



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:14 AM UTC

PDB ID : 7S2S / pdb_00007s2s
Title : nanobody bound to Interleukin-2Rbeta
Authors : Glassman, C.R.; Jude, K.M.; Yen, M.; Garcia, K.C.
Deposited on : 2021-09-03
Resolution : 1.93 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

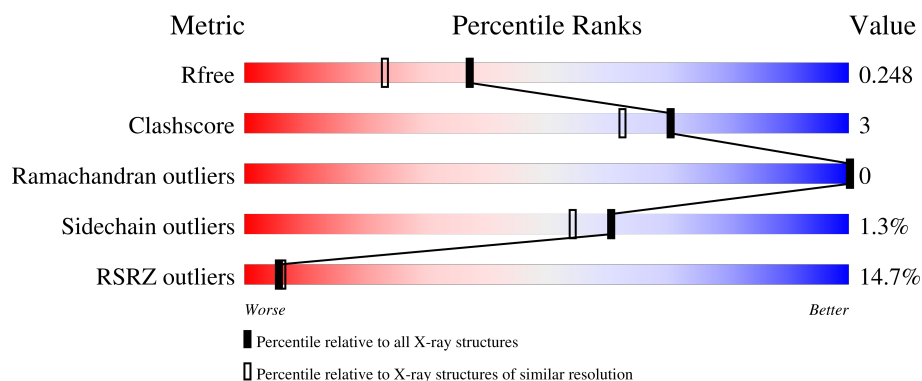
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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.



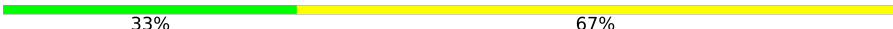
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	154	21% 75% 7% 18%
1	C	154	14% 72% 10% 18%
2	B	216	9% 84% 8% 8%
2	D	216	11% 85% 9% 6%
3	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	F	3	 67% 33%
3	H	3	 67% 33%
3	I	3	 33% 67%
4	G	3	 67% 33%
4	J	3	 67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5660 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 IL2Rb-binding nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	127	Total	C	N	O	S	0	0	0
			929	576	161	185	7			
1	A	127	Total	C	N	O	S	0	1	0
			948	589	166	186	7			

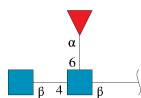
- Molecule 2 is a protein called Interleukin-2 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	199	Total	C	N	O	S	0	0	0
			1635	1045	289	291	10			
2	D	204	Total	C	N	O	S	0	0	0
			1659	1060	291	298	10			

There are 12 discrepancies between the modelled and reference sequences:

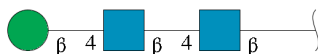
Chain	Residue	Modelled	Actual	Comment	Reference
B	237	HIS	-	expression tag	UNP P14784
B	238	HIS	-	expression tag	UNP P14784
B	239	HIS	-	expression tag	UNP P14784
B	240	HIS	-	expression tag	UNP P14784
B	241	HIS	-	expression tag	UNP P14784
B	242	HIS	-	expression tag	UNP P14784
D	237	HIS	-	expression tag	UNP P14784
D	238	HIS	-	expression tag	UNP P14784
D	239	HIS	-	expression tag	UNP P14784
D	240	HIS	-	expression tag	UNP P14784
D	241	HIS	-	expression tag	UNP P14784
D	242	HIS	-	expression tag	UNP P14784

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



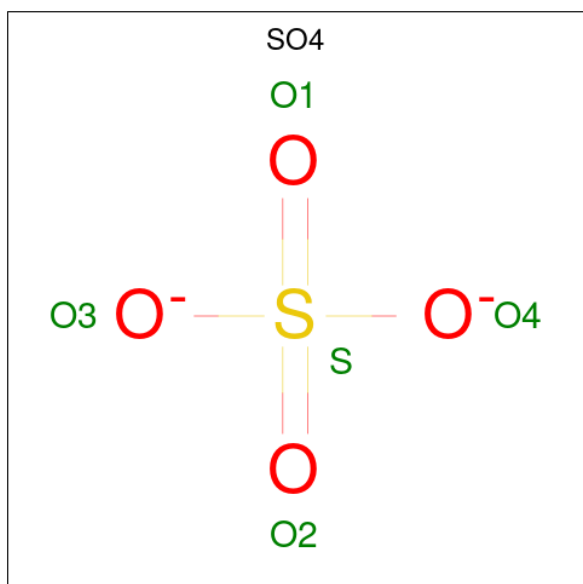
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	H	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 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
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

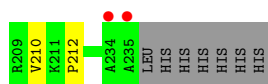
- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	12	Total O 12 12	0	0
6	B	82	Total O 82 82	0	0
6	A	7	Total O 7 7	0	0
6	D	92	Total O 93 93	0	1



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 33% 67%



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

Chain G: 67% 33%



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

Chain J: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.70Å 69.50Å 91.72Å 99.57° 99.85° 90.19°	Depositor
Resolution (Å)	44.53 – 1.93 44.53 – 1.93	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.53-1.93) 95.9 (44.53-1.93)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.213 , 0.247 0.214 , 0.248	Depositor DCC
R_{free} test set	2012 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5660	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 7.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, MLY, NAG, SO4

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	0.13	0/959	0.32	0/1298
1	C	0.13	0/937	0.32	0/1270
2	B	0.20	0/1661	0.43	0/2269
2	D	0.20	0/1686	0.43	0/2306
All	All	0.18	0/5243	0.39	0/7143

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	948	0	917	6	0
1	C	929	0	881	8	0
2	B	1635	0	1580	8	0
2	D	1659	0	1595	14	0
3	E	38	0	34	0	0
3	F	38	0	34	1	0
3	H	38	0	34	1	0
3	I	38	0	34	1	0
4	G	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	39	0	34	0	0
5	A	5	0	0	1	0
5	B	20	0	0	0	0
5	D	40	0	0	0	0
6	A	7	0	0	0	0
6	B	82	0	0	0	0
6	C	12	0	0	0	0
6	D	93	0	0	2	0
All	All	5660	0	5177	36	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 3.

All (36) 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:D:184:LEU:HD23	2:D:193:ILE:HD11	1.57	0.86
2:D:161:PHE:O	2:D:165:LEU:HG	1.96	0.66
2:D:54:LEU:HD13	4:G:3:BMA:H3	1.77	0.65
2:B:147:ARG:NH1	2:B:196:GLU:OE2	2.30	0.64
1:C:34:MET:HE2	1:C:78:LEU:HD22	1.79	0.64
2:D:117:ARG:HD3	2:D:119:MET:HE1	1.80	0.62
2:B:161:PHE:O	2:B:165:LEU:HG	2.02	0.60
2:D:166:GLU:HG3	2:D:187:LYS:HG3	1.84	0.59
2:B:167:PHE:CD1	2:B:210:VAL:HG12	2.39	0.57
2:D:165:LEU:HD13	2:D:210:VAL:HG21	1.85	0.57
1:A:66:ARG:NH2	1:A:89:ASP:OD2	2.38	0.56
2:B:79:VAL:HG11	2:B:85:ALA:HB3	1.89	0.54
1:A:87:PRO:O	1:A:90:THR:HG22	2.12	0.50
1:C:20:LEU:HG	1:C:82:MET:HE2	1.94	0.50
2:B:49:SER:HB3	2:B:83:SER:HB3	1.95	0.48
1:C:67:PHE:CE1	1:C:82:MET:HB3	2.49	0.47
1:C:92:MET:SD	1:C:123:GLN:HG2	2.55	0.46
1:A:37:PHE:CD2	1:A:47:GLY:HA2	2.52	0.45
2:D:107:ARG:NH1	6:D:401:HOH:O	2.35	0.45
2:D:135:PRO:HG2	2:D:208:VAL:HG13	1.98	0.45
1:A:6:GLU:HG3	1:A:95:CYS:SG	2.56	0.45
1:C:36:TRP:CD1	1:C:80:LEU:HB2	2.52	0.45
2:B:64:TRP:CE2	3:F:1:NAG:H5	2.52	0.44
2:B:135:PRO:HG2	2:B:208:VAL:HG13	2.00	0.44
1:C:37:PHE:CD2	1:C:47:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LEU:HB3	2:B:227:LEU:HD22	2.00	0.43
1:C:3:GLN:HB3	1:C:4:LEU:H	1.74	0.42
2:D:87:ASN:CG	3:H:1:NAG:H5	2.46	0.41
1:A:6:GLU:HB2	1:A:122:THR:HG23	2.02	0.41
1:C:38:ARG:HA	1:C:92:MET:O	2.21	0.41
2:D:165:LEU:HD23	2:D:212:PRO:HA	2.03	0.41
2:D:64:TRP:HE3	2:D:107:ARG:HH12	1.68	0.41
2:D:64:TRP:HH2	3:I:2:NAG:H82	1.85	0.41
2:D:53:ALA:C	2:D:55:GLN:H	2.29	0.40
1:A:64:LYS:HD2	5:A:201:SO4:O1	2.21	0.40
2:D:190:GLN:NE2	6:D:408:HOH:O	2.48	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	125/154 (81%)	122 (98%)	3 (2%)	0	100	100
1	C	124/154 (80%)	124 (100%)	0	0	100	100
2	B	193/216 (89%)	182 (94%)	11 (6%)	0	100	100
2	D	200/216 (93%)	190 (95%)	10 (5%)	0	100	100
All	All	642/740 (87%)	618 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	98/119 (82%)	97 (99%)	1 (1%)	68	64
1	C	94/119 (79%)	91 (97%)	3 (3%)	34	20
2	B	178/193 (92%)	176 (99%)	2 (1%)	65	60
2	D	179/193 (93%)	178 (99%)	1 (1%)	78	78
All	All	549/624 (88%)	542 (99%)	7 (1%)	61	54

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	11	SER
1	C	25	SER
1	C	82	MET
2	B	190	GLN
2	B	214	GLN
1	A	111	GLU
2	D	83	SER

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

Mol	Chain	Res	Type
1	C	81	GLN
1	C	83	ASN
2	B	139	GLN
2	B	142	HIS
2	B	176	HIS
2	B	188	GLN
2	B	190	GLN
1	A	81	GLN
1	A	123	GLN
2	D	87	ASN
2	D	122	GLN
2	D	142	HIS
2	D	176	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	MLY	D	211	2	9,10,11	0.58	0	6,11,13	0.85	0
2	MLY	D	97	2	9,10,11	0.55	0	6,11,13	0.97	0
1	MLY	C	71	1	9,10,11	0.56	0	6,11,13	0.79	0
2	MLY	B	211	2	9,10,11	0.48	0	6,11,13	0.87	0
2	MLY	B	97	2	9,10,11	0.64	0	6,11,13	0.78	0
1	MLY	A	71	1	9,10,11	0.53	0	6,11,13	0.83	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	MLY	D	211	2	-	3/8/9/11	-
2	MLY	D	97	2	-	0/8/9/11	-
1	MLY	C	71	1	-	4/8/9/11	-
2	MLY	B	211	2	-	3/8/9/11	-
2	MLY	B	97	2	-	2/8/9/11	-
1	MLY	A	71	1	-	3/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	71	MLY	N-CA-CB-CG
1	A	71	MLY	C-CA-CB-CG
2	B	97	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	C	71	MLY	CD-CE-NZ-CH1
1	C	71	MLY	CD-CE-NZ-CH2
2	B	97	MLY	CG-CD-CE-NZ
1	C	71	MLY	CE-CD-CG-CB
2	B	211	MLY	CA-CB-CG-CD
2	B	211	MLY	C-CA-CB-CG
2	D	211	MLY	C-CA-CB-CG
2	B	211	MLY	N-CA-CB-CG
2	D	211	MLY	N-CA-CB-CG
1	A	71	MLY	CE-CD-CG-CB
2	D	211	MLY	CA-CB-CG-CD
1	C	71	MLY	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
3	NAG	E	1	2,3	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.69	1 (5%)
3	FUC	E	3	3	10,10,11	0.75	0	14,14,16	0.68	0
3	NAG	F	1	2,3	14,14,15	0.20	0	17,19,21	0.65	1 (5%)
3	NAG	F	2	3	14,14,15	0.35	0	17,19,21	0.64	1 (5%)
3	FUC	F	3	3	10,10,11	0.90	1 (10%)	14,14,16	0.96	0
4	NAG	G	1	4,2	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	G	2	4	14,14,15	0.21	0	17,19,21	0.47	0
4	BMA	G	3	4	11,11,12	0.67	0	15,15,17	0.76	0
3	NAG	H	1	2,3	14,14,15	0.35	0	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.36	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	H	3	3	10,10,11	0.98	0	14,14,16	0.88	0
3	NAG	I	1	2,3	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
3	NAG	I	2	3	14,14,15	0.46	0	17,19,21	0.42	0
3	FUC	I	3	3	10,10,11	0.87	0	14,14,16	0.78	0
4	NAG	J	1	4,2	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	J	2	4	14,14,15	0.19	0	17,19,21	0.52	0
4	BMA	J	3	4	11,11,12	0.56	0	15,15,17	0.84	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
3	NAG	E	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
4	NAG	G	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
3	NAG	H	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	FUC	H	3	3	-	-	0/1/1/1
3	NAG	I	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
4	NAG	J	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	FUC	C1-C2	2.24	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	I	1	NAG	C1-O5-C5	2.45	115.47	112.19
3	E	2	NAG	C1-O5-C5	2.35	115.34	112.19
3	F	1	NAG	C1-O5-C5	2.19	115.12	112.19
3	F	2	NAG	C1-O5-C5	2.17	115.09	112.19
4	J	3	BMA	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

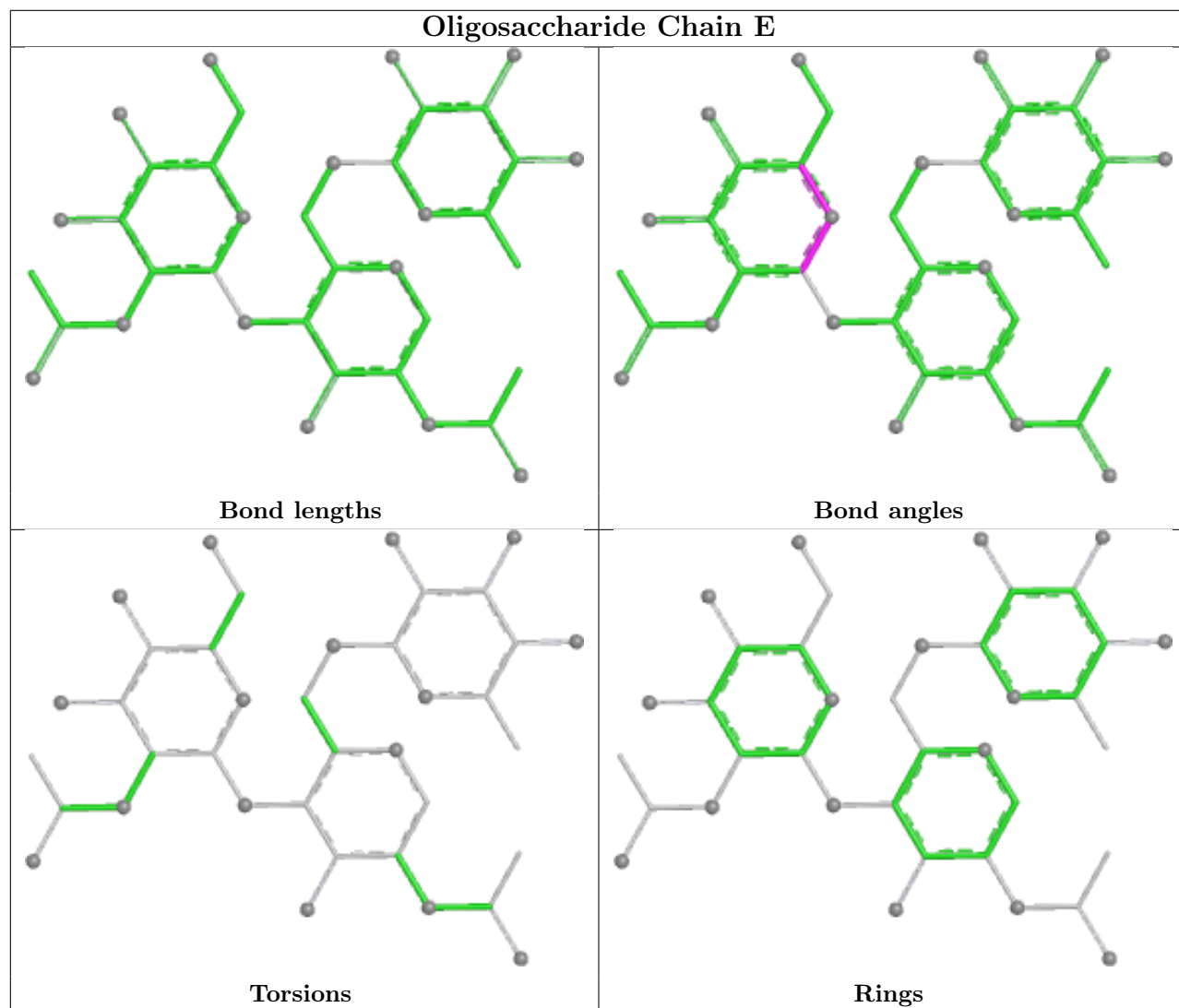
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7

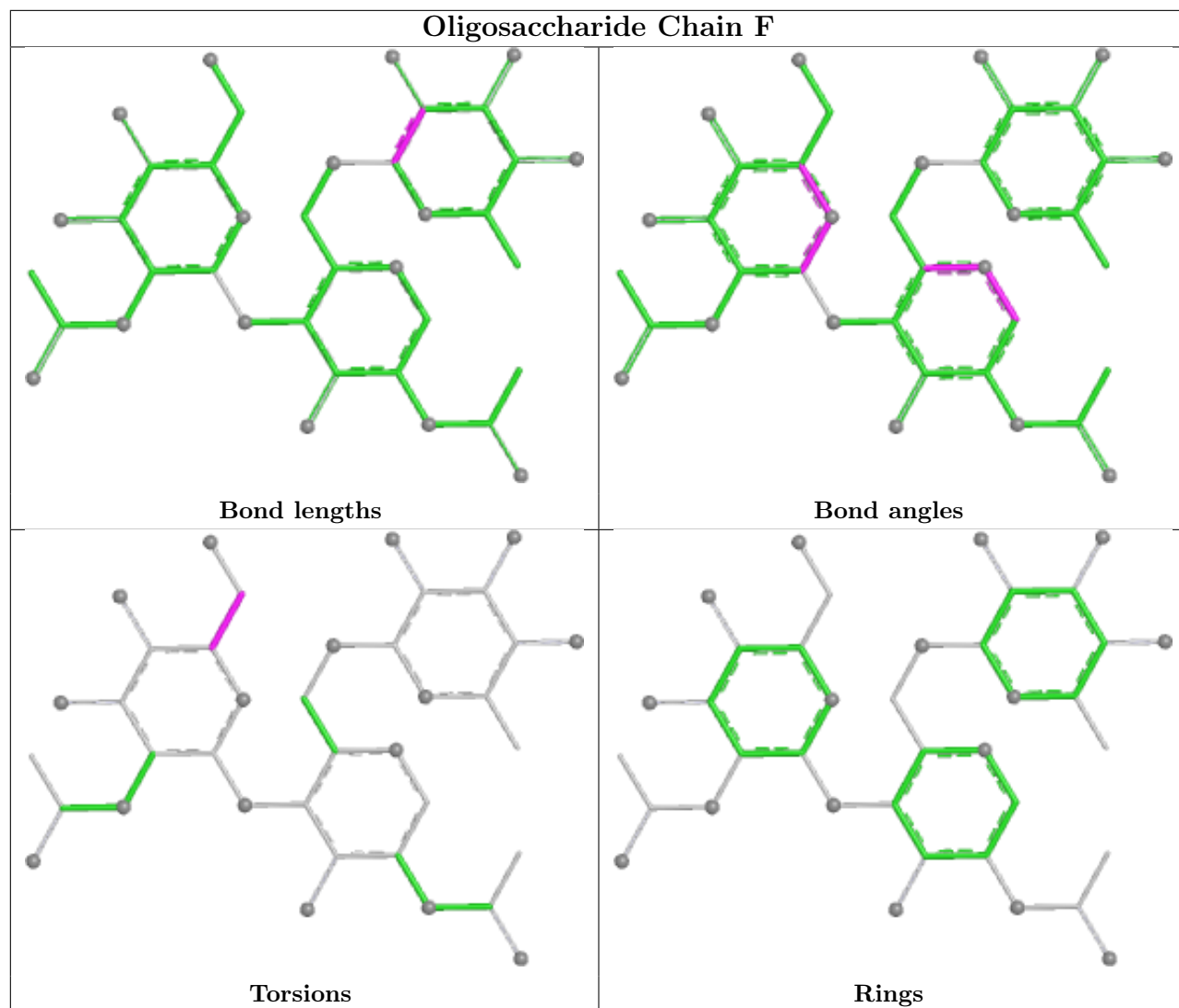
There are no ring outliers.

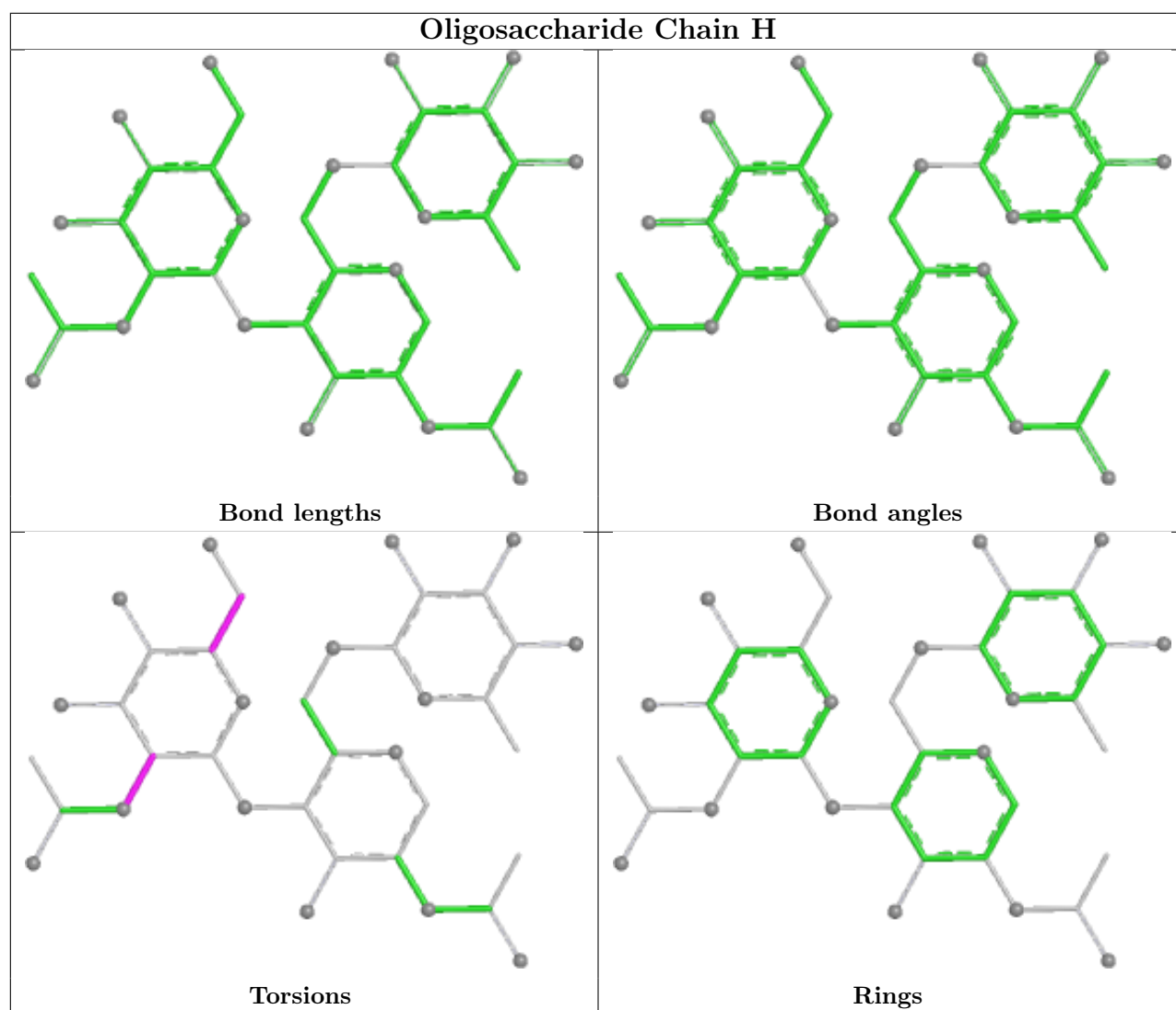
4 monomers are involved in 4 short contacts:

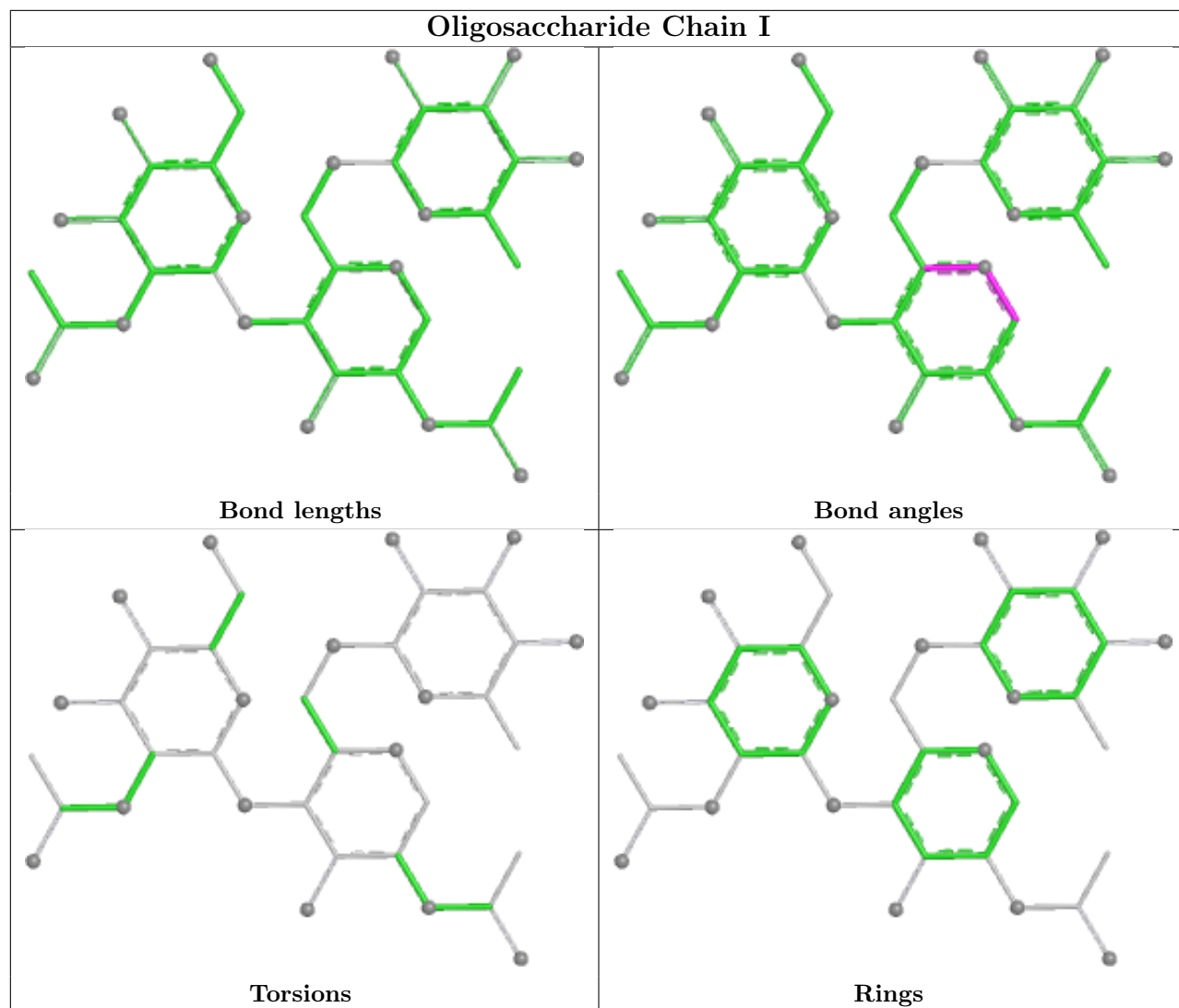
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
4	G	3	BMA	1	0
3	H	1	NAG	1	0
3	I	2	NAG	1	0

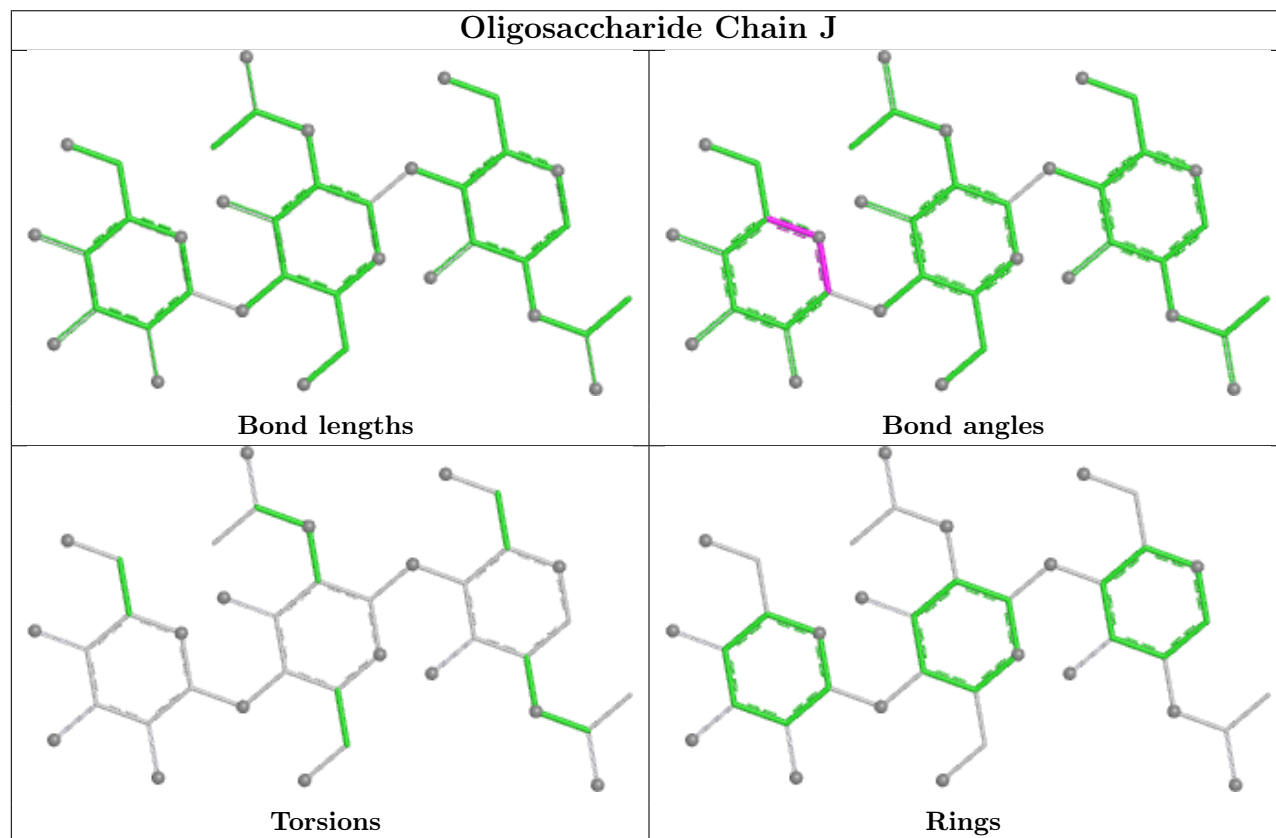
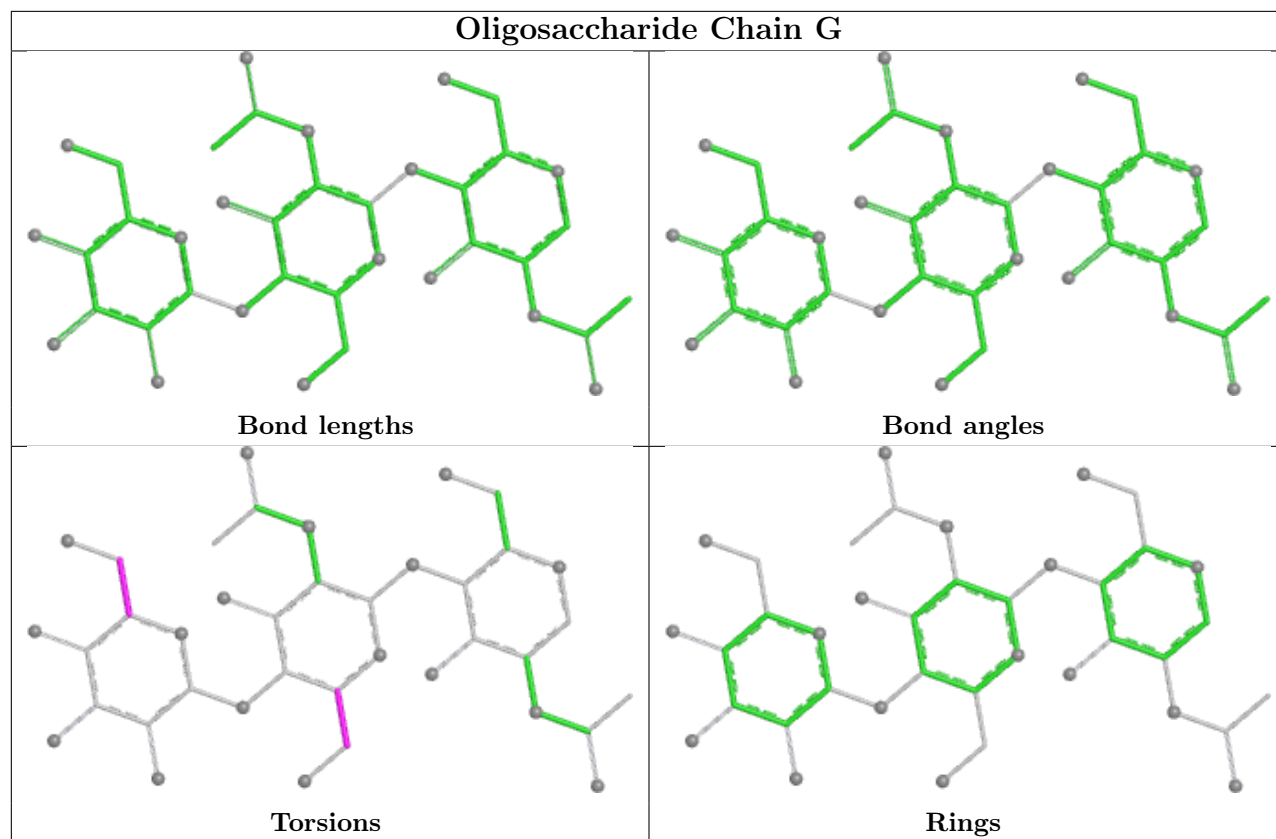
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry

13 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	$\# Z > 2$
5	SO4	D	303	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	D	307	-	4,4,4	0.26	0	6,6,6	0.09	0
5	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	D	304	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	D	301	-	4,4,4	0.26	0	6,6,6	0.10	0
5	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	D	308	-	4,4,4	0.24	0	6,6,6	0.18	0
5	SO4	A	201	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	D	302	-	4,4,4	0.25	0	6,6,6	0.06	0
5	SO4	D	305	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	D	306	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	B	304	-	4,4,4	0.24	0	6,6,6	0.09	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	201	SO4	1	0

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	126/154 (81%)	1.38	32 (25%) 1 1	22, 81, 110, 129	1 (0%)
1	C	126/154 (81%)	1.15	21 (16%) 4 4	35, 78, 101, 122	0
2	B	197/216 (91%)	0.60	19 (9%) 13 15	24, 37, 81, 115	0
2	D	202/216 (93%)	0.68	24 (11%) 9 10	25, 37, 94, 152	0
All	All	651/740 (87%)	0.88	96 (14%) 6 6	22, 47, 103, 152	1 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	54	LEU	8.4
2	D	53	ALA	6.5
1	A	2	VAL	6.0
2	D	55	GLN	5.9
2	D	56	ASP	5.4
2	B	114	VAL	5.0
1	C	129	GLY	4.3
2	D	114	VAL	4.1
2	B	167	PHE	4.1
2	D	57	THR	4.0
2	B	113	GLY	3.9
2	D	167	PHE	3.9
2	D	82	ALA	3.6
1	A	30	SER	3.6
2	D	235	ALA	3.6
1	A	128	SER	3.5
2	D	32	SER	3.5
1	C	74	ALA	3.4
1	A	116	TYR	3.3
2	B	235	ALA	3.3
2	B	186	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	27	TYR	3.2
2	D	52	GLY	3.2
2	D	116	TRP	3.2
1	A	40	ALA	3.1
1	A	18	LEU	3.0
2	B	116	TRP	3.0
2	B	189	LYS	3.0
1	A	73	ASN	3.0
2	B	57	THR	2.9
2	B	82	ALA	2.9
1	C	116	TYR	2.9
1	A	86	LYS	2.8
1	C	25	SER	2.8
2	B	81	GLN	2.8
1	A	67	PHE	2.7
2	B	51	ASP	2.6
2	B	111	ARG	2.6
2	B	201	ASP	2.6
1	C	18	LEU	2.6
1	A	122	THR	2.6
1	A	14	ALA	2.6
1	A	74	ALA	2.6
1	C	127	SER	2.6
1	A	13	GLN	2.5
1	A	27	TYR	2.5
1	C	29	ILE	2.5
2	D	115	ARG	2.5
1	C	13	GLN	2.5
1	C	126	VAL	2.5
1	A	12	VAL	2.5
2	D	77	LEU	2.5
1	A	10	GLY	2.4
1	C	21	SER	2.4
2	B	115	ARG	2.4
1	A	87	PRO	2.4
1	A	42	GLY	2.4
1	C	28	THR	2.4
2	D	197	THR	2.4
2	B	190	GLN	2.4
2	D	58	SER	2.4
1	A	88	GLU	2.3
1	A	125	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	2.3
2	D	234	ALA	2.3
1	A	16	GLY	2.3
2	B	32	SER	2.3
1	A	90	THR	2.3
1	C	40	ALA	2.3
1	A	127	SER	2.3
1	A	28	THR	2.3
1	A	31	SER	2.2
1	C	12	VAL	2.2
2	D	180	GLU	2.2
1	A	11	SER	2.2
1	A	119	GLY	2.2
1	C	43	LYS	2.2
1	C	87	PRO	2.2
1	A	5	GLN	2.1
2	B	145	THR	2.1
1	C	42	GLY	2.1
1	A	60	GLY	2.1
1	C	128	SER	2.1
2	D	49	SER	2.1
1	A	8	GLY	2.1
1	C	124	VAL	2.1
1	A	124	VAL	2.1
2	D	84	TRP	2.1
2	D	81	GLN	2.1
2	D	184	LEU	2.1
2	D	191	GLU	2.0
1	C	65	GLY	2.0
1	C	84	SER	2.0
2	B	188	GLN	2.0
2	B	197	THR	2.0
2	D	113	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	MLY	A	71	11/12	0.88	0.15	69,80,87,89	0
2	MLY	B	211	11/12	0.92	0.12	26,29,49,50	0
2	MLY	D	211	11/12	0.92	0.12	29,33,59,61	0
2	MLY	B	97	11/12	0.92	0.12	31,34,55,58	0
1	MLY	C	71	11/12	0.93	0.14	54,61,66,67	0
2	MLY	D	97	11/12	0.93	0.12	29,37,58,61	0

6.3 Carbohydrates

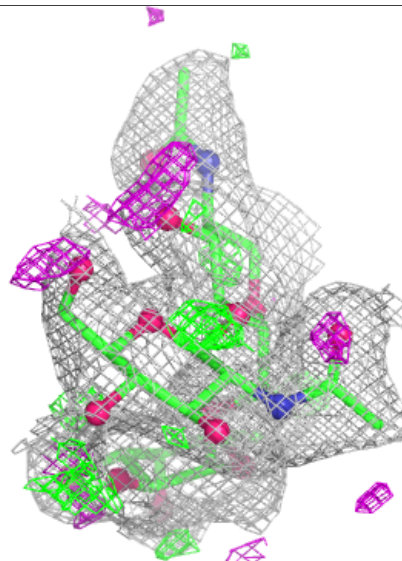
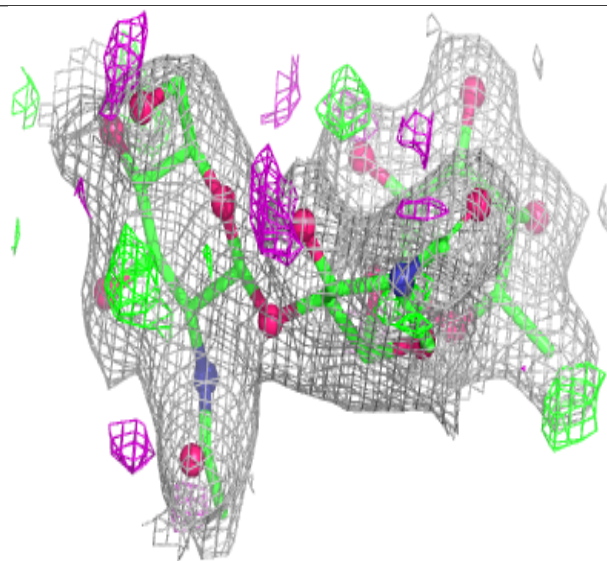
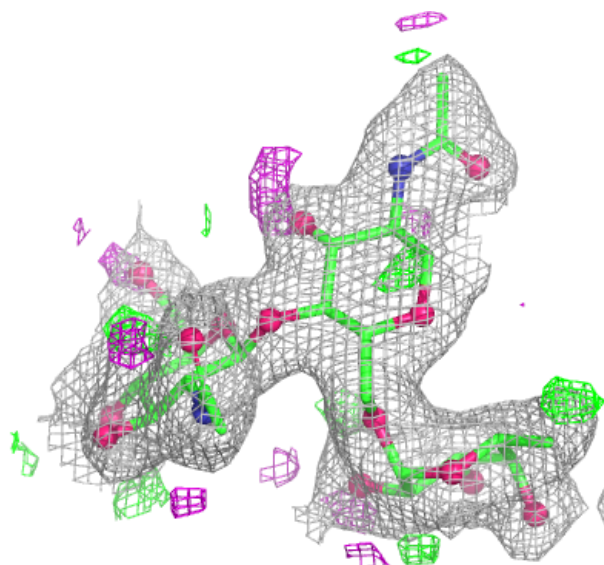
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	G	3	11/12	0.46	0.19	96,103,112,115	0
4	BMA	J	3	11/12	0.51	0.19	82,94,109,111	0
3	NAG	I	2	14/15	0.57	0.23	63,89,105,117	0
3	NAG	F	2	14/15	0.66	0.19	54,70,88,92	0
3	FUC	F	3	10/11	0.79	0.18	51,59,69,77	0
4	NAG	G	2	14/15	0.79	0.16	51,68,94,98	0
3	FUC	I	3	10/11	0.81	0.15	55,59,65,66	0
4	NAG	J	2	14/15	0.85	0.13	49,60,75,83	0
3	NAG	H	2	14/15	0.85	0.12	28,53,64,73	0
3	NAG	E	2	14/15	0.86	0.13	32,48,62,74	0
3	FUC	H	3	10/11	0.89	0.12	33,34,38,39	0
4	NAG	J	1	14/15	0.90	0.11	34,43,55,56	0
4	NAG	G	1	14/15	0.92	0.09	37,43,51,56	0
3	NAG	I	1	14/15	0.93	0.10	35,44,61,71	0
3	NAG	H	1	14/15	0.94	0.09	25,33,43,43	0
3	NAG	F	1	14/15	0.94	0.09	34,42,51,59	0
3	NAG	E	1	14/15	0.94	0.08	25,32,43,43	0
3	FUC	E	3	10/11	0.94	0.08	27,33,34,35	0

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

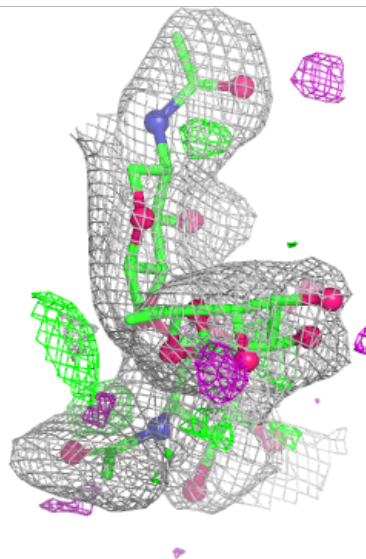
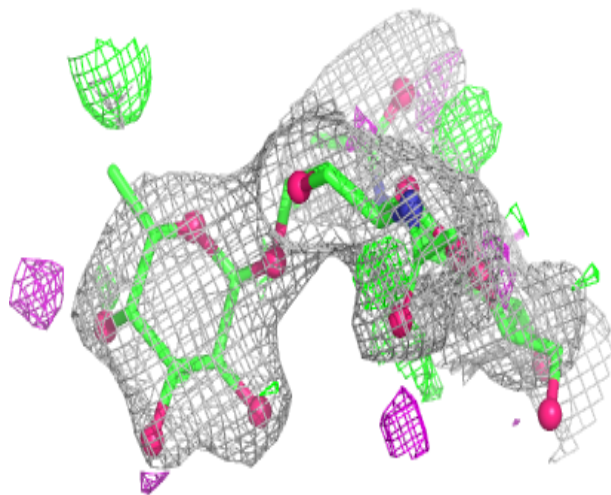
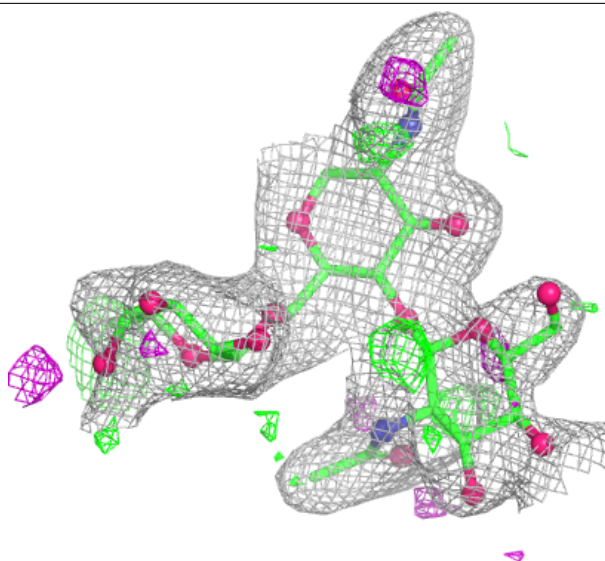
Electron density around Chain E:

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



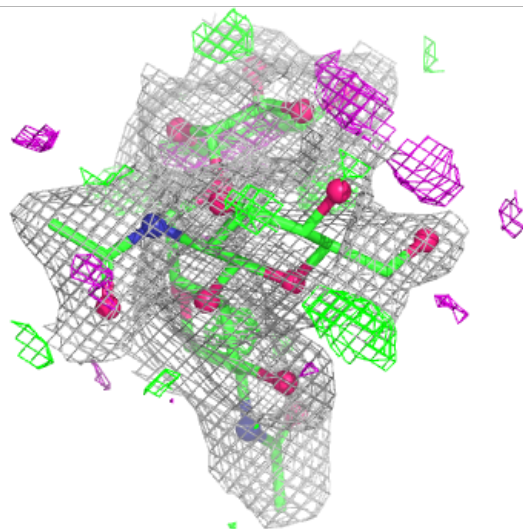
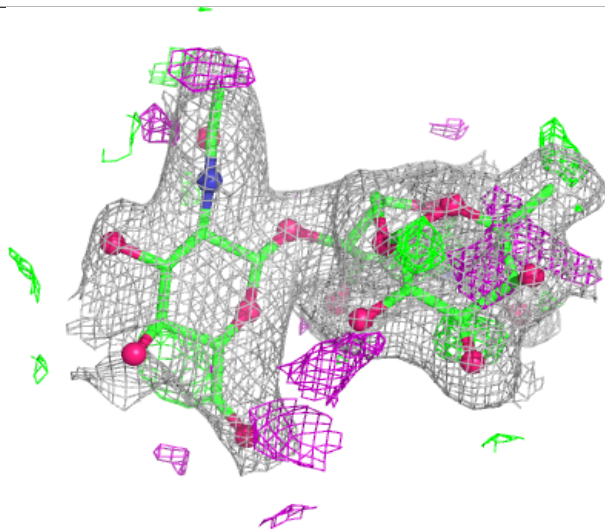
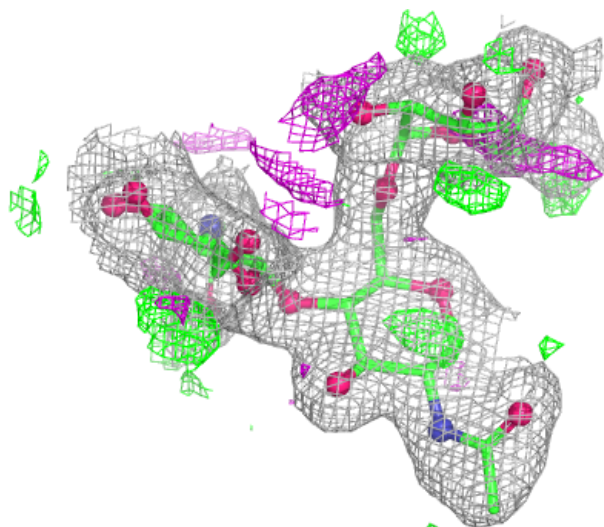
Electron density around Chain F:

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



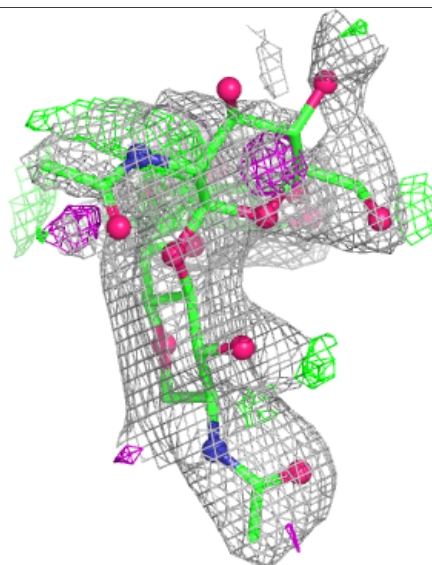
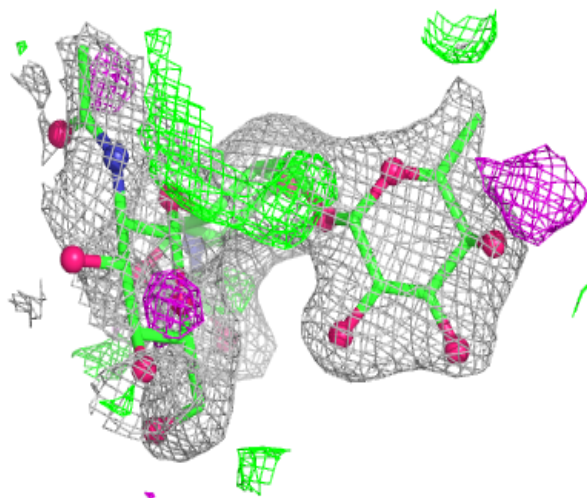
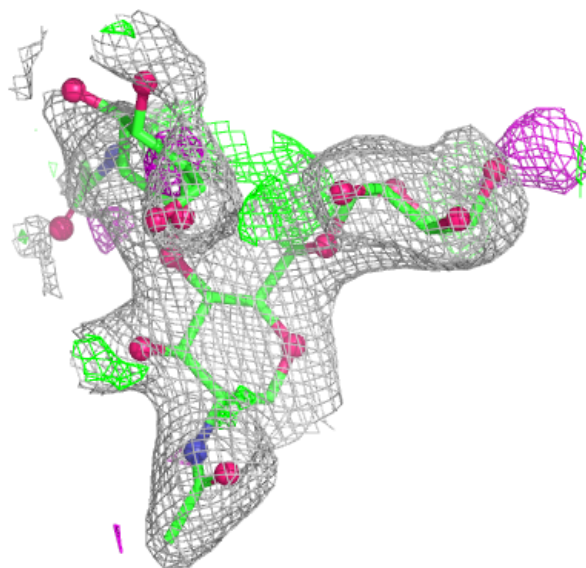
Electron density around Chain H:

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



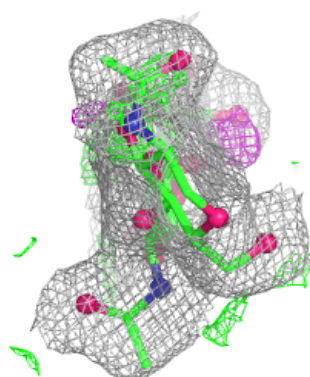
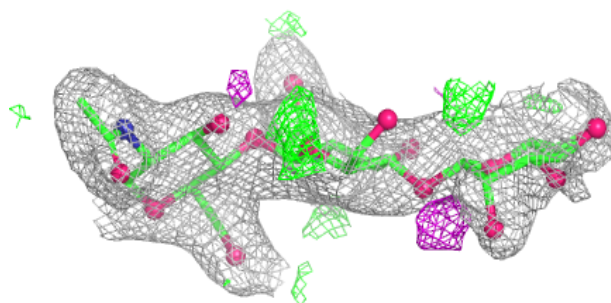
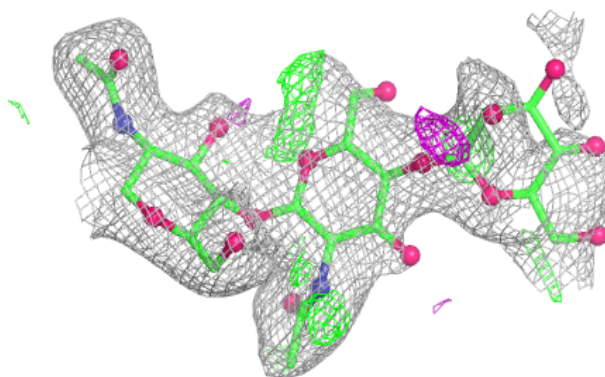
Electron density around Chain I:

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

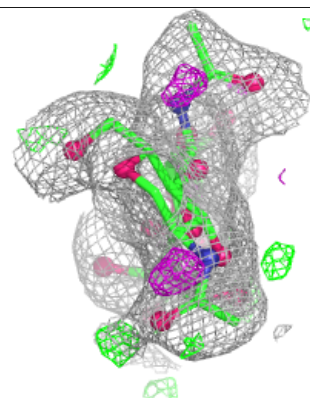
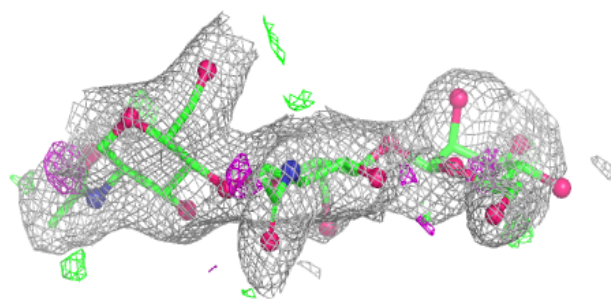
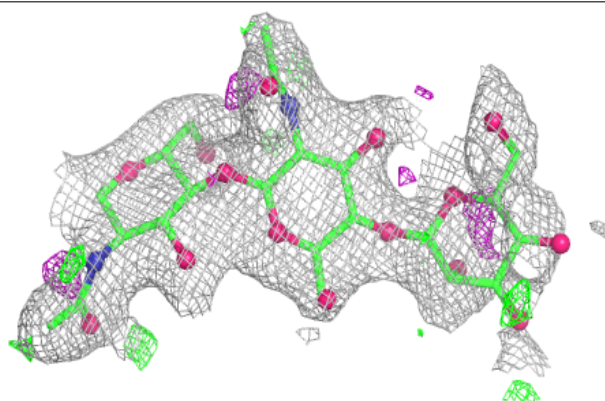


Electron density around Chain G:

$2mF_o-DF_c$ (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)



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	D	306	5/5	0.66	0.16	97,98,112,115	0
5	SO4	D	304	5/5	0.69	0.15	82,82,112,119	0
5	SO4	B	304	5/5	0.69	0.15	96,99,112,118	0
5	SO4	A	201	5/5	0.72	0.13	101,102,109,121	0
5	SO4	D	308	5/5	0.75	0.22	91,97,112,162	0
5	SO4	D	307	5/5	0.77	0.15	100,110,117,166	0
5	SO4	B	303	5/5	0.79	0.11	67,77,88,93	0
5	SO4	D	305	5/5	0.80	0.11	84,85,114,117	0
5	SO4	D	303	5/5	0.83	0.12	61,74,83,89	0
5	SO4	B	302	5/5	0.92	0.09	61,64,69,72	0
5	SO4	D	302	5/5	0.92	0.09	56,63,68,71	0
5	SO4	D	301	5/5	0.97	0.07	31,45,55,63	0
5	SO4	B	301	5/5	0.97	0.08	32,44,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.