



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 07:53 AM EDT

PDB ID : 1MWA
Title : 2C/H-2KBM3/DEV8 ALLOGENEIC COMPLEX
Authors : Luz, J.G.; Huang, M.D.; Garcia, K.C.; Rudolph, M.G.; Teyton, L.; Wilson, I.A.
Deposited on : 2002-09-27
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

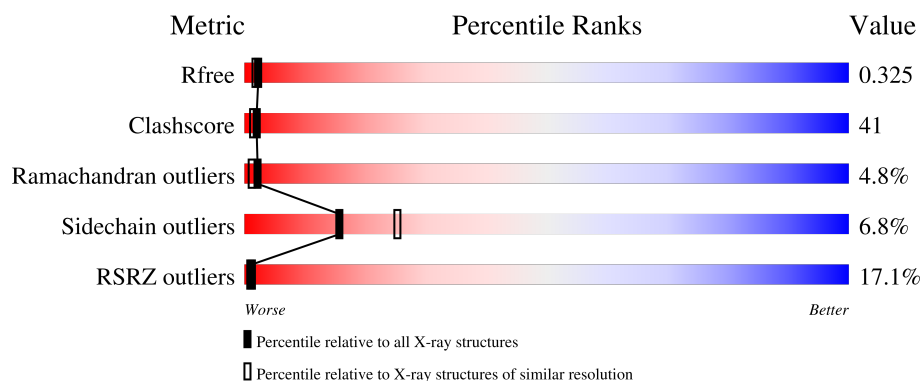
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



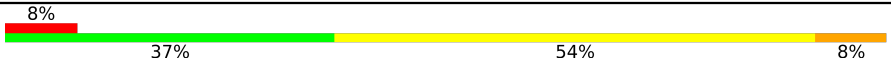

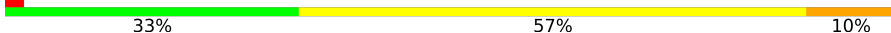



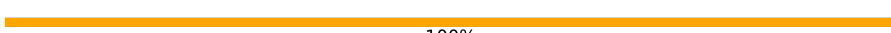



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	202	<div> <div>6%</div> <div>55%</div> <div>40%</div> <div>5%</div> </div>
1	C	202	<div> <div>44%</div> <div>33%</div> <div>56%</div> <div>9%</div> </div>
2	B	237	<div> <div>%</div> <div>60%</div> <div>36%</div> <div>%</div> </div>
2	D	237	<div> <div>60%</div> <div>28%</div> <div>60%</div> <div>11%</div> </div>
3	H	275	<div> <div>%</div> <div>55%</div> <div>39%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	275	
4	L	99	
4	M	99	
5	P	8	
5	Q	8	
6	E	2	
6	K	2	
7	F	3	
7	G	3	
7	J	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
10	ACY	P	1001	-	-	-	X
6	NAG	K	1	X	-	-	-
7	NAG	F	1	-	-	X	-
7	NAG	J	1	-	-	X	-
9	NAG	B	808	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13973 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 2C T CELL RECEPTOR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			
1	C	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	SEE REMARK 999	GB 224220
A	165	ALA	LYS	SEE REMARK 999	GB 224220
C	127	ALA	GLN	SEE REMARK 999	GB 224220
C	165	ALA	LYS	SEE REMARK 999	GB 224220

- Molecule 2 is a protein called 2C T CELL RECEPTOR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			
2	D	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	SEE REMARK 999	GB 1791255
B	?	-	ARG	SEE REMARK 999	GB 1791255
B	?	-	ALA	SEE REMARK 999	GB 1791255
B	105	THR	GLU	SEE REMARK 999	GB 1791255
B	106	LEU	GLN	SEE REMARK 999	GB 1791255
B	107	TYR	PHE	SEE REMARK 999	GB 1791255
B	110	ALA	PRO	SEE REMARK 999	GB 1791255
B	115	SER	THR	SEE REMARK 999	GB 1791255

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Chain	Residue	Modelled	Actual	Comment	Reference
D	97	GLY	GLN	SEE REMARK 999	GB 1791255
D	?	-	ARG	SEE REMARK 999	GB 1791255
D	?	-	ALA	SEE REMARK 999	GB 1791255
D	105	THR	GLU	SEE REMARK 999	GB 1791255
D	106	LEU	GLN	SEE REMARK 999	GB 1791255
D	107	TYR	PHE	SEE REMARK 999	GB 1791255
D	110	ALA	PRO	SEE REMARK 999	GB 1791255
D	115	SER	THR	SEE REMARK 999	GB 1791255

- Molecule 3 is a protein called H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	274	Total	C	N	O	S	0	0	0
			2225	1404	392	420	9			
3	I	274	Total	C	N	O	S	0	0	0
			2224	1404	392	419	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	77	SER	ASP	conflict	UNP P01901
H	89	ALA	LYS	conflict	UNP P01901
H	275	ARG	GLU	conflict	UNP P01901
I	77	SER	ASP	conflict	UNP P01901
I	89	ALA	LYS	conflict	UNP P01901
I	275	ARG	GLU	conflict	UNP P01901

- Molecule 4 is a protein called MICROGLOBULIN MHC LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
4	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 5 is a protein called DEV8.

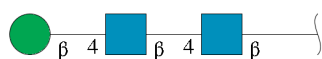
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	8	Total	C	N	O	0	0	0
			76	51	10	15			
5	Q	8	Total	C	N	O	0	0	0
			76	51	10	15			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



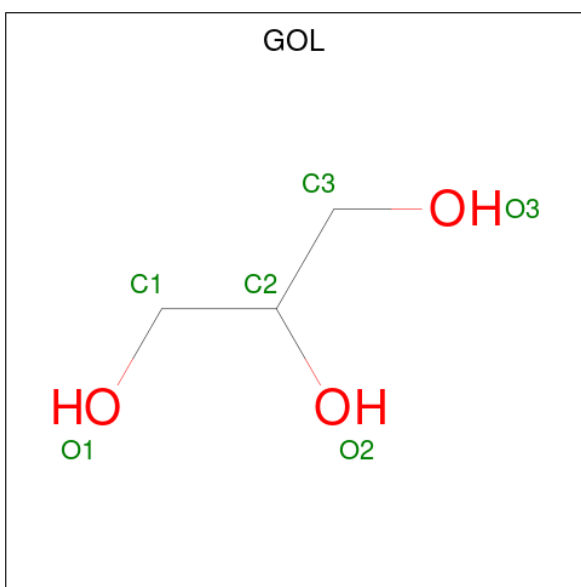
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



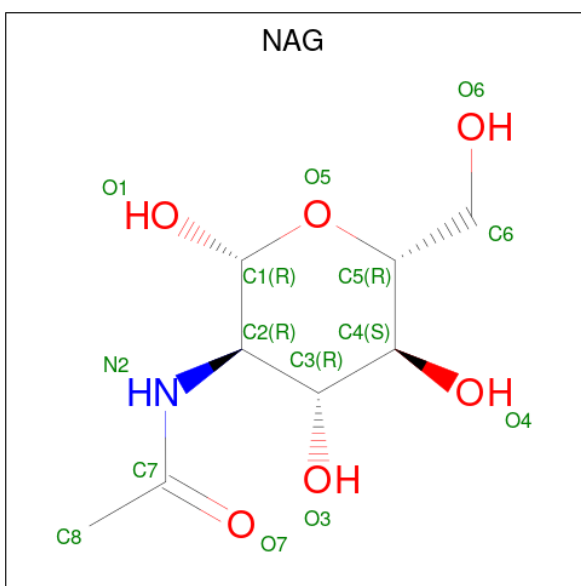
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



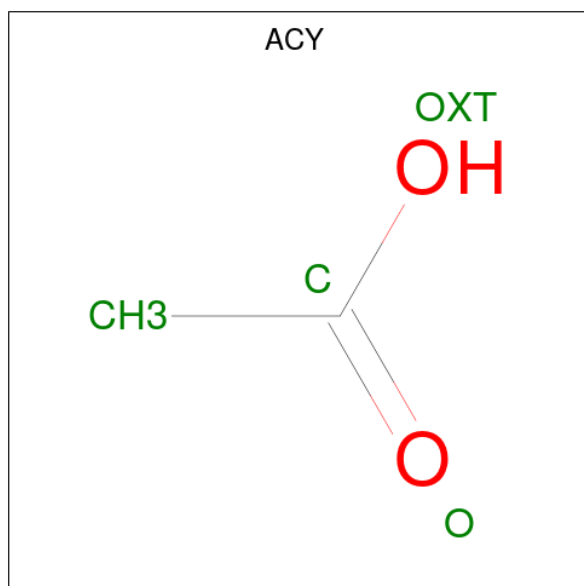
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	I	1	Total	C	O	0	0
			6	3	3		
8	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	106	Total	O	0	0
			106	106		
11	C	41	Total	O	0	0
			41	41		
11	B	118	Total	O	0	0
			118	118		
11	D	10	Total	O	0	0
			10	10		
11	H	183	Total	O	0	0
			183	183		
11	I	107	Total	O	0	0
			107	107		
11	L	62	Total	O	0	0
			62	62		
11	M	44	Total	O	0	0
			44	44		

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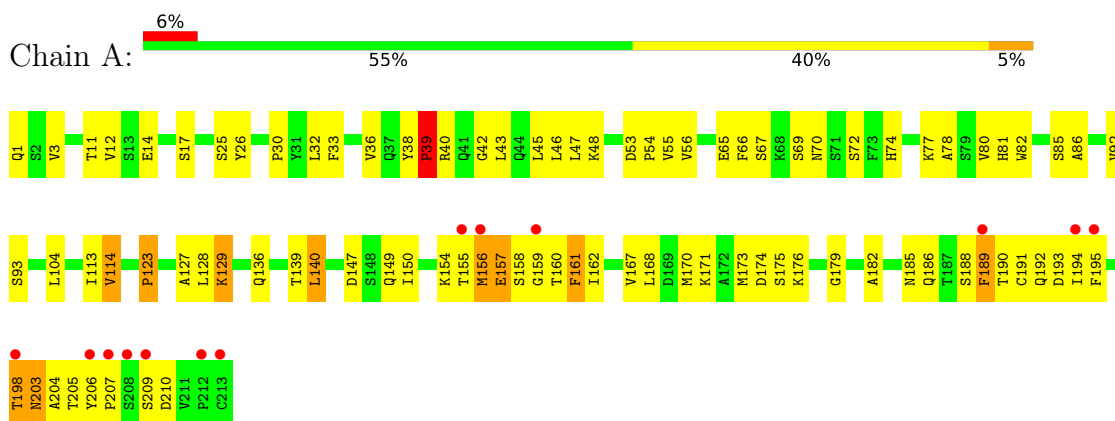
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	2	Total	O	0	0
			2	2		
11	Q	2	Total	O	0	0
			2	2		

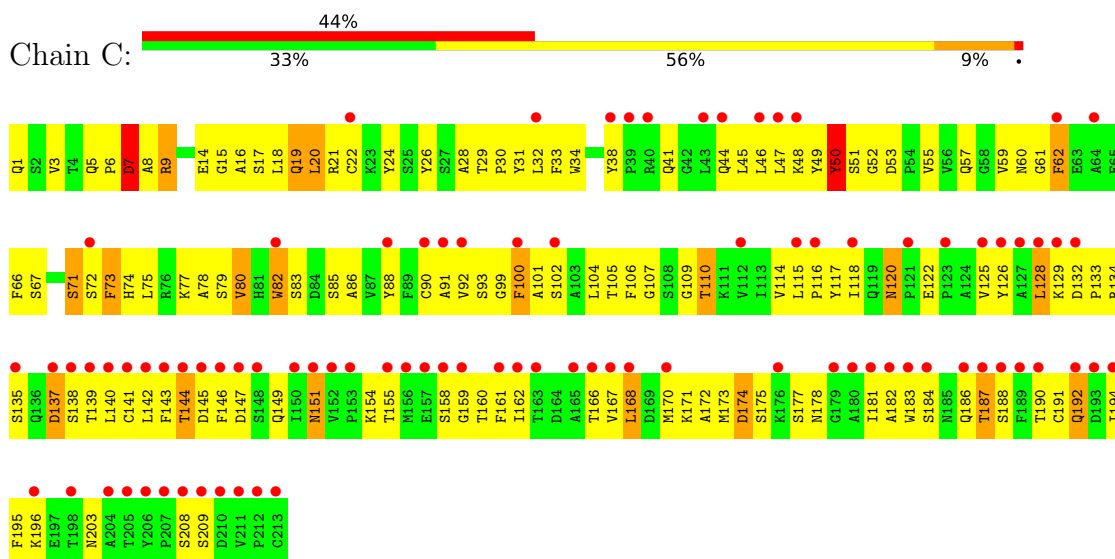
3 Residue-property plots

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.

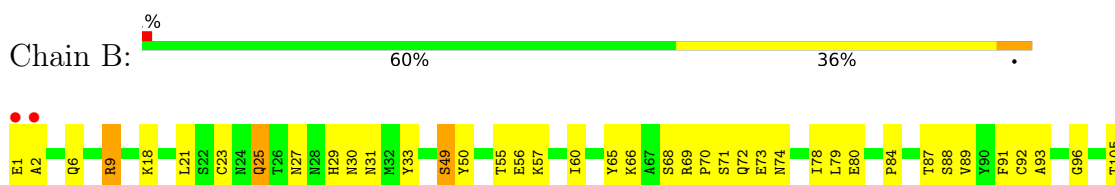
• Molecule 1: 2C T CELL RECEPTOR ALPHA CHAIN

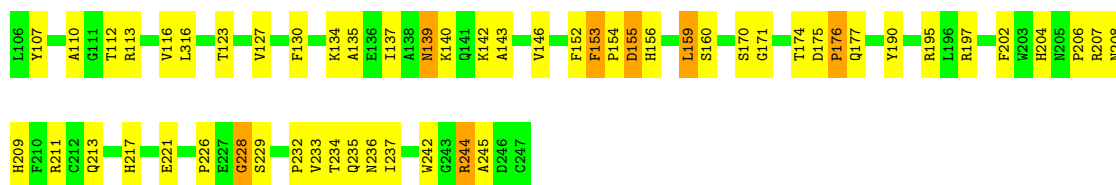


• Molecule 1: 2C T CELL RECEPTOR ALPHA CHAIN

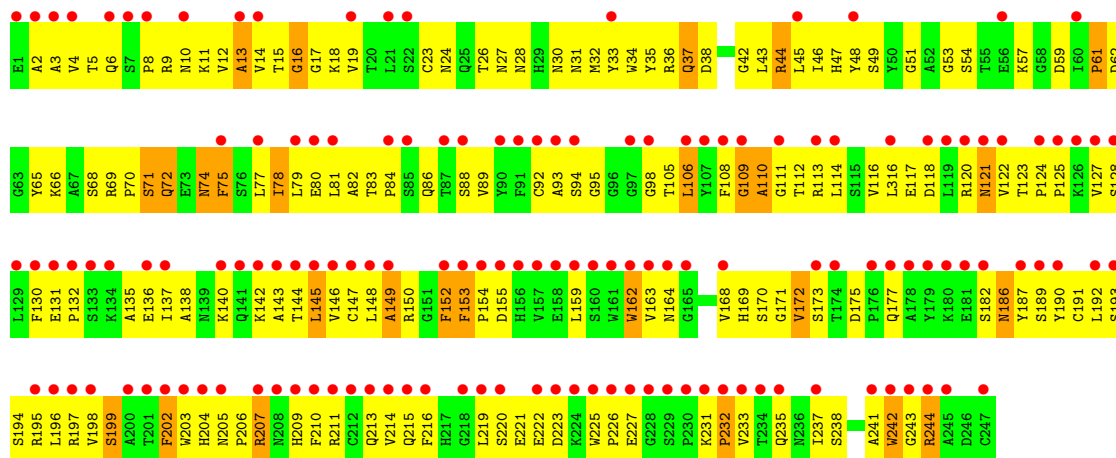


• Molecule 2: 2C T CELL RECEPTOR BETA CHAIN

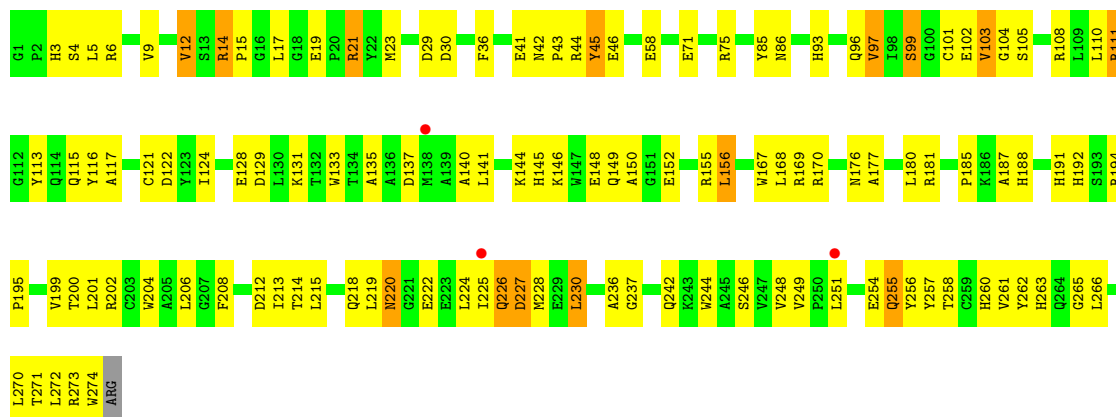




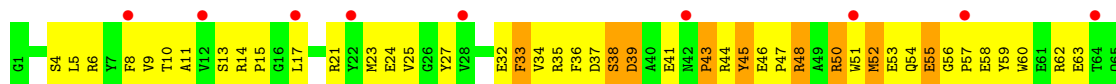
• Molecule 2: 2C T CELL RECEPTOR BETA CHAIN

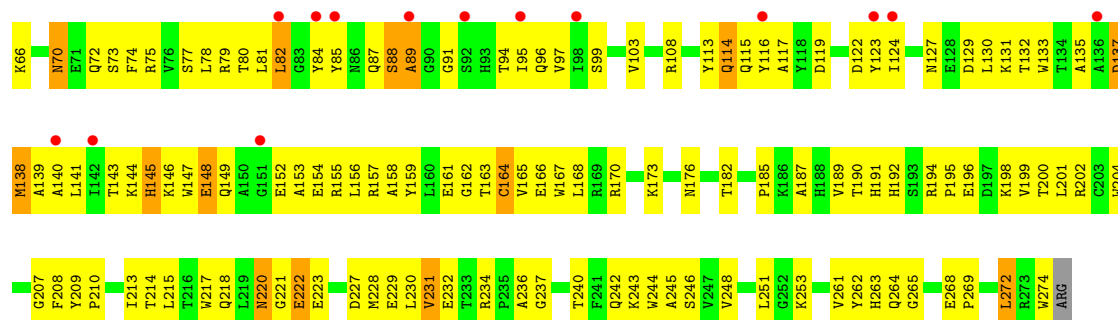


• Molecule 3: H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN



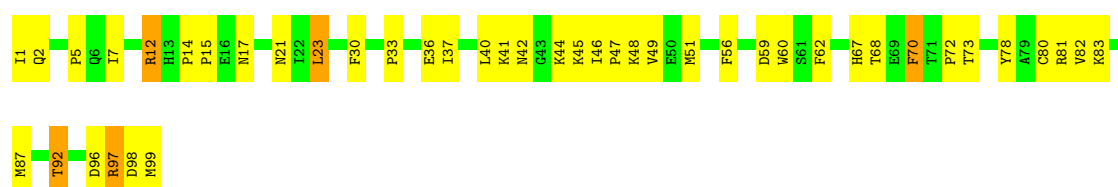
• Molecule 3: H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN





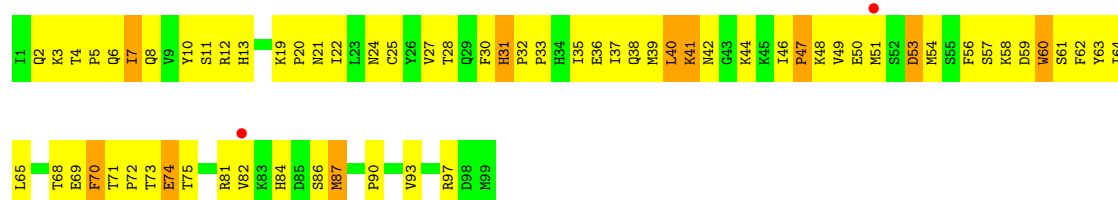
● Molecule 4: MICROGLOBULIN MHC LIGHT CHAIN

Chain L: 56% 39% 5%



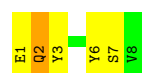
● Molecule 4: MICROGLOBULIN MHC LIGHT CHAIN

Chain M: 33% 57% 10%



● Molecule 5: DEV8

Chain P: 38% 50% 12%



● Molecule 5: DEV8

Chain Q: 75% 62% 38%



● Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%

MAG1
MAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	297.90Å 95.94Å 84.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.40 49.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-2.40) 99.6 (49.65-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.284 , 0.313 0.294 , 0.325	Depositor DCC
R_{free} test set	4781 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13973	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: ACY, NAG, GOL, BMA

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	0.44	0/1611	0.76	0/2193
1	C	0.34	0/1611	0.66	0/2193
2	B	0.43	0/1904	0.75	2/2586 (0.1%)
2	D	0.27	0/1904	0.56	0/2586
3	H	0.41	0/2286	0.71	0/3106
3	I	0.38	1/2285 (0.0%)	0.71	1/3105 (0.0%)
4	L	0.44	0/847	0.77	0/1148
4	M	0.33	0/847	0.72	0/1148
5	P	0.50	0/78	0.77	0/102
5	Q	0.61	0/78	0.88	0/102
All	All	0.39	1/13451 (0.0%)	0.70	3/18269 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
3	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	220	ASN	C-N	-5.16	1.23	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	228	GLY	N-CA-C	-7.15	95.22	113.10
3	I	220	ASN	CA-C-N	-6.59	103.03	116.20
2	B	9	ARG	NE-CZ-NH1	-5.36	117.62	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	50	TYR	Peptide
3	I	220	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1570	0	1503	91	0
1	C	1570	0	1503	153	1
2	B	1853	0	1761	102	0
2	D	1853	0	1763	229	0
3	H	2225	0	2115	120	0
3	I	2224	0	2113	236	0
4	L	821	0	796	39	0
4	M	821	0	796	98	0
5	P	76	0	70	8	0
5	Q	76	0	70	28	0
6	E	28	0	25	1	0
6	K	28	0	26	5	0
7	F	39	0	34	15	0
7	G	39	0	34	4	0
7	J	39	0	33	13	0
8	A	6	0	8	0	0
8	I	6	0	8	0	0
8	L	6	0	8	0	0
9	B	14	0	13	0	0
10	P	4	0	3	0	0
11	A	106	0	0	8	0
11	B	118	0	0	10	1
11	C	41	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	10	0	0	1	0
11	H	183	0	0	9	0
11	I	107	0	0	16	0
11	L	62	0	0	3	0
11	M	44	0	0	19	0
11	P	2	0	0	0	0
11	Q	2	0	0	0	0
All	All	13973	0	12682	1051	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

The worst 5 of 1051 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)
2:B:236:ASN:HD21	7:J:1:NAG:C1	1.18	1.50
7:J:2:NAG:H61	7:J:3:BMA:C2	1.52	1.34
7:J:2:NAG:C6	7:J:3:BMA:H2	1.32	1.32
1:A:185:ASN:HD21	7:F:1:NAG:C2	1.53	1.20
1:A:185:ASN:ND2	7:F:1:NAG:C2	2.07	1.18

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:SER:CB	11:B:859:HOH:O[4_555]	1.98	0.22

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	200/202 (99%)	169 (84%)	24 (12%)	7 (4%)	3	3
1	C	200/202 (99%)	134 (67%)	43 (22%)	23 (12%)	0	0
2	B	235/237 (99%)	214 (91%)	17 (7%)	4 (2%)	9	11
2	D	235/237 (99%)	154 (66%)	62 (26%)	19 (8%)	1	0
3	H	272/275 (99%)	246 (90%)	23 (8%)	3 (1%)	14	20
3	I	272/275 (99%)	226 (83%)	34 (12%)	12 (4%)	2	2
4	L	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
4	M	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	0
5	P	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
5	Q	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
All	All	1620/1642 (99%)	1319 (81%)	223 (14%)	78 (5%)	2	1

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	PRO
1	A	140	LEU
1	C	7	ASP
2	B	153	PHE
2	B	226	PRO

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	176/176 (100%)	165 (94%)	11 (6%)	18	28
1	C	176/176 (100%)	161 (92%)	15 (8%)	10	16
2	B	200/200 (100%)	194 (97%)	6 (3%)	41	61
2	D	200/200 (100%)	185 (92%)	15 (8%)	13	21
3	H	231/232 (100%)	215 (93%)	16 (7%)	15	25
3	I	230/232 (99%)	210 (91%)	20 (9%)	10	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	94/94 (100%)	89 (95%)	5 (5%)	22	37
4	M	94/94 (100%)	89 (95%)	5 (5%)	22	37
5	P	8/8 (100%)	7 (88%)	1 (12%)	4	5
5	Q	8/8 (100%)	6 (75%)	2 (25%)	0	0
All	All	1417/1420 (100%)	1321 (93%)	96 (7%)	16	25

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	111	ARG
3	I	87	GLN
3	H	212	ASP
3	I	45	TYR
3	I	114	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	235	GLN
4	M	29	GLN
3	H	220	ASN
4	M	21	ASN
3	I	255	GLN

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 ⓘ

13 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
6	NAG	E	1	1,6	14,14,15	1.08	0	17,19,21	1.78	2 (11%)
6	NAG	E	2	6	14,14,15	1.06	1 (7%)	17,19,21	1.82	5 (29%)
7	NAG	F	1	1,7	14,14,15	0.91	0	17,19,21	1.35	1 (5%)
7	NAG	F	2	7	14,14,15	0.62	0	17,19,21	1.16	1 (5%)
7	BMA	F	3	7	11,11,12	1.53	3 (27%)	15,15,17	2.80	6 (40%)
7	NAG	G	1	1,7	14,14,15	1.09	1 (7%)	17,19,21	1.61	3 (17%)
7	NAG	G	2	7	14,14,15	1.10	2 (14%)	17,19,21	2.28	4 (23%)
7	BMA	G	3	7	11,11,12	1.22	1 (9%)	15,15,17	1.06	0
7	NAG	J	1	2,7	14,14,15	1.00	0	17,19,21	1.64	3 (17%)
7	NAG	J	2	7	14,14,15	1.16	2 (14%)	17,19,21	2.18	4 (23%)
7	BMA	J	3	7	11,11,12	0.79	1 (9%)	15,15,17	1.92	3 (20%)
6	NAG	K	1	6,3	14,14,15	1.04	0	17,19,21	1.86	1 (5%)
6	NAG	K	2	6	14,14,15	0.62	0	17,19,21	1.07	3 (17%)

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
6	NAG	E	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
7	NAG	F	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	F	2	7	-	0/6/23/26	0/1/1/1
7	BMA	F	3	7	-	2/2/19/22	0/1/1/1
7	NAG	G	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,3	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3	BMA	O5-C5	-3.45	1.36	1.43
7	G	3	BMA	O5-C1	-3.30	1.38	1.43
7	J	2	NAG	O5-C1	-2.88	1.39	1.43
7	G	2	NAG	O5-C1	-2.78	1.39	1.43
6	E	2	NAG	O5-C1	-2.76	1.39	1.43

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	O5-C1-C2	-6.91	100.38	111.29
7	G	2	NAG	O5-C1-C2	-6.90	100.39	111.29
7	F	3	BMA	C1-O5-C5	6.76	121.34	112.19
6	E	1	NAG	O5-C1-C2	-6.09	101.67	111.29
7	J	2	NAG	O5-C1-C2	5.43	119.86	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	K	1	NAG	C1

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 38 short contacts:

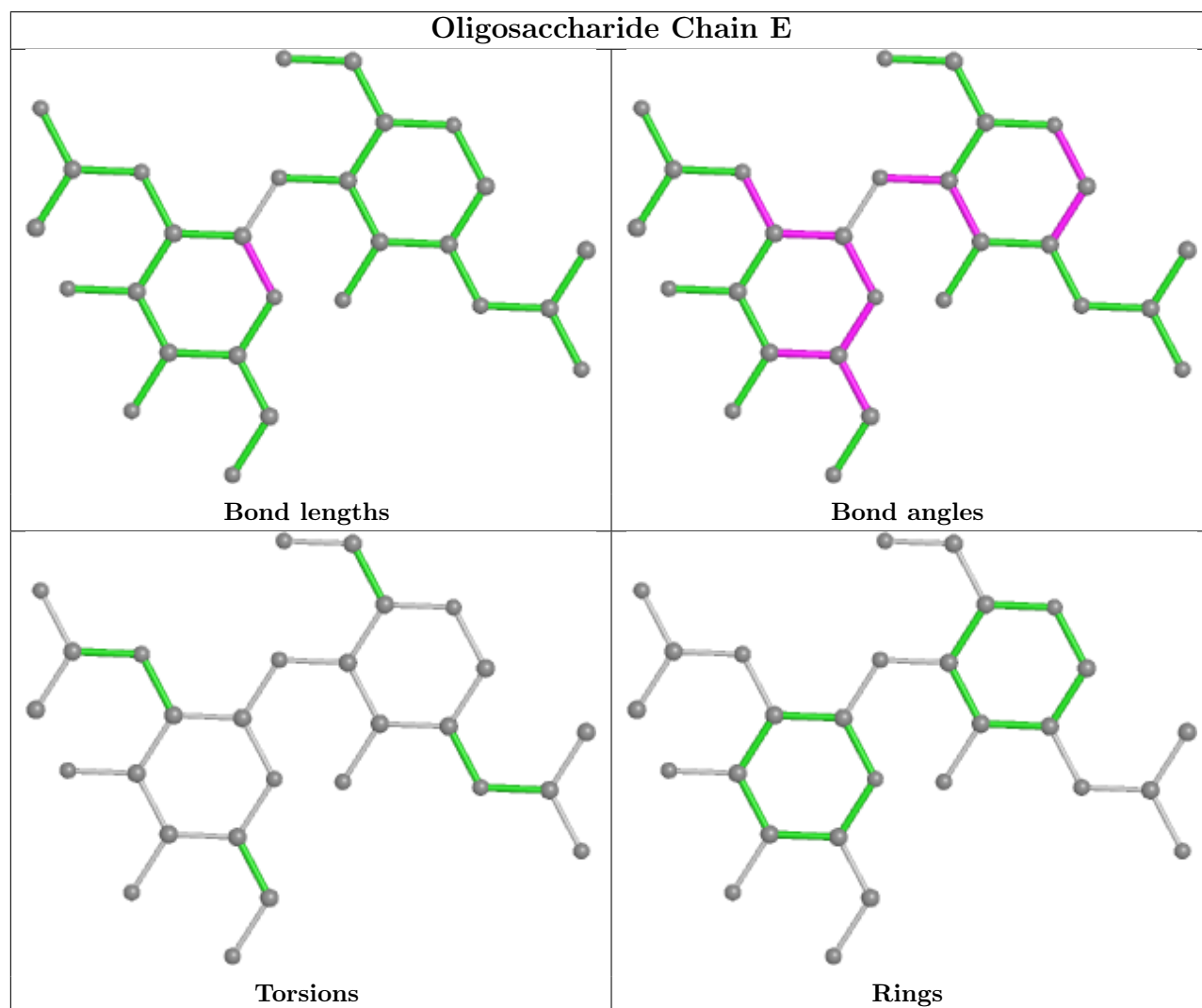
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	2	0
6	K	2	NAG	5	0
7	J	2	NAG	5	0
7	J	3	BMA	5	0
7	F	1	NAG	11	0
7	F	3	BMA	4	0
7	G	1	NAG	4	0
7	F	2	NAG	5	0

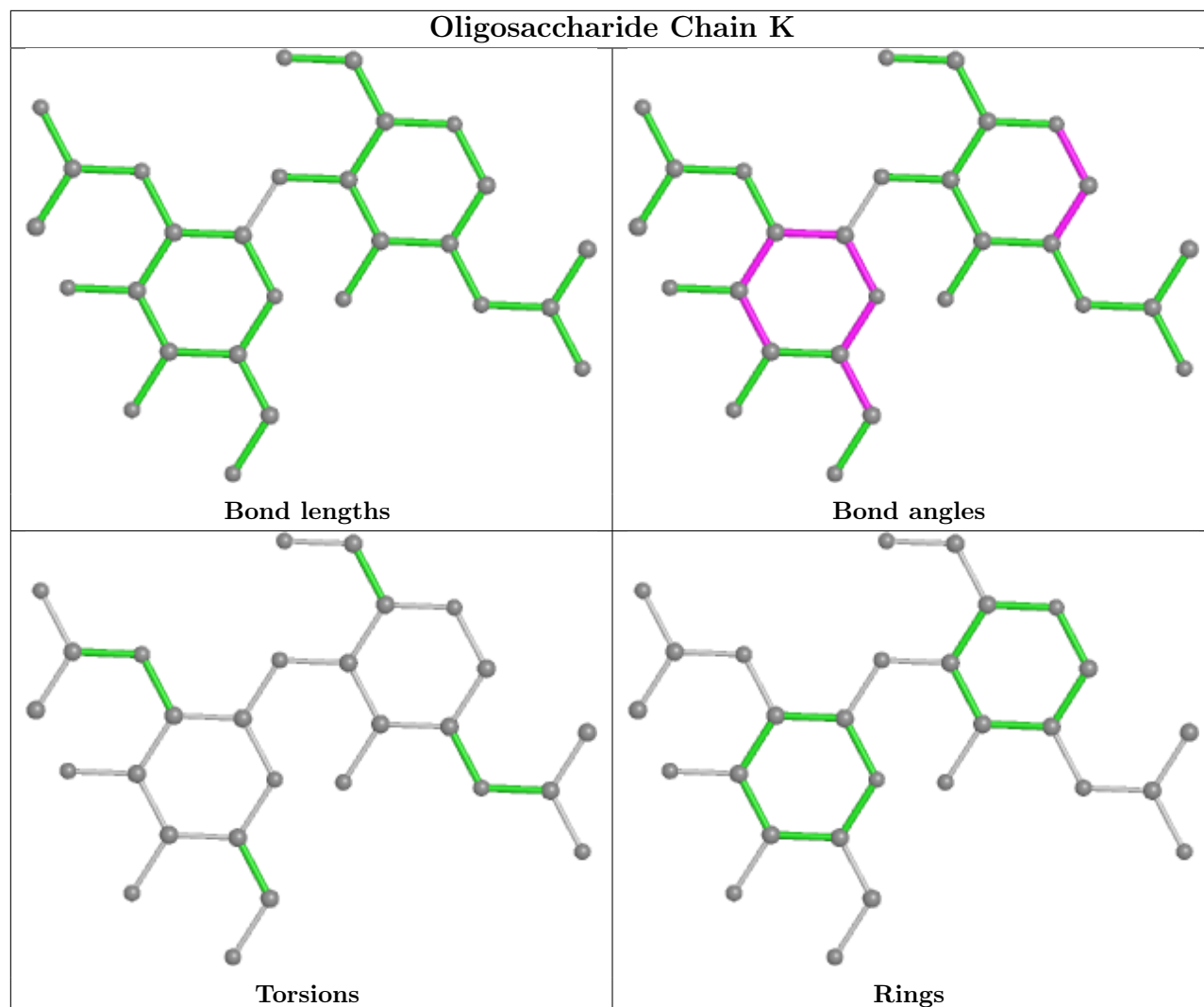
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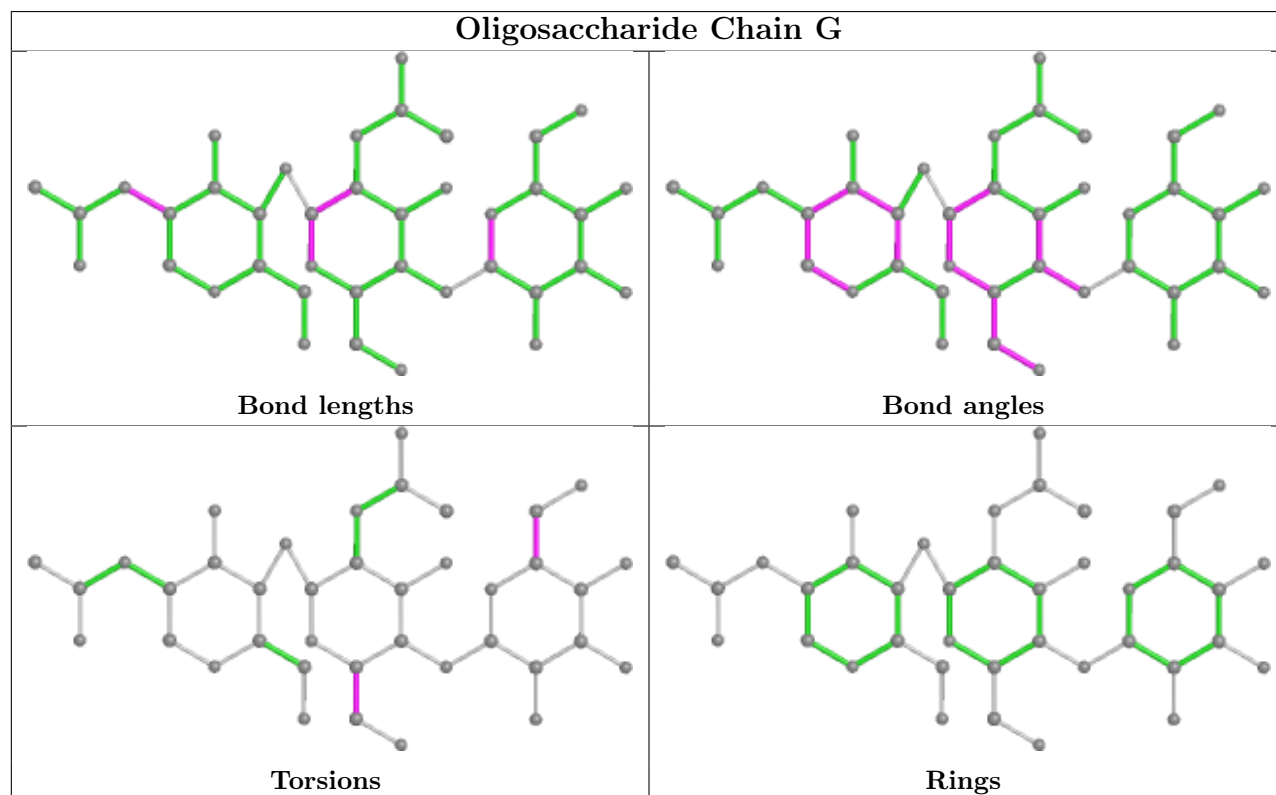
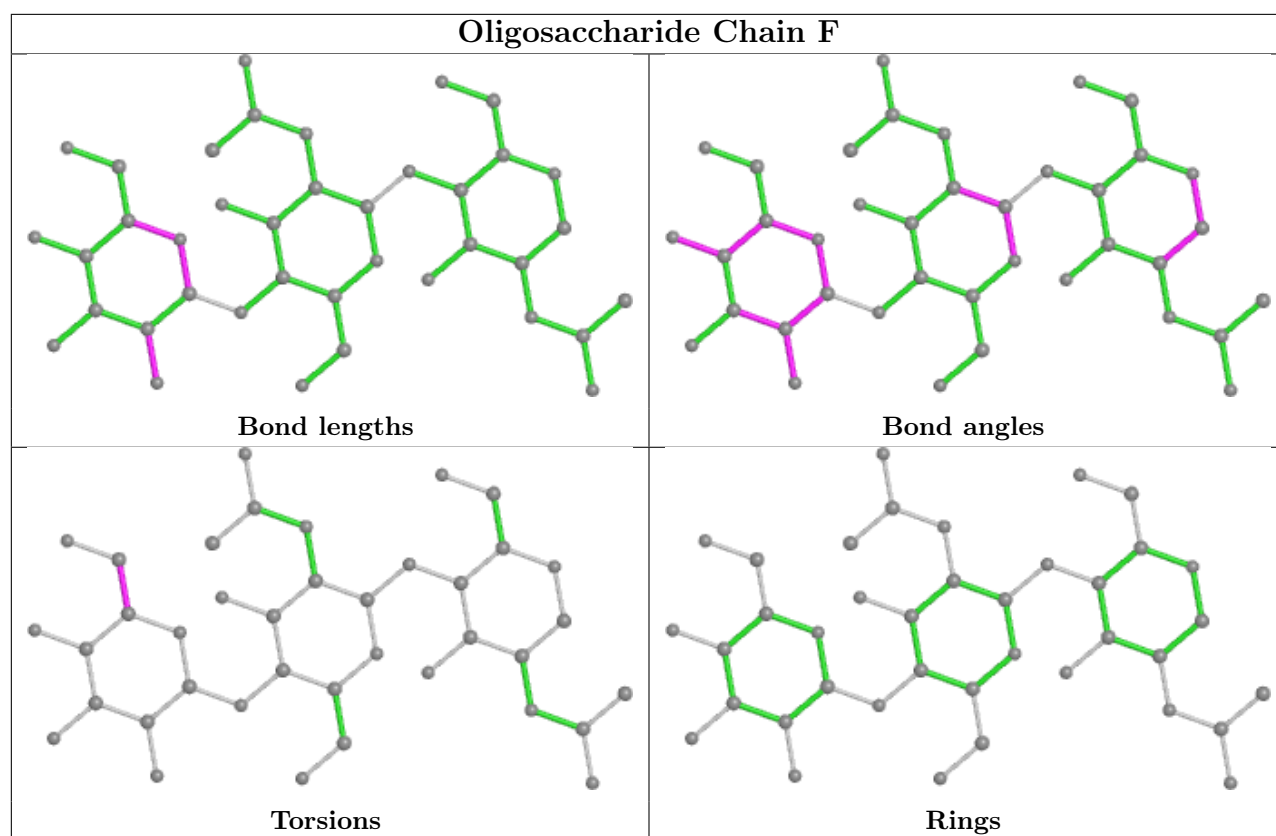
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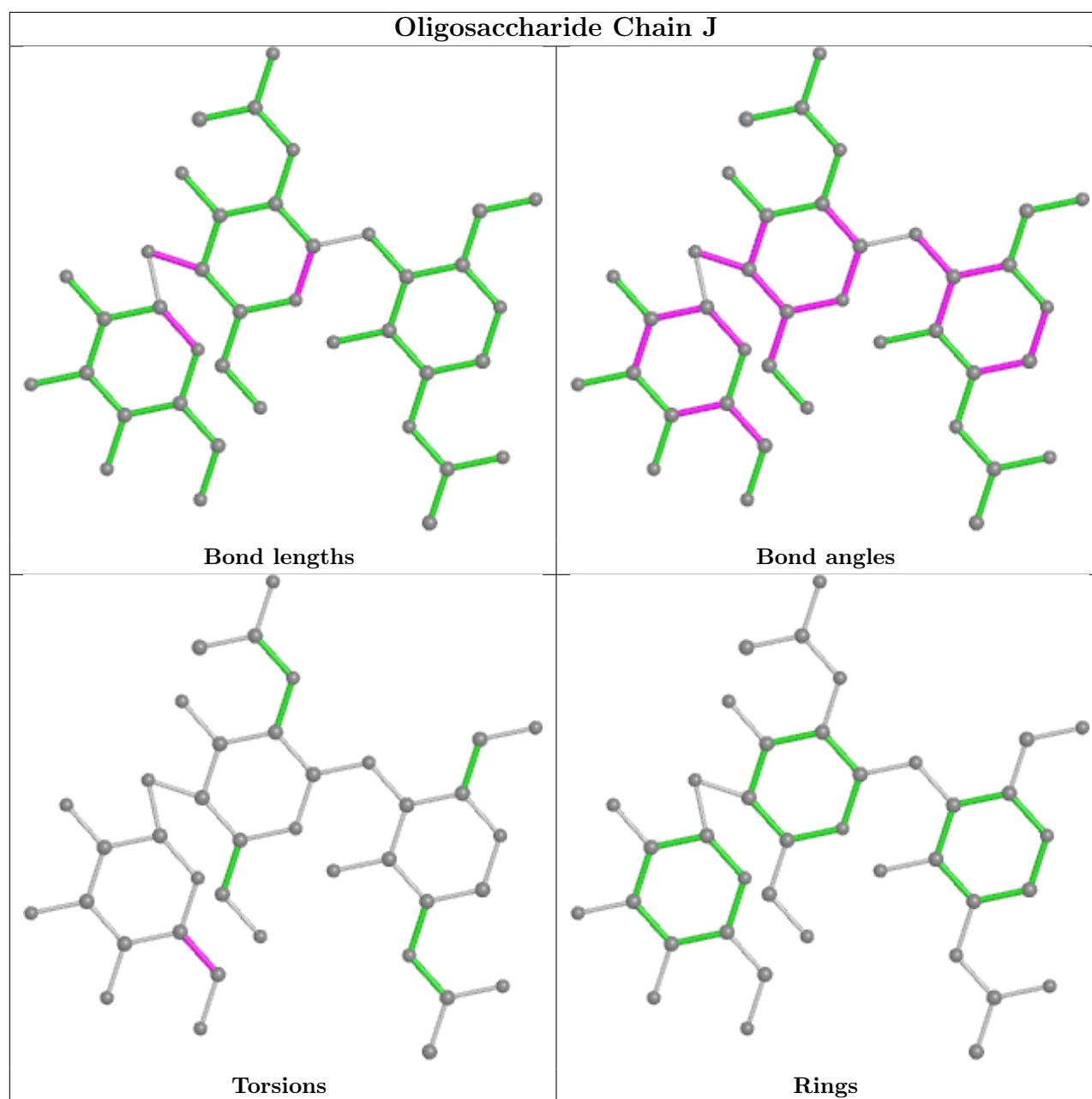
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1	NAG	8	0
7	G	2	NAG	3	0
6	E	1	NAG	1	0

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](#)

5 ligands 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
10	ACY	P	1001	-	3,3,3	0.81	0	3,3,3	1.13	0
9	NAG	B	808	2	14,14,15	0.91	1 (7%)	17,19,21	1.71	1 (5%)
8	GOL	A	902	-	5,5,5	0.28	0	5,5,5	0.70	0
8	GOL	L	901	-	5,5,5	0.34	0	5,5,5	0.68	0
8	GOL	I	903	-	5,5,5	0.66	0	5,5,5	0.79	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
8	GOL	A	902	-	-	2/4/4/4	-
8	GOL	L	901	-	-	2/4/4/4	-
8	GOL	I	903	-	-	2/4/4/4	-
9	NAG	B	808	2	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	808	NAG	C2-N2	-2.17	1.42	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	808	NAG	O5-C1-C2	-5.86	102.03	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	808	NAG	C1

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	902	GOL	C1-C2-C3-O3
8	I	903	GOL	C1-C2-C3-O3
8	L	901	GOL	C1-C2-C3-O3
8	A	902	GOL	O2-C2-C3-O3
8	I	903	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	202/202 (100%)	0.44	13 (6%) 19 18	4, 25, 74, 98	0
1	C	202/202 (100%)	2.33	89 (44%) 0 0	52, 82, 127, 136	0
2	B	237/237 (100%)	0.10	2 (0%) 86 84	14, 27, 47, 74	0
2	D	237/237 (100%)	3.22	143 (60%) 0 0	59, 113, 124, 141	0
3	H	274/275 (99%)	0.12	3 (1%) 80 79	7, 23, 43, 54	0
3	I	274/275 (99%)	0.57	23 (8%) 11 10	15, 47, 70, 77	0
4	L	99/99 (100%)	-0.11	0 100 100	9, 21, 36, 44	0
4	M	99/99 (100%)	0.57	2 (2%) 65 63	32, 47, 61, 65	0
5	P	8/8 (100%)	0.28	0 100 100	10, 14, 19, 19	0
5	Q	8/8 (100%)	3.46	6 (75%) 0 0	81, 84, 89, 91	0
All	All	1640/1642 (99%)	0.98	281 (17%) 1 1	4, 39, 122, 141	0

The worst 5 of 281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	145	LEU	15.6
1	C	211	VAL	14.1
2	D	218	GLY	13.3
2	D	214	VAL	12.7
1	C	127	ALA	11.6

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

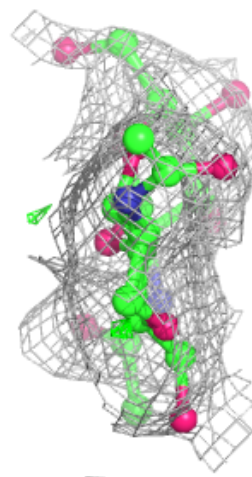
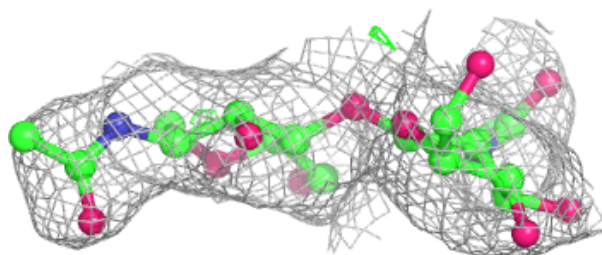
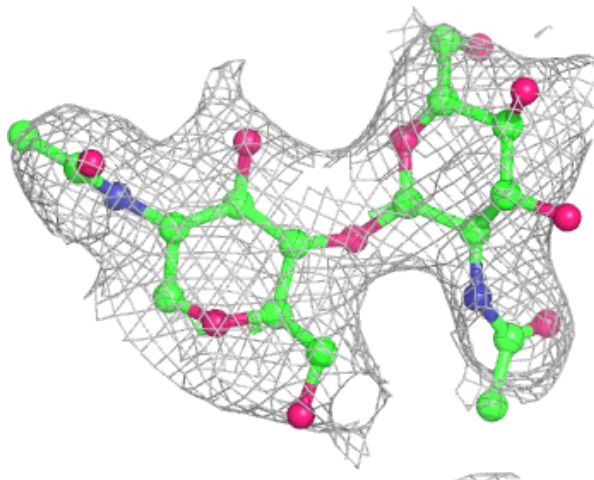
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	F	1	14/15	0.49	0.32	128,129,130,130	0
7	NAG	G	2	14/15	0.53	0.29	125,127,128,130	0
6	NAG	K	1	14/15	0.67	0.20	102,113,115,115	0
7	NAG	F	2	14/15	0.71	0.39	130,130,130,131	0
7	BMA	F	3	11/12	0.73	0.23	129,130,130,131	0
7	NAG	G	1	14/15	0.75	0.19	115,122,124,125	0
7	BMA	J	3	11/12	0.78	0.19	121,123,124,124	0
6	NAG	K	2	14/15	0.80	0.33	125,126,126,126	0
7	NAG	J	1	14/15	0.81	0.36	101,103,106,108	0
6	NAG	E	2	14/15	0.82	0.26	109,114,116,116	0
7	BMA	G	3	11/12	0.83	0.25	131,132,132,133	0
7	NAG	J	2	14/15	0.87	0.27	112,115,117,119	0
6	NAG	E	1	14/15	0.88	0.30	80,88,98,103	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.

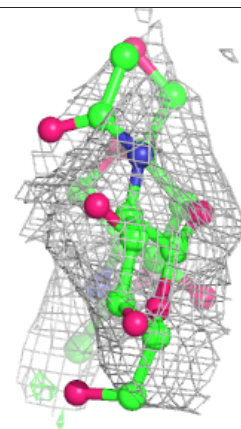
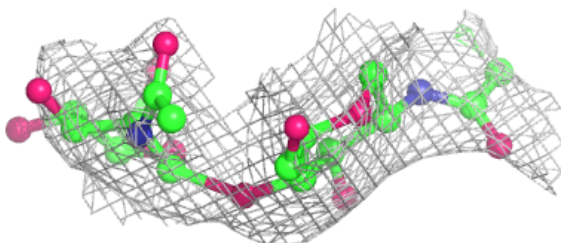
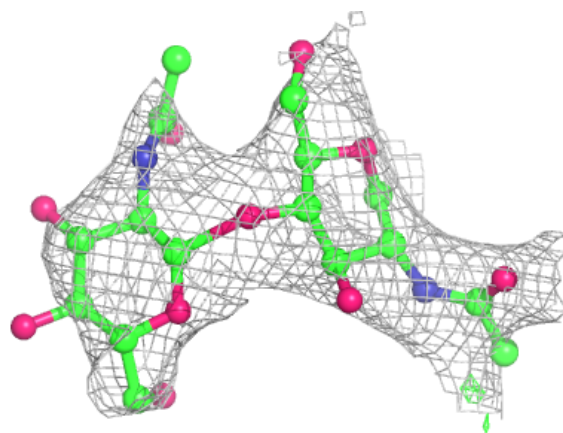
Electron density around Chain E:

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

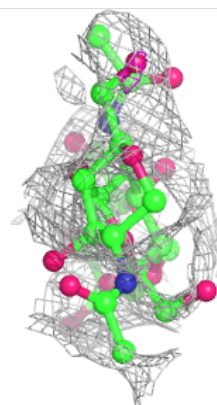
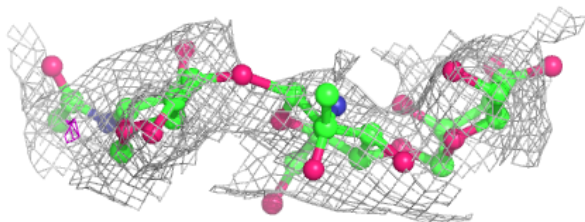
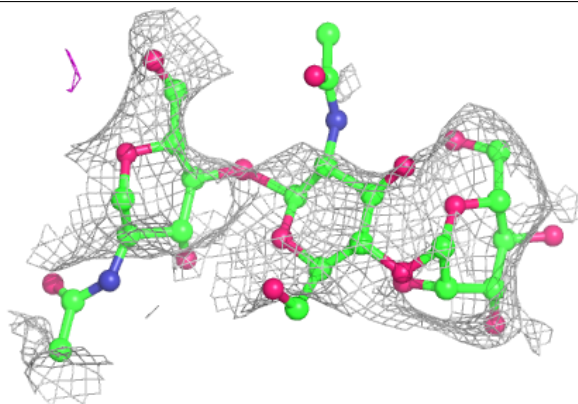


Electron density around Chain K:

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

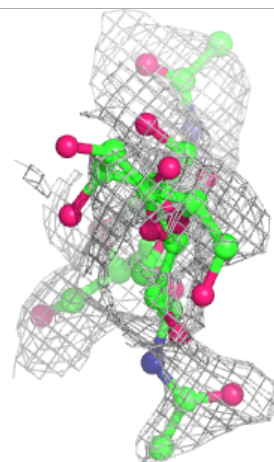
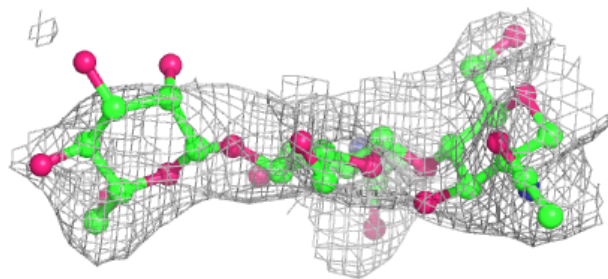
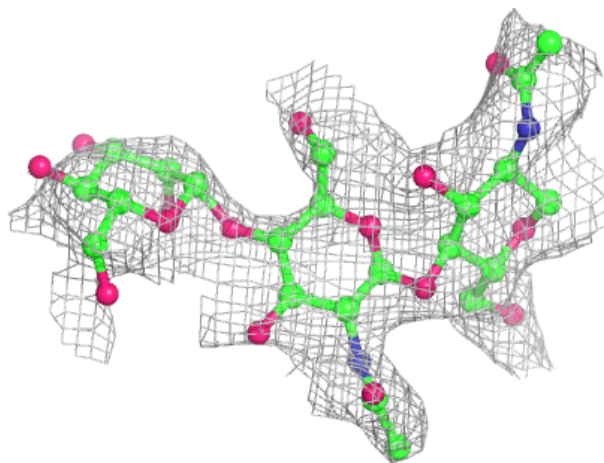
**Electron density around Chain F:**

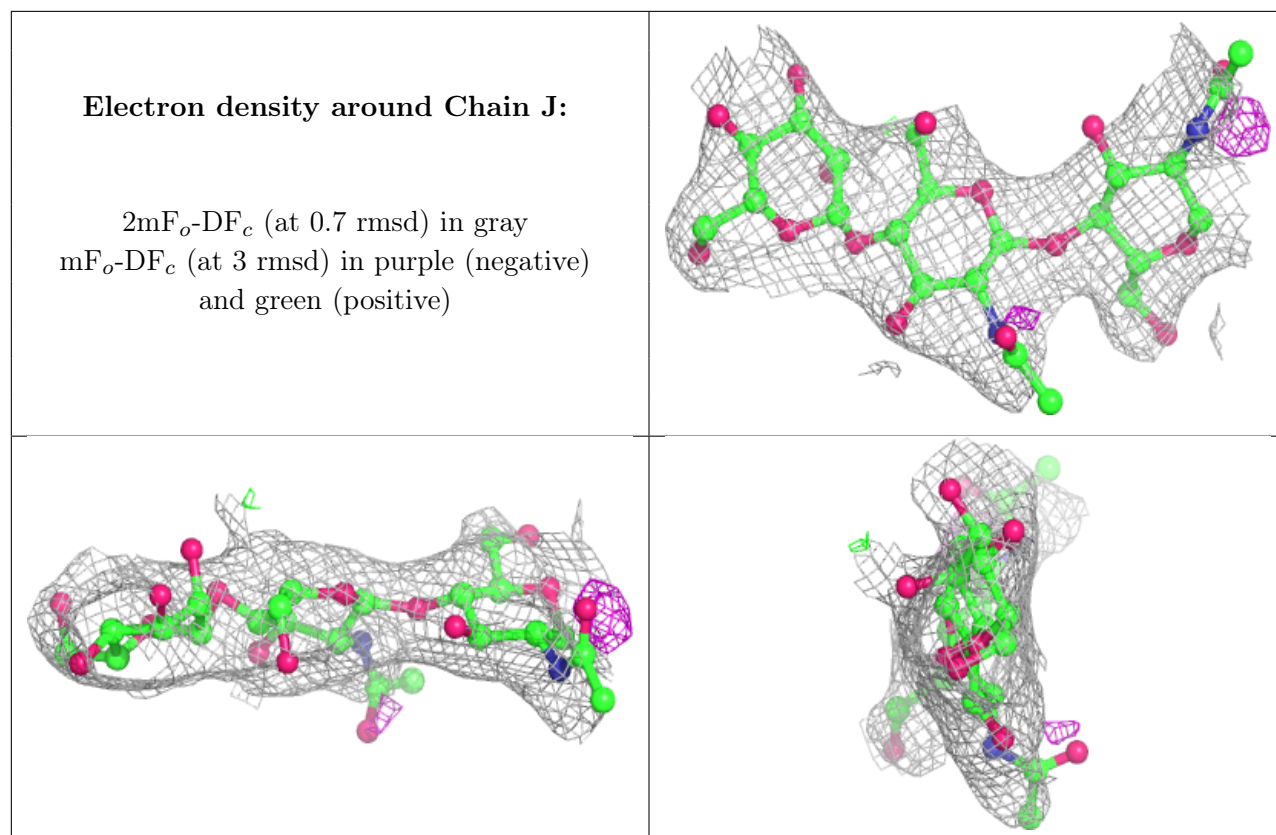
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(\AA^2)	Q<0.9
9	NAG	B	808	14/15	0.59	0.29	91,103,104,105	0
8	GOL	I	903	6/6	0.62	0.27	101,102,102,102	0
10	ACY	P	1001	4/4	0.69	0.56	84,84,84,85	0
8	GOL	L	901	6/6	0.81	0.34	101,101,101,101	0
8	GOL	A	902	6/6	0.82	0.53	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.