



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:32 PM UTC

PDB ID : 1ONA / pdb_00001ona
Title : CO-CRYSTALS OF CONCANAVALIN A WITH METHYL-3,6-DI-O-(ALPHA-D-MANNOPYRANOSYL)-ALPHA-D-MANNOPYRANOSIDE
Authors : Bouckaert, J.; Maes, D.; Poortmans, F.; Wyns, L.; Loris, R.
Deposited on : 1996-07-07
Resolution : 2.35 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

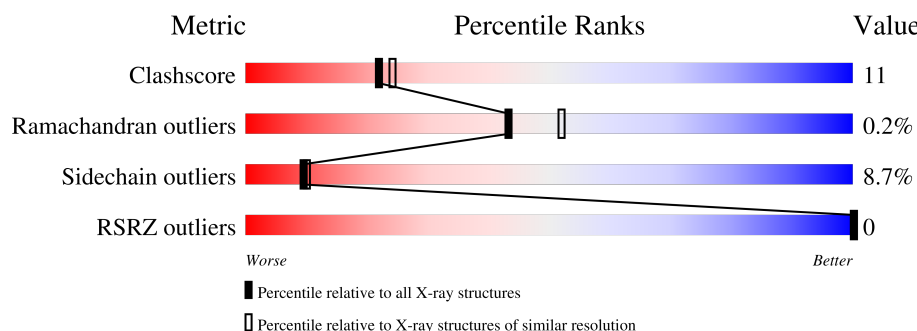
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



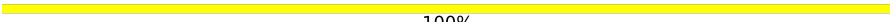
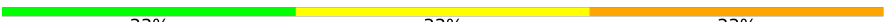
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	237	
1	B	237	
1	C	237	
1	D	237	
2	E	3	
2	F	3	

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Mol	Chain	Length	Quality of chain
2	G	3	 100%
2	H	3	 33%33%33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7368 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.

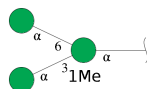
- Molecule 1 is a protein called CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1755	1111	291	351	2			
1	B	231	Total	C	N	O	S	0	0	0
			1755	1111	291	351	2			
1	C	231	Total	C	N	O	S	0	0	0
			1755	1111	291	351	2			
1	D	231	Total	C	N	O	S	0	0	0
			1755	1111	291	351	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	conflict	UNP P02866
A	155	GLU	ARG	conflict	UNP P02866
B	151	ASP	GLU	conflict	UNP P02866
B	155	GLU	ARG	conflict	UNP P02866
C	151	ASP	GLU	conflict	UNP P02866
C	155	GLU	ARG	conflict	UNP P02866
D	151	ASP	GLU	conflict	UNP P02866
D	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			35	19	16			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	3	Total	C	O	0	0	0
			35	19	16			
2	G	3	Total	C	O	0	0	0
			35	19	16			
2	H	3	Total	C	O	0	0	0
			35	19	16			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	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	D	1	Total	Ca	0	0
			1	1		

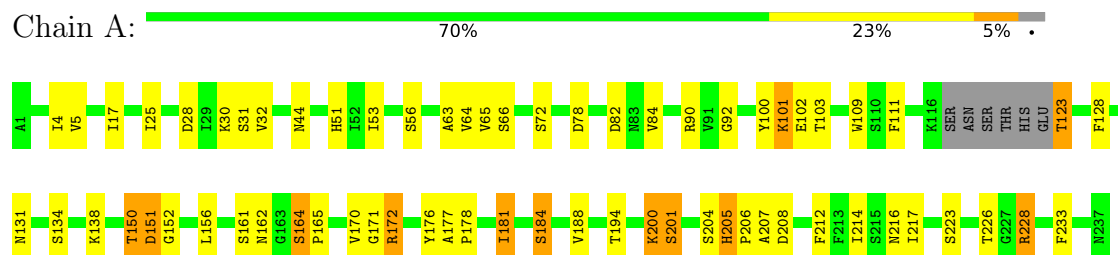
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	47	Total	O	0	0
			47	47		
5	C	50	Total	O	0	0
			50	50		
5	D	53	Total	O	0	0
			53	53		

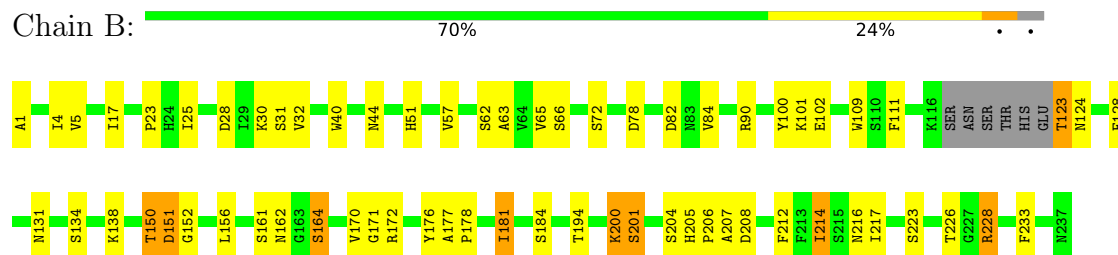
3 Residue-property plots

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.

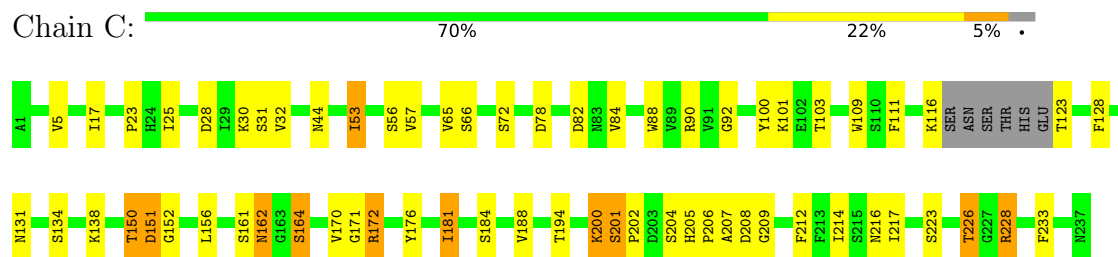
• Molecule 1: CONCANAVALIN A



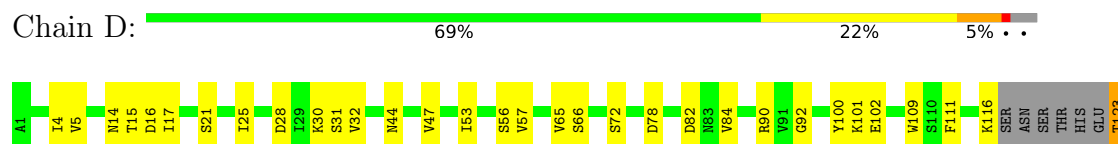
• Molecule 1: CONCANAVALIN A

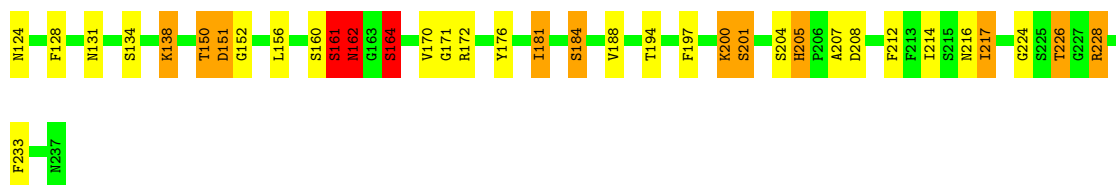


• Molecule 1: CONCANAVALIN A



• Molecule 1: CONCANAVALIN A





- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain E: 67% 33%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain F: 33% 67%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain G: 100%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain H: 33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.83Å 64.84Å 125.92Å 90.00° 93.87° 90.00°	Depositor
Resolution (Å)	8.00 – 2.35 8.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.35) 72.3 (8.00-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.32Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.282 0.306 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7368	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 21.40 % 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 7.0631e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, MN, CA, MMA

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	0/1795	1.09	12/2446 (0.5%)
1	B	0.72	0/1795	1.09	11/2446 (0.4%)
1	C	0.73	0/1795	1.09	13/2446 (0.5%)
1	D	0.76	2/1795 (0.1%)	1.13	14/2446 (0.6%)
All	All	0.74	2/7180 (0.0%)	1.10	50/9784 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162	ASN	CG-ND2	-5.89	1.20	1.33
1	D	161	SER	N-CA	5.71	1.53	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	TYR	N-CA-C	6.71	118.59	111.28
1	D	184	SER	N-CA-C	6.39	119.06	111.33
1	A	184	SER	N-CA-C	6.38	119.05	111.33
1	C	152	GLY	N-CA-C	-6.16	107.16	115.36
1	D	176	TYR	N-CA-C	6.13	118.47	111.11
1	C	212	PHE	N-CA-C	-6.12	99.72	109.76
1	B	176	TYR	N-CA-C	6.12	118.45	111.11
1	D	152	GLY	N-CA-C	-6.10	107.25	115.36
1	B	4	ILE	N-CA-C	6.09	116.64	108.11
1	B	212	PHE	N-CA-C	-6.09	99.77	109.76
1	A	4	ILE	N-CA-C	6.03	116.55	108.11
1	D	226	THR	N-CA-C	-6.02	102.05	110.35
1	B	152	GLY	N-CA-C	-5.99	107.39	115.36
1	A	176	TYR	N-CA-C	5.92	118.22	111.11
1	C	216	ASN	N-CA-C	-5.90	102.33	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASN	N-CA-C	-5.89	102.34	110.35
1	C	226	THR	N-CA-C	-5.82	102.32	110.35
1	B	216	ASN	N-CA-C	-5.81	102.45	110.35
1	C	172	ARG	CB-CG-CD	-5.76	98.05	111.30
1	D	216	ASN	N-CA-C	-5.75	102.53	110.35
1	A	152	GLY	N-CA-C	-5.74	107.73	115.36
1	A	172	ARG	CB-CG-CD	-5.72	98.14	111.30
1	D	212	PHE	N-CA-C	-5.70	100.41	109.76
1	D	4	ILE	N-CA-C	5.68	116.07	108.11
1	B	5	VAL	N-CA-C	-5.67	99.38	107.77
1	C	209	GLY	N-CA-C	5.62	118.20	110.56
1	D	172	ARG	CB-CG-CD	-5.56	98.51	111.30
1	A	212	PHE	N-CA-C	-5.55	100.66	109.76
1	D	201	SER	CA-C-N	5.54	125.07	119.19
1	D	201	SER	C-N-CA	5.54	125.07	119.19
1	B	172	ARG	CB-CG-CD	-5.54	98.56	111.30
1	A	5	VAL	N-CA-C	-5.46	99.69	107.77
1	C	5	VAL	N-CA-C	-5.44	99.72	107.77
1	B	201	SER	CA-C-N	5.39	124.91	119.19
1	B	201	SER	C-N-CA	5.39	124.91	119.19
1	C	103	THR	N-CA-C	-5.39	102.50	110.48
1	B	214	ILE	N-CA-C	-5.35	100.42	108.12
1	D	138	LYS	N-CA-C	5.31	118.86	112.38
1	A	103	THR	N-CA-C	-5.30	102.63	110.48
1	A	201	SER	CA-C-N	5.29	124.80	119.19
1	A	201	SER	C-N-CA	5.29	124.80	119.19
1	C	201	SER	CA-C-N	5.25	124.75	119.19
1	C	201	SER	C-N-CA	5.25	124.75	119.19
1	D	217	ILE	N-CA-C	5.23	116.58	110.62
1	D	5	VAL	N-CA-C	-5.19	100.09	107.77
1	A	138	LYS	N-CA-C	5.16	118.68	112.38
1	D	164	SER	O-C-N	5.12	128.14	121.64
1	C	23	PRO	N-CA-C	-5.06	103.17	111.21
1	B	138	LYS	N-CA-C	5.03	118.51	112.38
1	C	138	LYS	N-CA-C	5.02	118.50	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1755	0	1701	39	0
1	B	1755	0	1701	41	0
1	C	1755	0	1701	39	0
1	D	1755	0	1701	43	0
2	E	35	0	32	3	0
2	F	35	0	32	2	0
2	G	35	0	32	4	0
2	H	35	0	32	4	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
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
5	A	50	0	0	1	0
5	B	47	0	0	3	0
5	C	50	0	0	1	0
5	D	53	0	0	2	0
All	All	7368	0	6932	151	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 11.

All (151) 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:A:17:ILE:HD13	1:A:228:ARG:HD3	1.47	0.96
1:C:90:ARG:NH1	1:C:217:ILE:HG22	1.84	0.93
1:B:90:ARG:NH1	1:B:217:ILE:HG22	1.84	0.92
1:C:17:ILE:HD13	1:C:228:ARG:HD3	1.52	0.92
1:B:170:VAL:HG23	1:B:226:THR:HG22	1.52	0.92
1:A:170:VAL:HG23	1:A:226:THR:HG22	1.52	0.92
1:C:170:VAL:HG23	1:C:226:THR:HG22	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:NH1	1:A:217:ILE:HG22	1.87	0.90
1:D:90:ARG:NH1	1:D:217:ILE:HG22	1.86	0.90
1:B:17:ILE:HD13	1:B:228:ARG:HD3	1.54	0.89
1:D:170:VAL:HG23	1:D:226:THR:HG22	1.53	0.88
1:D:17:ILE:HD13	1:D:228:ARG:HD3	1.56	0.87
1:A:170:VAL:CG2	1:A:226:THR:HA	2.17	0.75
1:D:162:ASN:OD1	1:D:164:SER:HB2	1.87	0.75
1:C:131:ASN:HB2	1:D:123:THR:O	1.86	0.74
1:A:123:THR:HB	1:B:131:ASN:HD22	1.53	0.73
1:C:170:VAL:CG2	1:C:226:THR:HA	2.18	0.73
1:D:170:VAL:CG2	1:D:226:THR:HA	2.19	0.71
1:B:170:VAL:CG2	1:B:226:THR:HA	2.20	0.71
1:C:90:ARG:HH11	1:C:217:ILE:HG22	1.54	0.70
1:A:90:ARG:HH11	1:A:217:ILE:HG22	1.57	0.69
1:B:44:ASN:OD1	1:B:200:LYS:HA	1.94	0.68
1:A:100:TYR:CD2	2:E:3:MAN:H62	2.28	0.68
1:A:44:ASN:OD1	1:A:200:LYS:HA	1.94	0.67
1:A:100:TYR:HD2	2:E:3:MAN:H62	1.57	0.67
1:C:44:ASN:OD1	1:C:200:LYS:HA	1.93	0.67
1:B:90:ARG:HH11	1:B:217:ILE:HG22	1.55	0.67
1:D:44:ASN:OD1	1:D:200:LYS:HA	1.95	0.66
1:B:162:ASN:OD1	1:B:164:SER:HB2	1.96	0.66
1:D:90:ARG:HH11	1:D:217:ILE:HG22	1.59	0.66
1:B:1:ALA:HB1	5:B:245:HOH:O	1.96	0.66
1:A:162:ASN:OD1	1:A:164:SER:HB2	1.97	0.65
1:C:201:SER:HB3	1:C:206:PRO:HB3	1.79	0.64
1:A:123:THR:HB	1:B:131:ASN:ND2	2.13	0.62
1:C:162:ASN:OD1	1:C:164:SER:HB2	1.99	0.61
1:B:201:SER:HB3	1:B:206:PRO:HB3	1.82	0.61
1:D:16:ASP:N	2:H:2:MAN:O6	2.34	0.60
1:D:224:GLY:HA2	5:D:251:HOH:O	2.03	0.57
1:C:100:TYR:HB3	1:C:205:HIS:O	2.05	0.57
1:C:172:ARG:NH2	5:C:243:HOH:O	2.37	0.57
1:B:51:HIS:CD2	5:B:288:HOH:O	2.58	0.57
1:A:123:THR:CB	1:B:131:ASN:HD22	2.15	0.57
1:C:100:TYR:HD2	2:G:3:MAN:H62	1.70	0.56
1:D:17:ILE:CD1	1:D:228:ARG:HD3	2.30	0.56
1:B:100:TYR:HB3	1:B:205:HIS:O	2.06	0.56
1:D:170:VAL:CG2	1:D:226:THR:HG22	2.33	0.55
1:C:207:ALA:HB1	1:C:208:ASP:CG	2.31	0.55
1:A:150:THR:O	1:A:151:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASP:HA	5:B:269:HOH:O	2.07	0.54
1:A:100:TYR:HD2	2:E:3:MAN:C6	2.21	0.54
2:G:1:MMA:H3	2:G:1:MMA:H72	1.90	0.54
1:D:150:THR:O	1:D:151:ASP:HB2	2.08	0.53
1:A:100:TYR:HB3	1:A:205:HIS:O	2.07	0.53
1:C:100:TYR:CD2	2:G:3:MAN:H62	2.44	0.53
1:B:150:THR:O	1:B:151:ASP:HB2	2.09	0.53
1:C:150:THR:O	1:C:151:ASP:HB2	2.09	0.52
1:D:207:ALA:HB1	1:D:208:ASP:CG	2.34	0.52
1:B:62:SER:HB3	1:C:57:VAL:HG11	1.91	0.52
1:A:156:LEU:O	1:A:171:GLY:HA3	2.09	0.52
1:A:201:SER:HB3	1:A:206:PRO:HB3	1.90	0.52
1:B:28:ASP:HB3	1:B:31:SER:O	2.10	0.51
1:A:28:ASP:HB3	1:A:31:SER:O	2.10	0.51
1:A:17:ILE:CD1	1:A:228:ARG:HD3	2.29	0.51
1:D:156:LEU:O	1:D:171:GLY:HA3	2.11	0.51
1:A:131:ASN:HB2	1:B:123:THR:O	2.11	0.50
1:B:123:THR:O	1:B:124:ASN:OD1	2.28	0.50
1:B:207:ALA:HB1	1:B:208:ASP:CG	2.37	0.49
1:C:88:TRP:CG	1:D:138:LYS:HD2	2.48	0.49
1:A:25:ILE:HG21	1:A:65:VAL:HG21	1.94	0.49
1:B:17:ILE:CD1	1:B:228:ARG:HD3	2.37	0.49
1:D:100:TYR:HB3	1:D:205:HIS:O	2.12	0.49
1:C:156:LEU:O	1:C:171:GLY:HA3	2.13	0.48
1:B:181:ILE:HD12	1:B:181:ILE:HA	1.73	0.48
1:D:28:ASP:HB3	1:D:31:SER:O	2.13	0.48
1:B:156:LEU:O	1:B:171:GLY:HA3	2.12	0.48
1:D:123:THR:O	1:D:124:ASN:OD1	2.31	0.47
1:B:170:VAL:CG2	1:B:226:THR:HG22	2.33	0.47
1:C:111:PHE:HB3	1:C:128:PHE:CZ	2.49	0.47
1:C:28:ASP:HB3	1:C:31:SER:O	2.15	0.47
1:D:170:VAL:HG22	1:D:226:THR:HA	1.96	0.47
1:C:228:ARG:HG2	2:G:3:MAN:O3	2.14	0.47
1:C:25:ILE:HG21	1:C:65:VAL:HG21	1.97	0.46
1:B:170:VAL:HG22	1:B:226:THR:HA	1.98	0.46
1:D:102:GLU:HA	1:D:201:SER:HB2	1.98	0.46
1:B:66:SER:HB3	1:B:72:SER:HB3	1.98	0.45
1:C:116:LYS:HB3	1:C:123:THR:HG23	1.99	0.45
1:B:57:VAL:HB	1:C:53:ILE:HD11	1.99	0.45
1:A:170:VAL:CG2	1:A:226:THR:HG22	2.35	0.45
1:C:92:GLY:HA2	1:C:109:TRP:CH2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLU:HA	1:B:201:SER:HB2	1.97	0.45
1:C:170:VAL:HG22	1:C:226:THR:HA	1.96	0.45
1:C:88:TRP:CE3	1:D:138:LYS:HB2	2.51	0.45
1:D:14:ASN:HB3	5:D:288:HOH:O	2.17	0.44
1:D:25:ILE:HG21	1:D:65:VAL:HG21	2.00	0.44
1:B:23:PRO:HB2	1:B:40:TRP:O	2.17	0.44
1:C:88:TRP:CD2	1:D:138:LYS:HB2	2.53	0.44
1:A:172:ARG:NH2	5:A:278:HOH:O	2.50	0.44
1:C:181:ILE:HD12	1:C:181:ILE:HA	1.76	0.44
1:D:207:ALA:HA	1:D:208:ASP:HA	1.76	0.44
1:B:207:ALA:HA	1:B:208:ASP:HA	1.81	0.43
1:B:111:PHE:HB3	1:B:128:PHE:CZ	2.53	0.43
1:C:201:SER:CB	1:C:206:PRO:HB3	2.47	0.43
1:B:25:ILE:HG21	1:B:65:VAL:HG21	2.01	0.43
1:D:116:LYS:HB3	1:D:123:THR:HG23	2.00	0.43
1:A:170:VAL:HG22	1:A:226:THR:HA	1.96	0.43
1:B:30:LYS:HD2	1:B:84:VAL:HG13	2.01	0.43
1:D:16:ASP:H	2:H:2:MAN:HO6	1.66	0.43
1:A:181:ILE:HD12	1:A:181:ILE:HA	1.71	0.43
1:C:17:ILE:CD1	1:C:228:ARG:HD3	2.34	0.43
1:D:160:SER:O	1:D:161:SER:C	2.61	0.43
1:C:123:THR:O	1:D:131:ASN:HB2	2.19	0.43
1:A:66:SER:HB3	1:A:72:SER:HB3	2.01	0.42
1:C:56:SER:OG	1:C:188:VAL:HA	2.19	0.42
1:A:111:PHE:HB3	1:A:128:PHE:CZ	2.54	0.42
1:C:32:VAL:HB	1:C:233:PHE:CD2	2.53	0.42
1:D:56:SER:OG	1:D:188:VAL:HA	2.19	0.42
1:A:56:SER:OG	1:A:188:VAL:HA	2.18	0.42
1:A:109:TRP:HA	1:A:194:THR:O	2.20	0.42
1:C:201:SER:HA	1:C:202:PRO:HD2	1.85	0.42
1:A:101:LYS:HD2	1:A:165:PRO:O	2.20	0.42
1:C:170:VAL:CG2	1:C:226:THR:HG22	2.34	0.42
1:D:15:THR:HB	2:H:2:MAN:O6	2.19	0.42
1:D:111:PHE:HB3	1:D:128:PHE:CZ	2.55	0.42
1:D:217:ILE:HG21	1:D:217:ILE:HD13	1.83	0.42
1:B:177:ALA:HA	1:B:178:PRO:HD3	1.91	0.42
1:A:64:VAL:HG21	1:D:57:VAL:HG22	2.02	0.41
1:C:66:SER:HB3	1:C:72:SER:HB3	2.01	0.41
1:A:92:GLY:HA2	1:A:109:TRP:CH2	2.55	0.41
1:D:181:ILE:HD12	1:D:181:ILE:HA	1.72	0.41
1:B:32:VAL:HB	1:B:233:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:TYR:HD2	2:F:3:MAN:H62	1.84	0.41
1:B:109:TRP:HA	1:B:194:THR:O	2.20	0.41
1:D:32:VAL:HB	1:D:233:PHE:CD2	2.56	0.41
1:C:30:LYS:HD2	1:C:84:VAL:HG13	2.01	0.41
1:D:92:GLY:HA2	1:D:109:TRP:CH2	2.55	0.41
1:D:228:ARG:HG2	2:H:3:MAN:O3	2.21	0.41
1:A:207:ALA:HA	1:A:208:ASP:HA	1.79	0.41
1:B:228:ARG:HG2	2:F:3:MAN:O3	2.21	0.41
1:A:30:LYS:HD2	1:A:84:VAL:HG13	2.03	0.41
1:D:30:LYS:HD2	1:D:84:VAL:HG13	2.02	0.41
1:D:66:SER:HB3	1:D:72:SER:HB3	2.03	0.41
1:A:90:ARG:HG3	1:A:217:ILE:HG23	2.02	0.41
1:B:90:ARG:NH1	1:B:217:ILE:CG2	2.71	0.41
1:D:109:TRP:HA	1:D:194:THR:O	2.21	0.41
1:A:32:VAL:HB	1:A:233:PHE:CD2	2.56	0.40
1:A:51:HIS:O	1:A:63:ALA:HA	2.20	0.40
1:C:109:TRP:HA	1:C:194:THR:O	2.20	0.40
1:D:47:VAL:HA	1:D:197:PHE:O	2.20	0.40
1:A:177:ALA:HA	1:A:178:PRO:HD3	1.89	0.40
1:B:51:HIS:O	1:B:63:ALA:HA	2.21	0.40
1:A:102:GLU:HA	1:A:201:SER:HB2	2.04	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	227/237 (96%)	215 (95%)	12 (5%)	0	100	100
1	B	227/237 (96%)	212 (93%)	15 (7%)	0	100	100
1	C	227/237 (96%)	212 (93%)	14 (6%)	1 (0%)	30	34
1	D	227/237 (96%)	213 (94%)	13 (6%)	1 (0%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	908/948 (96%)	852 (94%)	54 (6%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	ASN
1	D	162	ASN

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	195/203 (96%)	177 (91%)	18 (9%)	8	9
1	B	195/203 (96%)	179 (92%)	16 (8%)	10	11
1	C	195/203 (96%)	179 (92%)	16 (8%)	10	11
1	D	195/203 (96%)	177 (91%)	18 (9%)	8	9
All	All	780/812 (96%)	712 (91%)	68 (9%)	9	10

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	78	ASP
1	A	82	ASP
1	A	101	LYS
1	A	123	THR
1	A	134	SER
1	A	150	THR
1	A	151	ASP
1	A	161	SER
1	A	164	SER
1	A	181	ILE
1	A	184	SER
1	A	200	LYS

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Mol	Chain	Res	Type
1	A	204	SER
1	A	205	HIS
1	A	214	ILE
1	A	223	SER
1	A	228	ARG
1	B	78	ASP
1	B	82	ASP
1	B	101	LYS
1	B	123	THR
1	B	134	SER
1	B	150	THR
1	B	151	ASP
1	B	161	SER
1	B	164	SER
1	B	181	ILE
1	B	184	SER
1	B	200	LYS
1	B	204	SER
1	B	214	ILE
1	B	223	SER
1	B	228	ARG
1	C	53	ILE
1	C	78	ASP
1	C	82	ASP
1	C	101	LYS
1	C	134	SER
1	C	150	THR
1	C	151	ASP
1	C	161	SER
1	C	164	SER
1	C	181	ILE
1	C	184	SER
1	C	200	LYS
1	C	204	SER
1	C	214	ILE
1	C	223	SER
1	C	228	ARG
1	D	21	SER
1	D	53	ILE
1	D	78	ASP
1	D	82	ASP
1	D	101	LYS

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Mol	Chain	Res	Type
1	D	123	THR
1	D	134	SER
1	D	150	THR
1	D	151	ASP
1	D	161	SER
1	D	164	SER
1	D	181	ILE
1	D	184	SER
1	D	200	LYS
1	D	204	SER
1	D	205	HIS
1	D	214	ILE
1	D	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	43	GLN
1	A	237	ASN
1	B	41	ASN
1	B	43	GLN
1	B	51	HIS
1	B	131	ASN
1	B	237	ASN
1	C	41	ASN
1	C	237	ASN
1	D	41	ASN
1	D	43	GLN
1	D	237	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 ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MMA	E	1	2	13,13,13	0.38	0	18,18,18	0.82	0
2	MAN	E	2	2	11,11,12	0.58	0	15,15,17	0.84	0
2	MAN	E	3	2	11,11,12	0.59	0	15,15,17	0.79	0
2	MMA	F	1	2	13,13,13	0.33	0	18,18,18	0.64	0
2	MAN	F	2	2	11,11,12	0.44	0	15,15,17	1.22	2 (13%)
2	MAN	F	3	2	11,11,12	0.78	0	15,15,17	0.88	0
2	MMA	G	1	2	13,13,13	0.36	0	18,18,18	0.91	0
2	MAN	G	2	2	11,11,12	0.58	0	15,15,17	1.07	2 (13%)
2	MAN	G	3	2	11,11,12	0.53	0	15,15,17	0.60	0
2	MMA	H	1	2	13,13,13	0.43	0	18,18,18	0.56	0
2	MAN	H	2	2	11,11,12	0.43	0	15,15,17	0.89	0
2	MAN	H	3	2	11,11,12	0.44	0	15,15,17	1.02	1 (6%)

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	MMA	E	1	2	-	2/4/24/24	0/1/1/1
2	MAN	E	2	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
2	MMA	F	1	2	-	0/4/24/24	0/1/1/1
2	MAN	F	2	2	-	0/2/19/22	0/1/1/1
2	MAN	F	3	2	-	1/2/19/22	0/1/1/1
2	MMA	G	1	2	-	2/4/24/24	0/1/1/1
2	MAN	G	2	2	-	2/2/19/22	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	0/1/1/1
2	MMA	H	1	2	-	2/4/24/24	0/1/1/1
2	MAN	H	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	H	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	MAN	C2-C3-C4	-3.11	105.40	110.86
2	F	2	MAN	C1-O5-C5	2.48	115.51	112.19
2	F	2	MAN	C1-C2-C3	2.22	112.87	109.64
2	G	2	MAN	C6-C5-C4	-2.09	107.89	113.02
2	G	2	MAN	O5-C5-C6	-2.01	103.75	107.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	MMA	C2-C1-O1-C7
2	G	1	MMA	O5-C1-O1-C7
2	H	2	MAN	O5-C5-C6-O6
2	G	2	MAN	O5-C5-C6-O6
2	H	2	MAN	C4-C5-C6-O6
2	G	2	MAN	C4-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
2	H	3	MAN	C4-C5-C6-O6
2	H	3	MAN	O5-C5-C6-O6
2	H	1	MMA	C4-C5-C6-O6
2	E	1	MMA	C4-C5-C6-O6
2	F	3	MAN	C4-C5-C6-O6
2	H	1	MMA	O5-C5-C6-O6
2	E	1	MMA	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 13 short contacts:

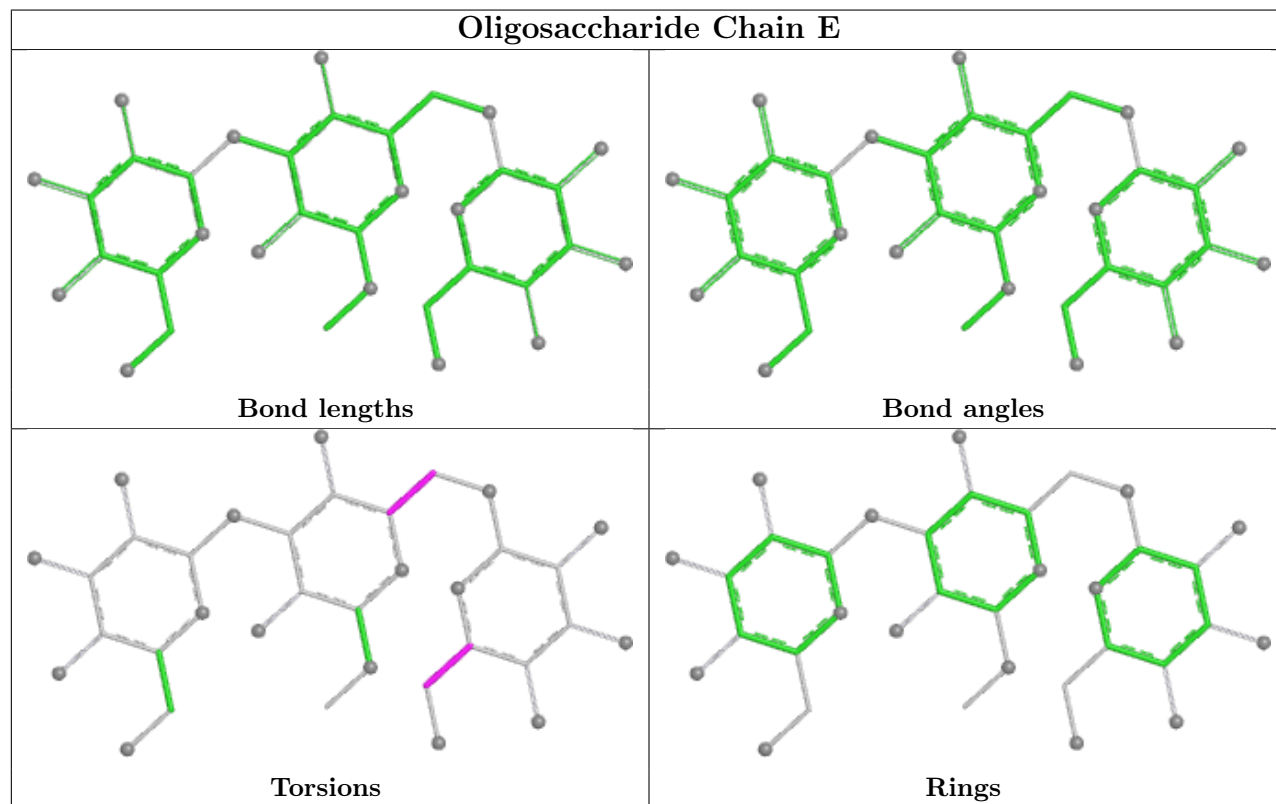
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	MAN	3	0
2	F	3	MAN	2	0
2	H	2	MAN	3	0
2	H	3	MAN	1	0

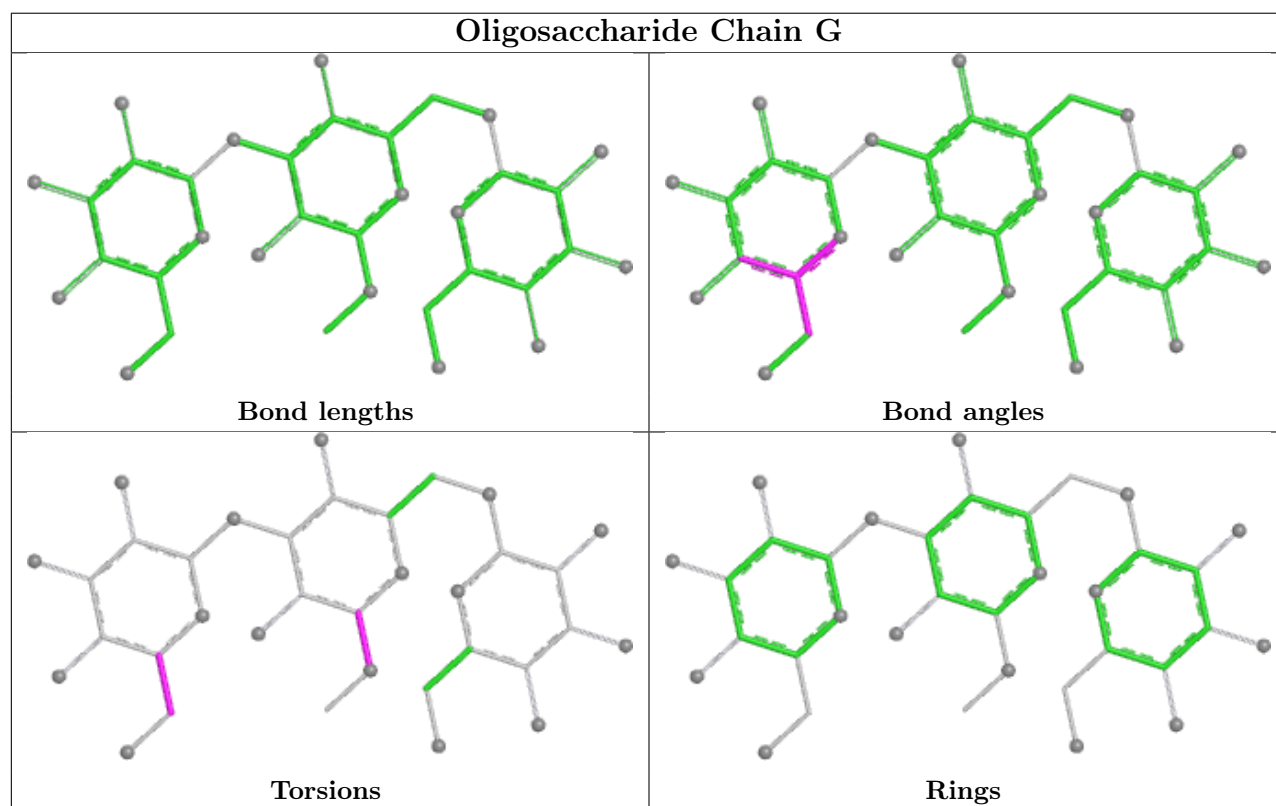
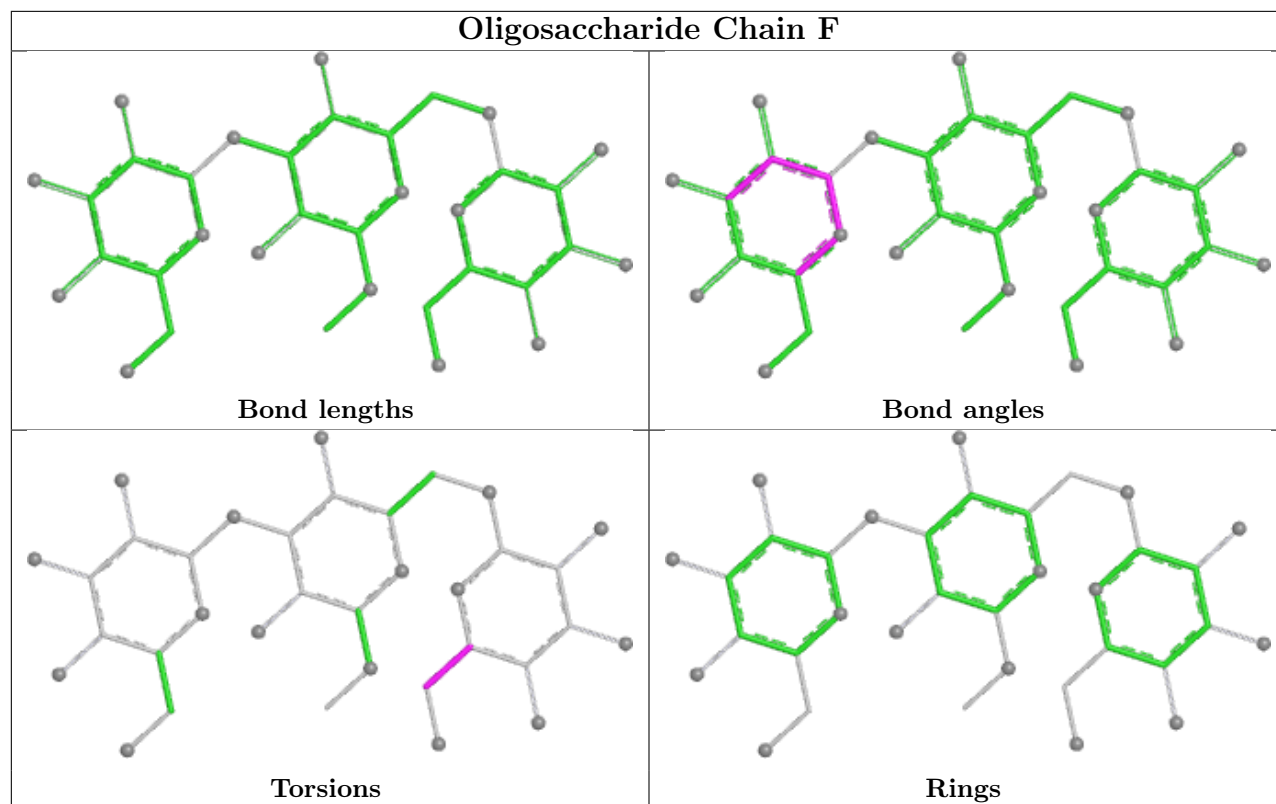
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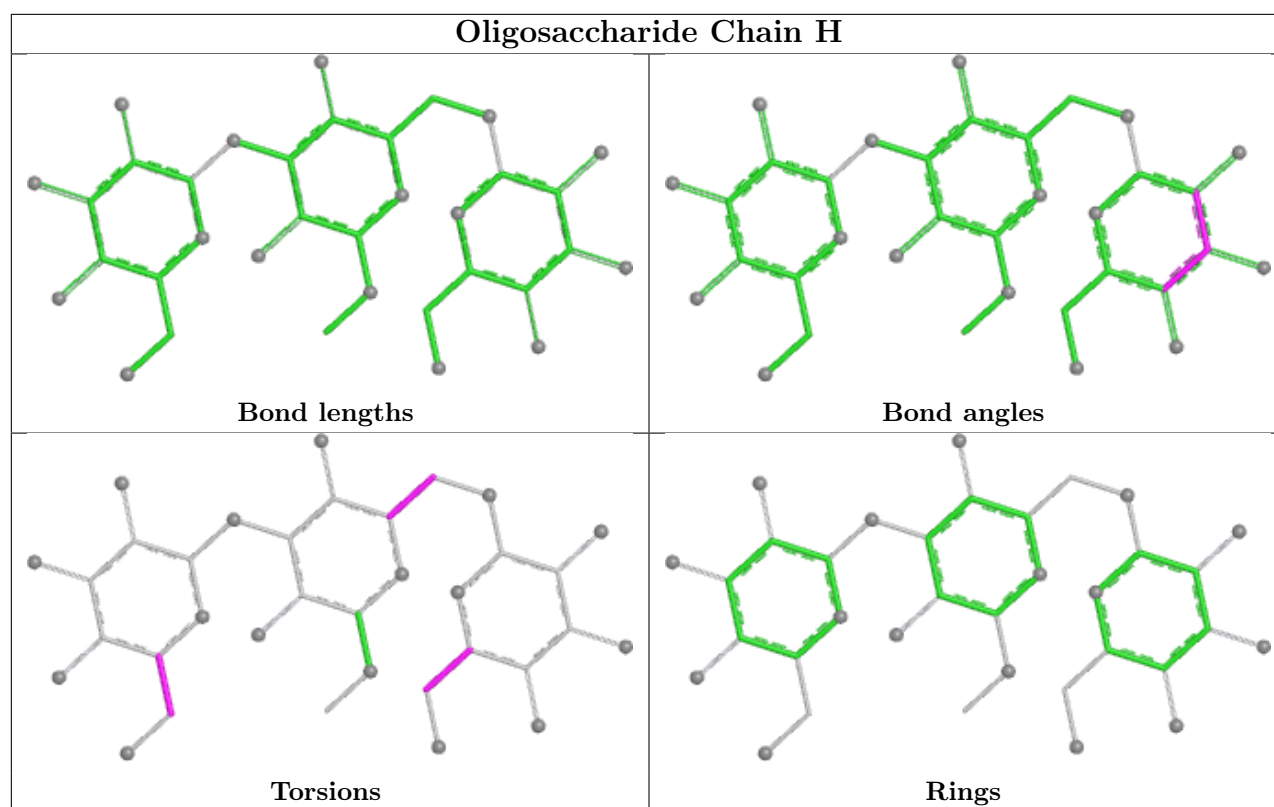
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	MMA	1	0
2	E	3	MAN	3	0

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 [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/237 (97%)	-1.40	0 100 100	2, 14, 51, 65	0
1	B	231/237 (97%)	-1.40	0 100 100	3, 14, 46, 67	0
1	C	231/237 (97%)	-1.40	0 100 100	2, 13, 48, 64	0
1	D	231/237 (97%)	-1.37	0 100 100	3, 15, 49, 70	0
All	All	924/948 (97%)	-1.39	0 100 100	2, 14, 49, 70	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	MAN	G	3	11/12	0.98	0.05	2,5,11,16	0
2	MAN	E	2	11/12	0.99	0.03	30,33,39,41	0
2	MAN	E	3	11/12	0.99	0.04	16,25,29,37	0
2	MMA	F	1	13/13	0.99	0.03	20,24,28,29	0
2	MAN	F	3	11/12	0.99	0.04	2,17,19,19	0
2	MMA	G	1	13/13	0.99	0.04	4,15,26,27	0
2	MAN	G	2	11/12	0.99	0.04	15,22,35,47	0
2	MMA	E	1	13/13	0.99	0.05	23,30,33,34	0
2	MMA	H	1	13/13	0.99	0.04	27,43,55,58	0

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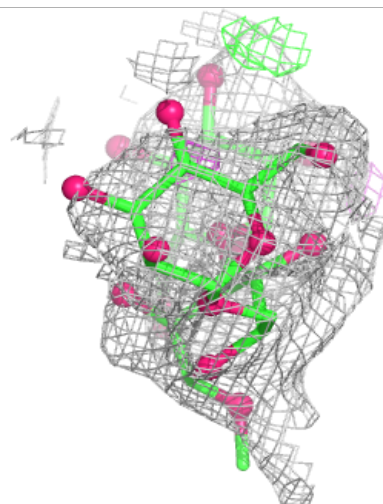
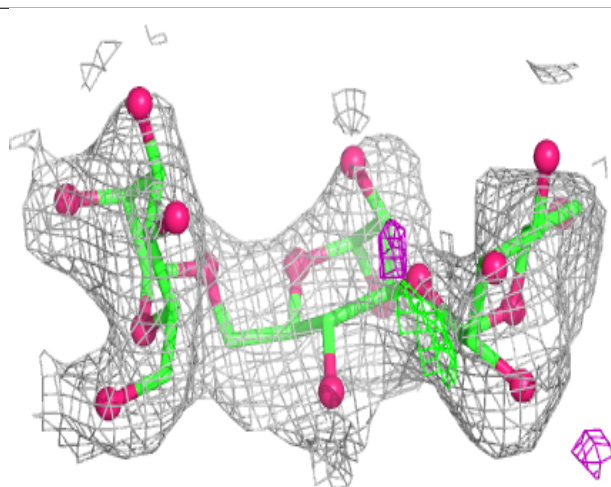
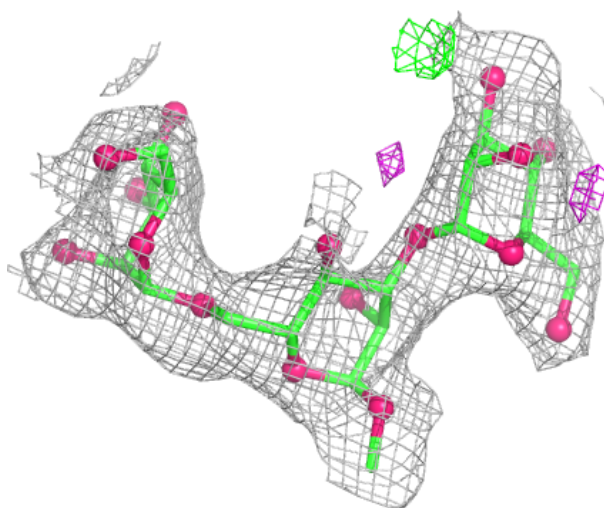
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	H	2	11/12	0.99	0.04	45,51,59,64	0
2	MAN	H	3	11/12	0.99	0.04	8,18,23,26	0
2	MAN	F	2	11/12	1.00	0.03	20,27,37,38	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

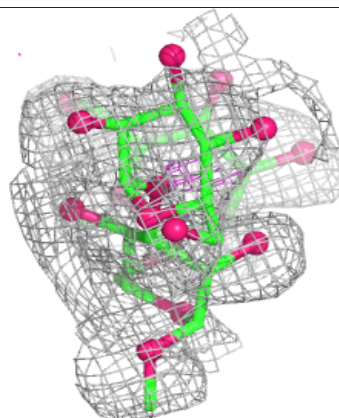
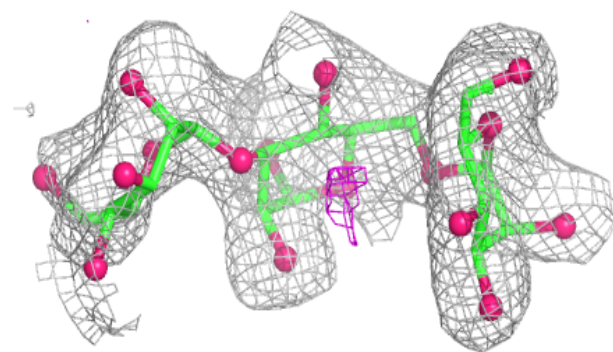
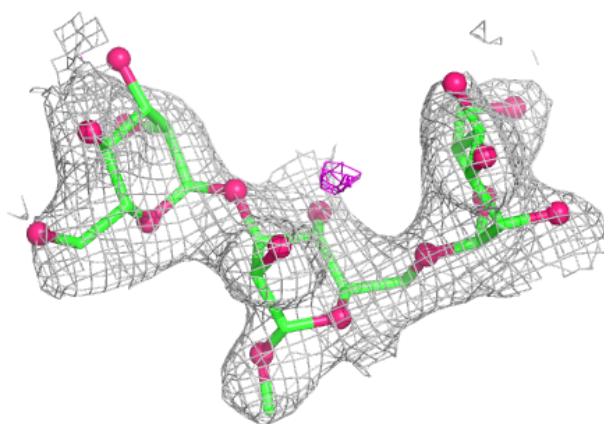
Electron density around Chain E:

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



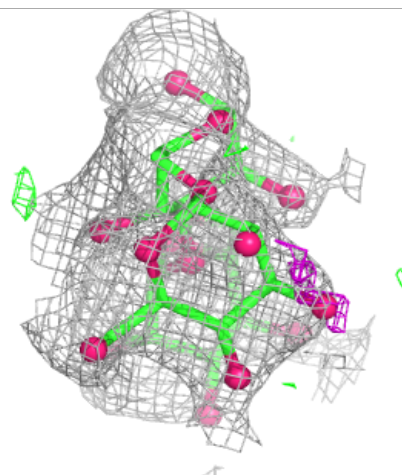
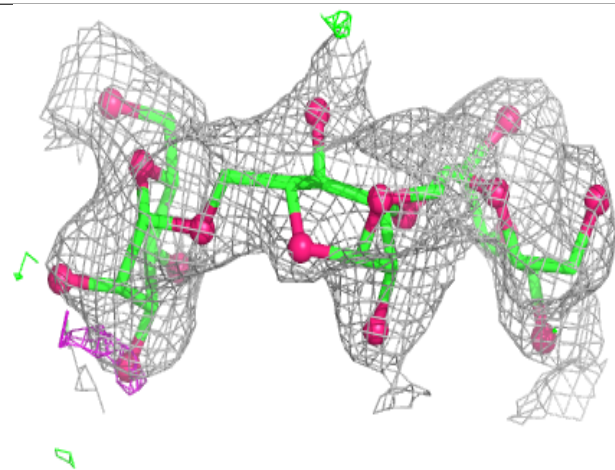
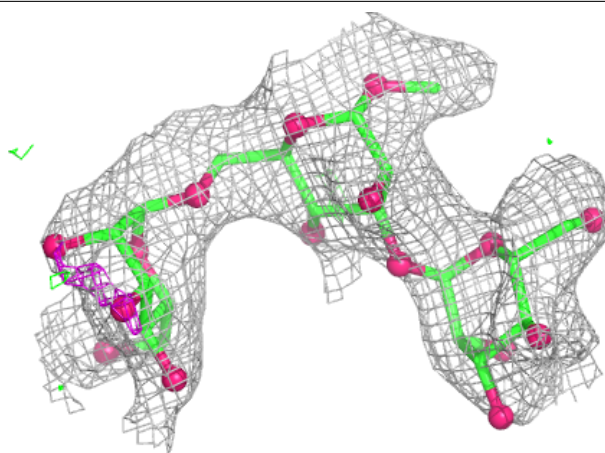
Electron density around Chain F:

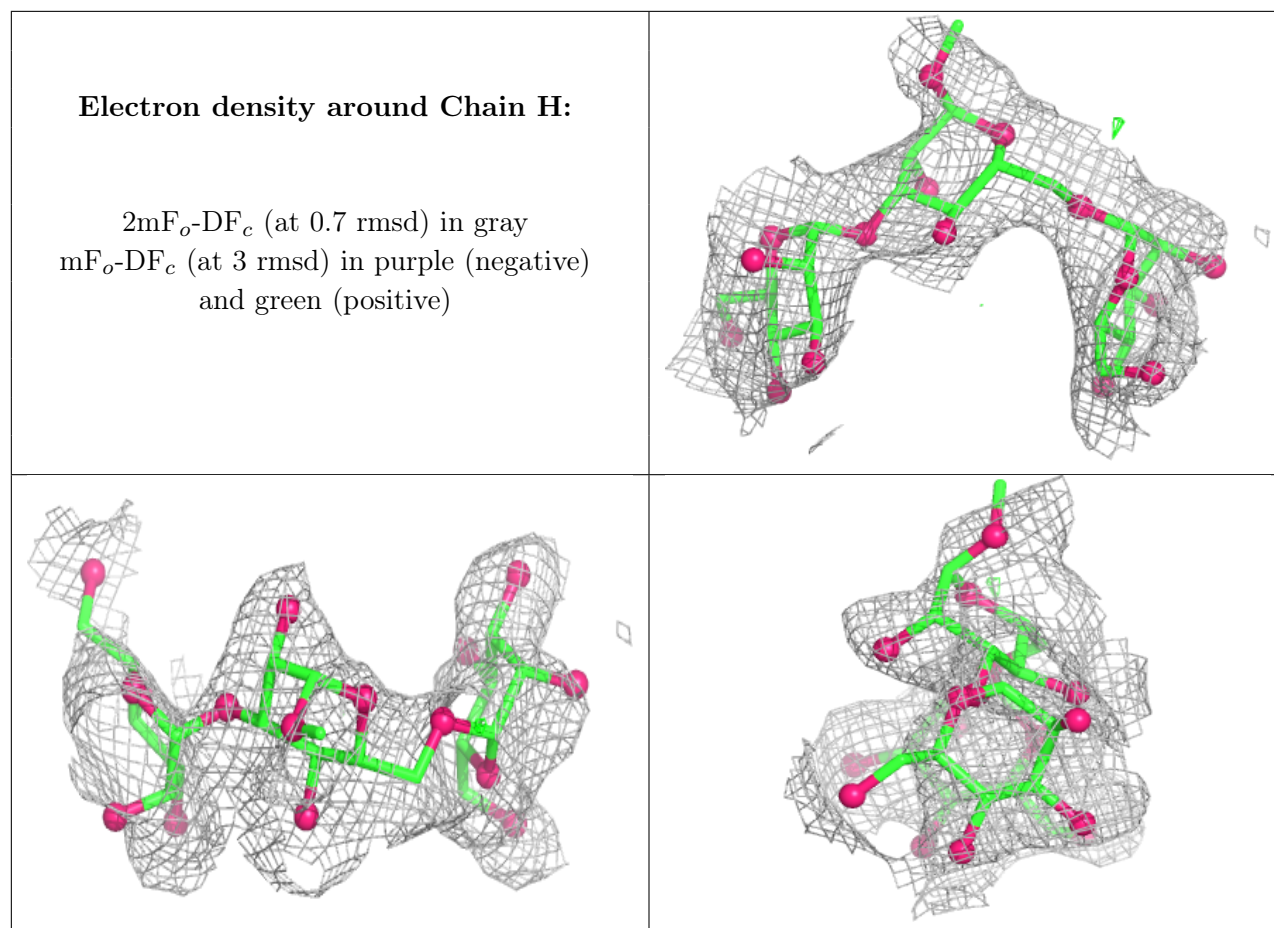
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands [i](#)

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
3	MN	C	238	1/1	0.99	0.02	21,21,21,21	0
4	CA	B	239	1/1	0.99	0.02	12,12,12,12	0
4	CA	D	239	1/1	0.99	0.03	14,14,14,14	0
3	MN	D	238	1/1	1.00	0.01	15,15,15,15	0
4	CA	A	239	1/1	1.00	0.02	10,10,10,10	0
3	MN	B	238	1/1	1.00	0.01	14,14,14,14	0
4	CA	C	239	1/1	1.00	0.02	18,18,18,18	0
3	MN	A	238	1/1	1.00	0.01	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.