



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:36 AM UTC

PDB ID : 1SL6 / pdb_00001sl6
Title : Crystal Structure of a fragment of DC-SIGNR (containing the carbohydrate recognition domain and two repeats of the neck) complexed with Lewis-x.
Authors : Guo, Y.; Feinberg, H.; Conroy, E.; Mitchell, D.A.; Alvarez, R.; Blixt, O.; Taylor, M.E.; Weis, W.I.; Drickamer, K.
Deposited on : 2004-03-05
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

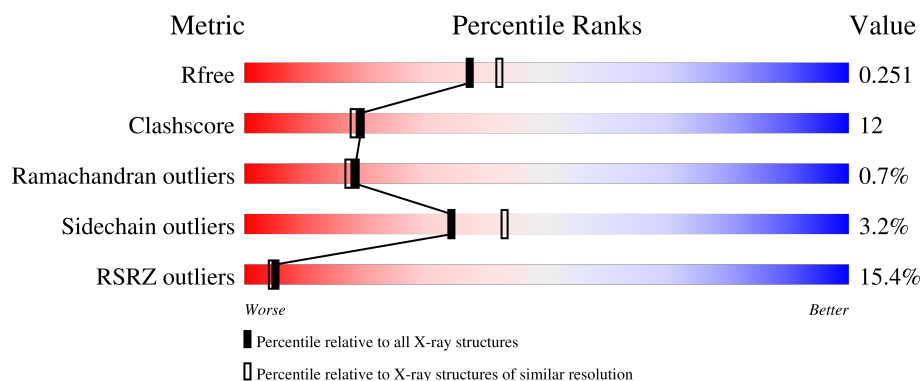
1 Overall quality at a glance

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))
R_{free}	180053	1898 (2.26-2.26)
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	184	11% 67% 21% .. 9%
1	B	184	15% 68% 21% .. 9%
1	C	184	13% 66% 22% . 9%
1	D	184	14% 62% 27% .. 9%
1	E	184	15% 67% 21% . 9%

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Mol	Chain	Length	Quality of chain
1	F	184	
2	G	3	
2	H	3	
2	I	3	
2	J	3	
2	K	3	
2	L	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDG	H	1	-	-	-	X

2 Entry composition [i](#)

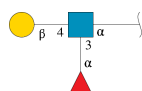
There are 4 unique types of molecules in this entry. The entry contains 8732 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 C-type lectin DC-SIGNR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1374	857	240	267	10			
1	B	168	Total	C	N	O	S	0	0	0
			1380	860	243	267	10			
1	C	168	Total	C	N	O	S	0	0	0
			1380	860	243	267	10			
1	D	168	Total	C	N	O	S	0	0	0
			1374	858	240	266	10			
1	E	168	Total	C	N	O	S	0	0	0
			1374	858	240	266	10			
1	F	168	Total	C	N	O	S	0	0	0
			1374	858	240	266	10			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	H	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	I	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	J	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	K	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	L	3	Total	C	N	O	0	0	0
			36	20	1	15			

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

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

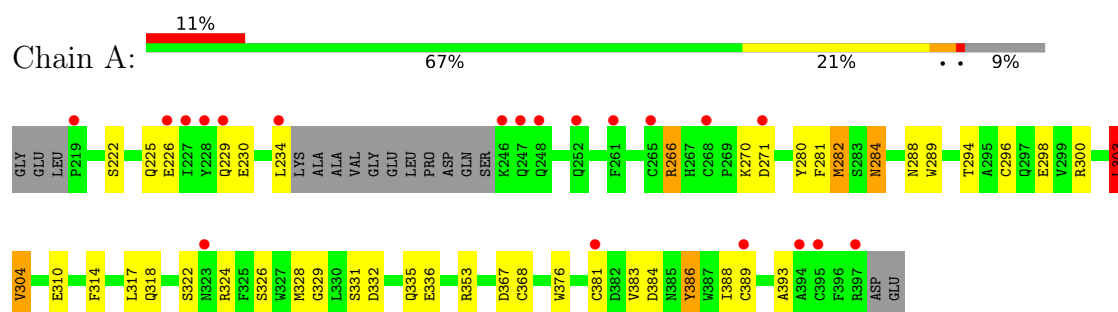
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total 42	O 42	0	0
4	B	34	Total 34	O 34	0	0
4	C	28	Total 28	O 28	0	0
4	D	37	Total 37	O 37	0	0
4	E	49	Total 49	O 49	0	0
4	F	46	Total 46	O 46	0	0

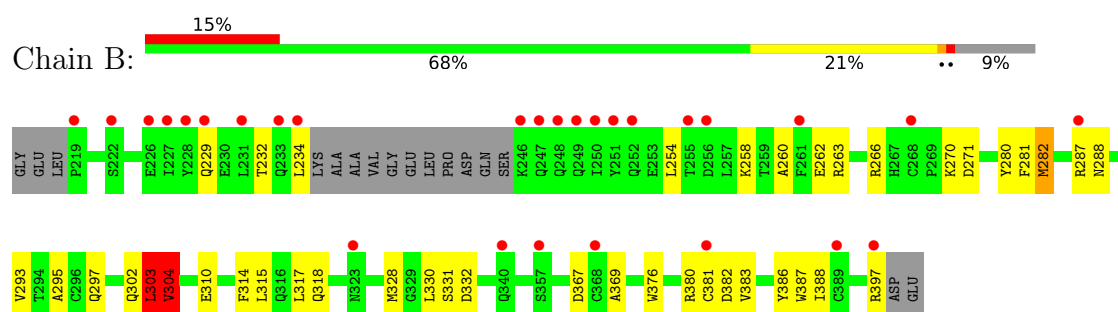
3 Residue-property plots [i](#)

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.

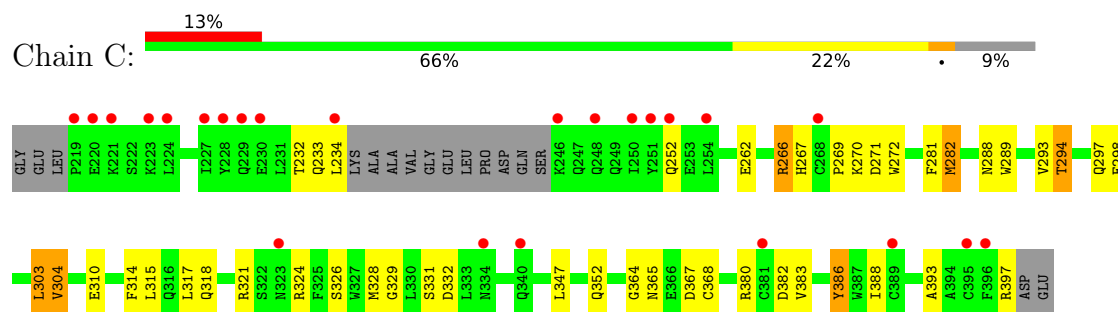
• Molecule 1: C-type lectin DC-SIGNR



• Molecule 1: C-type lectin DC-SIGNR

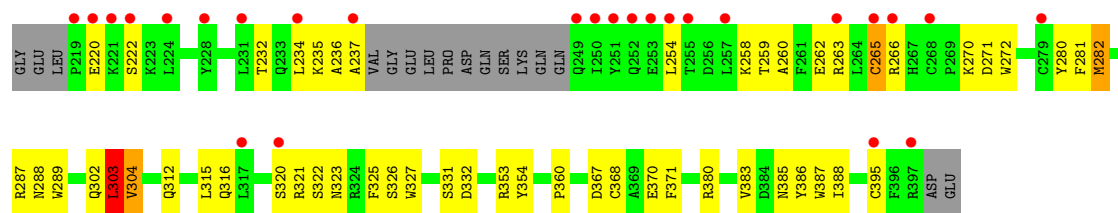


• Molecule 1: C-type lectin DC-SIGNR

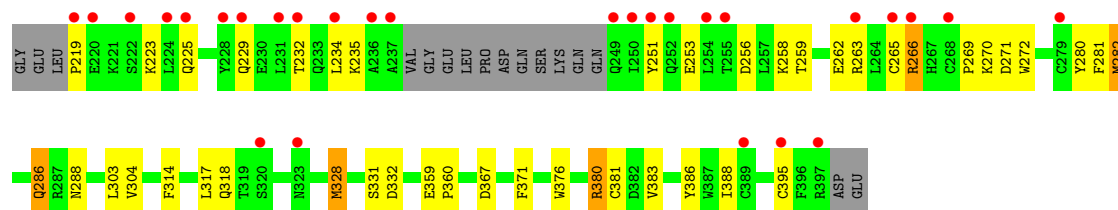


• Molecule 1: C-type lectin DC-SIGNR

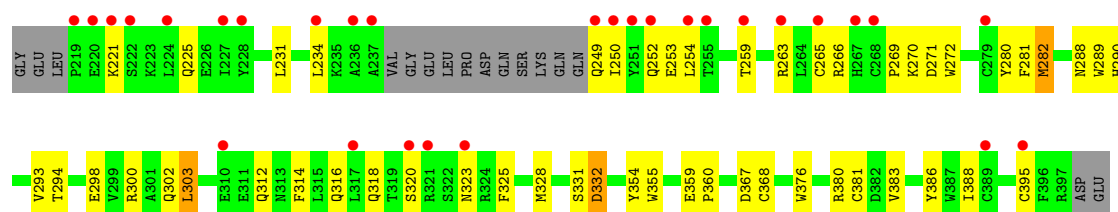




• Molecule 1: C-type lectin DC-SIGNR



• Molecule 1: C-type lectin DC-SIGNR



• Molecule 2: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose



• Molecule 2: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose



• Molecule 2: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose





- Molecule 2: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain J:  100%



- Molecule 2: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain K:  67% 33%



- Molecule 2: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain L:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.75Å 153.75Å 128.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.96 – 2.25 41.96 – 2.25	Depositor EDS
% Data completeness (in resolution range)	87.6 (41.96-2.25) 87.7 (41.96-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.256 (Not available) , 0.251	Depositor DCC
R_{free} test set	6701 reflections (8.35%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8732	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: FUC, NDG, CA, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/1410	0.82	3/1910 (0.2%)
1	B	0.37	0/1416	0.87	3/1917 (0.2%)
1	C	0.36	0/1416	0.84	3/1917 (0.2%)
1	D	0.36	0/1410	0.90	7/1909 (0.4%)
1	E	0.39	0/1410	0.87	4/1909 (0.2%)
1	F	0.38	0/1410	0.90	6/1909 (0.3%)
All	All	0.37	0/8472	0.87	26/11471 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	TYR	N-CA-C	-7.25	101.49	110.41
1	F	386	TYR	N-CA-C	-7.19	100.84	110.55
1	C	386	TYR	N-CA-C	-6.90	101.23	110.55
1	E	386	TYR	N-CA-C	-6.58	102.05	110.53
1	D	386	TYR	N-CA-C	-6.54	102.09	110.53
1	B	303	LEU	N-CA-C	-6.29	100.87	110.30
1	A	303	LEU	N-CA-C	-6.22	100.97	110.30
1	B	386	TYR	N-CA-C	-6.17	102.22	110.55
1	B	304	VAL	N-CA-C	5.94	121.70	109.34
1	F	325	PHE	N-CA-C	-5.75	101.14	109.59
1	D	325	PHE	N-CA-C	-5.69	101.22	109.59
1	F	231	LEU	N-CA-C	-5.39	105.48	111.36
1	C	328	MET	N-CA-C	-5.36	101.22	109.52
1	E	328	MET	N-CA-C	-5.35	101.40	109.85
1	E	371	PHE	N-CA-C	-5.35	101.26	109.76
1	D	304	VAL	N-CA-C	5.28	120.32	109.34
1	D	254	LEU	N-CA-C	-5.26	106.00	112.90
1	F	293	VAL	N-CA-C	-5.21	105.42	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	VAL	N-CA-C	5.20	120.16	109.34
1	F	254	LEU	N-CA-C	-5.18	106.96	113.28
1	D	265	CYS	N-CA-C	5.16	117.53	108.56
1	D	303	LEU	N-CA-C	-5.14	102.60	110.30
1	C	364	GLY	N-CA-C	-5.12	107.20	115.08
1	E	286	GLN	N-CA-C	5.08	118.02	110.14
1	F	332	ASP	N-CA-C	-5.04	104.10	111.30
1	D	371	PHE	N-CA-C	-5.00	101.81	109.76

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	1374	0	1250	28	0
1	B	1380	0	1257	28	0
1	C	1380	0	1259	35	0
1	D	1374	0	1259	33	0
1	E	1374	0	1259	33	0
1	F	1374	0	1259	42	0
2	G	36	0	28	2	0
2	H	36	0	28	0	0
2	I	36	0	28	0	0
2	J	36	0	28	0	0
2	K	36	0	28	0	0
2	L	36	0	28	1	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
4	A	42	0	0	1	0
4	B	34	0	0	0	0
4	C	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	37	0	0	0	0
4	E	49	0	0	1	0
4	F	46	0	0	1	0
All	All	8732	0	7711	189	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 12.

All (189) 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:E:282:MET:HE2	1:E:388:ILE:HG23	1.41	1.01
1:F:282:MET:HE2	1:F:388:ILE:HG23	1.45	0.98
1:A:296:CYS:SG	1:A:389:CYS:HB3	2.05	0.95
1:D:280:TYR:HB3	1:D:282:MET:HE1	1.47	0.94
1:D:282:MET:HE2	1:D:388:ILE:HG23	1.51	0.93
1:C:282:MET:HE2	1:C:388:ILE:HG12	1.55	0.89
1:D:281:PHE:C	1:D:282:MET:HE3	2.02	0.85
1:E:281:PHE:C	1:E:282:MET:HE3	2.03	0.83
1:A:282:MET:HE2	1:A:388:ILE:HG23	1.66	0.77
1:E:280:TYR:HB3	1:E:282:MET:HE1	1.67	0.76
1:F:280:TYR:HB3	1:F:282:MET:HE1	1.68	0.75
1:B:282:MET:N	1:B:282:MET:HE3	2.03	0.73
1:F:281:PHE:C	1:F:282:MET:HE3	2.14	0.73
1:B:397:ARG:HH12	1:E:270:LYS:HG2	1.54	0.73
1:B:397:ARG:NH1	1:E:270:LYS:HG2	2.05	0.71
1:F:380:ARG:HG3	1:F:380:ARG:HH11	1.56	0.71
1:B:281:PHE:C	1:B:282:MET:HE3	2.17	0.70
1:B:282:MET:HE2	1:B:388:ILE:HG23	1.73	0.69
1:C:281:PHE:C	1:C:282:MET:HE3	2.18	0.69
1:E:282:MET:CE	1:E:388:ILE:HG23	2.23	0.66
1:B:258:LYS:O	1:B:262:GLU:HG3	1.96	0.66
1:F:270:LYS:O	1:F:271:ASP:HB2	1.95	0.65
1:B:270:LYS:O	1:B:271:ASP:HB2	1.96	0.65
2:G:2:FUC:H3	2:G:3:GAL:H61	1.79	0.64
1:C:232:THR:C	1:C:234:LEU:H	2.06	0.63
1:B:280:TYR:HB3	1:B:282:MET:HE1	1.79	0.63
1:F:282:MET:HE2	1:F:388:ILE:CG2	2.25	0.62
1:F:282:MET:CE	1:F:388:ILE:HG23	2.26	0.62
1:E:331:SER:HB2	1:E:367:ASP:O	2.00	0.61
1:C:282:MET:CE	1:C:388:ILE:HG23	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:HB3	1:A:389:CYS:SG	2.41	0.60
1:C:310:GLU:CD	1:D:360:PRO:HG2	2.25	0.60
1:E:265:CYS:HA	1:E:395:CYS:HA	1.84	0.60
1:C:267:HIS:CE1	1:C:397:ARG:HE	2.20	0.59
1:E:380:ARG:HH11	1:E:380:ARG:CB	2.15	0.59
1:F:265:CYS:HA	1:F:395:CYS:HA	1.84	0.59
1:B:380:ARG:HB3	1:B:382:ASP:OD1	2.02	0.58
1:B:293:VAL:O	1:B:297:GLN:HG3	2.02	0.58
1:F:300:ARG:HG2	1:F:300:ARG:HH11	1.67	0.58
1:C:332:ASP:OD1	1:C:367:ASP:HA	2.04	0.58
1:E:282:MET:HE2	1:E:388:ILE:CG2	2.26	0.58
1:E:270:LYS:O	1:E:271:ASP:HB2	2.03	0.57
1:E:251:TYR:H	1:E:251:TYR:HD1	1.53	0.57
1:C:289:TRP:CG	1:C:368:CYS:HG	2.24	0.56
1:C:293:VAL:O	1:C:297:GLN:HG3	2.04	0.56
1:C:266:ARG:HA	1:C:393:ALA:HB1	1.87	0.56
1:C:324:ARG:HH12	1:F:323:ASN:ND2	2.04	0.56
4:A:428:HOH:O	2:G:3:GAL:H62	2.07	0.55
1:D:260:ALA:HA	1:D:263:ARG:NH1	2.21	0.55
1:B:380:ARG:HB2	1:B:383:VAL:HG23	1.88	0.55
1:C:397:ARG:HH12	1:F:270:LYS:HG2	1.70	0.55
1:E:280:TYR:CB	1:E:282:MET:HE1	2.34	0.55
1:C:347:LEU:HD23	1:C:352:GLN:HE22	1.70	0.55
1:D:282:MET:HE3	1:D:282:MET:N	2.22	0.55
1:E:263:ARG:O	1:E:266:ARG:HD2	2.06	0.55
1:D:280:TYR:CB	1:D:282:MET:HE1	2.28	0.55
1:C:282:MET:HE2	1:C:388:ILE:CG1	2.32	0.55
1:D:270:LYS:O	1:D:271:ASP:HB2	2.08	0.54
1:F:263:ARG:O	1:F:266:ARG:HD2	2.08	0.54
1:A:281:PHE:C	1:A:282:MET:HE3	2.33	0.54
1:C:380:ARG:HH11	1:C:380:ARG:HG2	1.72	0.53
1:E:314:PHE:O	1:E:318:GLN:HG2	2.08	0.53
1:A:328:MET:HE1	1:A:376:TRP:CD1	2.44	0.53
1:D:265:CYS:HA	1:D:395:CYS:HA	1.90	0.53
1:B:314:PHE:O	1:B:318:GLN:HG2	2.08	0.53
1:F:290:HIS:HD2	4:F:438:HOH:O	1.92	0.53
1:A:222:SER:O	1:A:225:GLN:HB2	2.09	0.53
1:B:287:ARG:NH1	1:B:295:ALA:HB2	2.23	0.53
1:C:324:ARG:NH1	1:F:323:ASN:ND2	2.56	0.53
1:C:397:ARG:NH1	1:F:270:LYS:HG2	2.24	0.53
1:A:310:GLU:CD	1:E:360:PRO:HG2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:O	1:C:298:GLU:HG3	2.09	0.53
1:F:234:LEU:HD23	1:F:234:LEU:O	2.09	0.52
1:A:331:SER:HB2	1:A:367:ASP:O	2.10	0.52
1:B:330:LEU:HB3	1:B:369:ALA:HB3	1.92	0.52
1:A:225:GLN:HB3	1:A:229:GLN:HE21	1.74	0.52
1:D:258:LYS:HG2	1:D:262:GLU:OE2	2.10	0.52
1:E:258:LYS:HG2	1:E:262:GLU:OE2	2.10	0.52
1:A:284:ASN:ND2	1:D:321:ARG:O	2.43	0.52
1:D:287:ARG:HG3	1:D:387:TRP:CZ3	2.45	0.52
1:F:269:PRO:HB2	1:F:272:TRP:CD1	2.44	0.51
1:F:280:TYR:CB	1:F:282:MET:HE1	2.38	0.51
1:C:269:PRO:HB2	1:C:272:TRP:CD1	2.45	0.51
1:F:332:ASP:OD1	1:F:367:ASP:HA	2.09	0.51
1:A:226:GLU:O	1:A:230:GLU:HG2	2.11	0.51
1:B:331:SER:HB2	1:B:367:ASP:O	2.10	0.51
1:D:259:THR:O	1:D:263:ARG:HG3	2.11	0.51
1:F:331:SER:HB2	1:F:367:ASP:O	2.11	0.51
1:C:314:PHE:O	1:C:318:GLN:HG2	2.11	0.51
1:E:288:ASN:HB2	1:E:381:CYS:O	2.11	0.51
1:F:294:THR:O	1:F:298:GLU:HG3	2.10	0.50
1:A:332:ASP:OD1	1:A:367:ASP:HA	2.11	0.50
1:A:282:MET:CE	1:A:388:ILE:HG23	2.39	0.50
1:C:270:LYS:O	1:C:271:ASP:HB2	2.12	0.50
1:F:302:GLN:O	1:F:303:LEU:C	2.55	0.50
1:C:252:GLN:HE22	1:D:353:ARG:NH1	2.11	0.49
1:E:328:MET:HE1	1:E:376:TRP:CD1	2.48	0.49
1:A:314:PHE:O	1:A:318:GLN:HG2	2.12	0.49
1:B:232:THR:C	1:B:234:LEU:H	2.19	0.49
1:B:328:MET:HE1	1:B:376:TRP:CD1	2.47	0.49
1:A:270:LYS:O	1:A:271:ASP:HB2	2.13	0.49
1:D:331:SER:HB2	1:D:367:ASP:O	2.13	0.48
1:E:234:LEU:HD23	1:E:234:LEU:O	2.14	0.48
1:C:282:MET:HE1	1:C:388:ILE:HG23	1.96	0.47
1:B:229:GLN:O	1:B:232:THR:HB	2.15	0.47
1:D:289:TRP:CG	1:D:368:CYS:HG	2.32	0.47
1:B:380:ARG:HH11	1:B:380:ARG:HG2	1.79	0.47
1:C:288:ASN:HA	1:C:383:VAL:O	2.15	0.47
1:C:331:SER:HB2	1:C:367:ASP:O	2.15	0.47
1:B:234:LEU:C	1:B:234:LEU:HD23	2.40	0.47
1:A:282:MET:HE3	1:A:282:MET:N	2.30	0.47
1:C:303:LEU:HD13	1:C:329:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:HA	1:B:263:ARG:NH1	2.30	0.47
1:C:324:ARG:HH12	1:F:323:ASN:HD21	1.62	0.47
1:D:282:MET:CE	1:D:388:ILE:HG23	2.36	0.46
1:F:314:PHE:O	1:F:318:GLN:HG2	2.15	0.46
1:D:235:LYS:C	1:D:237:ALA:H	2.22	0.46
1:D:332:ASP:OD1	1:D:367:ASP:HA	2.16	0.46
1:F:288:ASN:HB2	1:F:381:CYS:O	2.15	0.46
1:E:253:GLU:HA	1:E:256:ASP:HB2	1.98	0.46
1:B:332:ASP:OD1	1:B:367:ASP:HA	2.15	0.46
1:F:355:TRP:CD2	1:F:360:PRO:HD3	2.50	0.46
1:C:282:MET:HE3	1:C:282:MET:N	2.30	0.46
1:E:380:ARG:HH11	1:E:380:ARG:HB3	1.80	0.46
1:A:288:ASN:HA	1:A:383:VAL:O	2.15	0.46
1:B:234:LEU:HD22	1:B:254:LEU:HD11	1.98	0.46
1:C:234:LEU:C	1:C:234:LEU:HD23	2.41	0.46
1:F:380:ARG:HH11	1:F:380:ARG:CG	2.27	0.46
1:A:326:SER:HA	1:A:386:TYR:O	2.16	0.45
1:A:303:LEU:HD13	1:A:329:GLY:HA2	1.98	0.45
1:F:359:GLU:HB3	1:F:360:PRO:HA	1.97	0.45
1:E:282:MET:HE3	1:E:282:MET:N	2.30	0.45
1:F:259:THR:O	1:F:263:ARG:HG3	2.17	0.44
1:A:289:TRP:CG	1:A:368:CYS:HG	2.34	0.44
1:A:294:THR:O	1:A:298:GLU:HG3	2.17	0.44
1:A:266:ARG:HA	1:A:393:ALA:HB1	1.99	0.44
1:F:270:LYS:HE3	1:F:270:LYS:HB2	1.84	0.44
1:A:322:SER:O	1:A:324:ARG:HG3	2.18	0.44
1:C:304:VAL:HG21	1:C:315:LEU:CD1	2.48	0.44
1:D:259:THR:HG22	1:D:263:ARG:NE	2.33	0.43
1:A:280:TYR:HB3	1:A:282:MET:HE1	2.01	0.43
1:D:232:THR:O	1:D:235:LYS:HB3	2.18	0.43
1:D:312:GLN:HG2	1:D:354:TYR:CZ	2.52	0.43
1:F:253:GLU:HA	1:F:253:GLU:OE1	2.18	0.43
1:B:287:ARG:HG3	1:B:387:TRP:CZ3	2.54	0.43
1:C:281:PHE:O	1:C:282:MET:HE3	2.17	0.43
1:F:289:TRP:CG	1:F:368:CYS:HG	2.35	0.43
1:C:326:SER:HA	1:C:386:TYR:O	2.18	0.43
1:B:304:VAL:HG21	1:B:315:LEU:HD11	2.00	0.43
1:D:272:TRP:CE2	1:D:281:PHE:HB2	2.53	0.43
1:E:288:ASN:HA	1:E:383:VAL:O	2.18	0.43
1:A:300:ARG:HG2	1:A:300:ARG:HH11	1.83	0.43
1:E:219:PRO:O	1:E:223:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:GLN:HG3	1:F:250:ILE:N	2.33	0.43
1:A:288:ASN:HB2	1:A:381:CYS:O	2.19	0.42
1:C:380:ARG:HB3	1:C:382:ASP:OD1	2.19	0.42
1:B:310:GLU:CD	1:F:360:PRO:HG2	2.43	0.42
1:A:335:GLN:O	1:A:336:GLU:C	2.62	0.42
1:B:302:GLN:O	1:B:303:LEU:C	2.62	0.42
1:F:288:ASN:HA	1:F:383:VAL:O	2.18	0.42
1:F:300:ARG:HG2	1:F:300:ARG:NH1	2.34	0.42
1:C:347:LEU:HD23	1:C:352:GLN:NE2	2.33	0.42
1:E:269:PRO:HB2	1:E:272:TRP:CD1	2.55	0.42
1:E:251:TYR:CD1	1:E:251:TYR:N	2.88	0.42
1:D:302:GLN:O	1:D:303:LEU:C	2.62	0.42
1:D:316:GLN:O	1:D:320:SER:HB2	2.19	0.42
1:D:326:SER:O	1:D:370:GLU:HA	2.20	0.42
1:D:263:ARG:O	1:D:266:ARG:HD3	2.19	0.41
1:D:288:ASN:HA	1:D:383:VAL:O	2.20	0.41
1:D:304:VAL:HG21	1:D:315:LEU:HD11	2.00	0.41
1:E:232:THR:O	1:E:235:LYS:HB3	2.19	0.41
1:D:220:GLU:C	1:D:222:SER:H	2.27	0.41
1:E:359:GLU:HB3	1:E:360:PRO:HA	2.02	0.41
1:E:332:ASP:OD1	1:E:367:ASP:HA	2.21	0.41
1:D:327:TRP:NE1	1:D:385:ASN:HB2	2.36	0.41
1:E:286:GLN:NE2	4:E:442:HOH:O	2.48	0.41
1:F:328:MET:HE1	1:F:376:TRP:CD1	2.56	0.41
1:A:383:VAL:CG1	1:A:384:ASP:N	2.84	0.41
1:C:321:ARG:O	2:L:3:GAL:H3	2.20	0.41
1:D:322:SER:O	1:D:323:ASN:HB2	2.20	0.41
1:E:225:GLN:O	1:E:229:GLN:HB2	2.21	0.41
1:F:312:GLN:HG2	1:F:354:TYR:CE2	2.55	0.41
1:F:316:GLN:O	1:F:320:SER:HB2	2.21	0.41
1:D:235:LYS:O	1:D:237:ALA:N	2.51	0.40
1:F:221:LYS:HG2	1:F:225:GLN:OE1	2.21	0.40
1:F:380:ARG:CG	1:F:380:ARG:NH1	2.85	0.40
1:F:380:ARG:HG3	1:F:380:ARG:NH1	2.30	0.40
1:B:288:ASN:HB2	1:B:381:CYS:O	2.22	0.40
1:E:259:THR:O	1:E:263:ARG:HG3	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	164/184 (89%)	157 (96%)	6 (4%)	1 (1%)	21	21
1	B	164/184 (89%)	157 (96%)	6 (4%)	1 (1%)	21	21
1	C	164/184 (89%)	154 (94%)	7 (4%)	3 (2%)	6	3
1	D	164/184 (89%)	155 (94%)	8 (5%)	1 (1%)	21	21
1	E	164/184 (89%)	151 (92%)	12 (7%)	1 (1%)	21	21
1	F	164/184 (89%)	156 (95%)	8 (5%)	0	100	100
All	All	984/1104 (89%)	930 (94%)	47 (5%)	7 (1%)	18	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	233	GLN
1	D	236	ALA
1	C	304	VAL
1	C	365	ASN
1	A	304	VAL
1	B	304	VAL
1	E	304	VAL

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	150/165 (91%)	143 (95%)	7 (5%)	23	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	151/165 (92%)	147 (97%)	4 (3%)	40	50
1	C	151/165 (92%)	145 (96%)	6 (4%)	28	34
1	D	150/165 (91%)	146 (97%)	4 (3%)	39	49
1	E	150/165 (91%)	145 (97%)	5 (3%)	33	42
1	F	150/165 (91%)	147 (98%)	3 (2%)	48	59
All	All	902/990 (91%)	873 (97%)	29 (3%)	34	43

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
1	A	266	ARG
1	A	282	MET
1	A	284	ASN
1	A	303	LEU
1	A	317	LEU
1	A	353	ARG
1	B	266	ARG
1	B	282	MET
1	B	303	LEU
1	B	317	LEU
1	C	262	GLU
1	C	266	ARG
1	C	282	MET
1	C	294	THR
1	C	303	LEU
1	C	317	LEU
1	D	234	LEU
1	D	282	MET
1	D	303	LEU
1	D	380	ARG
1	E	266	ARG
1	E	282	MET
1	E	303	LEU
1	E	317	LEU
1	E	380	ARG
1	F	252	GLN
1	F	282	MET
1	F	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	286	GLN
1	A	290	HIS
1	A	313	ASN
1	A	323	ASN
1	A	340	GLN
1	A	352	GLN
1	A	385	ASN
1	B	276	GLN
1	B	286	GLN
1	B	290	HIS
1	B	297	GLN
1	B	323	ASN
1	B	340	GLN
1	B	352	GLN
1	C	267	HIS
1	C	286	GLN
1	C	290	HIS
1	C	297	GLN
1	C	340	GLN
1	D	233	GLN
1	D	278	ASN
1	D	286	GLN
1	D	302	GLN
1	D	323	ASN
1	E	233	GLN
1	E	286	GLN
1	E	318	GLN
1	E	340	GLN
1	F	233	GLN
1	F	278	ASN
1	F	302	GLN
1	F	323	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 ⓘ

18 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	NDG	G	1	2	15,15,15	0.57	0	21,21,21	0.57	0
2	FUC	G	2	2,3	10,10,11	0.47	0	14,14,16	0.43	0
2	GAL	G	3	2	11,11,12	0.48	0	15,15,17	0.32	0
2	NDG	H	1	2	15,15,15	0.40	0	21,21,21	0.63	0
2	FUC	H	2	2,3	10,10,11	0.38	0	14,14,16	0.43	0
2	GAL	H	3	2	11,11,12	0.43	0	15,15,17	0.27	0
2	NDG	I	1	2	15,15,15	0.48	0	21,21,21	0.59	0
2	FUC	I	2	2,3	10,10,11	0.56	0	14,14,16	0.39	0
2	GAL	I	3	2	11,11,12	0.43	0	15,15,17	0.31	0
2	NDG	J	1	2	15,15,15	0.54	0	21,21,21	0.63	0
2	FUC	J	2	2,3	10,10,11	0.44	0	14,14,16	0.47	0
2	GAL	J	3	2	11,11,12	0.46	0	15,15,17	0.31	0
2	NDG	K	1	2	15,15,15	0.50	0	21,21,21	0.91	1 (4%)
2	FUC	K	2	2,3	10,10,11	0.60	0	14,14,16	0.39	0
2	GAL	K	3	2	11,11,12	0.52	0	15,15,17	0.37	0
2	NDG	L	1	2	15,15,15	0.54	0	21,21,21	0.61	0
2	FUC	L	2	2,3	10,10,11	0.58	0	14,14,16	0.49	0
2	GAL	L	3	2	11,11,12	0.49	0	15,15,17	0.32	0

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	NDG	G	1	2	-	0/6/26/26	0/1/1/1
2	FUC	G	2	2,3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	NDG	H	1	2	-	0/6/26/26	0/1/1/1
2	FUC	H	2	2,3	-	-	0/1/1/1
2	GAL	H	3	2	-	2/2/19/22	0/1/1/1
2	NDG	I	1	2	-	0/6/26/26	0/1/1/1
2	FUC	I	2	2,3	-	-	0/1/1/1
2	GAL	I	3	2	-	2/2/19/22	0/1/1/1
2	NDG	J	1	2	-	4/6/26/26	0/1/1/1
2	FUC	J	2	2,3	-	-	0/1/1/1
2	GAL	J	3	2	-	1/2/19/22	0/1/1/1
2	NDG	K	1	2	-	2/6/26/26	0/1/1/1
2	FUC	K	2	2,3	-	-	0/1/1/1
2	GAL	K	3	2	-	1/2/19/22	0/1/1/1
2	NDG	L	1	2	-	2/6/26/26	0/1/1/1
2	FUC	L	2	2,3	-	-	0/1/1/1
2	GAL	L	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NDG	C4-C3-C2	2.10	113.47	110.40

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	3	GAL	C4-C5-C6-O6
2	J	1	NDG	C3-C2-N2-C7
2	J	3	GAL	O5-C5-C6-O6
2	I	3	GAL	O5-C5-C6-O6
2	H	3	GAL	O5-C5-C6-O6
2	L	1	NDG	C4-C5-C6-O6
2	K	3	GAL	O5-C5-C6-O6
2	L	3	GAL	O5-C5-C6-O6
2	L	1	NDG	O5-C5-C6-O6
2	J	1	NDG	C4-C5-C6-O6
2	K	1	NDG	C8-C7-N2-C2
2	J	1	NDG	O5-C5-C6-O6
2	J	1	NDG	C1-C2-N2-C7

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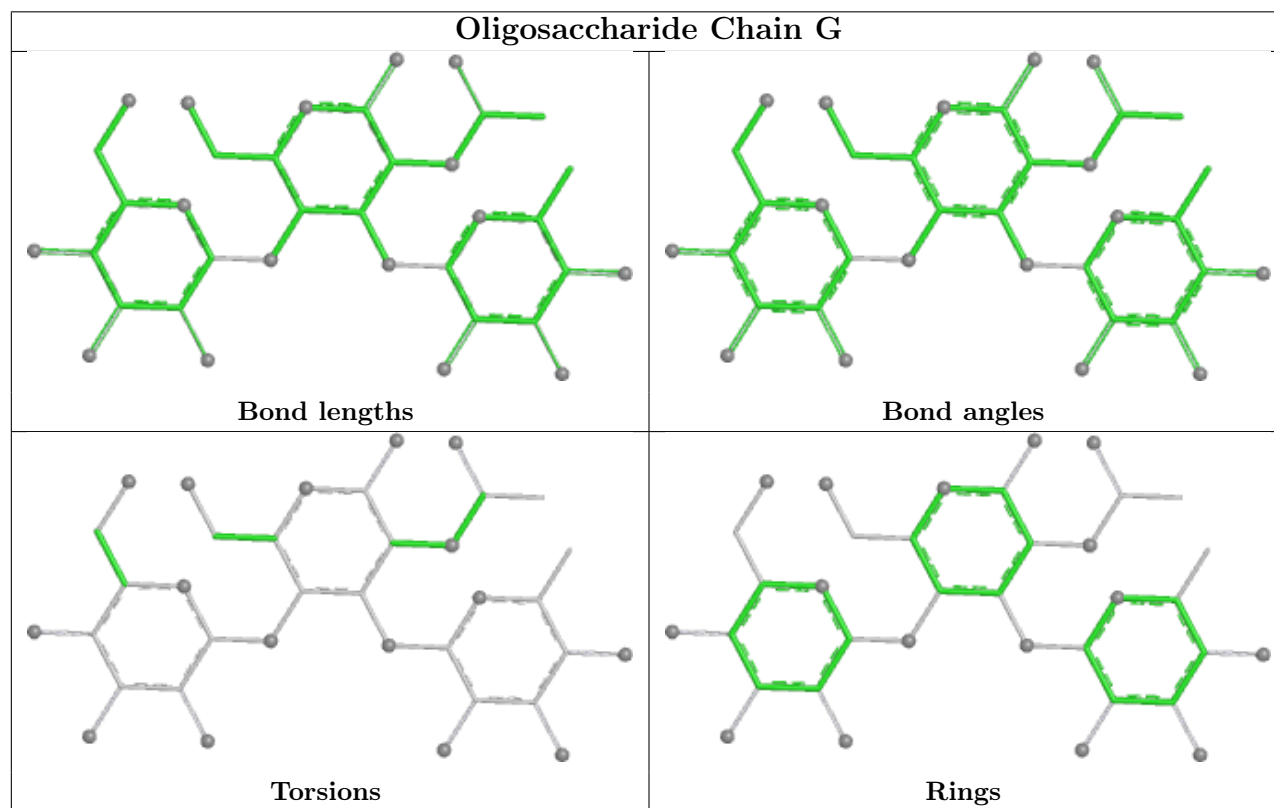
Mol	Chain	Res	Type	Atoms
2	K	1	NDG	O7-C7-N2-C2
2	I	3	GAL	C4-C5-C6-O6

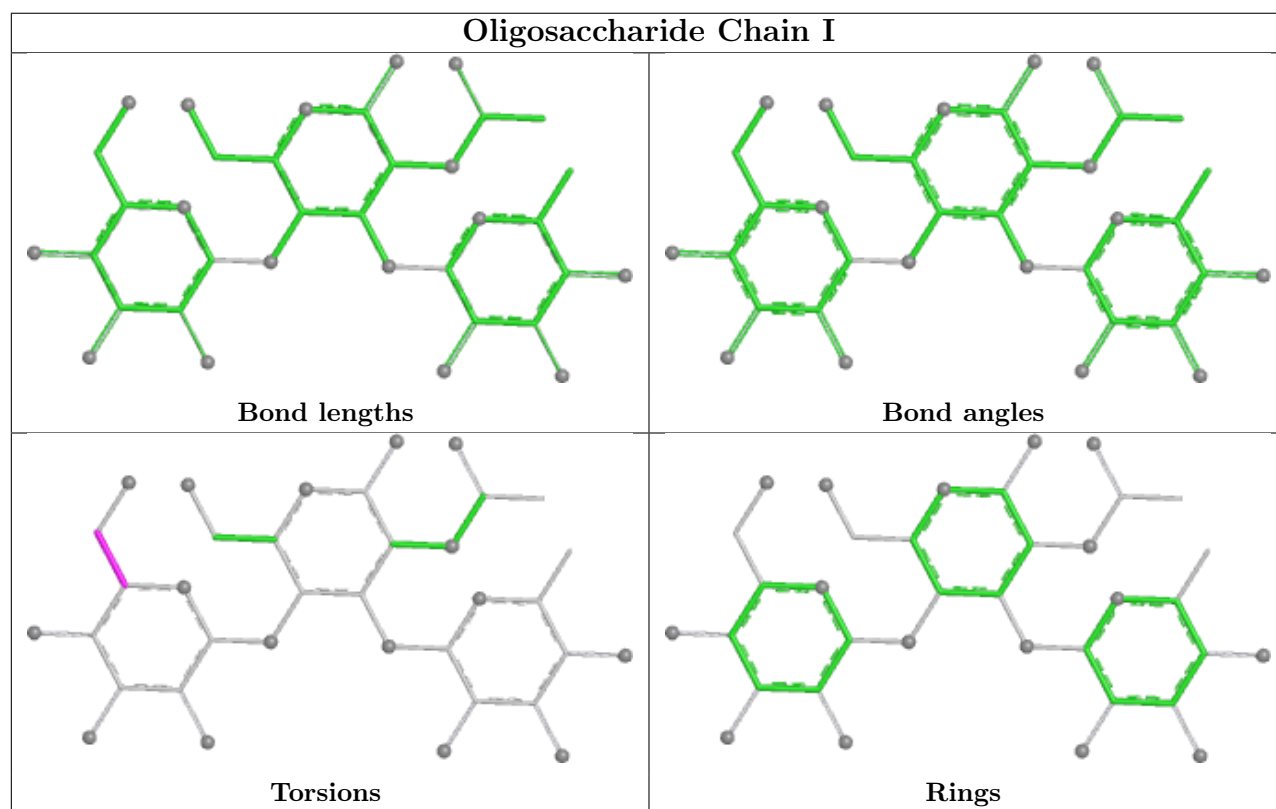
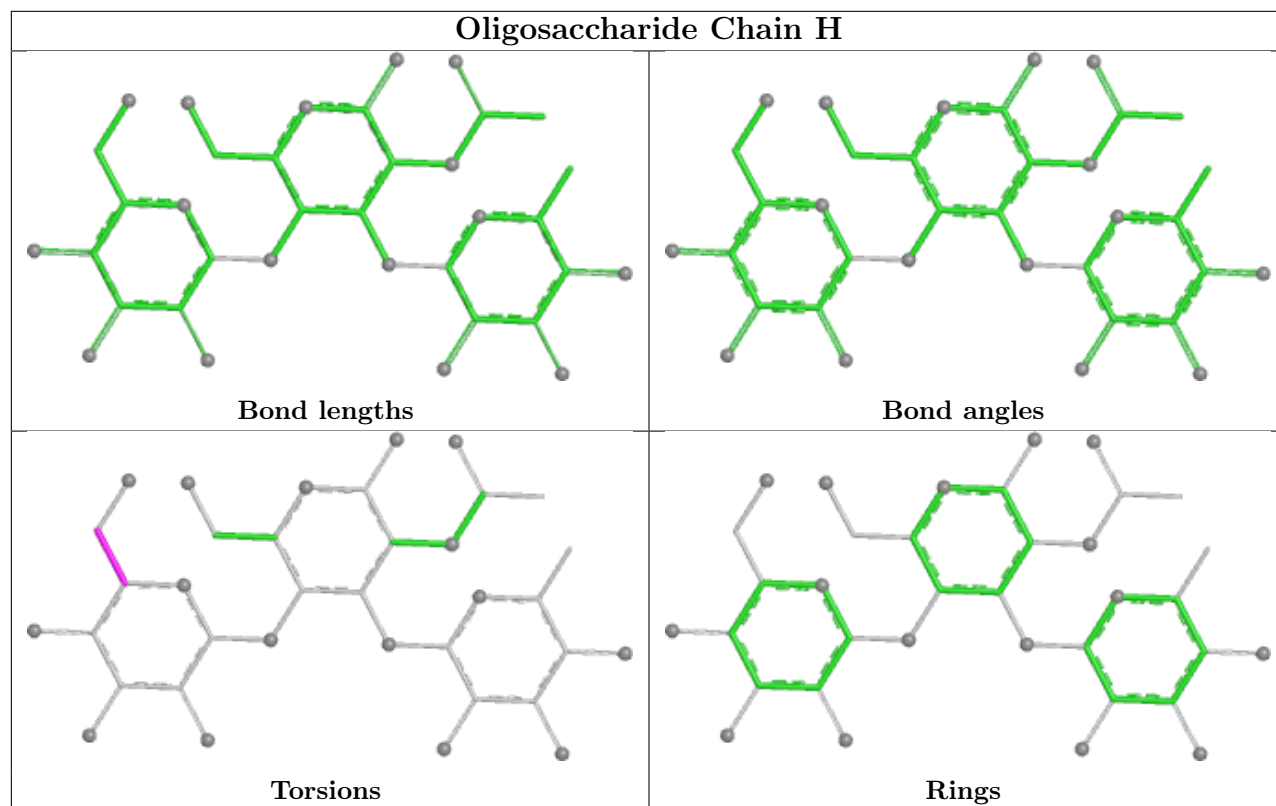
There are no ring outliers.

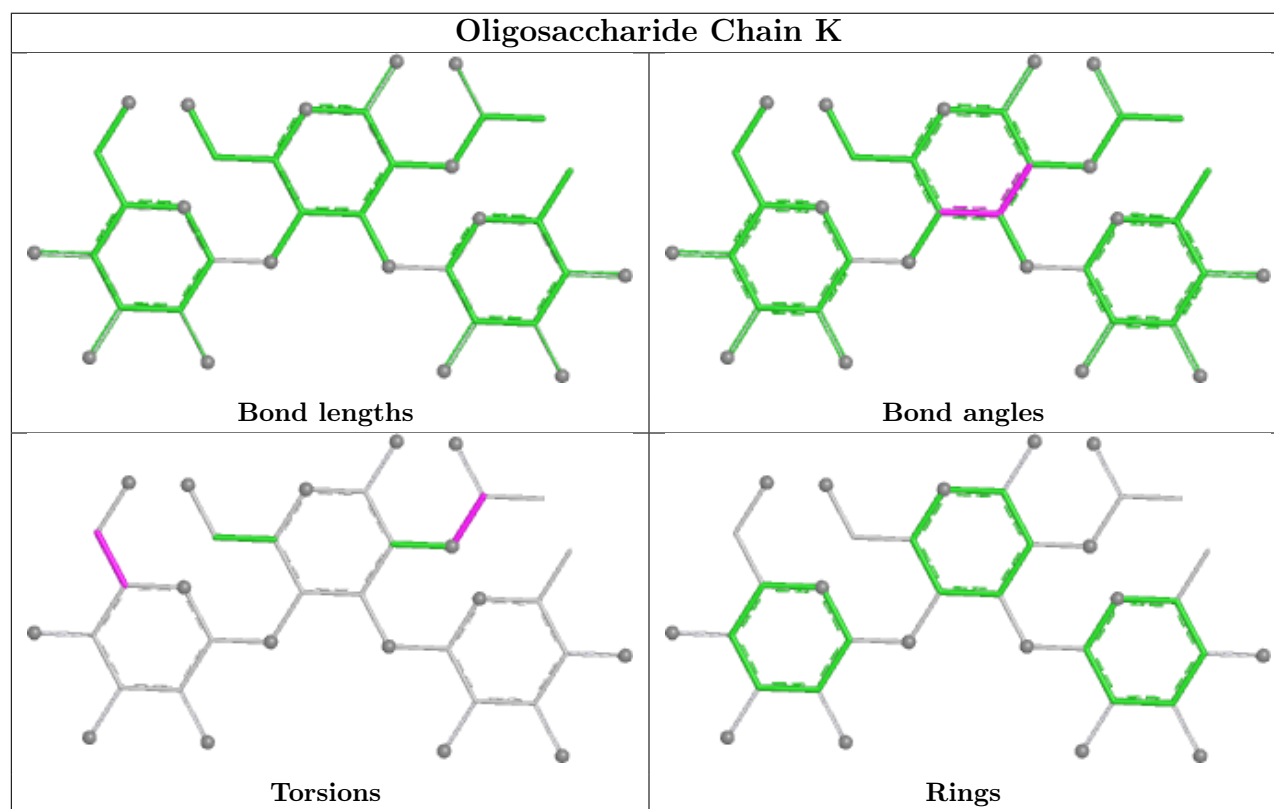
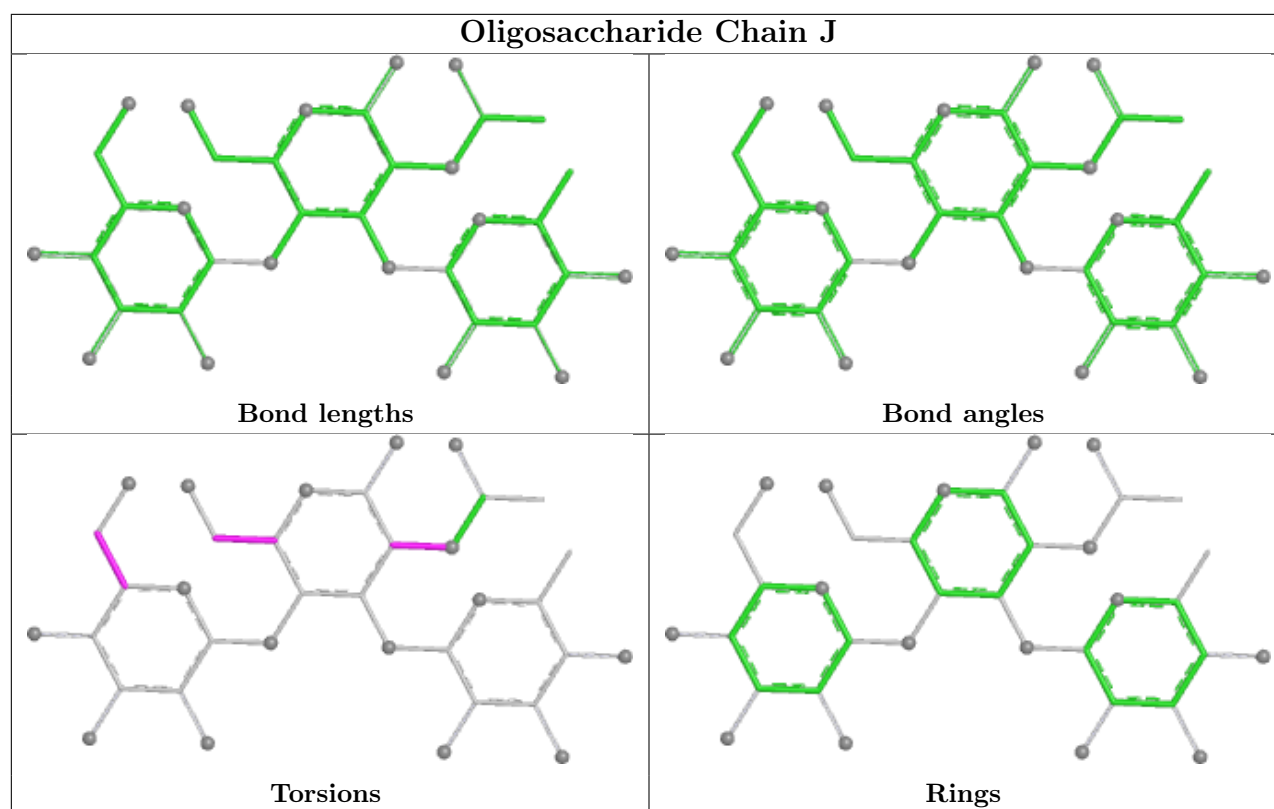
3 monomers are involved in 3 short contacts:

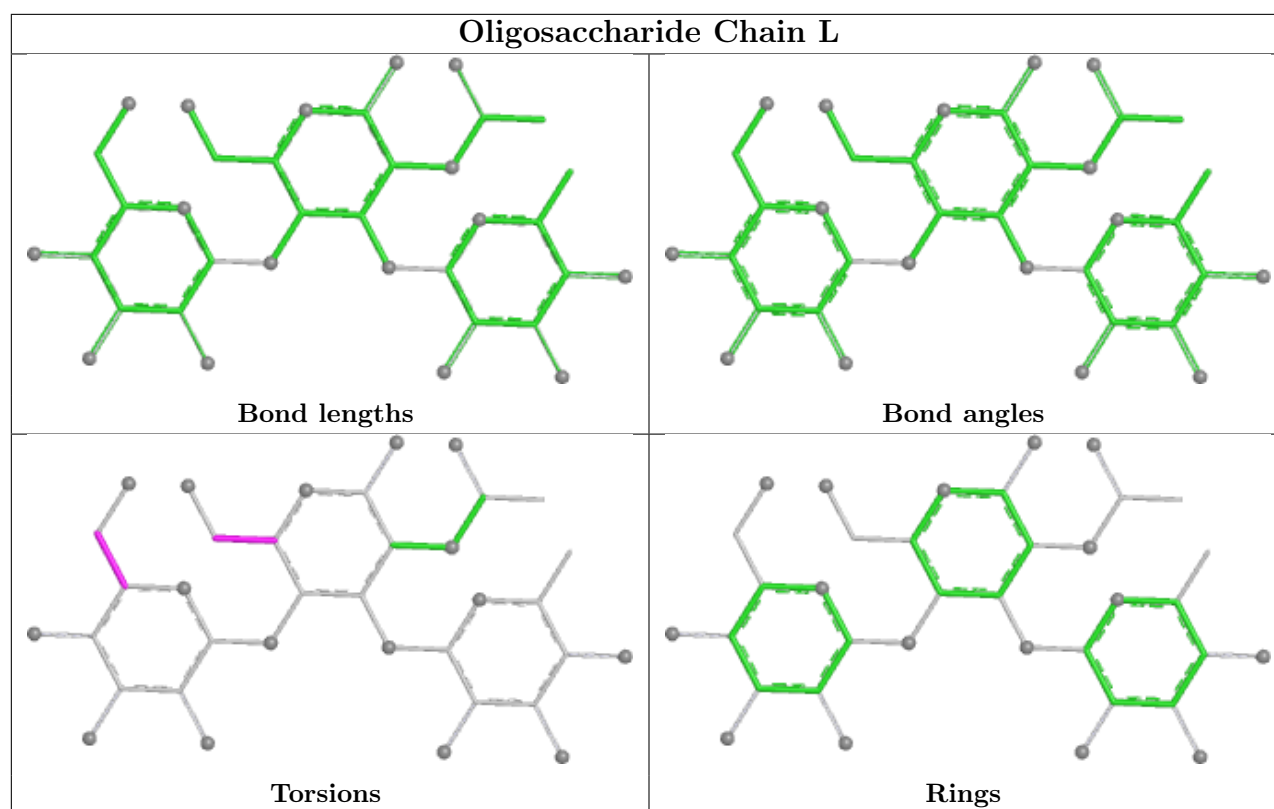
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	FUC	1	0
2	L	3	GAL	1	0
2	G	3	GAL	2	0

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 24 ligands modelled in this entry, 24 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 ⓘ

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	168/184 (91%)	0.92	20 (11%) 9 8	34, 50, 89, 100	0
1	B	168/184 (91%)	0.79	28 (16%) 4 3	33, 48, 90, 100	0
1	C	168/184 (91%)	1.00	24 (14%) 6 5	38, 53, 94, 100	0
1	D	168/184 (91%)	0.82	26 (15%) 5 4	31, 47, 90, 100	0
1	E	168/184 (91%)	0.79	28 (16%) 4 3	30, 43, 93, 100	0
1	F	168/184 (91%)	0.80	29 (17%) 4 3	30, 46, 88, 100	0
All	All	1008/1104 (91%)	0.85	155 (15%) 5 4	30, 48, 93, 100	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	LYS	6.0
1	C	248	GLN	5.7
1	B	246	LYS	5.7
1	E	237	ALA	5.7
1	C	246	LYS	5.3
1	B	381	CYS	5.3
1	E	250	ILE	4.9
1	C	251	TYR	4.8
1	E	252	GLN	4.7
1	E	219	PRO	4.7
1	D	237	ALA	4.6
1	B	234	LEU	4.5
1	F	219	PRO	4.5
1	B	250	ILE	4.5
1	C	250	ILE	4.5
1	D	219	PRO	4.4
1	F	222	SER	4.4
1	C	219	PRO	4.3
1	D	250	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	220	GLU	4.3
1	E	249	GLN	4.2
1	F	249	GLN	4.2
1	D	220	GLU	4.1
1	F	265	CYS	4.1
1	C	334	ASN	4.1
1	E	268	CYS	4.0
1	D	222	SER	3.9
1	E	251	TYR	3.9
1	F	250	ILE	3.9
1	C	234	LEU	3.9
1	F	228	TYR	3.8
1	C	389	CYS	3.8
1	A	234	LEU	3.8
1	F	251	TYR	3.7
1	D	397	ARG	3.7
1	A	219	PRO	3.7
1	B	226	GLU	3.7
1	D	221	LYS	3.7
1	E	279	CYS	3.6
1	B	228	TYR	3.6
1	D	254	LEU	3.6
1	E	254	LEU	3.6
1	D	249	GLN	3.5
1	E	224	LEU	3.5
1	A	397	ARG	3.5
1	B	248	GLN	3.5
1	E	263	ARG	3.3
1	F	224	LEU	3.2
1	B	251	TYR	3.2
1	F	236	ALA	3.2
1	C	268	CYS	3.2
1	C	220	GLU	3.1
1	F	268	CYS	3.1
1	E	320	SER	3.1
1	A	228	TYR	3.1
1	B	219	PRO	3.1
1	F	221	LYS	3.1
1	F	237	ALA	3.1
1	E	323	ASN	3.0
1	E	220	GLU	3.0
1	A	229	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	263	ARG	3.0
1	D	251	TYR	3.0
1	B	229	GLN	3.0
1	D	263	ARG	3.0
1	B	397	ARG	2.9
1	A	226	GLU	2.9
1	C	396	PHE	2.9
1	C	228	TYR	2.9
1	F	252	GLN	2.9
1	D	265	CYS	2.9
1	C	227	ILE	2.9
1	D	228	TYR	2.8
1	D	255	THR	2.8
1	B	357	SER	2.8
1	A	247	GLN	2.8
1	E	255	THR	2.8
1	B	249	GLN	2.8
1	D	252	GLN	2.8
1	B	247	GLN	2.7
1	E	229	GLN	2.7
1	C	221	LYS	2.7
1	B	340	GLN	2.7
1	D	320	SER	2.7
1	D	253	GLU	2.7
1	B	268	CYS	2.7
1	D	266	ARG	2.7
1	A	268	CYS	2.7
1	E	225	GLN	2.6
1	C	381	CYS	2.6
1	D	268	CYS	2.6
1	A	271	ASP	2.6
1	D	231	LEU	2.6
1	D	317	LEU	2.6
1	E	395	CYS	2.5
1	A	227	ILE	2.5
1	D	395	CYS	2.5
1	C	340	GLN	2.5
1	A	395	CYS	2.4
1	E	397	ARG	2.4
1	E	236	ALA	2.4
1	A	389	CYS	2.4
1	B	389	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	389	CYS	2.4
1	B	256	ASP	2.4
1	F	279	CYS	2.4
1	F	395	CYS	2.4
1	B	252	GLN	2.4
1	E	266	ARG	2.4
1	A	265	CYS	2.4
1	B	261	PHE	2.4
1	A	394	ALA	2.3
1	E	222	SER	2.3
1	F	234	LEU	2.3
1	F	267	HIS	2.3
1	B	233	GLN	2.3
1	A	381	CYS	2.3
1	E	232	THR	2.3
1	F	310	GLU	2.3
1	F	323	ASN	2.3
1	C	229	GLN	2.3
1	C	254	LEU	2.2
1	E	231	LEU	2.2
1	C	323	ASN	2.2
1	E	265	CYS	2.2
1	C	252	GLN	2.2
1	B	231	LEU	2.2
1	D	257	LEU	2.2
1	B	323	ASN	2.2
1	F	320	SER	2.2
1	A	261	PHE	2.2
1	B	368	CYS	2.2
1	F	227	ILE	2.2
1	A	323	ASN	2.2
1	B	255	THR	2.2
1	E	234	LEU	2.1
1	F	254	LEU	2.1
1	C	223	LYS	2.1
1	F	389	CYS	2.1
1	B	222	SER	2.1
1	D	224	LEU	2.1
1	C	230	GLU	2.1
1	C	395	CYS	2.1
1	E	228	TYR	2.1
1	D	234	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	287	ARG	2.1
1	F	321	ARG	2.1
1	F	255	THR	2.0
1	F	259	THR	2.0
1	A	248	GLN	2.0
1	A	252	GLN	2.0
1	D	279	CYS	2.0
1	C	224	LEU	2.0
1	F	317	LEU	2.0
1	B	227	ILE	2.0

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

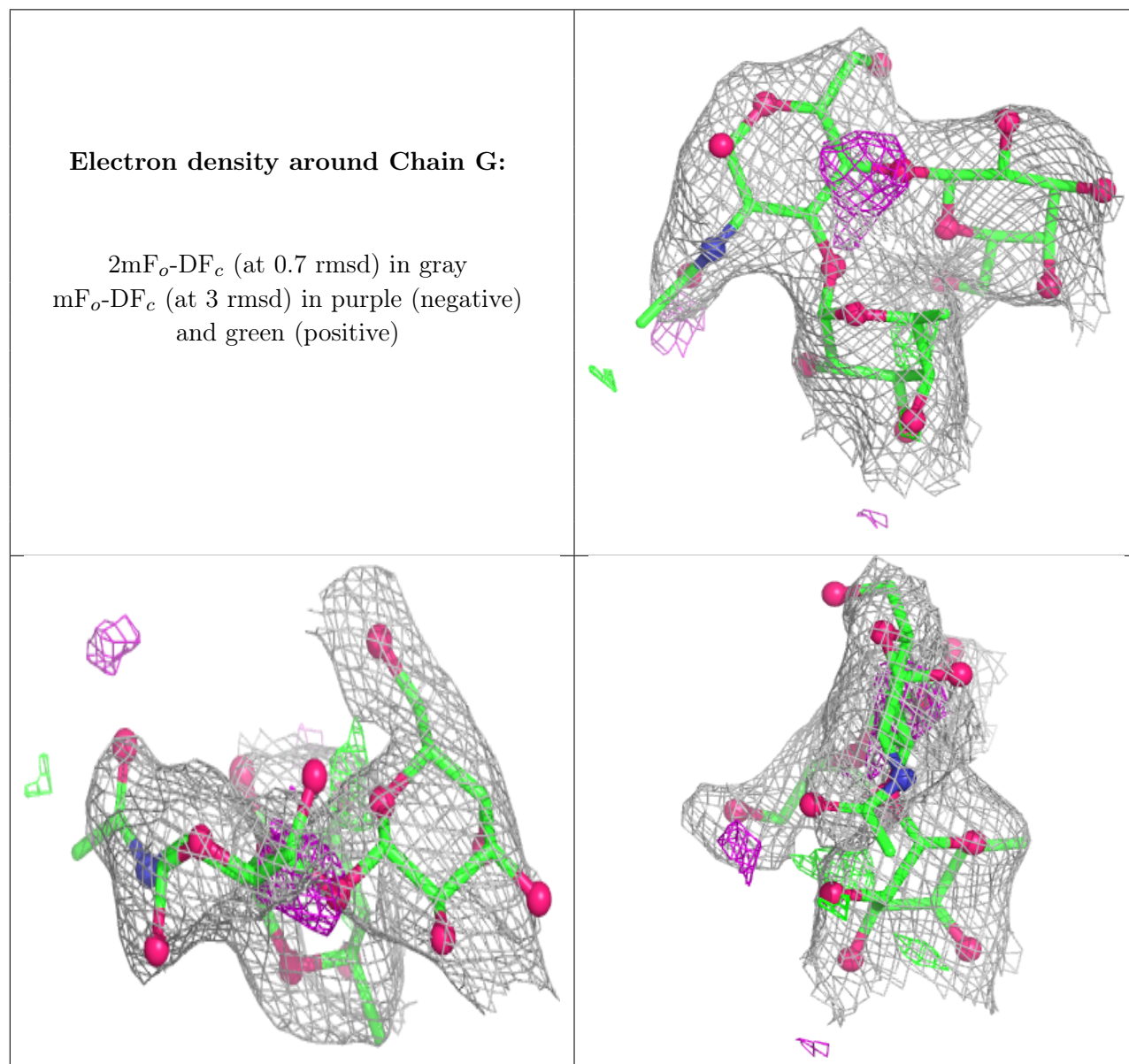
There are no non-standard protein/DNA/RNA residues in this entry.

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.

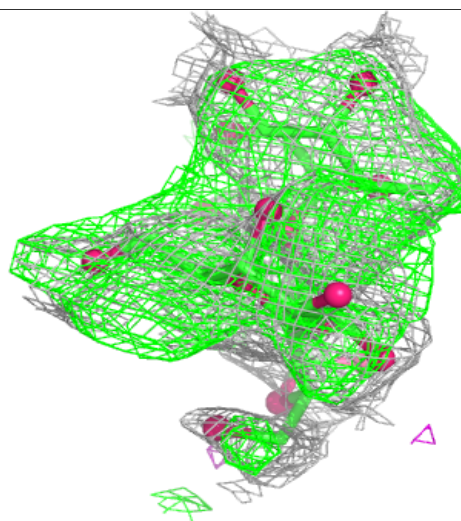
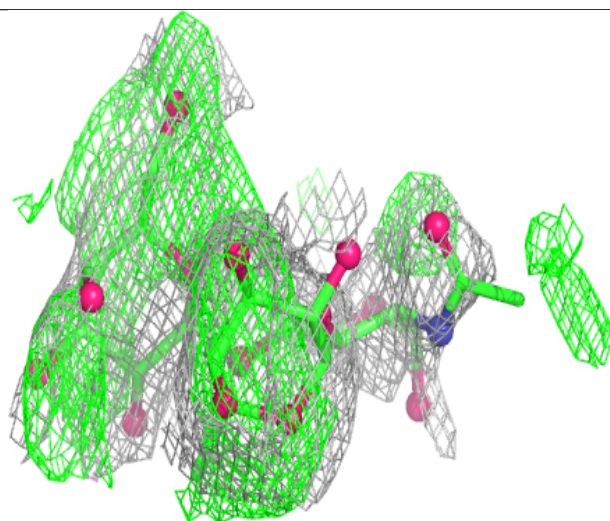
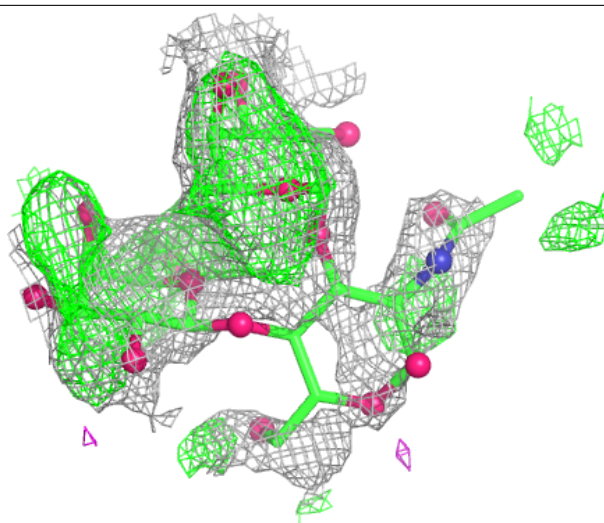
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NDG	H	1	15/15	0.62	0.46	62,69,70,72	15
2	NDG	I	1	15/15	0.71	0.21	89,97,97,99	0
2	NDG	G	1	15/15	0.72	0.17	81,90,90,91	0
2	GAL	H	3	11/12	0.75	0.39	73,73,74,75	11
2	GAL	I	3	11/12	0.77	0.19	99,99,100,100	0
2	NDG	J	1	15/15	0.78	0.16	69,78,82,84	0
2	GAL	G	3	11/12	0.80	0.16	89,91,92,92	0
2	NDG	L	1	15/15	0.80	0.18	65,78,82,82	0
2	NDG	K	1	15/15	0.82	0.15	61,73,78,80	0
2	FUC	H	2	10/11	0.82	0.38	47,52,56,57	10
2	GAL	K	3	11/12	0.83	0.19	75,76,77,77	0
2	FUC	I	2	10/11	0.87	0.21	76,80,82,84	0
2	GAL	L	3	11/12	0.88	0.17	76,78,79,80	0
2	GAL	J	3	11/12	0.89	0.15	75,77,78,80	0
2	FUC	G	2	10/11	0.91	0.16	60,68,71,74	0
2	FUC	J	2	10/11	0.92	0.15	53,58,61,64	0
2	FUC	L	2	10/11	0.94	0.11	45,49,53,55	0
2	FUC	K	2	10/11	0.96	0.11	39,46,50,53	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.



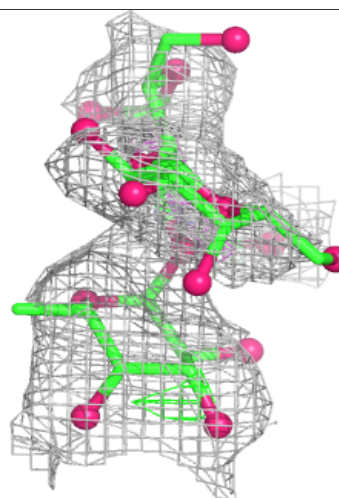
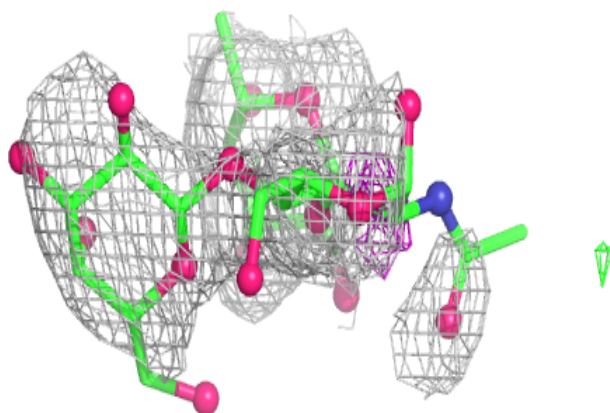
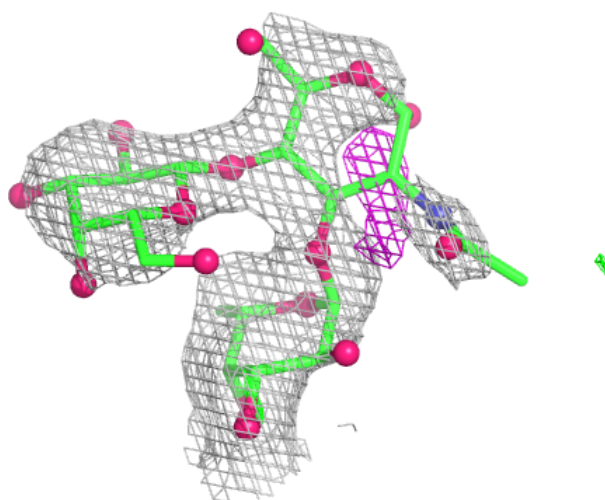
Electron density around Chain H:

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



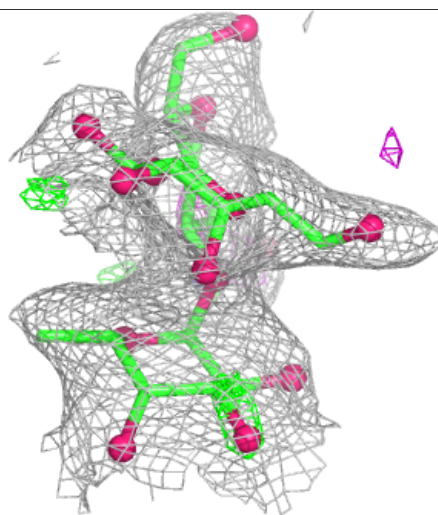
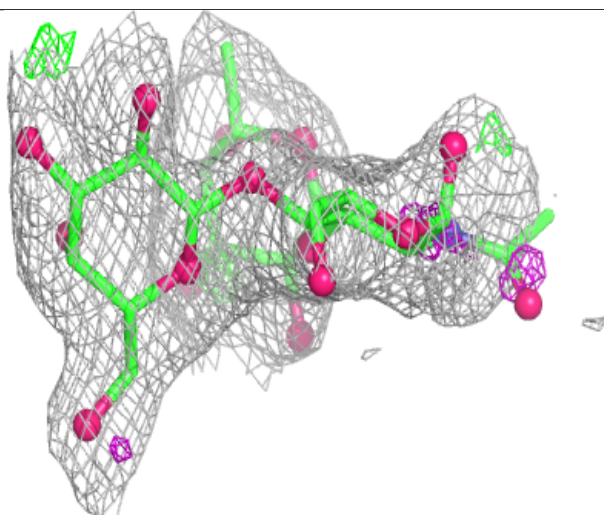
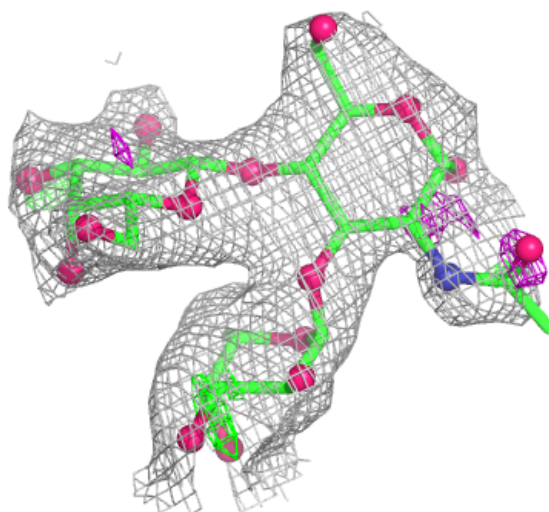
Electron density around Chain I:

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



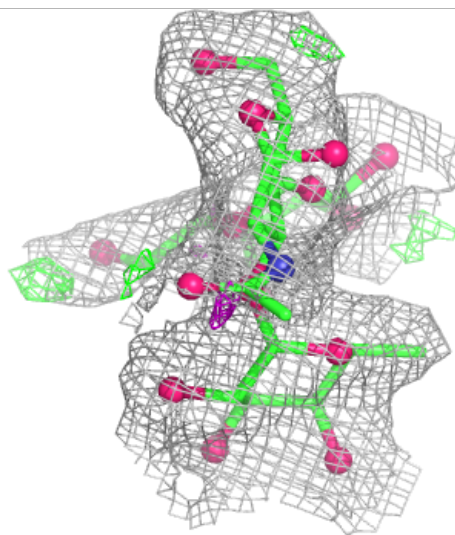
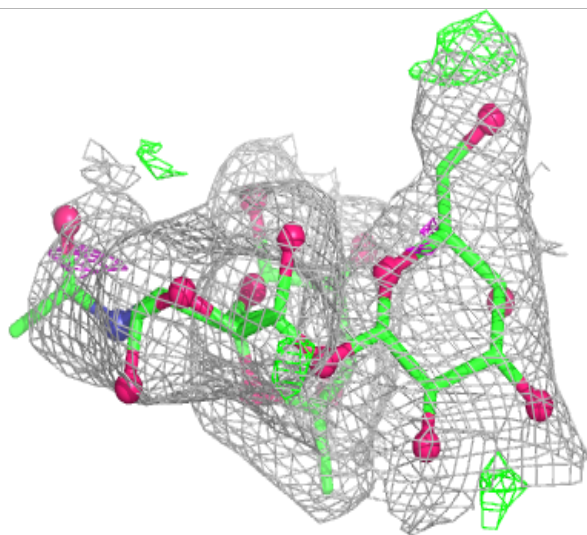
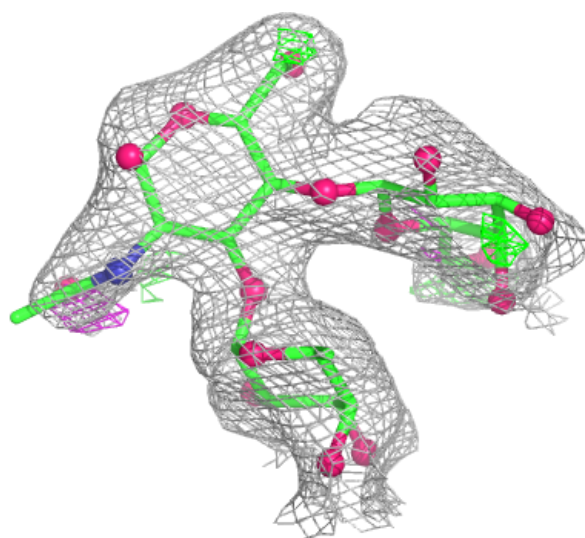
Electron density around Chain J:

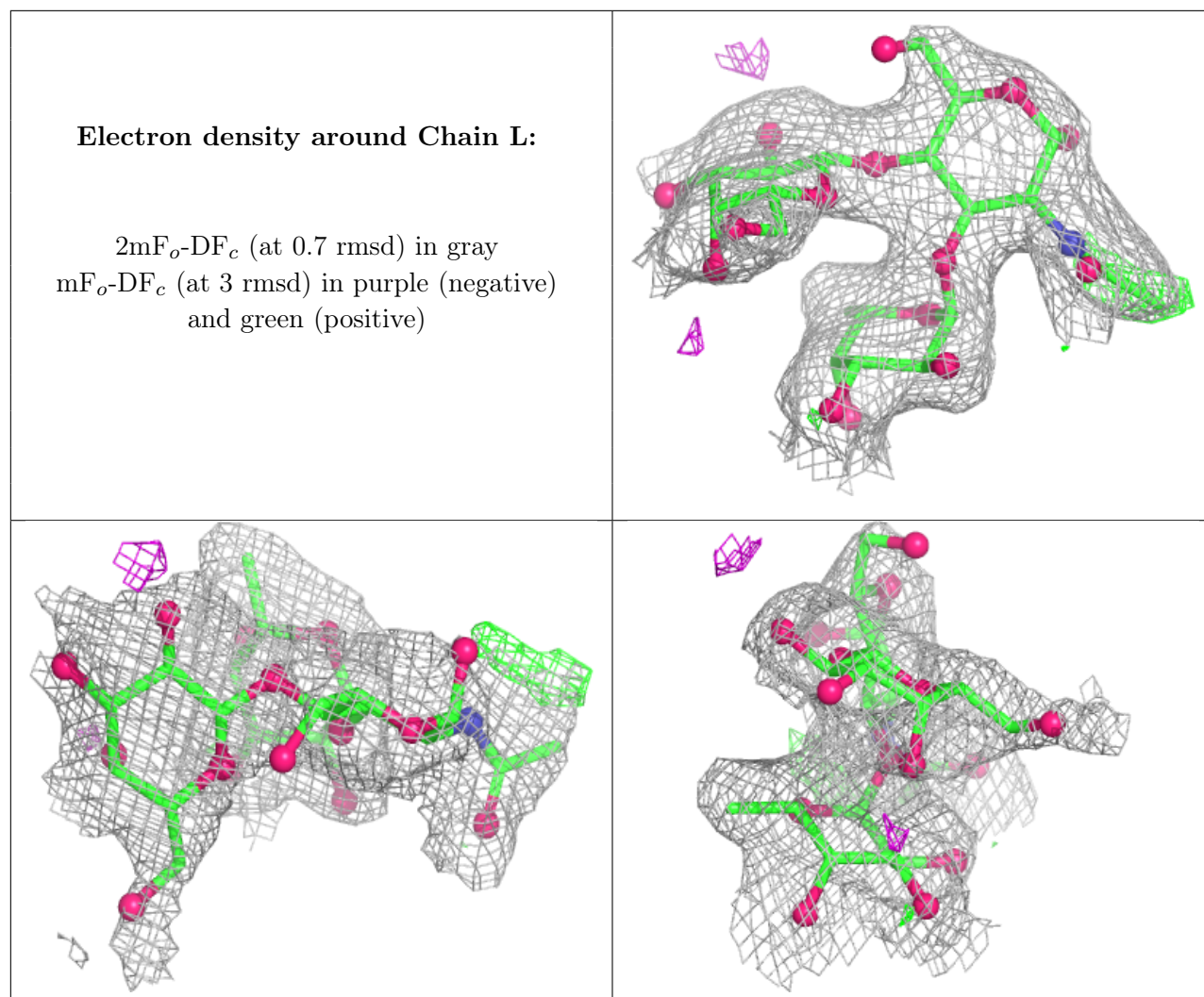
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	D	4	1/1	0.88	0.09	95,95,95,95	0
3	CA	E	4	1/1	0.92	0.07	100,100,100,100	0
3	CA	F	4	1/1	0.94	0.07	97,97,97,97	0
3	CA	C	4	1/1	0.97	0.05	73,73,73,73	0
3	CA	B	4	1/1	0.97	0.06	76,76,76,76	0
3	CA	B	3	1/1	0.99	0.03	46,46,46,46	0
3	CA	A	2	1/1	0.99	0.04	48,48,48,48	0
3	CA	C	1	1/1	0.99	0.03	46,46,46,46	0
3	CA	C	2	1/1	0.99	0.03	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	3	1/1	0.99	0.03	41,41,41,41	0
3	CA	A	3	1/1	0.99	0.05	56,56,56,56	0
3	CA	D	1	1/1	0.99	0.02	36,36,36,36	0
3	CA	D	3	1/1	0.99	0.02	35,35,35,35	0
3	CA	A	4	1/1	0.99	0.04	62,62,62,62	0
3	CA	E	1	1/1	0.99	0.05	32,32,32,32	0
3	CA	E	3	1/1	0.99	0.03	34,34,34,34	0
3	CA	B	1	1/1	0.99	0.03	40,40,40,40	0
3	CA	F	1	1/1	0.99	0.02	35,35,35,35	0
3	CA	F	2	1/1	0.99	0.03	32,32,32,32	0
3	CA	B	2	1/1	0.99	0.03	44,44,44,44	0
3	CA	E	2	1/1	1.00	0.04	31,31,31,31	0
3	CA	D	2	1/1	1.00	0.01	38,38,38,38	0
3	CA	F	3	1/1	1.00	0.03	33,33,33,33	0
3	CA	A	1	1/1	1.00	0.02	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.