



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 05:51 PM EDT

PDB ID : 4RZT
Title : Lac repressor engineered to bind sucralose, sucralose-bound tetramer
Authors : Arbing, M.A.; Cascio, D.; Sawaya, M.R.; Kosuri, S.; Church, G.M.
Deposited on : 2014-12-24
Resolution : 3.10 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

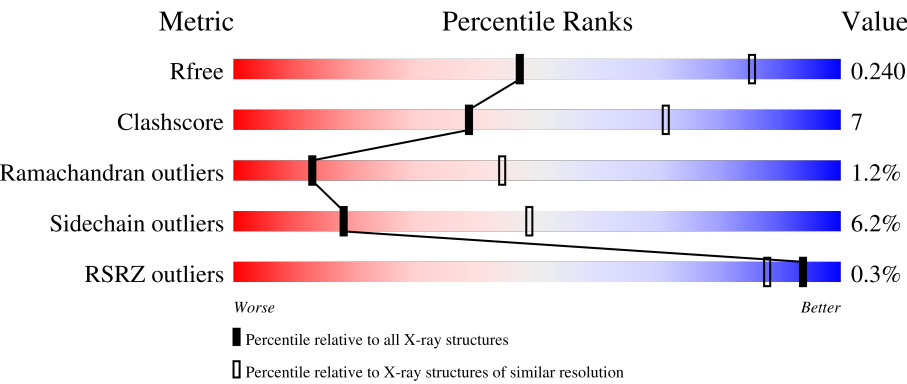
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



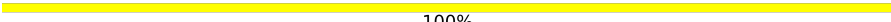
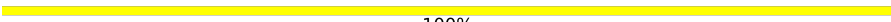

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	381	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>66%11%•21%</div></div>
1	B	381	<div><div></div><div></div><div></div><div></div><div></div></div> <div>66%10%•23%</div>
1	C	381	<div><div></div><div></div><div></div><div></div><div></div></div> <div>67%10%•21%</div>
1	D	381	<div><div></div><div></div><div></div><div></div><div></div></div> <div>66%10%•23%</div>
2	E	2	<div><div></div><div></div><div></div><div></div><div></div></div> <div>100%</div>

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8787 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 Lac repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2196	1369	386	430	11			
1	B	295	Total	C	N	O	S	0	0	0
			2127	1333	375	409	10			
1	C	301	Total	C	N	O	S	0	0	0
			2211	1377	392	431	11			
1	D	295	Total	C	N	O	S	0	0	0
			2145	1342	378	414	11			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP C9QQT3
A	-19	GLY	-	expression tag	UNP C9QQT3
A	-18	SER	-	expression tag	UNP C9QQT3
A	-17	SER	-	expression tag	UNP C9QQT3
A	-16	HIS	-	expression tag	UNP C9QQT3
A	-15	HIS	-	expression tag	UNP C9QQT3
A	-14	HIS	-	expression tag	UNP C9QQT3
A	-13	HIS	-	expression tag	UNP C9QQT3
A	-12	HIS	-	expression tag	UNP C9QQT3
A	-11	HIS	-	expression tag	UNP C9QQT3
A	-10	SER	-	expression tag	UNP C9QQT3
A	-9	SER	-	expression tag	UNP C9QQT3
A	-8	GLY	-	expression tag	UNP C9QQT3
A	-7	LEU	-	expression tag	UNP C9QQT3
A	-6	VAL	-	expression tag	UNP C9QQT3
A	-5	PRO	-	expression tag	UNP C9QQT3
A	-4	ARG	-	expression tag	UNP C9QQT3
A	-3	GLY	-	expression tag	UNP C9QQT3
A	-2	SER	-	expression tag	UNP C9QQT3
A	-1	HIS	-	expression tag	UNP C9QQT3
A	0	MET	-	expression tag	UNP C9QQT3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	149	THR	ASP	engineered mutation	UNP C9QQT3
A	150	ALA	VAL	engineered mutation	UNP C9QQT3
A	156	LEU	ILE	engineered mutation	UNP C9QQT3
A	193	ASP	SER	engineered mutation	UNP C9QQT3
B	-20	MET	-	expression tag	UNP C9QQT3
B	-19	GLY	-	expression tag	UNP C9QQT3
B	-18	SER	-	expression tag	UNP C9QQT3
B	-17	SER	-	expression tag	UNP C9QQT3
B	-16	HIS	-	expression tag	UNP C9QQT3
B	-15	HIS	-	expression tag	UNP C9QQT3
B	-14	HIS	-	expression tag	UNP C9QQT3
B	-13	HIS	-	expression tag	UNP C9QQT3
B	-12	HIS	-	expression tag	UNP C9QQT3
B	-11	HIS	-	expression tag	UNP C9QQT3
B	-10	SER	-	expression tag	UNP C9QQT3
B	-9	SER	-	expression tag	UNP C9QQT3
B	-8	GLY	-	expression tag	UNP C9QQT3
B	-7	LEU	-	expression tag	UNP C9QQT3
B	-6	VAL	-	expression tag	UNP C9QQT3
B	-5	PRO	-	expression tag	UNP C9QQT3
B	-4	ARG	-	expression tag	UNP C9QQT3
B	-3	GLY	-	expression tag	UNP C9QQT3
B	-2	SER	-	expression tag	UNP C9QQT3
B	-1	HIS	-	expression tag	UNP C9QQT3
B	0	MET	-	expression tag	UNP C9QQT3
B	149	THR	ASP	engineered mutation	UNP C9QQT3
B	150	ALA	VAL	engineered mutation	UNP C9QQT3
B	156	LEU	ILE	engineered mutation	UNP C9QQT3
B	193	ASP	SER	engineered mutation	UNP C9QQT3
C	-20	MET	-	expression tag	UNP C9QQT3
C	-19	GLY	-	expression tag	UNP C9QQT3
C	-18	SER	-	expression tag	UNP C9QQT3
C	-17	SER	-	expression tag	UNP C9QQT3
C	-16	HIS	-	expression tag	UNP C9QQT3
C	-15	HIS	-	expression tag	UNP C9QQT3
C	-14	HIS	-	expression tag	UNP C9QQT3
C	-13	HIS	-	expression tag	UNP C9QQT3
C	-12	HIS	-	expression tag	UNP C9QQT3
C	-11	HIS	-	expression tag	UNP C9QQT3
C	-10	SER	-	expression tag	UNP C9QQT3
C	-9	SER	-	expression tag	UNP C9QQT3
C	-8	GLY	-	expression tag	UNP C9QQT3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	expression tag	UNP C9QQT3
C	-6	VAL	-	expression tag	UNP C9QQT3
C	-5	PRO	-	expression tag	UNP C9QQT3
C	-4	ARG	-	expression tag	UNP C9QQT3
C	-3	GLY	-	expression tag	UNP C9QQT3
C	-2	SER	-	expression tag	UNP C9QQT3
C	-1	HIS	-	expression tag	UNP C9QQT3
C	0	MET	-	expression tag	UNP C9QQT3
C	149	THR	ASP	engineered mutation	UNP C9QQT3
C	150	ALA	VAL	engineered mutation	UNP C9QQT3
C	156	LEU	ILE	engineered mutation	UNP C9QQT3
C	193	ASP	SER	engineered mutation	UNP C9QQT3
D	-20	MET	-	expression tag	UNP C9QQT3
D	-19	GLY	-	expression tag	UNP C9QQT3
D	-18	SER	-	expression tag	UNP C9QQT3
D	-17	SER	-	expression tag	UNP C9QQT3
D	-16	HIS	-	expression tag	UNP C9QQT3
D	-15	HIS	-	expression tag	UNP C9QQT3
D	-14	HIS	-	expression tag	UNP C9QQT3
D	-13	HIS	-	expression tag	UNP C9QQT3
D	-12	HIS	-	expression tag	UNP C9QQT3
D	-11	HIS	-	expression tag	UNP C9QQT3
D	-10	SER	-	expression tag	UNP C9QQT3
D	-9	SER	-	expression tag	UNP C9QQT3
D	-8	GLY	-	expression tag	UNP C9QQT3
D	-7	LEU	-	expression tag	UNP C9QQT3
D	-6	VAL	-	expression tag	UNP C9QQT3
D	-5	PRO	-	expression tag	UNP C9QQT3
D	-4	ARG	-	expression tag	UNP C9QQT3
D	-3	GLY	-	expression tag	UNP C9QQT3
D	-2	SER	-	expression tag	UNP C9QQT3
D	-1	HIS	-	expression tag	UNP C9QQT3
D	0	MET	-	expression tag	UNP C9QQT3
D	149	THR	ASP	engineered mutation	UNP C9QQT3
D	150	ALA	VAL	engineered mutation	UNP C9QQT3
D	156	LEU	ILE	engineered mutation	UNP C9QQT3
D	193	ASP	SER	engineered mutation	UNP C9QQT3

- Molecule 2 is an oligosaccharide called 4-chloro-4-deoxy-alpha-D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total 23	C 12	Cl 3	O 8	0	0	0
2	F	2	Total 23	C 12	Cl 3	O 8	0	0	0
2	G	2	Total 23	C 12	Cl 3	O 8	0	0	0
2	H	2	Total 23	C 12	Cl 3	O 8	0	0	0

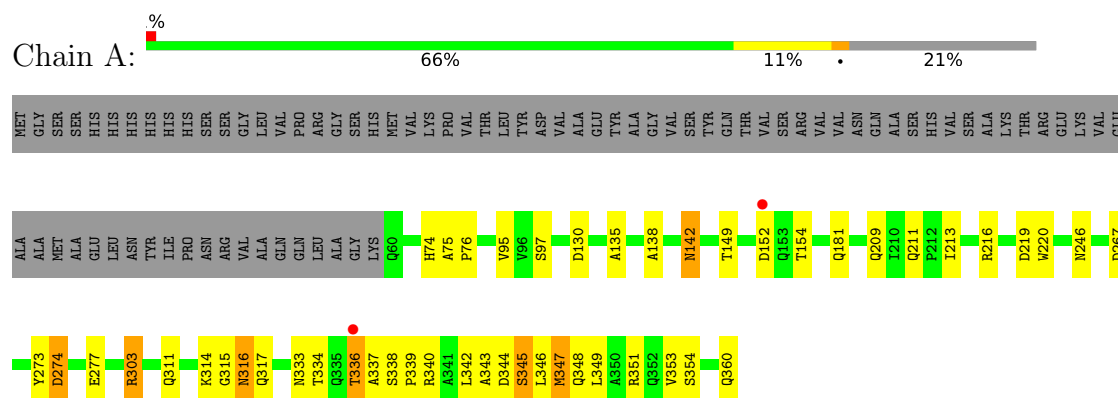
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	3	Total 3	O 3	0	0
3	C	5	Total 5	O 5	0	0
3	D	2	Total 2	O 2	0	0

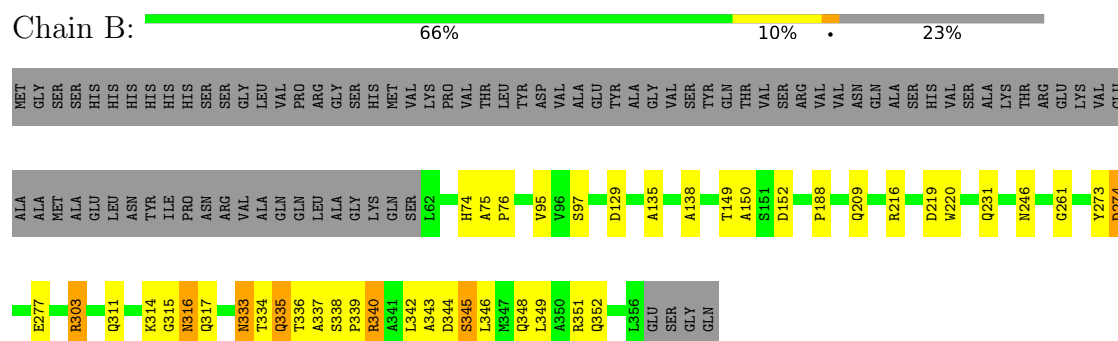
3 Residue-property plots

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.

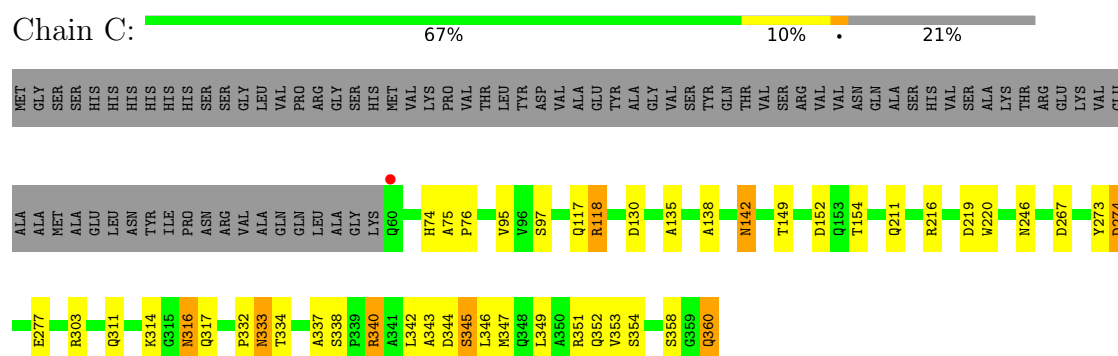
• Molecule 1: Lac repressor



• Molecule 1: Lac repressor

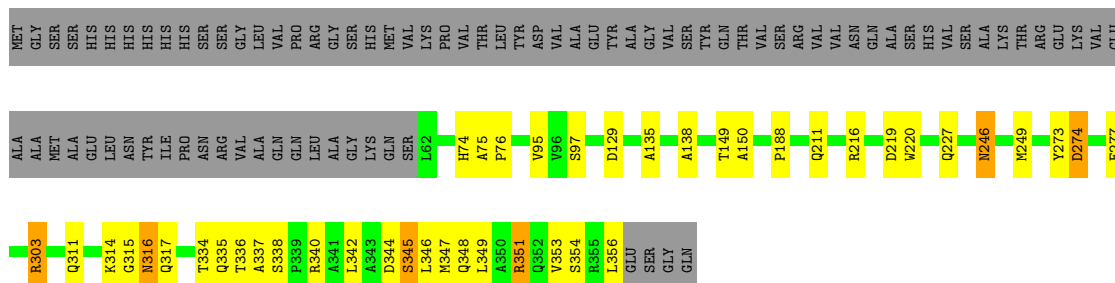


• Molecule 1: Lac repressor



- Molecule 1: Lac repressor

Chain D:  66% 10% 23%



- Molecule 2: 4-chloro-4-deoxy-alpha-D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose

Chain E:  100%



- Molecule 2: 4-chloro-4-deoxy-alpha-D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose

Chain F:  100%



- Molecule 2: 4-chloro-4-deoxy-alpha-D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose

Chain G:  100%



- Molecule 2: 4-chloro-4-deoxy-alpha-D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.59Å 74.08Å 149.16Å 90.00° 119.91° 90.00°	Depositor
Resolution (Å)	81.66 – 3.10 81.66 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.0 (81.66-3.10) 85.0 (81.66-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0049, BUSTER-TNT BUSTER 2.10.0	Depositor
R, R_{free}	0.205 , 0.243 0.204 , 0.240	Depositor DCC
R_{free} test set	1230 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8787	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: RRJ, RRY

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	0.54	0/2225	0.71	0/3032
1	B	0.51	0/2156	0.70	0/2945
1	C	0.51	0/2240	0.71	1/3051 (0.0%)
1	D	0.50	0/2174	0.71	0/2967
All	All	0.51	0/8795	0.71	1/11995 (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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	THR	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	150	ALA	Peptide
1	D	150	ALA	Peptide

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	2196	0	2195	43	0
1	B	2127	0	2118	31	0
1	C	2211	0	2221	43	0
1	D	2145	0	2145	33	0
2	E	23	0	0	0	0
2	F	23	0	0	0	0
2	G	23	0	0	0	0
2	H	23	0	0	0	0
3	A	6	0	0	0	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0
3	D	2	0	0	0	0
All	All	8787	0	8679	130	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 7.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:HA	1:A:333:ASN:HD21	1.55	0.71
1:C:345:SER:O	1:C:349:LEU:HG	1.94	0.68
1:A:339:PRO:HB3	1:C:360:GLN:HB3	1.75	0.67
1:A:343:ALA:O	1:A:347:MET:HB2	1.94	0.67
1:B:345:SER:O	1:B:349:LEU:HG	1.93	0.66
1:D:345:SER:O	1:D:349:LEU:HG	1.95	0.66
1:C:267:ASP:HA	1:C:333:ASN:HD21	1.61	0.65
1:A:345:SER:O	1:A:349:LEU:HG	1.97	0.65
1:D:347:MET:O	1:D:351:ARG:HD3	1.98	0.63
1:A:343:ALA:HB3	1:C:358:SER:OG	2.00	0.61
1:C:337:ALA:HB3	1:C:342:LEU:HD13	1.82	0.60
1:A:354:SER:HB2	1:C:347:MET:HG3	1.83	0.59
1:C:343:ALA:O	1:C:347:MET:HB2	2.03	0.58
1:A:211:GLN:HE21	1:A:211:GLN:HA	1.69	0.57
1:C:142:ASN:HD22	1:C:142:ASN:N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:SER:O	1:C:342:LEU:HB2	2.05	0.57
1:C:349:LEU:O	1:C:353:VAL:HG23	2.05	0.57
1:A:347:MET:SD	1:C:351:ARG:HG2	2.45	0.56
1:A:142:ASN:HD22	1:A:142:ASN:N	2.02	0.56
1:B:338:SER:O	1:B:342:LEU:HB2	2.06	0.56
1:B:343:ALA:HB2	1:D:353:VAL:HB	1.88	0.55
1:D:338:SER:O	1:D:342:LEU:HB2	2.06	0.55
1:D:348:GLN:O	1:D:349:LEU:C	2.44	0.55
1:C:349:LEU:O	1:C:352:GLN:HG2	2.05	0.55
1:A:351:ARG:O	1:A:354:SER:OG	2.10	0.55
1:B:348:GLN:O	1:B:349:LEU:C	2.45	0.55
1:C:337:ALA:CB	1:C:342:LEU:HD13	2.37	0.55
1:D:334:THR:O	1:D:336:THR:N	2.40	0.54
1:A:338:SER:O	1:A:342:LEU:HB2	2.08	0.54
1:C:211:GLN:HE21	1:C:211:GLN:HA	1.72	0.54
1:A:337:ALA:HB3	1:A:342:LEU:HD13	1.91	0.53
1:C:333:ASN:H	1:C:333:ASN:HD22	1.54	0.53
1:A:333:ASN:HD22	1:A:333:ASN:H	1.56	0.53
1:C:332:PRO:O	1:C:333:ASN:C	2.47	0.53
1:C:340:ARG:HH11	1:C:340:ARG:HB3	1.73	0.53
1:B:340:ARG:HB3	1:B:340:ARG:HH11	1.74	0.52
1:D:344:ASP:O	1:D:345:SER:C	2.46	0.52
1:C:75:ALA:HB3	1:C:76:PRO:HD3	1.92	0.52
1:D:316:ASN:HD22	1:D:317:GLN:N	2.06	0.52
1:B:344:ASP:O	1:B:345:SER:C	2.45	0.52
1:A:349:LEU:O	1:A:353:VAL:HG23	2.10	0.51
1:C:351:ARG:O	1:C:354:SER:OG	2.11	0.51
1:C:316:ASN:HD22	1:C:317:GLN:N	2.08	0.51
1:A:342:LEU:HG	1:A:346:LEU:HD12	1.94	0.50
1:B:337:ALA:HB3	1:B:342:LEU:HD13	1.93	0.50
1:A:311:GLN:O	1:A:311:GLN:HG3	2.12	0.50
1:A:337:ALA:CB	1:A:342:LEU:HD13	2.42	0.50
1:A:343:ALA:CB	1:C:354:SER:O	2.60	0.50
1:D:75:ALA:HB3	1:D:76:PRO:HD3	1.93	0.50
1:A:75:ALA:HB3	1:A:76:PRO:HD3	1.93	0.50
1:B:316:ASN:HD22	1:B:317:GLN:N	2.09	0.49
1:B:343:ALA:HB2	1:D:354:SER:N	2.28	0.49
1:A:316:ASN:HD22	1:A:317:GLN:N	2.10	0.49
1:B:337:ALA:CB	1:B:342:LEU:HD13	2.43	0.49
1:C:311:GLN:O	1:C:311:GLN:HG3	2.12	0.49
1:B:336:THR:HG23	1:B:336:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ALA:HB3	1:B:76:PRO:HD3	1.94	0.49
1:D:336:THR:O	1:D:336:THR:HG23	2.12	0.49
1:B:311:GLN:O	1:B:311:GLN:HG3	2.13	0.48
1:B:346:LEU:O	1:B:349:LEU:N	2.47	0.48
1:D:347:MET:O	1:D:351:ARG:CD	2.60	0.48
1:B:333:ASN:OD1	1:B:335:GLN:CB	2.62	0.48
1:D:337:ALA:CB	1:D:342:LEU:HD13	2.42	0.48
1:D:344:ASP:C	1:D:346:LEU:N	2.67	0.48
1:A:354:SER:CB	1:C:347:MET:HG3	2.44	0.48
1:D:337:ALA:HB3	1:D:342:LEU:HD13	1.96	0.48
1:A:340:ARG:HA	1:C:358:SER:HA	1.96	0.47
1:C:273:TYR:O	1:C:274:ASP:CB	2.63	0.47
1:D:311:GLN:O	1:D:311:GLN:HG3	2.14	0.47
1:B:348:GLN:O	1:B:351:ARG:N	2.48	0.46
1:C:342:LEU:HG	1:C:346:LEU:HD12	1.96	0.46
1:A:273:TYR:O	1:A:274:ASP:CB	2.63	0.46
1:A:343:ALA:CB	1:C:358:SER:OG	2.63	0.46
1:C:117:GLN:O	1:C:118:ARG:HB3	2.15	0.46
1:D:346:LEU:O	1:D:349:LEU:N	2.49	0.46
1:D:219:ASP:O	1:D:220:TRP:HB2	2.16	0.46
1:A:219:ASP:O	1:A:220:TRP:HB2	2.16	0.45
1:A:354:SER:HB2	1:C:347:MET:CG	2.43	0.45
1:C:316:ASN:HD22	1:C:317:GLN:H	1.65	0.45
1:B:273:TYR:O	1:B:274:ASP:CB	2.64	0.45
1:D:273:TYR:O	1:D:274:ASP:CB	2.64	0.45
1:B:339:PRO:HB3	1:D:356:LEU:O	2.17	0.45
1:D:246:ASN:HA	1:D:273:TYR:O	2.17	0.45
1:B:303:ARG:NH1	1:B:315:GLY:O	2.47	0.44
1:C:219:ASP:O	1:C:220:TRP:HB2	2.17	0.44
1:D:316:ASN:HD22	1:D:317:GLN:H	1.63	0.44
1:B:219:ASP:O	1:B:220:TRP:HB2	2.17	0.44
1:D:348:GLN:O	1:D:351:ARG:N	2.50	0.44
1:A:343:ALA:HB1	1:C:354:SER:O	2.16	0.44
1:A:347:MET:O	1:A:351:ARG:HB2	2.17	0.44
1:C:142:ASN:N	1:C:142:ASN:ND2	2.66	0.44
1:B:135:ALA:O	1:B:138:ALA:HB3	2.17	0.44
1:C:118:ARG:CD	1:C:118:ARG:O	2.65	0.44
1:D:246:ASN:ND2	1:D:249:MET:H	2.15	0.44
1:B:316:ASN:HD22	1:B:317:GLN:H	1.66	0.44
1:B:343:ALA:CB	1:D:354:SER:N	2.81	0.44
1:B:246:ASN:HA	1:B:273:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:N	1:A:142:ASN:ND2	2.65	0.43
1:A:74:HIS:CE1	1:B:74:HIS:CE1	3.06	0.43
1:A:303:ARG:NH1	1:A:315:GLY:O	2.48	0.43
1:B:349:LEU:HA	1:B:352:GLN:CD	2.39	0.43
1:A:316:ASN:HD22	1:A:317:GLN:H	1.67	0.43
1:D:246:ASN:HD21	1:D:249:MET:H	1.67	0.43
1:B:231:GLN:HG2	1:D:227:GLN:HG2	2.00	0.43
1:C:135:ALA:O	1:C:138:ALA:HB3	2.19	0.42
1:D:135:ALA:O	1:D:138:ALA:HB3	2.19	0.42
1:D:246:ASN:HD21	1:D:249:MET:HG3	1.84	0.42
1:A:347:MET:SD	1:C:354:SER:OG	2.77	0.42
1:A:354:SER:CB	1:C:347:MET:CG	2.96	0.42
1:B:348:GLN:C	1:B:352:GLN:OE1	2.58	0.42
1:A:246:ASN:HA	1:A:273:TYR:O	2.19	0.42
1:C:246:ASN:HA	1:C:273:TYR:O	2.19	0.42
1:C:360:GLN:HE21	1:C:360:GLN:HB2	1.68	0.42
1:C:347:MET:O	1:C:351:ARG:HB2	2.19	0.41
1:A:135:ALA:O	1:A:138:ALA:HB3	2.20	0.41
1:A:342:LEU:HA	1:A:345:SER:OG	2.21	0.41
1:B:349:LEU:HA	1:B:352:GLN:OE1	2.21	0.41
1:C:74:HIS:CE1	1:D:74:HIS:CE1	3.08	0.41
1:A:181:GLN:HE21	1:A:213:ILE:HG21	1.86	0.41
1:A:334:THR:OG1	1:A:336:THR:O	2.23	0.41
1:A:347:MET:O	1:A:351:ARG:CG	2.68	0.41
1:C:211:GLN:HA	1:C:211:GLN:NE2	2.36	0.41
1:C:219:ASP:O	1:C:220:TRP:CB	2.69	0.41
1:A:348:GLN:HA	1:A:351:ARG:HB2	2.03	0.41
1:A:351:ARG:HB3	1:B:261:GLY:HA3	2.02	0.41
1:A:211:GLN:HA	1:A:211:GLN:NE2	2.33	0.40
1:D:219:ASP:O	1:D:220:TRP:CB	2.69	0.40
1:B:188:PRO:HD2	1:B:220:TRP:CE2	2.56	0.40
1:D:303:ARG:NH1	1:D:315:GLY:O	2.47	0.40
1:D:188:PRO:HD2	1:D:220:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/381 (78%)	263 (88%)	33 (11%)	3 (1%)	15	49
1	B	293/381 (77%)	262 (89%)	27 (9%)	4 (1%)	11	40
1	C	299/381 (78%)	267 (89%)	28 (9%)	4 (1%)	12	42
1	D	293/381 (77%)	261 (89%)	29 (10%)	3 (1%)	15	49
All	All	1184/1524 (78%)	1053 (89%)	117 (10%)	14 (1%)	13	44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	ASP
1	B	274	ASP
1	C	274	ASP
1	D	274	ASP
1	B	335	GLN
1	C	333	ASN
1	A	314	LYS
1	C	314	LYS
1	D	335	GLN
1	A	152	ASP
1	B	152	ASP
1	B	314	LYS
1	D	314	LYS
1	C	152	ASP

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	233/311 (75%)	217 (93%)	16 (7%)	15	45
1	B	220/311 (71%)	207 (94%)	13 (6%)	19	50
1	C	236/311 (76%)	221 (94%)	15 (6%)	17	48
1	D	225/311 (72%)	212 (94%)	13 (6%)	20	51
All	All	914/1244 (74%)	857 (94%)	57 (6%)	18	49

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	97	SER
1	A	130	ASP
1	A	142	ASN
1	A	149	THR
1	A	154	THR
1	A	209	GLN
1	A	216	ARG
1	A	277	GLU
1	A	303	ARG
1	A	316	ASN
1	A	336	THR
1	A	344	ASP
1	A	345	SER
1	A	347	MET
1	A	360	GLN
1	B	95	VAL
1	B	97	SER
1	B	129	ASP
1	B	149	THR
1	B	209	GLN
1	B	216	ARG
1	B	277	GLU
1	B	303	ARG
1	B	316	ASN
1	B	333	ASN
1	B	334	THR
1	B	340	ARG
1	B	345	SER
1	C	95	VAL
1	C	97	SER
1	C	118	ARG
1	C	130	ASP

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Mol	Chain	Res	Type
1	C	142	ASN
1	C	149	THR
1	C	154	THR
1	C	216	ARG
1	C	277	GLU
1	C	303	ARG
1	C	316	ASN
1	C	340	ARG
1	C	344	ASP
1	C	345	SER
1	C	360	GLN
1	D	95	VAL
1	D	97	SER
1	D	129	ASP
1	D	149	THR
1	D	211	GLN
1	D	216	ARG
1	D	246	ASN
1	D	277	GLU
1	D	303	ARG
1	D	316	ASN
1	D	340	ARG
1	D	345	SER
1	D	351	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	181	GLN
1	A	209	GLN
1	A	211	GLN
1	A	231	GLN
1	A	316	ASN
1	A	333	ASN
1	A	360	GLN
1	B	209	GLN
1	B	309	GLN
1	B	316	ASN
1	C	142	ASN
1	C	180	GLN
1	C	181	GLN

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Mol	Chain	Res	Type
1	C	211	GLN
1	C	231	GLN
1	C	316	ASN
1	C	333	ASN
1	C	360	GLN
1	D	246	ASN
1	D	309	GLN
1	D	316	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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	RRY	E	1	2	10,12,12	1.56	3 (30%)	8,18,18	1.77	2 (25%)
2	RRJ	E	2	2	10,11,12	2.34	3 (30%)	11,15,17	3.16	6 (54%)
2	RRY	F	1	2	10,12,12	1.27	1 (10%)	8,18,18	1.76	2 (25%)
2	RRJ	F	2	2	10,11,12	1.03	0	11,15,17	2.95	6 (54%)
2	RRY	G	1	2	10,12,12	0.95	0	8,18,18	1.72	2 (25%)
2	RRJ	G	2	2	10,11,12	2.25	3 (30%)	11,15,17	2.41	3 (27%)
2	RRY	H	1	2	10,12,12	2.26	1 (10%)	8,18,18	2.27	2 (25%)
2	RRJ	H	2	2	10,11,12	3.07	4 (40%)	11,15,17	4.30	7 (63%)

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	RRY	E	1	2	-	3/5/24/24	0/1/1/1
2	RRJ	E	2	2	-	0/2/19/22	0/1/1/1
2	RRY	F	1	2	-	4/5/24/24	0/1/1/1
2	RRJ	F	2	2	-	0/2/19/22	0/1/1/1
2	RRY	G	1	2	-	5/5/24/24	0/1/1/1
2	RRJ	G	2	2	-	1/2/19/22	0/1/1/1
2	RRY	H	1	2	-	5/5/24/24	0/1/1/1
2	RRJ	H	2	2	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	RRJ	C4-CL4	7.85	1.95	1.79
2	H	1	RRY	O2-C2	6.67	1.52	1.40
2	E	2	RRJ	O5-C1	4.59	1.51	1.43
2	G	2	RRJ	C4-C5	-4.57	1.47	1.52
2	E	2	RRJ	C2-C3	-4.03	1.46	1.52
2	G	2	RRJ	C4-CL4	3.82	1.87	1.79
2	H	2	RRJ	C2-C3	-3.81	1.46	1.52
2	E	1	RRY	O3-C3	3.13	1.49	1.42
2	F	1	RRY	O2-C2	3.10	1.46	1.40
2	E	2	RRJ	C4-CL4	2.92	1.85	1.79
2	H	2	RRJ	O5-C1	2.72	1.48	1.43
2	G	2	RRJ	C2-C3	-2.62	1.48	1.52
2	H	2	RRJ	C1-C2	2.47	1.57	1.52
2	E	1	RRY	O5-C2	2.19	1.46	1.43
2	E	1	RRY	O2-C2	2.09	1.44	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	RRJ	C5-C4-CL4	10.05	123.66	109.96
2	E	2	RRJ	C1-O5-C5	6.87	121.50	112.19
2	G	2	RRJ	C3-C4-C5	-6.43	103.43	109.59
2	H	2	RRJ	C3-C4-C5	-6.35	103.50	109.59
2	F	2	RRJ	C1-O5-C5	5.76	120.00	112.19
2	E	2	RRJ	O3-C3-C2	-4.97	100.48	109.99
2	H	2	RRJ	C1-O5-C5	4.66	118.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	RRJ	C1-C2-C3	4.55	115.26	109.67
2	E	1	RRY	O2-C2-O5	4.48	118.15	109.50
2	H	1	RRY	O2-C2-O5	4.38	117.95	109.50
2	H	1	RRY	O2-C2-C1	3.93	117.36	108.69
2	E	2	RRJ	C5-C4-CL4	3.75	115.08	109.96
2	H	2	RRJ	C1-C2-C3	3.71	114.23	109.67
2	F	2	RRJ	C5-C4-CL4	3.68	114.98	109.96
2	F	1	RRY	O2-C2-O5	3.67	116.60	109.50
2	G	1	RRY	C5-C6-CL6	-3.18	105.89	111.33
2	H	2	RRJ	O3-C3-C2	-3.16	103.94	109.99
2	G	2	RRJ	O3-C3-C2	-3.03	104.19	109.99
2	G	1	RRY	O2-C2-O5	3.00	115.29	109.50
2	E	2	RRJ	O5-C5-C4	2.99	114.29	110.40
2	F	2	RRJ	O5-C5-C6	-2.95	102.58	107.20
2	G	2	RRJ	O6-C6-C5	-2.56	102.50	111.29
2	H	2	RRJ	O2-C2-C3	-2.40	105.34	110.14
2	F	2	RRJ	C3-C4-C5	-2.38	107.31	109.59
2	E	2	RRJ	C3-C4-C5	-2.32	107.37	109.59
2	E	2	RRJ	C1-C2-C3	2.21	112.38	109.67
2	F	1	RRY	C5-C6-CL6	-2.20	107.58	111.33
2	F	2	RRJ	O3-C3-C2	-2.10	105.98	109.99
2	E	1	RRY	O5-C5-C4	-2.05	100.38	105.49
2	H	2	RRJ	O5-C5-C6	-2.05	103.99	107.20

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	RRY	C4-C5-C6-CL6
2	E	1	RRY	O5-C5-C6-CL6
2	F	1	RRY	C4-C5-C6-CL6
2	F	1	RRY	O5-C5-C6-CL6
2	F	1	RRY	CL1-C1-C2-C3
2	F	1	RRY	CL1-C1-C2-O2
2	G	1	RRY	C4-C5-C6-CL6
2	G	1	RRY	O5-C5-C6-CL6
2	G	1	RRY	CL1-C1-C2-C3
2	G	1	RRY	CL1-C1-C2-O5
2	G	1	RRY	CL1-C1-C2-O2
2	H	1	RRY	C4-C5-C6-CL6
2	H	1	RRY	O5-C5-C6-CL6
2	H	1	RRY	CL1-C1-C2-C3

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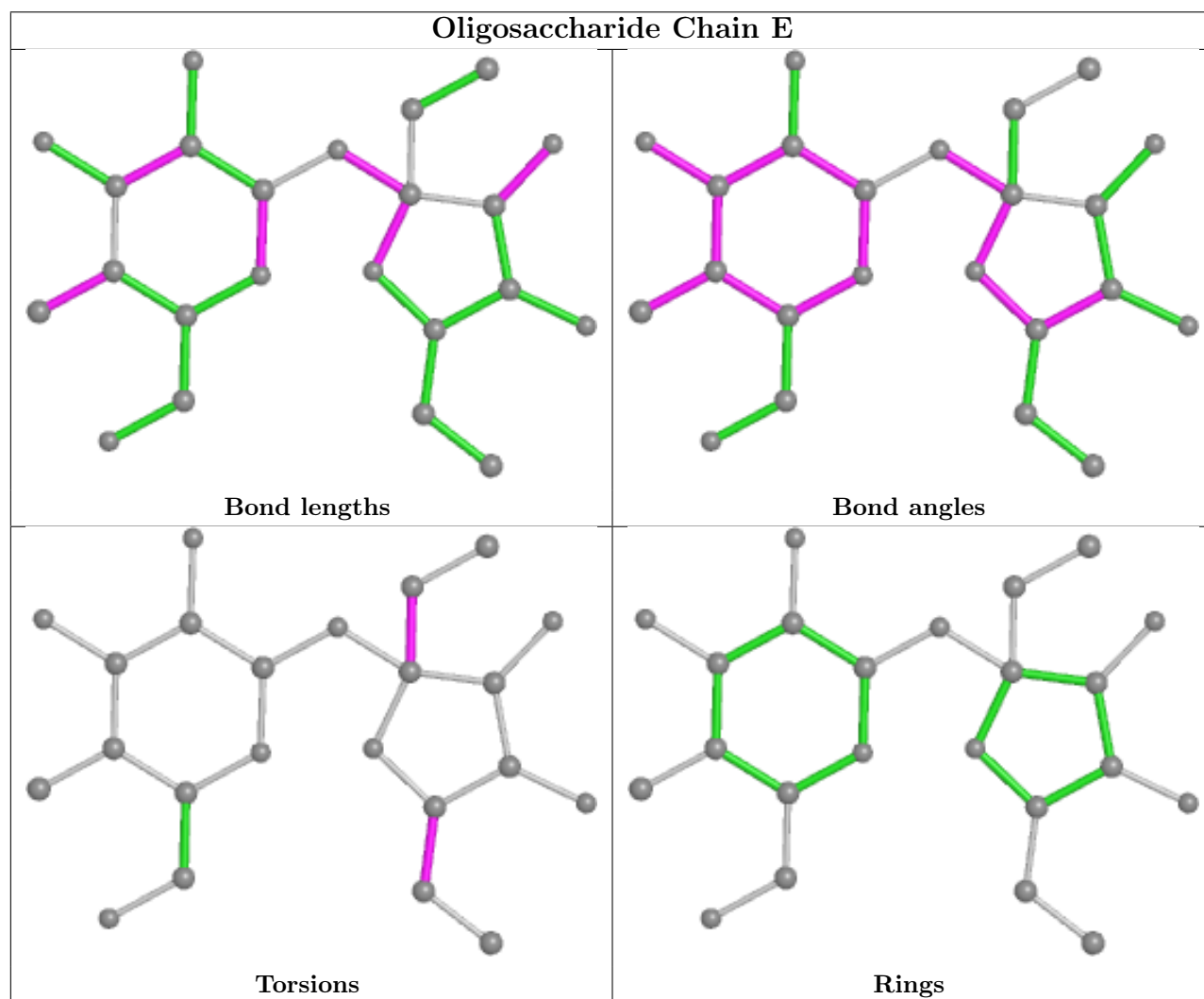
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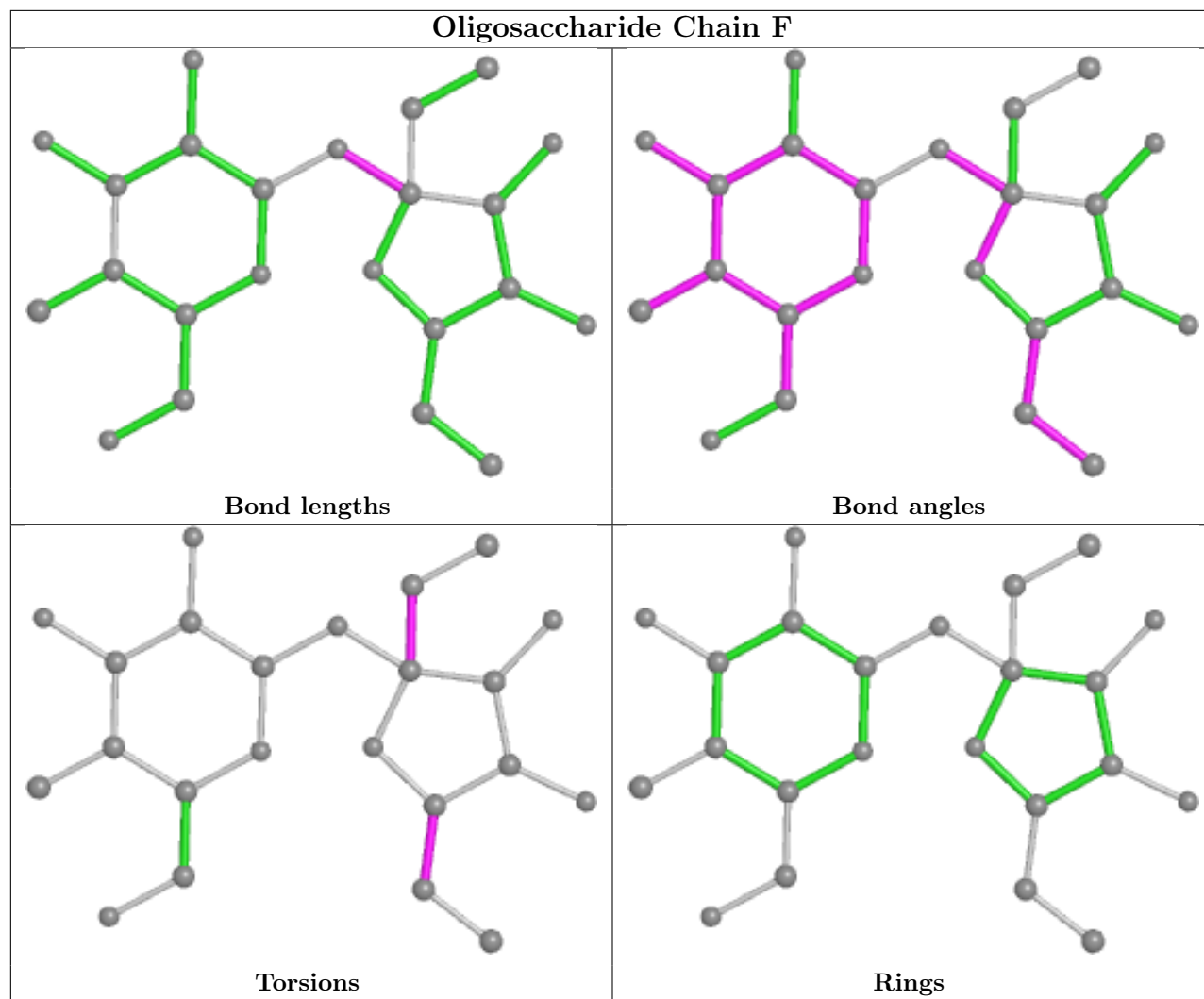
Mol	Chain	Res	Type	Atoms
2	H	1	RRY	CL1-C1-C2-O5
2	H	1	RRY	CL1-C1-C2-O2
2	G	2	RRJ	C4-C5-C6-O6
2	E	1	RRY	CL1-C1-C2-O2

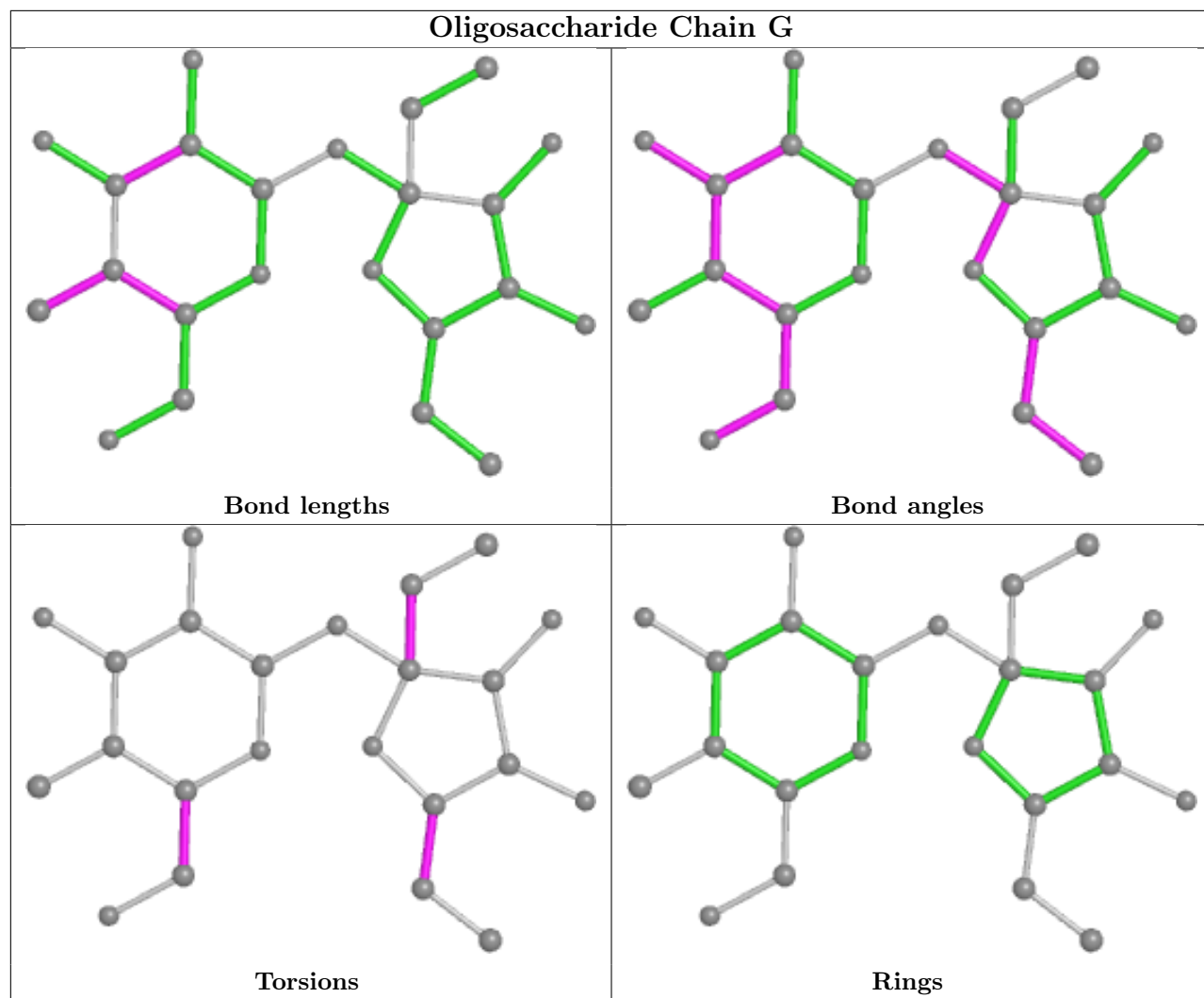
There are no ring outliers.

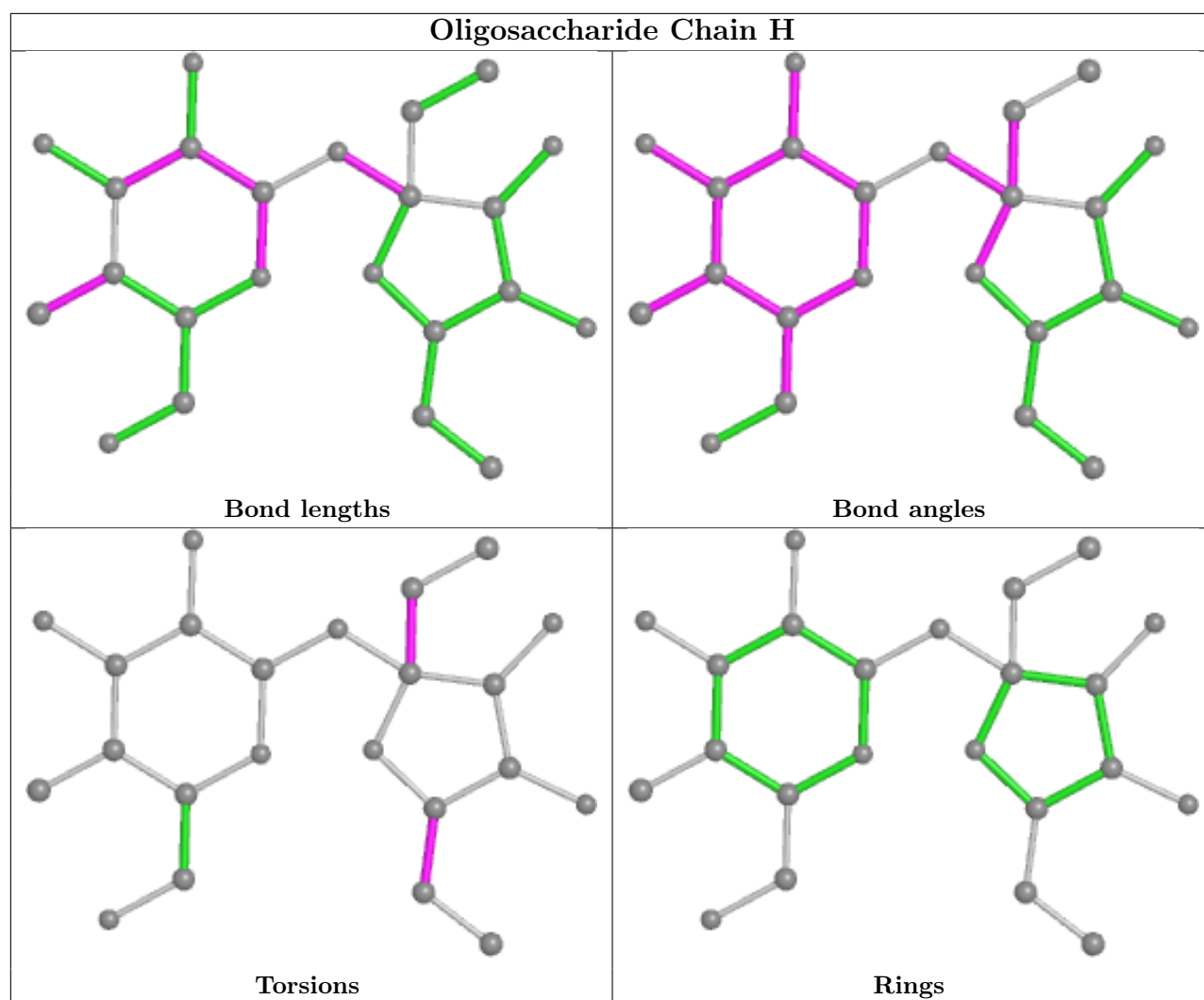
No monomer is involved in short contacts.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	301/381 (79%)	0.01	2 (0%) 87 75	50, 86, 161, 185	0
1	B	295/381 (77%)	-0.15	0 100 100	53, 100, 156, 184	0
1	C	301/381 (79%)	-0.09	1 (0%) 94 88	57, 89, 156, 183	0
1	D	295/381 (77%)	-0.06	0 100 100	61, 104, 155, 183	0
All	All	1192/1524 (78%)	-0.07	3 (0%) 94 88	50, 95, 158, 185	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	THR	2.7
1	A	152	ASP	2.5
1	C	60	GLN	2.2

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.

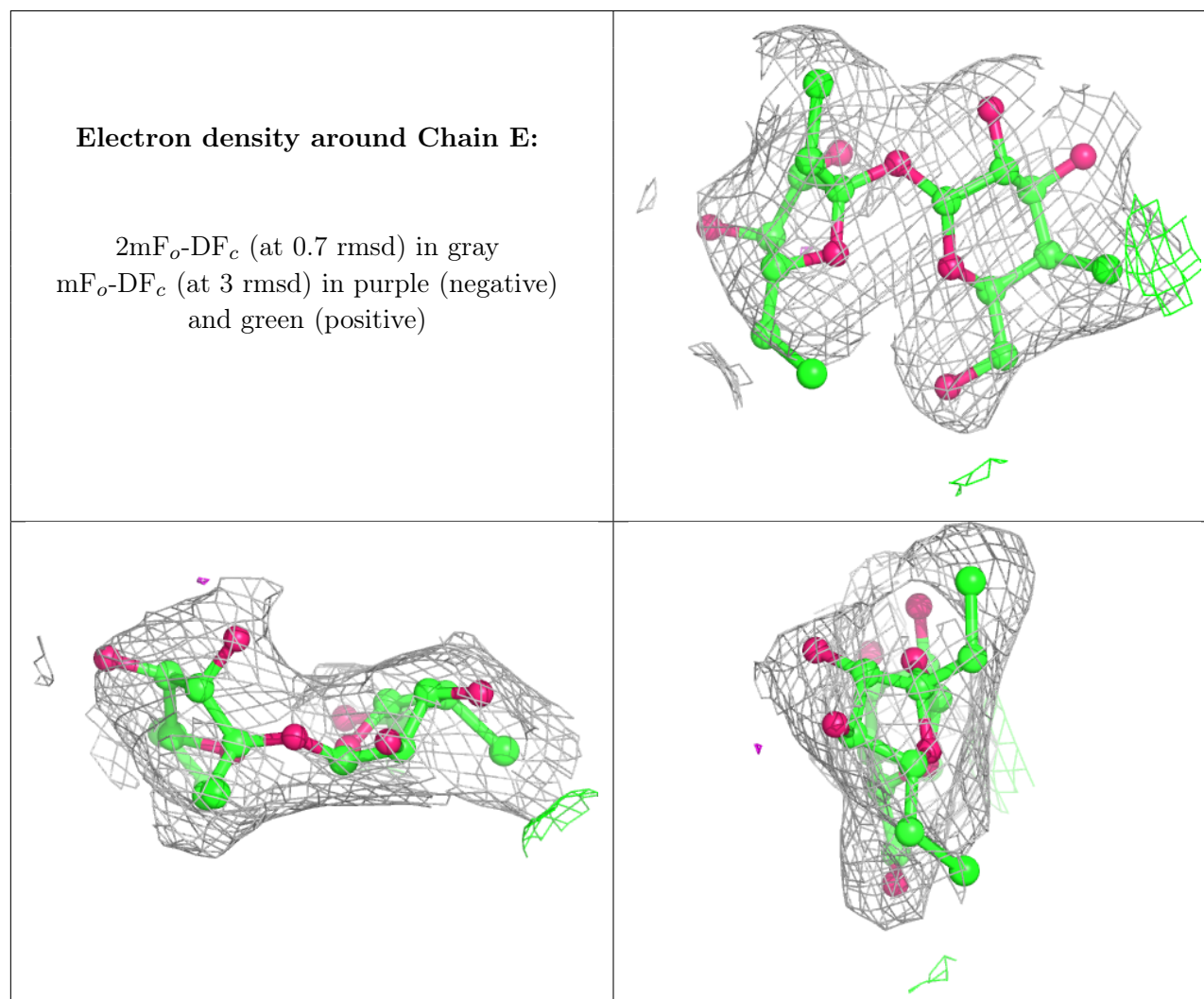
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	RRY	H	1	12/12	0.95	0.18	80,89,99,117	0
2	RRY	G	1	12/12	0.97	0.17	68,78,95,121	0
2	RRY	F	1	12/12	0.97	0.21	71,83,97,111	0
2	RRJ	F	2	11/12	0.98	0.20	68,70,75,80	0

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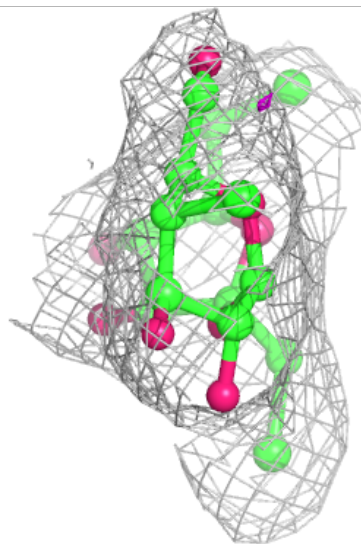
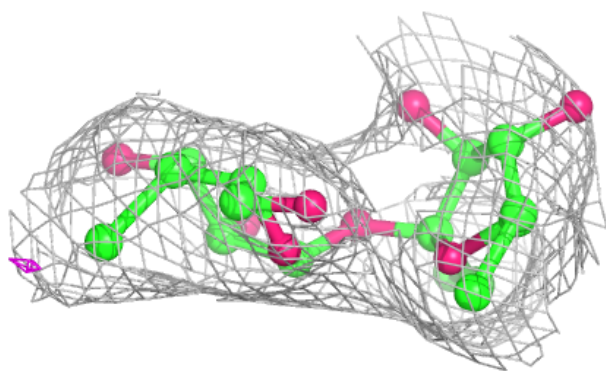
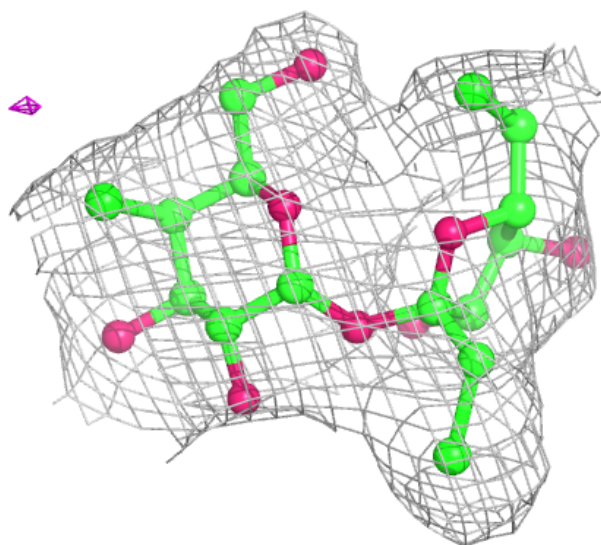
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	RRJ	E	2	11/12	0.98	0.20	51,55,59,60	0
2	RRJ	G	2	11/12	0.98	0.20	57,60,70,70	0
2	RRY	E	1	12/12	0.98	0.23	61,76,102,128	0
2	RRJ	H	2	11/12	0.98	0.23	71,76,81,89	0

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



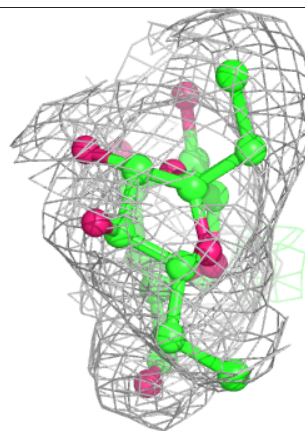
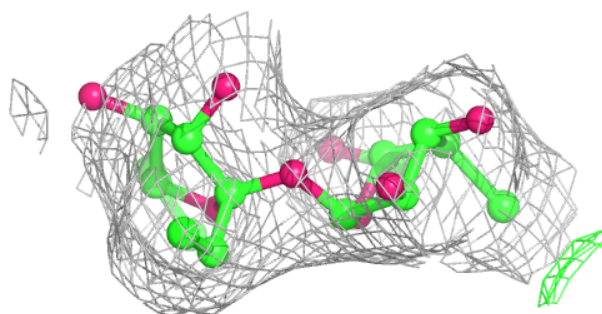
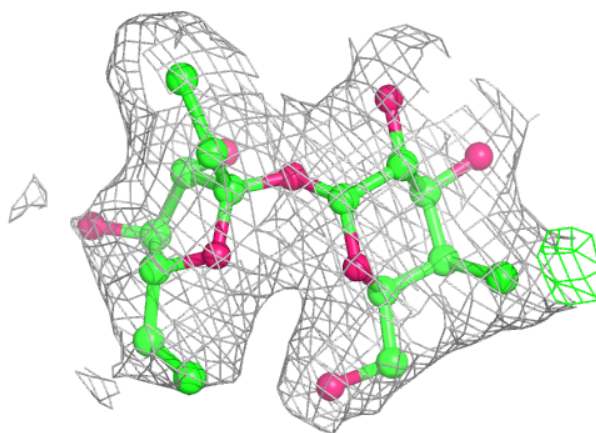
Electron density around Chain F:

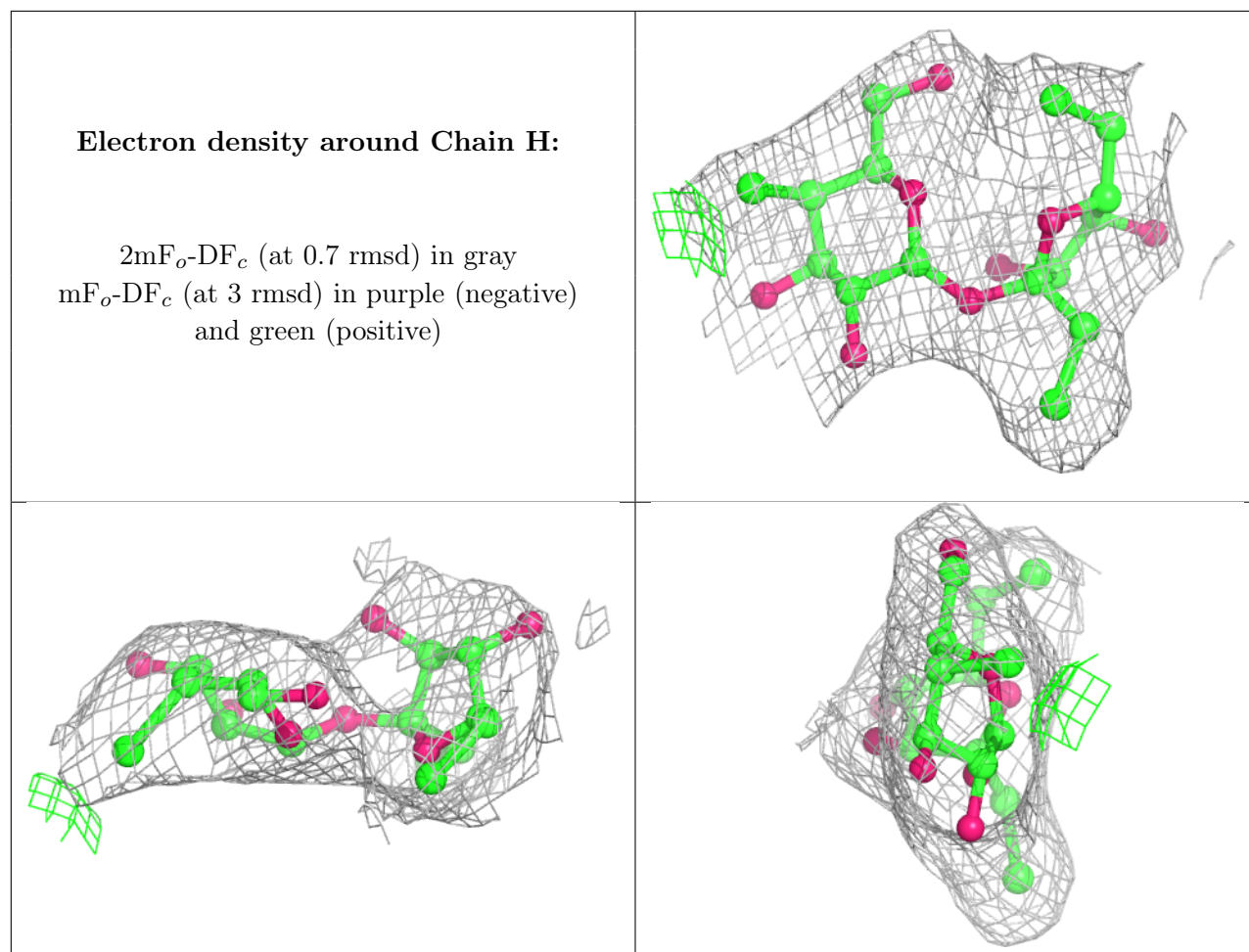
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.