



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:00 AM UTC

PDB ID : 5XQG / pdb_00005xqg
Title : Crystal structure of a PL 26 exo-rhamnogalacturonan lyase from *Penicillium chrysogenum* complexed with unsaturated galacturonosyl rhamnose
Authors : Kunishige, Y.; Iwai, M.; Tada, T.; Nishimura, S.; Sakamoto, T.
Deposited on : 2017-06-07
Resolution : 2.74 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

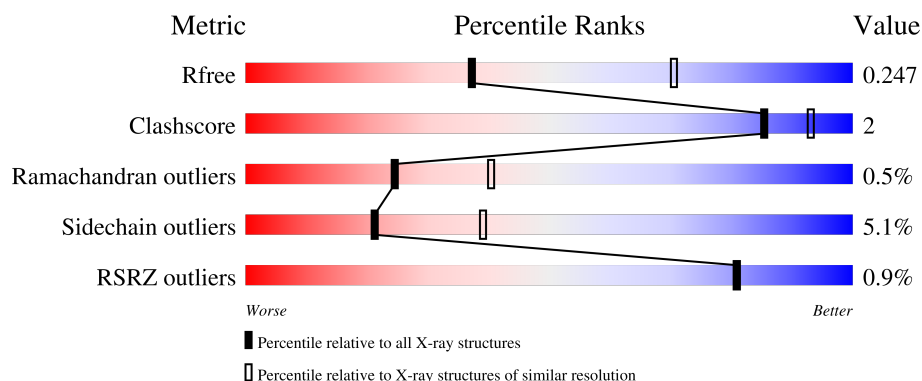
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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.



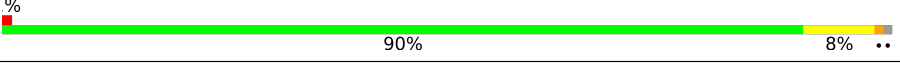
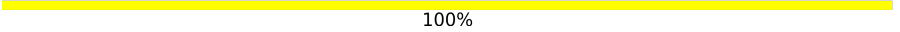
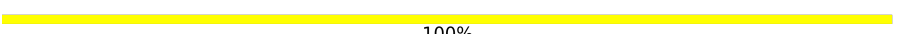
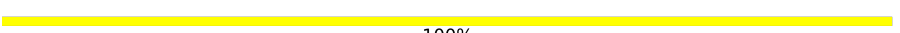
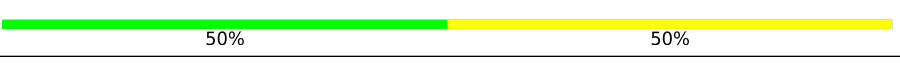
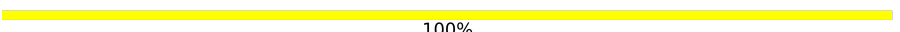
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	906	% 87% 10% ..
1	B	906	89% 9% ..
1	C	906	% 88% 9% ..
1	D	906	% 89% 6% ..
1	E	906	% 89% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	906	 90% 8% ..
1	G	906	 88% 8% . .
1	H	906	 89% 8% ..
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 50% 50%
2	M	2	 100%
2	N	2	 100%
2	O	2	 50% 50%
2	P	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 57208 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 Perglx 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
			6994	4464	1174	1350	6			
1	E	899	Total	C	N	O	S	0	1	0
			7054	4493	1183	1372	6			
1	F	900	Total	C	N	O	S	0	0	0
			7040	4487	1183	1364	6			
1	G	888	Total	C	N	O	S	0	1	0
			6989	4460	1170	1353	6			
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)-alpha-L-rhamnopyranose.



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	M	2	Total	C	O	0	0	0
			22	12	10			
2	N	2	Total	C	O	0	0	0
			22	12	10			
2	O	2	Total	C	O	0	0	0
			22	12	10			
2	P	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	128	Total	O	0	0
			128	128		
4	C	122	Total	O	0	0
			122	122		
4	D	95	Total	O	0	0
			95	95		
4	E	122	Total	O	0	0
			122	122		

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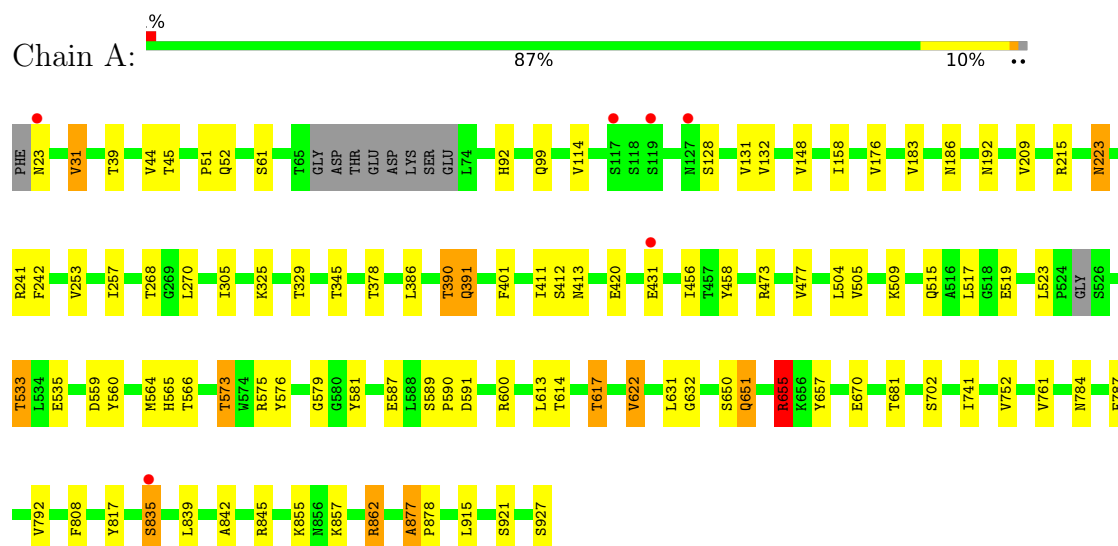
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	116	Total 116	O 116	0	0
4	G	72	Total 72	O 72	0	0
4	H	89	Total 89	O 89	0	0

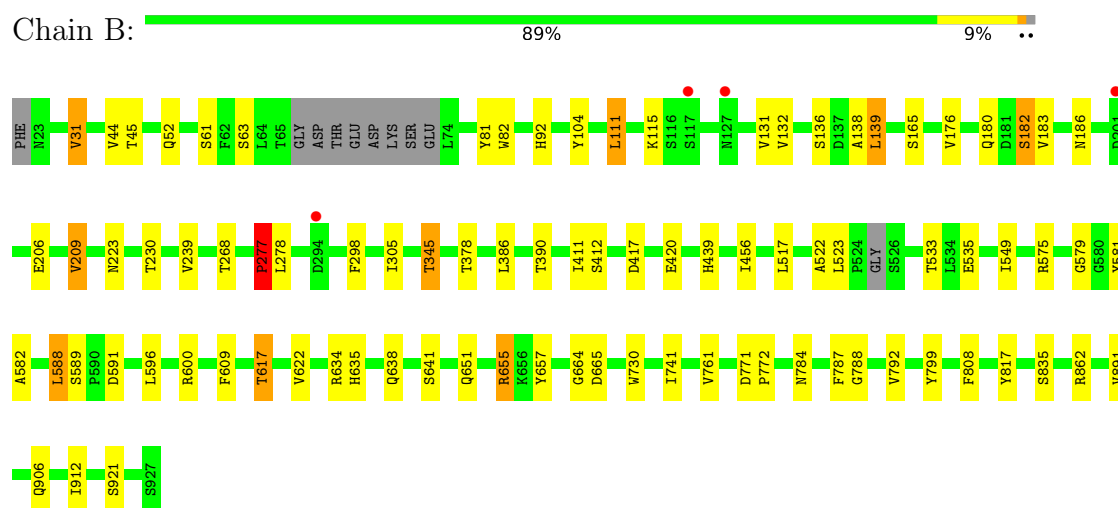
3 Residue-property plots [i](#)

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

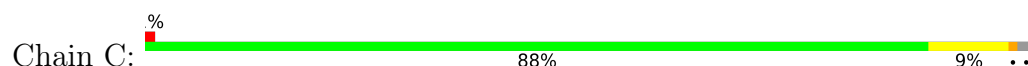
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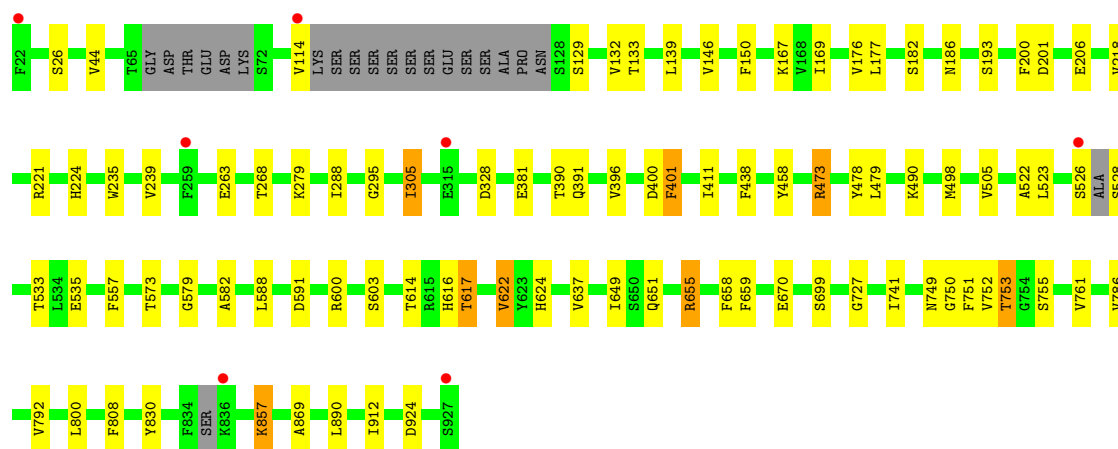


• Molecule 1: Pcrglx protein

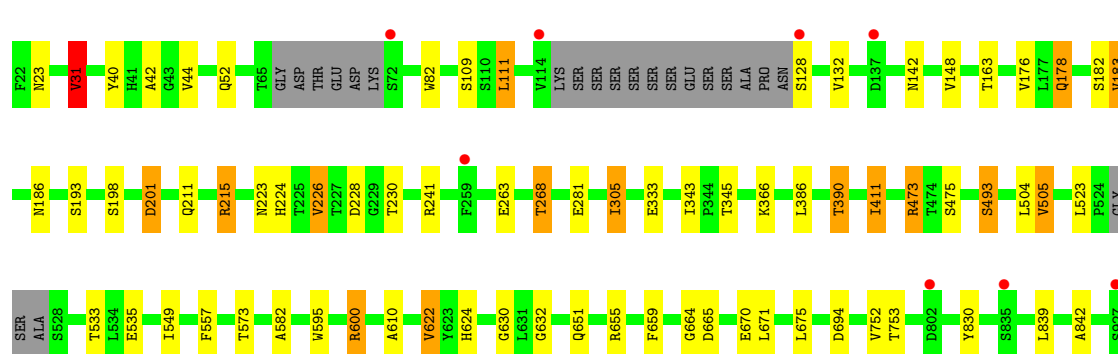
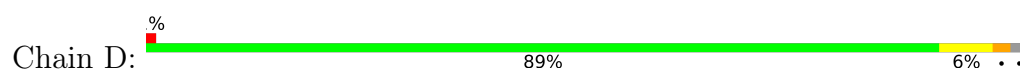


• Molecule 1: Pcrglx protein

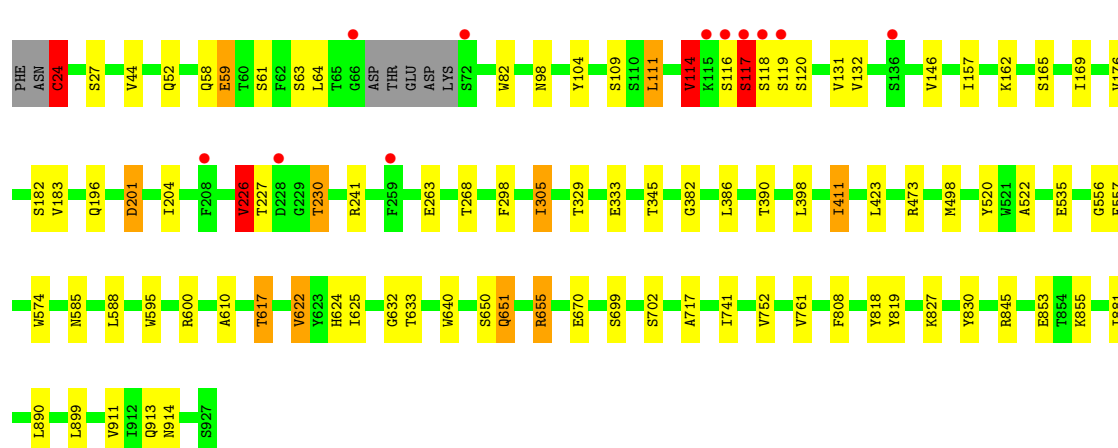
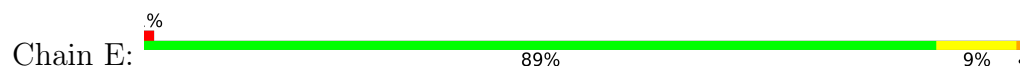




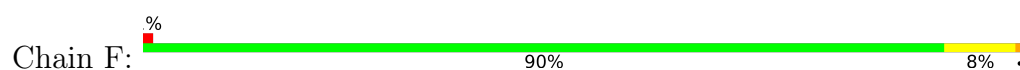
• Molecule 1: Pcrglx protein

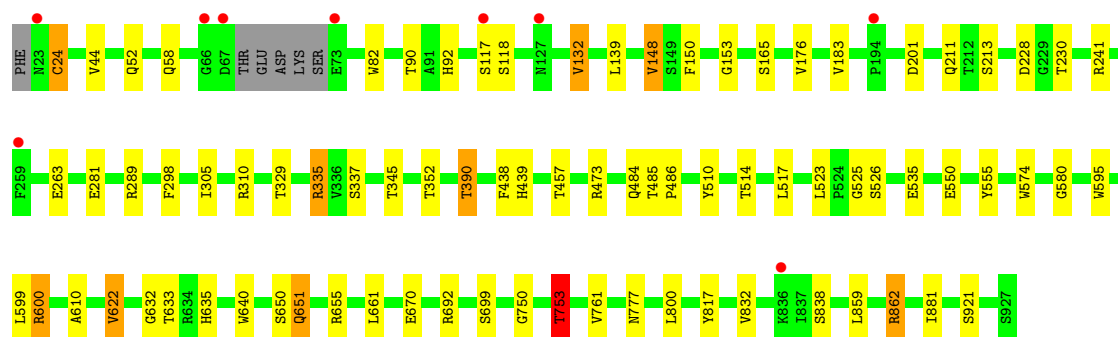


• Molecule 1: Pcrglx protein

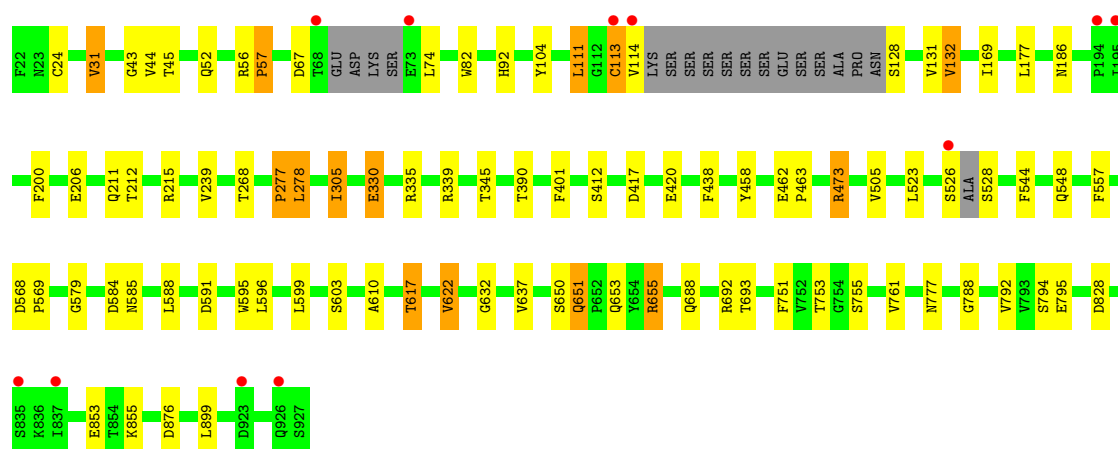
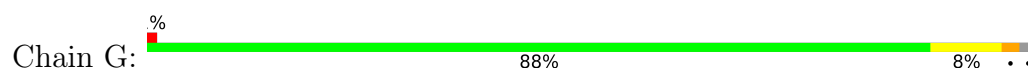


• Molecule 1: Pcrglx protein

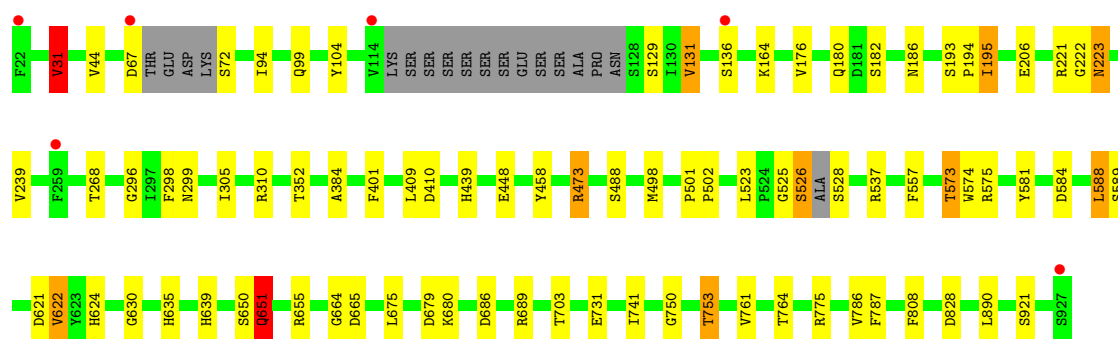
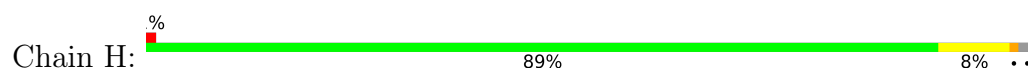




• Molecule 1: Pcrglx protein



• Molecule 1: Pcrglx protein



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



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

Chain J:  100%

RAM1
GAD2

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

Chain K:  100%

RAM1
GAD2

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

Chain L:  50%  50%

RAM1
GAD2

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

Chain M:  100%

RAM1
GAD2

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

Chain N:  100%

RAM1
GAD2

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

Chain O:  50%  50%

RAM1
GAD2

- Molecule 2: 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	167.88Å 171.94Å 342.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.19 – 2.74 171.19 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (171.19-2.74) 99.7 (171.19-2.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.08 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.188 , 0.247 0.193 , 0.247	Depositor DCC
R_{free} test set	12767 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	57208	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 46.86 % 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 1.0780e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.96	0/7232	1.06	11/9878 (0.1%)
1	B	0.96	1/7256 (0.0%)	1.04	9/9907 (0.1%)
1	C	0.95	0/7223	1.03	10/9857 (0.1%)
1	D	0.93	2/7218 (0.0%)	1.04	9/9854 (0.1%)
1	E	1.00	3/7262 (0.0%)	1.08	12/9914 (0.1%)
1	F	0.97	2/7245 (0.0%)	1.06	10/9892 (0.1%)
1	G	0.93	1/7196 (0.0%)	1.06	13/9822 (0.1%)
1	H	0.95	1/7204 (0.0%)	1.06	12/9833 (0.1%)
All	All	0.96	10/57836 (0.0%)	1.05	86/78957 (0.1%)

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	E	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	24	CYS	C-N	18.36	1.57	1.33
1	F	486	PRO	CA-C	-6.24	1.47	1.53
1	E	27	SER	C-O	-5.92	1.16	1.23
1	B	278	LEU	N-CA	5.81	1.53	1.46
1	G	74	LEU	N-CA	5.67	1.52	1.46
1	E	226	VAL	C-O	-5.53	1.18	1.24
1	F	153	GLY	C-O	5.48	1.29	1.23
1	D	343	ILE	N-CA	-5.41	1.42	1.46
1	H	310	ARG	CA-C	-5.40	1.46	1.52
1	D	366	LYS	CA-C	5.03	1.58	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	24	CYS	O-C-N	-21.80	88.12	123.00
1	E	114	VAL	CB-CA-C	-9.38	100.12	111.94
1	F	457	THR	N-CA-C	-9.31	98.52	110.53
1	C	305	ILE	N-CA-CB	-7.98	103.43	112.21
1	H	195	ILE	N-CA-CB	-7.97	100.41	111.41
1	F	753	THR	N-CA-C	-7.67	99.42	110.24
1	H	222	GLY	N-CA-C	7.50	121.02	110.74
1	F	574	TRP	N-CA-C	-7.04	101.23	110.53
1	B	183	VAL	CA-C-N	-6.97	113.47	120.31
1	B	183	VAL	C-N-CA	-6.97	113.47	120.31
1	E	226	VAL	CB-CA-C	-6.94	100.28	111.59
1	G	114	VAL	N-CA-CB	6.84	123.12	111.50
1	D	23	ASN	CB-CA-C	-6.76	96.97	110.42
1	A	456	ILE	N-CA-C	6.71	117.33	111.90
1	G	111	LEU	N-CA-C	6.68	119.41	111.33
1	G	74	LEU	N-CA-C	6.55	119.57	108.90
1	B	439	HIS	N-CA-C	6.51	119.07	109.24
1	E	116	SER	CA-C-N	6.46	133.88	121.54
1	E	116	SER	C-N-CA	6.46	133.88	121.54
1	G	43	GLY	N-CA-C	-6.44	103.55	112.18
1	E	117	SER	N-CA-C	6.43	124.49	110.80
1	A	784	ASN	N-CA-C	6.36	118.21	111.28
1	C	616	HIS	CA-C-N	6.35	128.69	120.44
1	C	616	HIS	C-N-CA	6.35	128.69	120.44
1	C	869	ALA	N-CA-C	6.30	117.84	110.41
1	D	31	VAL	CB-CA-C	6.22	120.07	110.50
1	D	215	ARG	N-CA-C	6.00	118.53	109.23
1	D	226	VAL	CB-CA-C	-5.99	101.47	111.29
1	F	24	CYS	N-CA-C	5.98	123.53	110.80
1	E	411	ILE	CB-CA-C	-5.93	102.77	110.84
1	A	877	ALA	CA-C-N	-5.90	112.50	119.05
1	A	877	ALA	C-N-CA	-5.90	112.50	119.05
1	G	57	PRO	N-CA-C	5.87	124.57	112.47
1	E	24	CYS	N-CA-CB	5.86	120.47	110.50
1	B	345	THR	CB-CA-C	5.83	119.12	110.14
1	E	574	TRP	N-CA-C	-5.83	102.84	110.53
1	A	533	THR	N-CA-CB	5.81	119.29	110.28
1	A	655	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	G	113	CYS	CA-C-N	5.78	132.11	121.70
1	G	113	CYS	C-N-CA	5.78	132.11	121.70
1	C	792	VAL	CB-CA-C	-5.77	104.58	111.97
1	G	278	LEU	N-CA-C	5.76	123.06	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	ILE	N-CA-C	5.73	116.54	111.90
1	H	31	VAL	CB-CA-C	5.71	119.30	110.50
1	H	223	ASN	N-CA-CB	-5.69	102.38	111.43
1	E	911	VAL	CB-CA-C	-5.69	104.56	112.02
1	H	296	GLY	N-CA-C	5.66	118.44	111.93
1	G	215	ARG	N-CA-C	5.63	117.75	109.24
1	E	305	ILE	N-CA-CB	-5.59	105.68	112.33
1	G	305	ILE	N-CA-CB	-5.57	105.71	112.33
1	G	277	PRO	N-CA-C	5.51	121.36	113.47
1	D	694	ASP	N-CA-C	5.49	119.69	113.15
1	A	431	GLU	N-CA-C	-5.44	102.57	110.08
1	D	493	SER	N-CA-C	5.40	116.85	111.07
1	D	305	ILE	N-CA-CB	-5.40	106.27	112.21
1	F	457	THR	CA-C-N	-5.39	113.02	122.62
1	F	457	THR	C-N-CA	-5.39	113.02	122.62
1	A	792	VAL	CB-CA-C	-5.38	104.97	112.02
1	B	784	ASN	N-CA-C	5.35	118.60	111.75
1	H	584	ASP	N-CA-C	5.35	117.19	111.36
1	G	56	ARG	CA-C-N	5.32	126.50	119.84
1	G	56	ARG	C-N-CA	5.32	126.50	119.84
1	H	439	HIS	N-CA-C	5.31	117.06	109.14
1	F	600	ARG	N-CA-C	5.27	117.78	111.71
1	F	201	ASP	N-CA-C	-5.26	101.98	110.14
1	C	727	GLY	CA-C-N	5.24	125.55	119.47
1	C	727	GLY	C-N-CA	5.24	125.55	119.47
1	B	891	VAL	N-CA-CB	5.23	115.44	111.83
1	A	573	THR	CB-CA-C	-5.21	98.62	110.07
1	F	580	GLY	N-CA-C	5.16	120.13	114.40
1	C	649	ILE	N-CA-C	-5.15	106.66	111.45
1	H	651	GLN	CA-C-N	5.15	124.81	119.56
1	H	651	GLN	C-N-CA	5.15	124.81	119.56
1	C	800	LEU	N-CA-C	5.14	116.89	111.28
1	A	223	ASN	CB-CA-C	-5.11	98.83	110.07
1	F	800	LEU	N-CA-C	5.10	117.58	111.71
1	E	717	ALA	N-CA-C	-5.10	105.91	111.82
1	C	235	TRP	N-CA-C	5.09	114.96	108.24
1	H	182	SER	N-CA-CB	-5.09	103.67	111.56
1	A	845	ARG	N-CA-C	5.08	117.55	111.71
1	D	183	VAL	CA-C-N	-5.08	114.72	119.85
1	D	183	VAL	C-N-CA	-5.08	114.72	119.85
1	H	131	VAL	CB-CA-C	5.07	118.14	110.63
1	B	730	TRP	N-CA-C	5.06	116.87	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	221	ARG	N-CA-C	5.04	117.96	109.95
1	B	138	ALA	N-CA-C	5.00	116.01	108.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	24	CYS	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7025	0	6584	36	0
1	B	7052	0	6618	31	0
1	C	7007	0	6587	31	0
1	D	6994	0	6572	23	1
1	E	7054	0	6633	39	1
1	F	7040	0	6601	23	0
1	G	6989	0	6553	37	0
1	H	6997	0	6567	25	0
2	I	22	0	17	0	0
2	J	22	0	17	0	0
2	K	22	0	16	0	0
2	L	22	0	17	0	0
2	M	22	0	17	0	0
2	N	22	0	17	0	0
2	O	22	0	17	2	0
2	P	22	0	17	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	122	0	0	2	0
4	B	128	0	0	1	0
4	C	122	0	0	1	0
4	D	95	0	0	0	0
4	E	122	0	0	2	0
4	F	116	0	0	0	0
4	G	72	0	0	1	0
4	H	89	0	0	1	0
All	All	57208	0	52850	241	1

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 (241) 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:G:24:CYS:CB	1:G:113:CYS:SG	2.14	1.34
1:G:526:SER:HG	1:G:528:SER:N	1.56	1.04
1:E:201:ASP:OD2	1:E:227:THR:HG21	1.73	0.88
1:E:119:SER:O	1:E:120:SER:C	2.23	0.81
1:G:24:CYS:HG	1:G:113:CYS:CB	1.95	0.78
1:G:24:CYS:HB2	1:G:113:CYS:SG	2.28	0.72
1:G:688:GLN:HE22	2:O:1:RAM:H62	1.57	0.69
1:G:526:SER:OG	1:G:528:SER:N	2.26	0.69
1:H:526:SER:O	1:H:528:SER:N	2.29	0.66
1:G:31:VAL:HG12	1:G:104:TYR:HB2	1.77	0.66
1:G:277:PRO:O	1:G:417:ASP:O	2.13	0.66
1:E:241:ARG:NH2	1:E:670:GLU:OE2	2.28	0.65
1:G:473:ARG:HD3	1:G:557:PHE:O	1.96	0.65
1:C:391:GLN:HG2	4:C:1214:HOH:O	1.97	0.65
1:E:196:GLN:NE2	1:E:230:THR:HG21	2.12	0.65
1:D:281:GLU:OE1	1:D:390:THR:HB	1.97	0.64
1:E:59:GLU:HA	1:E:111:LEU:HD22	1.79	0.63
1:A:591:ASP:OD2	1:A:617:THR:HG21	2.00	0.62
1:A:192:ASN:ND2	1:D:228:ASP:OD2	2.32	0.62
1:G:591:ASP:OD2	1:G:617:THR:HG21	2.00	0.61
1:B:591:ASP:OD2	1:B:617:THR:HG21	2.01	0.60
1:G:111:LEU:HD12	1:G:111:LEU:O	2.00	0.60
1:E:617:THR:HG23	1:E:655:ARG:NH1	2.17	0.60
1:E:752:VAL:HG21	1:E:830:TYR:CZ	2.35	0.59
1:F:753:THR:HG22	1:F:777:ASN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:THR:HG23	1:B:655:ARG:NH1	2.18	0.59
1:B:817:TYR:O	1:B:862:ARG:NH2	2.36	0.59
1:H:750:GLY:O	1:H:753:THR:HG23	2.02	0.59
1:D:31:VAL:HG13	1:D:504:LEU:HB3	1.85	0.59
1:B:600:ARG:HD3	1:B:912:ILE:HG23	1.85	0.58
1:D:178[A]:GLN:HG2	1:D:268:THR:HG22	1.85	0.58
1:D:386:LEU:HD22	1:D:411:ILE:HG23	1.85	0.58
1:G:688:GLN:NE2	2:O:1:RAM:H62	2.18	0.58
1:B:664:GLY:O	1:B:665:ASP:C	2.46	0.57
1:D:111:LEU:O	1:D:111:LEU:HD12	2.03	0.57
1:A:617:THR:CG2	1:A:655:ARG:NH1	2.68	0.57
1:C:288:ILE:HG23	1:C:411:ILE:CD1	2.35	0.56
1:A:535:GLU:CD	1:A:600:ARG:HH22	2.14	0.55
1:D:473:ARG:HD3	1:D:557:PHE:O	2.07	0.55
1:G:595:TRP:CE2	1:G:610:ALA:HB1	2.43	0.54
1:H:195:ILE:HG23	1:H:195:ILE:O	2.07	0.54
1:A:631:LEU:HG	1:A:681:THR:HG21	1.89	0.54
1:B:522:ALA:O	1:B:600:ARG:HD2	2.07	0.54
1:C:751:PHE:O	1:C:753:THR:O	2.26	0.54
1:A:535:GLU:OE1	1:A:600:ARG:NH2	2.40	0.54
1:G:412:SER:HB3	1:G:420:GLU:HB2	1.90	0.54
1:C:535:GLU:OE1	1:C:600:ARG:NH2	2.40	0.54
1:F:650:SER:O	1:F:651:GLN:C	2.51	0.54
1:G:751:PHE:O	1:G:753:THR:O	2.26	0.53
1:C:201:ASP:O	1:C:224:HIS:HA	2.09	0.53
1:F:599:LEU:HD21	1:F:661:LEU:HD11	1.89	0.53
1:A:564:MET:HE1	1:A:576:TYR:HB3	1.91	0.53
1:C:522:ALA:O	1:C:600:ARG:HD2	2.08	0.53
1:H:575:ARG:HD2	1:H:581:TYR:HB3	1.91	0.52
1:F:750:GLY:O	1:F:753:THR:OG1	2.27	0.52
1:B:139:LEU:HD11	1:B:209:VAL:HG21	1.91	0.52
1:E:196:GLN:HE21	1:E:230:THR:HG21	1.71	0.52
1:D:198:SER:OG	1:D:230:THR:HG22	2.10	0.52
1:E:741:ILE:HG23	1:E:808:PHE:CG	2.45	0.51
1:C:221:ARG:NH2	1:C:670:GLU:OE1	2.38	0.51
1:C:288:ILE:HG23	1:C:411:ILE:HD13	1.93	0.51
1:E:650:SER:O	1:E:651:GLN:C	2.53	0.51
1:C:473:ARG:HD3	1:C:557:PHE:O	2.11	0.51
1:B:277:PRO:O	1:B:417:ASP:O	2.28	0.51
1:E:114:VAL:O	1:E:117:SER:OG	2.21	0.51
1:E:169:ILE:C	1:E:169:ILE:HD12	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:GLU:OE1	1:F:600:ARG:NH2	2.43	0.51
1:B:517:LEU:HG	1:B:657:TYR:HD1	1.76	0.51
1:B:549:ILE:HD11	1:B:609:PHE:CE1	2.46	0.50
1:H:473:ARG:HD3	1:H:557:PHE:O	2.10	0.50
1:G:169:ILE:C	1:G:169:ILE:HD12	2.36	0.50
1:D:664:GLY:O	1:D:665:ASP:C	2.55	0.50
1:E:622:VAL:HA	1:E:632:GLY:HA2	1.93	0.49
1:F:241:ARG:NH2	1:F:670:GLU:OE2	2.45	0.49
1:F:622:VAL:HA	1:F:632:GLY:HA2	1.94	0.49
1:H:741:ILE:HG23	1:H:808:PHE:CD1	2.47	0.49
1:A:741:ILE:HG23	1:A:808:PHE:CD1	2.47	0.49
1:C:752:VAL:HG21	1:C:830:TYR:CZ	2.47	0.49
1:G:596:LEU:HD23	1:G:599:LEU:HD12	1.95	0.49
1:B:617:THR:CG2	1:B:655:ARG:NH1	2.75	0.49
1:C:857:LYS:NZ	1:C:924:ASP:OD2	2.45	0.49
1:H:31:VAL:HG12	1:H:104:TYR:HB2	1.95	0.49
1:H:630:GLY:HA2	1:H:675:LEU:HD23	1.95	0.49
1:E:157:ILE:HA	1:E:204:ILE:HD11	1.95	0.48
1:A:617:THR:HG23	4:A:1123:HOH:O	2.13	0.48
1:A:817:TYR:O	1:A:862:ARG:NH2	2.46	0.48
1:B:589:SER:OG	1:B:787:PHE:HA	2.14	0.48
1:E:535:GLU:OE1	1:E:600:ARG:NH2	2.47	0.48
1:E:52:GLN:HA	1:E:82:TRP:CD1	2.48	0.48
1:F:484:GLN:O	1:F:485:THR:C	2.56	0.48
1:G:622:VAL:HA	1:G:632:GLY:HA2	1.95	0.48
1:C:526:SER:O	1:C:528:SER:N	2.47	0.48
1:A:253:VAL:HB	1:A:477:VAL:HB	1.96	0.48
1:B:741:ILE:HG23	1:B:808:PHE:CD1	2.48	0.48
1:B:45:THR:HA	1:B:92:HIS:O	2.14	0.47
1:F:148:VAL:HG22	1:F:150:PHE:CE2	2.49	0.47
1:F:550:GLU:HG3	1:F:555:TYR:OH	2.15	0.47
1:A:31:VAL:HG13	1:A:504:LEU:HB3	1.97	0.47
1:B:386:LEU:HD22	1:B:411:ILE:HG23	1.94	0.47
1:E:226:VAL:HG22	4:E:1142:HOH:O	2.13	0.47
1:B:412:SER:HB3	1:B:420:GLU:HB2	1.96	0.47
1:D:241:ARG:NH2	1:D:670:GLU:OE2	2.48	0.47
1:D:624:HIS:CE1	1:D:671:LEU:HD22	2.49	0.47
1:F:535:GLU:CD	1:F:600:ARG:HH22	2.22	0.47
1:H:664:GLY:O	1:H:665:ASP:C	2.57	0.47
1:A:877:ALA:O	1:A:878:PRO:C	2.56	0.47
1:B:81:TYR:O	1:B:799:TYR:OH	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:ARG:O	1:G:339:ARG:HD2	2.14	0.47
1:F:595:TRP:CE2	1:F:610:ALA:HB1	2.49	0.46
1:H:180:GLN:NE2	1:H:195:ILE:HD11	2.30	0.46
1:B:182:SER:HB2	4:B:1217:HOH:O	2.14	0.46
1:D:630:GLY:HA2	1:D:675:LEU:HD23	1.97	0.46
1:F:438:PHE:CZ	1:F:439:HIS:HD2	2.34	0.46
1:B:298:PHE:HB2	1:C:890:LEU:HD13	1.97	0.46
1:C:295:GLY:H	1:C:381[A]:GLU:CD	2.23	0.46
1:B:535:GLU:CD	1:B:600:ARG:HH22	2.24	0.46
1:C:169:ILE:C	1:C:169:ILE:HD12	2.40	0.46
1:C:741:ILE:HG23	1:C:808:PHE:CD1	2.50	0.46
1:C:588:LEU:HD22	1:C:786:VAL:CG2	2.46	0.46
1:E:520:TYR:O	1:E:913:GLN:HG2	2.17	0.46
1:F:132:VAL:HG13	1:F:211:GLN:NE2	2.30	0.46
1:E:382:GLY:O	1:E:498:MET:HE1	2.16	0.45
1:E:114:VAL:O	1:E:117:SER:CB	2.64	0.45
1:E:633:THR:HG21	1:E:640:TRP:HA	1.97	0.45
1:B:31:VAL:HG12	1:B:104:TYR:HB2	1.98	0.45
1:G:462:GLU:HG3	1:G:463:PRO:HD2	1.97	0.45
1:F:310:ARG:HG3	1:F:335:ARG:HB3	1.99	0.45
1:G:52:GLN:HA	1:G:82:TRP:CD1	2.51	0.45
1:H:650:SER:O	1:H:651:GLN:C	2.59	0.45
1:A:158:ILE:HD11	1:A:242:PHE:CE2	2.52	0.45
1:C:396:VAL:HG23	1:C:479:LEU:HD23	1.99	0.45
1:C:478:TYR:CD2	1:C:498:MET:HG3	2.51	0.45
1:E:111:LEU:HD12	1:E:111:LEU:HA	1.63	0.45
1:B:111:LEU:HD23	1:B:115:LYS:HE3	1.99	0.45
1:C:591:ASP:OD2	1:C:617:THR:HG21	2.17	0.45
1:G:585:ASN:N	1:G:585:ASN:HD22	2.15	0.45
1:A:517:LEU:HG	1:A:657:TYR:HD1	1.81	0.44
1:B:588:LEU:HD13	1:B:906:GLN:HG3	1.99	0.44
1:A:589:SER:OG	1:A:787:PHE:HA	2.18	0.44
1:D:839:LEU:HB3	1:D:842:ALA:HB3	1.98	0.44
1:E:845:ARG:HA	1:E:914:ASN:OD1	2.17	0.44
1:H:384:ALA:HB2	1:H:409:LEU:HD13	1.99	0.44
1:A:559:ASP:O	1:A:560:TYR:C	2.60	0.44
1:B:634:ARG:HG3	1:B:635:HIS:CD2	2.52	0.44
1:F:510:TYR:O	1:F:514:THR:HG23	2.18	0.44
1:A:413:ASN:ND2	1:A:420:GLU:OE1	2.42	0.44
1:A:839:LEU:HB3	1:A:842:ALA:HB3	1.99	0.44
1:F:817:TYR:O	1:F:862:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:568:ASP:C	1:G:568:ASP:OD1	2.60	0.44
1:H:589:SER:OG	1:H:787:PHE:HA	2.17	0.44
1:E:298:PHE:HB2	1:H:890:LEU:HD13	2.00	0.44
1:F:633:THR:HG21	1:F:640:TRP:HA	1.99	0.44
1:A:752:VAL:O	1:A:752:VAL:HG12	2.18	0.43
1:H:621:ASP:OD1	1:H:639:HIS:HB3	2.19	0.43
1:A:509:LYS:HB3	4:A:1207:HOH:O	2.18	0.43
1:G:650:SER:O	1:G:651:GLN:C	2.61	0.43
1:C:438:PHE:CE1	1:C:637:VAL:HB	2.54	0.43
1:G:438:PHE:CE1	1:G:637:VAL:HB	2.54	0.43
1:D:40:TYR:OH	1:D:42:ALA:HB2	2.19	0.43
1:E:595:TRP:CE2	1:E:610:ALA:HB1	2.54	0.43
1:B:549:ILE:HD11	1:B:609:PHE:HE1	1.84	0.43
1:E:398:LEU:HB2	1:E:423:LEU:HD21	2.00	0.43
1:F:281:GLU:CD	1:F:390:THR:HB	2.44	0.43
1:A:45:THR:HA	1:A:92:HIS:O	2.19	0.43
1:A:915:LEU:HD23	1:A:915:LEU:HA	1.93	0.43
1:D:31:VAL:HG22	1:D:505:VAL:C	2.44	0.43
1:E:622:VAL:HG22	1:E:624:HIS:CE1	2.54	0.43
1:D:535:GLU:OE1	1:D:600:ARG:NH2	2.47	0.42
1:E:117:SER:HB3	1:E:118:SER:H	1.35	0.42
1:G:653:GLN:NE2	1:G:795:GLU:OE1	2.48	0.42
1:H:299:ASN:OD1	1:H:488:SER:OG	2.35	0.42
1:H:588:LEU:HD22	1:H:786:VAL:HG21	2.01	0.42
1:B:596:LEU:O	1:B:600:ARG:HG3	2.18	0.42
1:G:569:PRO:HD2	4:G:1120:HOH:O	2.20	0.42
1:H:622:VAL:HG22	1:H:624:HIS:CE1	2.54	0.42
1:A:515:GLN:HE21	1:A:519:GLU:HG2	1.84	0.42
1:A:587:GLU:O	1:A:590:PRO:HD3	2.18	0.42
1:G:45:THR:HA	1:G:92:HIS:O	2.19	0.42
1:E:535:GLU:CD	1:E:600:ARG:HH22	2.27	0.42
1:E:818:TYR:O	1:E:819:TYR:C	2.62	0.42
1:H:679:ASP:OD1	1:H:680:LYS:N	2.53	0.42
1:A:257:ILE:HD13	1:A:270:LEU:HD21	2.02	0.42
1:A:613:LEU:O	1:A:617:THR:HB	2.19	0.42
1:B:638:GLN:HB2	1:B:641:SER:HB3	2.01	0.42
1:C:749:ASN:O	1:C:750:GLY:C	2.62	0.42
1:F:52:GLN:HA	1:F:82:TRP:CD1	2.54	0.42
1:F:289:ARG:HA	1:F:298:PHE:O	2.20	0.42
1:C:617:THR:CG2	1:C:655:ARG:NH1	2.83	0.42
1:H:501:PRO:HA	1:H:502:PRO:HD3	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:741:ILE:HG23	1:H:808:PHE:CG	2.55	0.42
1:B:788:GLY:O	1:B:792:VAL:HG23	2.19	0.42
1:D:622:VAL:HA	1:D:632:GLY:HA2	2.00	0.42
1:D:752:VAL:HG21	1:D:830:TYR:CZ	2.55	0.42
1:A:51:PRO:O	1:A:52:GLN:C	2.62	0.42
1:C:535:GLU:CD	1:C:600:ARG:HH22	2.27	0.42
1:G:24:CYS:CA	1:G:113:CYS:SG	3.01	0.42
1:G:132:VAL:HG13	1:G:211:GLN:CD	2.45	0.42
1:G:584:ASP:O	1:G:585:ASN:C	2.62	0.42
1:A:617:THR:HG23	1:A:655:ARG:NH1	2.35	0.42
1:C:600:ARG:HD3	1:C:912:ILE:HG23	2.01	0.42
1:D:659:PHE:CE1	1:D:664:GLY:HA2	2.54	0.42
1:F:90:THR:OG1	1:F:92:HIS:NE2	2.50	0.42
1:G:617:THR:HG23	1:G:655:ARG:NH1	2.35	0.42
1:D:142:ASN:C	1:D:142:ASN:OD1	2.63	0.41
1:G:544:PHE:O	1:G:548:GLN:HG2	2.20	0.41
1:G:899:LEU:HD12	1:G:899:LEU:C	2.45	0.41
1:B:575:ARG:HD2	1:B:581:TYR:HB3	2.02	0.41
1:E:24:CYS:O	1:E:24:CYS:SG	2.78	0.41
1:E:556:GLY:O	1:E:557:PHE:C	2.63	0.41
1:D:595:TRP:CE2	1:D:610:ALA:HB1	2.56	0.41
1:E:386:LEU:HB2	1:E:411:ILE:HD12	2.01	0.41
1:E:899:LEU:HD12	1:E:899:LEU:C	2.46	0.41
1:A:622:VAL:HA	1:A:632:GLY:HA2	2.03	0.41
1:C:150:PHE:CE2	1:C:218:VAL:HG21	2.55	0.41
1:A:241:ARG:NH2	1:A:670:GLU:OE2	2.53	0.41
1:C:400:ASP:O	1:C:401:PHE:C	2.64	0.41
1:E:241:ARG:NH1	4:E:1115:HOH:O	2.54	0.41
1:H:573:THR:HB	1:H:574:TRP:O	2.20	0.41
1:E:146:VAL:HA	1:E:162:LYS:O	2.20	0.41
1:A:575:ARG:HD2	1:A:581:TYR:HB3	2.03	0.41
1:C:622:VAL:HG22	1:C:624:HIS:CE1	2.55	0.41
1:E:522:ALA:O	1:E:600:ARG:HG2	2.21	0.41
1:F:859:LEU:O	1:F:862:ARG:HB3	2.20	0.41
1:H:525:GLY:N	4:H:1105:HOH:O	2.53	0.41
1:A:386:LEU:HD22	1:A:411:ILE:HG23	2.02	0.41
1:C:617:THR:CG2	1:C:655:ARG:HH11	2.34	0.41
1:D:52:GLN:HA	1:D:82:TRP:CD1	2.56	0.41
1:E:64:LEU:HD11	1:E:104:TYR:HB3	2.02	0.41
1:E:890:LEU:HD13	1:H:298:PHE:HB2	2.02	0.41
1:G:177:LEU:HB3	1:G:200:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:SER:O	1:A:651:GLN:C	2.64	0.41
1:C:658:PHE:O	1:C:659:PHE:C	2.63	0.41
1:A:390:THR:HG22	1:A:391[B]:GLN:OE1	2.20	0.40
1:G:111:LEU:HD12	1:G:111:LEU:C	2.43	0.40
1:A:565:HIS:ND1	1:A:566:THR:OG1	2.52	0.40
1:H:686:ASP:HB3	1:H:689:ARG:HB3	2.02	0.40
1:D:201:ASP:O	1:D:224:HIS:HA	2.22	0.40
1:B:52:GLN:HA	1:B:82:TRP:CD1	2.56	0.40
1:B:771:ASP:N	1:B:772:PRO:CD	2.84	0.40
1:C:177:LEU:HB3	1:C:200:PHE:HB2	2.02	0.40
1:G:788:GLY:O	1:G:792:VAL:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:GLN:O	1:E:117:SER:CB[3_644]	2.15	0.05

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	891/906 (98%)	850 (95%)	37 (4%)	4 (0%)	30	47
1	B	892/906 (98%)	856 (96%)	31 (4%)	5 (1%)	21	36
1	C	880/906 (97%)	842 (96%)	34 (4%)	4 (0%)	24	40
1	D	882/906 (97%)	830 (94%)	50 (6%)	2 (0%)	43	62
1	E	896/906 (99%)	851 (95%)	41 (5%)	4 (0%)	30	47
1	F	896/906 (99%)	849 (95%)	39 (4%)	8 (1%)	14	26
1	G	881/906 (97%)	839 (95%)	35 (4%)	7 (1%)	16	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	881/906 (97%)	841 (96%)	37 (4%)	3 (0%)	36	54
All	All	7099/7248 (98%)	6758 (95%)	304 (4%)	37 (0%)	24	40

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	117	SER
1	E	263	GLU
1	F	526	SER
1	A	401	PHE
1	F	24	CYS
1	H	401	PHE
1	A	835	SER
1	B	582	ALA
1	C	582	ALA
1	F	117	SER
1	G	401	PHE
1	A	579	GLY
1	A	651	GLN
1	B	165	SER
1	B	277	PRO
1	B	579	GLY
1	B	651	GLN
1	C	579	GLY
1	D	582	ALA
1	F	635	HIS
1	F	651	GLN
1	F	692	ARG
1	G	67	ASP
1	G	330	GLU
1	G	828	ASP
1	H	651	GLN
1	C	401	PHE
1	C	651	GLN
1	E	329	THR
1	E	651	GLN
1	F	263	GLU
1	F	525	GLY
1	G	278	LEU
1	G	651	GLN
1	H	635	HIS
1	D	651	GLN

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Mol	Chain	Res	Type
1	G	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	724/745 (97%)	679 (94%)	45 (6%)	16	30
1	B	731/745 (98%)	698 (96%)	33 (4%)	24	44
1	C	726/745 (97%)	688 (95%)	38 (5%)	21	38
1	D	724/745 (97%)	684 (94%)	40 (6%)	19	35
1	E	732/745 (98%)	692 (94%)	40 (6%)	19	35
1	F	724/745 (97%)	692 (96%)	32 (4%)	25	45
1	G	721/745 (97%)	688 (95%)	33 (5%)	24	43
1	H	724/745 (97%)	684 (94%)	40 (6%)	19	35
All	All	5806/5960 (97%)	5505 (95%)	301 (5%)	21	38

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	31	VAL
1	A	39	THR
1	A	44	VAL
1	A	61	SER
1	A	99	GLN
1	A	114	VAL
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

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Mol	Chain	Res	Type
1	A	209	VAL
1	A	215	ARG
1	A	223	ASN
1	A	268	THR
1	A	305	ILE
1	A	325	LYS
1	A	329	THR
1	A	345	THR
1	A	378	THR
1	A	390	THR
1	A	391[A]	GLN
1	A	391[B]	GLN
1	A	412	SER
1	A	458	TYR
1	A	473	ARG
1	A	505	VAL
1	A	523	LEU
1	A	533	THR
1	A	573	THR
1	A	614	THR
1	A	617	THR
1	A	622	VAL
1	A	655	ARG
1	A	702	SER
1	A	761	VAL
1	A	835	SER
1	A	855	LYS
1	A	857	LYS
1	A	862	ARG
1	A	921	SER
1	A	927	SER
1	B	31	VAL
1	B	44	VAL
1	B	61	SER
1	B	63	SER
1	B	111	LEU
1	B	131	VAL
1	B	132	VAL
1	B	136	SER
1	B	139	LEU
1	B	176	VAL
1	B	180	GLN

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Mol	Chain	Res	Type
1	B	182	SER
1	B	186	ASN
1	B	206	GLU
1	B	209	VAL
1	B	223	ASN
1	B	230	THR
1	B	239	VAL
1	B	268	THR
1	B	277	PRO
1	B	305	ILE
1	B	345	THR
1	B	378	THR
1	B	390	THR
1	B	523	LEU
1	B	533	THR
1	B	588	LEU
1	B	617	THR
1	B	622	VAL
1	B	655	ARG
1	B	761	VAL
1	B	835	SER
1	B	921	SER
1	C	26	SER
1	C	44	VAL
1	C	114	VAL
1	C	129	SER
1	C	132	VAL
1	C	133	THR
1	C	139	LEU
1	C	146	VAL
1	C	167	LYS
1	C	176	VAL
1	C	182	SER
1	C	186	ASN
1	C	193	SER
1	C	206	GLU
1	C	239	VAL
1	C	263	GLU
1	C	268	THR
1	C	279	LYS
1	C	305	ILE
1	C	328	ASP

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Mol	Chain	Res	Type
1	C	390	THR
1	C	458	TYR
1	C	473	ARG
1	C	490	LYS
1	C	505	VAL
1	C	523	LEU
1	C	533	THR
1	C	573	THR
1	C	603	SER
1	C	614	THR
1	C	617	THR
1	C	622	VAL
1	C	655	ARG
1	C	699	SER
1	C	753	THR
1	C	755	SER
1	C	761	VAL
1	C	857	LYS
1	D	31	VAL
1	D	44	VAL
1	D	109	SER
1	D	111	LEU
1	D	128	SER
1	D	132	VAL
1	D	148	VAL
1	D	163	THR
1	D	176	VAL
1	D	178[A]	GLN
1	D	178[B]	GLN
1	D	182	SER
1	D	183	VAL
1	D	186	ASN
1	D	193	SER
1	D	201	ASP
1	D	215	ARG
1	D	223[A]	ASN
1	D	223[B]	ASN
1	D	226	VAL
1	D	263[A]	GLU
1	D	263[B]	GLU
1	D	268	THR
1	D	305	ILE

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Mol	Chain	Res	Type
1	D	333	GLU
1	D	345	THR
1	D	390	THR
1	D	411	ILE
1	D	473	ARG
1	D	475	SER
1	D	493	SER
1	D	505	VAL
1	D	523	LEU
1	D	533	THR
1	D	549	ILE
1	D	573	THR
1	D	600	ARG
1	D	622	VAL
1	D	655	ARG
1	D	753	THR
1	E	24	CYS
1	E	44	VAL
1	E	58[A]	GLN
1	E	58[B]	GLN
1	E	59	GLU
1	E	61	SER
1	E	63	SER
1	E	98	ASN
1	E	109	SER
1	E	111	LEU
1	E	114	VAL
1	E	117	SER
1	E	131	VAL
1	E	132	VAL
1	E	165	SER
1	E	176	VAL
1	E	182	SER
1	E	183	VAL
1	E	201	ASP
1	E	226	VAL
1	E	230	THR
1	E	268	THR
1	E	305	ILE
1	E	333	GLU
1	E	345	THR
1	E	390	THR

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Mol	Chain	Res	Type
1	E	473	ARG
1	E	585	ASN
1	E	588	LEU
1	E	617	THR
1	E	622	VAL
1	E	625	ILE
1	E	655	ARG
1	E	699	SER
1	E	702	SER
1	E	761	VAL
1	E	827	LYS
1	E	853	GLU
1	E	855	LYS
1	E	881	ILE
1	F	44	VAL
1	F	58	GLN
1	F	118	SER
1	F	132	VAL
1	F	139	LEU
1	F	148	VAL
1	F	165	SER
1	F	176	VAL
1	F	183	VAL
1	F	213	SER
1	F	228	ASP
1	F	230	THR
1	F	305	ILE
1	F	329	THR
1	F	335	ARG
1	F	337	SER
1	F	345	THR
1	F	352	THR
1	F	390	THR
1	F	473	ARG
1	F	517	LEU
1	F	523	LEU
1	F	622	VAL
1	F	655	ARG
1	F	699	SER
1	F	753	THR
1	F	761	VAL
1	F	832	VAL

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Mol	Chain	Res	Type
1	F	838	SER
1	F	862	ARG
1	F	881	ILE
1	F	921	SER
1	G	31	VAL
1	G	44	VAL
1	G	57	PRO
1	G	128	SER
1	G	131	VAL
1	G	132	VAL
1	G	186	ASN
1	G	206	GLU
1	G	212	THR
1	G	239	VAL
1	G	268	THR
1	G	305	ILE
1	G	330	GLU
1	G	345	THR
1	G	390	THR
1	G	458	TYR
1	G	473	ARG
1	G	505	VAL
1	G	523	LEU
1	G	588	LEU
1	G	603	SER
1	G	617	THR
1	G	622	VAL
1	G	655	ARG
1	G	692	ARG
1	G	693	THR
1	G	755	SER
1	G	761	VAL
1	G	777	ASN
1	G	794	SER
1	G	853	GLU
1	G	855	LYS
1	G	876	ASP
1	H	31	VAL
1	H	44	VAL
1	H	67	ASP
1	H	72	SER
1	H	94	ILE

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Mol	Chain	Res	Type
1	H	99	GLN
1	H	129	SER
1	H	131	VAL
1	H	136	SER
1	H	164	LYS
1	H	176	VAL
1	H	186	ASN
1	H	193	SER
1	H	194	PRO
1	H	206	GLU
1	H	223	ASN
1	H	239	VAL
1	H	268	THR
1	H	305	ILE
1	H	352	THR
1	H	410	ASP
1	H	448	GLU
1	H	458	TYR
1	H	473	ARG
1	H	498	MET
1	H	523	LEU
1	H	526	SER
1	H	537	ARG
1	H	573	THR
1	H	588	LEU
1	H	622	VAL
1	H	655	ARG
1	H	703	THR
1	H	731	GLU
1	H	753	THR
1	H	761	VAL
1	H	764	THR
1	H	775	ARG
1	H	828	ASP
1	H	921	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	178	GLN
1	A	199	ASN

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Mol	Chain	Res	Type
1	A	223	ASN
1	A	369	GLN
1	A	515	GLN
1	A	585	ASN
1	A	688	GLN
1	A	810	GLN
1	B	99	GLN
1	B	189	ASN
1	B	192	ASN
1	B	223	ASN
1	B	303	GLN
1	B	324	GLN
1	B	369	GLN
1	B	373	ASN
1	B	512	HIS
1	C	98	ASN
1	C	180	GLN
1	C	373	ASN
1	C	391	GLN
1	C	777	ASN
1	C	810	GLN
1	D	23	ASN
1	D	103	GLN
1	D	155	ASN
1	D	264	ASN
1	D	303	GLN
1	D	324	GLN
1	D	373	ASN
1	D	391	GLN
1	D	512	HIS
1	D	515	GLN
1	D	585	ASN
1	D	777	ASN
1	D	810	GLN
1	E	75	GLN
1	E	98	ASN
1	E	103	GLN
1	E	172	ASN
1	E	178	GLN
1	E	196	GLN
1	E	264	ASN
1	E	303	GLN

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Mol	Chain	Res	Type
1	E	324	GLN
1	E	373	ASN
1	E	391	GLN
1	E	515	GLN
1	E	585	ASN
1	E	638	GLN
1	E	688	GLN
1	F	75	GLN
1	F	223	ASN
1	F	264	ASN
1	F	299	ASN
1	F	303	GLN
1	F	324	GLN
1	F	391	GLN
1	F	539	GLN
1	F	688	GLN
1	F	810	GLN
1	G	32	HIS
1	G	98	ASN
1	G	103	GLN
1	G	178	GLN
1	G	180	GLN
1	G	189	ASN
1	G	211	GLN
1	G	303	GLN
1	G	373	ASN
1	G	391	GLN
1	G	512	HIS
1	G	515	GLN
1	G	688	GLN
1	G	784	ASN
1	G	820	HIS
1	H	23	ASN
1	H	98	ASN
1	H	103	GLN
1	H	155	ASN
1	H	180	GLN
1	H	303	GLN
1	H	373	ASN
1	H	391	GLN
1	H	512	HIS
1	H	539	GLN

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Mol	Chain	Res	Type
1	H	585	ASN
1	H	688	GLN
1	H	746	ASN

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 ⓘ

16 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	0.54	0	16,16,16	1.35	2 (12%)
2	GAD	I	2	2	10,11,11	2.12	3 (30%)	12,15,15	1.82	2 (16%)
2	RAM	J	1	2	11,11,11	0.43	0	16,16,16	1.24	2 (12%)
2	GAD	J	2	2	10,11,11	2.16	3 (30%)	12,15,15	1.90	2 (16%)
2	RAM	K	1	2	11,11,11	0.55	0	16,16,16	1.24	2 (12%)
2	GAD	K	2	2	10,11,11	2.26	1 (10%)	12,15,15	2.24	4 (33%)
2	RAM	L	1	2	11,11,11	0.54	0	16,16,16	0.85	0
2	GAD	L	2	2	10,11,11	2.08	2 (20%)	12,15,15	1.88	4 (33%)
2	RAM	M	1	2	11,11,11	0.50	0	16,16,16	1.21	2 (12%)
2	GAD	M	2	2	10,11,11	2.29	1 (10%)	12,15,15	1.76	2 (16%)
2	RAM	N	1	2	11,11,11	0.82	0	16,16,16	1.43	1 (6%)
2	GAD	N	2	2	10,11,11	2.29	2 (20%)	12,15,15	2.45	4 (33%)
2	RAM	O	1	2	11,11,11	0.70	0	16,16,16	1.95	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAD	O	2	2	10,11,11	2.24	1 (10%)	12,15,15	1.38	3 (25%)
2	RAM	P	1	2	11,11,11	0.43	0	16,16,16	1.44	4 (25%)
2	GAD	P	2	2	10,11,11	2.08	1 (10%)	12,15,15	2.05	3 (25%)

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	-	0/4/17/17	0/1/1/1
2	RAM	J	1	2	-	-	0/1/1/1
2	GAD	J	2	2	-	0/4/17/17	0/1/1/1
2	RAM	K	1	2	-	-	0/1/1/1
2	GAD	K	2	2	-	3/4/17/17	0/1/1/1
2	RAM	L	1	2	-	-	0/1/1/1
2	GAD	L	2	2	-	0/4/17/17	0/1/1/1
2	RAM	M	1	2	-	-	0/1/1/1
2	GAD	M	2	2	-	0/4/17/17	0/1/1/1
2	RAM	N	1	2	-	-	0/1/1/1
2	GAD	N	2	2	-	0/4/17/17	0/1/1/1
2	RAM	O	1	2	-	-	0/1/1/1
2	GAD	O	2	2	-	0/4/17/17	0/1/1/1
2	RAM	P	1	2	-	-	0/1/1/1
2	GAD	P	2	2	-	0/4/17/17	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	2	GAD	O5-C5	6.25	1.45	1.37
2	N	2	GAD	O5-C5	6.21	1.45	1.37
2	K	2	GAD	O5-C5	6.21	1.45	1.37
2	O	2	GAD	O5-C5	5.98	1.45	1.37
2	P	2	GAD	O5-C5	5.38	1.44	1.37
2	J	2	GAD	O5-C5	5.22	1.44	1.37
2	L	2	GAD	O5-C5	5.17	1.44	1.37
2	I	2	GAD	O5-C5	5.17	1.44	1.37
2	I	2	GAD	C5-C6	-2.53	1.43	1.48
2	I	2	GAD	O6B-C6	-2.48	1.23	1.30
2	J	2	GAD	O6B-C6	-2.42	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	GAD	C3-C4	2.29	1.53	1.50
2	L	2	GAD	O5-C1	-2.14	1.41	1.45
2	N	2	GAD	O6B-C6	-2.09	1.24	1.30

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	GAD	O5-C5-C4	-5.82	119.59	124.94
2	P	2	GAD	O5-C5-C4	-5.56	119.84	124.94
2	N	2	GAD	O5-C5-C4	-5.45	119.94	124.94
2	J	2	GAD	O5-C5-C4	-4.95	120.40	124.94
2	I	2	GAD	O5-C5-C4	-4.55	120.76	124.94
2	L	2	GAD	O5-C5-C4	-4.24	121.05	124.94
2	M	2	GAD	O5-C5-C4	-4.18	121.10	124.94
2	O	1	RAM	C1-O5-C5	4.03	120.65	114.37
2	O	1	RAM	O5-C1-C2	4.03	117.38	110.30
2	N	2	GAD	O5-C5-C6	3.98	119.17	111.85
2	I	1	RAM	O4-C4-C5	3.49	117.43	109.74
2	K	2	GAD	O5-C5-C6	3.36	118.02	111.85
2	M	2	GAD	O5-C5-C6	3.19	117.70	111.85
2	P	2	GAD	O5-C5-C6	3.08	117.51	111.85
2	J	2	GAD	C1-O5-C5	3.05	121.88	115.42
2	N	1	RAM	C1-O5-C5	2.88	118.86	114.37
2	O	1	RAM	O5-C5-C4	2.86	114.71	109.55
2	P	1	RAM	C6-C5-C4	-2.85	107.88	113.08
2	I	2	GAD	C1-O5-C5	2.83	121.42	115.42
2	O	2	GAD	O5-C5-C4	-2.81	122.36	124.94
2	P	1	RAM	C1-O5-C5	2.58	118.39	114.37
2	P	1	RAM	O5-C5-C4	2.57	114.17	109.55
2	P	1	RAM	C1-C2-C3	2.50	115.45	110.36
2	N	2	GAD	O6B-C6-C5	2.47	119.67	114.06
2	L	2	GAD	C1-C2-C3	-2.40	106.14	109.64
2	L	2	GAD	O3-C3-C2	2.40	113.71	109.44
2	N	2	GAD	O3-C3-C2	2.33	113.60	109.44
2	M	1	RAM	C6-C5-C4	-2.32	108.84	113.08
2	O	1	RAM	C1-C2-C3	2.30	115.05	110.36
2	I	1	RAM	O4-C4-C3	-2.22	105.15	110.38
2	K	1	RAM	O4-C4-C3	-2.21	105.17	110.38
2	O	2	GAD	O3-C3-C2	2.20	113.36	109.44
2	O	2	GAD	C1-O5-C5	2.18	120.04	115.42
2	J	1	RAM	O5-C1-C2	-2.17	106.48	110.30
2	M	1	RAM	O1-C1-C2	-2.14	102.76	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	RAM	O2-C2-C3	-2.10	105.42	110.38
2	P	2	GAD	C1-C2-C3	-2.07	106.63	109.64
2	J	1	RAM	C4-C3-C2	2.07	114.46	110.83
2	O	1	RAM	O5-C5-C6	-2.06	102.17	106.74
2	O	1	RAM	C6-C5-C4	-2.06	109.32	113.08
2	K	2	GAD	O3-C3-C4	-2.04	104.66	109.27
2	L	2	GAD	O6B-C6-C5	2.02	118.65	114.06
2	K	2	GAD	C1-C2-C3	-2.01	106.71	109.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

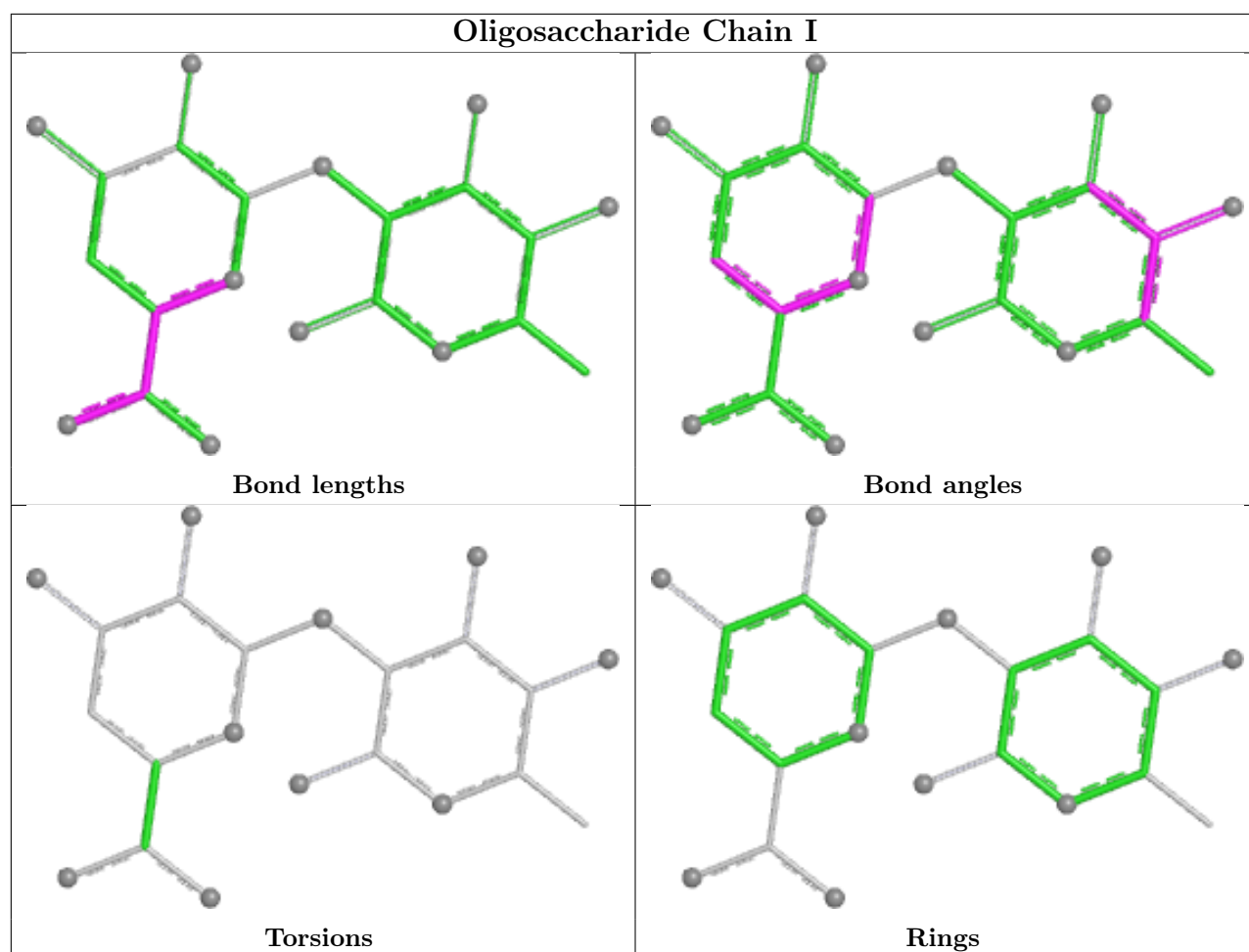
Mol	Chain	Res	Type	Atoms
2	K	2	GAD	C4-C5-C6-O6A
2	K	2	GAD	O5-C5-C6-O6A
2	K	2	GAD	O5-C5-C6-O6B

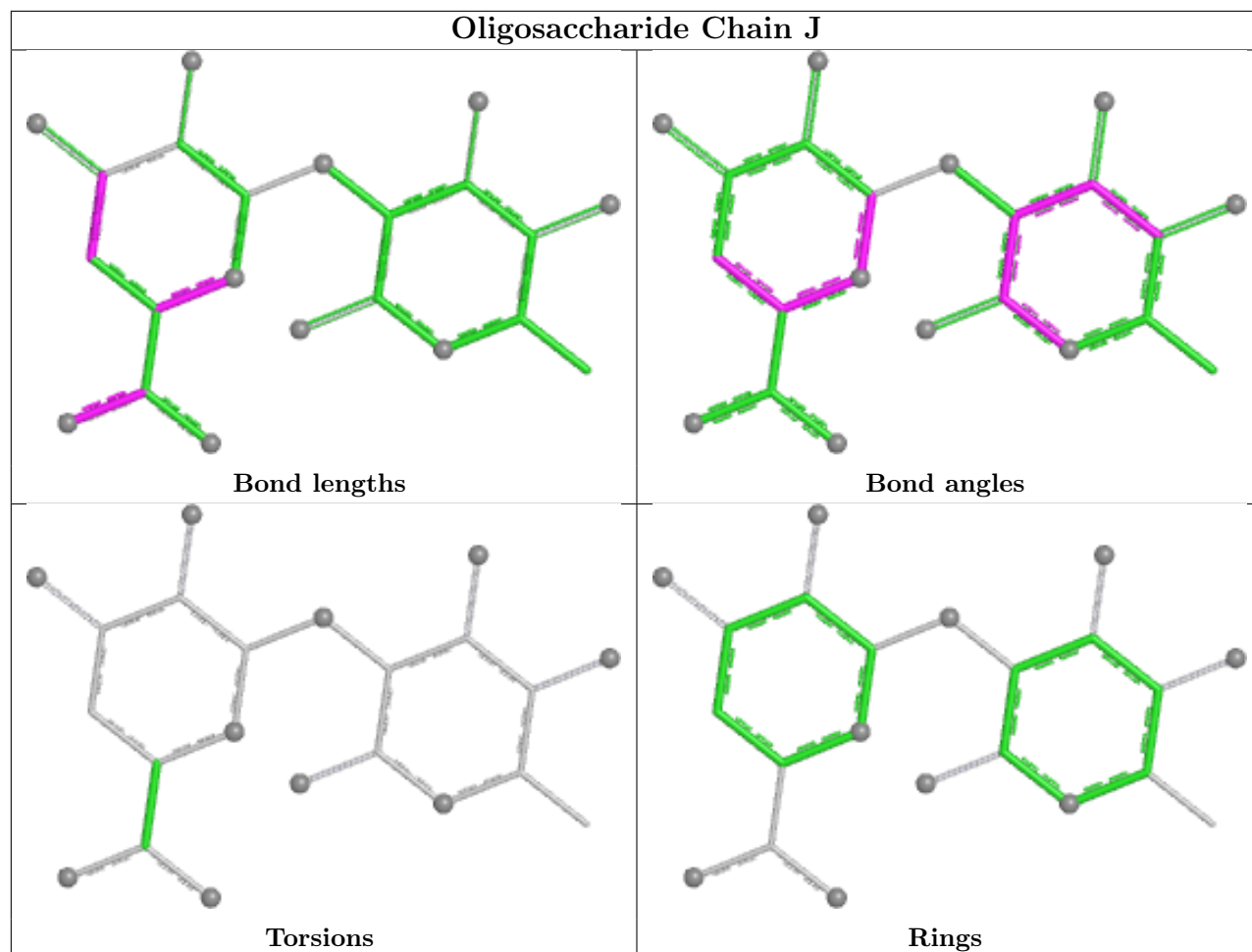
There are no ring outliers.

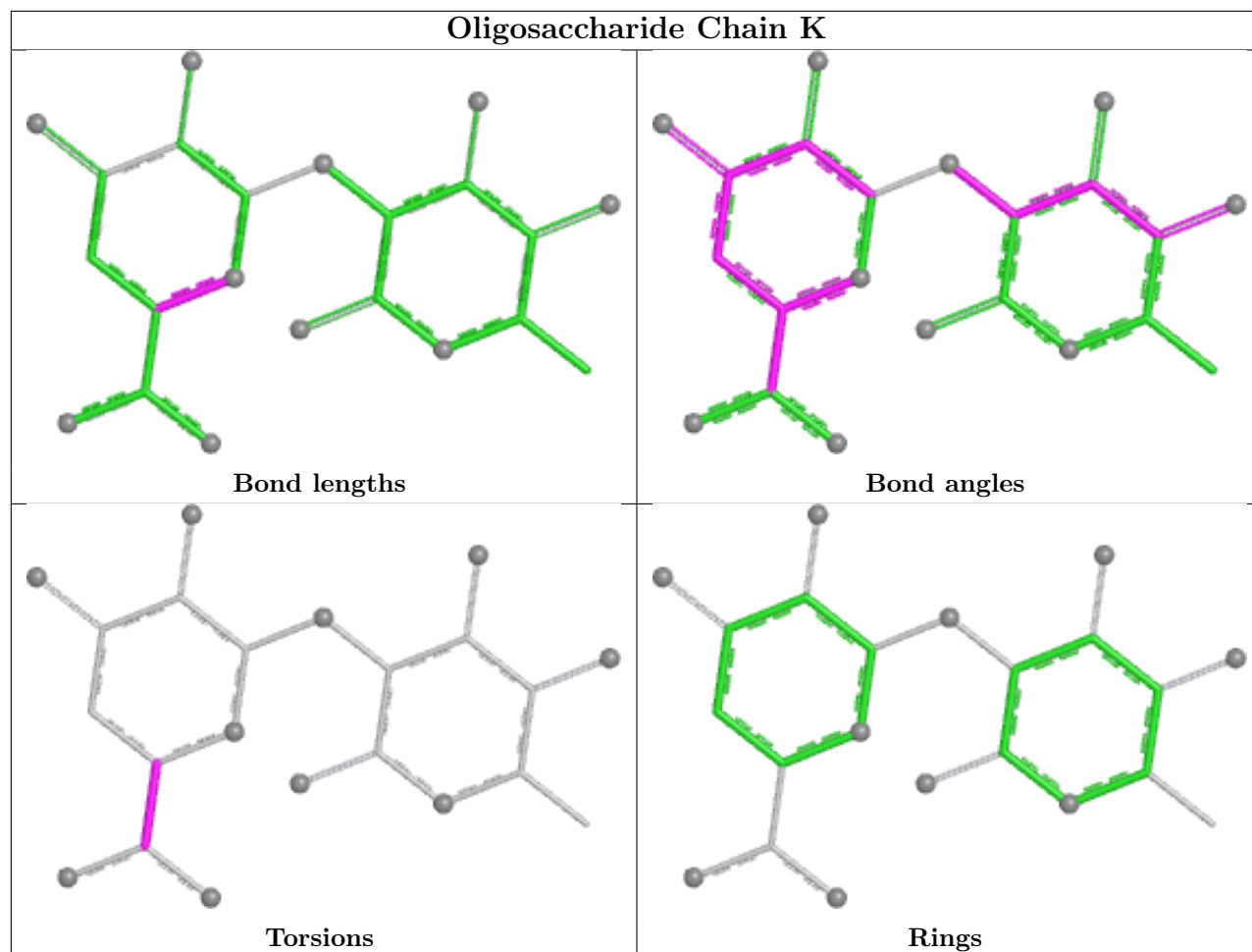
1 monomer is involved in 2 short contacts:

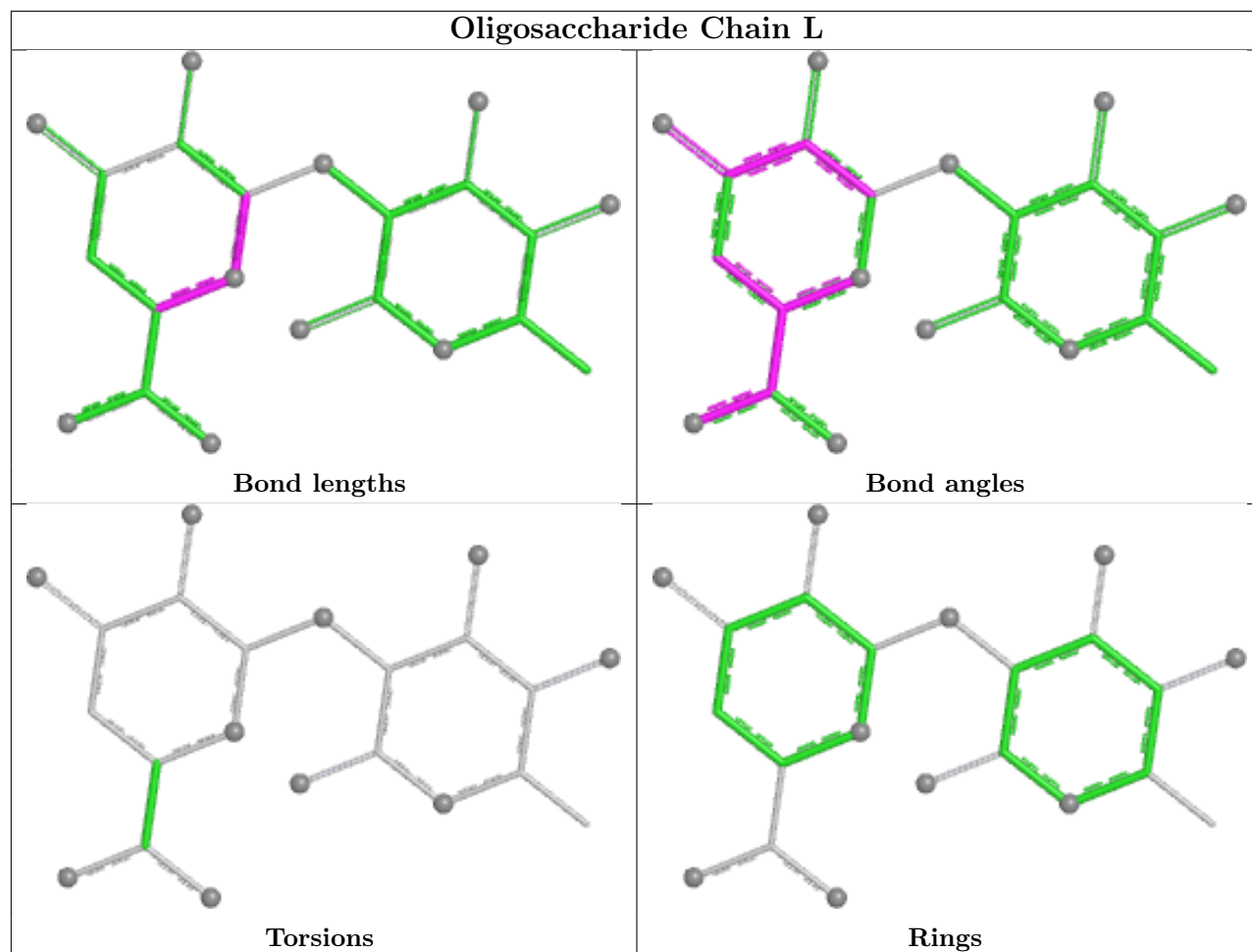
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	RAM	2	0

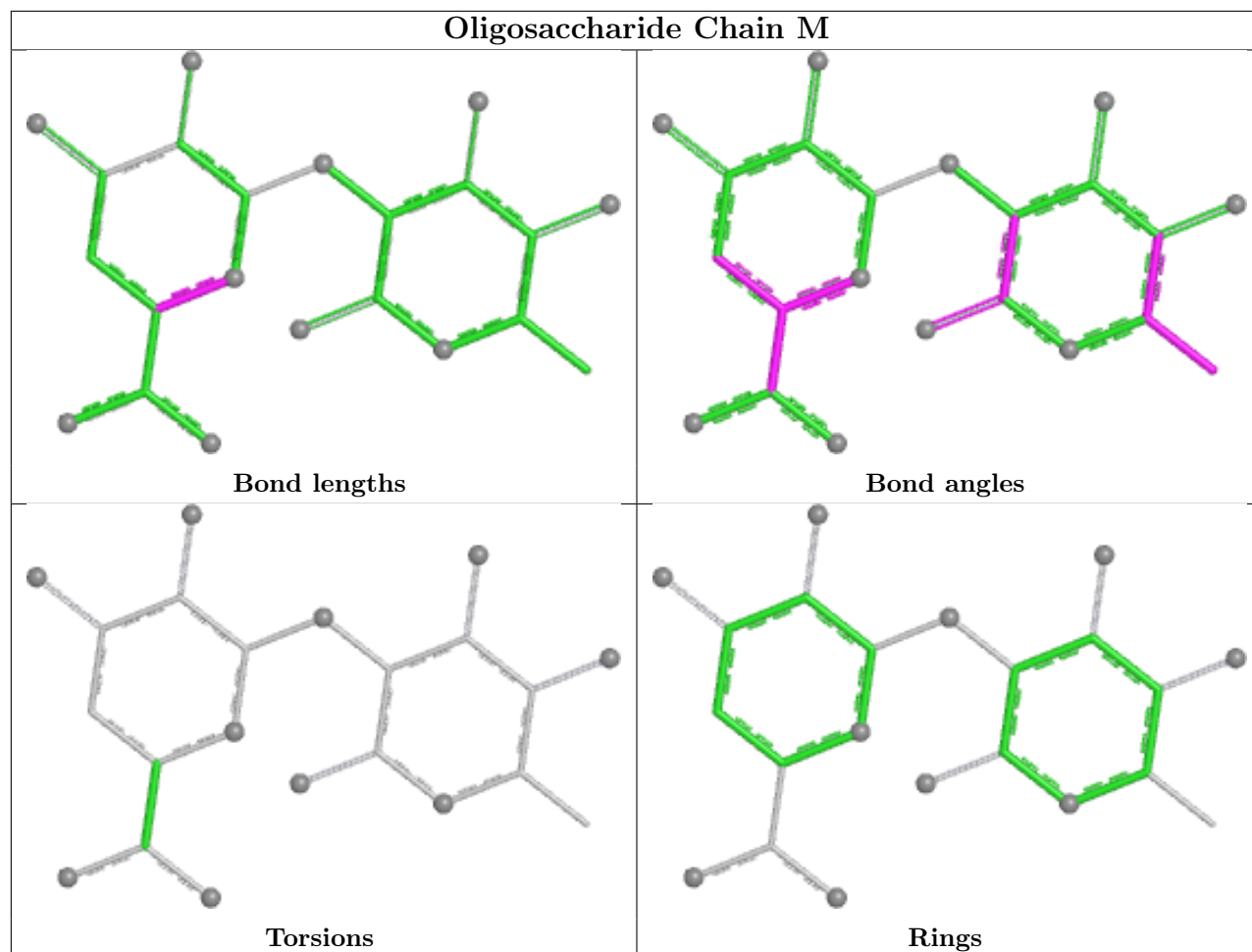
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

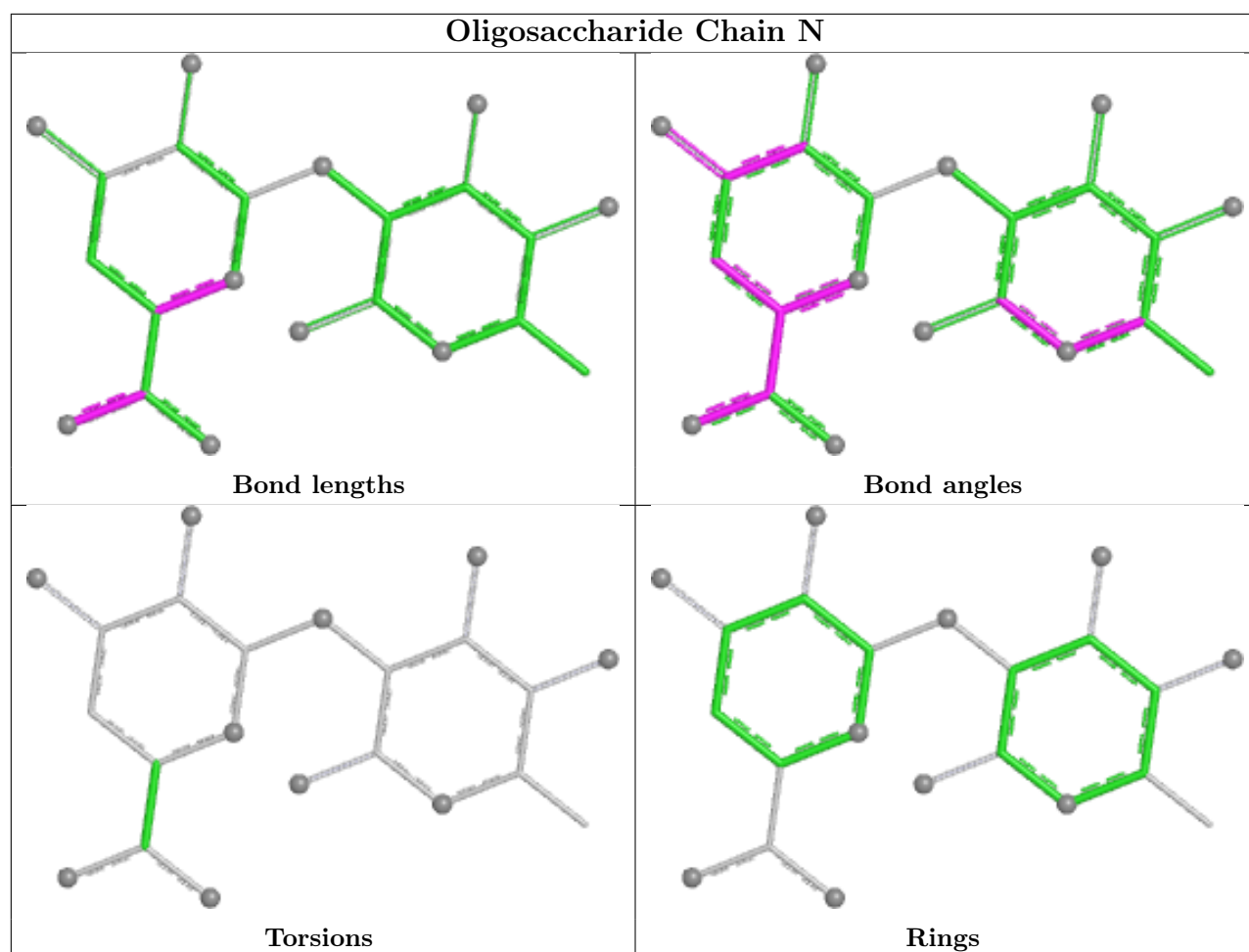


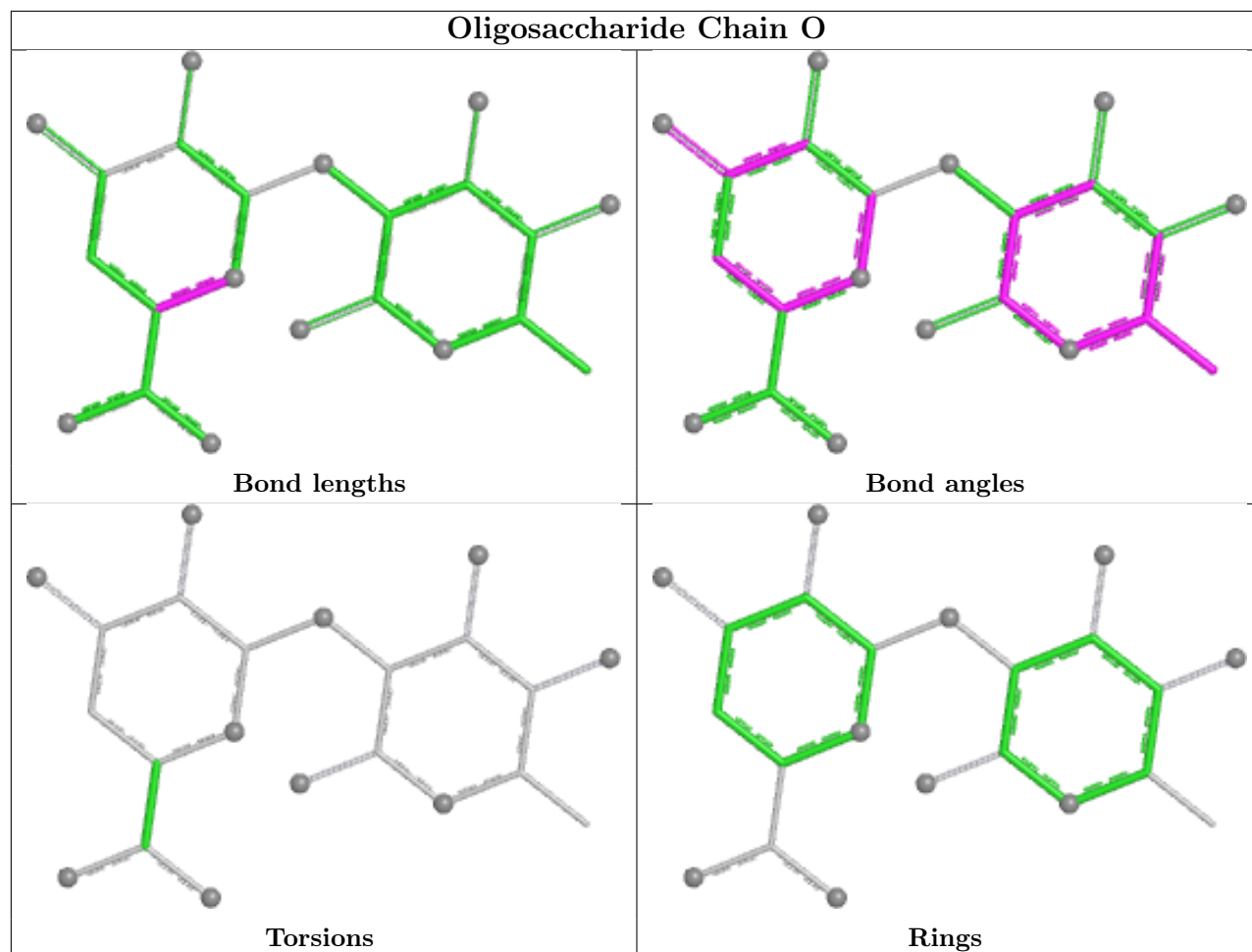


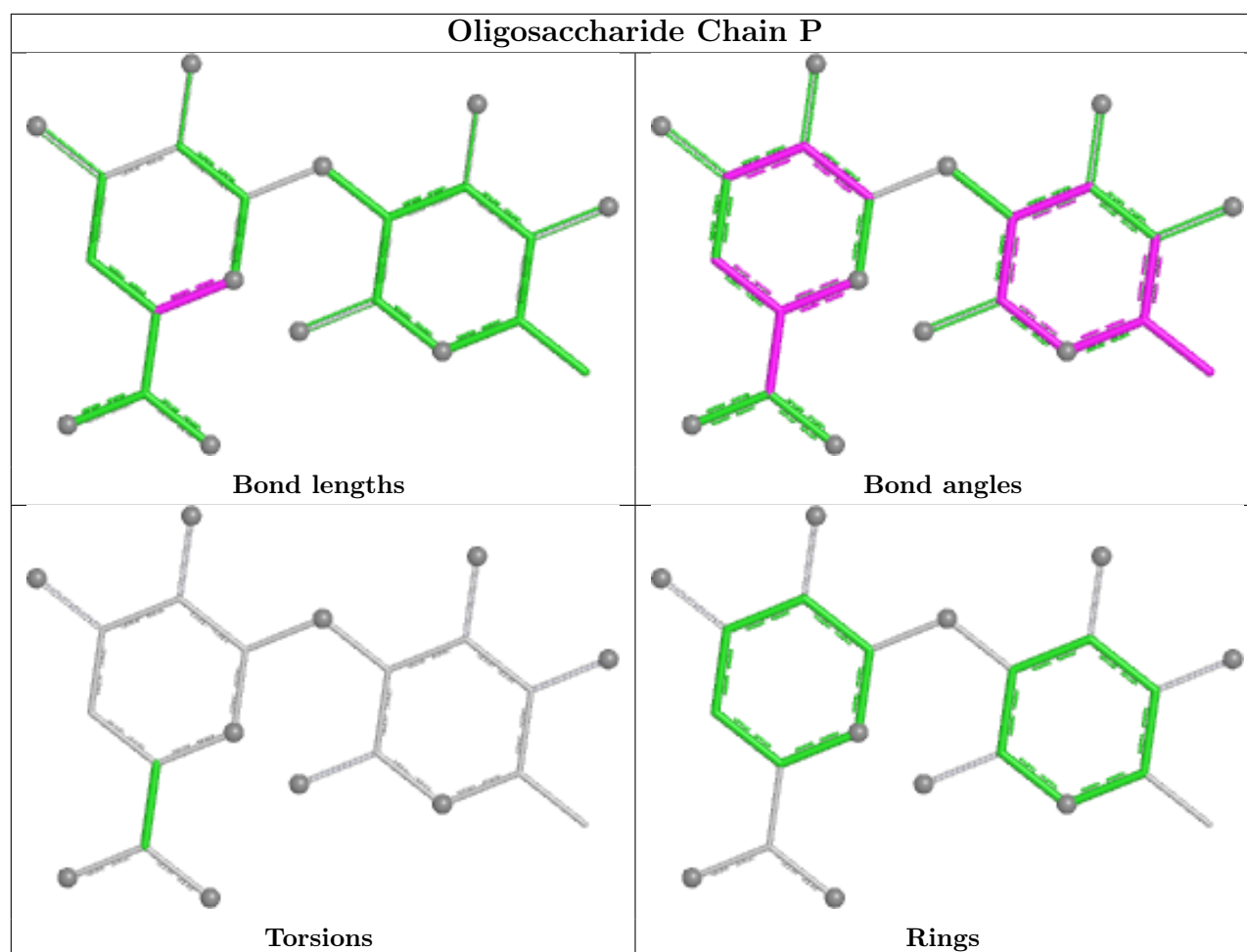












5.6 Ligand geometry [i](#)

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%)	-0.46	6 (0%) 84 84	16, 26, 45, 71	1 (0%)
1	B	896/906 (98%)	-0.45	4 (0%) 88 89	11, 26, 45, 68	2 (0%)
1	C	885/906 (97%)	-0.42	7 (0%) 82 82	10, 28, 47, 74	5 (0%)
1	D	884/906 (97%)	-0.36	8 (0%) 81 81	15, 30, 49, 71	6 (0%)
1	E	899/906 (99%)	-0.36	11 (1%) 76 75	16, 28, 49, 72	1 (0%)
1	F	900/906 (99%)	-0.34	9 (1%) 79 79	16, 28, 49, 75	0
1	G	888/906 (98%)	-0.22	11 (1%) 76 75	16, 32, 56, 84	1 (0%)
1	H	888/906 (98%)	-0.23	6 (0%) 84 84	16, 32, 55, 79	1 (0%)
All	All	7136/7248 (98%)	-0.35	62 (0%) 81 81	10, 29, 50, 84	17 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	114	VAL	5.8
1	H	114	VAL	4.8
1	G	526	SER	4.8
1	H	927	SER	4.7
1	C	114	VAL	4.3
1	E	118	SER	4.1
1	F	259	PHE	4.1
1	F	67	ASP	4.0
1	F	73	GLU	3.7
1	H	67	ASP	3.4
1	F	127	ASN	3.4
1	A	117	SER	3.3
1	E	66	GLY	3.3
1	C	927	SER	3.2
1	D	835	SER	3.2
1	E	117	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	526	SER	3.0
1	H	259	PHE	3.0
1	E	119	SER	3.0
1	D	72	SER	2.9
1	F	117	SER	2.9
1	F	23	ASN	2.8
1	E	72	SER	2.8
1	E	259	PHE	2.7
1	D	114	VAL	2.7
1	B	117	SER	2.7
1	D	137	ASP	2.7
1	C	259[A]	PHE	2.6
1	F	836	LYS	2.6
1	C	836	LYS	2.6
1	G	923	ASP	2.6
1	G	68	THR	2.5
1	A	119	SER	2.5
1	F	66	GLY	2.5
1	B	127	ASN	2.5
1	D	927	SER	2.5
1	G	837	ILE	2.4
1	A	835	SER	2.4
1	B	201[A]	ASP	2.4
1	B	294	ASP	2.4
1	C	315	GLU	2.4
1	D	128	SER	2.3
1	G	113	CYS	2.3
1	G	926	GLN	2.3
1	C	22	PHE	2.3
1	G	73	GLU	2.2
1	H	136	SER	2.2
1	G	195	ILE	2.2
1	D	802	ASP	2.2
1	D	259	PHE	2.2
1	A	431	GLU	2.2
1	G	194	PRO	2.2
1	E	136	SER	2.2
1	G	835	SER	2.2
1	A	127	ASN	2.1
1	E	228	ASP	2.1
1	E	116	SER	2.1
1	F	194	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	208	PHE	2.1
1	H	22	PHE	2.1
1	E	115	LYS	2.0
1	A	23	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

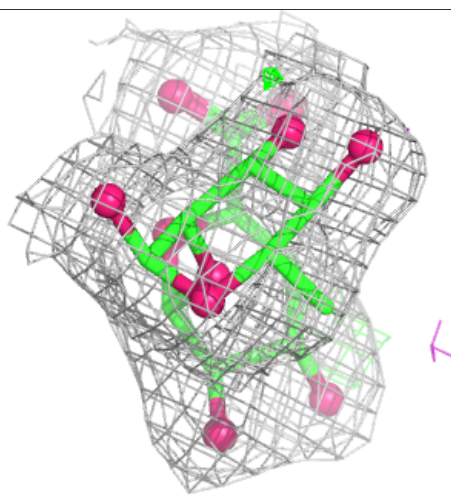
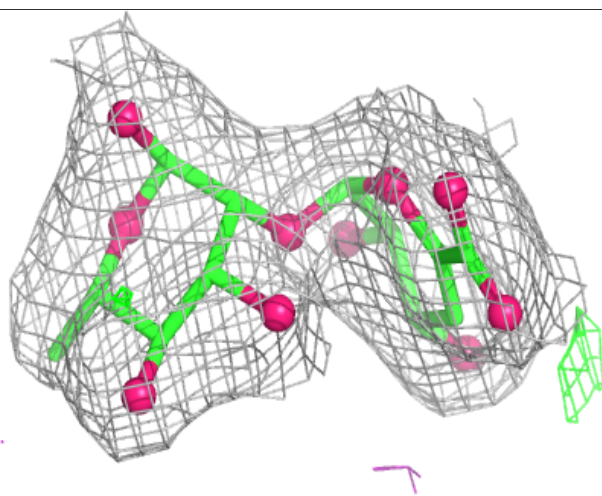
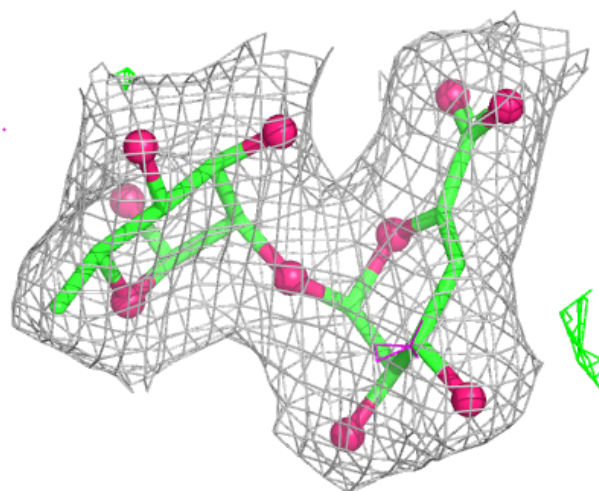
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAD	P	2	11/11	0.94	0.08	30,35,38,39	0
2	GAD	L	2	11/11	0.95	0.07	27,30,32,34	0
2	GAD	M	2	11/11	0.95	0.07	29,31,33,33	0
2	GAD	N	2	11/11	0.95	0.07	25,29,30,30	0
2	GAD	O	2	11/11	0.95	0.08	30,38,42,45	0
2	GAD	K	2	11/11	0.95	0.07	29,32,34,36	0
2	RAM	O	1	11/11	0.96	0.08	40,44,46,50	0
2	RAM	N	1	11/11	0.96	0.07	23,24,26,29	0
2	RAM	K	1	11/11	0.96	0.08	31,34,36,41	0
2	RAM	J	1	11/11	0.97	0.07	21,23,24,25	0
2	RAM	L	1	11/11	0.97	0.06	28,32,34,37	0
2	GAD	J	2	11/11	0.97	0.06	22,25,26,29	0
2	RAM	M	1	11/11	0.97	0.06	26,27,30,34	0
2	RAM	P	1	11/11	0.97	0.07	31,34,36,38	0
2	GAD	I	2	11/11	0.97	0.06	19,23,24,26	0
2	RAM	I	1	11/11	0.98	0.06	21,23,24,24	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.

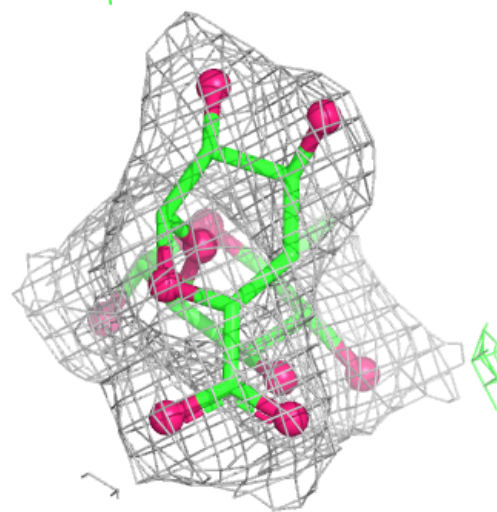
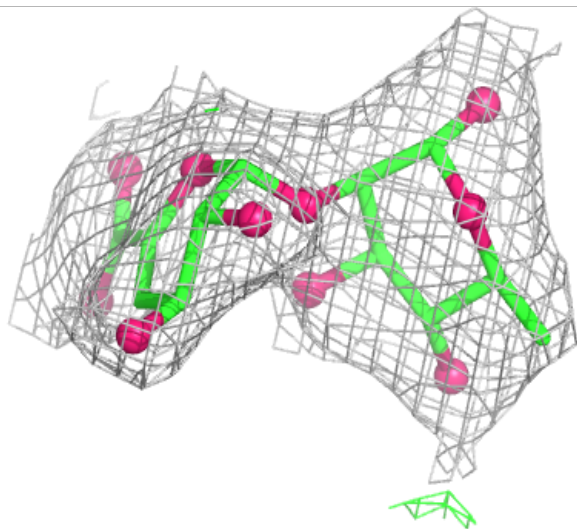
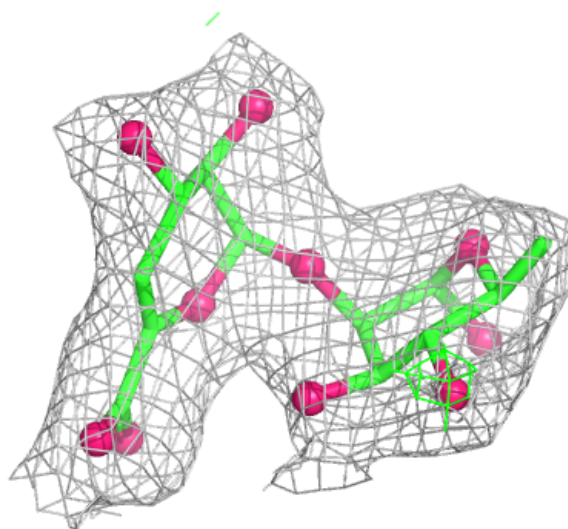
Electron density around Chain I:

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



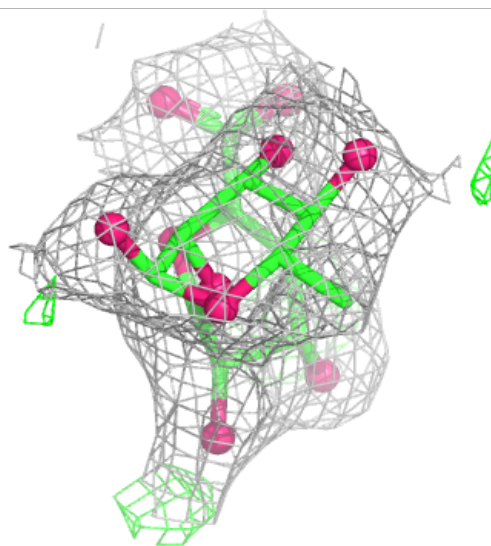
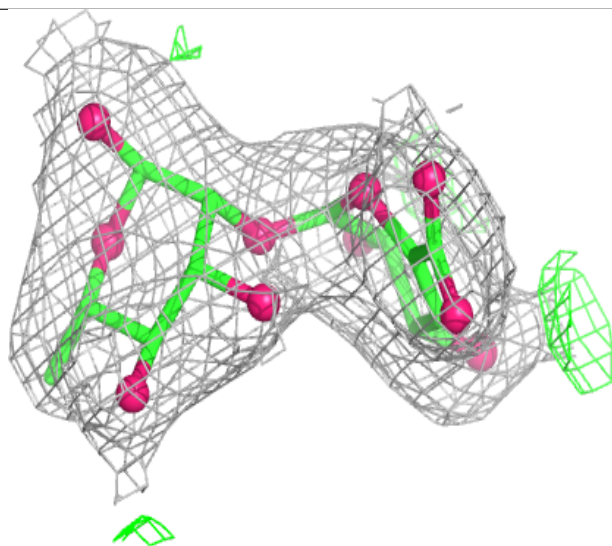
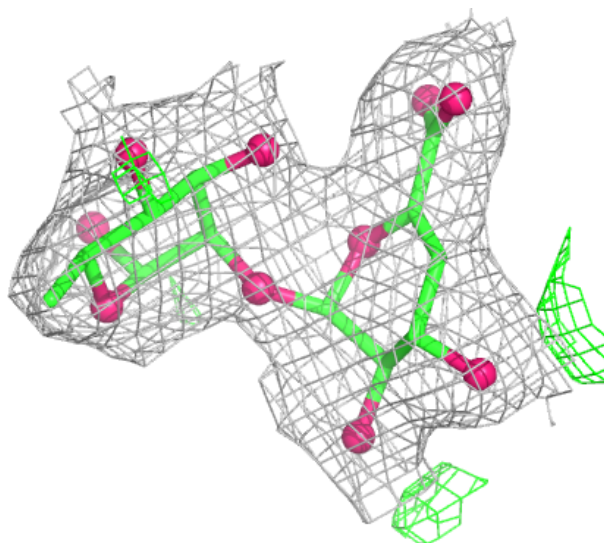
Electron density around Chain J:

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



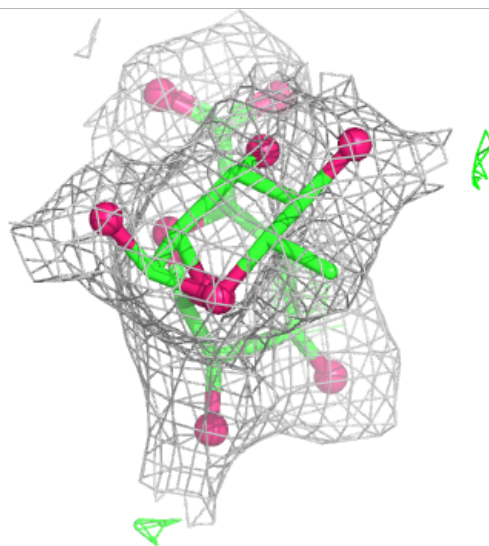
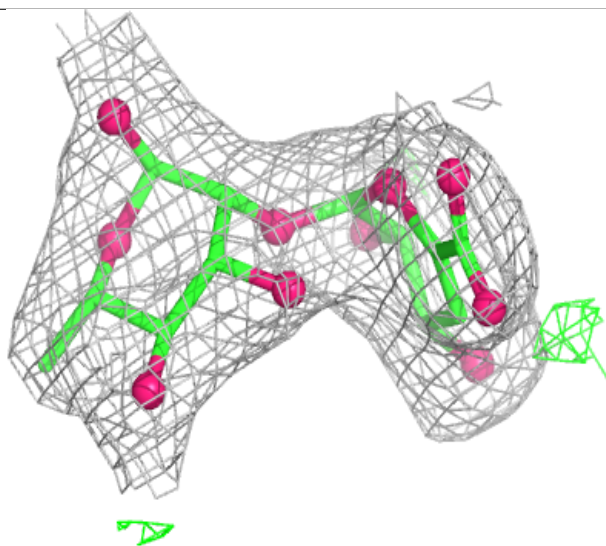
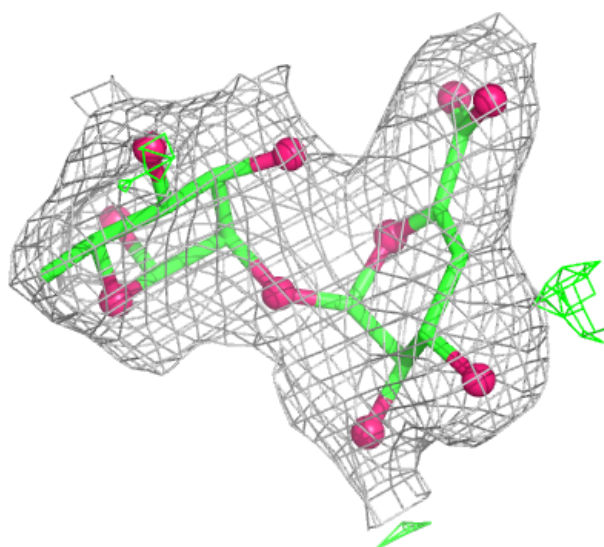
Electron density around Chain K:

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



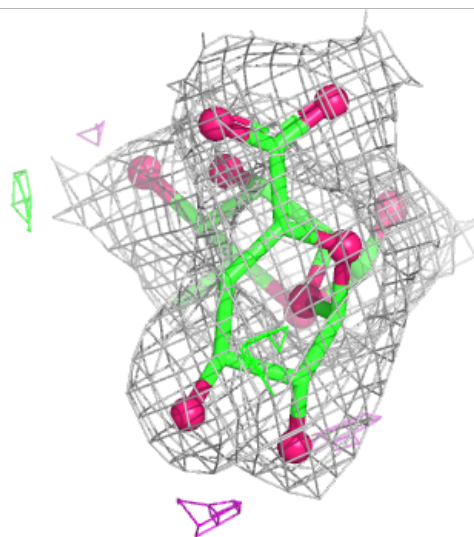
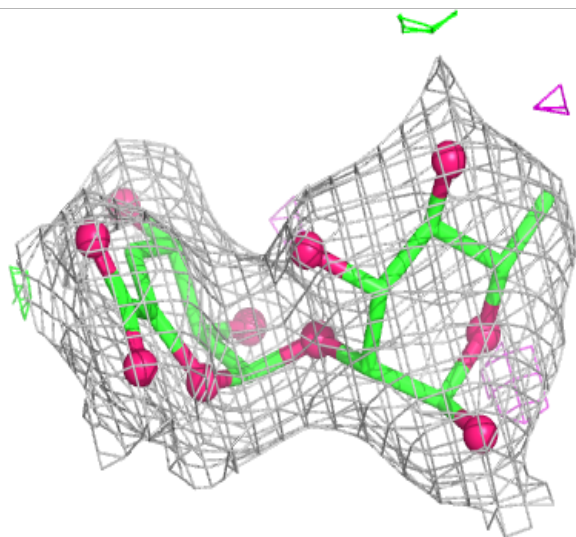
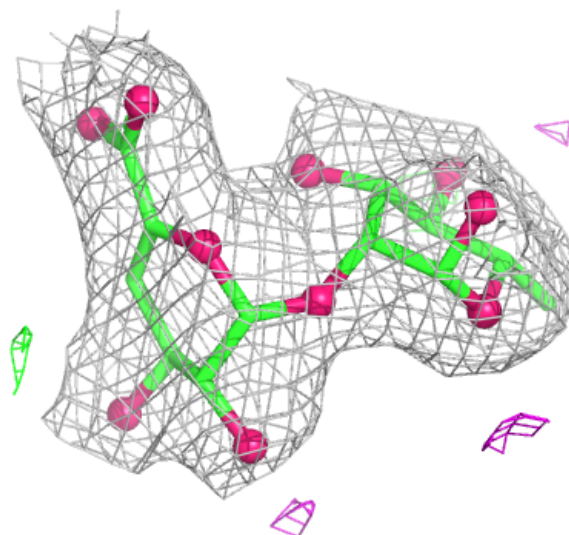
Electron density around Chain L:

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



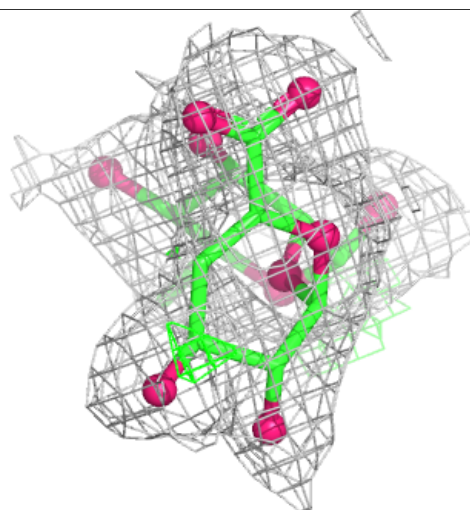
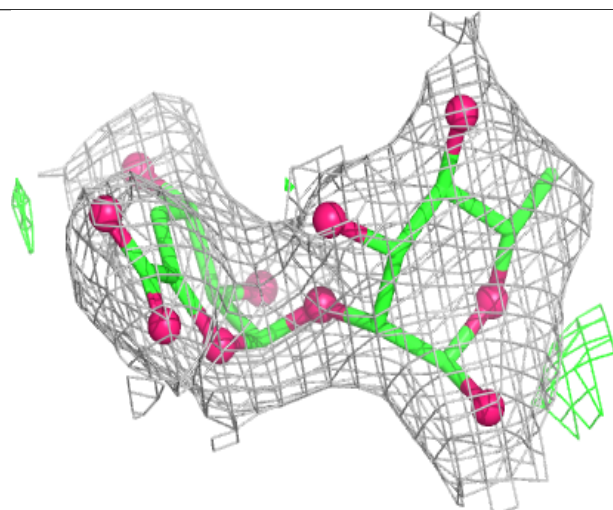
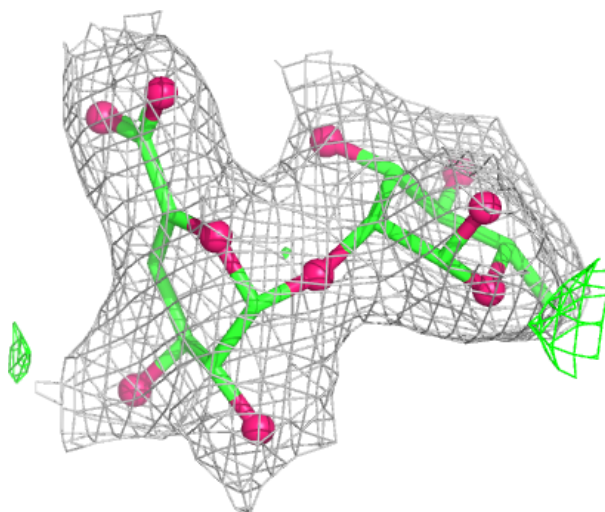
Electron density around Chain M:

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



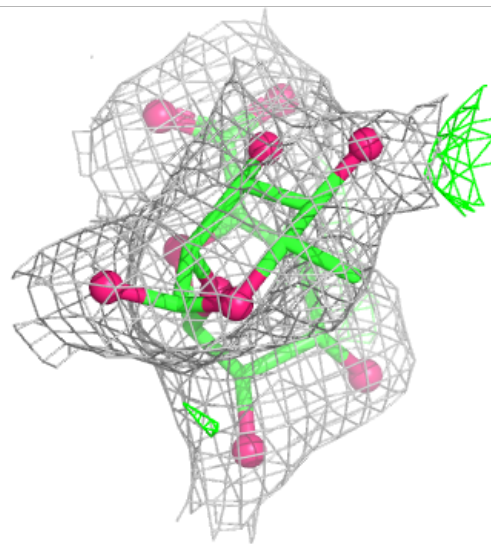
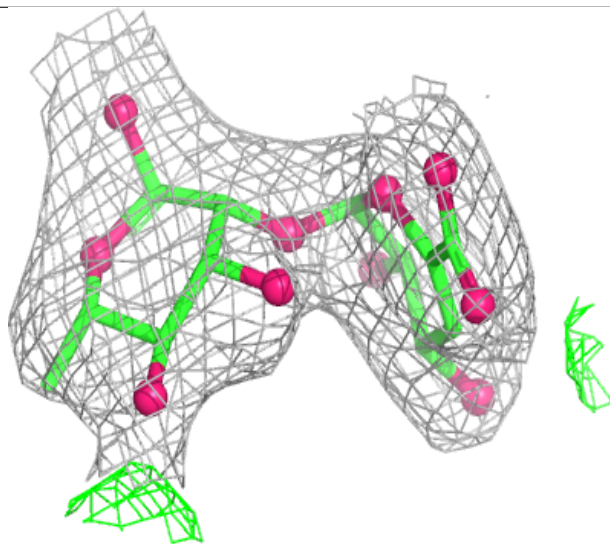
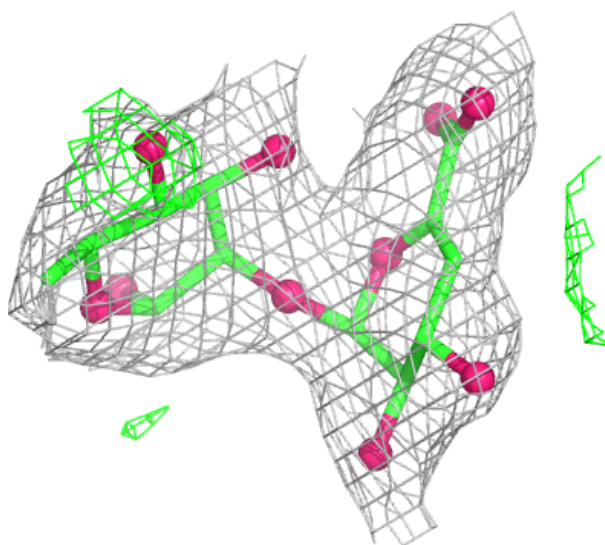
Electron density around Chain N:

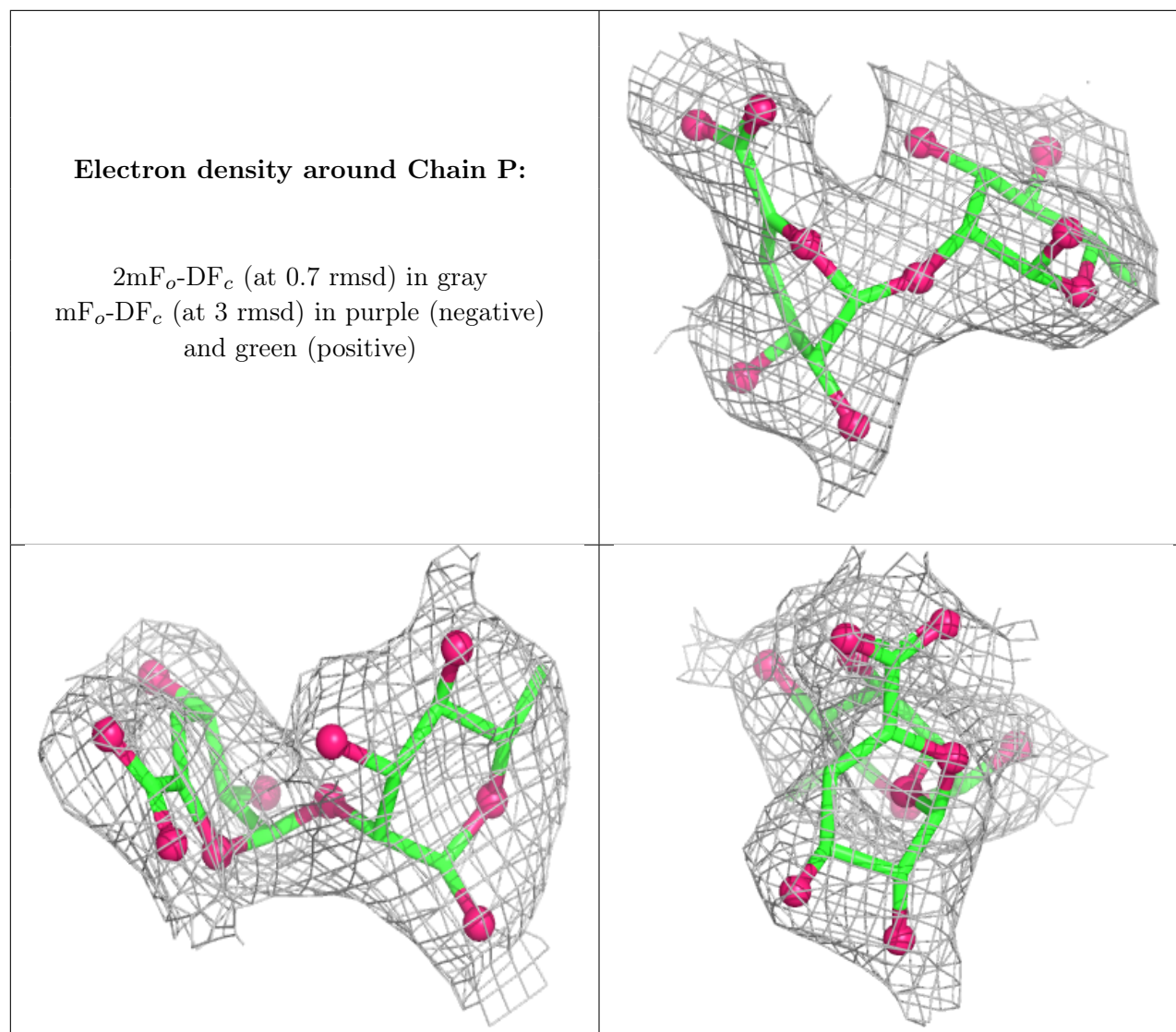
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	E	1003	1/1	0.98	0.04	12,12,12,12	0
3	CA	B	1003	1/1	0.99	0.04	11,11,11,11	0
3	CA	F	1003	1/1	0.99	0.03	11,11,11,11	0
3	CA	G	1003	1/1	0.99	0.04	18,18,18,18	0
3	CA	H	1003	1/1	0.99	0.05	19,19,19,19	0
3	CA	C	1003	1/1	1.00	0.03	9,9,9,9	0
3	CA	D	1003	1/1	1.00	0.03	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	1003	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.