



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:58 PM UTC

PDB ID : 2PEL / pdb_00002pel
Title : PEANUT LECTIN
Authors : Banerjee, R.; Das, K.; Ravishankar, R.; Suguna, K.; Surolia, A.; Vijayan, M.
Deposited on : 1995-08-23
Resolution : 2.25 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

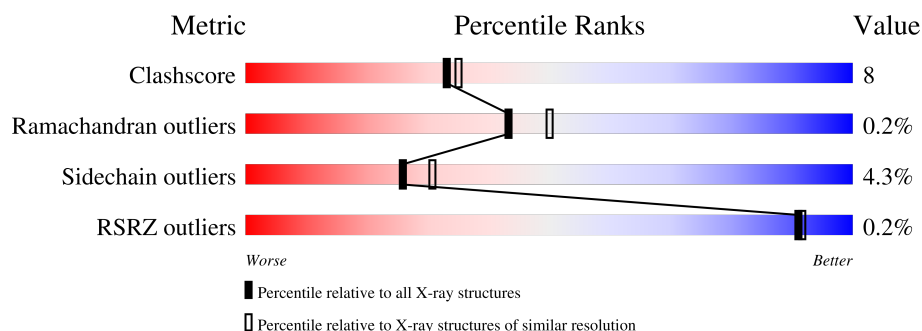
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	236	
1	B	236	
1	C	236	
1	D	236	
2	E	2	
2	F	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	2	 100%
3	G	2	 50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7635 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 PEANUT LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	B	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	C	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	D	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	2	Total	C	O	0	0	0
			23	12	11			

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

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

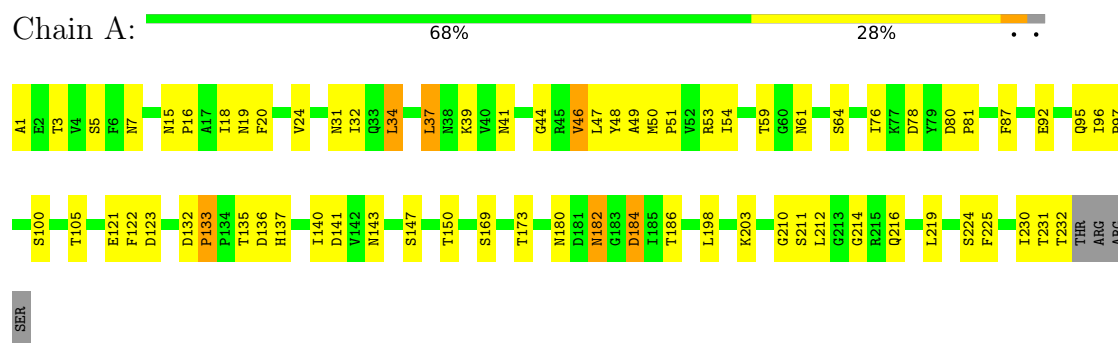
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	165	Total	O	0	0
			165	165		
6	C	122	Total	O	0	0
			122	122		
6	D	129	Total	O	0	0
			129	129		

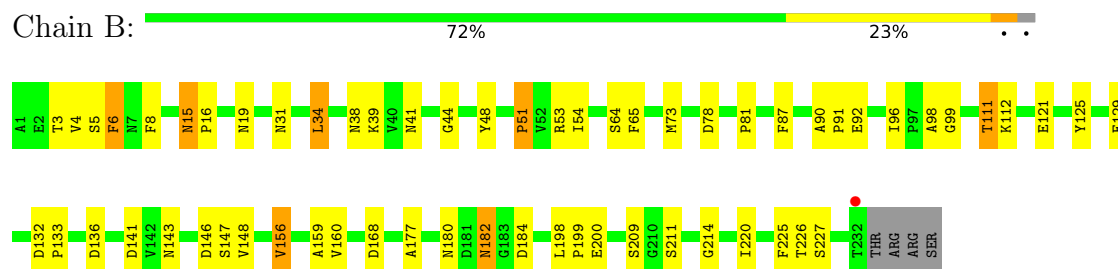
3 Residue-property plots

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.

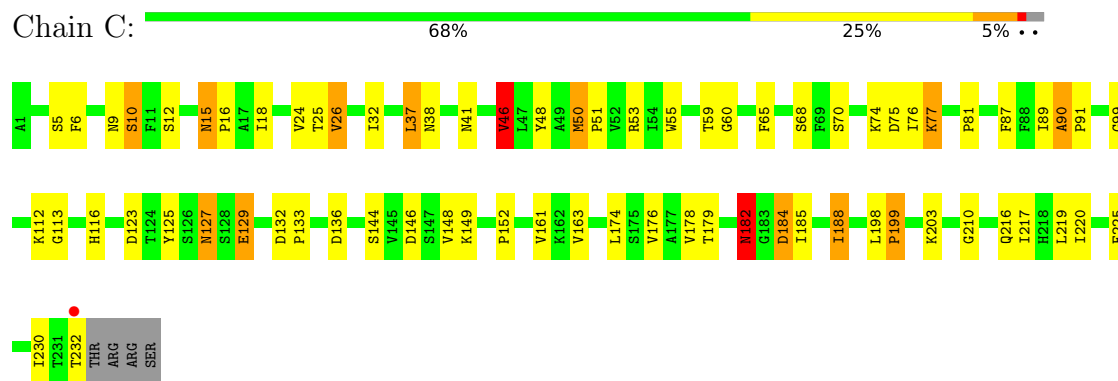
• Molecule 1: PEANUT LECTIN



• Molecule 1: PEANUT LECTIN

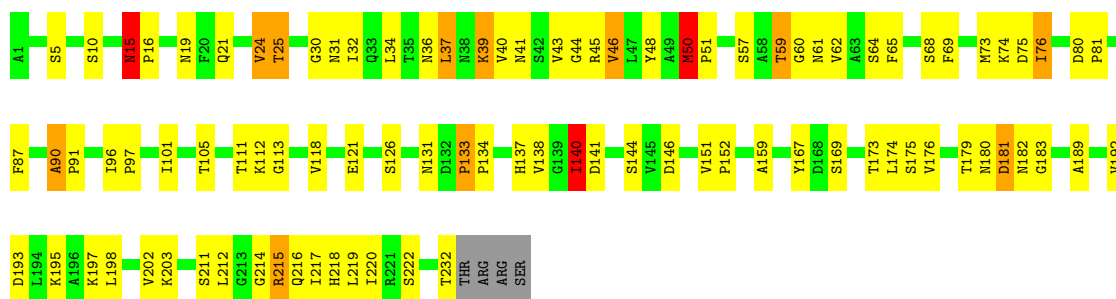


• Molecule 1: PEANUT LECTIN



• Molecule 1: PEANUT LECTIN

Chain D:  58% 34% 5% ..



- Molecule 2: beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  50% 50%

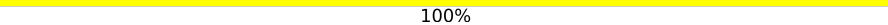


- Molecule 2: beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  50% 50%



- Molecule 2: beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  100%



- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain G:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.30Å 126.90Å 76.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.25 10.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	78.0 (10.00-2.25) 73.2 (10.00-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 2.26Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.164 , (Not available) 0.157 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7635	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, CA, GLC, MN, 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	1.08	2/1779 (0.1%)	1.99	46/2426 (1.9%)
1	B	1.11	1/1779 (0.1%)	1.97	41/2426 (1.7%)
1	C	1.02	0/1779	1.96	49/2426 (2.0%)
1	D	1.04	0/1779	2.00	56/2426 (2.3%)
All	All	1.06	3/7116 (0.0%)	1.98	192/9704 (2.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	GLY	N-CA	6.85	1.55	1.45
1	A	212	LEU	CA-C	-5.21	1.46	1.52
1	A	135	THR	CA-CB	5.08	1.60	1.53

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ALA	CA-C-O	-10.27	109.00	121.02
1	A	19	ASN	CA-CB-CG	8.93	121.53	112.60
1	D	40	VAL	CA-C-O	-8.69	111.10	121.18
1	B	19	ASN	CA-CB-CG	8.66	121.26	112.60
1	D	181	ASP	CA-C-N	8.31	132.24	120.28
1	D	181	ASP	C-N-CA	8.31	132.24	120.28
1	D	121	GLU	CA-C-N	8.09	134.37	123.20
1	D	121	GLU	C-N-CA	8.09	134.37	123.20
1	C	37	LEU	N-CA-C	8.02	120.93	111.71
1	A	59	THR	CA-C-O	-7.85	112.70	121.89
1	D	181	ASP	CA-CB-CG	7.82	120.42	112.60
1	D	131	ASN	CA-CB-CG	7.74	120.34	112.60
1	A	80	ASP	O-C-N	7.70	128.34	121.18
1	B	48	TYR	N-CA-C	-7.68	98.43	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ASP	N-CA-C	-7.60	100.47	110.43
1	A	230	ILE	N-CA-CB	7.54	119.19	110.82
1	A	198	LEU	O-C-N	7.50	126.51	121.71
1	C	87	PHE	CA-C-O	-7.42	112.64	120.58
1	A	48	TYR	N-CA-C	-7.39	98.73	109.59
1	C	182	ASN	CA-CB-CG	7.31	119.91	112.60
1	A	143	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	C	136	ASP	CA-CB-CG	7.22	119.82	112.60
1	D	133	PRO	N-CA-C	-6.97	102.19	110.70
1	C	146	ASP	CA-CB-CG	6.97	119.57	112.60
1	C	127	ASN	OD1-CG-ND2	6.91	129.51	122.60
1	D	169	SER	N-CA-C	6.88	118.78	111.28
1	C	26	VAL	CA-C-O	-6.87	113.22	120.57
1	B	129	GLU	CA-CB-CG	6.82	127.75	114.10
1	D	87	PHE	CA-C-O	-6.78	112.84	120.43
1	D	111	THR	CA-CB-OG1	-6.74	99.49	109.60
1	B	6	PHE	O-C-N	6.73	130.62	123.42
1	D	202	VAL	O-C-N	6.68	130.37	122.95
1	B	220	ILE	N-CA-CB	6.67	119.86	111.46
1	C	174	LEU	CA-C-O	-6.63	113.64	120.54
1	C	116	HIS	CA-CB-CG	6.55	120.35	113.80
1	C	48	TYR	N-CA-C	-6.49	100.23	109.96
1	C	220	ILE	CA-C-O	-6.46	113.61	120.53
1	A	87	PHE	N-CA-C	-6.46	98.20	108.73
1	C	132	ASP	O-C-N	6.41	127.90	121.30
1	C	50	MET	CA-C-O	6.38	125.44	119.76
1	D	218	HIS	CA-CB-CG	6.35	120.15	113.80
1	C	129	GLU	CB-CG-CD	6.30	123.32	112.60
1	C	133	PRO	N-CA-C	-6.30	103.01	110.70
1	D	80	ASP	CA-CB-CG	6.30	118.90	112.60
1	D	180	ASN	CB-CG-ND2	6.30	125.86	116.40
1	B	73	MET	CA-C-O	-6.28	113.58	120.36
1	C	53	ARG	CD-NE-CZ	6.25	133.16	124.40
1	A	133	PRO	N-CA-C	-6.24	103.09	110.70
1	A	231	THR	N-CA-C	-6.23	99.25	109.40
1	A	59	THR	N-CA-C	-6.21	101.59	110.59
1	C	9	ASN	N-CA-C	-6.20	105.54	113.23
1	C	136	ASP	N-CA-C	-6.13	102.27	110.24
1	D	31	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	184	ASP	CA-CB-CG	6.11	118.71	112.60
1	D	87	PHE	N-CA-C	-6.11	99.25	108.96
1	A	180	ASN	CA-C-N	6.11	128.46	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASN	C-N-CA	6.11	128.46	120.28
1	A	143	ASN	CA-CB-CG	6.09	118.69	112.60
1	B	65	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	39	LYS	N-CA-CB	-6.05	100.95	110.69
1	A	231	THR	N-CA-CB	6.04	121.33	110.83
1	D	198	LEU	O-C-N	6.03	126.16	121.88
1	B	4	VAL	O-C-N	6.02	129.70	123.20
1	D	48	TYR	N-CA-C	-6.02	100.93	109.96
1	D	90	ALA	N-CA-C	6.00	113.41	108.07
1	C	184	ASP	CA-CB-CG	5.98	118.58	112.60
1	C	176	VAL	N-CA-C	5.96	117.06	108.48
1	A	34	LEU	CA-C-O	-5.95	114.11	120.42
1	B	78	ASP	CA-C-O	-5.93	112.03	120.51
1	D	118	VAL	CB-CA-C	5.91	118.96	110.33
1	D	220	ILE	CA-C-O	-5.91	114.21	120.48
1	C	46	VAL	CB-CA-C	5.91	119.61	110.50
1	A	232	THR	CA-C-O	-5.91	110.76	120.80
1	D	75	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	136	ASP	N-CA-C	-5.89	102.71	110.43
1	B	133	PRO	N-CA-C	-5.89	103.51	110.70
1	D	141	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	179	THR	CA-C-O	-5.82	114.06	120.70
1	B	200	GLU	CA-C-O	-5.82	114.38	120.55
1	D	101	ILE	CA-C-O	-5.81	113.51	120.78
1	C	90	ALA	O-C-N	5.79	126.46	121.54
1	A	49	ALA	N-CA-C	5.78	118.36	111.71
1	D	59	THR	CA-C-O	-5.78	114.45	120.70
1	B	38	ASN	OD1-CG-ND2	5.78	128.38	122.60
1	B	143	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	140	ILE	O-C-N	5.76	129.23	123.18
1	B	177	ALA	CA-C-O	-5.75	114.12	120.33
1	C	60	GLY	N-CA-C	-5.75	106.72	115.00
1	B	31	ASN	OD1-CG-ND2	5.75	128.35	122.60
1	C	38	ASN	CA-CB-CG	-5.74	106.86	112.60
1	B	147	SER	N-CA-C	5.73	118.37	110.35
1	A	78	ASP	CA-C-O	-5.70	112.36	120.51
1	A	147	SER	CA-C-O	5.70	127.42	121.15
1	D	105	THR	CA-C-N	5.67	131.46	122.61
1	D	105	THR	C-N-CA	5.67	131.46	122.61
1	B	160	VAL	CA-C-O	-5.65	114.53	120.57
1	B	87	PHE	N-CA-C	-5.64	99.99	108.96
1	C	6	PHE	O-C-N	5.64	129.59	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASP	N-CA-C	-5.64	98.04	108.24
1	D	65	PHE	CA-C-N	5.62	130.70	122.77
1	D	65	PHE	C-N-CA	5.62	130.70	122.77
1	B	6	PHE	CA-C-O	-5.62	115.22	121.23
1	D	183	GLY	N-CA-C	-5.62	108.01	114.69
1	A	186	THR	CA-CB-CG2	5.60	120.03	110.50
1	D	21	GLN	CA-C-O	-5.59	114.11	120.32
1	C	99	GLY	CA-C-N	5.59	128.70	120.82
1	C	99	GLY	C-N-CA	5.59	128.70	120.82
1	D	134	PRO	N-CA-C	5.59	120.91	114.20
1	D	90	ALA	O-C-N	5.58	127.09	121.56
1	C	55	TRP	CA-CB-CG	5.58	124.19	113.60
1	D	76	ILE	CB-CA-C	5.57	118.92	110.62
1	A	141	ASP	CA-C-O	-5.54	114.34	120.38
1	B	34	LEU	N-CA-C	5.54	117.39	111.36
1	B	98	ALA	CA-C-N	-5.53	110.58	121.41
1	B	98	ALA	C-N-CA	-5.53	110.58	121.41
1	C	220	ILE	CB-CA-C	5.52	119.02	110.96
1	D	138	VAL	N-CA-C	-5.52	100.53	108.53
1	A	150	THR	CA-CB-OG1	-5.51	101.34	109.60
1	D	126	SER	N-CA-C	5.51	117.28	108.41
1	A	184	ASP	CA-C-O	-5.50	115.00	121.16
1	A	186	THR	CA-CB-OG1	-5.50	101.35	109.60
1	B	226	THR	CA-C-N	-5.50	114.04	122.62
1	B	226	THR	C-N-CA	-5.50	114.04	122.62
1	D	64	SER	N-CA-C	-5.49	101.23	109.95
1	D	176	VAL	N-CA-CB	-5.49	101.78	111.93
1	D	140	ILE	CB-CA-C	5.48	118.97	110.96
1	A	46	VAL	CB-CA-C	5.48	118.94	110.50
1	C	65	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	15	ASN	CA-CB-CG	5.46	118.06	112.60
1	C	129	GLU	CA-CB-CG	5.46	125.03	114.10
1	C	152	PRO	N-CA-CB	5.45	108.16	103.31
1	A	18	ILE	CB-CA-C	-5.45	102.57	110.63
1	B	132	ASP	O-C-N	5.44	127.53	121.43
1	A	105	THR	CA-CB-CG2	5.43	119.74	110.50
1	C	179	THR	N-CA-CB	5.43	118.85	110.21
1	C	89	ILE	O-C-N	5.43	129.06	123.20
1	B	96	ILE	CA-C-N	5.42	125.43	119.90
1	B	96	ILE	C-N-CA	5.42	125.43	119.90
1	B	168	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	122	PHE	CA-CB-CG	-5.41	108.39	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	SER	N-CA-C	5.41	117.60	111.11
1	C	48	TYR	CB-CA-C	5.40	118.52	109.89
1	A	122	PHE	N-CA-C	-5.39	97.46	107.71
1	A	92	GLU	N-CA-C	5.39	118.95	112.38
1	B	156	VAL	CB-CA-C	5.38	118.81	110.96
1	C	146	ASP	N-CA-C	-5.36	97.17	107.57
1	B	87	PHE	CA-C-O	-5.35	114.44	120.43
1	C	75	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	8	PHE	N-CA-CB	5.34	118.98	110.65
1	D	197	LYS	N-CA-C	5.33	120.06	113.50
1	C	188	ILE	O-C-N	5.33	128.31	123.19
1	A	140	ILE	N-CA-C	-5.33	100.71	108.17
1	A	51	PRO	CA-C-O	-5.32	114.93	121.31
1	C	199	PRO	CA-C-N	5.31	127.40	120.28
1	C	199	PRO	C-N-CA	5.31	127.40	120.28
1	A	64	SER	N-CA-C	-5.31	102.19	110.42
1	B	15	ASN	O-C-N	5.27	125.79	121.31
1	D	220	ILE	N-CA-C	-5.26	100.81	108.17
1	C	15	ASN	O-C-N	5.25	125.77	121.31
1	C	188	ILE	CA-C-O	-5.24	116.03	120.96
1	C	24	VAL	O-C-N	5.24	128.19	122.63
1	D	167	TYR	O-C-N	5.24	129.35	123.27
1	A	122	PHE	CB-CA-C	5.23	119.45	111.76
1	D	193	ASP	CB-CA-C	5.23	119.89	111.05
1	A	31	ASN	CA-CB-CG	5.22	117.82	112.60
1	D	50	MET	N-CA-C	5.21	116.22	109.65
1	A	61	ASN	N-CA-C	5.21	117.44	110.35
1	A	3	THR	CA-CB-OG1	-5.19	101.82	109.60
1	D	146	ASP	N-CA-C	-5.17	98.87	108.24
1	A	51	PRO	N-CA-C	-5.15	103.11	111.19
1	D	46	VAL	CB-CA-C	5.14	117.84	110.33
1	D	69	PHE	CA-C-O	-5.14	115.78	121.33
1	A	216	GLN	CA-C-O	-5.14	115.93	121.38
1	C	90	ALA	N-CA-CB	-5.13	104.84	111.35
1	C	116	HIS	CA-C-O	5.12	127.03	120.57
1	D	192	VAL	CB-CA-C	-5.12	103.15	110.12
1	B	209	SER	CA-C-N	5.12	128.58	122.03
1	B	209	SER	C-N-CA	5.12	128.58	122.03
1	C	178	VAL	CA-C-O	-5.12	115.05	120.53
1	D	192	VAL	O-C-N	5.11	128.29	123.03
1	D	222	SER	CA-C-O	-5.11	115.77	121.23
1	A	105	THR	N-CA-C	-5.10	107.06	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	10	SER	N-CA-CB	5.08	120.28	111.39
1	C	123	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	50	MET	CA-CB-CG	-5.07	103.95	114.10
1	D	15	ASN	O-C-N	5.05	126.87	121.12
1	B	51	PRO	N-CA-CB	5.04	108.01	103.33
1	B	73	MET	CA-CB-CG	-5.03	104.04	114.10
1	C	59	THR	CA-CB-OG1	-5.03	102.06	109.60
1	B	180	ASN	CB-CG-OD1	-5.02	110.77	120.80
1	D	36	ASN	CA-CB-CG	-5.00	107.60	112.60

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	1743	0	1699	25	0
1	B	1743	0	1699	18	0
1	C	1743	0	1699	31	0
1	D	1743	0	1699	39	0
2	E	23	0	21	1	0
2	F	23	0	20	2	0
2	H	23	0	21	0	0
3	G	23	0	21	1	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	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	147	0	0	3	0
6	B	165	0	0	1	0
6	C	122	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	129	0	0	5	0
All	All	7635	0	6879	109	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 8.

All (109) 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:37:LEU:HG	1:D:76:ILE:HD13	1.55	0.87
1:B:111:THR:HG22	1:B:112:LYS:HD3	1.62	0.79
1:A:15:ASN:HD22	1:A:16:PRO:HD2	1.49	0.78
1:C:77:LYS:H	1:C:77:LYS:HD2	1.50	0.76
1:C:15:ASN:HD22	1:C:16:PRO:HD2	1.51	0.75
1:A:182:ASN:HD21	1:A:184:ASP:HB2	1.55	0.70
1:A:41:ASN:HD22	1:A:211:SER:HA	1.58	0.69
1:C:182:ASN:HD21	1:C:184:ASP:HB2	1.58	0.68
1:D:175:SER:HB3	1:D:189:ALA:HB2	1.76	0.67
1:B:182:ASN:ND2	1:B:184:ASP:H	1.93	0.66
1:C:77:LYS:H	1:C:77:LYS:CD	2.05	0.66
1:D:10:SER:HB2	1:D:30:GLY:HA3	1.82	0.62
1:D:62:VAL:HG21	6:D:328:HOH:O	1.99	0.62
1:A:34:LEU:O	1:A:44:GLY:HA3	2.00	0.61
1:D:90:ALA:HB1	1:D:91:PRO:HD2	1.83	0.61
1:D:15:ASN:HD22	1:D:16:PRO:HD2	1.65	0.61
1:D:60:GLY:HA2	1:D:195:LYS:HZ2	1.68	0.59
1:D:25:THR:HG22	6:D:271:HOH:O	2.04	0.58
1:A:50:MET:HG3	6:B:248:HOH:O	2.02	0.57
1:A:15:ASN:HD22	1:A:16:PRO:CD	2.17	0.57
1:C:149:LYS:HG2	1:C:188:ILE:HD11	1.87	0.57
1:A:37:LEU:HG	1:A:76:ILE:HD13	1.87	0.57
1:D:34:LEU:O	1:D:44:GLY:HA3	2.05	0.57
1:B:34:LEU:O	1:B:44:GLY:HA3	2.05	0.57
1:D:90:ALA:HB1	1:D:91:PRO:CD	2.35	0.56
1:D:133:PRO:HD2	1:D:137:HIS:CE1	2.40	0.56
1:A:133:PRO:HD2	1:A:137:HIS:CE1	2.41	0.56
1:C:12:SER:HA	1:C:26:VAL:HG11	1.88	0.55
1:C:32:ILE:O	1:C:219:LEU:HA	2.06	0.55
1:C:10:SER:HB3	1:D:74:LYS:HE2	1.88	0.55
1:D:32:ILE:HD13	1:D:46:VAL:HG21	1.89	0.55
1:B:41:ASN:HD22	1:B:211:SER:HA	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ASN:ND2	1:C:16:PRO:HD2	2.21	0.54
1:D:10:SER:HA	6:D:245:HOH:O	2.07	0.54
1:D:19:ASN:ND2	1:D:203:LYS:NZ	2.57	0.53
1:A:173:THR:HG21	1:D:173:THR:HG21	1.89	0.53
1:C:32:ILE:HD13	1:C:46:VAL:HG21	1.90	0.53
1:C:74:LYS:HE2	1:D:10:SER:HB3	1.89	0.53
1:C:37:LEU:HG	1:C:76:ILE:HD13	1.89	0.53
1:D:43:VAL:HG12	1:D:96:ILE:HD13	1.90	0.53
1:D:60:GLY:HA2	1:D:195:LYS:NZ	2.25	0.51
1:B:51:PRO:HB3	1:B:92:GLU:HG3	1.93	0.51
1:C:113:GLY:O	1:C:144:SER:HA	2.11	0.51
1:C:198:LEU:HB3	1:C:199:PRO:HD2	1.93	0.50
1:D:19:ASN:HD21	1:D:203:LYS:HZ1	1.56	0.50
1:D:41:ASN:ND2	1:D:211:SER:HA	2.26	0.50
1:A:47:LEU:HD23	1:A:203:LYS:HB3	1.92	0.50
1:A:182:ASN:ND2	1:A:184:ASP:HB2	2.25	0.50
1:A:95:GLN:NE2	6:A:279:HOH:O	2.44	0.50
1:D:24:VAL:HG21	1:D:45:ARG:O	2.12	0.49
1:C:70:SER:HA	1:C:161:VAL:O	2.13	0.48
1:B:15:ASN:HD22	1:B:16:PRO:HD2	1.77	0.48
1:B:91:PRO:HB3	1:B:199:PRO:HG3	1.95	0.48
1:D:113:GLY:O	1:D:144:SER:HA	2.13	0.48
1:A:32:ILE:HD13	1:A:46:VAL:HG21	1.95	0.48
1:C:41:ASN:HD22	1:C:41:ASN:N	2.11	0.48
1:C:37:LEU:HB2	6:C:334:HOH:O	2.12	0.48
1:D:140:ILE:HD13	1:D:174:LEU:HD23	1.96	0.48
1:B:90:ALA:HB1	1:B:91:PRO:HD2	1.96	0.48
1:D:50:MET:HG2	1:D:51:PRO:HD2	1.94	0.48
1:D:175:SER:HB3	1:D:189:ALA:CB	2.44	0.48
1:D:214:GLY:O	1:D:215:ARG:HG2	2.15	0.47
1:D:19:ASN:ND2	1:D:203:LYS:HZ1	2.12	0.47
1:D:59:THR:C	1:D:61:ASN:H	2.23	0.47
1:C:68:SER:HA	1:C:163:VAL:O	2.15	0.47
1:C:90:ALA:HB1	1:C:91:PRO:HD2	1.96	0.47
1:B:39:LYS:HE2	1:B:39:LYS:HB3	1.66	0.46
1:D:203:LYS:HA	6:D:246:HOH:O	2.14	0.46
1:B:125:TYR:CZ	2:F:2:GAL:H5	2.50	0.46
1:D:32:ILE:O	1:D:219:LEU:HA	2.16	0.46
1:A:20:PHE:HD1	1:A:24:VAL:HG11	1.81	0.45
1:A:214:GLY:HA3	2:E:2:GAL:H61	1.99	0.45
1:D:73:MET:HA	1:D:217:ILE:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLY:HA3	2:F:2:GAL:H61	1.97	0.45
1:B:6:PHE:CZ	1:B:225:PHE:HB3	2.52	0.45
1:D:159:ALA:HB1	1:D:181:ASP:HB2	1.99	0.45
1:C:50:MET:HA	1:C:51:PRO:HD3	1.72	0.45
1:A:1:ALA:HB2	6:A:341:HOH:O	2.17	0.44
1:D:181:ASP:HB3	6:D:308:HOH:O	2.16	0.44
1:A:5:SER:HA	1:A:225:PHE:O	2.17	0.44
1:C:18:ILE:CG2	1:C:46:VAL:HG22	2.47	0.44
1:B:121:GLU:OE1	1:B:141:ASP:OD2	2.36	0.43
1:D:81:PRO:HA	1:D:216:GLN:HB3	2.00	0.43
1:A:100:SER:HA	6:A:357:HOH:O	2.18	0.43
1:A:7:ASN:OD1	1:A:224:SER:HB3	2.19	0.43
1:A:41:ASN:ND2	1:A:211:SER:HA	2.29	0.43
1:B:156:VAL:HG12	1:B:159:ALA:HB2	2.00	0.43
1:C:77:LYS:CD	1:C:77:LYS:N	2.79	0.43
1:C:127:ASN:HB3	1:C:129:GLU:CD	2.43	0.43
1:D:39:LYS:HE2	1:D:39:LYS:HB3	1.66	0.43
1:C:217:ILE:HG22	1:C:219:LEU:HG	2.01	0.42
1:C:5:SER:HA	1:C:225:PHE:O	2.20	0.42
1:D:151:VAL:CG2	1:D:152:PRO:HD2	2.50	0.41
1:C:81:PRO:HA	1:C:216:GLN:HB3	2.02	0.41
1:A:121:GLU:OE2	1:A:123:ASP:HB2	2.20	0.41
1:C:41:ASN:HA	1:C:210:GLY:O	2.21	0.41
1:C:125:TYR:CZ	3:G:2:GAL:H5	2.56	0.41
1:C:90:ALA:HB1	1:C:91:PRO:CD	2.49	0.41
1:C:203:LYS:HA	6:C:362:HOH:O	2.20	0.41
1:A:96:ILE:HA	1:A:97:PRO:HD3	1.96	0.41
1:A:32:ILE:O	1:A:219:LEU:HA	2.21	0.41
1:A:41:ASN:HA	1:A:210:GLY:O	2.22	0.40
1:B:41:ASN:ND2	1:B:211:SER:HA	2.36	0.40
1:B:198:LEU:HB3	1:B:199:PRO:HD2	2.03	0.40
1:A:132:ASP:HA	1:A:133:PRO:HD3	1.96	0.40
1:B:3:THR:HA	1:B:227:SER:O	2.22	0.40
1:B:5:SER:HA	1:B:225:PHE:O	2.21	0.40
1:C:74:LYS:CE	1:D:10:SER:HB3	2.51	0.40
1:D:174:LEU:O	1:D:189:ALA:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/236 (98%)	223 (97%)	6 (3%)	1 (0%)	30	31
1	B	230/236 (98%)	224 (97%)	5 (2%)	1 (0%)	30	31
1	C	230/236 (98%)	217 (94%)	13 (6%)	0	100	100
1	D	230/236 (98%)	220 (96%)	10 (4%)	0	100	100
All	All	920/944 (98%)	884 (96%)	34 (4%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	81	PRO
1	A	81	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/201 (98%)	193 (98%)	4 (2%)	48	59
1	B	197/201 (98%)	191 (97%)	6 (3%)	36	45
1	C	197/201 (98%)	188 (95%)	9 (5%)	24	28
1	D	197/201 (98%)	182 (92%)	15 (8%)	12	10
All	All	788/804 (98%)	754 (96%)	34 (4%)	26	31

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	53	ARG
1	A	54	ILE
1	A	182	ASN
1	B	53	ARG
1	B	54	ILE
1	B	64	SER
1	B	111	THR
1	B	148	VAL
1	B	182	ASN
1	C	25	THR
1	C	46	VAL
1	C	77	LYS
1	C	112	LYS
1	C	148	VAL
1	C	182	ASN
1	C	185	ILE
1	C	230	ILE
1	C	232	THR
1	D	5	SER
1	D	15	ASN
1	D	24	VAL
1	D	25	THR
1	D	37	LEU
1	D	39	LYS
1	D	50	MET
1	D	57	SER
1	D	68	SER
1	D	97	PRO
1	D	112	LYS
1	D	140	ILE
1	D	182	ASN
1	D	212	LEU
1	D	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	19	ASN
1	A	33	GLN
1	A	41	ASN
1	A	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	GLN
1	A	180	ASN
1	A	182	ASN
1	A	216	GLN
1	B	9	ASN
1	B	15	ASN
1	B	31	ASN
1	B	41	ASN
1	B	61	ASN
1	B	95	GLN
1	B	182	ASN
1	B	216	GLN
1	C	15	ASN
1	C	31	ASN
1	C	33	GLN
1	C	41	ASN
1	C	61	ASN
1	C	182	ASN
1	D	15	ASN
1	D	19	ASN
1	D	33	GLN
1	D	41	ASN
1	D	61	ASN
1	D	95	GLN
1	D	182	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](#)

8 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	GLC	E	1	2	12,12,12	1.09	2 (16%)	17,17,17	1.77	5 (29%)
2	GAL	E	2	2	11,11,12	0.87	0	15,15,17	1.32	1 (6%)
2	GLC	F	1	2	12,12,12	1.05	0	17,17,17	2.65	7 (41%)
2	GAL	F	2	2	11,11,12	0.73	0	15,15,17	1.12	1 (6%)
3	BGC	G	1	3	12,12,12	1.25	2 (16%)	17,17,17	1.72	4 (23%)
3	GAL	G	2	3	11,11,12	0.92	1 (9%)	15,15,17	1.74	6 (40%)
2	GLC	H	1	2	12,12,12	0.91	0	17,17,17	2.31	8 (47%)
2	GAL	H	2	2	11,11,12	0.81	0	15,15,17	1.18	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	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
3	BGC	G	1	3	-	0/2/22/22	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	BGC	O1-C1	2.66	1.47	1.39
2	E	1	GLC	O1-C1	2.37	1.47	1.39
3	G	2	GAL	O5-C1	-2.36	1.39	1.43
3	G	1	BGC	O2-C2	2.32	1.48	1.43
2	E	1	GLC	O2-C2	2.28	1.48	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	GLC	O5-C1-C2	4.85	118.82	110.30
2	F	1	GLC	O2-C2-C3	4.63	121.30	110.38
2	F	1	GLC	C1-C2-C3	4.56	119.66	110.36
2	H	1	GLC	O2-C2-C1	4.44	119.48	109.25
2	F	1	GLC	C1-O5-C5	4.16	121.69	113.65
2	H	1	GLC	C1-O5-C5	4.11	121.61	113.65
3	G	1	BGC	C3-C4-C5	4.09	117.64	110.23
2	H	1	GLC	C3-C4-C5	3.96	117.40	110.23
2	E	1	GLC	O3-C3-C4	-3.83	101.35	110.38
3	G	1	BGC	C1-C2-C3	3.34	117.16	110.36
2	F	1	GLC	O2-C2-C1	3.27	116.80	109.25
2	E	1	GLC	O4-C4-C5	3.22	117.24	109.32
2	F	2	GAL	C1-O5-C5	3.16	116.42	112.19
2	H	1	GLC	O2-C2-C3	3.03	117.51	110.38
2	H	1	GLC	C1-C2-C3	3.01	116.50	110.36
2	F	1	GLC	C3-C4-C5	2.97	115.61	110.23
3	G	2	GAL	C6-C5-C4	2.92	120.20	113.02
2	E	2	GAL	O4-C4-C3	2.87	117.15	110.38
2	E	1	GLC	C1-O5-C5	2.76	118.99	113.65
2	F	1	GLC	O3-C3-C4	-2.73	103.93	110.38
3	G	2	GAL	O3-C3-C2	2.51	115.17	110.05
2	H	1	GLC	O3-C3-C4	-2.48	104.52	110.38
3	G	2	GAL	O5-C1-C2	2.46	116.65	110.79
2	E	1	GLC	O1-C1-C2	-2.41	101.98	108.98
3	G	1	BGC	O5-C1-C2	2.37	114.47	110.30
3	G	2	GAL	O4-C4-C3	2.32	115.84	110.38
3	G	2	GAL	C2-C3-C4	2.29	114.89	110.86
3	G	2	GAL	O2-C2-C3	2.29	114.89	110.15
2	H	2	GAL	O2-C2-C3	2.28	114.87	110.15
3	G	1	BGC	O3-C3-C2	-2.18	105.25	110.38
2	H	1	GLC	O4-C4-C5	2.10	114.49	109.32
2	H	1	GLC	O5-C1-C2	2.07	113.93	110.30
2	E	1	GLC	O2-C2-C3	2.03	115.17	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

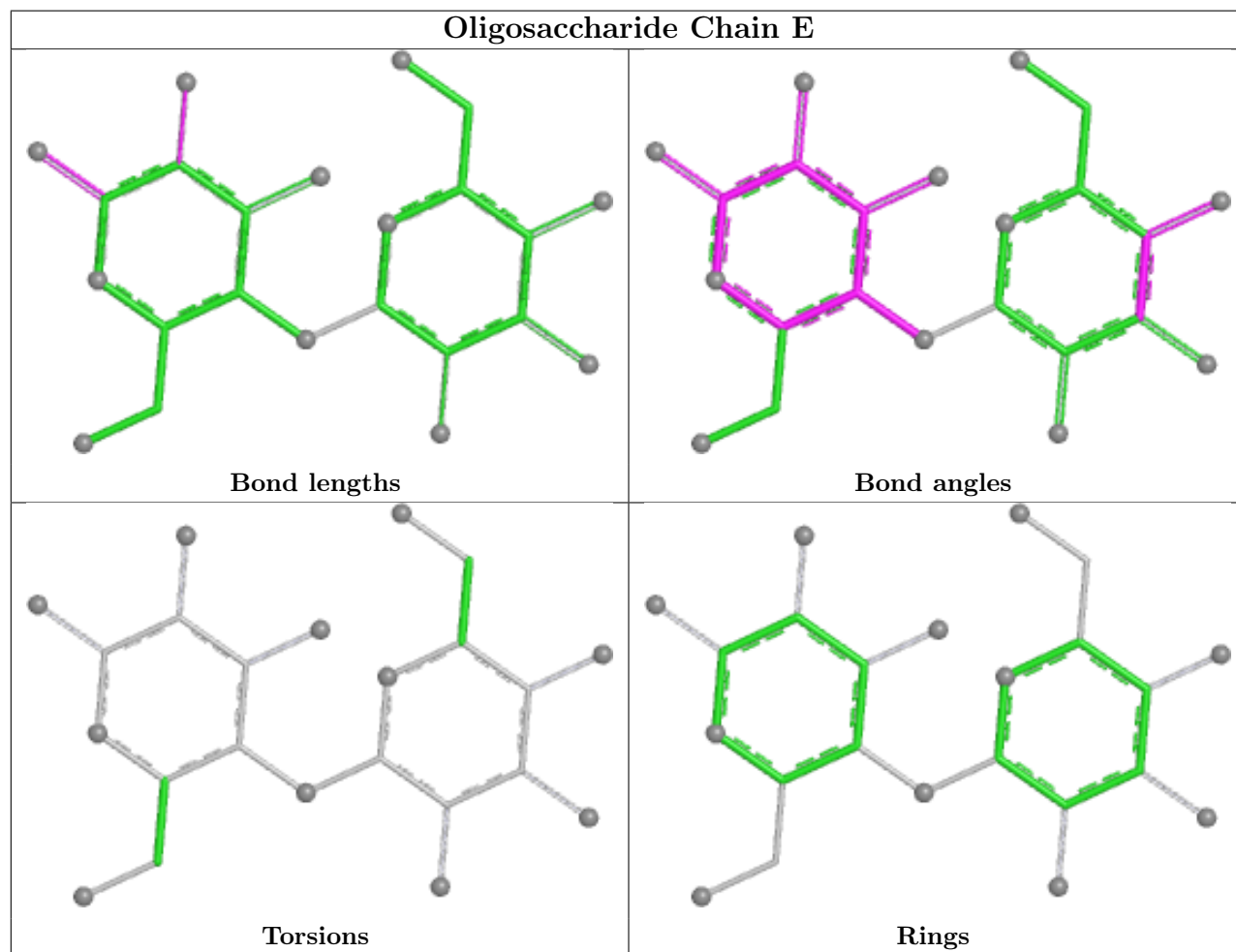
Mol	Chain	Res	Type	Atoms
2	H	1	GLC	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6

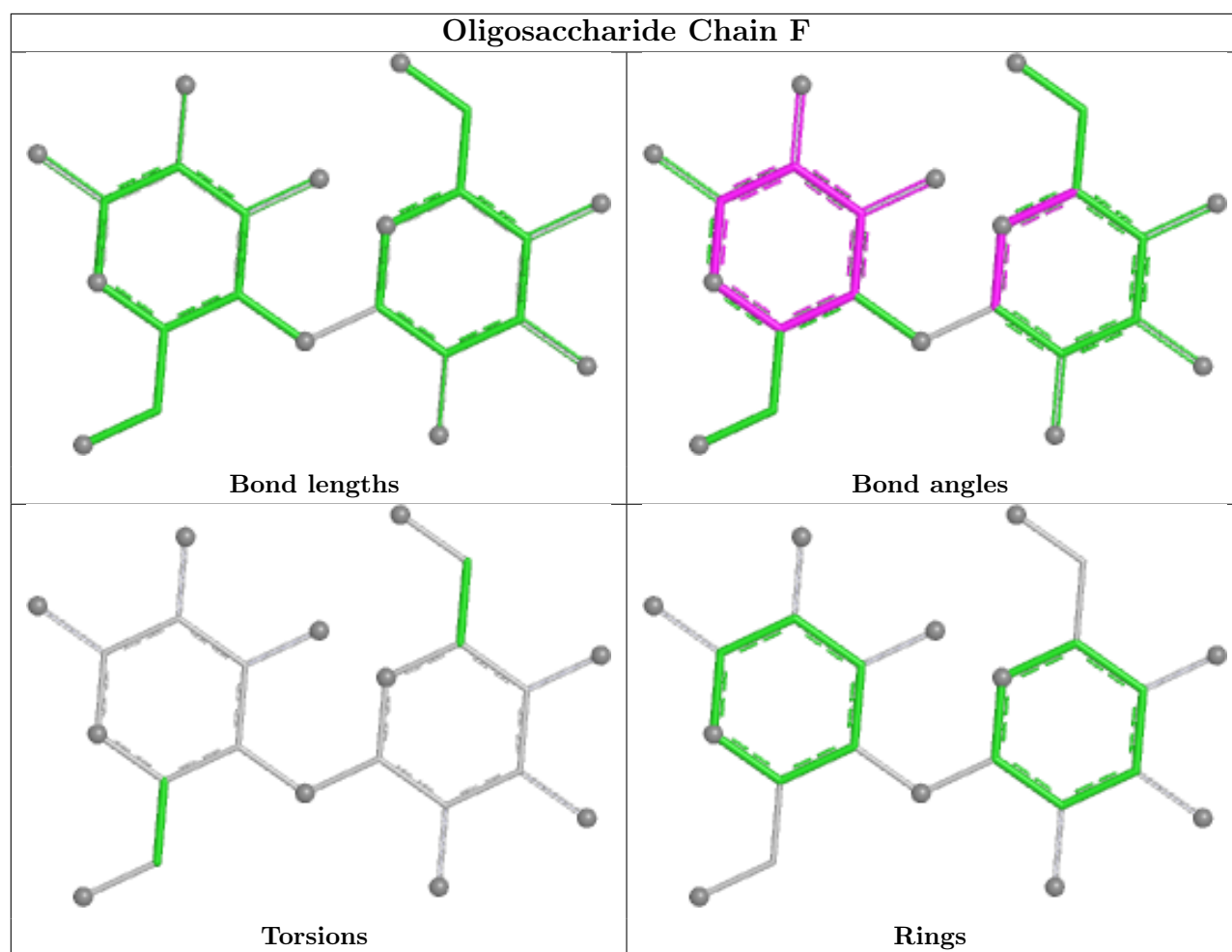
There are no ring outliers.

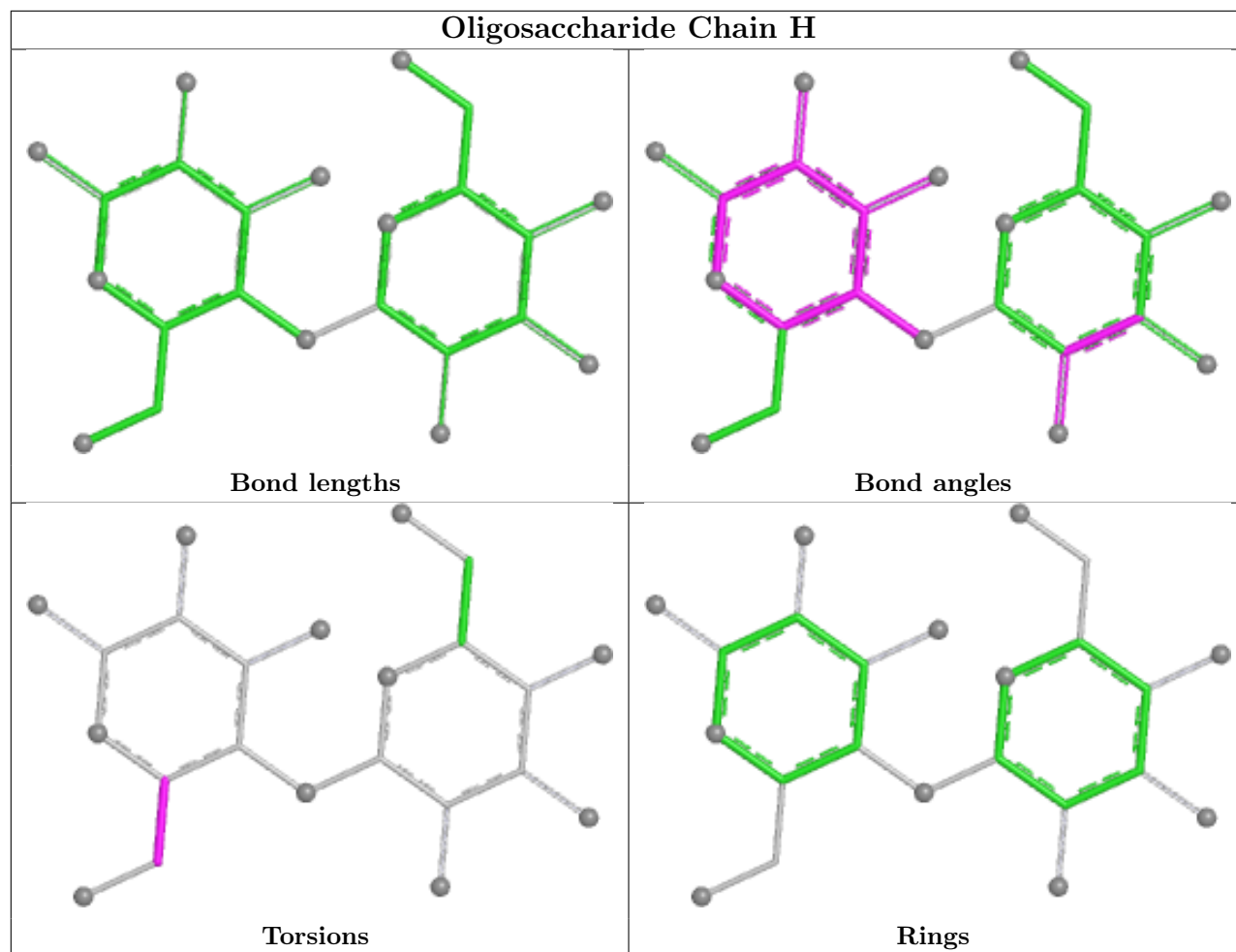
3 monomers are involved in 4 short contacts:

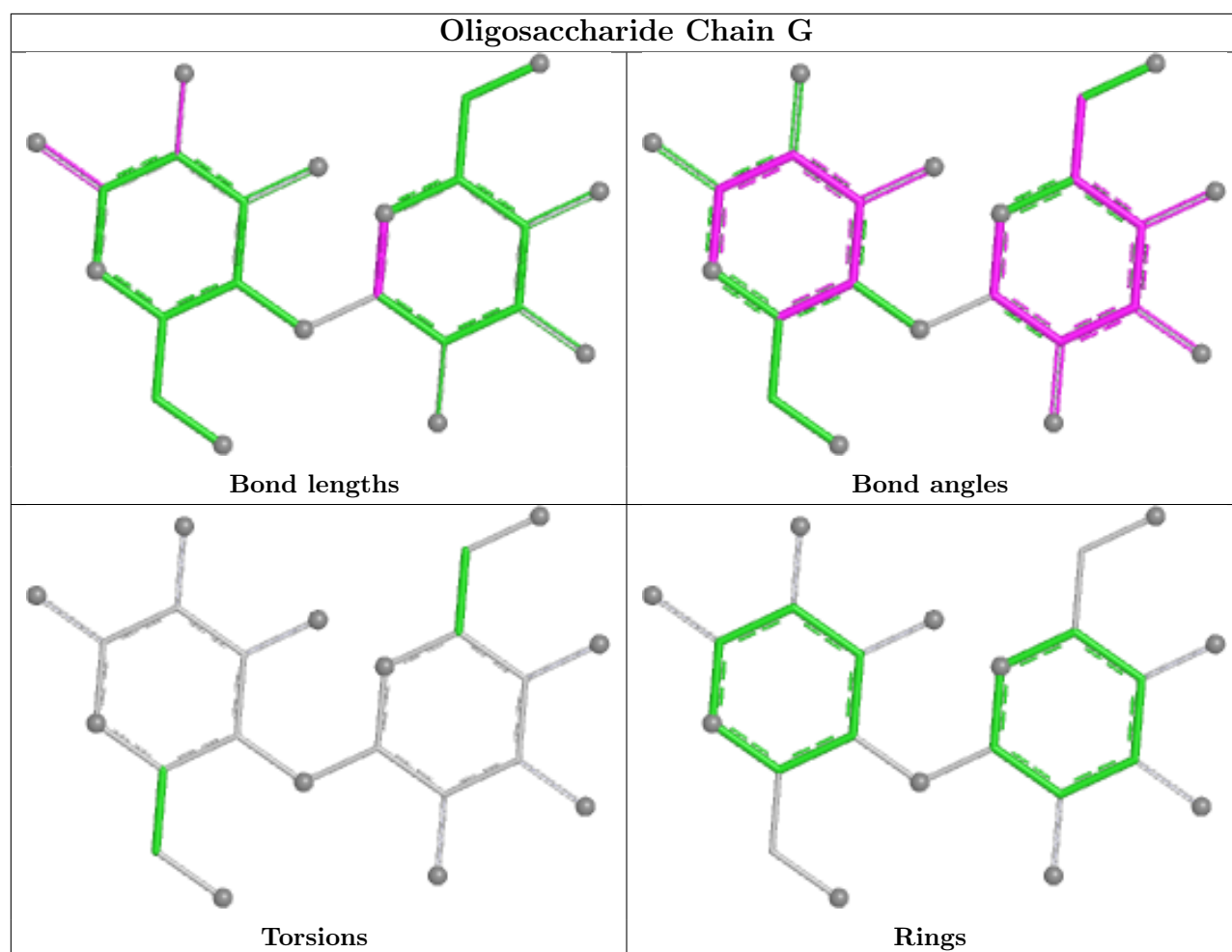
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GAL	2	0
3	G	2	GAL	1	0
2	E	2	GAL	1	0

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









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 [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	232/236 (98%)	-0.77	0 100 100	7, 18, 35, 56	0
1	B	232/236 (98%)	-0.82	1 (0%) 88 89	7, 17, 33, 60	0
1	C	232/236 (98%)	-0.57	1 (0%) 88 89	8, 22, 38, 54	0
1	D	232/236 (98%)	-0.53	0 100 100	8, 19, 40, 62	0
All	All	928/944 (98%)	-0.67	2 (0%) 91 92	7, 19, 37, 62	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	THR	2.7
1	C	232	THR	2.4

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.

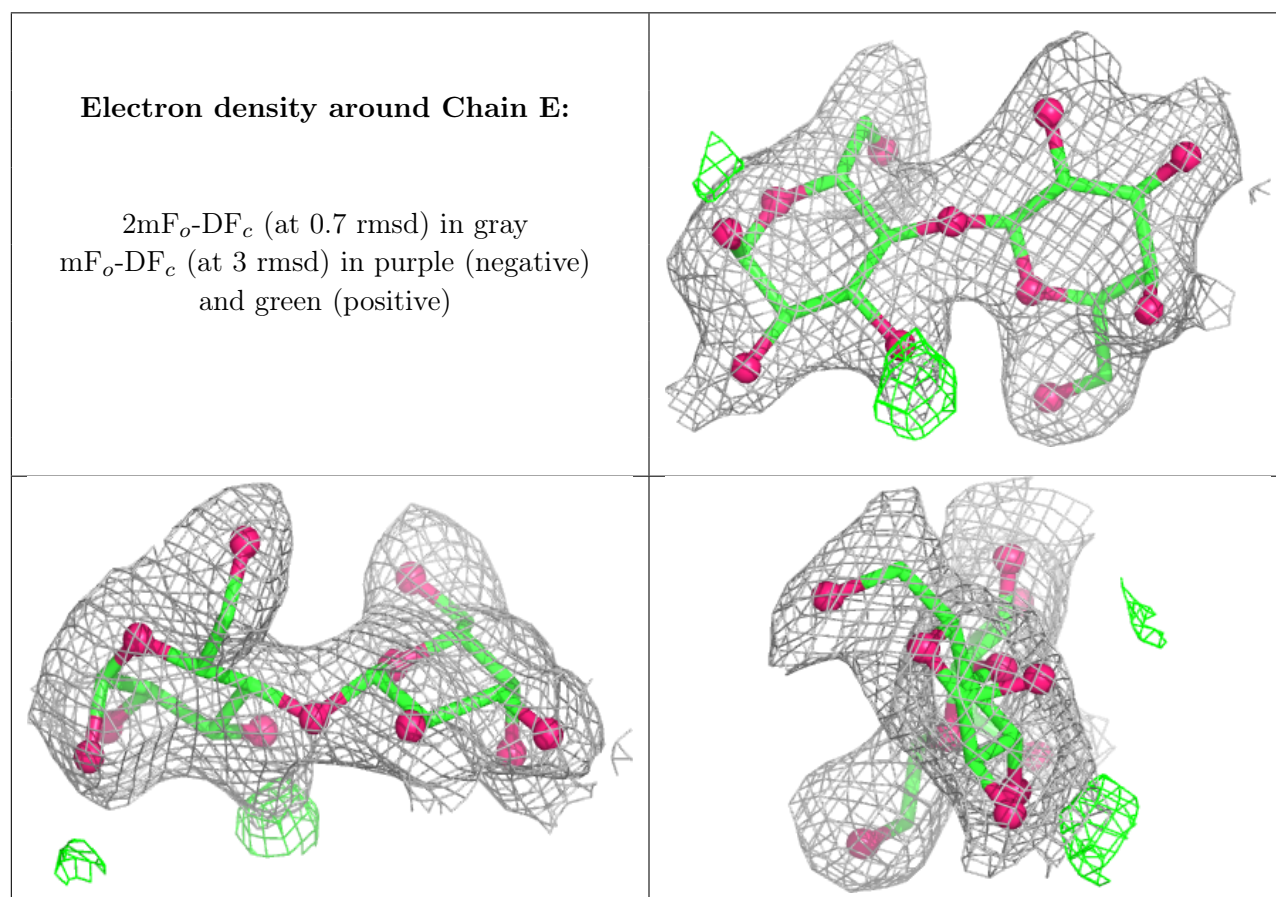
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	G	1	12/12	0.78	0.09	47,51,55,57	0
2	GLC	H	1	12/12	0.81	0.10	37,47,51,53	0
3	GAL	G	2	11/12	0.83	0.10	38,42,44,47	0
2	GLC	F	1	12/12	0.86	0.09	30,41,46,51	0
2	GLC	E	1	12/12	0.92	0.07	29,37,40,42	0

Continued on next page...

Continued from previous page...

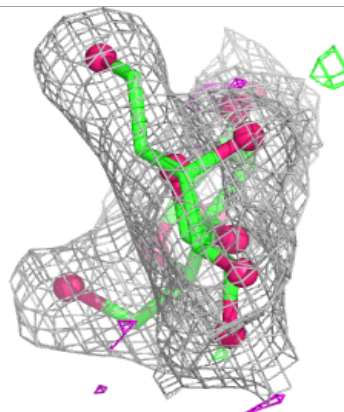
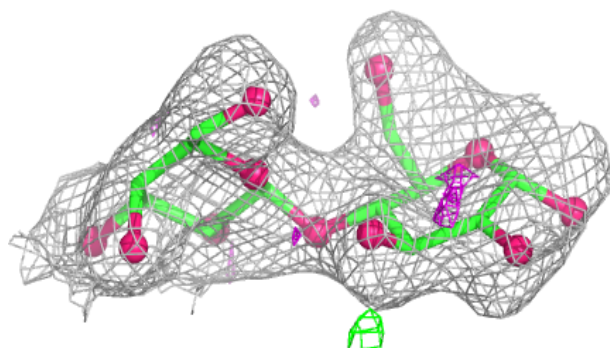
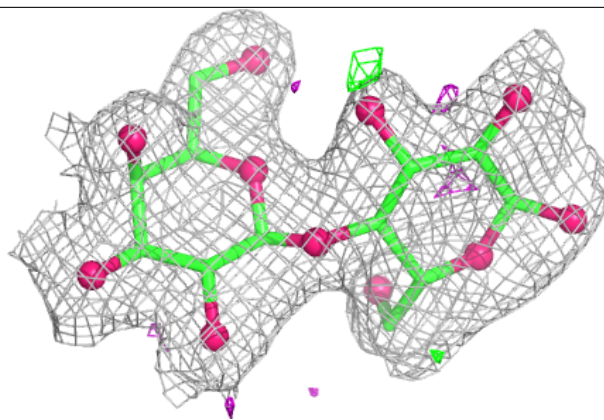
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	H	2	11/12	0.93	0.07	23,26,32,34	0
2	GAL	E	2	11/12	0.96	0.06	18,20,23,24	0
2	GAL	F	2	11/12	0.97	0.05	17,20,23,25	0

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

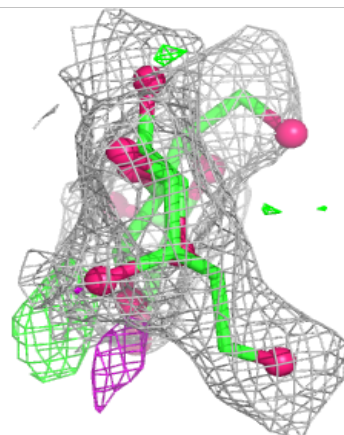
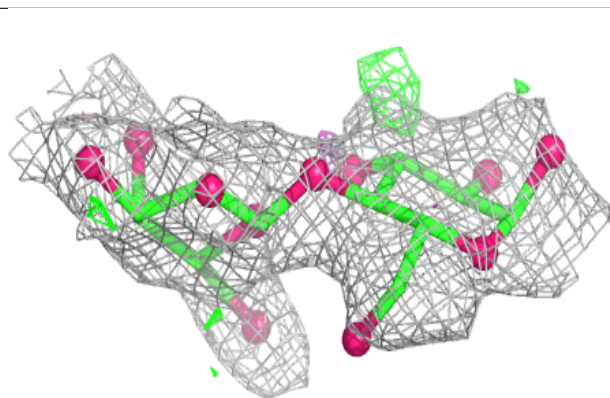
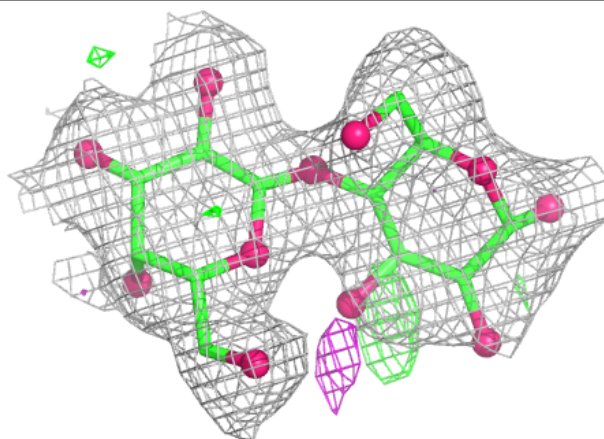


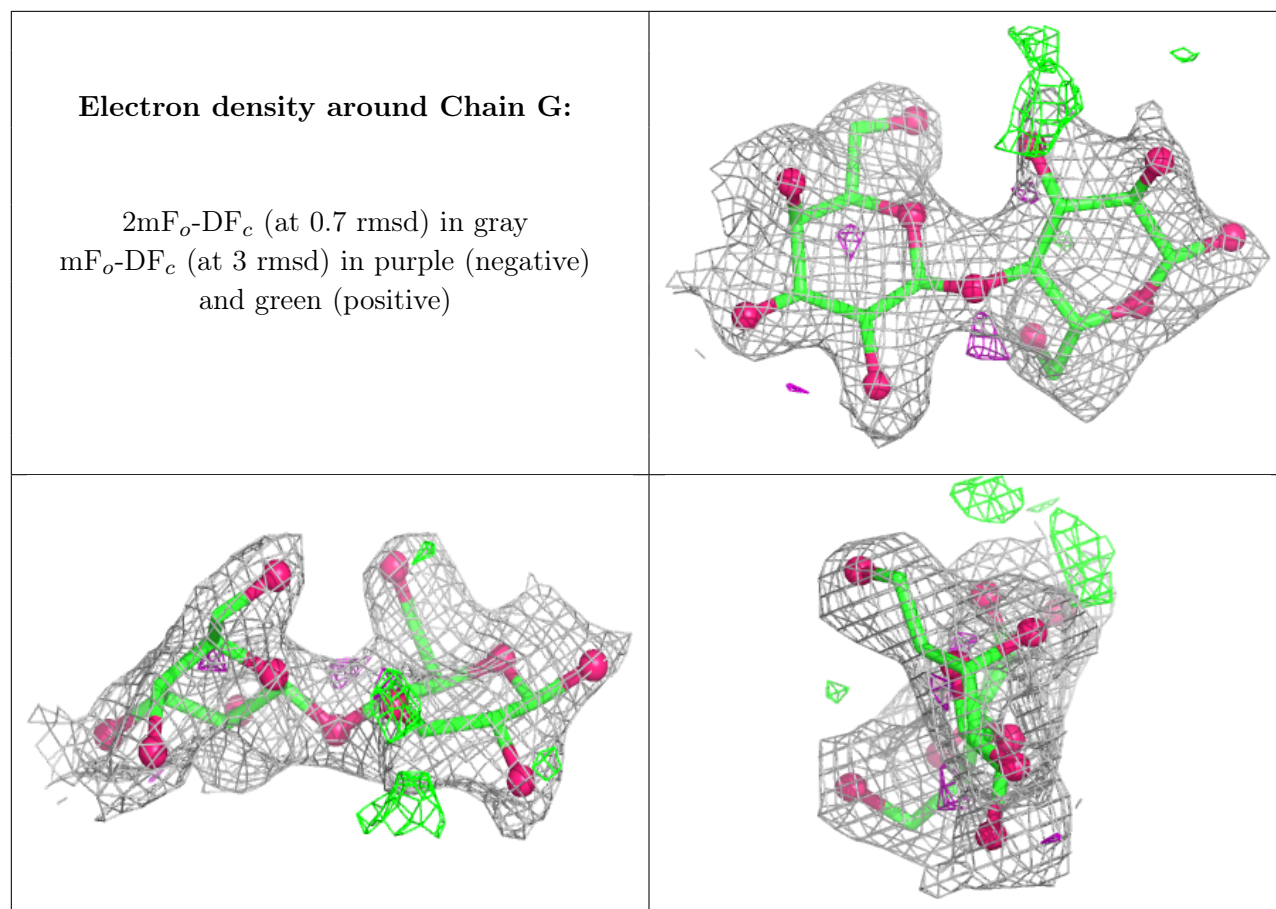
Electron density around Chain F:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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
5	MN	C	238	1/1	0.87	0.10	37,37,37,37	0
5	MN	B	238	1/1	0.93	0.09	34,34,34,34	0
4	CA	D	237	1/1	0.93	0.04	17,17,17,17	0
4	CA	C	237	1/1	0.95	0.03	18,18,18,18	0
5	MN	D	238	1/1	0.95	0.13	35,35,35,35	0
5	MN	A	238	1/1	0.97	0.08	35,35,35,35	0
4	CA	B	237	1/1	0.98	0.03	16,16,16,16	0
4	CA	A	237	1/1	0.99	0.04	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.