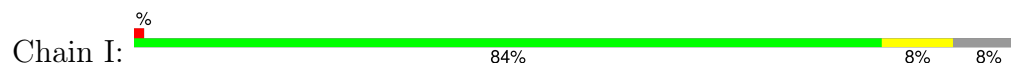


• Molecule 2: FIBRE PROTEIN

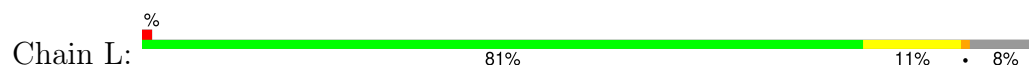




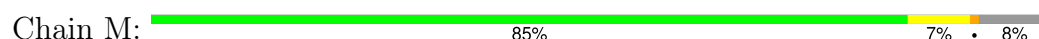
• Molecule 2: FIBRE PROTEIN



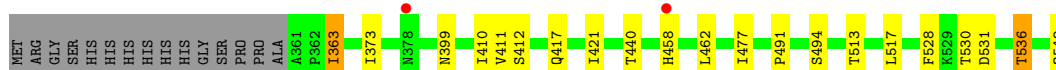
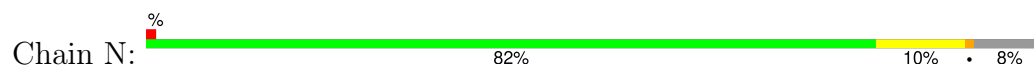
• Molecule 2: FIBRE PROTEIN



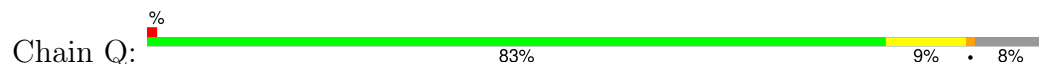
• Molecule 2: FIBRE PROTEIN



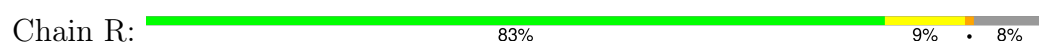
• Molecule 2: FIBRE PROTEIN



• Molecule 2: FIBRE PROTEIN



• Molecule 2: FIBRE PROTEIN

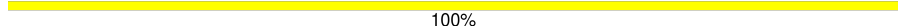


• Molecule 2: FIBRE PROTEIN

Chain S:  83% 9% 8%

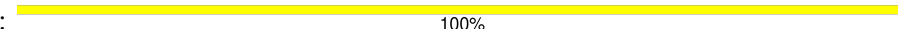


- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain U:  100%

GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain W:  100%

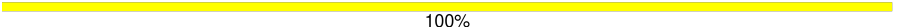
GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain a:  50% 50%

GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain c:  100%

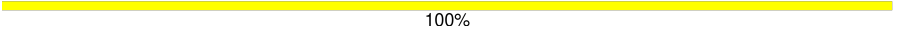
GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain d:  50% 50%

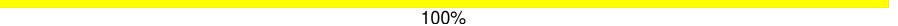
GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain e:  100%

GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain f:  100%

GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain h:  100%GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain i:  50%  50%GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain j:  100%GAL1
SIA2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-gulopyranose

Chain b:  100%GL01
SIA2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-gulopyranose

Chain g:  100%GL01
SIA2

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	221.15Å 221.15Å 391.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.91 49.63 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.63-2.91) 99.0 (49.63-2.91)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.254 0.196 , 0.246	Depositor DCC
R_{free} test set	1034 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28671	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, GL0, SIA

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	0/932	0.79	2/1264 (0.2%)
1	B	0.83	2/932 (0.2%)	1.03	3/1265 (0.2%)
1	G	0.69	0/977	0.88	2/1326 (0.2%)
1	J	0.65	0/977	0.82	0/1326
1	K	0.68	0/982	0.83	1/1332 (0.1%)
1	O	0.67	0/934	0.79	0/1268
1	P	0.62	0/977	0.79	0/1326
1	T	0.62	0/946	0.87	1/1284 (0.1%)
1	V	0.62	0/962	0.83	0/1305
1	X	0.64	0/977	0.75	0/1326
1	Y	0.68	0/946	0.81	1/1284 (0.1%)
1	Z	0.62	0/932	0.83	0/1264
2	C	0.68	0/1441	0.82	0/1964
2	D	0.64	0/1441	0.80	1/1964 (0.1%)
2	E	0.61	0/1441	0.77	0/1964
2	F	0.66	0/1441	0.81	0/1964
2	H	0.65	0/1441	0.80	0/1964
2	I	0.63	0/1441	0.80	0/1964
2	L	0.65	0/1441	0.78	0/1964
2	M	0.65	0/1441	0.78	0/1964
2	N	0.66	0/1441	0.81	0/1964
2	Q	0.64	0/1441	0.79	1/1964 (0.1%)
2	R	0.67	0/1441	0.80	0/1964
2	S	0.63	0/1441	0.80	1/1964 (0.1%)
All	All	0.65	2/28766 (0.0%)	0.81	13/39138 (0.0%)

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	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	THR	CA-C	6.47	1.61	1.53
1	B	114	ASP	N-CA	5.07	1.52	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	GLN	OE1-CD-NE2	-9.14	113.46	122.60
1	G	83	TYR	N-CA-C	6.94	118.93	111.36
1	B	111	GLN	CG-CD-NE2	6.41	126.01	116.40
2	D	384	ARG	CB-CA-C	5.88	120.18	110.78
1	B	114	ASP	N-CA-C	5.87	118.90	111.69
1	A	55	ILE	CB-CA-C	-5.79	102.81	110.98
1	K	62	ALA	N-CA-C	-5.45	104.75	111.40
1	A	130	ASN	N-CA-C	5.40	117.06	108.79
1	Y	130	ASN	N-CA-C	5.38	117.36	109.24
2	S	437	ASN	N-CA-C	5.34	116.11	108.74
1	G	18	ARG	N-CA-C	5.24	117.90	111.82
1	T	95	SER	N-CA-C	5.24	116.95	108.41
2	Q	437	ASN	N-CA-C	5.18	115.89	108.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	82	ASP	Peptide

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	914	0	910	25	0
1	B	914	0	914	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	959	0	966	13	0
1	J	959	0	966	18	0
1	K	963	0	966	20	0
1	O	917	0	920	16	0
1	P	959	0	966	18	0
1	T	928	0	928	22	0
1	V	944	0	946	24	0
1	X	959	0	966	21	0
1	Y	928	0	928	13	0
1	Z	914	0	910	20	0
2	C	1406	0	1382	17	0
2	D	1406	0	1382	10	0
2	E	1406	0	1382	16	0
2	F	1406	0	1382	12	0
2	H	1406	0	1382	16	0
2	I	1406	0	1382	19	0
2	L	1406	0	1382	16	0
2	M	1406	0	1382	10	0
2	N	1406	0	1382	20	0
2	Q	1406	0	1382	14	0
2	R	1406	0	1382	15	0
2	S	1406	0	1382	18	0
3	U	32	0	27	0	0
3	W	32	0	27	0	0
3	a	32	0	28	1	0
3	c	32	0	28	0	0
3	d	32	0	27	1	0
3	e	32	0	27	0	0
3	f	32	0	27	0	0
3	h	32	0	27	0	0
3	i	32	0	27	1	0
3	j	32	0	27	0	0
4	b	32	0	27	0	0
4	g	32	0	28	0	0
5	A	2	0	0	0	0
5	B	4	0	0	1	0
5	C	5	0	0	0	0
5	D	5	0	0	2	0
5	E	4	0	0	2	0
5	F	12	0	0	3	0
5	G	9	0	0	3	0
5	H	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	10	0	0	2	0
5	J	2	0	0	1	0
5	K	1	0	0	1	0
5	L	11	0	0	3	0
5	M	14	0	0	0	0
5	N	17	0	0	4	0
5	O	5	0	0	0	0
5	P	1	0	0	0	0
5	Q	13	0	0	7	0
5	R	10	0	0	2	0
5	S	7	0	0	0	0
5	T	5	0	0	2	0
5	V	1	0	0	0	0
5	X	3	0	0	1	0
5	Y	2	0	0	0	0
5	Z	5	0	0	2	0
All	All	28671	0	28197	389	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 (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:458:HIS:CD2	5:N:703:HOH:O	1.84	1.27
1:X:28:MET:HB3	5:X:203:HOH:O	1.48	1.14
1:B:90:ARG:HD2	1:B:108:THR:O	1.48	1.10
2:Q:467:ARG:HD2	5:Q:713:HOH:O	1.51	1.09
2:I:373:ILE:HD11	1:P:70:VAL:HG21	1.10	1.08
2:L:399:ASN:HD22	2:N:536:THR:HG22	1.25	1.02
1:B:36:THR:HA	1:B:107:VAL:O	1.58	1.01
1:B:90:ARG:HB3	1:B:108:THR:O	1.60	1.01
1:B:90:ARG:HD3	1:B:109:ASN:HB3	1.40	1.00
1:B:90:ARG:CD	1:B:109:ASN:HB3	1.96	0.95
2:D:467:ARG:HD2	5:D:703:HOH:O	1.63	0.95
1:B:36:THR:HG23	1:B:107:VAL:C	1.90	0.95
2:M:536:THR:HG22	2:N:399:ASN:HD22	1.32	0.95
1:B:34:GLY:O	1:B:35:GLU:HB2	1.63	0.95
1:K:37:ALA:HB2	1:K:110:LEU:HD11	1.50	0.94
1:B:36:THR:HG23	1:B:107:VAL:O	1.67	0.93
1:B:34:GLY:O	1:B:35:GLU:CB	2.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:536:THR:HG22	2:N:399:ASN:ND2	1.87	0.90
2:Q:531:ASP:OD2	2:S:477:ILE:HG22	1.71	0.89
5:G:2005:HOH:O	2:R:440:THR:HG22	1.72	0.89
2:H:536:THR:HG22	2:I:399:ASN:HD22	1.35	0.89
2:C:536:THR:HG22	2:H:399:ASN:HD22	1.38	0.89
2:E:536:THR:HG22	2:F:399:ASN:HD22	1.38	0.86
2:C:536:THR:HG22	2:H:399:ASN:ND2	1.90	0.86
2:H:467:ARG:HD2	5:H:708:HOH:O	1.74	0.86
5:I:710:HOH:O	3:d:1:GAL:H5	1.75	0.86
2:S:377:ILE:HG22	2:S:378:ASN:ND2	1.90	0.85
1:B:90:ARG:HA	1:B:108:THR:HB	1.60	0.84
1:B:36:THR:CG2	1:B:107:VAL:O	2.26	0.84
2:R:491:PRO:HD2	5:R:708:HOH:O	1.78	0.82
2:S:377:ILE:HG22	2:S:378:ASN:HD22	1.45	0.81
2:I:373:ILE:CD1	1:P:70:VAL:HG21	2.03	0.81
2:I:373:ILE:HD11	1:P:70:VAL:CG2	2.04	0.78
1:T:137:VAL:O	5:T:201:HOH:O	2.00	0.78
2:L:399:ASN:ND2	2:N:536:THR:HG22	1.98	0.77
1:P:139:VAL:HG12	1:P:139:VAL:O	1.85	0.77
1:J:98:LEU:C	1:J:98:LEU:HD23	2.10	0.76
2:E:536:THR:HG22	2:F:399:ASN:ND2	2.00	0.76
2:H:536:THR:HG22	2:I:399:ASN:ND2	2.01	0.76
1:K:55:ILE:HD12	1:K:122:VAL:HG22	1.67	0.76
1:B:90:ARG:CD	1:B:108:THR:O	2.32	0.75
2:E:373:ILE:HD12	1:O:73:LEU:HD11	1.68	0.75
2:L:531:ASP:OD2	2:N:477:ILE:HG22	1.87	0.74
2:N:491:PRO:HD2	5:N:706:HOH:O	1.87	0.73
2:C:399:ASN:HD22	2:I:536:THR:HG22	1.53	0.73
2:N:373:ILE:HD11	1:Y:70:VAL:HG11	1.71	0.72
1:A:121:LYS:HD3	5:Q:707:HOH:O	1.89	0.72
1:O:37:ALA:HB2	1:O:110:LEU:HD11	1.69	0.72
2:F:454:PRO:HD2	5:F:710:HOH:O	1.89	0.72
2:H:477:ILE:HG22	2:I:531:ASP:OD2	1.90	0.72
1:B:36:THR:CA	1:B:107:VAL:O	2.36	0.71
1:T:28:MET:HE1	1:T:136:VAL:HG23	1.73	0.71
1:J:99:LYS:HE2	5:J:2002:HOH:O	1.91	0.70
1:B:55:ILE:HD13	1:B:103:ALA:HB2	1.73	0.69
1:P:17:ALA:HB1	1:P:45:LEU:O	1.93	0.69
2:Q:477:ILE:HG22	2:R:531:ASP:OD2	1.94	0.68
1:Y:55:ILE:HD12	1:Y:98:LEU:HD21	1.75	0.68
1:A:59:ILE:HD12	1:A:60:SER:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:536:THR:CG2	2:N:399:ASN:HD22	2.05	0.68
1:T:36:THR:HB	1:T:108:THR:HA	1.75	0.68
1:B:86:ASP:OD2	1:B:113:SER:HB2	1.94	0.67
1:B:90:ARG:O	1:B:108:THR:N	2.27	0.67
1:T:28:MET:HE1	1:T:136:VAL:CG2	2.25	0.67
1:K:53:LEU:HD11	1:K:55:ILE:HD11	1.75	0.67
1:V:37:ALA:HB2	1:V:110:LEU:HD11	1.77	0.66
1:P:55:ILE:CD1	1:P:122:VAL:HG13	2.25	0.66
1:B:108:THR:HG22	1:B:109:ASN:N	2.09	0.66
1:V:92:HIS:CE1	1:V:106:ASN:HD21	2.12	0.66
1:P:55:ILE:HD12	1:P:122:VAL:HG22	1.78	0.66
2:L:399:ASN:HD22	2:N:536:THR:CG2	2.04	0.66
2:M:382:VAL:HG23	2:M:383:ILE:HG12	1.77	0.66
1:B:110:LEU:HD12	1:B:114:ASP:OD2	1.95	0.65
2:E:373:ILE:HD11	1:O:70:VAL:HG21	1.78	0.65
1:A:121:LYS:HE2	5:Q:707:HOH:O	1.96	0.64
1:Z:98:LEU:CD1	5:Z:204:HOH:O	2.45	0.64
1:A:55:ILE:HD12	1:A:122:VAL:HG22	1.80	0.64
2:C:498:MET:HE3	2:C:500:ILE:HD11	1.78	0.64
2:H:521:ARG:HH21	2:I:491:PRO:HB3	1.63	0.64
1:V:56:GLU:HB3	1:V:73:LEU:HD12	1.80	0.64
1:V:36:THR:HG22	1:V:108:THR:HA	1.79	0.63
2:N:531:ASP:OD1	5:N:701:HOH:O	2.16	0.62
2:C:399:ASN:ND2	2:I:536:THR:HG22	2.13	0.62
1:T:60:SER:HB3	1:T:67:VAL:HG23	1.81	0.62
1:A:106:ASN:C	1:A:106:ASN:HD22	2.06	0.62
2:L:421:ILE:HG12	2:L:513:THR:HG23	1.81	0.62
2:F:377:ILE:HD12	2:F:382:VAL:HG21	1.82	0.62
1:Z:58:LEU:HD12	1:Z:58:LEU:N	2.15	0.61
1:B:110:LEU:CD1	1:B:114:ASP:OD2	2.47	0.61
2:C:536:THR:CG2	2:H:399:ASN:HD22	2.12	0.61
2:L:467:ARG:HD2	5:L:2011:HOH:O	2.00	0.61
1:X:29:ILE:HD12	1:X:133:ILE:HG21	1.83	0.61
2:L:477:ILE:HG22	2:M:531:ASP:OD2	2.00	0.61
1:A:37:ALA:HB2	1:A:110:LEU:HD11	1.83	0.61
1:B:90:ARG:HD2	1:B:109:ASN:HB3	1.80	0.61
1:G:57:TRP:HB2	1:G:72:ILE:HG22	1.81	0.61
1:X:123:LYS:HG2	1:X:128:VAL:HG13	1.83	0.60
1:B:90:ARG:HD3	1:B:109:ASN:CB	2.26	0.60
2:R:536:THR:HG22	2:S:399:ASN:ND2	2.15	0.60
1:B:90:ARG:CB	1:B:108:THR:O	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:CA	1:B:108:THR:HB	2.32	0.60
1:J:55:ILE:CD1	1:J:98:LEU:HD21	2.32	0.60
1:K:17:ALA:HB2	1:K:44:THR:HG21	1.84	0.59
2:C:531:ASP:OD2	2:I:477:ILE:HG22	2.02	0.59
1:O:55:ILE:HD12	1:O:98:LEU:HD21	1.82	0.59
1:Y:93:PHE:HA	1:Y:105:ILE:HG22	1.84	0.59
1:T:57:TRP:HB2	1:T:72:ILE:HG22	1.84	0.59
1:T:123:LYS:HG2	1:T:128:VAL:HG13	1.84	0.59
1:B:34:GLY:O	1:B:35:GLU:CG	2.50	0.59
1:B:74:TYR:CE1	1:B:98:LEU:HD22	2.38	0.59
1:B:90:ARG:HB3	1:B:108:THR:C	2.26	0.59
2:C:373:ILE:HD11	1:T:70:VAL:HG11	1.84	0.59
2:D:458:HIS:HB3	5:I:708:HOH:O	2.03	0.58
1:J:39:LEU:HD22	1:J:133:ILE:HG21	1.85	0.58
1:X:94:THR:HG22	1:X:106:ASN:HD22	1.67	0.58
1:T:98:LEU:C	1:T:98:LEU:HD23	2.27	0.58
1:V:67:VAL:HG22	1:V:68:ASP:OD1	2.02	0.58
1:B:67:VAL:HG12	1:B:68:ASP:OD2	2.04	0.58
1:J:37:ALA:HB2	1:J:110:LEU:HD11	1.84	0.58
1:Y:37:ALA:HB2	1:Y:110:LEU:HD11	1.86	0.58
2:Q:491:PRO:HD2	5:Q:702:HOH:O	2.04	0.57
1:A:55:ILE:CD1	1:A:122:VAL:HG22	2.35	0.57
1:P:123:LYS:HG2	1:P:128:VAL:HG13	1.85	0.57
2:L:374:ASN:HB2	2:L:440:THR:HG21	1.84	0.57
1:K:71:ILE:HG22	1:K:84:TYR:CB	2.35	0.57
2:L:483:ASP:O	2:L:487:VAL:HG22	2.05	0.57
1:A:70:VAL:HG11	2:Q:373:ILE:HD11	1.86	0.57
1:T:20:LEU:HD12	1:T:21:SER:N	2.20	0.57
1:G:70:VAL:HG21	2:R:373:ILE:HD11	1.86	0.56
5:D:705:HOH:O	2:I:458:HIS:HB3	2.05	0.56
1:J:17:ALA:CB	1:J:44:THR:HG21	2.35	0.56
1:B:34:GLY:C	1:B:35:GLU:HG3	2.30	0.56
1:O:112:LEU:HD23	1:O:137:VAL:HG12	1.88	0.56
1:X:67:VAL:HG12	1:X:68:ASP:OD1	2.05	0.56
1:B:39:LEU:HD12	1:B:105:ILE:HD11	1.88	0.56
2:Q:363:ILE:HD13	2:Q:364:THR:N	2.21	0.56
1:K:31:LYS:O	1:K:137:VAL:HA	2.05	0.56
1:X:36:THR:HB	1:X:108:THR:HA	1.88	0.56
1:B:108:THR:CG2	1:B:109:ASN:N	2.69	0.55
1:V:60:SER:OG	1:V:67:VAL:HG23	2.06	0.55
1:B:73:LEU:CD2	2:D:373:ILE:HD12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:411:VAL:HG13	2:S:528:PHE:HB2	1.88	0.55
1:V:106:ASN:HD22	1:V:106:ASN:C	2.14	0.55
1:Z:98:LEU:HD12	5:Z:204:HOH:O	2.07	0.55
1:A:87:LEU:HD23	1:A:90:ARG:NH2	2.22	0.55
2:E:373:ILE:CD1	1:O:73:LEU:HD11	2.37	0.55
2:M:477:ILE:HG22	2:N:531:ASP:OD2	2.05	0.55
1:Y:55:ILE:CD1	1:Y:98:LEU:HD21	2.37	0.55
2:R:458:HIS:HD2	5:R:705:HOH:O	1.89	0.55
1:Y:98:LEU:C	1:Y:98:LEU:HD23	2.32	0.55
2:D:536:THR:HG22	2:E:399:ASN:HD22	1.72	0.54
2:S:421:ILE:HG12	2:S:513:THR:HG23	1.89	0.54
2:N:373:ILE:CD1	1:Y:70:VAL:HG11	2.37	0.54
2:H:511:THR:O	2:H:512:LEU:HD23	2.08	0.54
1:B:115:ILE:HA	5:B:201:HOH:O	2.07	0.54
5:G:2005:HOH:O	2:R:440:THR:CG2	2.44	0.54
1:O:20:LEU:C	1:O:20:LEU:HD23	2.33	0.54
1:G:33:LYS:NZ	5:G:2001:HOH:O	2.39	0.54
2:S:373:ILE:HD11	1:Z:70:VAL:HG11	1.90	0.54
1:T:20:LEU:HD12	1:T:20:LEU:C	2.32	0.54
1:X:74:TYR:CZ	1:X:77:ASP:HA	2.43	0.54
1:A:110:LEU:HD21	1:A:135:LEU:HD21	1.90	0.54
1:G:54:ASP:HB3	1:G:123:LYS:HB2	1.90	0.53
2:H:437:ASN:OD1	2:H:439:THR:HB	2.08	0.53
1:P:36:THR:HG21	1:P:108:THR:HG22	1.91	0.53
1:X:37:ALA:HB2	1:X:110:LEU:HD11	1.90	0.53
1:K:59:ILE:HD13	1:K:118:TYR:CZ	2.44	0.52
1:Z:59:ILE:HG23	1:Z:59:ILE:O	2.09	0.52
2:Q:505:LYS:HD2	5:Q:709:HOH:O	2.08	0.52
1:V:17:ALA:HB2	1:V:44:THR:HG21	1.90	0.52
2:R:374:ASN:HA	2:R:440:THR:HG21	1.91	0.52
2:C:482:LEU:HD12	2:C:522:LEU:HD21	1.92	0.52
2:N:363:ILE:C	2:N:363:ILE:HD13	2.34	0.52
2:Q:363:ILE:HD13	2:Q:363:ILE:C	2.35	0.52
2:I:373:ILE:HB	1:P:73:LEU:HD11	1.92	0.52
2:N:458:HIS:HD2	5:N:703:HOH:O	1.47	0.51
1:G:22:ILE:HG13	1:G:129:ALA:HB1	1.92	0.51
1:B:36:THR:CG2	1:B:107:VAL:C	2.74	0.51
2:F:389:LEU:CD2	2:F:398:VAL:HG22	2.40	0.51
1:B:90:ARG:CD	1:B:109:ASN:CB	2.81	0.51
1:J:98:LEU:C	1:J:98:LEU:CD2	2.81	0.51
1:X:43:PHE:CZ	1:X:101:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:LEU:HD11	1:G:55:ILE:HD11	1.93	0.51
2:H:483:ASP:O	2:H:487:VAL:HG22	2.10	0.51
1:P:87:LEU:HD23	1:P:90:ARG:NH2	2.25	0.51
2:Q:458:HIS:CE1	2:Q:459:THR:HG23	2.46	0.51
1:V:93:PHE:HA	1:V:105:ILE:HG22	1.93	0.51
1:J:32:ALA:HB3	1:J:35:GLU:HG2	1.93	0.51
1:X:56:GLU:OE2	1:X:58:LEU:HD21	2.11	0.51
2:H:536:THR:CG2	2:I:399:ASN:HD22	2.16	0.51
1:X:30:GLU:HG2	1:X:138:LEU:HD11	1.93	0.51
1:B:34:GLY:O	1:B:35:GLU:HG3	2.12	0.50
2:E:452:VAL:O	1:O:125:ALA:HB1	2.11	0.50
1:K:70:VAL:HG12	5:K:2001:HOH:O	2.11	0.50
1:K:36:THR:HB	1:K:108:THR:HA	1.94	0.50
1:B:39:LEU:HB3	1:B:133:ILE:HD12	1.93	0.50
1:B:54:ASP:HB3	1:B:123:LYS:HB2	1.93	0.50
1:V:20:LEU:C	1:V:20:LEU:HD23	2.37	0.50
1:B:31:LYS:HG3	1:B:37:ALA:HB2	1.92	0.50
2:R:536:THR:HG22	2:S:399:ASN:HD22	1.75	0.50
1:Z:29:ILE:HG22	1:Z:31:LYS:CE	2.41	0.50
1:Z:55:ILE:HG12	1:Z:122:VAL:HG22	1.94	0.50
1:A:123:LYS:HG2	1:A:128:VAL:HG22	1.94	0.49
2:L:440:THR:HG22	5:L:2003:HOH:O	2.12	0.49
2:S:477:ILE:HG23	2:S:477:ILE:O	2.12	0.49
1:B:86:ASP:OD2	1:B:113:SER:CB	2.59	0.49
1:O:57:TRP:HB2	1:O:72:ILE:HG22	1.94	0.49
1:K:130:ASN:OD1	1:K:130:ASN:N	2.46	0.49
1:J:32:ALA:HB3	1:J:35:GLU:CG	2.41	0.49
2:R:387:ILE:HD11	2:R:436:ILE:HD13	1.93	0.49
1:A:121:LYS:CD	5:Q:707:HOH:O	2.56	0.49
2:C:477:ILE:HG22	2:H:531:ASP:OD2	2.13	0.49
1:J:98:LEU:HD23	1:J:98:LEU:O	2.11	0.49
1:B:57:TRP:HB2	1:B:72:ILE:HG22	1.95	0.49
1:J:74:TYR:CZ	1:J:77:ASP:HA	2.47	0.49
1:V:93:PHE:CD1	1:V:98:LEU:HD21	2.48	0.49
1:K:71:ILE:HG22	1:K:84:TYR:HB2	1.95	0.49
2:D:531:ASP:OD2	2:F:477:ILE:HG22	2.13	0.49
2:S:373:ILE:HD12	1:Z:73:LEU:CD2	2.43	0.49
1:A:91:VAL:HG13	1:A:107:VAL:HG22	1.95	0.49
1:B:43:PHE:CZ	1:B:101:GLY:HA2	2.48	0.49
1:O:28:MET:HE3	1:O:134:HIS:HB2	1.95	0.48
1:O:87:LEU:HD22	1:O:91:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:373:ILE:CD1	1:T:70:VAL:HG11	2.43	0.48
2:E:374:ASN:HB2	2:E:440:THR:HG21	1.95	0.48
2:Q:429:GLN:HE21	2:Q:456:PRO:CB	2.26	0.48
1:B:84:TYR:CD2	1:B:87:LEU:HD12	2.48	0.48
1:V:20:LEU:HD11	1:V:122:VAL:HG12	1.93	0.48
1:V:59:ILE:HG22	1:V:69:GLN:O	2.13	0.48
2:C:387:ILE:HD13	2:C:514:PHE:CE2	2.48	0.48
2:C:483:ASP:O	2:C:487:VAL:HG22	2.14	0.48
2:F:382:VAL:HG23	2:F:383:ILE:HG12	1.95	0.48
1:B:20:LEU:HD23	1:B:20:LEU:C	2.39	0.48
2:E:455:ARG:HB3	5:E:703:HOH:O	2.13	0.48
1:V:17:ALA:HB2	1:V:44:THR:CG2	2.43	0.48
1:T:31:LYS:HD2	1:T:37:ALA:HA	1.95	0.48
1:P:36:THR:CG2	1:P:108:THR:HG22	2.44	0.48
1:Z:20:LEU:HD11	1:Z:122:VAL:HG12	1.96	0.48
2:L:363:ILE:HD12	2:L:459:THR:OG1	2.14	0.47
1:G:98:LEU:HD23	1:G:98:LEU:C	2.40	0.47
1:Z:28:MET:HE3	1:Z:28:MET:N	2.28	0.47
1:Z:29:ILE:HG22	1:Z:31:LYS:HE2	1.96	0.47
2:H:377:ILE:HG22	2:H:378:ASN:ND2	2.28	0.47
1:Y:43:PHE:CZ	1:Y:101:GLY:HA2	2.49	0.47
1:P:55:ILE:HD13	1:P:122:VAL:HG13	1.94	0.47
1:B:74:TYR:CZ	1:B:77:ASP:HA	2.49	0.47
1:K:87:LEU:HB3	1:K:91:VAL:HG23	1.97	0.47
5:L:2001:HOH:O	1:V:73:LEU:HD11	2.15	0.47
1:X:20:LEU:HD23	1:X:20:LEU:C	2.39	0.47
1:B:74:TYR:CZ	1:B:98:LEU:HD22	2.50	0.47
1:B:90:ARG:HD2	1:B:108:THR:C	2.30	0.47
2:Q:483:ASP:O	2:Q:487:VAL:HG22	2.14	0.47
2:R:477:ILE:HG22	2:S:531:ASP:OD2	2.14	0.47
1:T:31:LYS:O	1:T:137:VAL:HA	2.15	0.47
2:L:383:ILE:HD12	2:L:528:PHE:HE2	1.80	0.47
1:X:87:LEU:HD23	1:X:90:ARG:NH2	2.30	0.47
1:Z:43:PHE:CZ	1:Z:101:GLY:HA2	2.49	0.47
1:K:98:LEU:C	1:K:98:LEU:HD23	2.40	0.47
1:T:57:TRP:CH2	1:T:120:CYS:HB2	2.50	0.47
1:B:109:ASN:O	1:B:111:GLN:HG2	2.15	0.46
1:X:20:LEU:HD23	1:X:21:SER:N	2.30	0.46
1:J:36:THR:HG22	1:J:109:ASN:H	1.81	0.46
1:T:95:SER:HB3	5:T:202:HOH:O	2.16	0.46
1:O:112:LEU:HD23	1:O:137:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:98:LEU:C	1:P:98:LEU:HD23	2.41	0.46
1:G:36:THR:HG21	1:G:108:THR:HG22	1.98	0.46
1:Z:106:ASN:HD22	1:Z:106:ASN:HA	1.63	0.46
2:M:373:ILE:HD11	1:X:70:VAL:HG21	1.97	0.46
1:P:55:ILE:HD11	1:P:122:VAL:HG13	1.95	0.46
1:V:58:LEU:HD23	1:V:70:VAL:HA	1.97	0.46
1:A:131:LYS:HE3	1:A:133:ILE:HD11	1.97	0.46
2:I:483:ASP:O	2:I:487:VAL:HG22	2.16	0.46
1:V:61:PRO:HG2	1:V:64:ASN:HB2	1.96	0.46
2:C:417:GLN:HB2	2:C:517:LEU:HD23	1.98	0.45
1:A:54:ASP:HB3	1:A:123:LYS:HB2	1.98	0.45
2:E:536:THR:CG2	2:F:399:ASN:HD22	2.20	0.45
2:N:417:GLN:HB2	2:N:517:LEU:HD23	1.98	0.45
1:P:55:ILE:O	1:P:73:LEU:HD23	2.16	0.45
2:I:520:ASN:H	2:I:520:ASN:HD22	1.64	0.45
1:A:87:LEU:HB3	1:A:91:VAL:HG23	1.97	0.45
1:G:36:THR:CG2	1:G:108:THR:HG22	2.46	0.45
2:E:455:ARG:CB	5:E:703:HOH:O	2.64	0.45
2:E:419:SER:O	3:a:2:SIA:O9	2.35	0.45
2:R:417:GLN:HB2	2:R:517:LEU:HD23	1.99	0.45
2:S:430:LEU:HD21	2:S:437:ASN:C	2.41	0.45
1:A:121:LYS:CE	5:Q:707:HOH:O	2.61	0.45
1:J:55:ILE:HD12	1:J:98:LEU:HD21	1.99	0.45
2:H:500:ILE:HB	2:H:513:THR:HB	1.99	0.45
1:X:64:ASN:HD22	1:X:66:LYS:H	1.65	0.45
1:B:36:THR:HG23	1:B:108:THR:N	2.32	0.44
1:T:60:SER:CB	1:T:67:VAL:HG23	2.45	0.44
1:V:57:TRP:HB2	1:V:72:ILE:HG22	2.00	0.44
1:X:73:LEU:HD11	1:X:80:TYR:HB2	2.00	0.44
1:K:38:TYR:O	1:K:40:PRO:HD3	2.17	0.44
1:Y:24:THR:HG22	1:Y:26:GLU:O	2.18	0.44
2:C:498:MET:HE3	2:C:500:ILE:CD1	2.48	0.44
2:E:365:LEU:HD21	2:E:460:TRP:CD2	2.53	0.44
2:I:425:ASP:OD1	2:I:425:ASP:C	2.61	0.44
2:S:498:MET:HE3	2:S:500:ILE:HD11	1.98	0.44
1:B:59:ILE:HD13	1:B:60:SER:N	2.33	0.44
1:K:55:ILE:CD1	1:K:122:VAL:HG13	2.48	0.44
1:V:59:ILE:HG23	1:V:59:ILE:O	2.18	0.44
1:A:20:LEU:HD11	1:A:122:VAL:HG12	2.00	0.44
2:M:383:ILE:HD12	2:M:528:PHE:HE2	1.81	0.44
1:X:57:TRP:HB2	1:X:72:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:373:ILE:HD11	1:V:70:VAL:HG21	1.99	0.43
1:K:59:ILE:HG22	1:K:71:ILE:HG23	1.99	0.43
1:G:57:TRP:O	1:G:58:LEU:HD23	2.19	0.43
2:N:373:ILE:HB	1:Y:73:LEU:HD11	2.00	0.43
2:H:373:ILE:HD11	1:J:70:VAL:HG11	2.00	0.43
2:Q:464:MET:HA	2:Q:464:MET:HE2	1.99	0.43
1:T:28:MET:HE1	1:T:136:VAL:HG21	2.01	0.43
2:F:425:ASP:C	2:F:425:ASP:OD1	2.61	0.43
1:J:17:ALA:HB3	1:J:44:THR:HG21	1.99	0.43
1:B:50:GLN:HB2	2:D:454:PRO:HG2	2.00	0.43
1:B:84:TYR:HD2	1:B:87:LEU:HD12	1.84	0.43
1:J:59:ILE:HD13	1:J:61:PRO:HD3	2.00	0.43
1:X:43:PHE:CE1	1:X:101:GLY:HA2	2.54	0.43
1:X:94:THR:CG2	1:X:106:ASN:HD22	2.32	0.43
1:K:71:ILE:HG22	1:K:84:TYR:CG	2.54	0.43
2:N:462:LEU:HD21	2:N:542:GLN:HB2	2.01	0.43
1:O:91:VAL:HA	1:O:106:ASN:O	2.18	0.43
2:L:498:MET:HE3	2:L:500:ILE:HD11	2.00	0.43
2:Q:429:GLN:HE21	2:Q:456:PRO:HB3	1.84	0.43
2:S:373:ILE:HD12	1:Z:73:LEU:HD21	2.01	0.42
1:B:35:GLU:O	1:B:110:LEU:N	2.47	0.42
2:D:541:ASN:ND2	2:E:450:ASN:OD1	2.49	0.42
1:K:124:LYS:O	1:K:125:ALA:C	2.62	0.42
2:C:373:ILE:HD11	1:T:70:VAL:HG21	2.01	0.42
1:J:17:ALA:HB2	1:J:44:THR:HG21	2.01	0.42
2:L:370:GLY:O	1:V:123:LYS:NZ	2.52	0.42
2:R:416:SER:OG	3:i:2:SIA:H113	2.19	0.42
1:B:59:ILE:HD13	1:B:60:SER:C	2.44	0.42
1:A:87:LEU:HB3	1:A:91:VAL:CG2	2.49	0.42
2:F:491:PRO:HD2	5:F:701:HOH:O	2.18	0.42
2:N:411:VAL:HG13	2:N:528:PHE:HB2	2.01	0.42
1:X:73:LEU:C	1:X:73:LEU:HD12	2.45	0.42
1:Y:57:TRP:HB2	1:Y:72:ILE:HG22	2.01	0.42
1:A:59:ILE:HD12	1:A:60:SER:H	1.84	0.42
2:S:466:ASN:OD1	2:S:469:VAL:HG23	2.20	0.42
1:Z:20:LEU:HD23	1:Z:21:SER:N	2.35	0.42
1:A:124:LYS:O	1:A:125:ALA:C	2.62	0.42
1:G:43:PHE:CZ	1:G:101:GLY:HA2	2.54	0.42
1:Z:60:SER:OG	1:Z:67:VAL:HG23	2.19	0.42
2:D:417:GLN:HB2	2:D:517:LEU:HD23	2.02	0.41
1:G:55:ILE:CD1	1:G:122:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:HG12	1:A:68:ASP:CG	2.45	0.41
1:V:55:ILE:HD13	1:V:103:ALA:HB2	2.02	0.41
1:O:24:THR:HG22	1:O:26:GLU:O	2.21	0.41
1:P:55:ILE:CD1	1:P:122:VAL:HG22	2.48	0.41
1:Z:22:ILE:HD13	1:Z:41:CYS:SG	2.60	0.41
1:A:20:LEU:C	1:A:20:LEU:HD23	2.45	0.41
1:B:90:ARG:NH2	1:B:111:GLN:HG3	2.36	0.41
2:F:425:ASP:HA	5:F:706:HOH:O	2.19	0.41
1:Y:40:PRO:HA	1:Y:104:SER:OG	2.20	0.41
1:T:98:LEU:HD23	1:T:99:LYS:N	2.34	0.41
1:B:73:LEU:HD23	2:D:373:ILE:HD12	2.02	0.41
2:L:452:VAL:O	1:V:125:ALA:HB1	2.21	0.41
1:A:127:GLY:O	1:A:128:VAL:HG23	2.21	0.41
1:G:19:SER:OG	1:G:20:LEU:N	2.53	0.41
2:I:376:PHE:CZ	2:I:381:PRO:HG3	2.56	0.41
2:I:520:ASN:H	2:I:520:ASN:ND2	2.19	0.41
1:J:24:THR:O	1:J:24:THR:HG22	2.20	0.41
1:O:55:ILE:HB	1:O:74:TYR:HB3	2.03	0.41
2:Q:536:THR:HG22	2:R:399:ASN:HD22	1.86	0.41
2:S:373:ILE:CD1	1:Z:70:VAL:HG11	2.51	0.41
1:A:106:ASN:C	1:A:106:ASN:ND2	2.78	0.41
1:B:98:LEU:C	1:B:98:LEU:HD23	2.46	0.41
2:E:414:THR:HG21	2:S:378:ASN:CB	2.51	0.41
2:F:413:PRO:HB2	2:M:378:ASN:HB3	2.02	0.41
1:K:29:ILE:HD12	1:K:39:LEU:HD23	2.03	0.41
2:N:421:ILE:HG12	2:N:513:THR:HG23	2.03	0.41
2:S:498:MET:HE3	2:S:500:ILE:CD1	2.51	0.41
1:T:37:ALA:HB2	1:T:110:LEU:HD11	2.02	0.41
1:Y:91:VAL:HG12	1:Y:107:VAL:HG22	2.03	0.41
1:Z:74:TYR:CZ	1:Z:77:ASP:HA	2.56	0.41
1:B:108:THR:CG2	1:B:109:ASN:H	2.34	0.41
2:R:422:MET:HG2	2:R:436:ILE:HB	2.03	0.41
1:T:53:LEU:HD12	1:T:54:ASP:H	1.86	0.41
1:V:56:GLU:CB	1:V:73:LEU:HD12	2.49	0.41
2:D:387:ILE:HD13	2:D:514:PHE:CE2	2.55	0.40
1:O:36:THR:HG22	1:O:109:ASN:H	1.85	0.40
1:P:29:ILE:O	1:P:135:LEU:HD12	2.21	0.40
2:E:391:ARG:HB2	2:E:396:VAL:HG22	2.03	0.40
1:Z:29:ILE:O	1:Z:135:LEU:HD12	2.22	0.40
2:I:389:LEU:HD22	2:I:398:VAL:HG22	2.02	0.40
2:M:387:ILE:HD11	2:M:436:ILE:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:HG13	1:B:81:ASP:HB3	2.02	0.40
2:C:456:PRO:HA	2:C:460:TRP:CZ2	2.57	0.40
1:K:29:ILE:HD12	1:K:39:LEU:CD2	2.51	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	115/124 (93%)	104 (90%)	11 (10%)	0	100	100
1	B	115/124 (93%)	104 (90%)	10 (9%)	1 (1%)	14	40
1	G	121/124 (98%)	110 (91%)	11 (9%)	0	100	100
1	J	121/124 (98%)	113 (93%)	8 (7%)	0	100	100
1	K	121/124 (98%)	107 (88%)	14 (12%)	0	100	100
1	O	114/124 (92%)	106 (93%)	8 (7%)	0	100	100
1	P	121/124 (98%)	111 (92%)	8 (7%)	2 (2%)	7	24
1	T	117/124 (94%)	104 (89%)	13 (11%)	0	100	100
1	V	119/124 (96%)	113 (95%)	6 (5%)	0	100	100
1	X	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
1	Y	117/124 (94%)	113 (97%)	4 (3%)	0	100	100
1	Z	115/124 (93%)	104 (90%)	10 (9%)	1 (1%)	14	40
2	C	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	D	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	E	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	F	180/197 (91%)	169 (94%)	11 (6%)	0	100	100
2	H	180/197 (91%)	170 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	L	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	M	180/197 (91%)	170 (94%)	10 (6%)	0	100	100
2	N	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	Q	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	R	180/197 (91%)	170 (94%)	10 (6%)	0	100	100
2	S	180/197 (91%)	170 (94%)	10 (6%)	0	100	100
All	All	3577/3852 (93%)	3353 (94%)	220 (6%)	4 (0%)	48	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	GLU
1	P	63	ASP
1	Z	65	GLN
1	P	24	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	104/110 (94%)	94 (90%)	10 (10%)	8	25
1	B	104/110 (94%)	97 (93%)	7 (7%)	15	41
1	G	109/110 (99%)	101 (93%)	8 (7%)	13	37
1	J	109/110 (99%)	98 (90%)	11 (10%)	7	23
1	K	109/110 (99%)	95 (87%)	14 (13%)	4	13
1	O	105/110 (96%)	95 (90%)	10 (10%)	8	25
1	P	109/110 (99%)	99 (91%)	10 (9%)	8	26
1	T	106/110 (96%)	94 (89%)	12 (11%)	5	18
1	V	107/110 (97%)	100 (94%)	7 (6%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	109/110 (99%)	100 (92%)	9 (8%)	10	30
1	Y	106/110 (96%)	96 (91%)	10 (9%)	8	25
1	Z	104/110 (94%)	92 (88%)	12 (12%)	5	17
2	C	159/171 (93%)	152 (96%)	7 (4%)	25	57
2	D	159/171 (93%)	155 (98%)	4 (2%)	42	73
2	E	159/171 (93%)	154 (97%)	5 (3%)	35	67
2	F	159/171 (93%)	152 (96%)	7 (4%)	25	57
2	H	159/171 (93%)	155 (98%)	4 (2%)	42	73
2	I	159/171 (93%)	158 (99%)	1 (1%)	78	92
2	L	159/171 (93%)	154 (97%)	5 (3%)	35	67
2	M	159/171 (93%)	153 (96%)	6 (4%)	29	62
2	N	159/171 (93%)	152 (96%)	7 (4%)	25	57
2	Q	159/171 (93%)	157 (99%)	2 (1%)	61	84
2	R	159/171 (93%)	154 (97%)	5 (3%)	35	67
2	S	159/171 (93%)	156 (98%)	3 (2%)	50	78
All	All	3189/3372 (95%)	3013 (94%)	176 (6%)	19	49

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	MET
1	A	42	LYS
1	A	59	ILE
1	A	70	VAL
1	A	82	ASP
1	A	92	HIS
1	A	99	LYS
1	A	106	ASN
1	A	121	LYS
1	A	128	VAL
1	B	28	MET
1	B	59	ILE
1	B	98	LEU
1	B	110	LEU
1	B	112	LEU
1	B	130	ASN
1	B	136	VAL

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Mol	Chain	Res	Type
2	C	363	ILE
2	C	372	SER
2	C	397	THR
2	C	416	SER
2	C	426	GLN
2	C	455	ARG
2	C	536	THR
2	D	363	ILE
2	D	433	THR
2	D	494	SER
2	D	529	LYS
2	E	372	SER
2	E	440	THR
2	E	455	ARG
2	E	472	THR
2	E	536	THR
2	F	363	ILE
2	F	383	ILE
2	F	416	SER
2	F	440	THR
2	F	455	ARG
2	F	472	THR
2	F	494	SER
1	G	22	ILE
1	G	24	THR
1	G	44	THR
1	G	66	LYS
1	G	67	VAL
1	G	71	ILE
1	G	130	ASN
1	G	134	HIS
2	H	363	ILE
2	H	410	ILE
2	H	439	THR
2	H	536	THR
2	I	382	VAL
1	J	20	LEU
1	J	29	ILE
1	J	33	LYS
1	J	59	ILE
1	J	73	LEU
1	J	75	SER

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Mol	Chain	Res	Type
1	J	100	SER
1	J	121	LYS
1	J	128	VAL
1	J	130	ASN
1	J	139	VAL
1	K	18	ARG
1	K	23	THR
1	K	30	GLU
1	K	36	THR
1	K	46	SER
1	K	50	GLN
1	K	67	VAL
1	K	70	VAL
1	K	71	ILE
1	K	106	ASN
1	K	112	LEU
1	K	113	SER
1	K	128	VAL
1	K	130	ASN
2	L	372	SER
2	L	411	VAL
2	L	440	THR
2	L	455	ARG
2	L	472	THR
2	M	363	ILE
2	M	372	SER
2	M	455	ARG
2	M	472	THR
2	M	478	SER
2	M	536	THR
2	N	363	ILE
2	N	410	ILE
2	N	412	SER
2	N	440	THR
2	N	494	SER
2	N	530	THR
2	N	536	THR
1	O	22	ILE
1	O	23	THR
1	O	33	LYS
1	O	44	THR
1	O	48	GLU

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Mol	Chain	Res	Type
1	O	67	VAL
1	O	77	ASP
1	O	92	HIS
1	O	111	GLN
1	O	128	VAL
1	P	21	SER
1	P	46	SER
1	P	65	GLN
1	P	67	VAL
1	P	77	ASP
1	P	82	ASP
1	P	98	LEU
1	P	106	ASN
1	P	108	THR
1	P	128	VAL
2	Q	363	ILE
2	Q	472	THR
2	R	363	ILE
2	R	372	SER
2	R	410	ILE
2	R	412	SER
2	R	536	THR
2	S	363	ILE
2	S	372	SER
2	S	472	THR
1	T	20	LEU
1	T	28	MET
1	T	36	THR
1	T	48	GLU
1	T	58	LEU
1	T	59	ILE
1	T	66	LYS
1	T	70	VAL
1	T	71	ILE
1	T	73	LEU
1	T	128	VAL
1	T	130	ASN
1	V	28	MET
1	V	44	THR
1	V	64	ASN
1	V	70	VAL
1	V	106	ASN

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Mol	Chain	Res	Type
1	V	128	VAL
1	V	136	VAL
1	X	23	THR
1	X	36	THR
1	X	48	GLU
1	X	64	ASN
1	X	70	VAL
1	X	75	SER
1	X	96	ASN
1	X	98	LEU
1	X	128	VAL
1	Y	44	THR
1	Y	67	VAL
1	Y	70	VAL
1	Y	71	ILE
1	Y	73	LEU
1	Y	75	SER
1	Y	77	ASP
1	Y	113	SER
1	Y	130	ASN
1	Y	136	VAL
1	Z	23	THR
1	Z	26	GLU
1	Z	28	MET
1	Z	29	ILE
1	Z	31	LYS
1	Z	58	LEU
1	Z	67	VAL
1	Z	70	VAL
1	Z	71	ILE
1	Z	73	LEU
1	Z	91	VAL
1	Z	106	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	111	GLN
1	B	109	ASN
1	B	134	HIS
2	C	378	ASN

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Mol	Chain	Res	Type
2	C	394	ASN
2	C	399	ASN
2	D	378	ASN
2	D	399	ASN
2	D	458	HIS
2	D	542	GLN
2	E	394	ASN
2	F	394	ASN
2	F	399	ASN
1	G	106	ASN
1	G	119	GLN
1	G	130	ASN
2	H	378	ASN
2	H	399	ASN
2	H	542	GLN
2	I	378	ASN
2	I	399	ASN
2	I	520	ASN
1	K	50	GLN
1	K	64	ASN
1	K	119	GLN
2	L	378	ASN
2	L	394	ASN
2	L	399	ASN
2	L	429	GLN
2	L	458	HIS
2	M	394	ASN
2	M	399	ASN
2	N	378	ASN
2	N	394	ASN
2	N	399	ASN
2	N	458	HIS
2	N	542	GLN
1	O	111	GLN
1	O	130	ASN
1	P	50	GLN
1	P	64	ASN
1	P	65	GLN
1	P	119	GLN
2	Q	394	ASN
2	Q	429	GLN
2	Q	542	GLN

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Mol	Chain	Res	Type
2	R	399	ASN
2	R	458	HIS
2	R	520	ASN
2	R	542	GLN
2	S	378	ASN
2	S	394	ASN
2	S	399	ASN
2	S	542	GLN
1	T	64	ASN
1	T	109	ASN
1	T	130	ASN
1	V	50	GLN
1	V	64	ASN
1	V	92	HIS
1	V	106	ASN
1	V	109	ASN
1	X	64	ASN
1	X	96	ASN
1	X	106	ASN
1	X	119	GLN
1	X	130	ASN
1	X	134	HIS
1	Y	69	GLN
1	Y	111	GLN
1	Y	130	ASN
1	Z	50	GLN
1	Z	92	HIS
1	Z	106	ASN
1	Z	119	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GAL	U	1	3	12,12,12	0.83	0	17,17,17	2.46	5 (29%)
3	SIA	U	2	3	20,20,21	0.69	0	21,28,31	1.43	3 (14%)
3	GAL	W	1	3	12,12,12	0.82	0	17,17,17	2.37	4 (23%)
3	SIA	W	2	3	20,20,21	0.67	0	21,28,31	1.24	3 (14%)
3	GAL	a	1	3	12,12,12	0.72	0	17,17,17	1.10	1 (5%)
3	SIA	a	2	3	20,20,21	0.73	0	21,28,31	1.53	5 (23%)
4	GL0	b	1	4	12,12,12	1.09	1 (8%)	17,17,17	2.92	5 (29%)
4	SIA	b	2	4	20,20,21	0.59	0	21,28,31	0.99	1 (4%)
3	GAL	c	1	3	12,12,12	0.50	0	17,17,17	1.22	1 (5%)
3	SIA	c	2	3	20,20,21	0.67	0	21,28,31	1.39	4 (19%)
3	GAL	d	1	3	12,12,12	0.70	0	17,17,17	2.02	4 (23%)
3	SIA	d	2	3	20,20,21	0.63	0	21,28,31	1.22	1 (4%)
3	GAL	e	1	3	12,12,12	0.95	0	17,17,17	2.81	3 (17%)
3	SIA	e	2	3	20,20,21	0.87	0	21,28,31	1.18	2 (9%)
3	GAL	f	1	3	12,12,12	0.87	0	17,17,17	2.35	5 (29%)
3	SIA	f	2	3	20,20,21	0.80	1 (5%)	21,28,31	1.73	5 (23%)
4	GL0	g	1	4	12,12,12	0.77	0	17,17,17	2.35	5 (29%)
4	SIA	g	2	4	20,20,21	0.77	0	21,28,31	1.50	4 (19%)
3	GAL	h	1	3	12,12,12	0.74	0	17,17,17	2.36	5 (29%)
3	SIA	h	2	3	20,20,21	0.68	0	21,28,31	1.24	3 (14%)
3	GAL	i	1	3	12,12,12	0.76	0	17,17,17	2.52	4 (23%)
3	SIA	i	2	3	20,20,21	0.71	0	21,28,31	1.62	6 (28%)
3	GAL	j	1	3	12,12,12	0.96	1 (8%)	17,17,17	2.29	5 (29%)
3	SIA	j	2	3	20,20,21	0.69	0	21,28,31	1.23	3 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	U	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	U	2	3	-	4/18/34/38	0/1/1/1
3	GAL	W	1	3	1/1/5/5	0/2/22/22	0/1/1/1
3	SIA	W	2	3	-	3/18/34/38	0/1/1/1
3	GAL	a	1	3	-	2/2/22/22	0/1/1/1
3	SIA	a	2	3	-	3/18/34/38	0/1/1/1
4	GL0	b	1	4	-	0/2/22/22	0/1/1/1
4	SIA	b	2	4	-	0/18/34/38	0/1/1/1
3	GAL	c	1	3	-	2/2/22/22	0/1/1/1
3	SIA	c	2	3	-	5/18/34/38	0/1/1/1
3	GAL	d	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	d	2	3	-	0/18/34/38	0/1/1/1
3	GAL	e	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	e	2	3	-	3/18/34/38	0/1/1/1
3	GAL	f	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	f	2	3	-	1/18/34/38	0/1/1/1
4	GL0	g	1	4	-	2/2/22/22	0/1/1/1
4	SIA	g	2	4	-	5/18/34/38	0/1/1/1
3	GAL	h	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	h	2	3	-	0/18/34/38	0/1/1/1
3	GAL	i	1	3	1/1/5/5	0/2/22/22	0/1/1/1
3	SIA	i	2	3	-	4/18/34/38	0/1/1/1
3	GAL	j	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	j	2	3	-	3/18/34/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	1	GAL	O3-C3	2.38	1.48	1.43
3	f	2	SIA	C4-C5	-2.30	1.51	1.53
4	b	1	GL0	O3-C3	-2.03	1.37	1.43

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	1	GAL	O3-C3-C4	8.77	131.04	110.38
4	b	1	GL0	O3-C3-C2	7.86	128.91	110.38
3	W	1	GAL	O3-C3-C4	7.11	127.15	110.38
3	U	1	GAL	O3-C3-C4	6.35	125.33	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	1	GAL	O3-C3-C2	6.23	125.07	110.38
3	i	1	GAL	O3-C3-C2	6.05	124.64	110.38
3	e	1	GAL	C4-C3-C2	5.94	121.25	110.83
4	b	1	GL0	C3-C4-C5	-5.93	99.48	110.23
3	i	1	GAL	C3-C4-C5	-5.41	100.42	110.23
3	j	1	GAL	O3-C3-C4	5.31	122.89	110.38
3	f	1	GAL	O3-C3-C2	5.15	122.52	110.38
3	d	1	GAL	O3-C3-C2	5.14	122.49	110.38
4	g	1	GL0	C3-C4-C5	-5.09	101.00	110.23
4	g	1	GL0	O3-C3-C2	4.93	122.00	110.38
3	d	1	GAL	O3-C3-C4	4.91	121.95	110.38
3	j	1	GAL	O3-C3-C2	4.70	121.46	110.38
3	i	1	GAL	O3-C3-C4	4.70	121.45	110.38
3	h	1	GAL	C3-C4-C5	-4.63	101.83	110.23
3	U	1	GAL	O3-C3-C2	4.50	120.99	110.38
3	f	1	GAL	C4-C3-C2	4.41	118.58	110.83
3	f	2	SIA	O1A-C1-C2	-4.32	113.51	122.85
3	j	1	GAL	C3-C4-C5	-4.21	102.61	110.23
3	W	1	GAL	O3-C3-C2	4.19	120.24	110.38
3	h	1	GAL	O3-C3-C4	4.13	120.11	110.38
3	U	1	GAL	C3-C4-C5	-4.10	102.79	110.23
4	g	1	GL0	O3-C3-C4	3.96	119.72	110.38
3	f	2	SIA	O1B-C1-C2	3.80	122.58	112.71
3	i	2	SIA	O6-C2-C3	-3.70	105.58	110.56
3	f	1	GAL	C1-O5-C5	3.67	120.75	113.65
3	f	1	GAL	O3-C3-C4	3.57	118.79	110.38
4	b	1	GL0	C1-O5-C5	3.47	120.37	113.65
3	f	1	GAL	O5-C1-C2	3.41	116.30	110.30
4	g	1	GL0	C1-O5-C5	3.41	120.25	113.65
4	g	2	SIA	O6-C2-C3	-3.36	106.04	110.56
3	U	1	GAL	C1-O5-C5	3.35	120.14	113.65
3	a	1	GAL	O3-C3-C2	3.35	118.28	110.38
4	b	1	GL0	C1-C2-C3	-3.33	103.56	110.36
3	W	1	GAL	C3-C4-C5	-3.22	104.39	110.23
3	f	2	SIA	C4-C5-N5	-3.21	104.12	110.44
3	c	1	GAL	O3-C3-C4	3.17	117.86	110.38
3	a	2	SIA	C4-C5-N5	-3.15	104.22	110.44
3	c	2	SIA	O1B-C1-C2	3.14	120.87	112.71
4	b	1	GL0	C4-C3-C2	3.06	116.21	110.83
3	U	2	SIA	O1B-C1-C2	3.03	120.60	112.71
3	c	2	SIA	O1A-C1-C2	-2.97	116.43	122.85
3	h	2	SIA	O6-C2-C3	-2.96	106.58	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	j	2	SIA	O1B-C1-C2	2.90	120.25	112.71
3	j	2	SIA	O1A-C1-C2	-2.84	116.71	122.85
3	i	1	GAL	O5-C5-C6	2.84	113.48	106.44
3	f	2	SIA	O9-C9-C8	-2.83	105.20	111.16
3	e	1	GAL	C3-C4-C5	-2.79	105.17	110.23
3	i	2	SIA	O1B-C1-C2	2.78	119.94	112.71
3	a	2	SIA	O7-C7-C8	2.76	115.20	108.93
4	g	2	SIA	O1B-C1-C2	2.76	119.88	112.71
3	i	2	SIA	C4-C5-N5	-2.75	105.02	110.44
3	j	1	GAL	C4-C3-C2	2.74	115.64	110.83
3	W	2	SIA	C4-C5-N5	-2.71	105.10	110.44
3	i	2	SIA	O1A-C1-C2	-2.71	117.00	122.85
3	e	2	SIA	O1B-C1-C2	2.66	119.63	112.71
3	d	1	GAL	C4-C3-C2	2.60	115.40	110.83
3	U	1	GAL	O5-C5-C6	2.59	112.87	106.44
3	a	2	SIA	O7-C7-C6	-2.59	103.85	109.44
3	d	1	GAL	C3-C4-C5	-2.57	105.57	110.23
3	c	2	SIA	O6-C2-C3	-2.56	107.11	110.56
3	U	2	SIA	C4-C5-N5	-2.55	105.41	110.44
3	j	1	GAL	O5-C5-C6	2.54	112.75	106.44
3	d	2	SIA	O6-C2-C3	-2.52	107.16	110.56
3	e	2	SIA	O6-C2-C3	-2.40	107.33	110.56
3	a	2	SIA	O6-C2-C3	-2.39	107.35	110.56
3	W	2	SIA	O1B-C1-C2	2.36	118.84	112.71
4	g	1	GL0	C4-C3-C2	2.29	114.85	110.83
3	h	1	GAL	C4-C3-C2	2.27	114.82	110.83
4	g	2	SIA	C9-C8-C7	-2.27	107.56	112.17
3	h	2	SIA	C4-C5-N5	-2.23	106.05	110.44
3	a	2	SIA	O1B-C1-C2	2.22	118.48	112.71
3	h	1	GAL	O5-C5-C6	2.22	111.93	106.44
3	W	2	SIA	C6-C5-N5	-2.13	107.50	110.91
3	W	1	GAL	C1-O5-C5	2.12	117.75	113.65
4	b	2	SIA	O1B-C1-C2	2.10	118.16	112.71
3	f	2	SIA	C8-C7-C6	-2.07	109.16	113.05
3	c	2	SIA	C5-N5-C10	2.07	127.95	123.11
4	g	2	SIA	O8-C8-C7	2.07	114.09	109.25
3	i	2	SIA	O6-C2-C1	2.05	111.59	107.72
3	h	2	SIA	O1B-C1-C2	2.05	118.03	112.71
3	i	2	SIA	C8-C7-C6	-2.03	109.24	113.05
3	U	2	SIA	C9-C8-C7	-2.02	108.06	112.17
3	j	2	SIA	O6-C2-C3	-2.01	107.86	110.56

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	U	1	GAL	C3
3	W	1	GAL	C3
3	d	1	GAL	C3
3	e	1	GAL	C3
3	f	1	GAL	C3
3	h	1	GAL	C3
3	i	1	GAL	C3
3	j	1	GAL	C3

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	a	2	SIA	O8-C8-C9-O9
3	c	2	SIA	O1A-C1-C2-O6
3	e	2	SIA	O1A-C1-C2-O6
3	i	2	SIA	O1A-C1-C2-O6
3	j	2	SIA	O1A-C1-C2-C3
3	i	2	SIA	O8-C8-C9-O9
3	a	2	SIA	C7-C8-C9-O9
3	h	1	GAL	C4-C5-C6-O6
3	f	1	GAL	O5-C5-C6-O6
3	f	1	GAL	C4-C5-C6-O6
3	h	1	GAL	O5-C5-C6-O6
3	a	1	GAL	C4-C5-C6-O6
3	c	1	GAL	O5-C5-C6-O6
3	i	2	SIA	C7-C8-C9-O9
4	g	2	SIA	C7-C8-C9-O9
3	a	1	GAL	O5-C5-C6-O6
3	c	1	GAL	C4-C5-C6-O6
3	U	1	GAL	C4-C5-C6-O6
4	g	1	GL0	C4-C5-C6-O6
3	d	1	GAL	C4-C5-C6-O6
4	g	2	SIA	O8-C8-C9-O9
3	e	1	GAL	C4-C5-C6-O6
3	d	1	GAL	O5-C5-C6-O6
3	U	1	GAL	O5-C5-C6-O6
3	U	2	SIA	O1A-C1-C2-O6
3	j	2	SIA	O1A-C1-C2-O6
4	g	1	GL0	O5-C5-C6-O6
3	e	1	GAL	O5-C5-C6-O6
3	W	2	SIA	O8-C8-C9-O9
3	j	1	GAL	C4-C5-C6-O6
4	g	2	SIA	C6-C7-C8-O8

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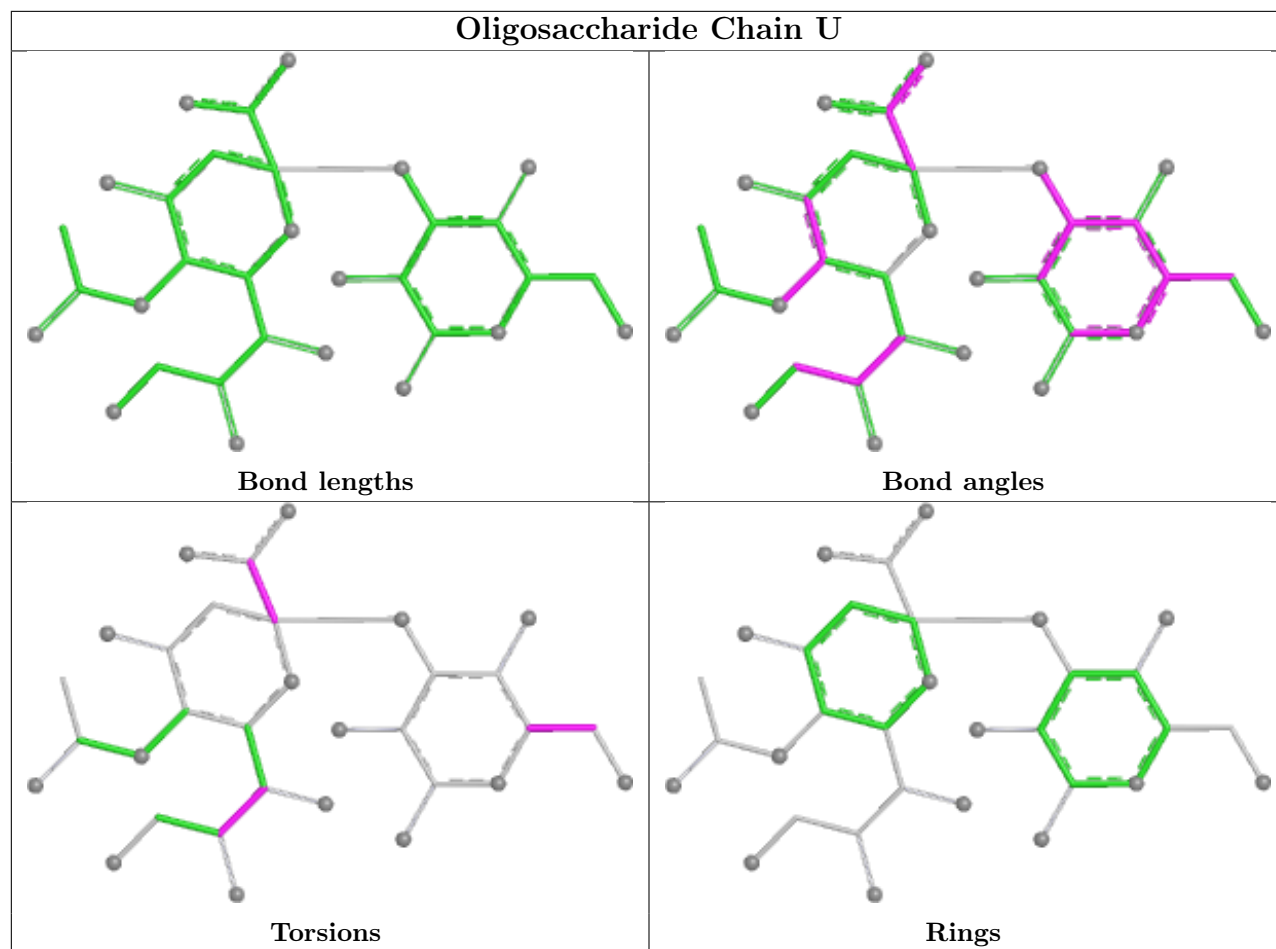
Mol	Chain	Res	Type	Atoms
3	U	2	SIA	C6-C7-C8-O8
3	c	2	SIA	C6-C7-C8-O8
3	e	2	SIA	O1A-C1-C2-C3
3	e	2	SIA	O1B-C1-C2-C3
3	i	2	SIA	O1A-C1-C2-C3
3	j	2	SIA	O1B-C1-C2-C3
3	W	2	SIA	C7-C8-C9-O9
3	f	2	SIA	O1A-C1-C2-O6
3	W	2	SIA	C6-C7-C8-O8
4	g	2	SIA	O7-C7-C8-O8
3	U	2	SIA	C6-C7-C8-C9
4	g	2	SIA	O7-C7-C8-C9
3	c	2	SIA	O7-C7-C8-C9
3	a	2	SIA	O1A-C1-C2-O6
3	c	2	SIA	O1A-C1-C2-C3
3	c	2	SIA	O7-C7-C8-O8
3	U	2	SIA	O7-C7-C8-C9
3	j	1	GAL	O5-C5-C6-O6

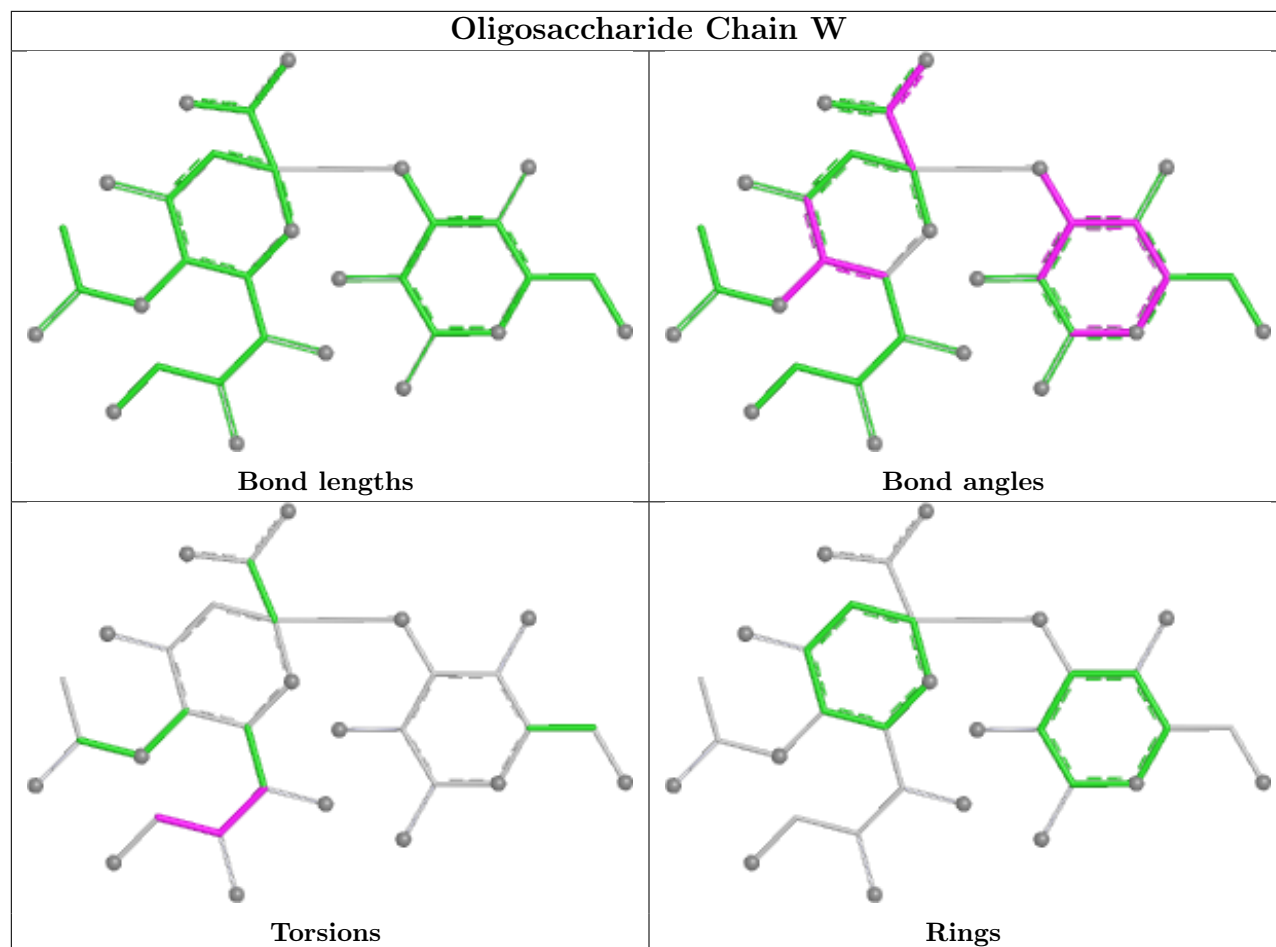
There are no ring outliers.

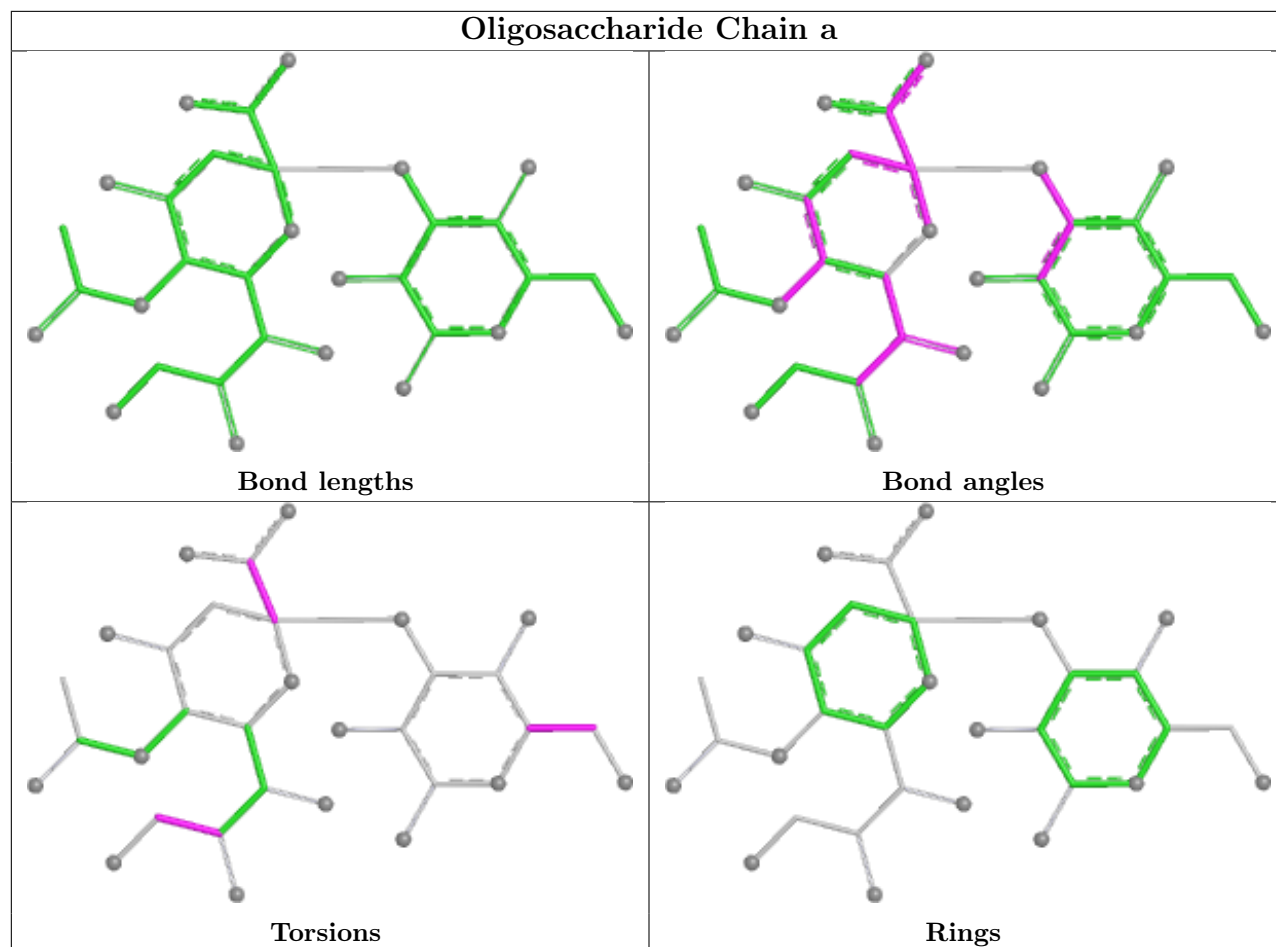
3 monomers are involved in 3 short contacts:

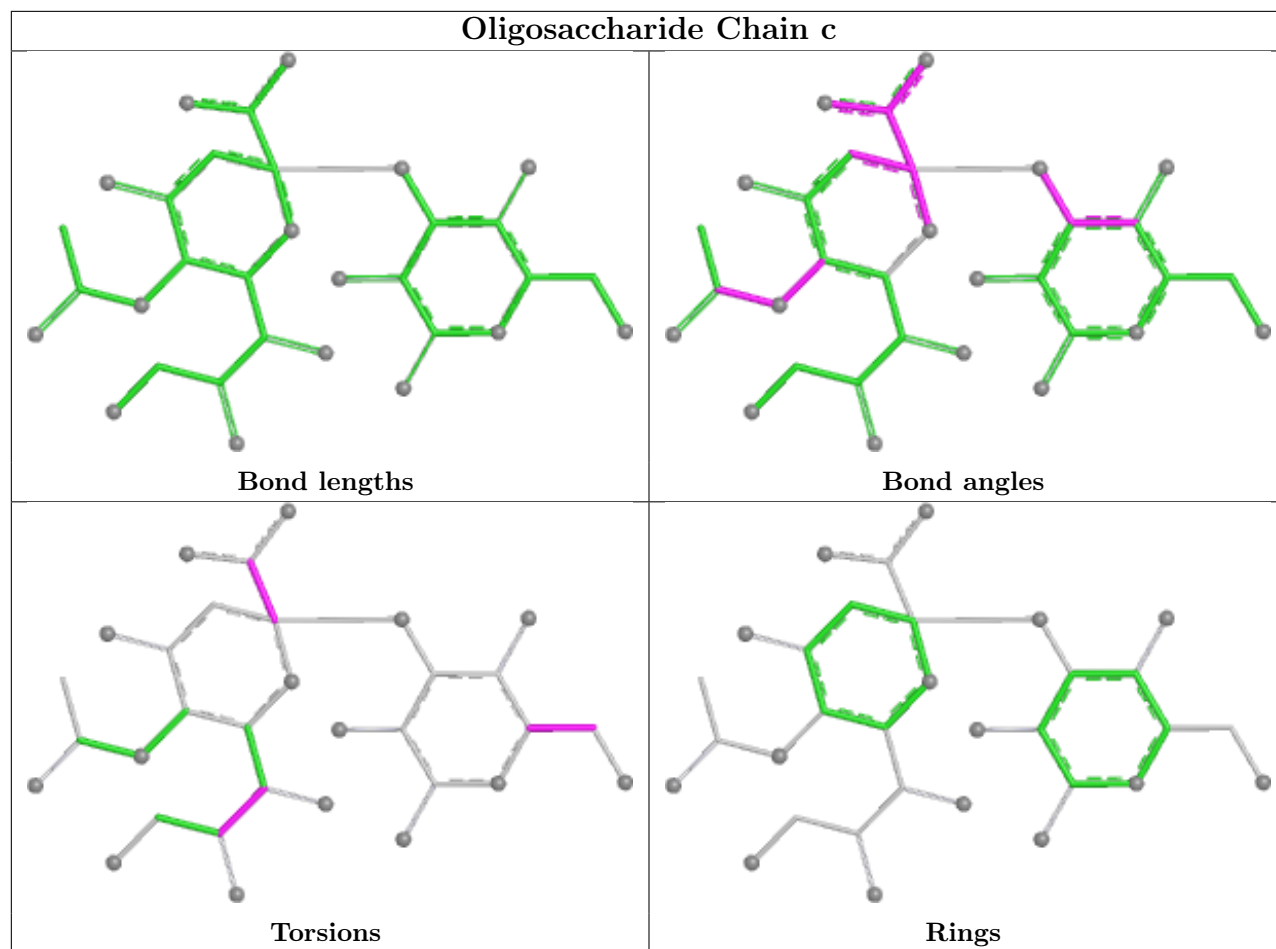
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	i	2	SIA	1	0
3	d	1	GAL	1	0
3	a	2	SIA	1	0

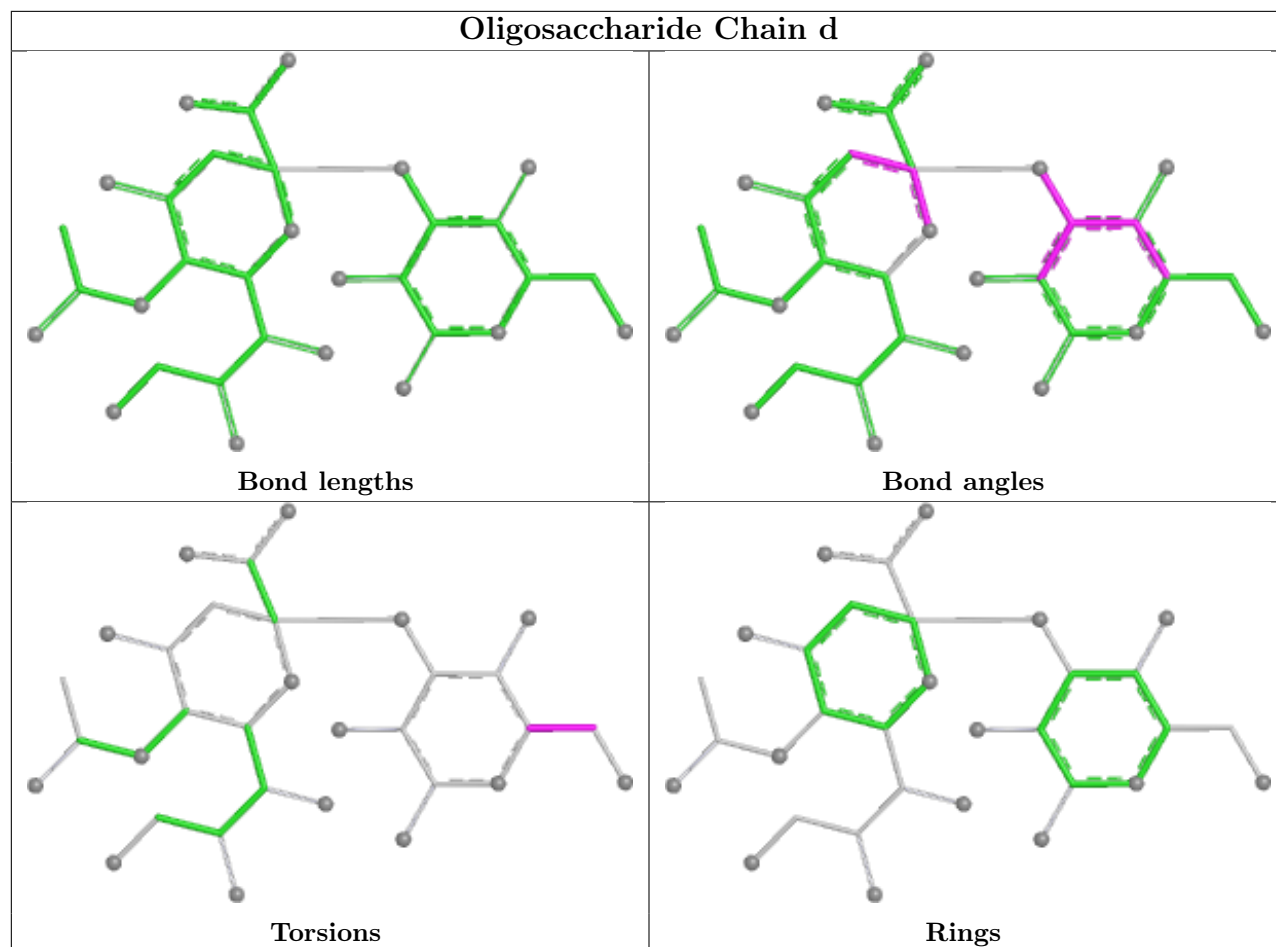
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

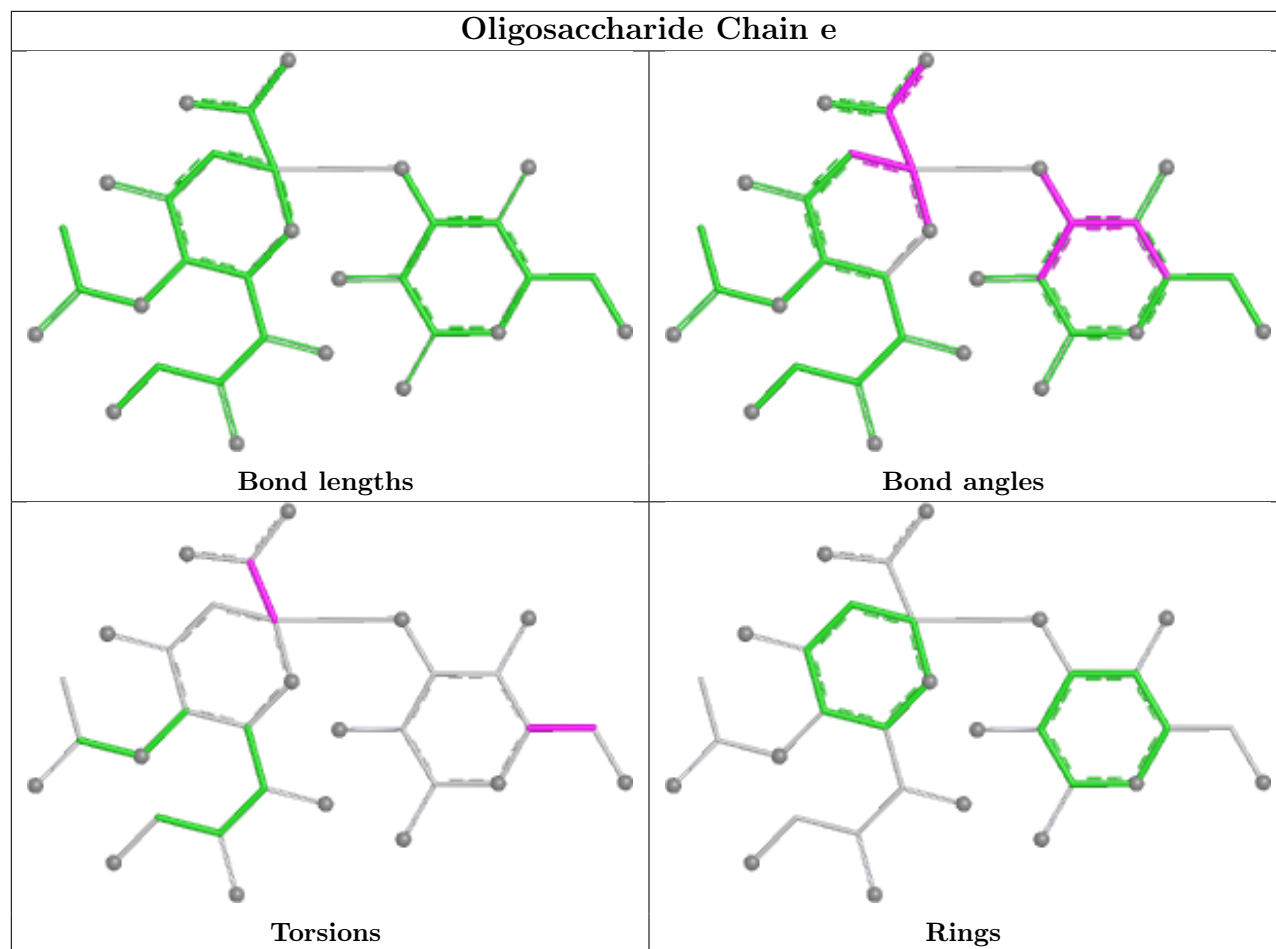


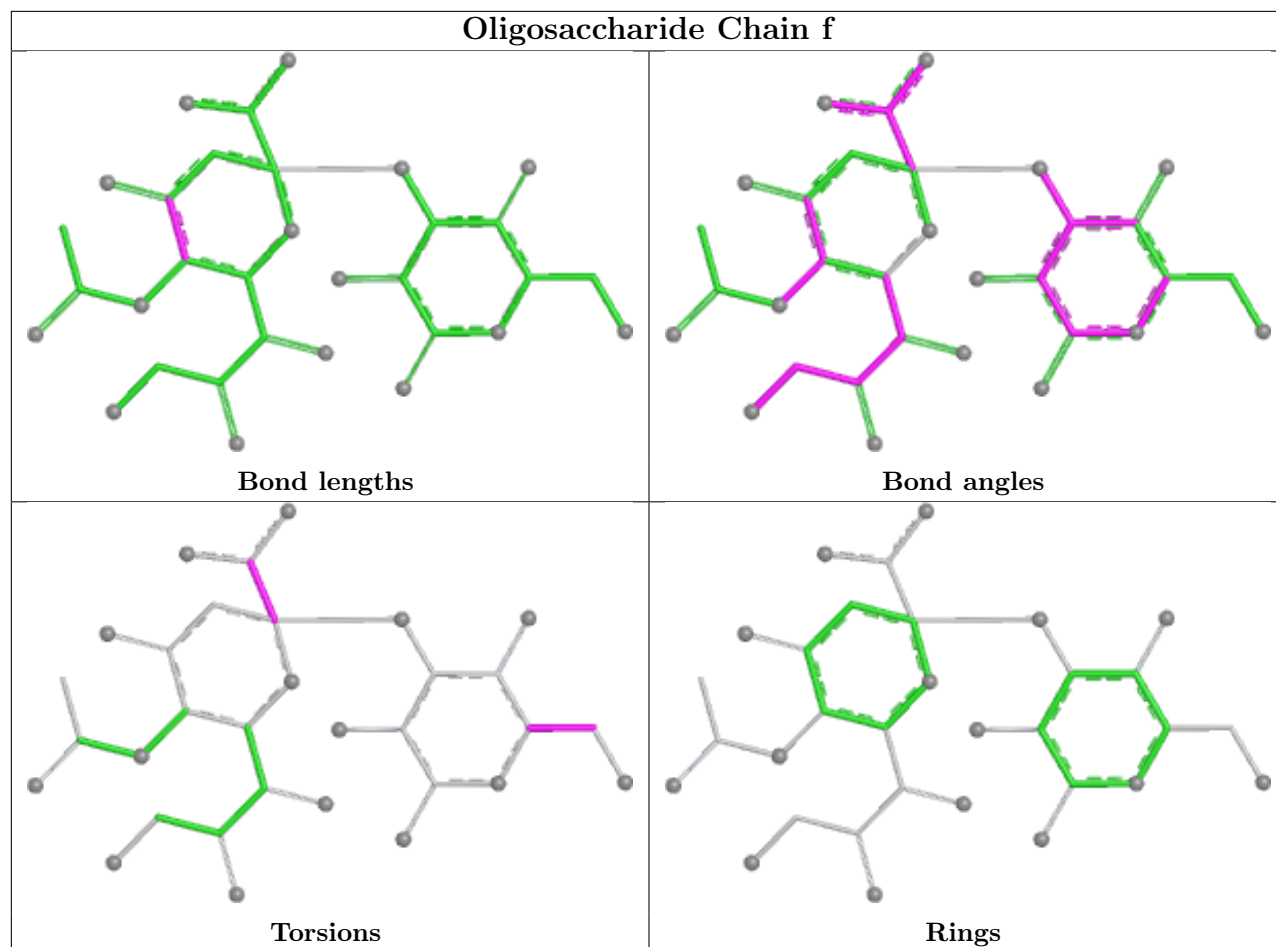


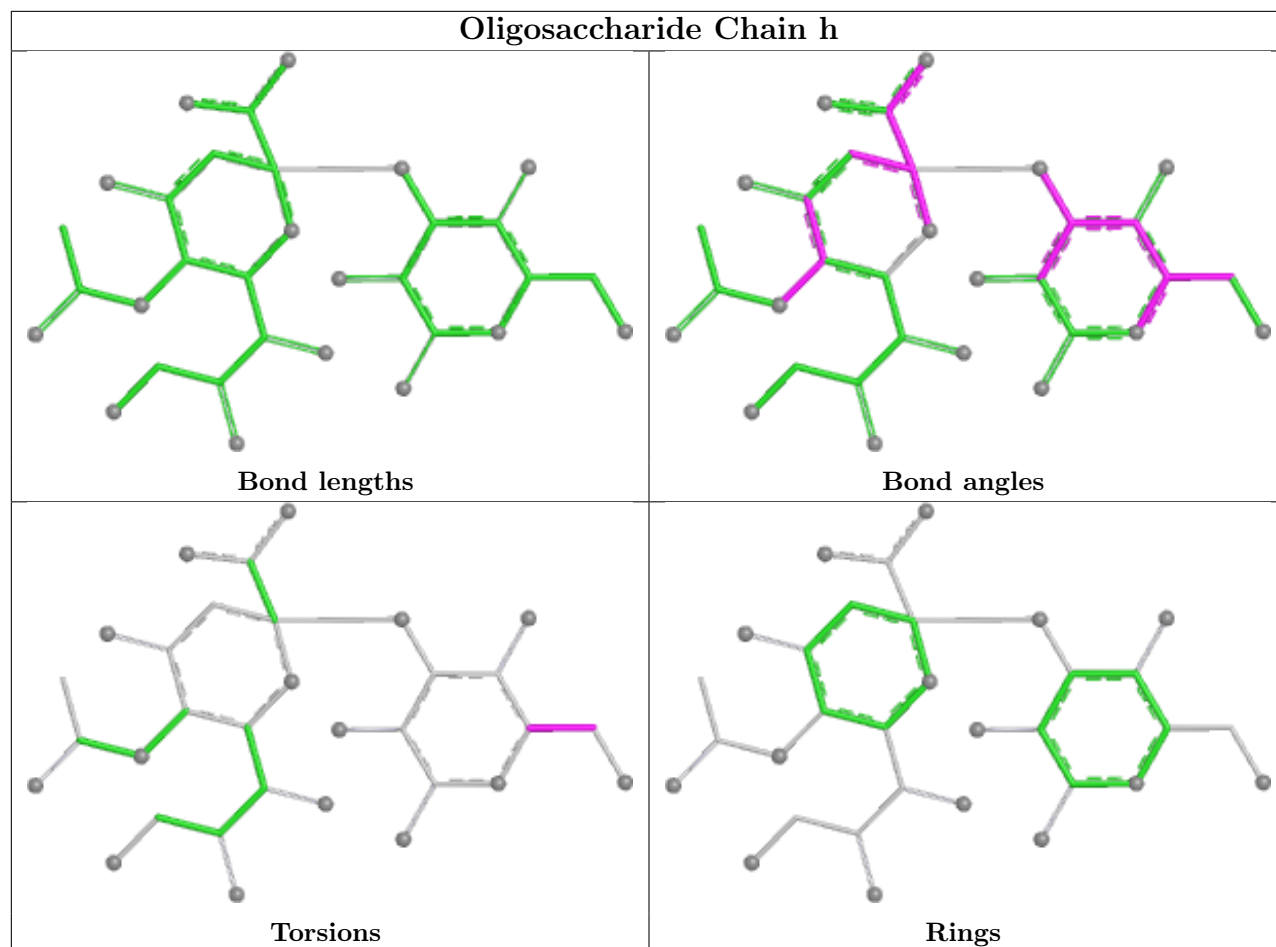


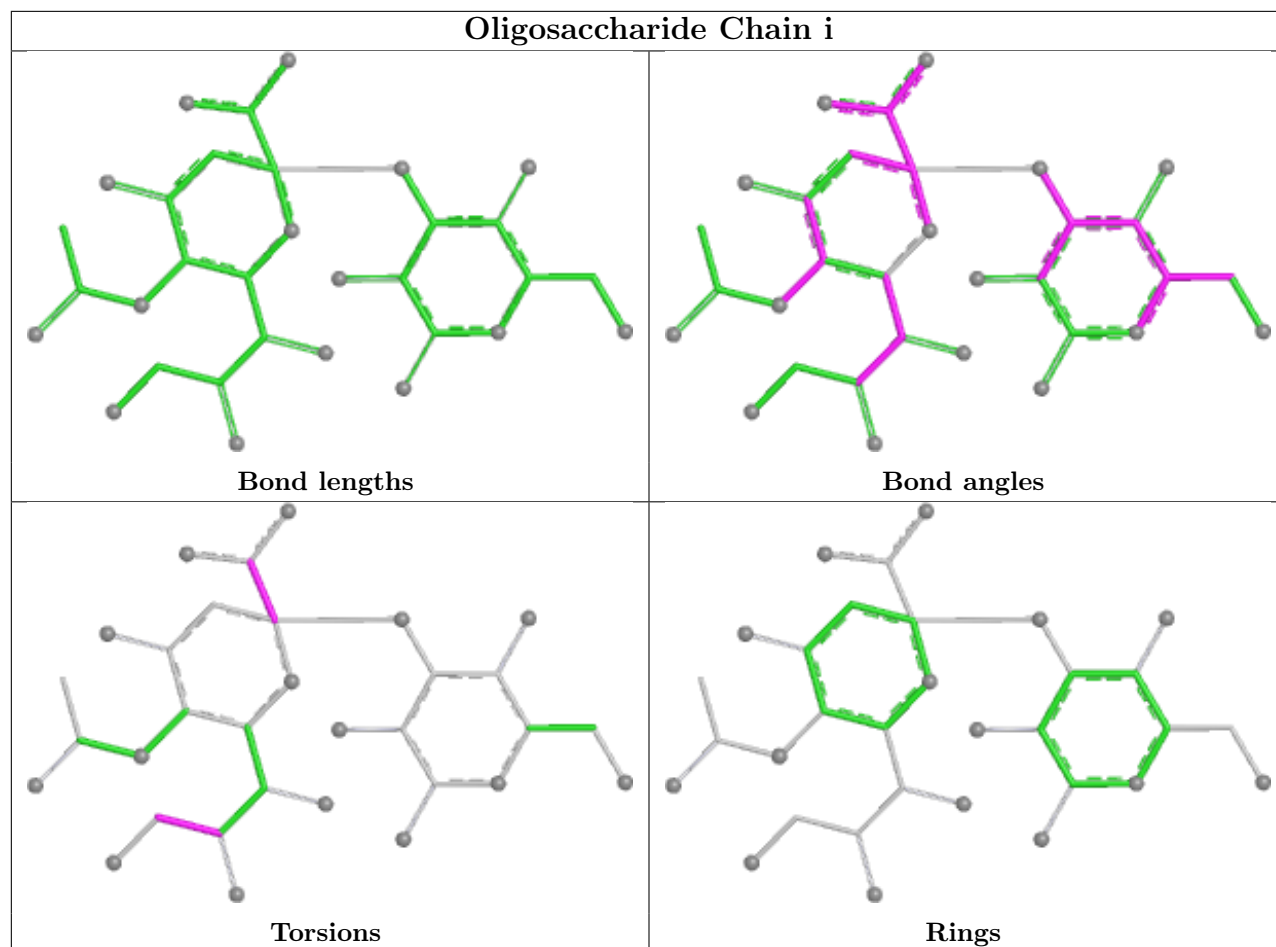




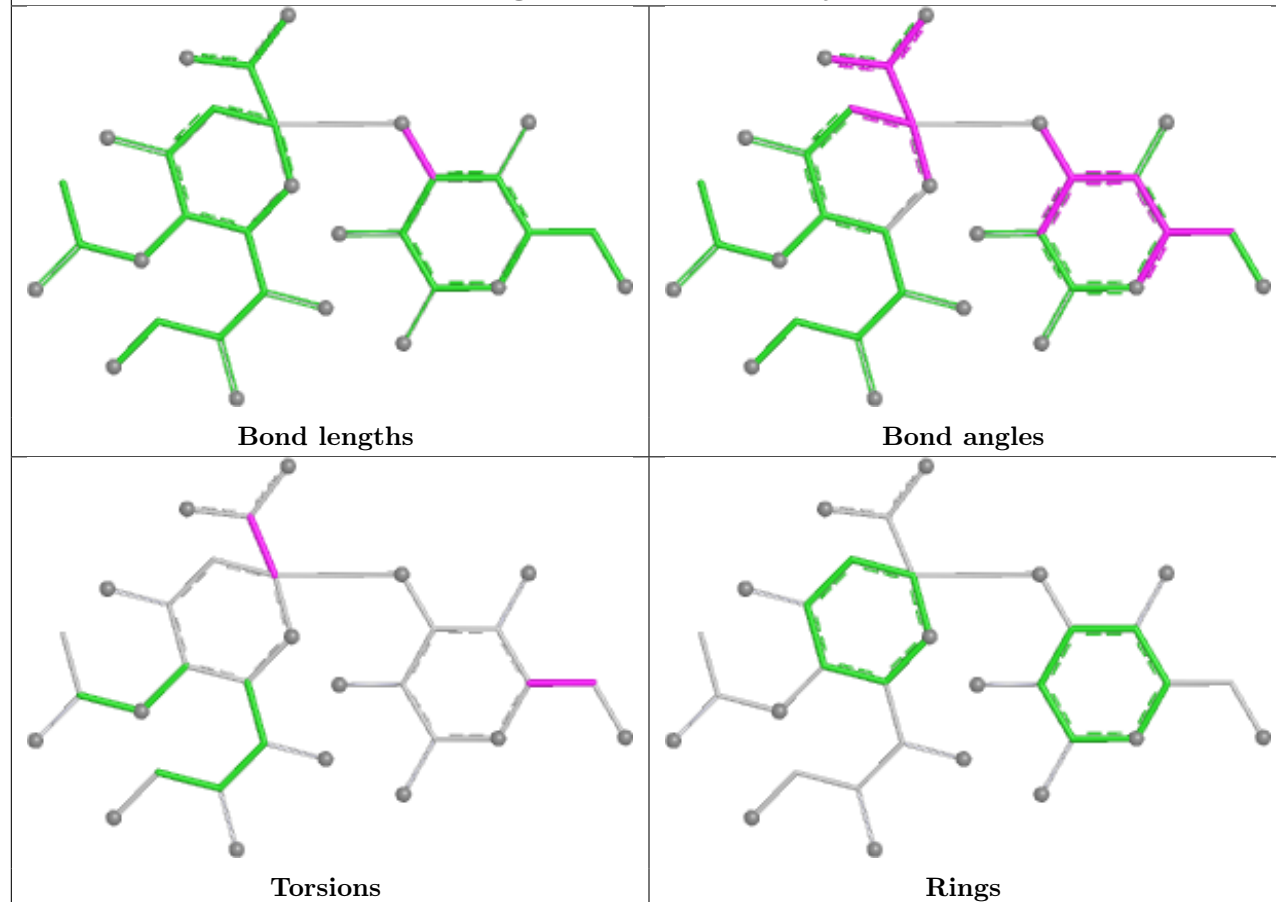




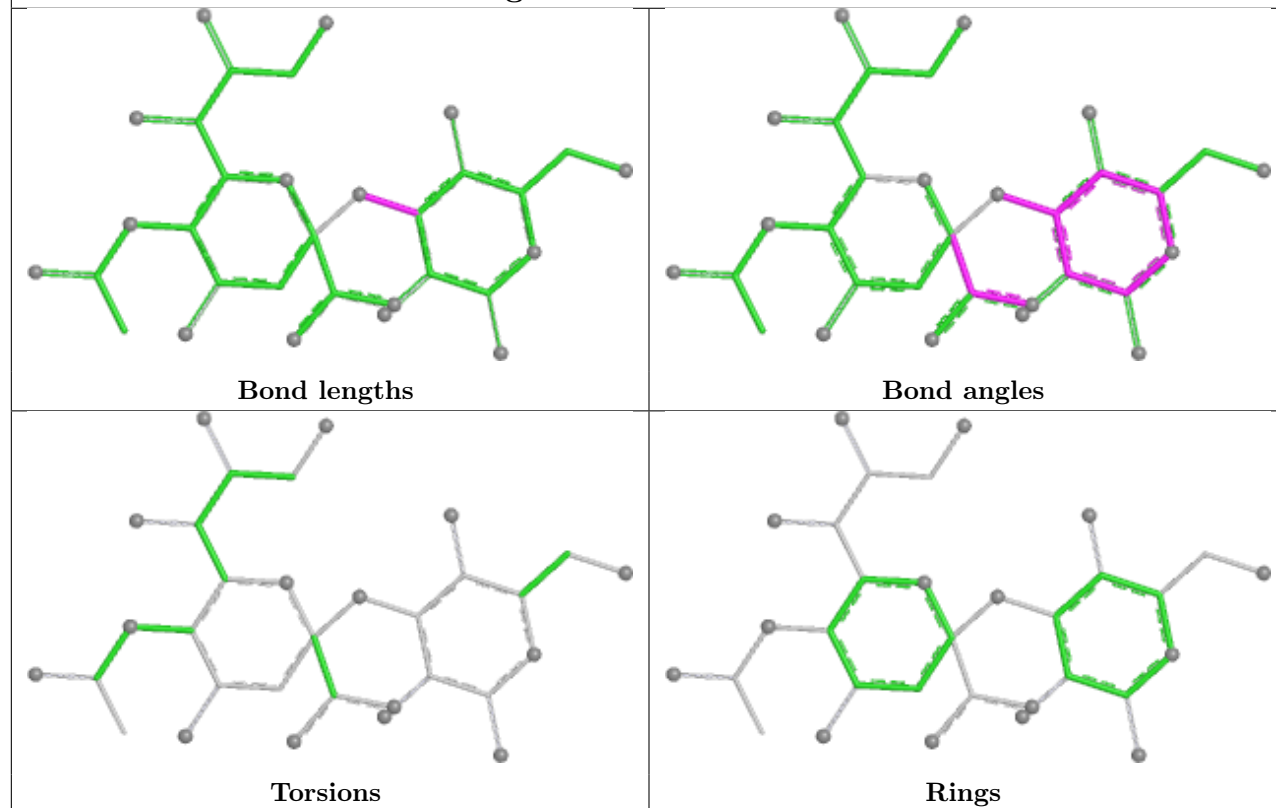


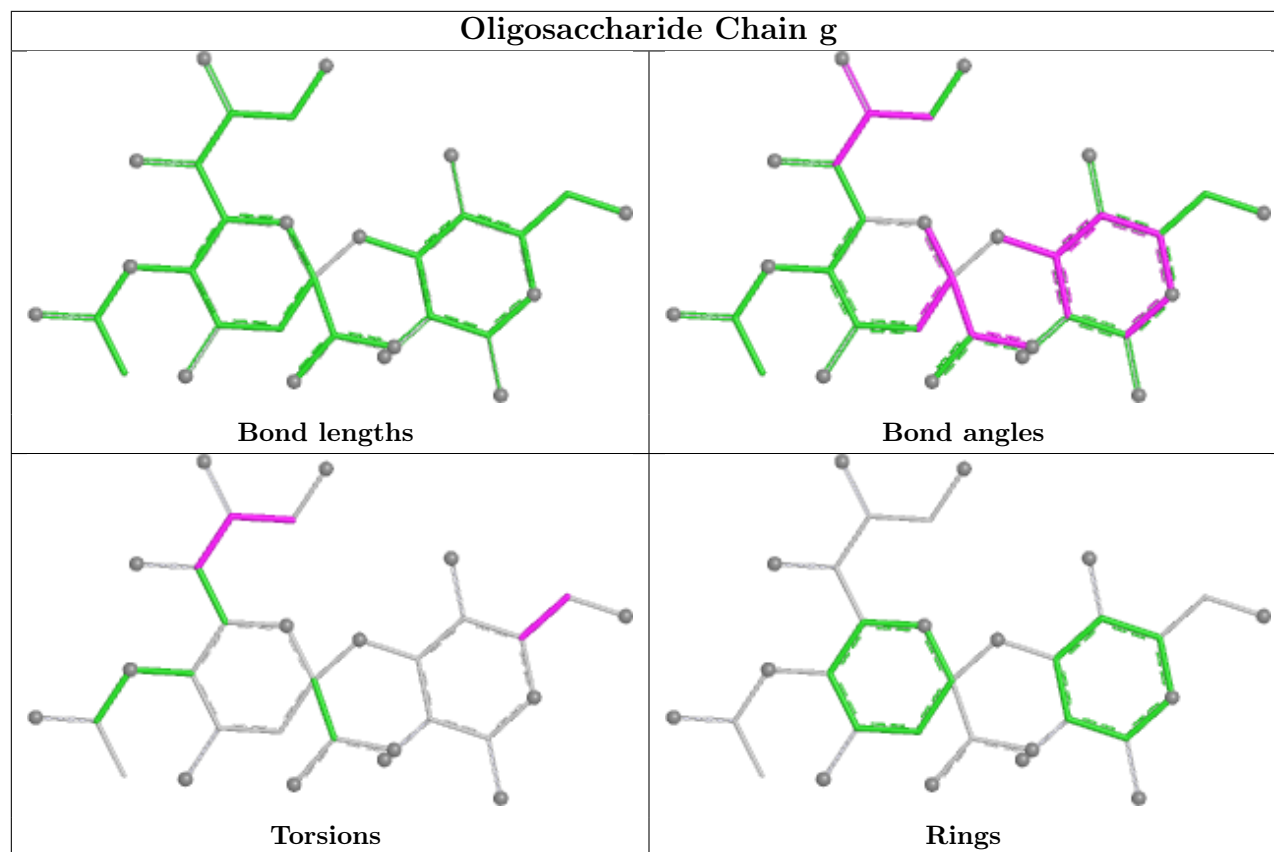


Oligosaccharide Chain j



Oligosaccharide Chain b





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, 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	117/124 (94%)	0.82	7 (5%) 27 21	36, 40, 43, 44	0
1	B	117/124 (94%)	2.76	68 (58%) 0 0	27, 34, 40, 42	0
1	G	123/124 (99%)	0.17	3 (2%) 59 50	35, 40, 44, 47	0
1	J	123/124 (99%)	0.34	2 (1%) 70 62	35, 40, 44, 47	0
1	K	123/124 (99%)	0.30	3 (2%) 59 50	35, 40, 44, 48	0
1	O	118/124 (95%)	0.24	1 (0%) 82 76	37, 40, 43, 43	0
1	P	123/124 (99%)	0.23	2 (1%) 70 62	36, 40, 43, 46	0
1	T	119/124 (95%)	0.44	4 (3%) 48 38	37, 40, 43, 45	0
1	V	121/124 (97%)	0.69	7 (5%) 29 22	36, 40, 43, 47	0
1	X	123/124 (99%)	0.22	1 (0%) 82 76	36, 40, 44, 47	0
1	Y	119/124 (95%)	0.35	1 (0%) 82 76	35, 40, 43, 45	0
1	Z	117/124 (94%)	0.56	5 (4%) 40 31	37, 40, 43, 44	0
2	C	182/197 (92%)	-0.13	0 100 100	38, 40, 42, 46	0
2	D	182/197 (92%)	0.19	2 (1%) 78 71	39, 40, 42, 44	0
2	E	182/197 (92%)	-0.12	0 100 100	38, 40, 42, 44	0
2	F	182/197 (92%)	-0.17	0 100 100	39, 40, 42, 47	0
2	H	182/197 (92%)	-0.12	0 100 100	39, 40, 42, 46	0
2	I	182/197 (92%)	0.18	2 (1%) 78 71	39, 40, 42, 44	0
2	L	182/197 (92%)	-0.07	1 (0%) 87 83	39, 40, 42, 45	0
2	M	182/197 (92%)	-0.09	0 100 100	39, 40, 41, 44	0
2	N	182/197 (92%)	-0.07	2 (1%) 78 71	39, 40, 42, 47	0
2	Q	182/197 (92%)	-0.05	1 (0%) 87 83	39, 40, 42, 45	0
2	R	182/197 (92%)	-0.17	0 100 100	39, 40, 42, 45	0
2	S	182/197 (92%)	-0.03	0 100 100	39, 40, 42, 45	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	3627/3852 (94%)	0.20	112 (3%)	51	41	27, 40, 43, 48	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	LEU	8.3
1	B	46	SER	7.6
1	B	136	VAL	7.4
1	B	126	PRO	6.9
1	B	47	PRO	6.5
1	B	109	ASN	6.4
1	B	52	PRO	6.3
1	B	50	GLN	6.3
1	B	21	SER	6.0
1	B	127	GLY	5.8
1	B	49	ASP	5.6
1	B	32	ALA	5.6
1	B	114	ASP	5.2
1	B	124	LYS	5.1
1	B	125	ALA	5.0
1	B	45	LEU	5.0
1	B	51	GLY	4.9
1	B	48	GLU	4.6
1	B	112	LEU	4.3
1	G	17	ALA	4.3
1	B	128	VAL	4.1
1	B	35	GLU	4.1
1	B	123	LYS	4.0
1	B	106	ASN	3.9
1	B	129	ALA	3.9
1	B	75	SER	3.8
1	B	44	THR	3.8
1	B	108	THR	3.7
1	B	89	GLY	3.6
1	B	22	ILE	3.5
1	B	91	VAL	3.5
1	B	53	LEU	3.4
1	P	139	VAL	3.4
1	B	63	ASP	3.3
1	B	80	TYR	3.2
1	Y	82	ASP	3.2
1	B	33	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	Z	48	GLU	3.2
1	B	121	LYS	3.1
1	B	99	LYS	3.1
1	B	37	ALA	3.1
1	B	28	MET	3.1
1	B	84	TYR	3.0
1	V	17	ALA	3.0
1	B	130	ASN	3.0
1	B	74	TYR	2.9
1	B	54	ASP	2.9
1	B	43	PHE	2.9
1	B	122	VAL	2.8
1	B	87	LEU	2.7
1	B	90	ARG	2.7
1	B	135	LEU	2.7
1	B	118	TYR	2.7
1	B	110	LEU	2.7
1	B	76	GLY	2.6
1	B	78	LYS	2.6
1	B	102	ASP	2.6
1	J	52	PRO	2.6
1	V	52	PRO	2.6
1	B	64	ASN	2.6
1	B	66	LYS	2.6
1	B	103	ALA	2.6
1	Z	31	LYS	2.6
1	B	113	SER	2.6
1	B	107	VAL	2.5
2	L	458	HIS	2.5
1	A	126	PRO	2.5
1	G	28	MET	2.4
1	V	28	MET	2.4
1	G	25	PRO	2.4
1	B	83	TYR	2.4
2	N	378	ASN	2.4
1	V	65	GLN	2.4
1	A	82	ASP	2.3
1	B	36	THR	2.3
1	K	82	ASP	2.3
1	P	82	ASP	2.3
1	K	16	PHE	2.3
1	X	28	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLN	2.3
2	N	458	HIS	2.3
1	B	55	ILE	2.3
1	J	139	VAL	2.3
1	V	137	VAL	2.3
1	A	34	GLY	2.3
1	T	30	GLU	2.2
1	B	77	ASP	2.2
1	B	61	PRO	2.2
1	B	67	VAL	2.2
1	T	64	ASN	2.2
2	I	378	ASN	2.2
1	Z	28	MET	2.2
2	D	361	ALA	2.2
1	A	47	PRO	2.2
1	O	63	ASP	2.2
1	T	136	VAL	2.2
1	B	27	GLU	2.2
1	B	79	ILE	2.1
1	V	115	ILE	2.1
2	D	458	HIS	2.1
1	B	31	LYS	2.1
1	B	34	GLY	2.1
1	A	45	LEU	2.1
2	Q	542	GLN	2.1
1	V	51	GLY	2.0
1	A	36	THR	2.0
1	B	94	THR	2.0
1	K	63	ASP	2.0
2	I	361	ALA	2.0
1	Z	46	SER	2.0
1	T	76	GLY	2.0
1	Z	63	ASP	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 ⓘ

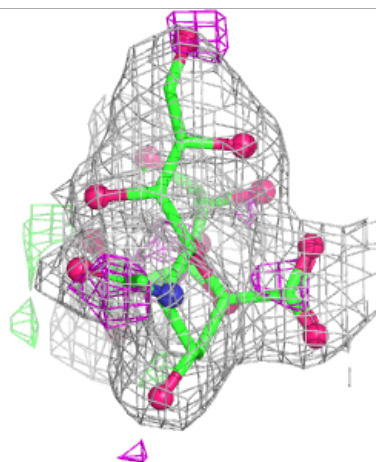
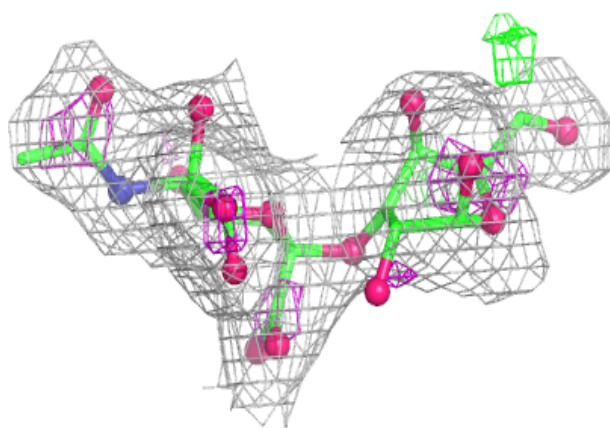
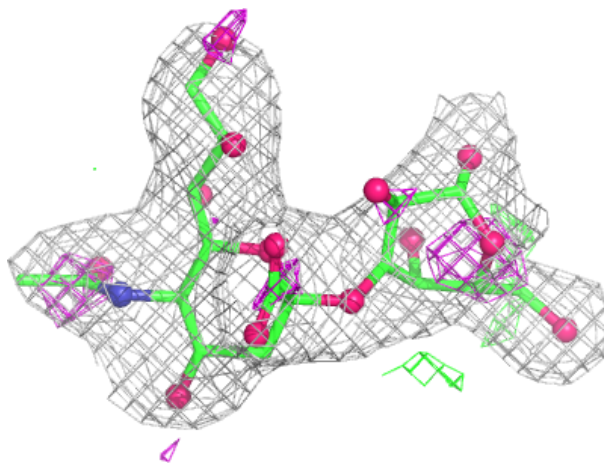
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GAL	U	1	12/12	-	-	45,53,54,55	0
3	SIA	U	2	20/21	-	-	34,37,39,39	0
3	GAL	W	1	12/12	-	-	58,68,69,69	0
3	SIA	W	2	20/21	-	-	41,46,54,54	0
3	GAL	a	1	12/12	-	-	48,53,54,54	0
3	SIA	a	2	20/21	-	-	32,40,42,42	0
3	GAL	c	1	12/12	-	-	46,51,53,54	0
3	SIA	c	2	20/21	-	-	33,38,41,41	0
3	GAL	d	1	12/12	-	-	50,60,64,65	0
3	SIA	d	2	20/21	-	-	31,36,43,43	0
3	GAL	e	1	12/12	-	-	50,59,60,61	0
3	SIA	e	2	20/21	-	-	36,39,43,44	0
3	GAL	f	1	12/12	-	-	45,52,56,56	0
3	SIA	f	2	20/21	-	-	31,34,39,40	0
3	GAL	h	1	12/12	-	-	53,61,64,65	0
3	SIA	h	2	20/21	-	-	38,42,48,48	0
3	GAL	i	1	12/12	-	-	48,57,59,60	0
3	SIA	i	2	20/21	-	-	31,37,43,45	0
3	GAL	j	1	12/12	-	-	54,62,63,64	0
3	SIA	j	2	20/21	-	-	42,44,49,49	0
4	GL0	b	1	12/12	-	-	51,60,63,63	0
4	SIA	b	2	20/21	-	-	36,40,45,45	0
4	GL0	g	1	12/12	-	-	43,51,56,58	0
4	SIA	g	2	20/21	-	-	31,35,38,38	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.

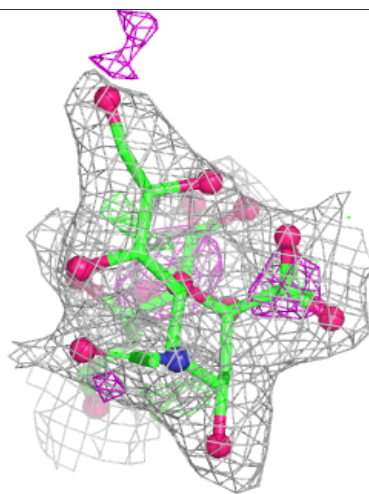
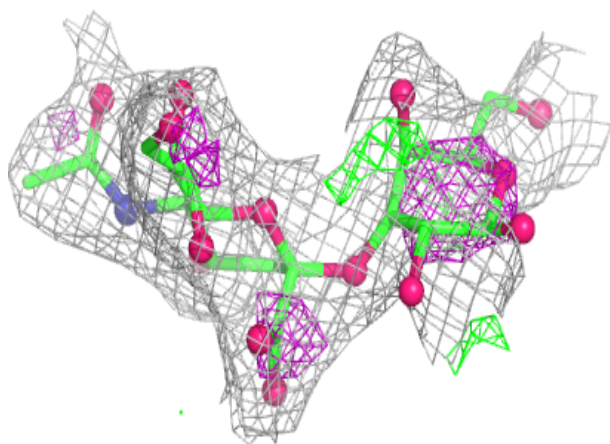
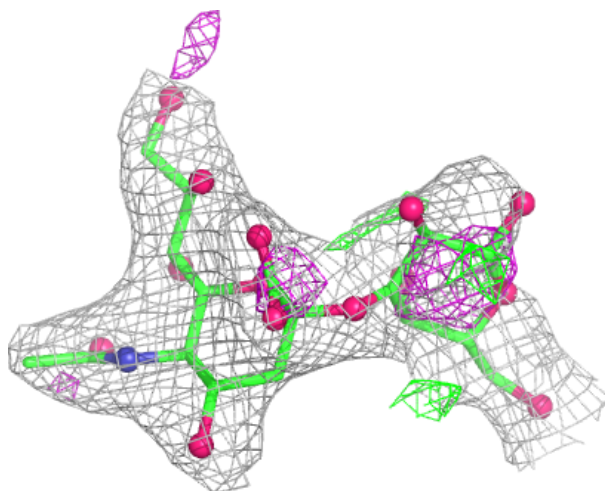
Electron density around Chain U:

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



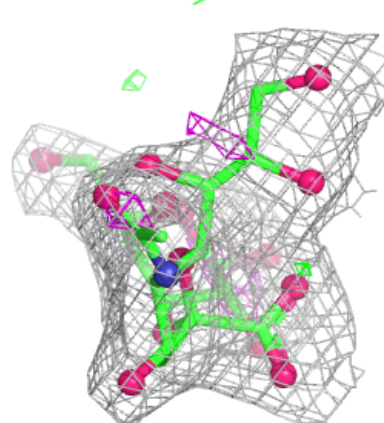
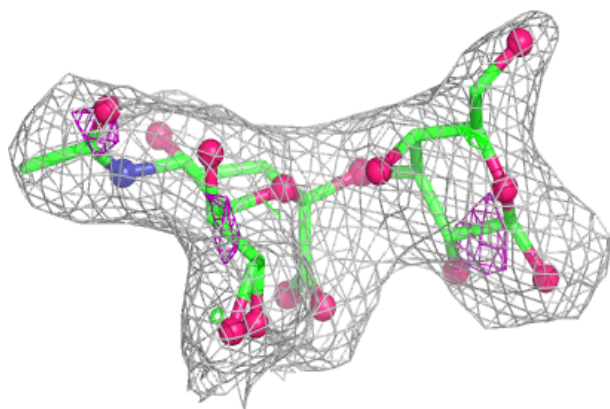
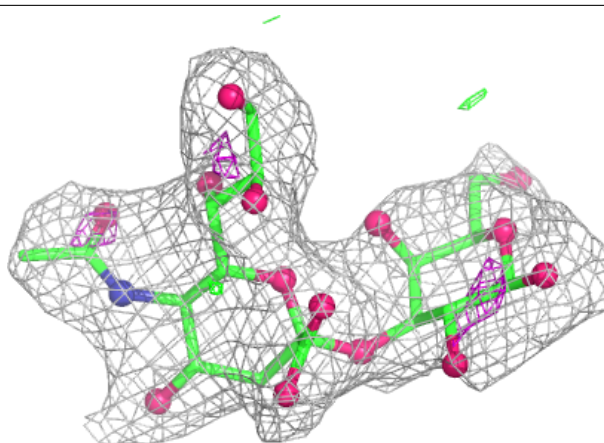
Electron density around Chain W:

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



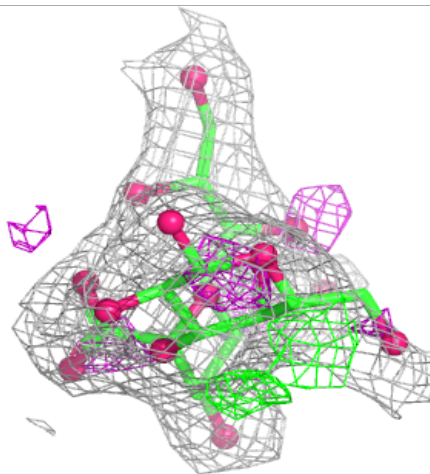
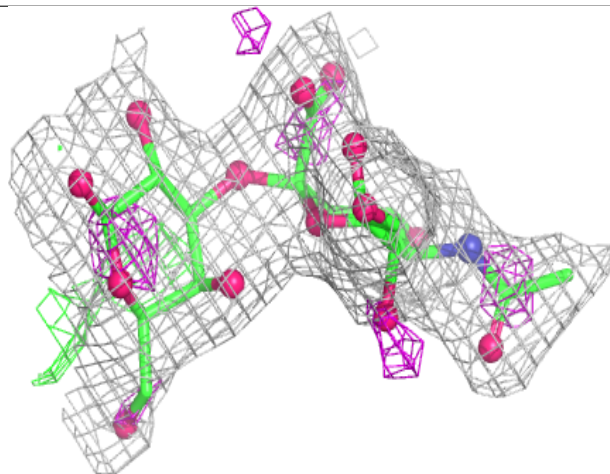
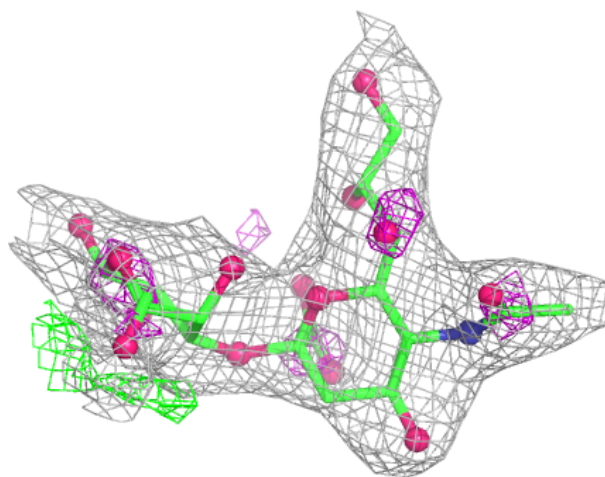
Electron density around Chain a:

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



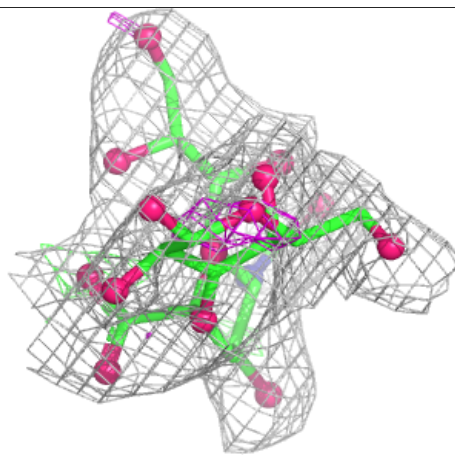
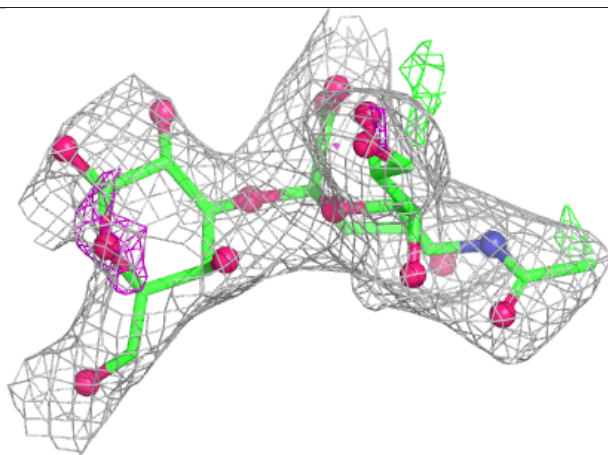
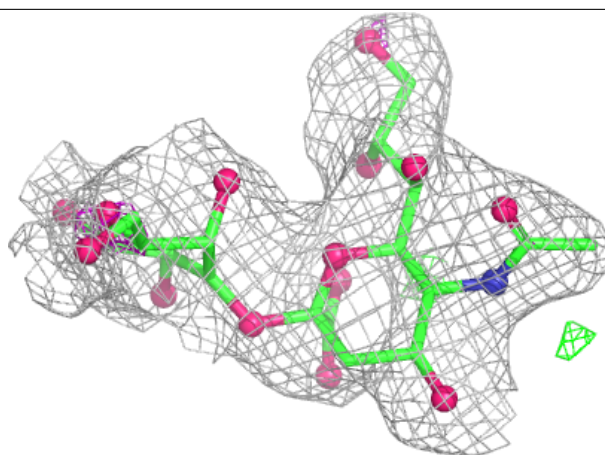
Electron density around Chain c:

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



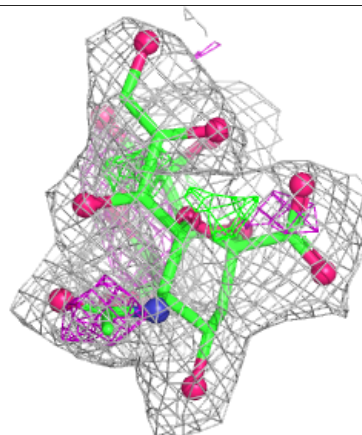
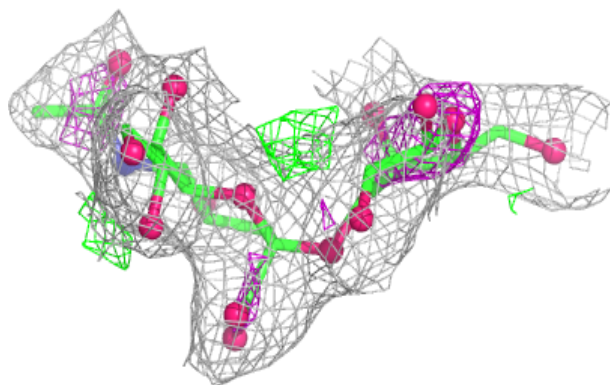
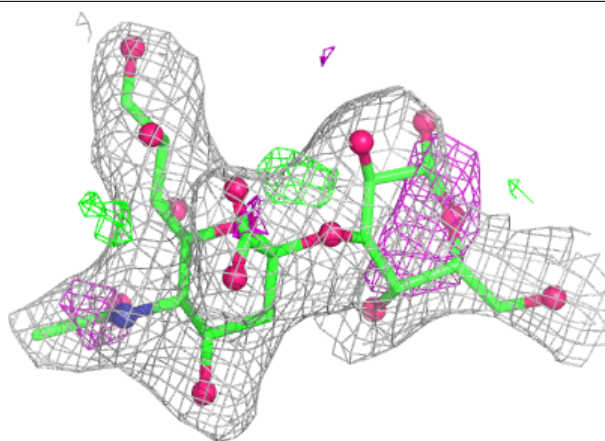
Electron density around Chain d:

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



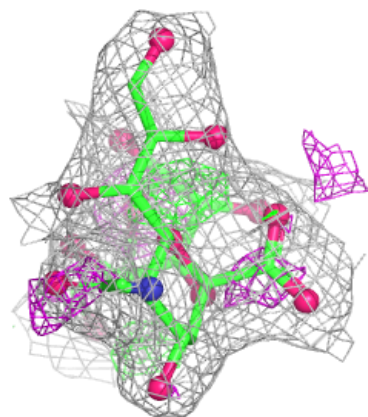
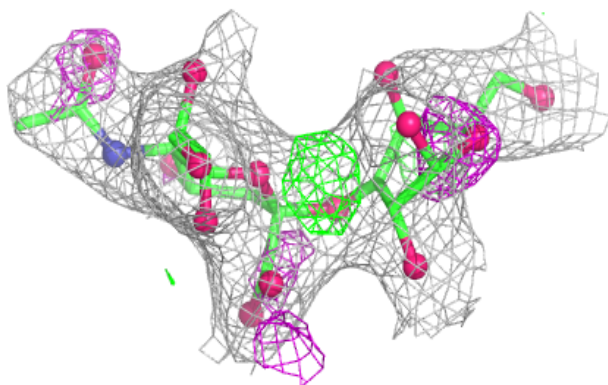
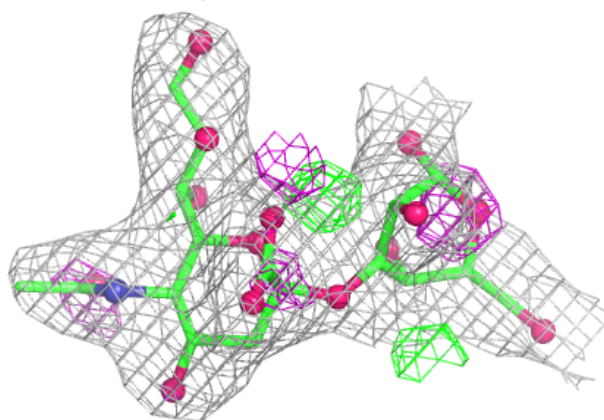
Electron density around Chain e:

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



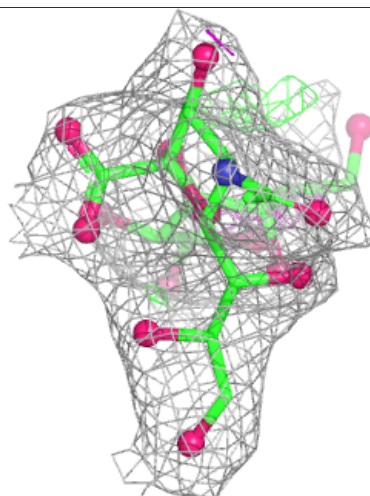
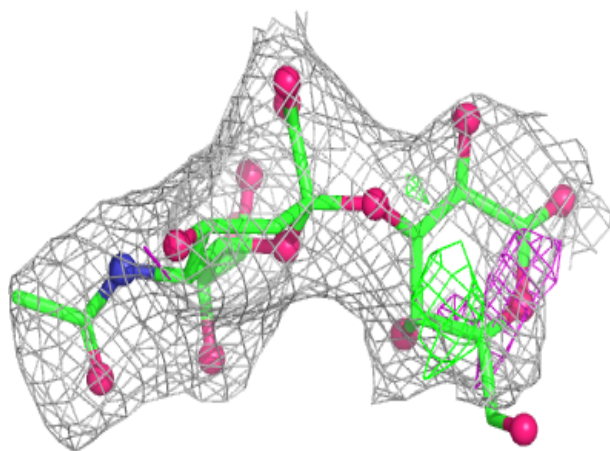
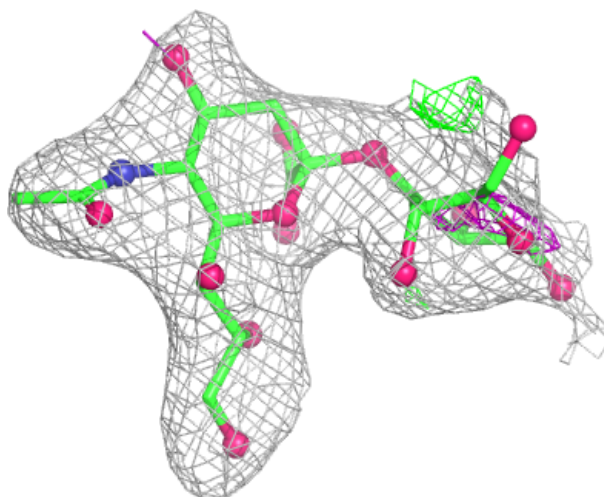
Electron density around Chain f:

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



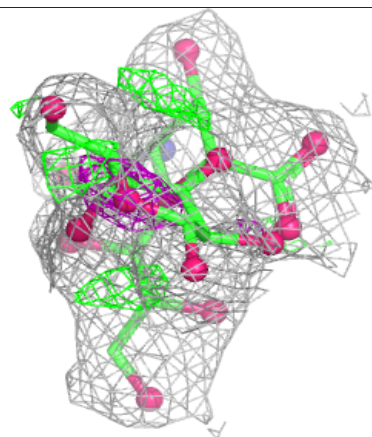
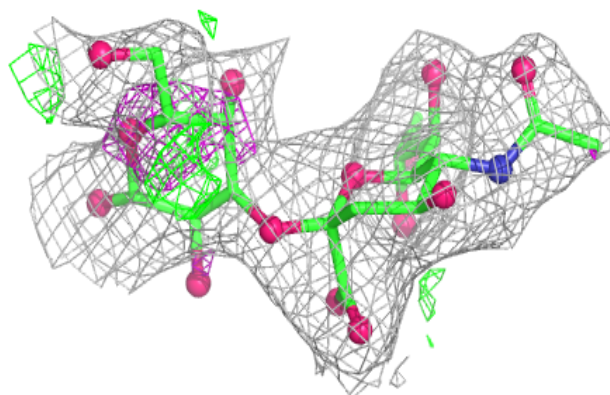
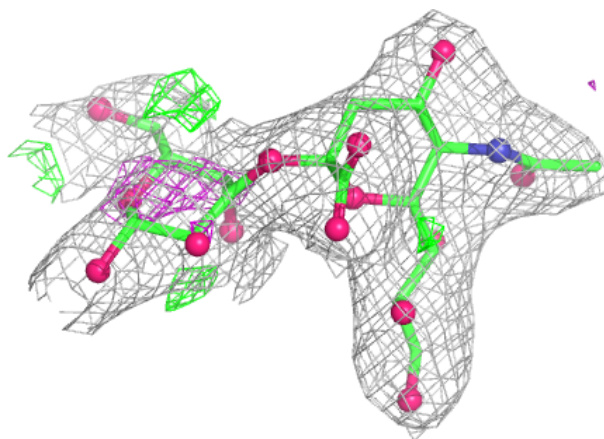
Electron density around Chain h:

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



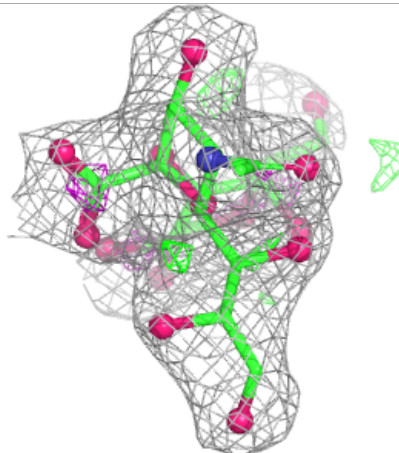
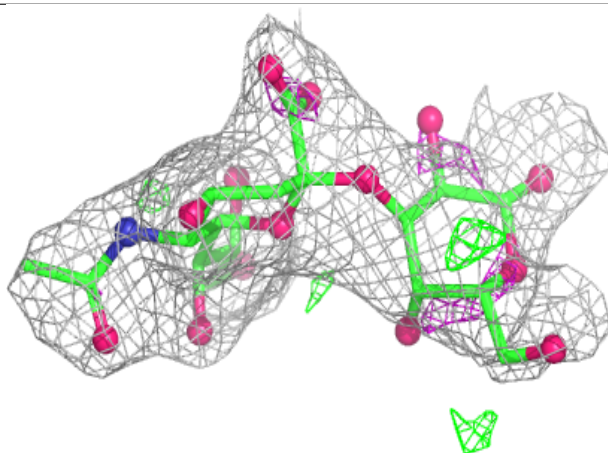
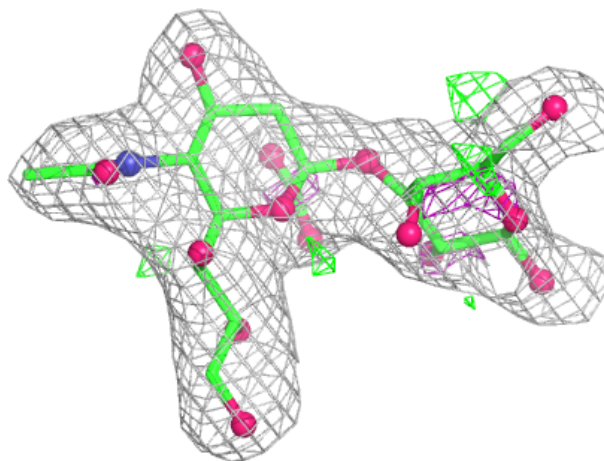
Electron density around Chain i:

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



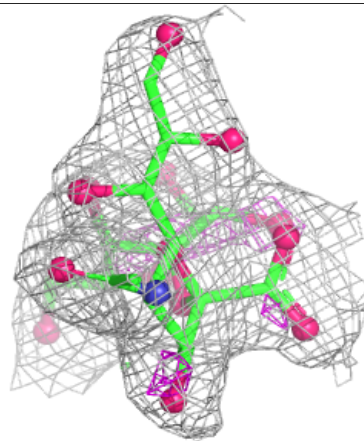
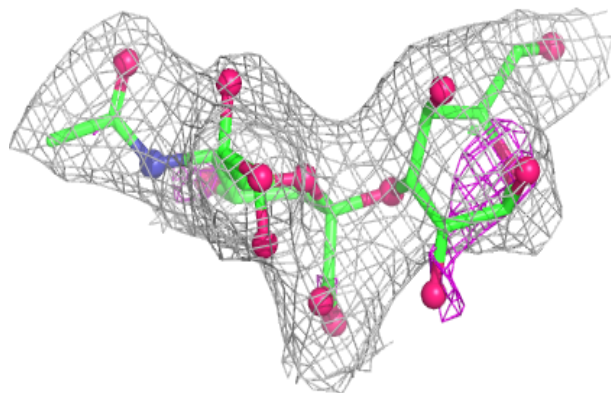
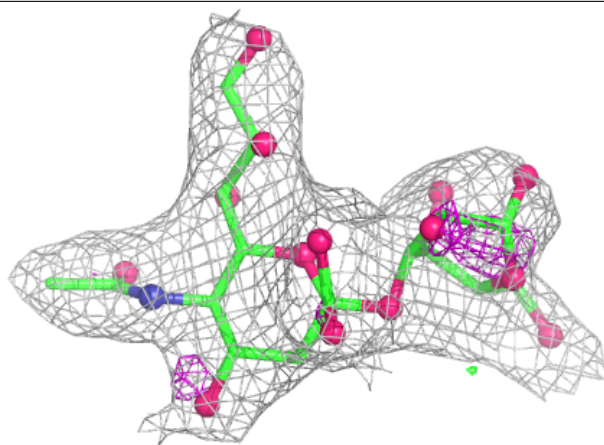
Electron density around Chain j:

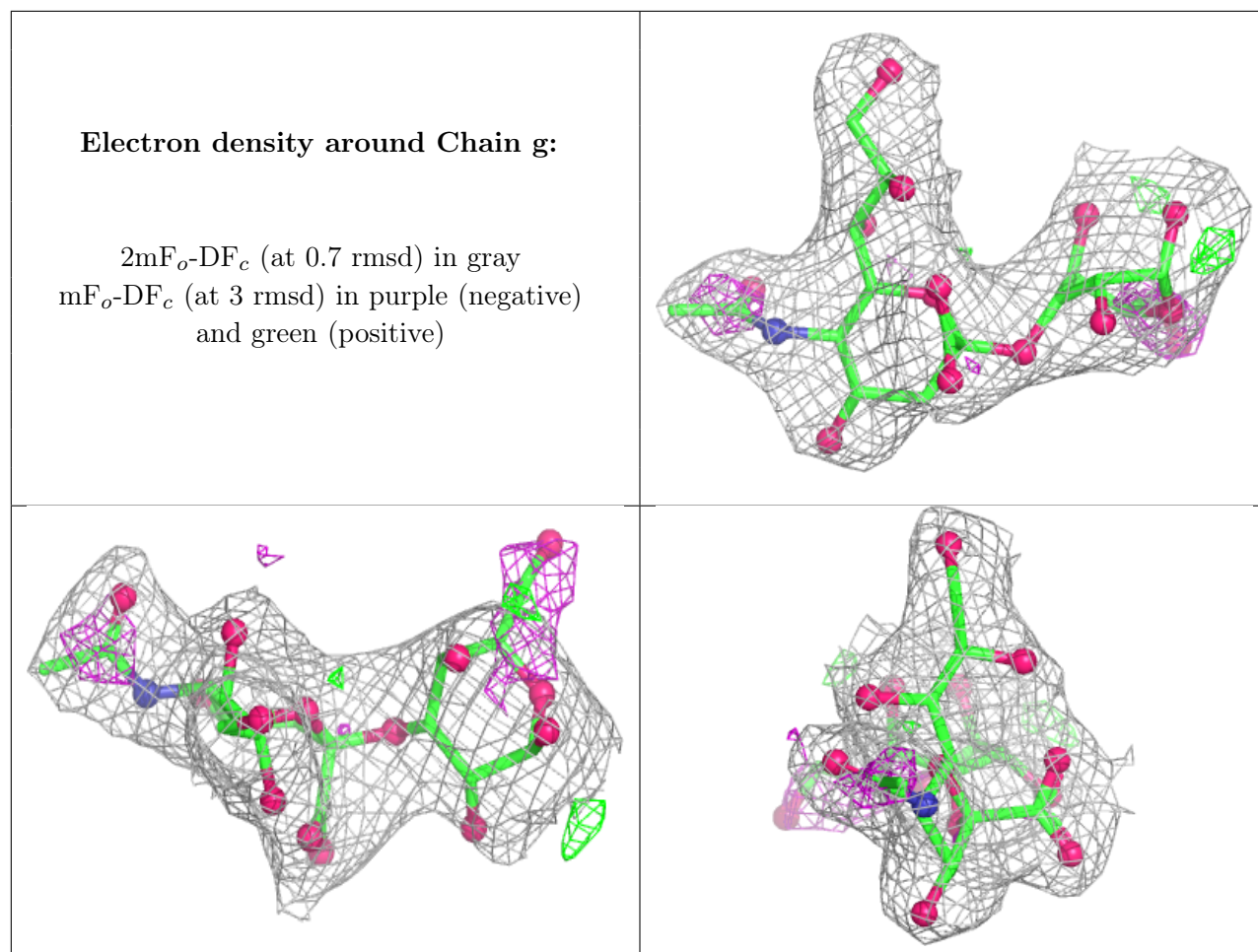
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain b:

$2mF_o-DF_c$ (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.