



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:51 AM BST

PDB ID : 5XQJ
Title : Crystal structure of a PL 26 exo-rhamnogalacturonan lyase from *Penicillium chrysogenum* complexed with unsaturated galacturonosyl rhamnose substituted with galactose
Authors : Kunishige, Y.; Iwai, M.; Tada, T.; Nishimura, S.; Sakamoto, T.
Deposited on : 2017-06-07
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

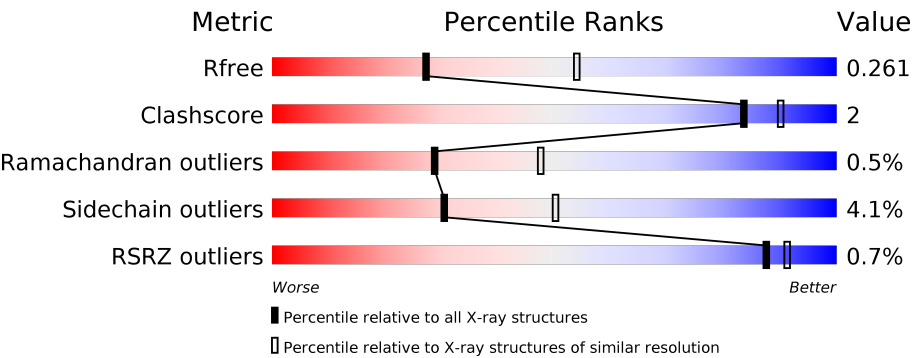
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





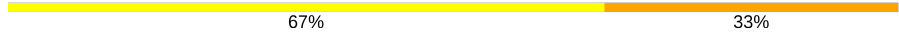
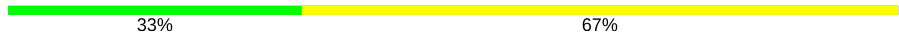



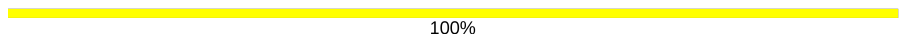
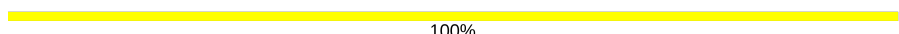
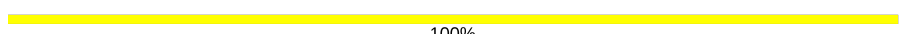
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	906	<div><div></div><div>88%10%..</div></div>
1	B	906	<div><div></div><div>90%8%..</div></div>
1	C	906	<div><div>%</div><div>88%9%..</div></div>
1	D	906	<div><div>%</div><div>89%8%..</div></div>
1	E	906	<div><div>%</div><div>90%8%..</div></div>
1	F	906	<div><div></div><div>90%9%. </div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	906	 88% 9% ..
1	H	906	 89% 8% ..
2	I	3	 67% 33%
2	K	3	 33% 67%
2	M	3	 33% 67%
2	N	3	 67% 33%
2	O	3	 67% 33%
3	J	2	 100%
3	L	2	 100%
3	P	2	 100%

2 Entry composition [i](#)

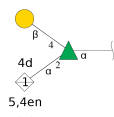
There are 5 unique types of molecules in this entry. The entry contains 57136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Percglx protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	896	Total	C	N	O	S	0	1	0
			7025	4479	1178	1362	6			
1	B	896	Total	C	N	O	S	0	2	0
			7052	4492	1182	1372	6			
1	C	885	Total	C	N	O	S	0	5	0
			7007	4473	1176	1352	6			
1	D	884	Total	C	N	O	S	0	6	0
			6992	4463	1174	1349	6			
1	E	900	Total	C	N	O	S	0	1	0
			7062	4497	1185	1374	6			
1	F	900	Total	C	N	O	S	0	0	0
			7040	4487	1183	1364	6			
1	G	886	Total	C	N	O	S	0	1	0
			6976	4452	1168	1351	5			
1	H	888	Total	C	N	O	S	0	1	0
			6997	4462	1174	1355	6			

- Molecule 2 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose.



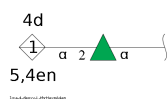
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	3	Total	C	O	0	0	0
			33	18	15			
2	K	3	Total	C	O	0	0	0
			33	18	15			
2	M	3	Total	C	O	0	0	0
			33	18	15			
2	N	3	Total	C	O	0	0	0
			33	18	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	O	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 3 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	J	2	Total	C	O	0	0	0
			22	12	10			
3	L	2	Total	C	O	0	0	0
			22	12	10			
3	P	2	Total	C	O	0	0	0
			22	12	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	H	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		

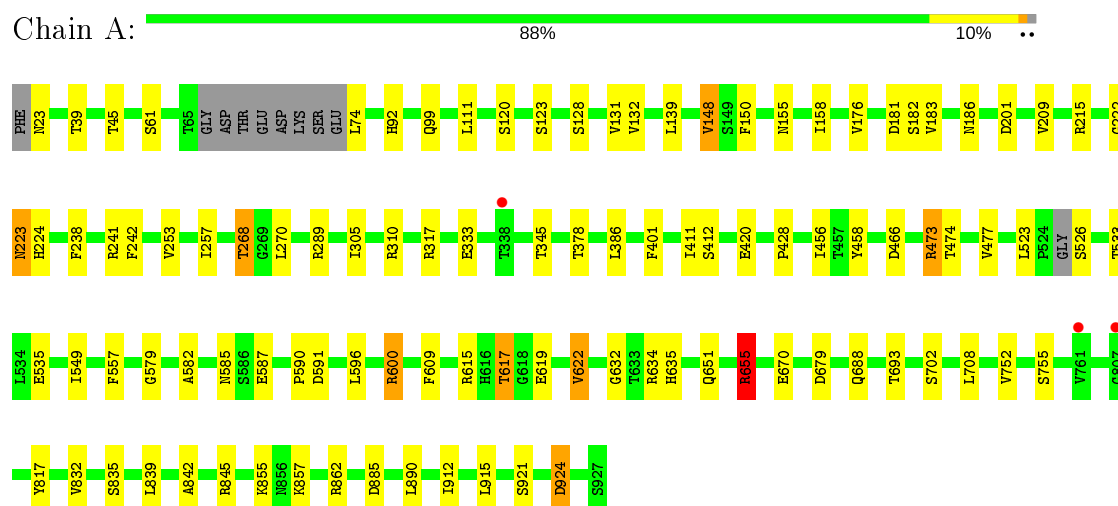
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total 119	O 119	0	0
5	B	108	Total 108	O 108	0	0
5	C	103	Total 103	O 103	0	0
5	D	92	Total 92	O 92	0	0
5	E	92	Total 92	O 92	0	0
5	F	98	Total 98	O 98	0	0
5	G	72	Total 72	O 72	0	0
5	H	62	Total 62	O 62	0	0

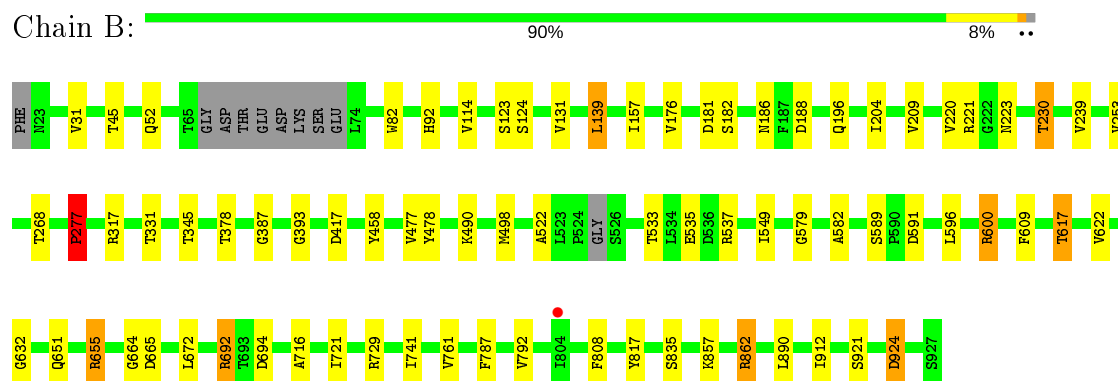
3 Residue-property plots

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.

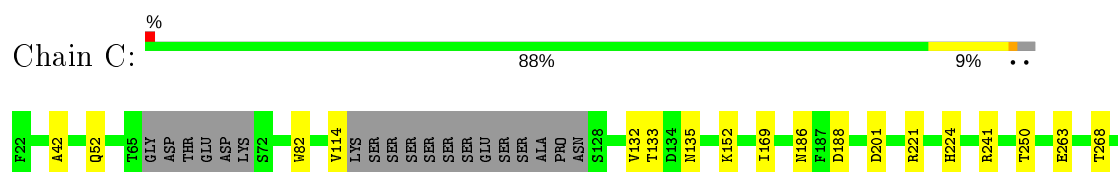
• Molecule 1: Pcrglx protein

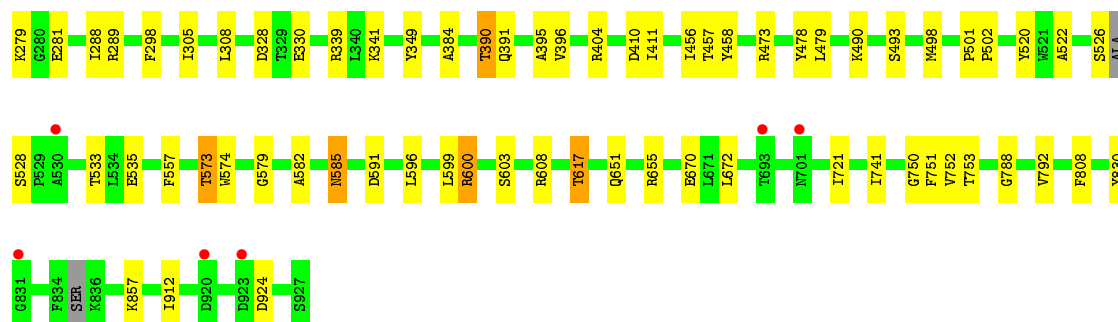


• Molecule 1: Pcrglx protein

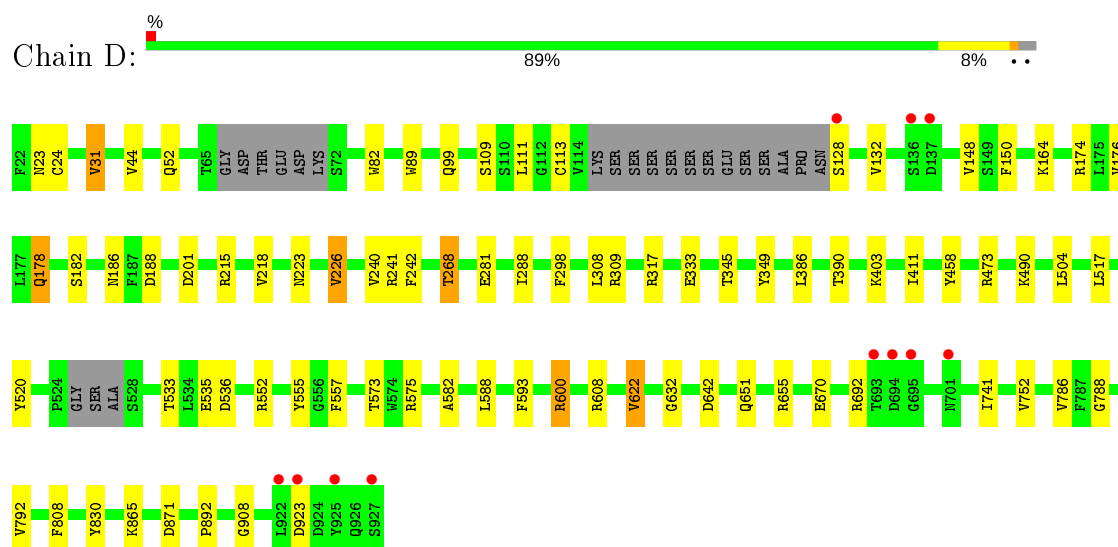


• Molecule 1: Pcrglx protein

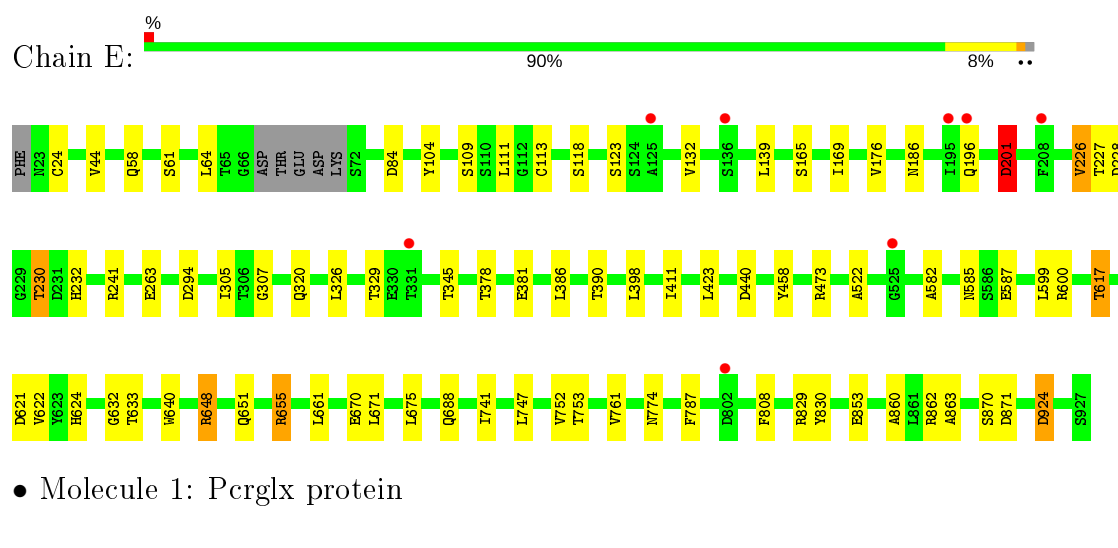




● Molecule 1: Pcrglx protein

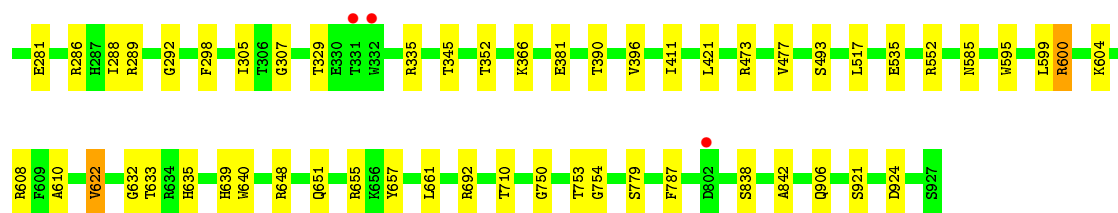


● Molecule 1: Pcrglx protein

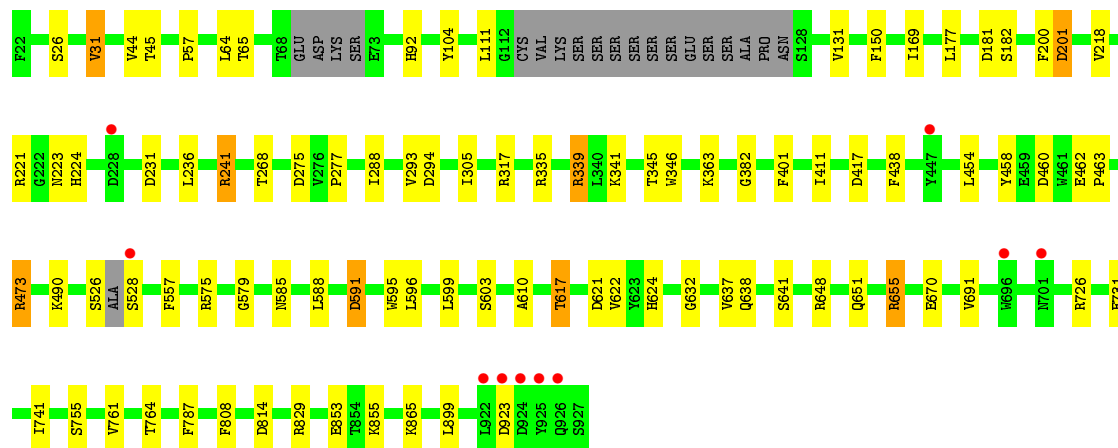
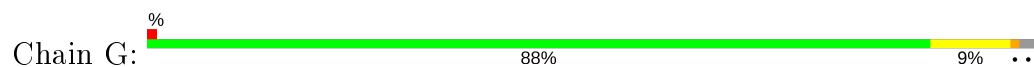


● Molecule 1: Pcrglx protein

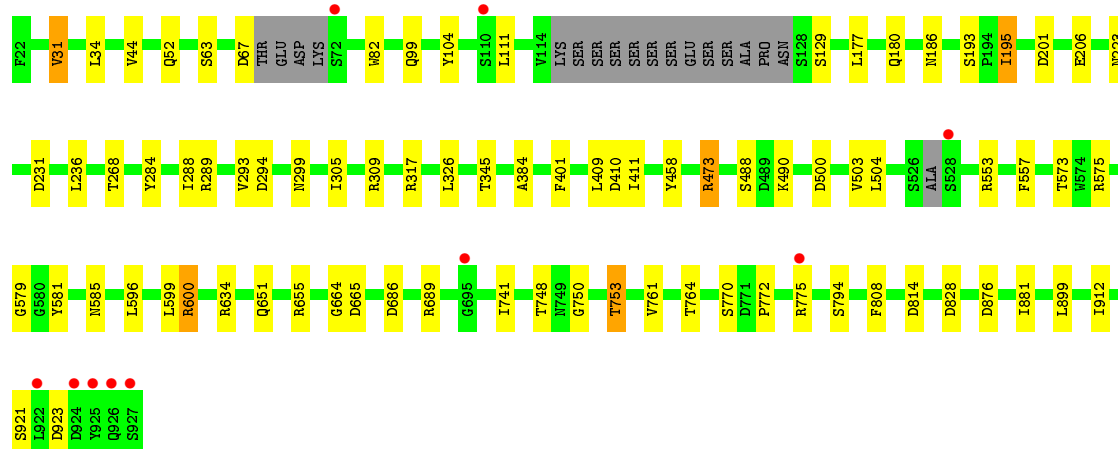
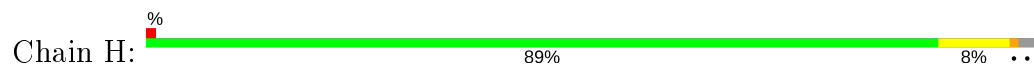




• Molecule 1: Pcrglx protein



• Molecule 1: Pcrglx protein



• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose



- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain K:  33% 67%

RAM1
GAD2
GAL3

- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain M:  33% 67%

RAM1
GAD2
GAL3

- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain N:  67% 33%

RAM1
GAD2
GAL3

- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain O:  67% 33%

RAM1
GAD2
GAL3

- Molecule 3: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain J:  100%

RAM1
GAD2

- Molecule 3: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain L:  100%

RAM1
GAD2

- Molecule 3: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain P:  100%

RAM1
GAD2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	167.62Å 171.80Å 342.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.17 – 2.75 49.12 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (171.17-2.75) 99.9 (49.12-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.196 , 0.262 0.200 , 0.261	Depositor DCC
R_{free} test set	12900 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	57136	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4459e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RAM, CA, GAD, GAL

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	0.73	0/7232	0.88	14/9878 (0.1%)
1	B	0.73	0/7256	0.87	11/9907 (0.1%)
1	C	0.70	0/7223	0.84	5/9857 (0.1%)
1	D	0.71	0/7218	0.86	16/9854 (0.2%)
1	E	0.71	0/7270	0.84	7/9925 (0.1%)
1	F	0.72	0/7245	0.88	10/9892 (0.1%)
1	G	0.69	0/7183	0.86	13/9804 (0.1%)
1	H	0.71	0/7204	0.87	15/9833 (0.2%)
All	All	0.71	0/57831	0.86	91/78950 (0.1%)

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	F	552	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	E	924	ASP	CB-CG-OD1	7.73	125.26	118.30
1	G	317	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	692	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	600	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	600	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	G	814	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	H	473	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	H	309	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	G	382	GLY	N-CA-C	7.10	130.84	113.10
1	H	309	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	D	317	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	317	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	D	23	ASN	CB-CA-C	-6.82	96.77	110.40
1	B	181	ASP	CB-CG-OD1	6.79	124.41	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	600	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	F	600	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	655	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	D	600	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	F	608	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	H	317	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	H	317	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	H	500	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	H	289	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	E	862	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	692	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	466	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	608	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	600	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	F	600	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	G	726	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	537	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	G	317	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	D	692	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	H	473	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	F	286	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	C	339	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	F	221	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	317	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	289	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	221	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	E	226	VAL	CB-CA-C	-5.88	100.22	111.40
1	E	862	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	G	814	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	473	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	G	473	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	G	181	ASP	CB-CG-OD1	5.81	123.53	118.30
1	F	74	LEU	N-CA-C	5.79	126.64	111.00
1	D	575	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	729	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	E	829	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	575	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	600	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	H	553	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	139	LEU	CA-CB-CG	5.68	128.37	115.30
1	G	275	ASP	CB-CG-OD1	5.68	123.41	118.30
1	D	309	ARG	NE-CZ-NH2	-5.66	117.47	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	862	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	H	600	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	885	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	174	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	H	814	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	404	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	G	221	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	E	440	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	845	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	H	634	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	289	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	309	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	181	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	H	500	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	600	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	552	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	G	829	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	G	241	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	F	473	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	226	VAL	CB-CA-C	-5.27	101.38	111.40
1	A	223	ASN	CB-CA-C	-5.27	99.85	110.40
1	G	339	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	679	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	181	ASP	CB-CG-OD1	5.25	123.03	118.30
1	F	221	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	F	692	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	D	536	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	871	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	201	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	600	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	H	553	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	317	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	615	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7025	0	6584	41	0
1	B	7052	0	6618	30	0
1	C	7007	0	6588	35	0
1	D	6992	0	6570	27	0
1	E	7062	0	6638	32	0
1	F	7040	0	6601	24	0
1	G	6976	0	6539	37	0
1	H	6997	0	6567	35	0
2	I	33	0	26	2	0
2	K	33	0	25	0	0
2	M	33	0	26	3	0
2	N	33	0	26	1	0
2	O	33	0	25	1	0
3	J	22	0	17	0	0
3	L	22	0	17	0	0
3	P	22	0	17	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	119	0	0	4	0
5	B	108	0	0	0	0
5	C	103	0	0	3	0
5	D	92	0	0	0	0
5	E	92	0	0	3	0
5	F	98	0	0	1	0
5	G	72	0	0	1	0
5	H	62	0	0	0	0
All	All	57136	0	52884	256	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 2.

All (256) 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:D:24:CYS:SG	1:D:113:CYS:CB	2.21	1.27
1:H:180:GLN:CD	1:H:195:ILE:CD1	2.44	0.86
1:D:24:CYS:CB	1:D:113:CYS:SG	2.67	0.83
1:C:526:SER:O	1:C:528:SER:N	2.17	0.78
1:F:73:GLU:CA	5:F:1191:HOH:O	2.32	0.77
1:D:178[A]:GLN:HG3	1:D:268:THR:HG22	1.72	0.71
1:H:180:GLN:NE2	1:H:195:ILE:CD1	2.54	0.71
1:B:522:ALA:O	1:B:600:ARG:HD2	1.91	0.71
1:H:180:GLN:CD	1:H:195:ILE:HD12	2.10	0.70
1:E:688:GLN:HE22	2:M:3:GAL:H2	1.56	0.70
1:G:648:ARG:HG2	1:G:787:PHE:CD2	2.25	0.70
1:A:241:ARG:NH2	1:A:670:GLU:OE2	2.25	0.69
1:B:617:THR:HG23	1:B:655:ARG:NH1	2.07	0.69
1:G:591:ASP:OD2	1:G:617:THR:HG21	1.94	0.67
1:D:281:GLU:OE1	1:D:390:THR:HB	1.98	0.64
1:A:591:ASP:OD2	1:A:617:THR:HG21	1.98	0.63
1:F:648:ARG:HG2	1:F:787:PHE:CD1	2.34	0.63
1:B:157:ILE:HD13	1:B:204:ILE:HD11	1.80	0.63
1:E:381:GLU:HG3	5:E:1103:HOH:O	1.99	0.63
1:F:599:LEU:HD21	1:F:661:LEU:HD11	1.81	0.62
1:G:277:PRO:O	1:G:417:ASP:O	2.18	0.62
1:A:617:THR:HG23	1:A:655:ARG:NH1	2.16	0.61
1:D:473:ARG:HD3	1:D:557:PHE:O	2.01	0.61
1:C:535:GLU:OE1	1:C:600:ARG:NH2	2.34	0.61
1:E:752:VAL:HG21	1:E:830:TYR:CZ	2.36	0.61
1:H:180:GLN:NE2	1:H:195:ILE:HD12	2.16	0.61
1:D:52:GLN:HA	1:D:82:TRP:CD1	2.37	0.60
1:A:155:ASN:HD22	1:A:201:ASP:HB3	1.68	0.58
1:E:741:ILE:HG23	1:E:808:PHE:CG	2.38	0.58
1:H:299:ASN:OD1	1:H:488:SER:OG	2.21	0.58
1:A:622:VAL:HA	1:A:632:GLY:HA2	1.86	0.57
1:C:391:GLN:HG2	5:C:1196:HOH:O	2.03	0.57
1:C:522:ALA:O	1:C:600:ARG:HD2	2.04	0.57
1:E:241:ARG:NH2	1:E:670:GLU:OE2	2.37	0.57
1:A:74:LEU:N	5:A:1101:HOH:O	2.37	0.57
1:D:111:LEU:HD12	1:D:111:LEU:O	2.04	0.56
1:E:307:GLY:O	1:H:575:ARG:HD3	2.06	0.56
1:C:857:LYS:NZ	1:C:924:ASP:OD2	2.35	0.56
1:B:549:ILE:HD11	1:B:609:PHE:CE1	2.41	0.55
1:D:752:VAL:HG21	1:D:830:TYR:CZ	2.42	0.55
1:G:473:ARG:HD3	1:G:557:PHE:O	2.07	0.54
1:C:752:VAL:HG21	1:C:830:TYR:CZ	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:LYS:NZ	1:B:924:ASP:OD2	2.39	0.54
1:F:750:GLY:O	1:F:753:THR:OG1	2.26	0.53
1:C:135:ASN:O	1:C:152:LYS:NZ	2.40	0.53
1:A:596:LEU:O	1:A:600:ARG:HG3	2.09	0.53
1:G:31:VAL:HG12	1:G:104:TYR:HB2	1.90	0.53
1:B:817:TYR:O	1:B:862:ARG:NH2	2.42	0.53
1:E:386:LEU:HD22	1:E:411:ILE:HG23	1.91	0.53
1:H:31:VAL:HG12	1:H:104:TYR:HB2	1.90	0.53
1:B:139:LEU:HD11	1:B:209:VAL:HG21	1.91	0.52
1:H:177:LEU:HD22	1:H:236:LEU:HD22	1.92	0.52
1:G:691:VAL:HG21	2:O:3:GAL:H61	1.91	0.52
1:E:196:GLN:NE2	1:E:230:THR:HG21	2.24	0.52
1:C:201:ASP:O	1:C:224:HIS:HA	2.10	0.52
1:H:111:LEU:O	1:H:111:LEU:HD12	2.09	0.52
1:E:648:ARG:HG2	1:E:787:PHE:CD1	2.44	0.52
1:F:148:VAL:HG22	1:F:150:PHE:CE1	2.45	0.51
1:A:535:GLU:OE1	1:A:600:ARG:NH2	2.44	0.51
1:G:585:ASN:N	1:G:585:ASN:HD22	2.08	0.51
1:E:522:ALA:O	1:E:600:ARG:HG2	2.10	0.51
1:G:648:ARG:CG	1:G:787:PHE:CD2	2.94	0.51
1:A:310:ARG:NE	5:A:1102:HOH:O	2.40	0.51
1:E:196:GLN:HE21	1:E:230:THR:HG21	1.76	0.51
1:E:870:SER:OG	1:E:871:ASP:N	2.43	0.51
1:H:180:GLN:HB2	1:H:195:ILE:HD12	1.92	0.51
1:D:241:ARG:NH2	1:D:670:GLU:OE2	2.43	0.51
1:H:180:GLN:OE1	1:H:195:ILE:HD11	2.10	0.51
1:A:268:THR:O	1:A:428:PRO:HA	2.12	0.50
1:D:31:VAL:HG13	1:D:504:LEU:HB3	1.94	0.50
1:H:180:GLN:NE2	1:H:195:ILE:HD13	2.23	0.50
1:D:788:GLY:O	1:D:792:VAL:HG23	2.12	0.50
1:G:526:SER:CB	1:G:528:SER:N	2.75	0.50
1:C:288:ILE:HG23	1:C:411:ILE:CD1	2.41	0.50
1:G:622:VAL:HA	1:G:632:GLY:HA2	1.92	0.50
1:E:648:ARG:CG	1:E:787:PHE:CD1	2.95	0.50
1:G:617:THR:HG23	1:G:655:ARG:NH1	2.27	0.50
1:H:575:ARG:HD2	1:H:581:TYR:HB3	1.94	0.50
1:A:139:LEU:HD11	1:A:209:VAL:HG21	1.94	0.49
1:A:688:GLN:HE22	2:I:3:GAL:H2	1.77	0.49
1:H:31:VAL:HG13	1:H:504:LEU:HB3	1.94	0.49
1:D:535:GLU:OE1	1:D:600:ARG:NH2	2.39	0.49
1:G:169:ILE:C	1:G:169:ILE:HD12	2.32	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:HB2	1:A:420:GLU:HB2	1.94	0.49
1:B:277:PRO:O	1:B:417:ASP:O	2.30	0.49
1:E:587:GLU:OE1	2:M:2:GAD:O6A	2.31	0.49
1:E:860:ALA:O	1:E:863:ALA:HB3	2.13	0.49
1:G:111:LEU:HD12	1:G:111:LEU:O	2.12	0.49
5:A:1135:HOH:O	1:D:892:PRO:HD3	2.13	0.49
1:C:473:ARG:HD3	1:C:557:PHE:O	2.13	0.48
1:G:182:SER:HB2	5:G:1164:HOH:O	2.12	0.48
1:F:622:VAL:HA	1:F:632:GLY:HA2	1.95	0.48
1:C:788:GLY:O	1:C:792:VAL:HG23	2.14	0.48
1:F:633:THR:HG21	1:F:640:TRP:HA	1.94	0.48
1:D:288:ILE:HG13	1:D:349:TYR:CE1	2.49	0.48
1:G:585:ASN:H	1:G:585:ASN:HD22	1.60	0.48
1:A:474:THR:OG1	1:A:619:GLU:OE2	2.26	0.47
1:G:224:HIS:CE1	1:G:236:LEU:HD23	2.49	0.47
1:B:52:GLN:HA	1:B:82:TRP:CD1	2.49	0.47
1:A:158:ILE:HD11	1:A:242:PHE:CE2	2.49	0.47
1:D:386:LEU:HD22	1:D:411:ILE:HG23	1.96	0.47
1:C:52:GLN:HA	1:C:82:TRP:CD1	2.50	0.47
1:D:24:CYS:SG	1:D:113:CYS:CA	2.98	0.47
1:C:478:TYR:CD2	1:C:498:MET:HG3	2.48	0.47
1:C:396:VAL:HG23	1:C:479:LEU:HD23	1.96	0.47
1:C:600:ARG:HD3	1:C:912:ILE:HG23	1.96	0.47
1:C:672:LEU:HD22	1:C:721:ILE:HD13	1.97	0.47
1:F:307:GLY:O	1:G:575:ARG:HD3	2.14	0.47
1:B:157:ILE:HD12	1:B:220:VAL:HG11	1.96	0.47
1:B:589:SER:OG	1:B:787:PHE:HA	2.15	0.47
1:A:890:LEU:HD13	1:D:298:PHE:HB2	1.96	0.47
1:B:622:VAL:HA	1:B:632:GLY:HA2	1.97	0.46
1:H:180:GLN:CB	1:H:195:ILE:HD12	2.45	0.46
1:B:45:THR:HA	1:B:92:HIS:O	2.15	0.46
1:B:549:ILE:HD11	1:B:609:PHE:HE1	1.80	0.46
1:G:45:THR:HA	1:G:92:HIS:O	2.16	0.46
1:A:617:THR:CG2	1:A:655:ARG:NH1	2.78	0.46
1:A:473:ARG:HD3	1:A:557:PHE:O	2.16	0.46
1:G:899:LEU:HD12	1:G:899:LEU:C	2.36	0.46
1:A:549:ILE:CD1	1:A:609:PHE:HE1	2.29	0.46
1:B:600:ARG:HD3	1:B:912:ILE:HG23	1.98	0.45
1:H:52:GLN:HA	1:H:82:TRP:CD1	2.51	0.45
1:H:899:LEU:HD12	1:H:899:LEU:C	2.36	0.45
1:G:595:TRP:CE2	1:G:610:ALA:HB1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:GLN:OE1	1:H:195:ILE:CD1	2.64	0.45
1:G:241:ARG:HH22	1:G:670:GLU:CD	2.19	0.45
1:A:148:VAL:HG22	1:A:150:PHE:CE1	2.52	0.45
1:A:817:TYR:O	1:A:862:ARG:NH2	2.50	0.45
1:D:622:VAL:HA	1:D:632:GLY:HA2	1.98	0.45
1:C:384:ALA:O	1:C:395:ALA:HA	2.17	0.45
1:H:180:GLN:CD	1:H:195:ILE:HD11	2.30	0.45
1:B:196:GLN:HB3	1:B:230:THR:HG21	1.98	0.45
1:D:588:LEU:HD22	1:D:786:VAL:CG2	2.47	0.45
1:A:752:VAL:O	1:A:752:VAL:HG12	2.16	0.45
1:C:573:THR:HB	1:C:574:TRP:O	2.16	0.45
1:D:24:CYS:SG	1:D:113:CYS:HB3	2.43	0.45
1:F:34:LEU:HG	1:F:604:LYS:HA	1.99	0.45
1:F:710:THR:OG1	2:N:3:GAL:O3	2.25	0.45
1:G:177:LEU:HB3	1:G:200:PHE:HB2	1.99	0.45
1:G:293:VAL:O	1:G:294:ASP:C	2.55	0.45
1:E:688:GLN:NE2	2:M:3:GAL:H2	2.28	0.45
1:A:253:VAL:HB	1:A:477:VAL:HB	1.98	0.45
1:C:221:ARG:NH2	1:C:670:GLU:OE1	2.36	0.45
1:A:45:THR:HA	1:A:92:HIS:O	2.16	0.45
1:H:596:LEU:HD23	1:H:599:LEU:HD12	1.99	0.45
1:A:182:SER:HB2	5:A:1215:HOH:O	2.15	0.44
1:C:241:ARG:NH1	5:C:1105:HOH:O	2.50	0.44
1:E:294:ASP:N	5:E:1103:HOH:O	2.48	0.44
1:D:741:ILE:HG23	1:D:808:PHE:CD1	2.52	0.44
1:E:648:ARG:HG3	1:E:787:PHE:CG	2.52	0.44
1:H:741:ILE:HG23	1:H:808:PHE:CG	2.51	0.44
1:B:157:ILE:HD13	1:B:204:ILE:CD1	2.47	0.44
1:C:169:ILE:HD12	1:C:169:ILE:C	2.37	0.44
1:E:622:VAL:HA	1:E:632:GLY:HA2	1.98	0.44
1:G:150:PHE:CE2	1:G:218:VAL:HG21	2.53	0.44
1:G:335:ARG:O	1:G:339:ARG:HD2	2.18	0.44
1:E:622:VAL:HG22	1:E:624:HIS:CE1	2.52	0.44
1:B:664:GLY:O	1:B:665:ASP:C	2.56	0.44
1:E:64:LEU:HD11	1:E:104:TYR:HB3	1.98	0.44
1:C:281:GLU:OE1	1:C:390:THR:HB	2.18	0.44
1:B:253:VAL:HB	1:B:477:VAL:HB	2.00	0.44
1:C:585:ASN:HD22	1:C:585:ASN:N	2.16	0.44
1:C:741:ILE:HG23	1:C:808:PHE:CD1	2.52	0.44
1:F:639:HIS:HB2	1:F:640:TRP:CE3	2.53	0.44
1:A:535:GLU:CD	1:A:600:ARG:HH22	2.20	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ASP:OD2	1:B:617:THR:HG21	2.18	0.43
1:A:456:ILE:HD11	1:D:308:LEU:HD13	2.00	0.43
1:F:396:VAL:HG12	1:F:421:LEU:HD21	2.00	0.43
1:H:600:ARG:HD3	1:H:912:ILE:HG23	2.00	0.43
1:B:741:ILE:HG23	1:B:808:PHE:CD1	2.53	0.43
1:E:617:THR:HG23	1:E:655:ARG:NH1	2.33	0.43
1:E:747:LEU:HD13	1:E:753:THR:HG21	2.00	0.43
1:C:751:PHE:O	1:C:753:THR:O	2.37	0.43
1:B:535:GLU:OE1	1:B:600:ARG:NH2	2.51	0.43
1:B:617:THR:CG2	1:B:655:ARG:NH1	2.77	0.43
1:H:473:ARG:HD3	1:H:557:PHE:O	2.18	0.43
1:G:462:GLU:HG3	1:G:463:PRO:HD2	2.01	0.43
1:H:34:LEU:HB2	1:H:503:VAL:HB	2.01	0.43
1:A:201:ASP:O	1:A:224:HIS:HA	2.18	0.43
1:C:501:PRO:O	1:C:608:ARG:NH2	2.51	0.43
1:A:688:GLN:NE2	2:I:3:GAL:H2	2.33	0.43
1:C:591:ASP:OD2	1:C:617:THR:HG21	2.19	0.42
1:C:288:ILE:HG13	1:C:349:TYR:CE1	2.53	0.42
1:G:201:ASP:O	1:G:224:HIS:HA	2.19	0.42
1:A:600:ARG:HD3	1:A:912:ILE:HG23	2.01	0.42
1:C:305:ILE:HA	1:C:308:LEU:HD11	2.00	0.42
1:F:201:ASP:OD2	1:F:227:THR:HG21	2.18	0.42
1:F:595:TRP:CE2	1:F:610:ALA:HB1	2.54	0.42
1:G:622:VAL:HG22	1:G:624:HIS:CE1	2.54	0.42
1:A:839:LEU:HB3	1:A:842:ALA:HB3	2.00	0.42
1:G:638:GLN:HB2	1:G:641:SER:HB3	2.01	0.42
1:A:924:ASP:OD1	1:A:924:ASP:N	2.52	0.42
1:H:284:TYR:CD1	1:H:326:LEU:HD12	2.55	0.42
1:B:596:LEU:O	1:B:600:ARG:HG3	2.20	0.42
1:C:456:ILE:HG23	1:C:457:THR:HG23	2.01	0.42
1:E:320:GLN:HB2	1:E:326:LEU:HD21	2.01	0.42
1:H:664:GLY:O	1:H:665:ASP:C	2.58	0.42
1:C:390:THR:HG22	5:C:1196:HOH:O	2.20	0.42
1:D:89:TRP:CZ2	1:D:517:LEU:HD22	2.55	0.42
1:A:634:ARG:HG3	1:A:635:HIS:CD2	2.54	0.42
1:F:754:GLY:HA3	1:F:779:SER:HB3	2.02	0.41
1:G:64:LEU:HD11	1:G:104:TYR:HB3	2.01	0.41
1:H:750:GLY:O	1:H:753:THR:CG2	2.68	0.41
1:A:386:LEU:HD13	1:A:411:ILE:CG2	2.50	0.41
1:C:501:PRO:HA	1:C:502:PRO:HD3	1.94	0.41
1:E:381:GLU:CG	5:E:1103:HOH:O	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:617:THR:O	1:E:621:ASP:HB2	2.20	0.41
1:F:288:ILE:HG23	1:F:411:ILE:CD1	2.50	0.41
1:H:686:ASP:HB3	1:H:689:ARG:HB3	2.02	0.41
1:C:42:ALA:HB1	1:C:250:THR:HB	2.02	0.41
1:F:517:LEU:HG	1:F:657:TYR:HD1	1.86	0.41
1:G:438:PHE:CE1	1:G:637:VAL:HB	2.55	0.41
1:B:890:LEU:HD13	1:C:298:PHE:HB2	2.02	0.41
1:E:201:ASP:OD2	1:E:227:THR:HG21	2.20	0.41
1:F:52:GLN:HA	1:F:82:TRP:CD1	2.55	0.41
1:F:289:ARG:HA	1:F:298:PHE:O	2.20	0.41
1:H:293:VAL:O	1:H:294:ASP:C	2.59	0.41
1:H:384:ALA:HB2	1:H:409:LEU:HD13	2.03	0.41
1:A:155:ASN:HD22	1:A:201:ASP:CB	2.33	0.41
1:A:915:LEU:HA	1:A:915:LEU:HD23	1.95	0.41
1:F:253:VAL:HB	1:F:477:VAL:HB	2.01	0.41
1:F:842:ALA:HB1	1:F:906:GLN:OE1	2.20	0.41
1:H:881:ILE:HD12	1:H:881:ILE:O	2.20	0.41
1:E:633:THR:HG21	1:E:640:TRP:HA	2.03	0.41
1:G:454:LEU:HD13	1:G:460:ASP:HB2	2.02	0.41
1:H:750:GLY:O	1:H:753:THR:HG23	2.21	0.41
1:C:596:LEU:HD23	1:C:599:LEU:HD12	2.03	0.41
1:D:240:VAL:HG12	1:D:242:PHE:CE1	2.56	0.41
1:F:206:GLU:OE2	1:F:221:ARG:HD2	2.20	0.41
1:F:292:GLY:O	1:F:381:GLU:HB2	2.21	0.41
1:A:708:LEU:HG	1:A:755:SER:HA	2.02	0.41
1:B:478:TYR:CD2	1:B:498:MET:HG3	2.55	0.41
1:E:398:LEU:HB2	1:E:423:LEU:HD21	2.02	0.41
1:B:716:ALA:HB3	1:B:792:VAL:HG11	2.02	0.41
1:D:403:LYS:HG2	1:D:555:TYR:CE1	2.56	0.41
1:G:741:ILE:HG23	1:G:808:PHE:CG	2.56	0.41
1:A:587:GLU:O	1:A:590:PRO:HD3	2.20	0.41
1:B:387:GLY:HA3	1:B:393:GLY:HA3	2.03	0.41
1:F:535:GLU:OE1	1:F:600:ARG:NH2	2.45	0.41
1:G:288:ILE:HG23	1:G:411:ILE:HD13	2.03	0.41
1:H:177:LEU:HD22	1:H:236:LEU:CD2	2.51	0.41
1:A:222:GLY:HA3	1:A:238:PHE:CZ	2.56	0.40
1:D:150:PHE:CE1	1:D:218:VAL:HG21	2.56	0.40
1:D:593:PHE:CD1	1:D:908:GLY:HA3	2.57	0.40
1:G:346:TRP:CD2	1:G:363:LYS:HE3	2.55	0.40
1:E:671:LEU:O	1:E:675:LEU:HG	2.21	0.40
1:A:257:ILE:HD13	1:A:270:LEU:HD21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:ARG:HD3	1:B:694:ASP:OD1	2.20	0.40
1:E:169:ILE:C	1:E:169:ILE:HD12	2.42	0.40
1:E:599:LEU:HD21	1:E:661:LEU:HD11	2.04	0.40
1:B:672:LEU:HD13	1:B:721:ILE:HG21	2.02	0.40
1:G:596:LEU:HD23	1:G:599:LEU:HD12	2.03	0.40
1:A:752:VAL:CG1	1:A:752:VAL:O	2.69	0.40
1:G:617:THR:O	1:G:621:ASP:HB2	2.22	0.40
1:H:288:ILE:HG23	1:H:411:ILE:CD1	2.52	0.40
1:H:770:SER:C	1:H:772:PRO:HD3	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	891/906 (98%)	852 (96%)	35 (4%)	4 (0%)	34	53
1	B	892/906 (98%)	846 (95%)	42 (5%)	4 (0%)	34	53
1	C	880/906 (97%)	841 (96%)	35 (4%)	4 (0%)	29	47
1	D	882/906 (97%)	831 (94%)	49 (6%)	2 (0%)	47	69
1	E	897/906 (99%)	842 (94%)	48 (5%)	7 (1%)	19	34
1	F	896/906 (99%)	849 (95%)	42 (5%)	5 (1%)	25	42
1	G	879/906 (97%)	836 (95%)	40 (5%)	3 (0%)	41	60
1	H	881/906 (97%)	831 (94%)	47 (5%)	3 (0%)	41	60
All	All	7098/7248 (98%)	6728 (95%)	338 (5%)	32 (0%)	29	47

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	263	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	579	GLY
1	C	750	GLY
1	E	232	HIS
1	E	774	ASN
1	F	74	LEU
1	F	263	GLU
1	F	635	HIS
1	G	579	GLY
1	H	401	PHE
1	A	401	PHE
1	E	329	THR
1	G	401	PHE
1	H	579	GLY
1	A	651	GLN
1	B	277	PRO
1	B	651	GLN
1	D	582	ALA
1	E	582	ALA
1	E	651	GLN
1	A	582	ALA
1	B	582	ALA
1	C	582	ALA
1	C	651	GLN
1	F	117	SER
1	F	651	GLN
1	G	651	GLN
1	H	651	GLN
1	D	164	LYS
1	E	378	THR
1	A	579	GLY
1	C	579	GLY

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	724/745 (97%)	687 (95%)	37 (5%)	24	41
1	B	731/745 (98%)	705 (96%)	26 (4%)	35	55
1	C	726/745 (97%)	703 (97%)	23 (3%)	39	59
1	D	724/745 (97%)	692 (96%)	32 (4%)	28	47
1	E	733/745 (98%)	701 (96%)	32 (4%)	28	47
1	F	724/745 (97%)	695 (96%)	29 (4%)	31	51
1	G	719/745 (96%)	691 (96%)	28 (4%)	32	52
1	H	724/745 (97%)	692 (96%)	32 (4%)	28	47
All	All	5805/5960 (97%)	5566 (96%)	239 (4%)	30	50

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	39	THR
1	A	61	SER
1	A	99	GLN
1	A	111	LEU
1	A	120	SER
1	A	123	SER
1	A	128	SER
1	A	131	VAL
1	A	132	VAL
1	A	148	VAL
1	A	176	VAL
1	A	183	VAL
1	A	186	ASN
1	A	215	ARG
1	A	223	ASN
1	A	268	THR
1	A	305	ILE
1	A	333	GLU
1	A	345	THR
1	A	378	THR
1	A	458	TYR
1	A	523	LEU
1	A	526	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	533	THR
1	A	585	ASN
1	A	617	THR
1	A	622	VAL
1	A	655	ARG
1	A	693	THR
1	A	702	SER
1	A	832	VAL
1	A	835	SER
1	A	855	LYS
1	A	857	LYS
1	A	921	SER
1	A	924	ASP
1	B	31	VAL
1	B	114	VAL
1	B	123	SER
1	B	124	SER
1	B	131	VAL
1	B	176	VAL
1	B	182	SER
1	B	186	ASN
1	B	188	ASP
1	B	223	ASN
1	B	230	THR
1	B	239	VAL
1	B	268	THR
1	B	277	PRO
1	B	331	THR
1	B	345	THR
1	B	378	THR
1	B	458	TYR
1	B	490	LYS
1	B	533	THR
1	B	617	THR
1	B	655	ARG
1	B	761	VAL
1	B	835	SER
1	B	921	SER
1	B	924	ASP
1	C	114	VAL
1	C	132	VAL
1	C	133	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	186	ASN
1	C	188	ASP
1	C	263	GLU
1	C	268	THR
1	C	279	LYS
1	C	328	ASP
1	C	330	GLU
1	C	341	LYS
1	C	390	THR
1	C	410	ASP
1	C	458	TYR
1	C	490	LYS
1	C	493	SER
1	C	520	TYR
1	C	533	THR
1	C	573	THR
1	C	585	ASN
1	C	603	SER
1	C	617	THR
1	C	655	ARG
1	D	31	VAL
1	D	44	VAL
1	D	99	GLN
1	D	109	SER
1	D	128	SER
1	D	132	VAL
1	D	148	VAL
1	D	176	VAL
1	D	178[A]	GLN
1	D	178[B]	GLN
1	D	182	SER
1	D	186	ASN
1	D	188	ASP
1	D	201	ASP
1	D	215	ARG
1	D	223[A]	ASN
1	D	223[B]	ASN
1	D	226	VAL
1	D	268	THR
1	D	333	GLU
1	D	345	THR
1	D	458	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	490	LYS
1	D	520	TYR
1	D	533	THR
1	D	573	THR
1	D	622	VAL
1	D	642	ASP
1	D	651	GLN
1	D	655	ARG
1	D	865	LYS
1	D	923	ASP
1	E	24	CYS
1	E	44	VAL
1	E	58[A]	GLN
1	E	58[B]	GLN
1	E	61	SER
1	E	84	ASP
1	E	109	SER
1	E	111	LEU
1	E	113	CYS
1	E	118	SER
1	E	123	SER
1	E	132	VAL
1	E	139	LEU
1	E	165	SER
1	E	176	VAL
1	E	186	ASN
1	E	201	ASP
1	E	226	VAL
1	E	228	ASP
1	E	230	THR
1	E	305	ILE
1	E	345	THR
1	E	390	THR
1	E	458	TYR
1	E	473	ARG
1	E	585	ASN
1	E	617	THR
1	E	648	ARG
1	E	655	ARG
1	E	761	VAL
1	E	853	GLU
1	E	924	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	44	VAL
1	F	58	GLN
1	F	76	SER
1	F	84	ASP
1	F	109	SER
1	F	118	SER
1	F	119	SER
1	F	132	VAL
1	F	165	SER
1	F	186	ASN
1	F	193	SER
1	F	228	ASP
1	F	230	THR
1	F	268	THR
1	F	281	GLU
1	F	305	ILE
1	F	329	THR
1	F	335	ARG
1	F	345	THR
1	F	352	THR
1	F	366	LYS
1	F	390	THR
1	F	493	SER
1	F	585	ASN
1	F	622	VAL
1	F	655	ARG
1	F	838	SER
1	F	921	SER
1	F	924	ASP
1	G	26	SER
1	G	31	VAL
1	G	44	VAL
1	G	57	PRO
1	G	65	THR
1	G	131	VAL
1	G	201	ASP
1	G	223	ASN
1	G	231	ASP
1	G	268	THR
1	G	305	ILE
1	G	341	LYS
1	G	345	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	458	TYR
1	G	490	LYS
1	G	588	LEU
1	G	591	ASP
1	G	603	SER
1	G	617	THR
1	G	655	ARG
1	G	731	GLU
1	G	755	SER
1	G	761	VAL
1	G	764	THR
1	G	853	GLU
1	G	855	LYS
1	G	865	LYS
1	G	923	ASP
1	H	31	VAL
1	H	44	VAL
1	H	63	SER
1	H	67	ASP
1	H	99	GLN
1	H	129	SER
1	H	186	ASN
1	H	193	SER
1	H	195	ILE
1	H	201	ASP
1	H	206	GLU
1	H	223	ASN
1	H	231	ASP
1	H	268	THR
1	H	305	ILE
1	H	345	THR
1	H	410	ASP
1	H	458	TYR
1	H	490	LYS
1	H	573	THR
1	H	585	ASN
1	H	655	ARG
1	H	748	THR
1	H	753	THR
1	H	761	VAL
1	H	764	THR
1	H	775	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	794	SER
1	H	828	ASP
1	H	876	ASP
1	H	921	SER
1	H	923	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	155	ASN
1	A	178	GLN
1	A	186	ASN
1	A	223	ASN
1	A	515	GLN
1	A	539	GLN
1	A	585	ASN
1	A	688	GLN
1	A	746	ASN
1	B	23	ASN
1	B	99	GLN
1	B	178	GLN
1	B	186	ASN
1	B	210	ASN
1	B	324	GLN
1	B	585	ASN
1	C	75	GLN
1	C	98	ASN
1	C	186	ASN
1	C	223	ASN
1	C	324	GLN
1	C	391	GLN
1	C	515	GLN
1	C	585	ASN
1	C	688	GLN
1	D	23	ASN
1	D	75	GLN
1	D	203	ASN
1	D	324	GLN
1	D	391	GLN
1	D	515	GLN
1	D	585	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	186	ASN
1	E	196	GLN
1	E	324	GLN
1	E	515	GLN
1	E	688	GLN
1	E	810	GLN
1	F	58	GLN
1	F	178	GLN
1	F	186	ASN
1	F	223	ASN
1	F	324	GLN
1	G	75	GLN
1	G	178	GLN
1	G	186	ASN
1	G	189	ASN
1	G	324	GLN
1	G	369	GLN
1	G	391	GLN
1	H	23	ASN
1	H	98	ASN
1	H	186	ASN
1	H	324	GLN
1	H	391	GLN
1	H	585	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

21 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	RAM	I	1	2	11,11,11	0.75	0	15,16,16	1.55	2 (13%)
2	GAD	I	2	2	7,11,11	2.32	2 (28%)	8,15,15	2.51	2 (25%)
2	GAL	I	3	2	11,11,12	1.21	1 (9%)	15,15,17	3.17	6 (40%)
3	RAM	J	1	3	11,11,11	0.66	0	15,16,16	1.62	2 (13%)
3	GAD	J	2	3	7,11,11	2.61	2 (28%)	8,15,15	2.73	2 (25%)
2	RAM	K	1	2	11,11,11	0.66	0	15,16,16	0.70	0
2	GAD	K	2	2	7,11,11	3.16	2 (28%)	8,15,15	2.91	3 (37%)
2	GAL	K	3	2	11,11,12	0.69	0	15,15,17	1.83	5 (33%)
3	RAM	L	1	3	11,11,11	0.95	0	15,16,16	1.21	1 (6%)
3	GAD	L	2	3	7,11,11	2.86	2 (28%)	8,15,15	2.52	3 (37%)
2	RAM	M	1	2	11,11,11	0.69	0	15,16,16	1.48	2 (13%)
2	GAD	M	2	2	7,11,11	2.89	2 (28%)	8,15,15	2.42	2 (25%)
2	GAL	M	3	2	11,11,12	0.88	0	15,15,17	2.86	5 (33%)
2	RAM	N	1	2	11,11,11	0.56	0	15,16,16	1.52	3 (20%)
2	GAD	N	2	2	7,11,11	3.18	3 (42%)	8,15,15	3.30	4 (50%)
2	GAL	N	3	2	11,11,12	0.96	0	15,15,17	1.70	2 (13%)
2	RAM	O	1	2	11,11,11	0.82	0	15,16,16	1.14	1 (6%)
2	GAD	O	2	2	7,11,11	2.59	2 (28%)	8,15,15	2.18	3 (37%)
2	GAL	O	3	1,2	11,11,12	1.80	2 (18%)	15,15,17	3.40	8 (53%)
3	RAM	P	1	3	11,11,11	0.94	0	15,16,16	1.83	3 (20%)
3	GAD	P	2	3	7,11,11	2.77	3 (42%)	8,15,15	3.14	3 (37%)

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	RAM	I	1	2	-	-	0/1/1/1
2	GAD	I	2	2	-	0/0/17/17	0/1/1/1
2	GAL	I	3	2	-	1/2/19/22	0/1/1/1
3	RAM	J	1	3	-	-	0/1/1/1
3	GAD	J	2	3	-	0/0/17/17	0/1/1/1
2	RAM	K	1	2	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAD	K	2	2	-	0/0/17/17	0/1/1/1
2	GAL	K	3	2	-	2/2/19/22	0/1/1/1
3	RAM	L	1	3	-	-	0/1/1/1
3	GAD	L	2	3	-	0/0/17/17	0/1/1/1
2	RAM	M	1	2	-	-	0/1/1/1
2	GAD	M	2	2	-	0/0/17/17	0/1/1/1
2	GAL	M	3	2	-	0/2/19/22	0/1/1/1
2	RAM	N	1	2	-	-	0/1/1/1
2	GAD	N	2	2	-	0/0/17/17	0/1/1/1
2	GAL	N	3	2	-	2/2/19/22	0/1/1/1
2	RAM	O	1	2	-	-	0/1/1/1
2	GAD	O	2	2	-	0/0/17/17	0/1/1/1
2	GAL	O	3	1,2	-	0/2/19/22	0/1/1/1
3	RAM	P	1	3	-	-	0/1/1/1
3	GAD	P	2	3	-	0/0/17/17	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	GAD	O5-C5	6.93	1.47	1.37
2	M	2	GAD	O5-C5	6.51	1.46	1.37
3	L	2	GAD	O5-C5	6.50	1.46	1.37
2	N	2	GAD	O5-C5	6.38	1.46	1.37
2	O	2	GAD	O5-C5	5.89	1.45	1.37
3	P	2	GAD	O5-C5	5.74	1.45	1.37
3	J	2	GAD	O5-C5	5.55	1.45	1.37
2	I	2	GAD	O5-C5	5.33	1.44	1.37
2	O	3	GAL	O4-C4	4.40	1.53	1.43
2	K	2	GAD	C4-C5	3.89	1.37	1.32
2	N	2	GAD	C4-C5	3.89	1.37	1.32
3	P	2	GAD	C4-C5	3.55	1.37	1.32
3	J	2	GAD	C3-C4	3.43	1.54	1.50
2	M	2	GAD	C4-C5	3.37	1.36	1.32
3	L	2	GAD	C4-C5	3.15	1.36	1.32
2	N	2	GAD	C3-C4	3.08	1.54	1.50
2	O	2	GAD	C4-C5	2.90	1.36	1.32
2	O	3	GAL	C4-C3	2.33	1.58	1.52
2	I	3	GAL	C1-C2	2.16	1.57	1.52
2	I	2	GAD	C3-C4	2.10	1.53	1.50
3	P	2	GAD	C3-C4	2.03	1.53	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	GAL	C1-O5-C5	7.42	122.25	112.19
2	O	3	GAL	C1-O5-C5	7.29	122.07	112.19
2	N	2	GAD	O5-C5-C4	-7.26	118.68	124.81
3	P	2	GAD	O5-C5-C4	-7.20	118.73	124.81
3	J	2	GAD	O5-C5-C4	-7.12	118.80	124.81
2	K	2	GAD	O5-C5-C4	-6.90	118.98	124.81
2	O	3	GAL	C3-C4-C5	-6.82	98.07	110.24
2	I	2	GAD	O5-C5-C4	-6.10	119.66	124.81
2	M	2	GAD	O5-C5-C4	-5.87	119.86	124.81
2	M	3	GAL	C1-O5-C5	5.73	119.96	112.19
2	I	3	GAL	O2-C2-C1	5.72	120.86	109.15
2	O	3	GAL	O4-C4-C3	5.40	122.84	110.35
2	I	3	GAL	O5-C1-C2	-5.36	102.50	110.77
2	M	3	GAL	O5-C1-C2	-4.96	103.11	110.77
2	M	3	GAL	O2-C2-C1	4.91	119.19	109.15
3	L	2	GAD	O5-C5-C4	-4.81	120.75	124.81
3	P	1	RAM	O5-C5-C4	4.56	117.70	109.52
2	N	3	GAL	O5-C5-C6	4.44	114.17	107.20
2	O	2	GAD	O5-C5-C4	-4.27	121.20	124.81
2	N	2	GAD	C2-C3-C4	-4.00	106.85	112.32
2	M	3	GAL	C1-C2-C3	-3.98	104.77	109.67
3	P	2	GAD	C1-C2-C3	-3.74	105.06	109.67
2	M	1	RAM	O5-C5-C4	3.56	115.91	109.52
3	L	2	GAD	O3-C3-C2	3.53	115.55	109.42
2	K	3	GAL	O2-C2-C1	3.53	116.38	109.15
2	N	1	RAM	O5-C5-C4	3.51	115.83	109.52
2	I	1	RAM	O4-C4-C5	3.51	117.44	109.67
2	O	3	GAL	O3-C3-C4	3.51	118.46	110.35
2	M	3	GAL	O5-C5-C6	3.48	112.66	107.20
2	I	3	GAL	C1-C2-C3	-3.46	105.41	109.67
2	I	3	GAL	C3-C4-C5	3.26	116.06	110.24
3	J	1	RAM	C3-C4-C5	-3.25	104.72	109.77
2	K	2	GAD	C2-C3-C4	-3.18	107.97	112.32
3	J	1	RAM	O4-C4-C5	3.10	116.53	109.67
3	L	2	GAD	C1-O5-C5	3.05	121.97	115.58
2	O	3	GAL	C1-C2-C3	-2.81	106.21	109.67
2	M	2	GAD	C2-C3-C4	-2.75	108.56	112.32
2	O	1	RAM	C1-C2-C3	2.73	115.98	110.31
2	M	1	RAM	C6-C5-C4	-2.70	108.09	113.07
2	O	2	GAD	C1-C2-C3	2.67	112.94	109.67
2	N	2	GAD	O3-C3-C2	2.59	113.91	109.42
2	K	3	GAL	C1-O5-C5	2.56	115.67	112.19
3	P	1	RAM	C6-C5-C4	-2.56	108.35	113.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	GAL	O5-C5-C6	2.56	111.21	107.20
2	N	2	GAD	C1-C2-C3	-2.53	106.56	109.67
2	I	2	GAD	O3-C3-C4	2.41	114.73	109.31
2	K	3	GAL	O5-C1-C2	-2.40	107.07	110.77
2	K	2	GAD	C1-C2-C3	-2.38	106.74	109.67
3	J	2	GAD	C1-O5-C5	2.37	120.56	115.58
2	K	3	GAL	C2-C3-C4	2.36	114.98	110.89
2	N	1	RAM	O4-C4-C3	-2.35	104.91	110.35
3	P	1	RAM	C1-C2-C3	2.33	115.16	110.31
2	O	3	GAL	O5-C5-C6	2.32	110.84	107.20
2	I	3	GAL	O4-C4-C3	-2.29	105.05	110.35
2	N	3	GAL	O3-C3-C4	-2.23	105.19	110.35
2	O	3	GAL	O2-C2-C1	2.21	113.67	109.15
2	O	2	GAD	C1-O5-C5	2.17	120.13	115.58
2	I	1	RAM	O1-C1-O5	2.13	116.78	110.38
3	P	2	GAD	C2-C3-C4	-2.13	109.41	112.32
2	N	1	RAM	O5-C5-C6	-2.11	102.15	106.70
2	O	3	GAL	C2-C3-C4	-2.11	107.25	110.89
3	L	1	RAM	O5-C1-C2	2.10	114.04	110.28

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	3	GAL	O5-C5-C6-O6
2	K	3	GAL	C4-C5-C6-O6
2	K	3	GAL	O5-C5-C6-O6
2	N	3	GAL	C4-C5-C6-O6
2	I	3	GAL	O5-C5-C6-O6

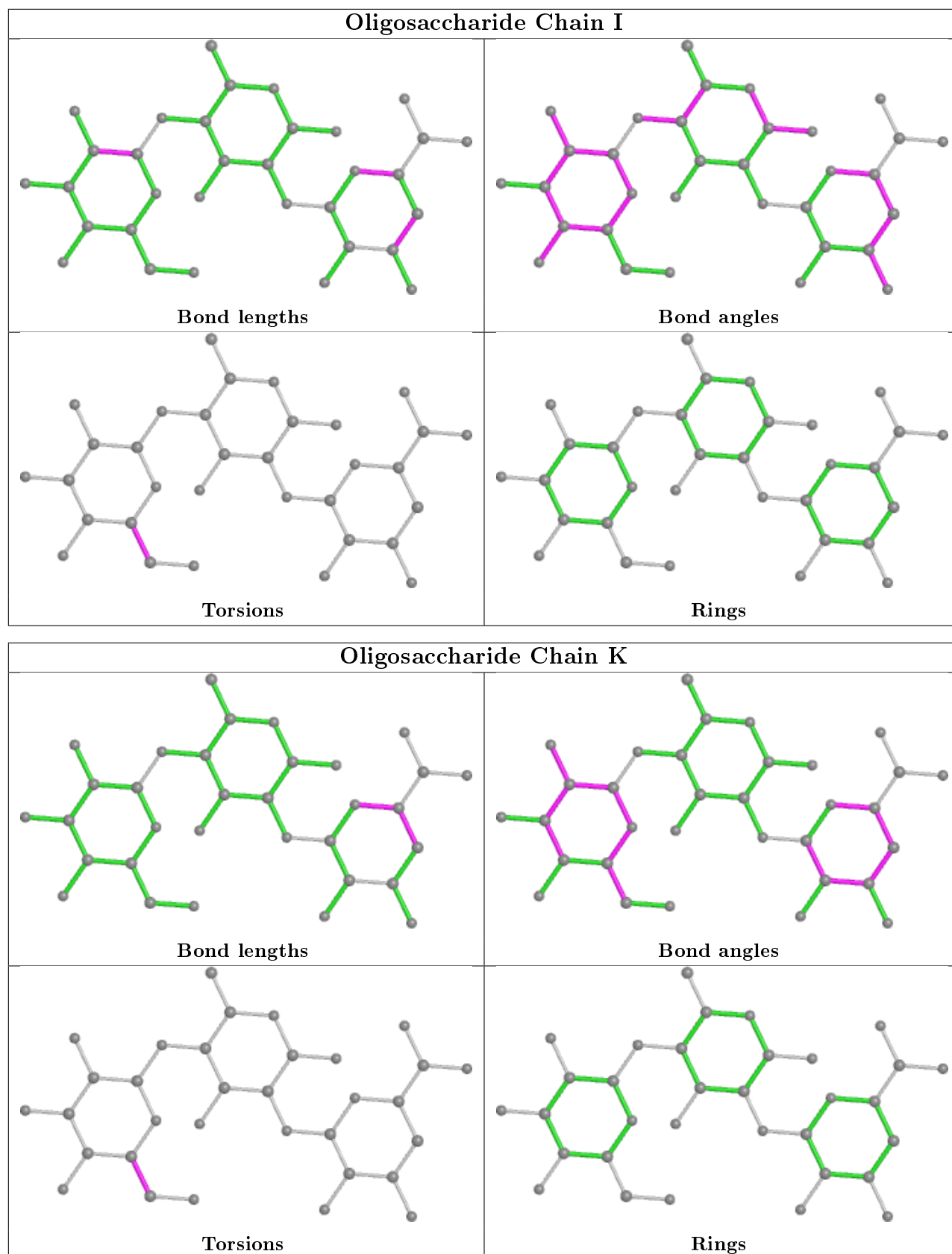
There are no ring outliers.

5 monomers are involved in 7 short contacts:

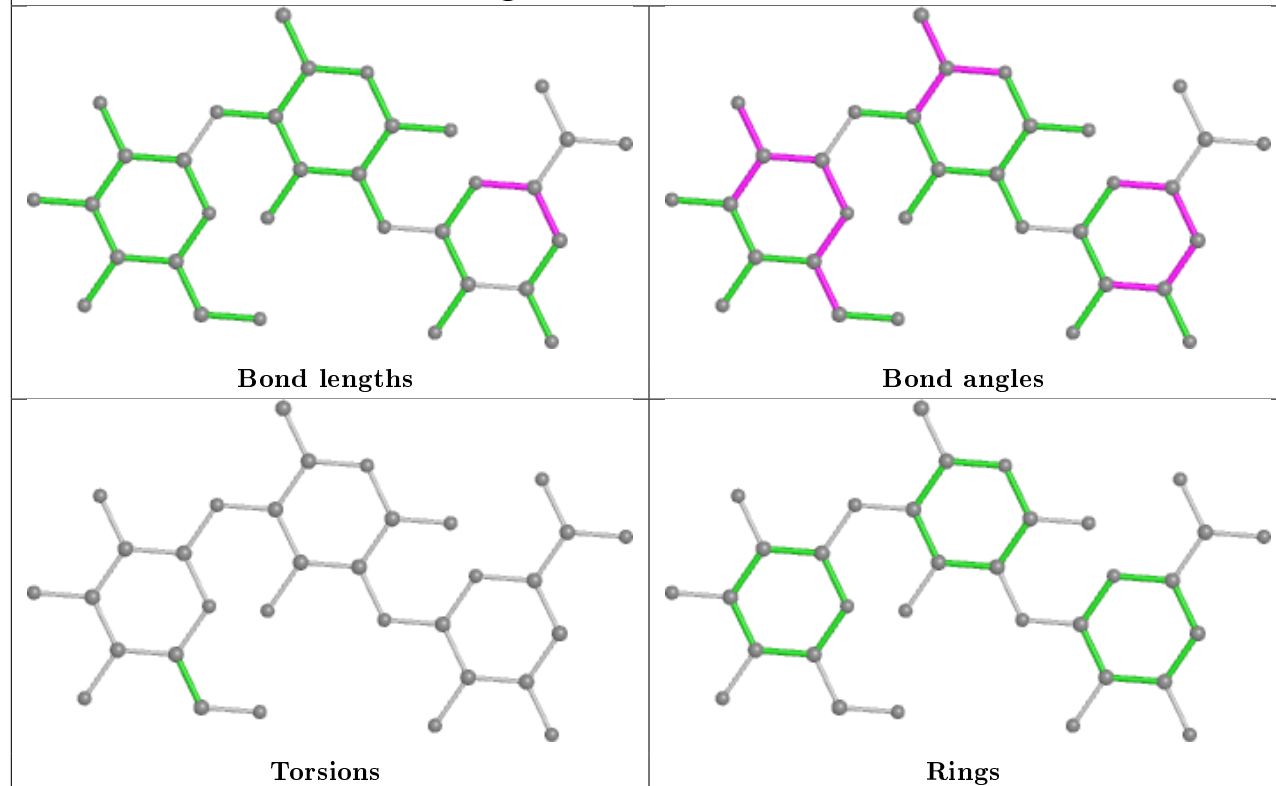
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	GAD	1	0
2	I	3	GAL	2	0
2	N	3	GAL	1	0
2	M	3	GAL	2	0
2	O	3	GAL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

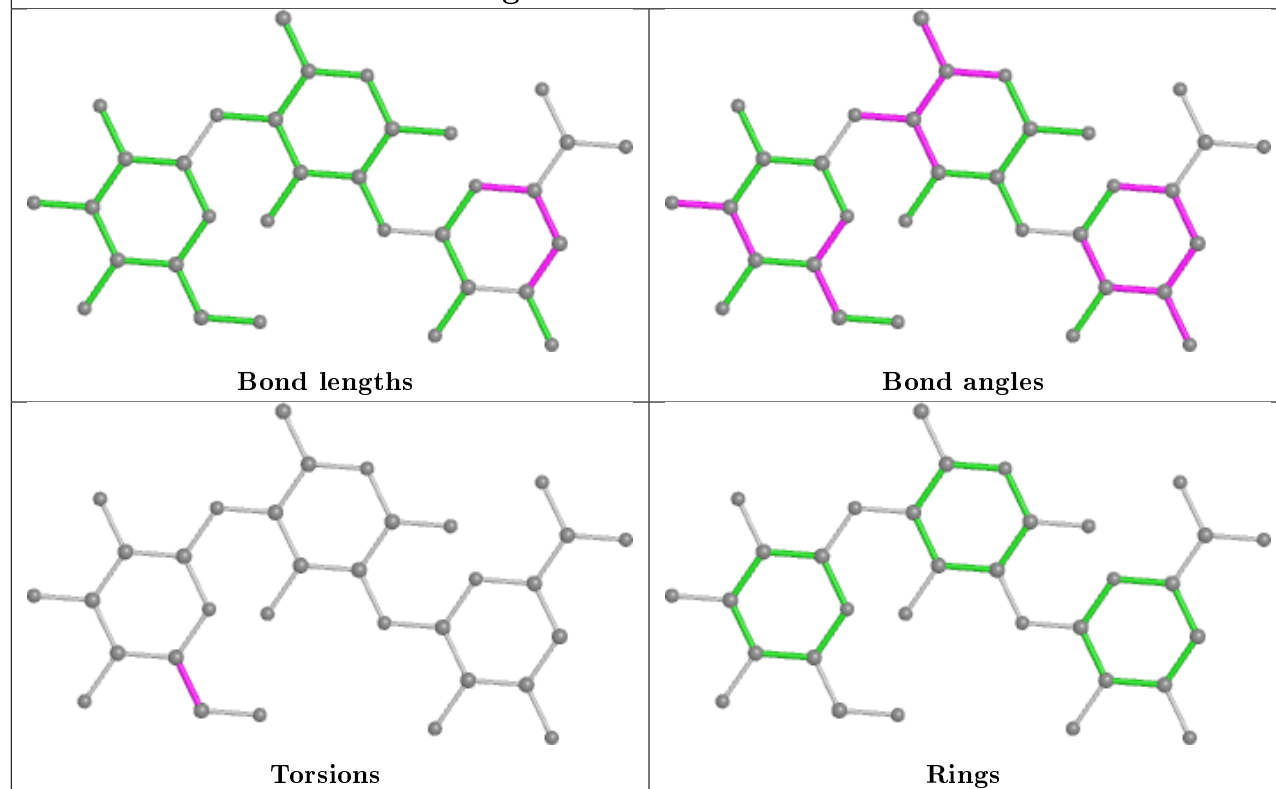
bond angles, torsion angles, and ring geometry for oligosaccharide.



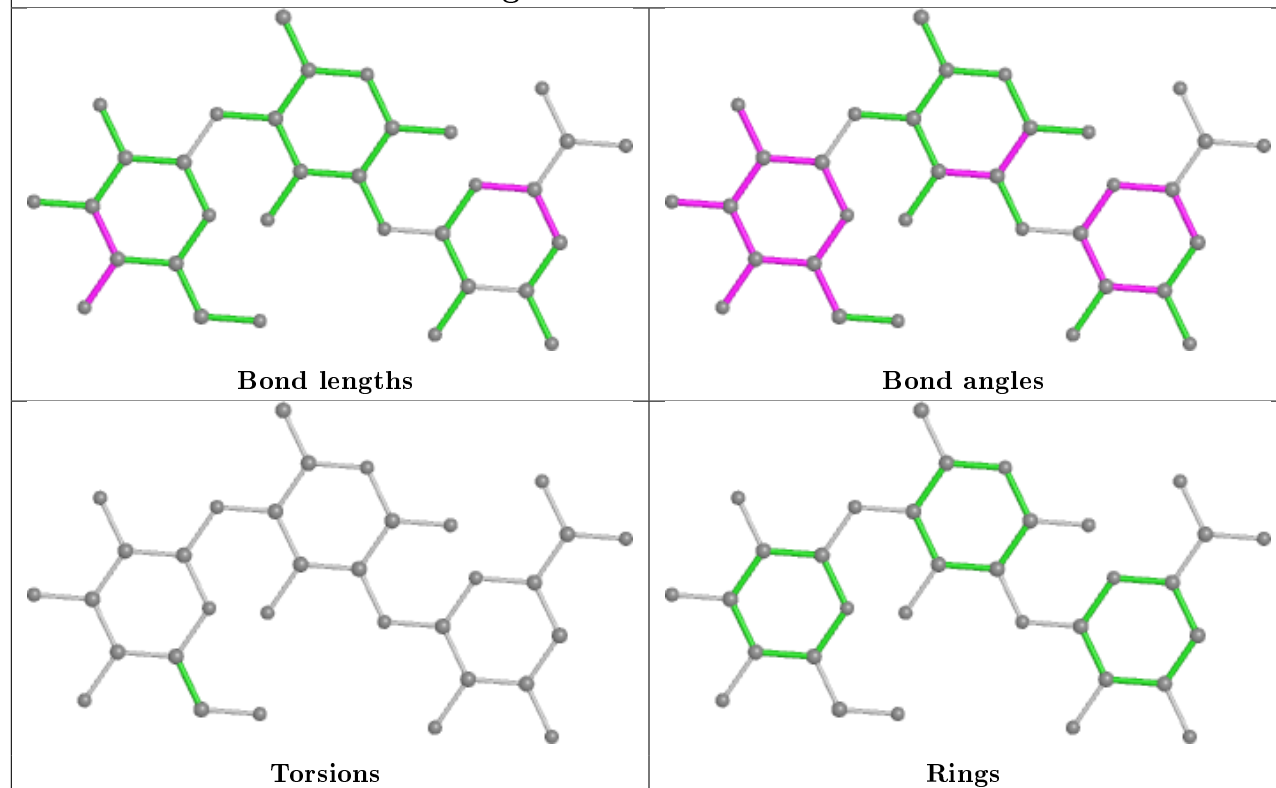
Oligosaccharide Chain M



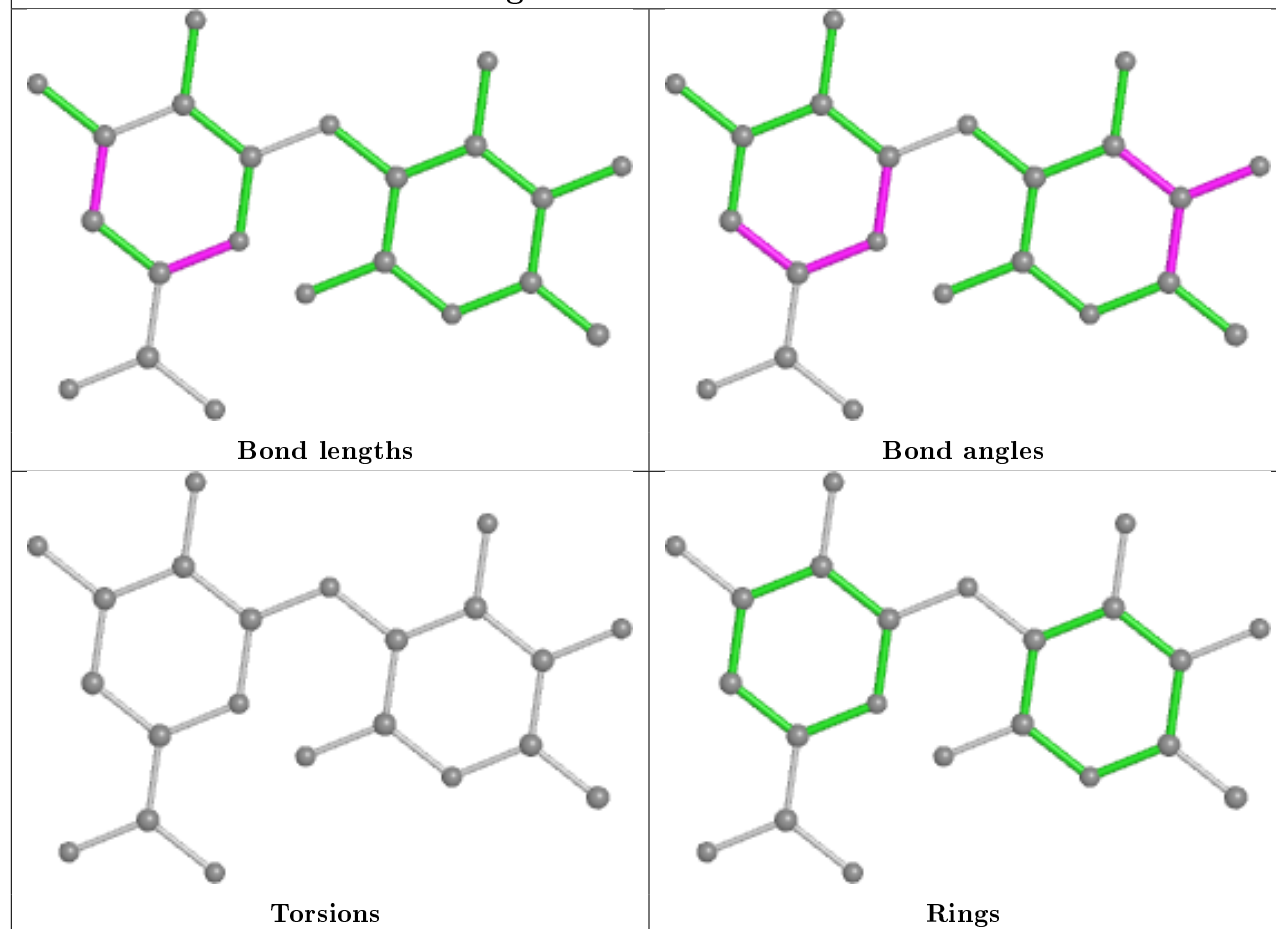
Oligosaccharide Chain N

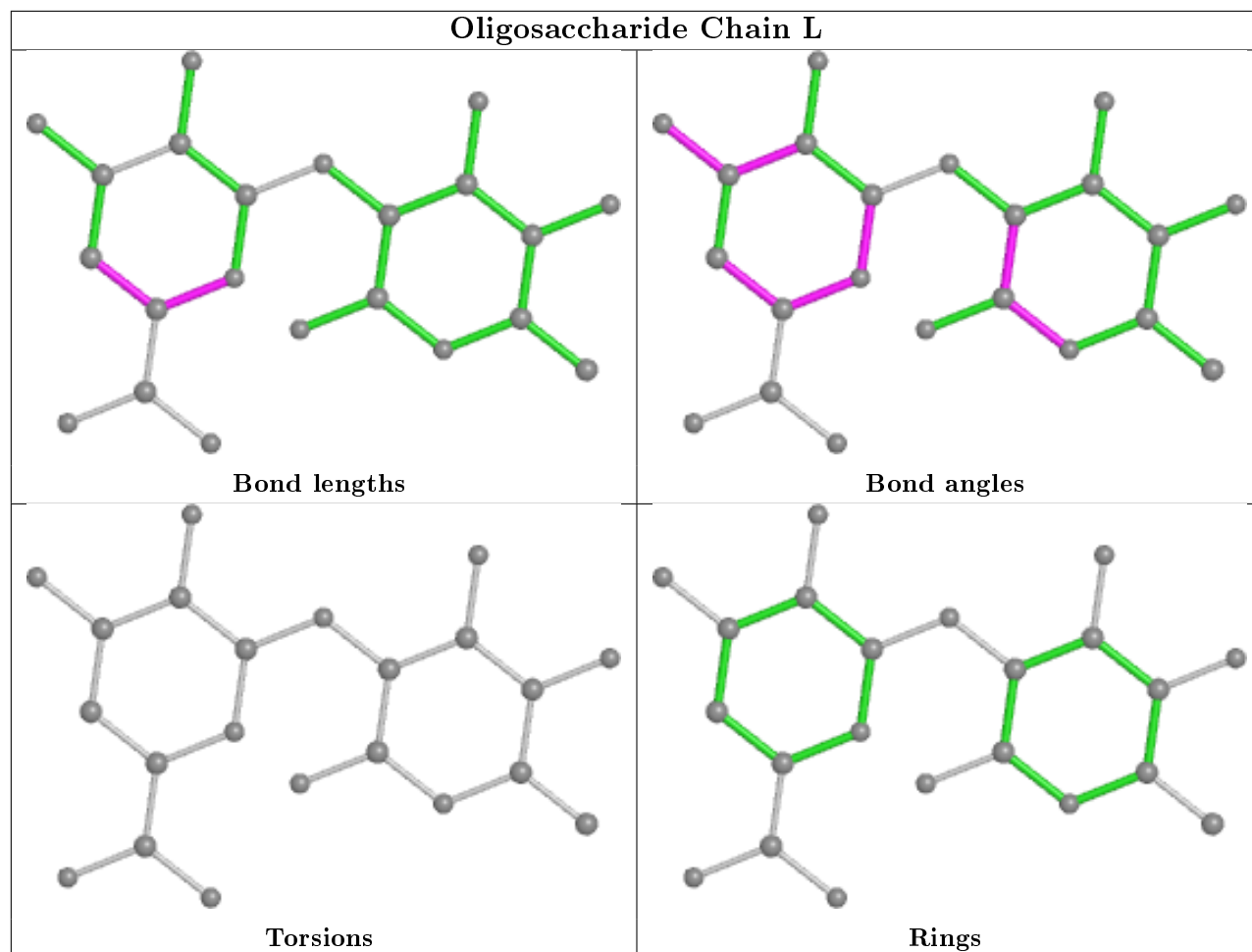


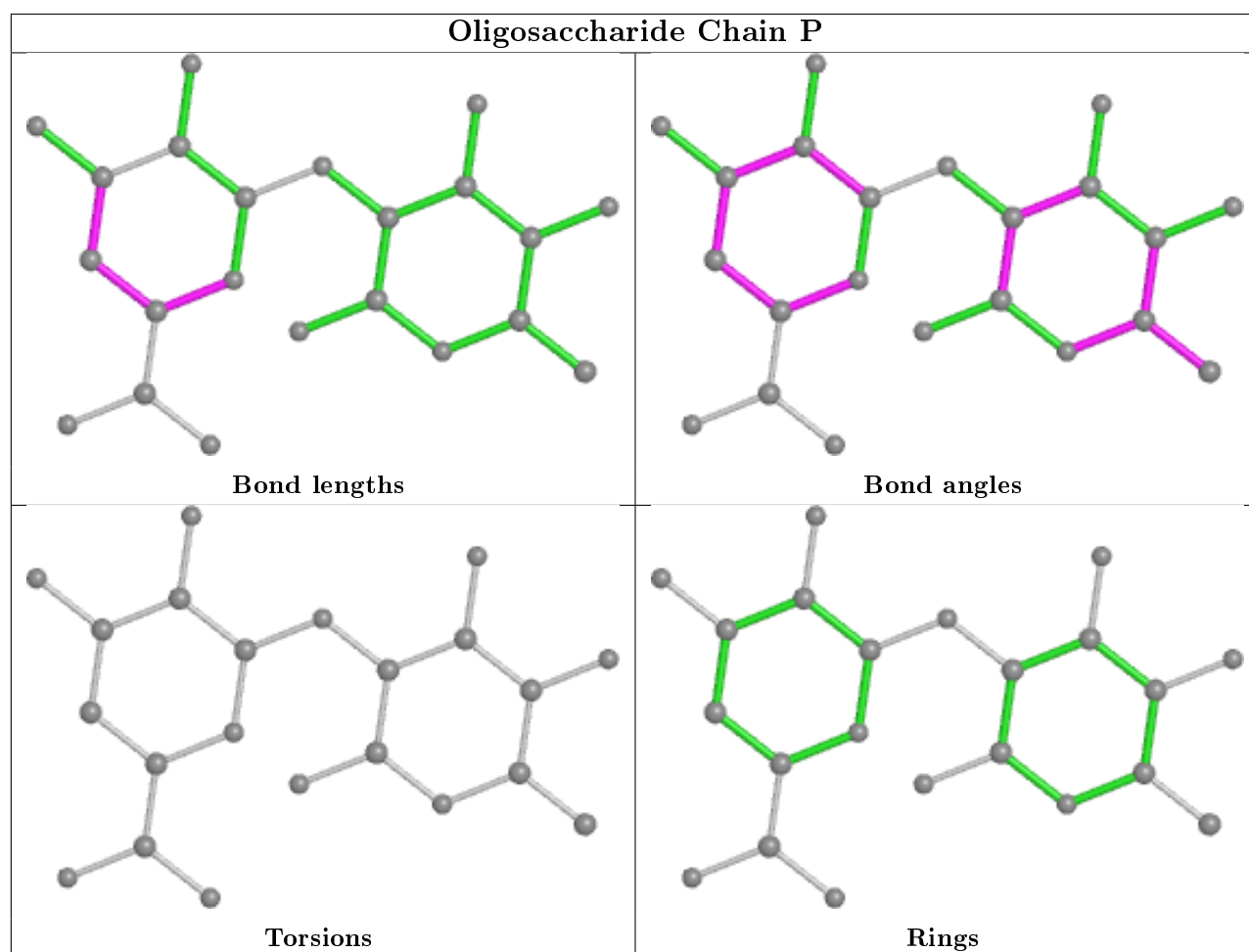
Oligosaccharide Chain O



Oligosaccharide Chain J







5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	896/906 (98%)	-0.35	3 (0%) 94 96	21, 33, 52, 76	0
1	B	896/906 (98%)	-0.34	1 (0%) 95 97	20, 32, 51, 78	0
1	C	885/906 (97%)	-0.31	6 (0%) 87 91	22, 35, 55, 81	0
1	D	884/906 (97%)	-0.28	11 (1%) 79 85	20, 37, 58, 81	0
1	E	900/906 (99%)	-0.26	8 (0%) 84 89	23, 36, 57, 84	0
1	F	900/906 (99%)	-0.33	4 (0%) 92 95	22, 34, 56, 79	0
1	G	886/906 (97%)	-0.19	10 (1%) 80 86	21, 39, 65, 86	0
1	H	888/906 (98%)	-0.17	10 (1%) 80 86	19, 39, 66, 90	0
All	All	7135/7248 (98%)	-0.28	53 (0%) 87 91	19, 35, 59, 90	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	923	ASP	3.7
1	F	23	ASN	3.6
1	G	926	GLN	3.5
1	A	761	VAL	3.4
1	D	693	THR	3.3
1	H	528	SER	3.3
1	C	701	ASN	3.2
1	H	925	TYR	2.9
1	G	528	SER	2.9
1	E	525	GLY	2.8
1	G	924	ASP	2.7
1	D	925	TYR	2.7
1	H	72	SER	2.7
1	H	924	ASP	2.7
1	B	804	ILE	2.5
1	H	927	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	920	ASP	2.5
1	C	831	GLY	2.5
1	F	331	THR	2.5
1	H	695	GLY	2.5
1	G	696	TRP	2.5
1	C	923	ASP	2.4
1	D	694	ASP	2.4
1	C	693	THR	2.4
1	E	195	ILE	2.4
1	D	137	ASP	2.4
1	G	701	ASN	2.4
1	E	125	ALA	2.4
1	E	208	PHE	2.4
1	H	926	GLN	2.3
1	D	695	GLY	2.3
1	H	110	SER	2.3
1	D	927	SER	2.3
1	A	807	GLY	2.3
1	D	701	ASN	2.2
1	E	196	GLN	2.2
1	E	331	THR	2.2
1	D	128	SER	2.2
1	E	136	SER	2.2
1	H	922	LEU	2.2
1	E	802	ASP	2.2
1	C	530	ALA	2.2
1	G	228	ASP	2.1
1	G	925	TYR	2.1
1	D	922	LEU	2.1
1	G	447	TYR	2.1
1	H	775	ARG	2.0
1	D	923	ASP	2.0
1	F	332	TRP	2.0
1	D	136	SER	2.0
1	F	802	ASP	2.0
1	A	338	THR	2.0
1	G	922	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

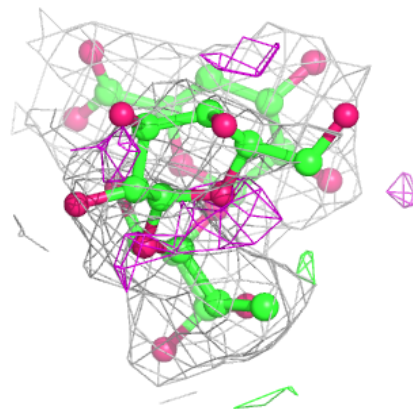
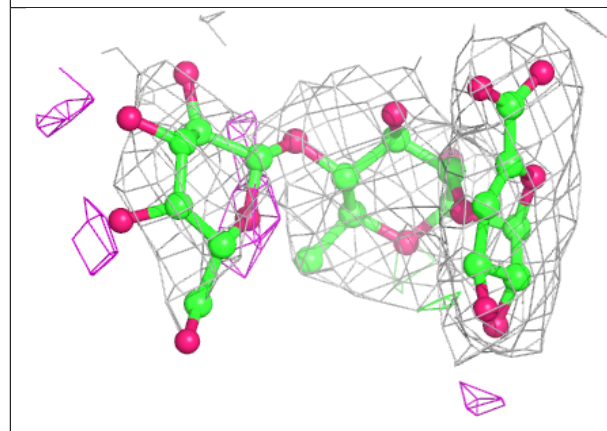
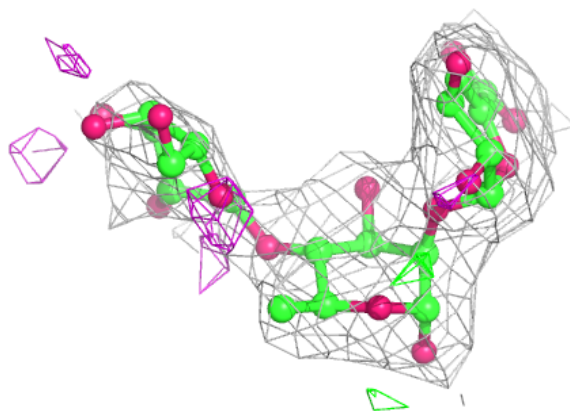
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	O	3	11/12	0.79	0.38	71,79,95,96	0
2	GAL	N	3	11/12	0.80	0.43	70,78,88,89	0
2	GAL	K	3	11/12	0.88	0.41	82,94,105,107	0
2	GAL	M	3	11/12	0.89	0.28	52,60,76,77	0
2	GAL	I	3	11/12	0.90	0.42	59,63,68,68	0
2	GAD	K	2	11/11	0.93	0.14	49,53,55,58	0
2	GAD	O	2	11/11	0.94	0.17	46,57,62,64	0
3	GAD	L	2	11/11	0.94	0.13	47,57,62,65	0
3	GAD	P	2	11/11	0.94	0.18	46,52,55,56	0
2	RAM	K	1	11/11	0.95	0.18	63,67,73,78	0
2	RAM	O	1	11/11	0.95	0.16	49,61,68,69	0
3	RAM	P	1	11/11	0.95	0.14	45,55,60,64	0
2	GAD	N	2	11/11	0.95	0.15	37,47,51,51	0
2	RAM	M	1	11/11	0.95	0.14	37,41,51,51	0
2	GAD	M	2	11/11	0.95	0.14	43,48,49,50	0
3	RAM	L	1	11/11	0.96	0.14	48,52,57,65	0
2	RAM	N	1	11/11	0.96	0.13	43,47,52,58	0
3	RAM	J	1	11/11	0.96	0.12	30,32,35,36	0
2	RAM	I	1	11/11	0.96	0.14	34,35,39,46	0
3	GAD	J	2	11/11	0.97	0.11	29,37,42,44	0
2	GAD	I	2	11/11	0.97	0.13	33,37,38,46	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.

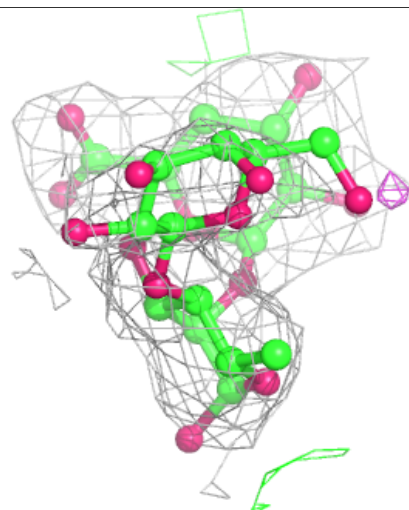
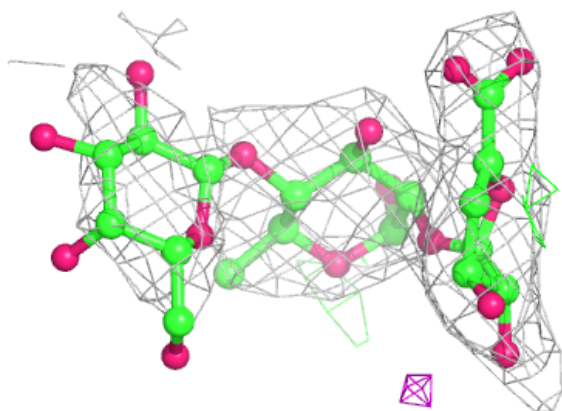
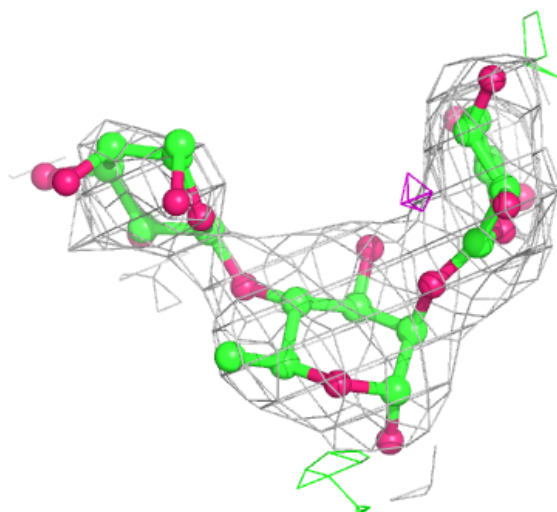
Electron density around Chain I:

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



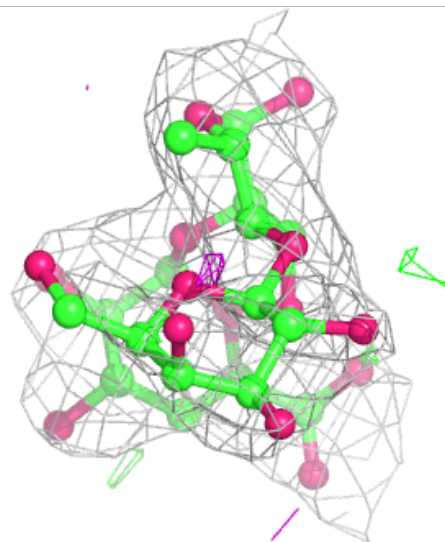
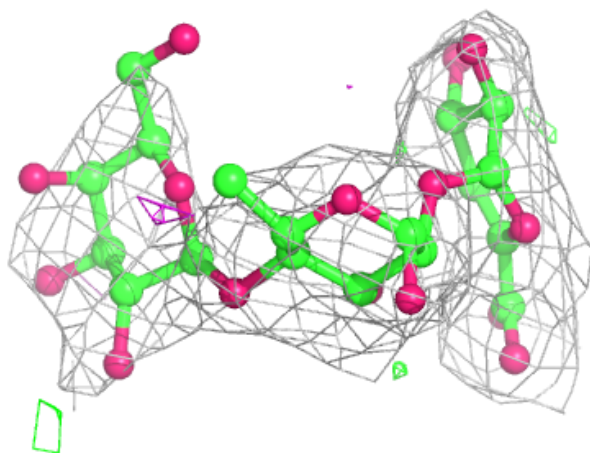
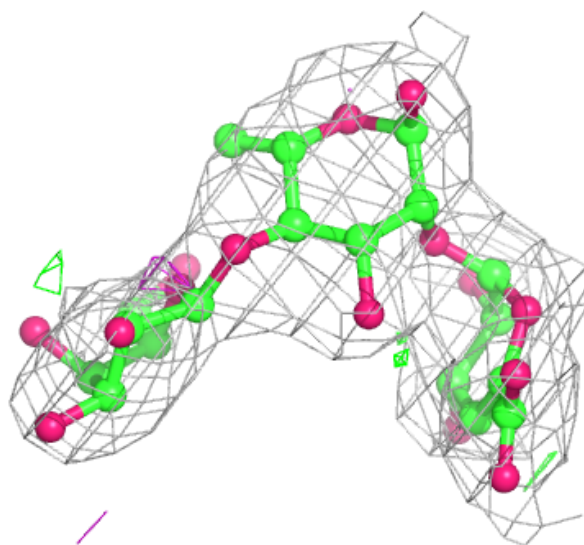
Electron density around Chain K:

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



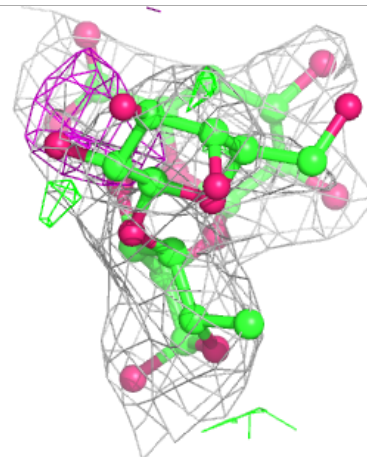
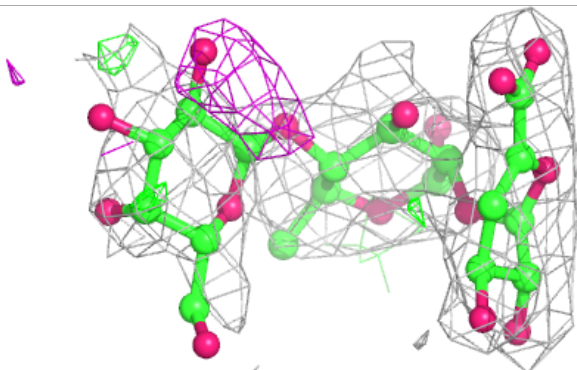
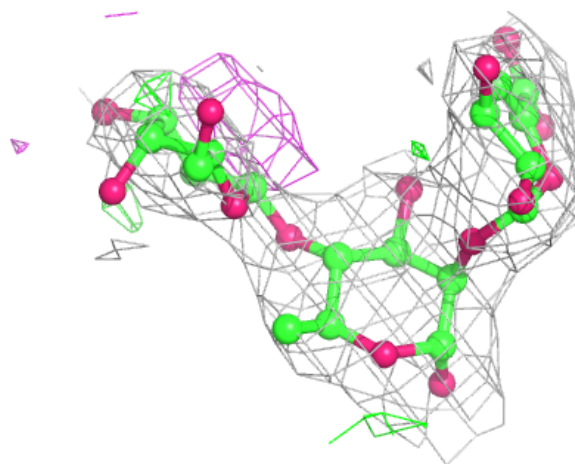
Electron density around Chain M:

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



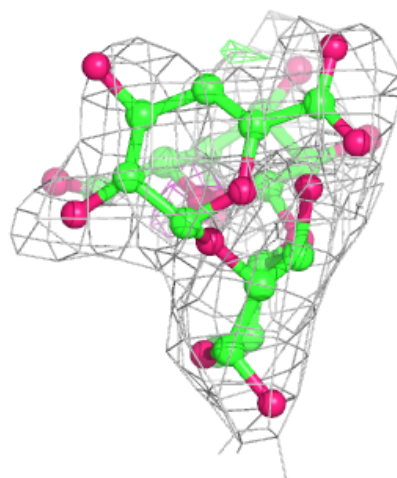
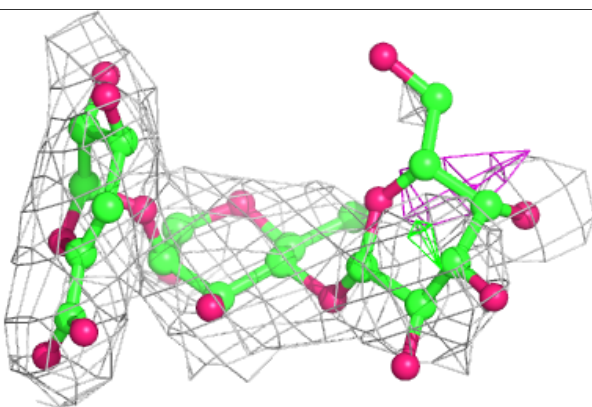
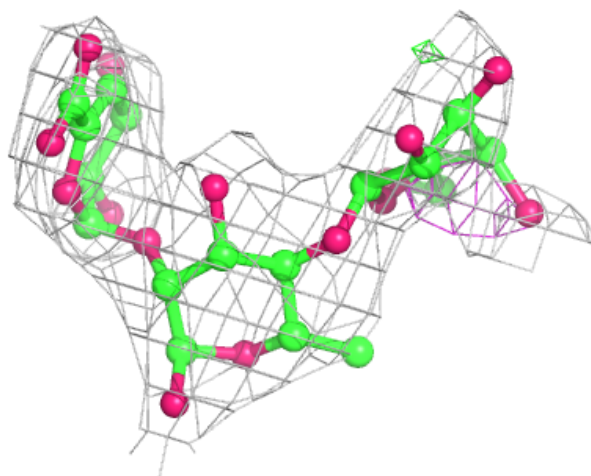
Electron density around Chain N:

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



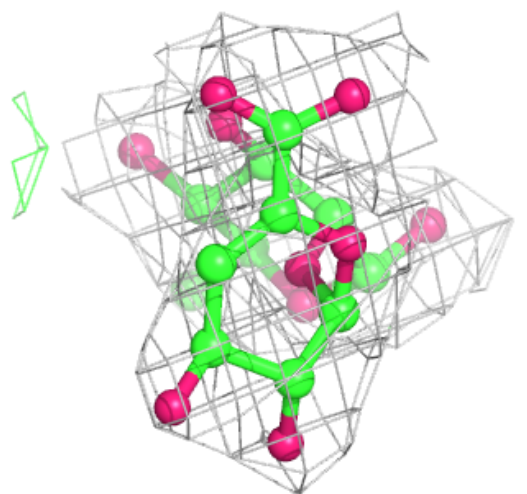
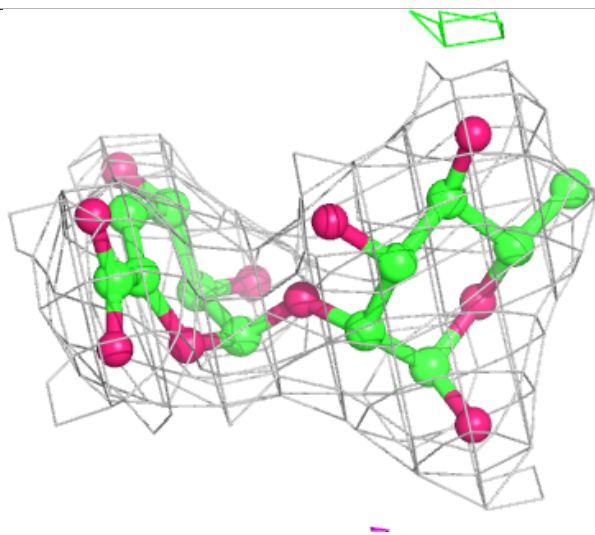
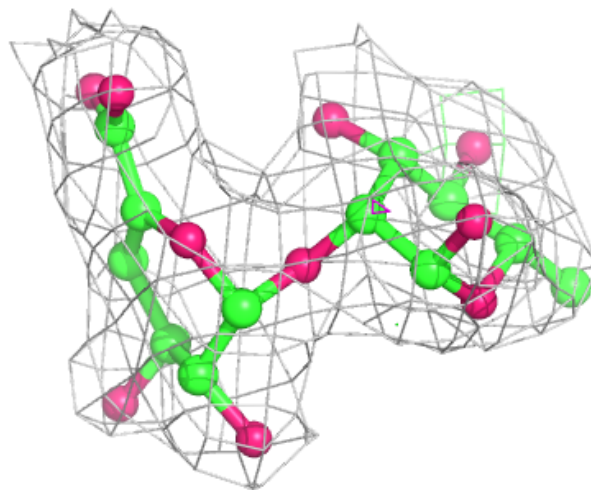
Electron density around Chain O:

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



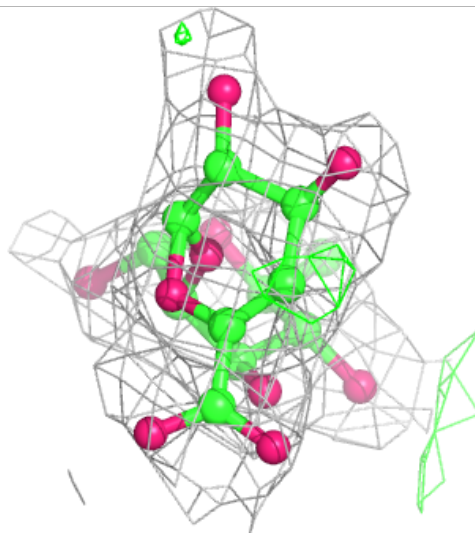
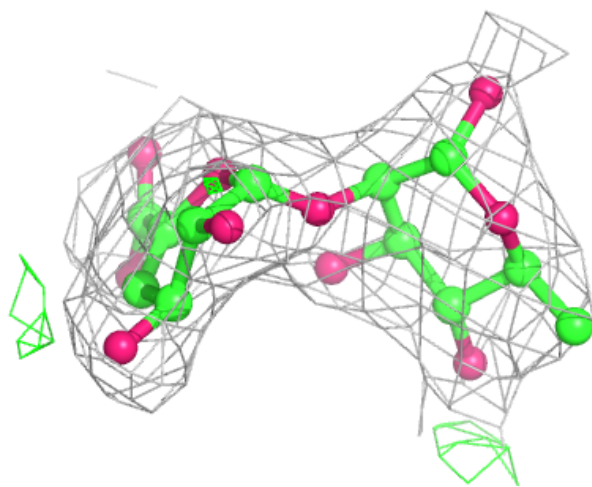
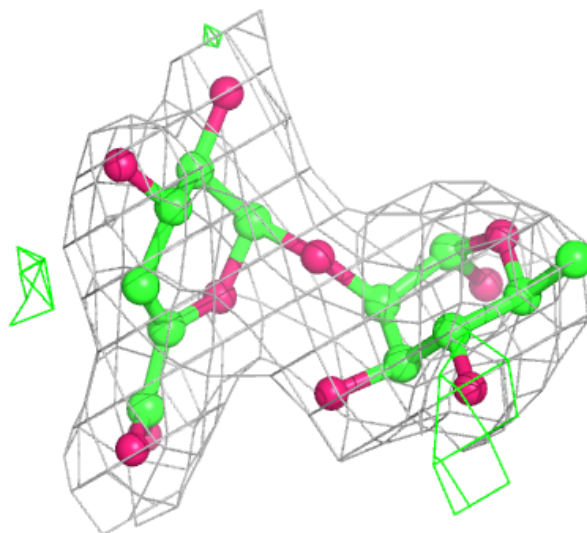
Electron density around Chain J:

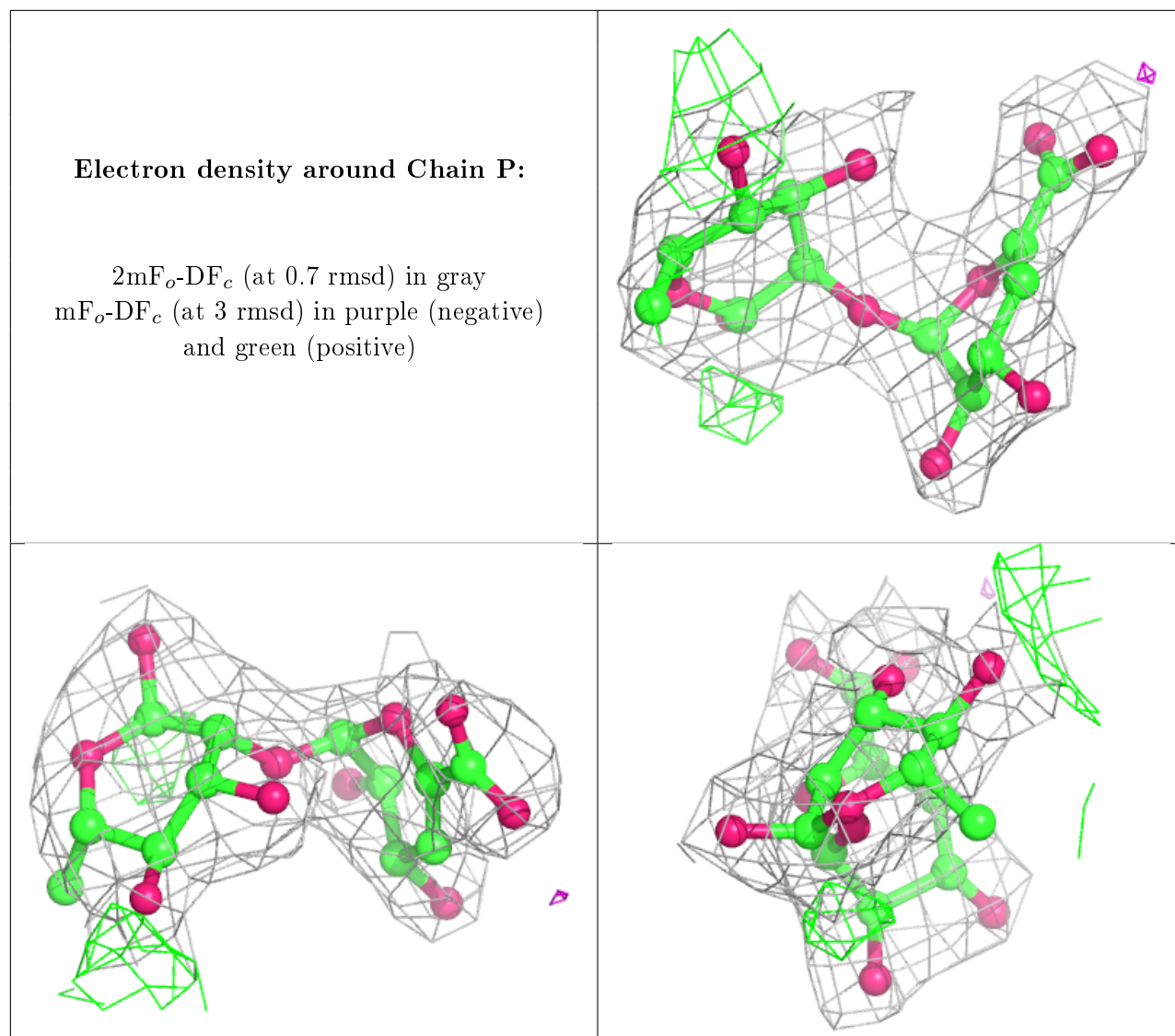
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	CA	E	1004	1/1	0.97	0.19	20,20,20,20	0
4	CA	F	1004	1/1	0.98	0.18	19,19,19,19	0
4	CA	A	1004	1/1	0.98	0.17	15,15,15,15	0
4	CA	H	1003	1/1	0.98	0.19	22,22,22,22	0
4	CA	G	1004	1/1	0.99	0.17	23,23,23,23	0
4	CA	B	1003	1/1	0.99	0.17	16,16,16,16	0
4	CA	C	1004	1/1	1.00	0.17	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	D	1003	1/1	1.00	0.18	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.