



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2024 – 03:48 AM EDT

PDB ID : 6RUQ
Title : Structure of GluA2cryst in complex the antagonist ZK200775 and the negative allosteric modulator GYKI53655 at 4.65 Å resolution
Authors : Krintel, C.; Venskutonyte, R.; Mirza, O.A.; Gajhede, M.; Kastrop, J.S.
Deposited on : 2019-05-28
Resolution : 4.65 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 : 2.37.1
buster-report : 1.1.7 (2018)
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

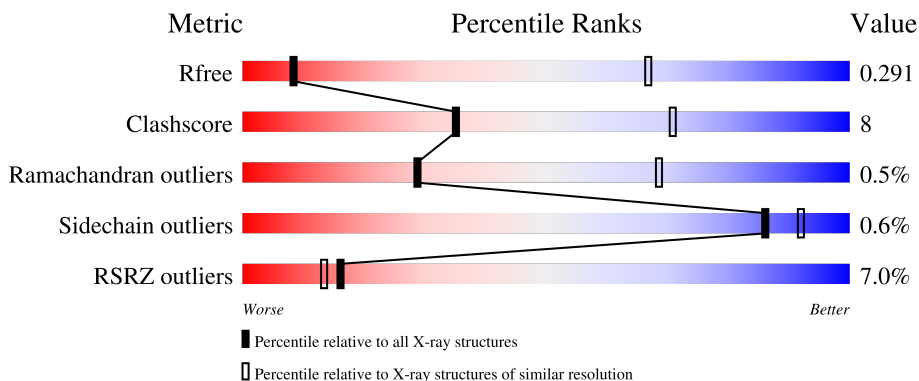
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.65 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	1083 (5.52-3.80)
Clashscore	141614	1156 (5.52-3.80)
Ramachandran outliers	138981	1092 (5.52-3.80)
Sidechain outliers	138945	1072 (5.50-3.80)
RSRZ outliers	127900	1114 (5.54-3.70)

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	823	 4% (poor fit), 76% (0 outliers), 19% (1 outlier), 5% (2 outliers)
1	B	823	 4% (poor fit), 76% (0 outliers), 18% (1 outlier), 5% (2 outliers)
1	C	823	 12% (poor fit), 78% (0 outliers), 18% (1 outlier), 2% (2 outliers)
1	D	823	 7% (poor fit), 78% (0 outliers), 17% (1 outlier), 5% (2 outliers)
2	E	3	 100% (0 outliers)

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Mol	Chain	Length	Quality of chain
2	G	3	 67% 33%
3	F	4	 100%

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
3	BMA	F	4	-	-	-	X
4	GYK	A	901	-	-	-	X
4	GYK	B	901	-	-	-	X
4	GYK	C	901	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25050 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	784	6156	3952	1023	1153	28	0	0	0
1	B	781	6130	3934	1019	1149	28	0	0	0
1	C	796	6255	4013	1039	1175	28	0	0	0
1	D	786	6169	3960	1025	1156	28	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	410	ALA	LYS	engineered mutation	UNP P19491
A	413	ALA	GLU	conflict	UNP P19491
A	414	ALA	MET	conflict	UNP P19491
A	416	ALA	GLU	conflict	UNP P19491
A	572	ALA	GLY	conflict	UNP P19491
A	575	GLN	ASN	conflict	UNP P19491
A	577	ALA	LEU	conflict	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	758	LEU	VAL	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
A	832	GLY	-	expression tag	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	410	ALA	LYS	engineered mutation	UNP P19491
B	413	ALA	GLU	conflict	UNP P19491
B	414	ALA	MET	conflict	UNP P19491
B	416	ALA	GLU	conflict	UNP P19491
B	572	ALA	GLY	conflict	UNP P19491
B	575	GLN	ASN	conflict	UNP P19491
B	577	ALA	LEU	conflict	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	758	LEU	VAL	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
B	832	GLY	-	expression tag	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491

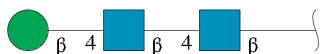
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Chain	Residue	Modelled	Actual	Comment	Reference
C	410	ALA	LYS	engineered mutation	UNP P19491
C	413	ALA	GLU	conflict	UNP P19491
C	414	ALA	MET	conflict	UNP P19491
C	416	ALA	GLU	conflict	UNP P19491
C	572	ALA	GLY	conflict	UNP P19491
C	575	GLN	ASN	conflict	UNP P19491
C	577	ALA	LEU	conflict	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	758	LEU	VAL	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
C	832	GLY	-	expression tag	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	410	ALA	LYS	engineered mutation	UNP P19491
D	413	ALA	GLU	conflict	UNP P19491
D	414	ALA	MET	conflict	UNP P19491
D	416	ALA	GLU	conflict	UNP P19491
D	572	ALA	GLY	conflict	UNP P19491
D	575	GLN	ASN	conflict	UNP P19491
D	577	ALA	LEU	conflict	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	758	LEU	VAL	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491
D	832	GLY	-	expression tag	UNP P19491

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

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



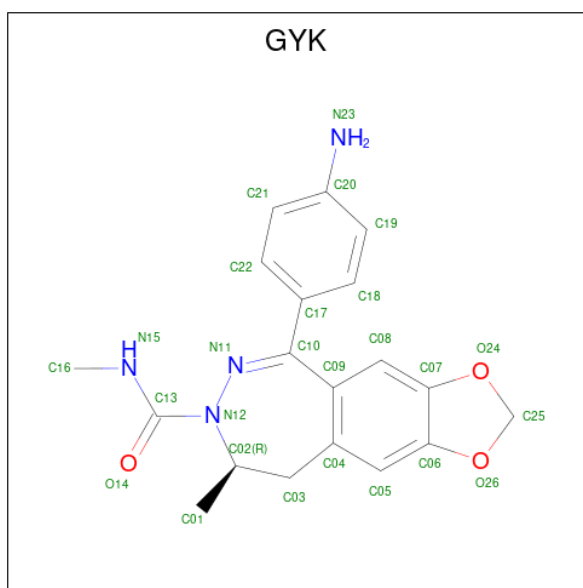
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	39	22	2	15	0	0	0
2	G	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



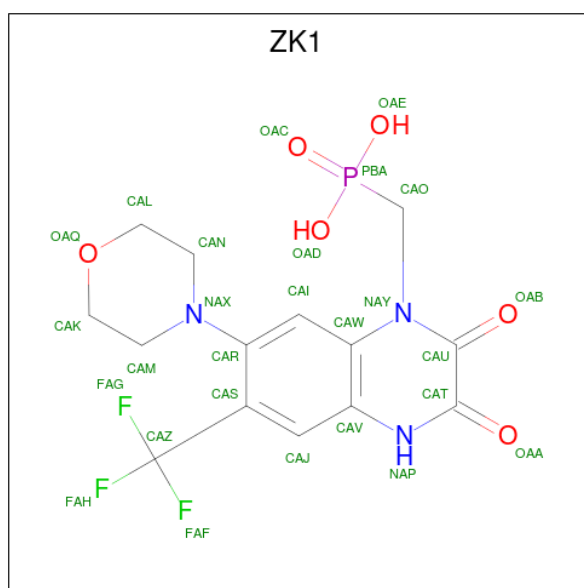
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	4	50	28	2	20	0	0	0

- Molecule 4 is (8R)-5-(4-aminophenyl)-N,8-dimethyl-8,9-dihydro-2H,7H-[1,3]dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide (three-letter code: GYK) (formula: C₁₉H₂₀N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	19	4	3		
4	B	1	Total	C	N	O	0	0
			26	19	4	3		
4	C	1	Total	C	N	O	0	0
			26	19	4	3		
4	D	1	Total	C	N	O	0	0
			26	19	4	3		

- Molecule 5 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P) (labeled as "Ligand of Interest" by depositor).

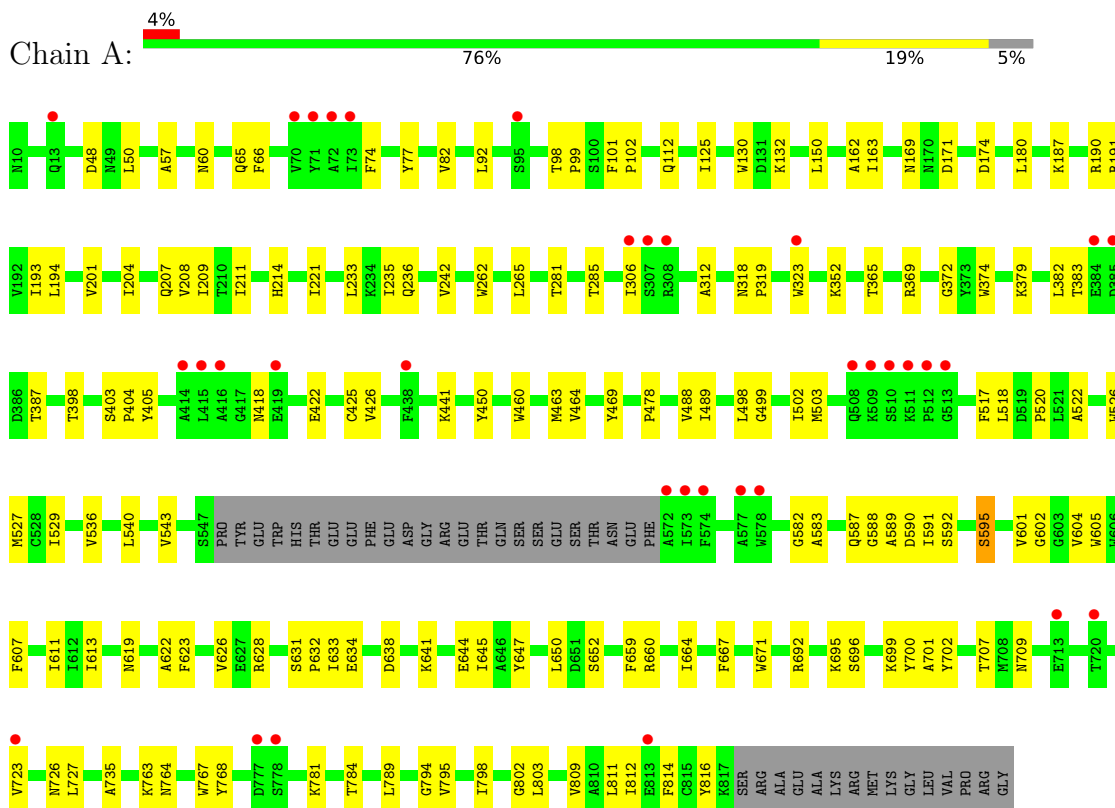


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
5	B	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
5	C	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
5	D	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		

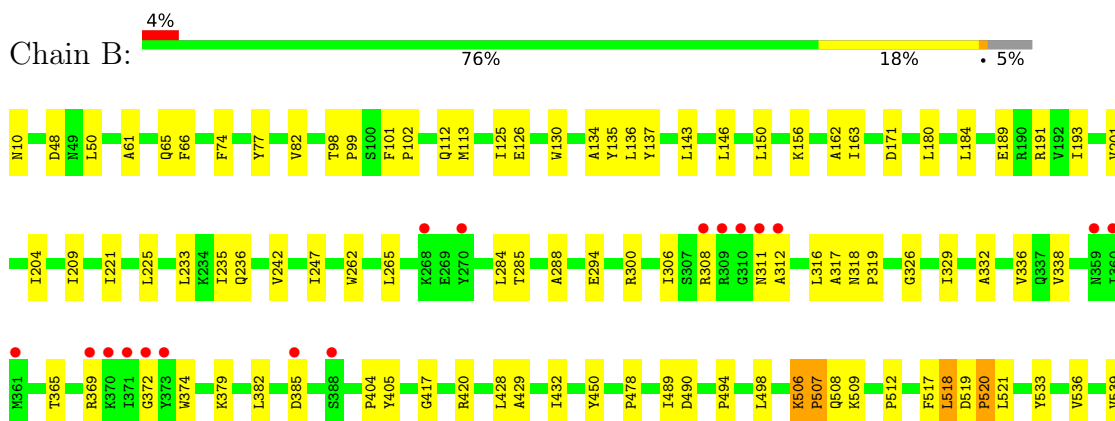
3 Residue-property plots

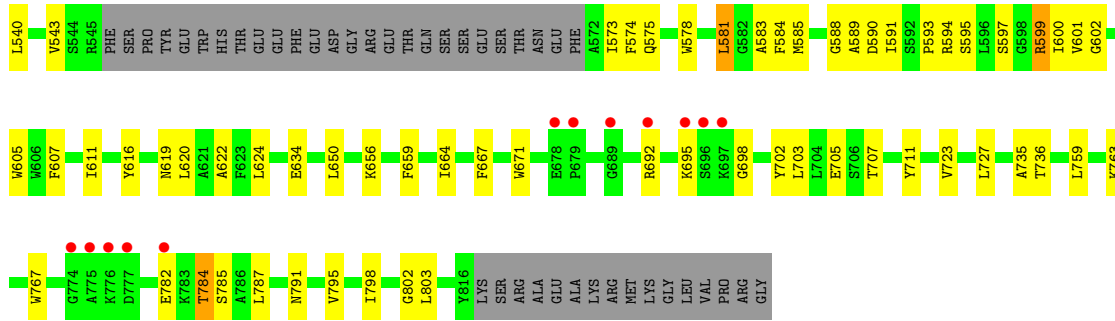
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate receptor 2

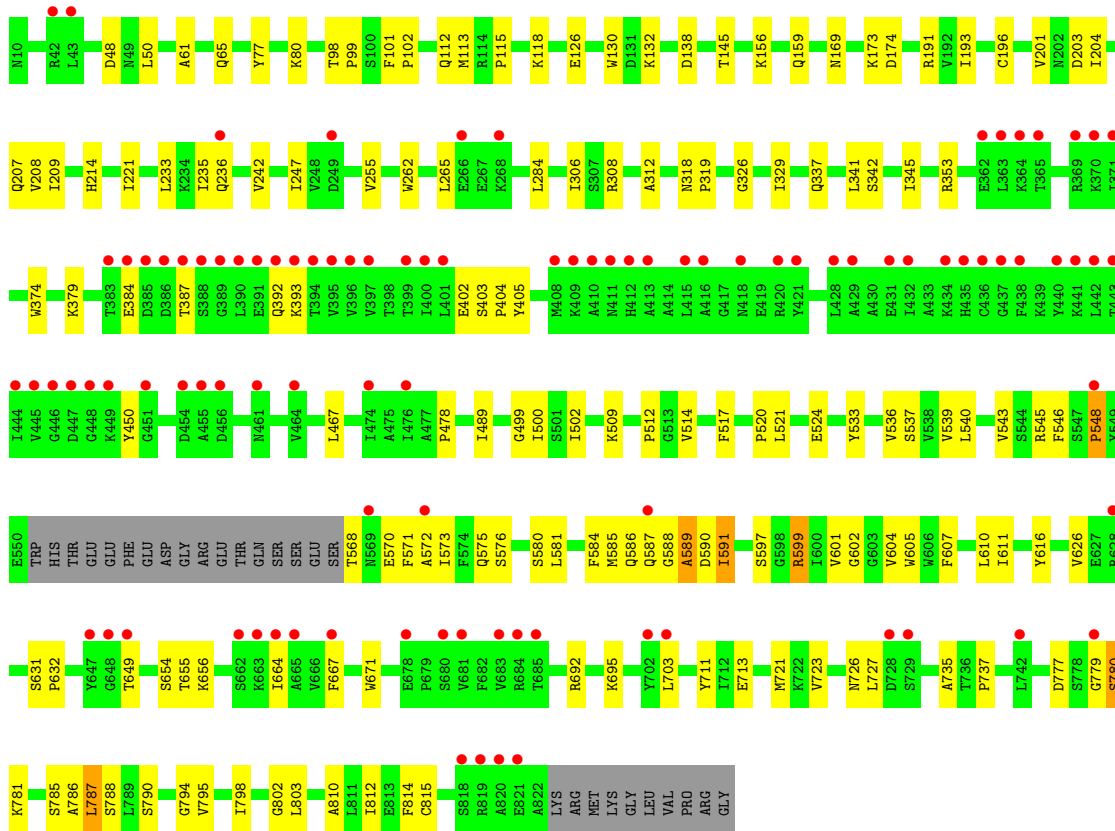
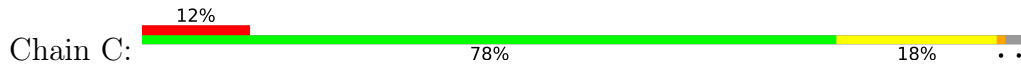


- Molecule 1: Glutamate receptor 2

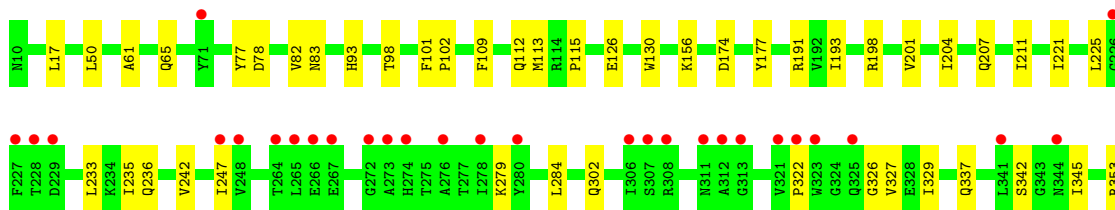
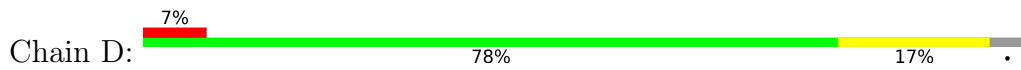


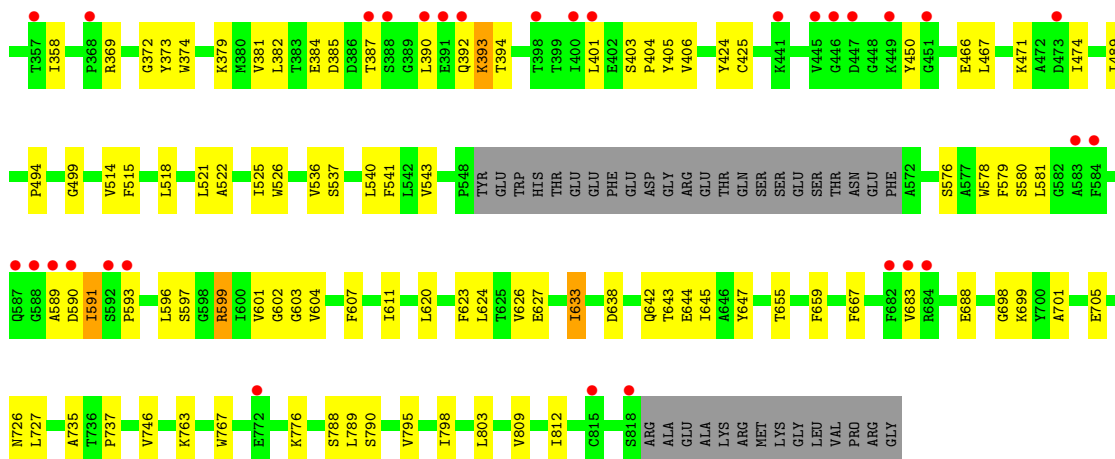


• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2





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

Chain E: 100%

MAG1
MAG2
BMA3

- Molecule 2: 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%

MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-3)-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
BMA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.77Å 306.60Å 107.73Å 90.00° 94.26° 90.00°	Depositor
Resolution (Å)	51.10 – 4.65 53.71 – 4.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (51.10-4.65) 99.1 (53.71-4.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 4.65Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.242 , 0.291 0.243 , 0.291	Depositor DCC
R_{free} test set	1561 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	167.3	Xtrriage
Anisotropy	0.165	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 127.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	25050	wwPDB-VP
Average B, all atoms (Å ²)	210.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: ZK1, BMA, GYK, NAG

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	0.24	0/6285	0.44	0/8493
1	B	0.25	0/6258	0.45	2/8458 (0.0%)
1	C	0.25	0/6387	0.44	0/8632
1	D	0.24	0/6299	0.43	0/8513
All	All	0.25	0/25229	0.44	2/34096 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	581	LEU	CA-CB-CG	5.42	127.76	115.30

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	6156	0	6156	116	0
1	B	6130	0	6129	116	0
1	C	6255	0	6240	112	0
1	D	6169	0	6169	105	0
2	E	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	39	0	34	0	0
3	F	50	0	43	2	0
4	A	26	0	0	0	0
4	B	26	0	0	2	0
4	C	26	0	0	0	0
4	D	26	0	0	1	0
5	A	27	0	13	1	0
5	B	27	0	13	1	0
5	C	27	0	13	3	0
5	D	27	0	13	2	0
All	All	25050	0	24857	407	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 407 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:498:LEU:HD21	1:A:707:THR:HG23	1.49	0.92
1:B:784:THR:OG1	1:B:785:SER:N	2.07	0.86
1:C:785:SER:O	1:C:787:LEU:N	2.09	0.84
1:C:781:LYS:NZ	1:D:627:GLU:OE2	2.11	0.83
1:D:372:GLY:HA2	1:D:382:LEU:HB3	1.64	0.79

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	780/823 (95%)	729 (94%)	49 (6%)	2 (0%)	41 76
1	B	777/823 (94%)	715 (92%)	57 (7%)	5 (1%)	25 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	792/823 (96%)	742 (94%)	44 (6%)	6 (1%)	19	60
1	D	782/823 (95%)	730 (93%)	48 (6%)	4 (0%)	29	68
All	All	3131/3292 (95%)	2916 (93%)	198 (6%)	17 (0%)	29	68

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	593	PRO
1	B	784	THR
1	C	786	ALA
1	D	522	ALA
1	B	507	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	662/696 (95%)	658 (99%)	4 (1%)	86	92
1	B	659/696 (95%)	652 (99%)	7 (1%)	73	85
1	C	672/696 (97%)	669 (100%)	3 (0%)	91	94
1	D	664/696 (95%)	661 (100%)	3 (0%)	88	93
All	All	2657/2784 (95%)	2640 (99%)	17 (1%)	86	92

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	393	LYS
1	D	599	ARG
1	B	509	LYS
1	B	594	ARG
1	B	595	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	344	ASN
1	D	366	ASN
1	D	756	GLN
1	D	508	GLN
1	A	756	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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	NAG	E	1	2,1	14,14,15	0.30	0	17,19,21	0.55	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.44	0
2	BMA	E	3	2	11,11,12	0.62	0	15,15,17	0.78	0
3	NAG	F	1	1,3	14,14,15	0.49	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.51	0
3	BMA	F	3	3	11,11,12	1.15	1 (9%)	15,15,17	1.02	1 (6%)
3	BMA	F	4	3	11,11,12	0.98	0	15,15,17	1.42	1 (6%)
2	NAG	G	1	2,1	14,14,15	0.89	1 (7%)	17,19,21	1.40	1 (5%)
2	NAG	G	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	BMA	G	3	2	11,11,12	0.63	0	15,15,17	0.75	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	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	BMA	F	4	3	-	1/2/19/22	1/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	3.24	1.48	1.43
3	F	3	BMA	C4-C3	2.16	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	5.52	119.67	112.19
3	F	4	BMA	C1-O5-C5	4.51	118.30	112.19
3	F	3	BMA	C2-C3-C4	2.13	114.57	110.89

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

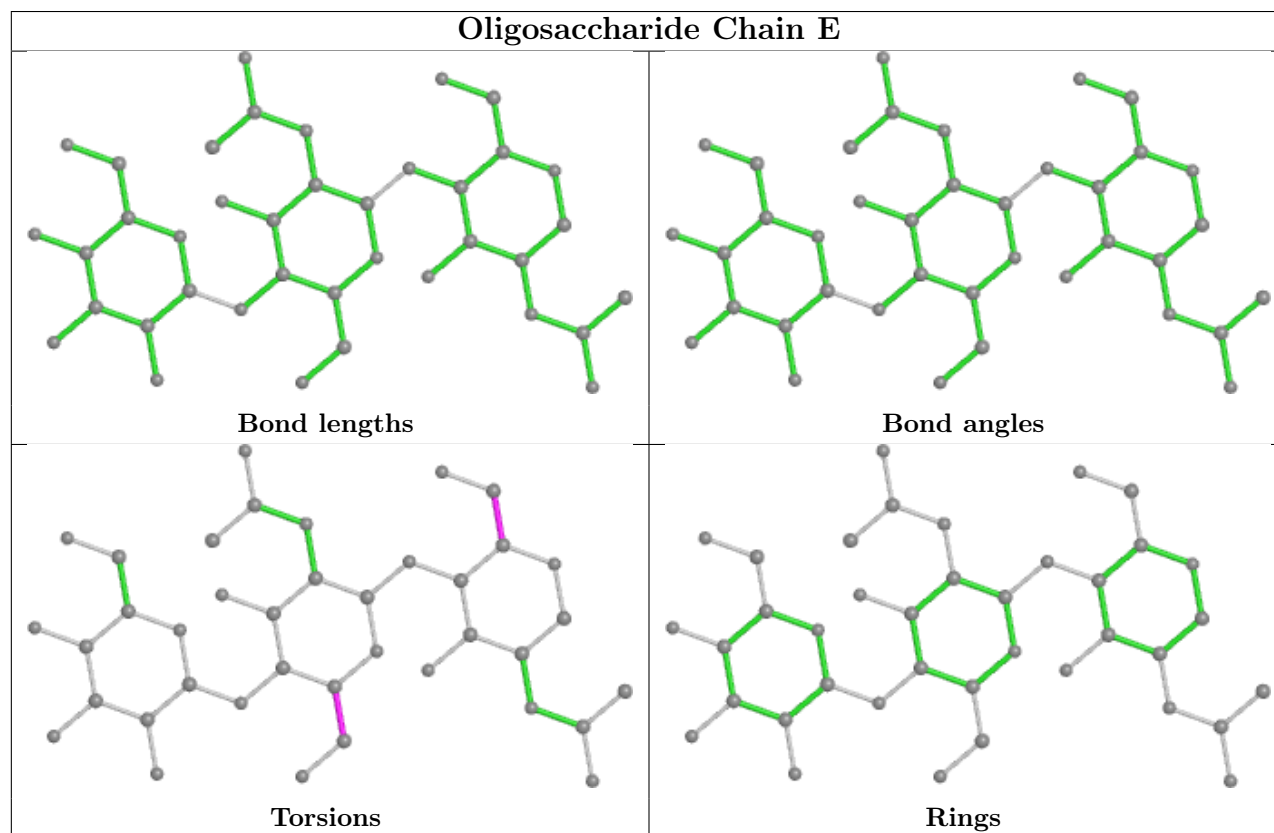
All (1) ring outliers are listed below:

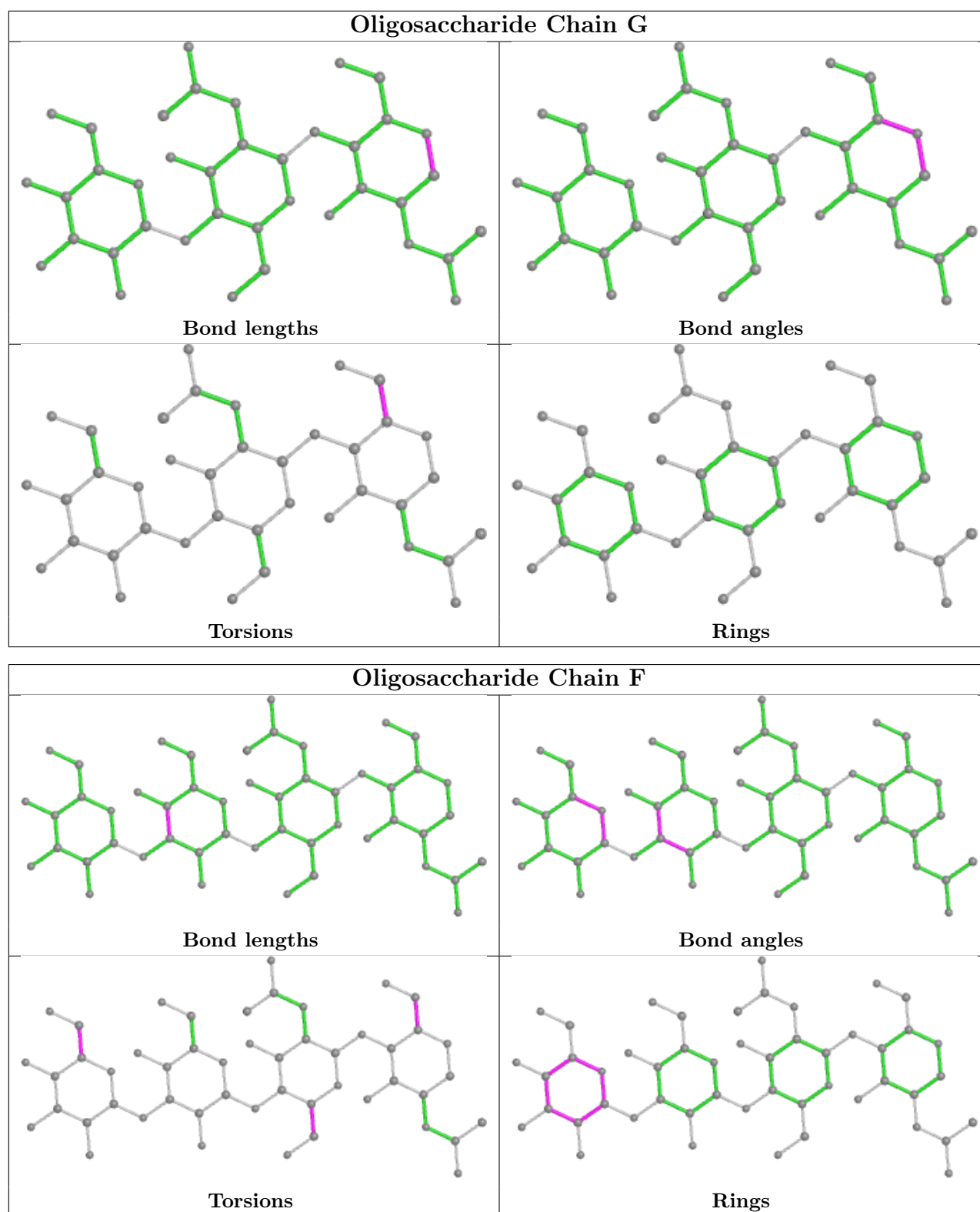
Mol	Chain	Res	Type	Atoms
3	F	4	BMA	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
3	F	2	NAG	2	0

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





5.6 Ligand geometry [i](#)

8 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
4	GYK	D	901	-	27,29,29	3.79	10 (37%)	30,42,42	2.02	6 (20%)
4	GYK	A	901	-	27,29,29	3.80	9 (33%)	30,42,42	2.03	6 (20%)
5	ZK1	B	902	-	28,29,29	3.50	13 (46%)	42,45,45	1.60	8 (19%)
4	GYK	C	901	-	27,29,29	3.84	11 (40%)	30,42,42	2.16	11 (36%)
5	ZK1	C	902	-	28,29,29	3.47	12 (42%)	42,45,45	1.67	9 (21%)
4	GYK	B	901	-	27,29,29	3.85	11 (40%)	30,42,42	2.22	11 (36%)
5	ZK1	A	902	-	28,29,29	3.49	12 (42%)	42,45,45	1.64	9 (21%)
5	ZK1	D	902	-	28,29,29	3.29	12 (42%)	42,45,45	1.61	7 (16%)

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
4	GYK	D	901	-	-	2/6/32/32	0/3/4/4
4	GYK	A	901	-	-	2/6/32/32	0/3/4/4
5	ZK1	B	902	-	-	5/13/23/23	0/3/3/3
4	GYK	C	901	-	-	2/6/32/32	0/3/4/4
5	ZK1	C	902	-	-	5/13/23/23	0/3/3/3
4	GYK	B	901	-	-	2/6/32/32	0/3/4/4
5	ZK1	A	902	-	-	4/13/23/23	0/3/3/3
5	ZK1	D	902	-	-	5/13/23/23	0/3/3/3

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	GYK	C10-N11	13.88	1.45	1.30
4	C	901	GYK	C10-N11	13.76	1.45	1.30
4	A	901	GYK	C10-N11	13.72	1.45	1.30
4	D	901	GYK	C10-N11	13.60	1.45	1.30
5	D	902	ZK1	OAA-CAT	9.28	1.41	1.23

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	901	GYK	O24-C07-C08	5.17	134.77	127.85
4	B	901	GYK	O24-C07-C08	5.17	134.76	127.85
4	D	901	GYK	O24-C07-C08	5.14	134.73	127.85
4	A	901	GYK	O24-C07-C08	5.09	134.66	127.85
4	D	901	GYK	O24-C07-C06	-4.58	104.57	109.78

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

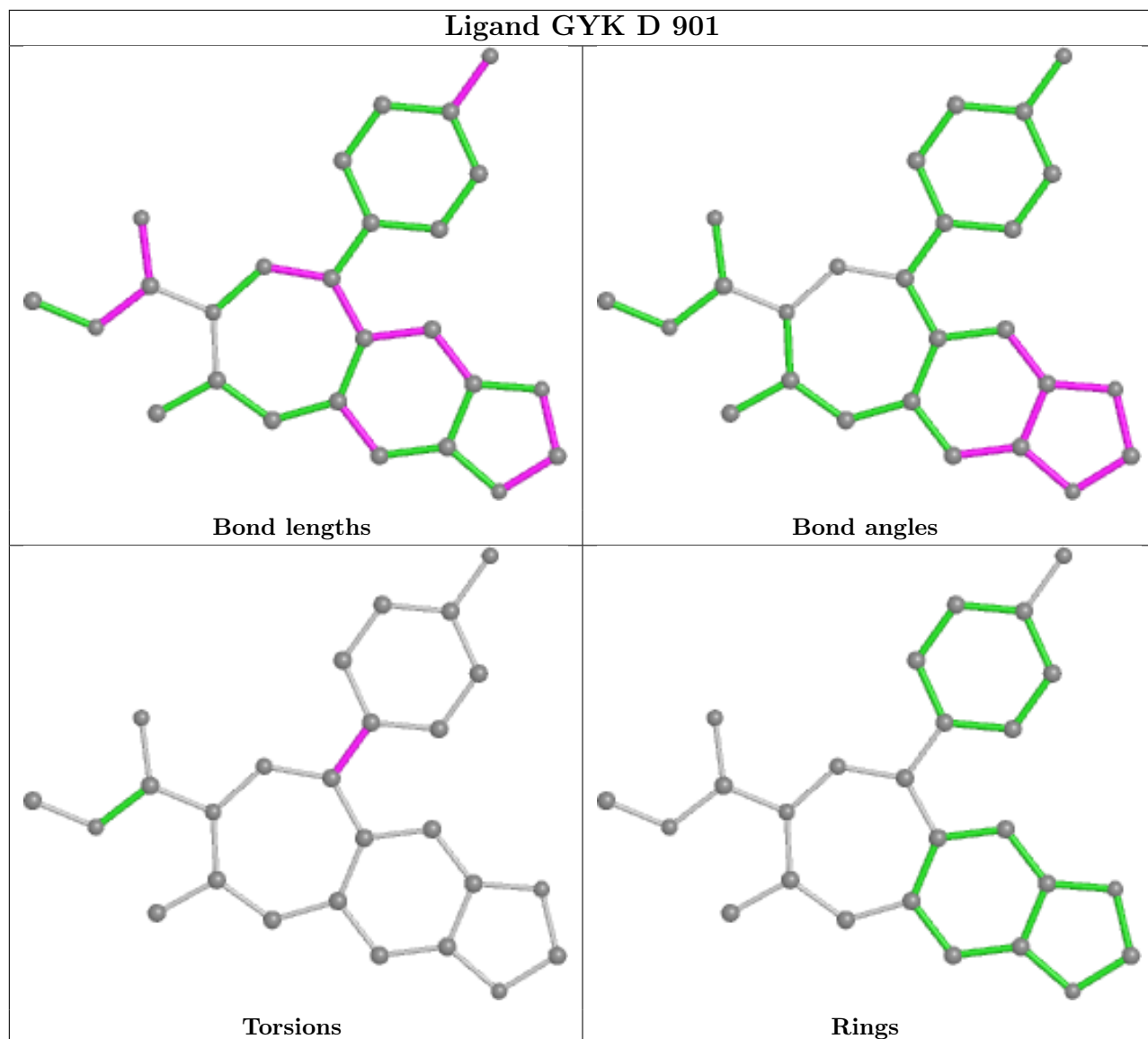
Mol	Chain	Res	Type	Atoms
4	A	901	GYK	C09-C10-C17-C18
4	A	901	GYK	C09-C10-C17-C22
4	B	901	GYK	N11-C10-C17-C18
4	B	901	GYK	N11-C10-C17-C22
4	C	901	GYK	N11-C10-C17-C18

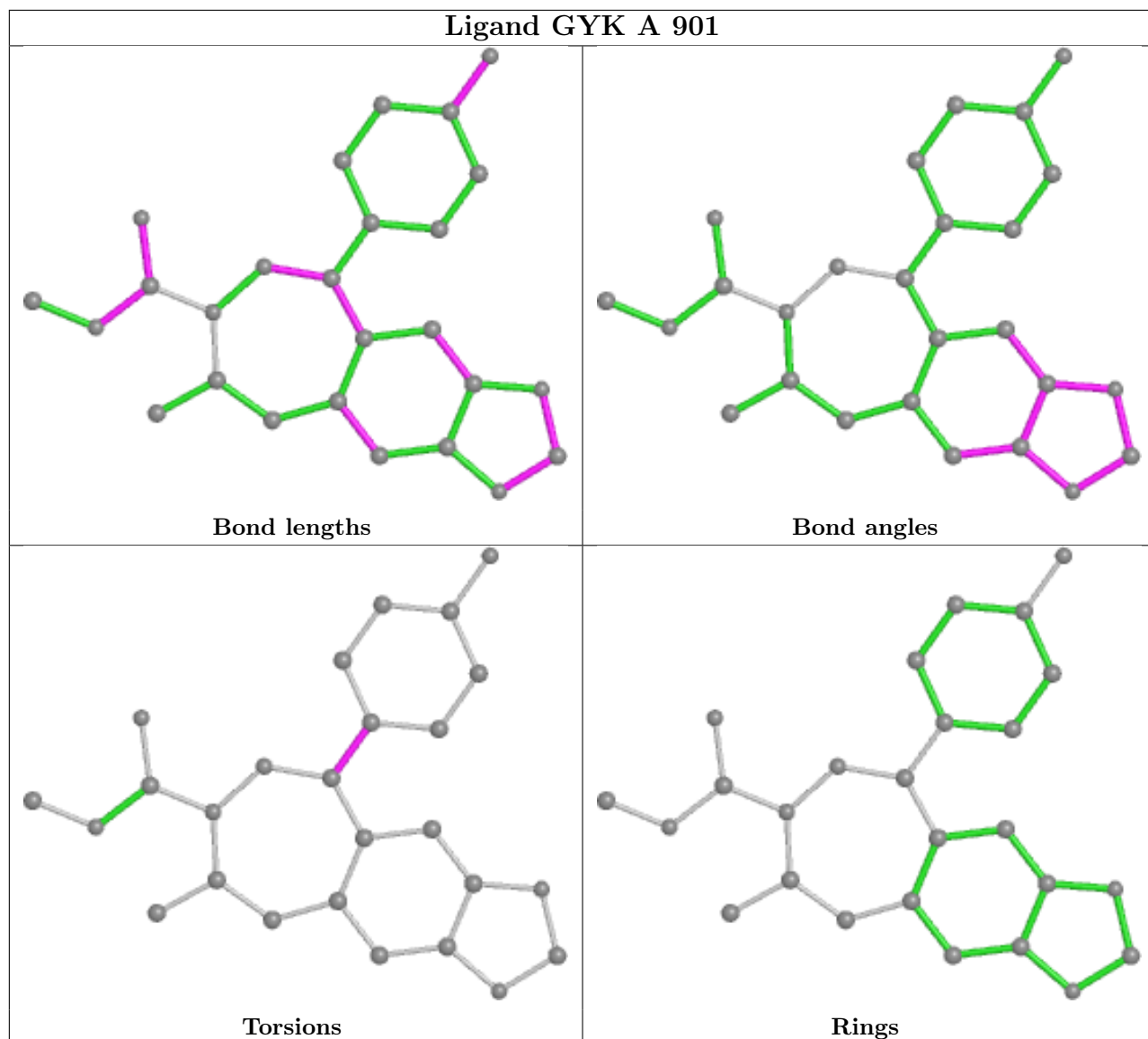
There are no ring outliers.

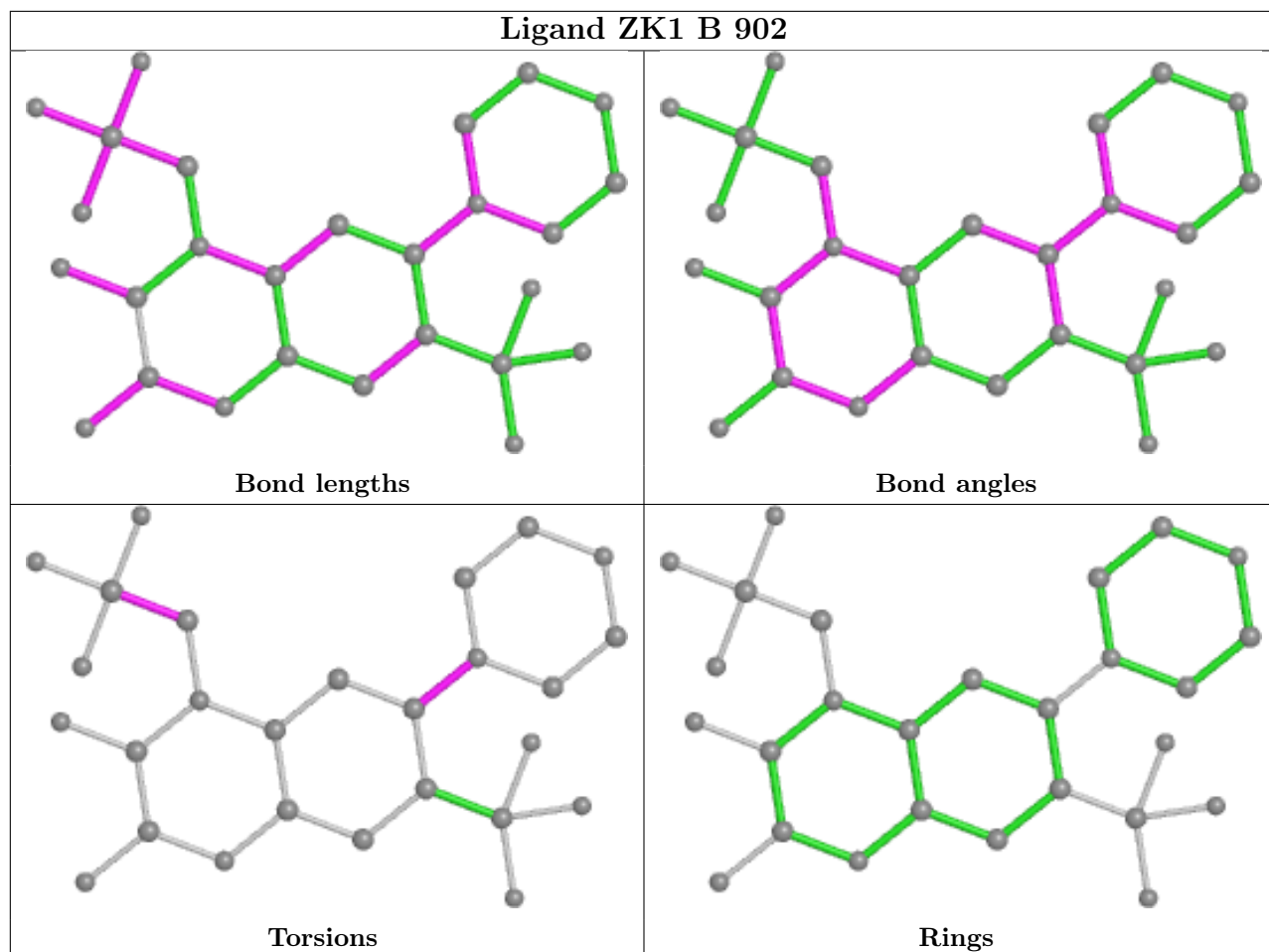
6 monomers are involved in 10 short contacts:

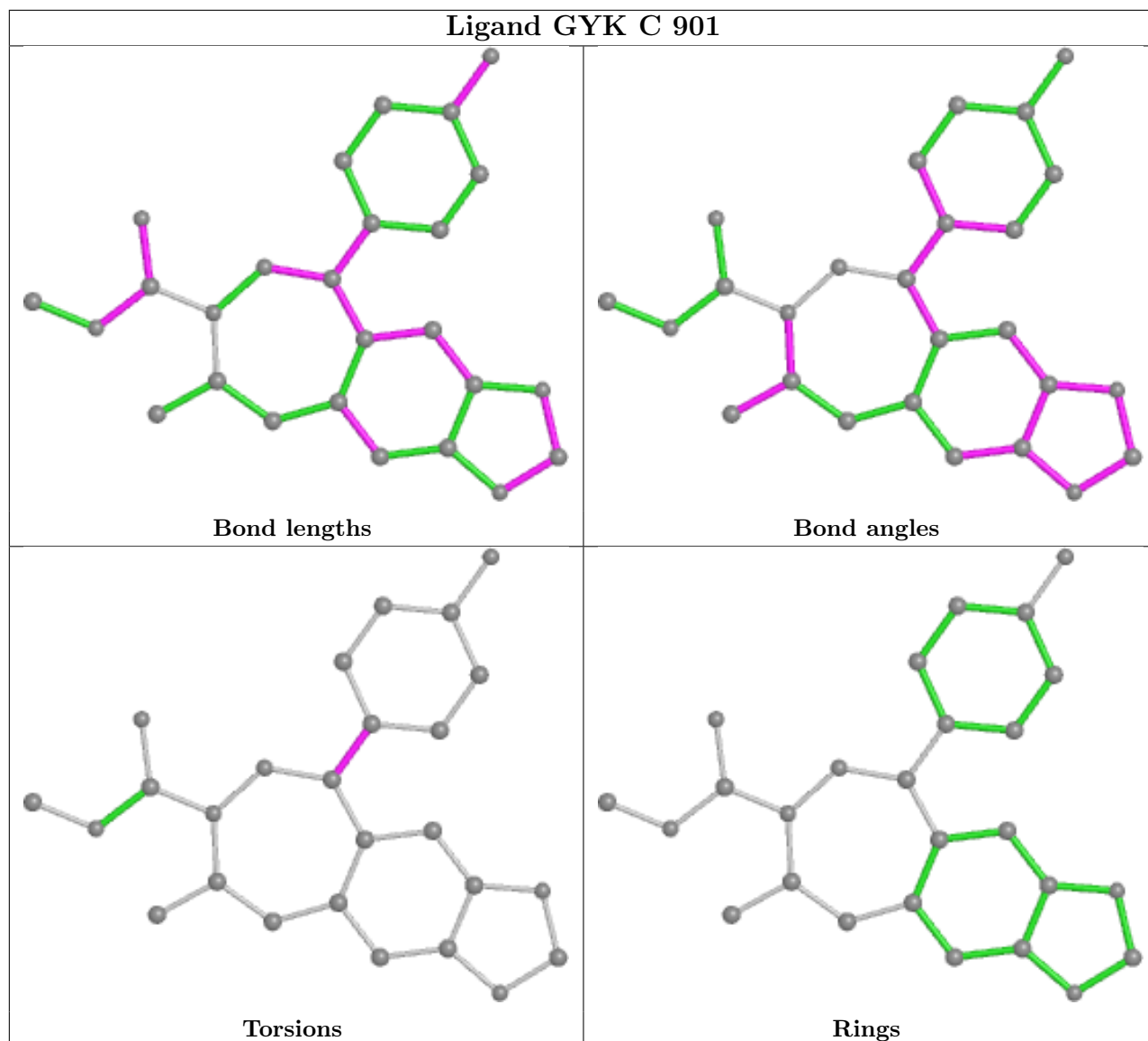
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	GYK	1	0
5	B	902	ZK1	1	0
5	C	902	ZK1	3	0
4	B	901	GYK	2	0
5	A	902	ZK1	1	0
5	D	902	ZK1	2	0

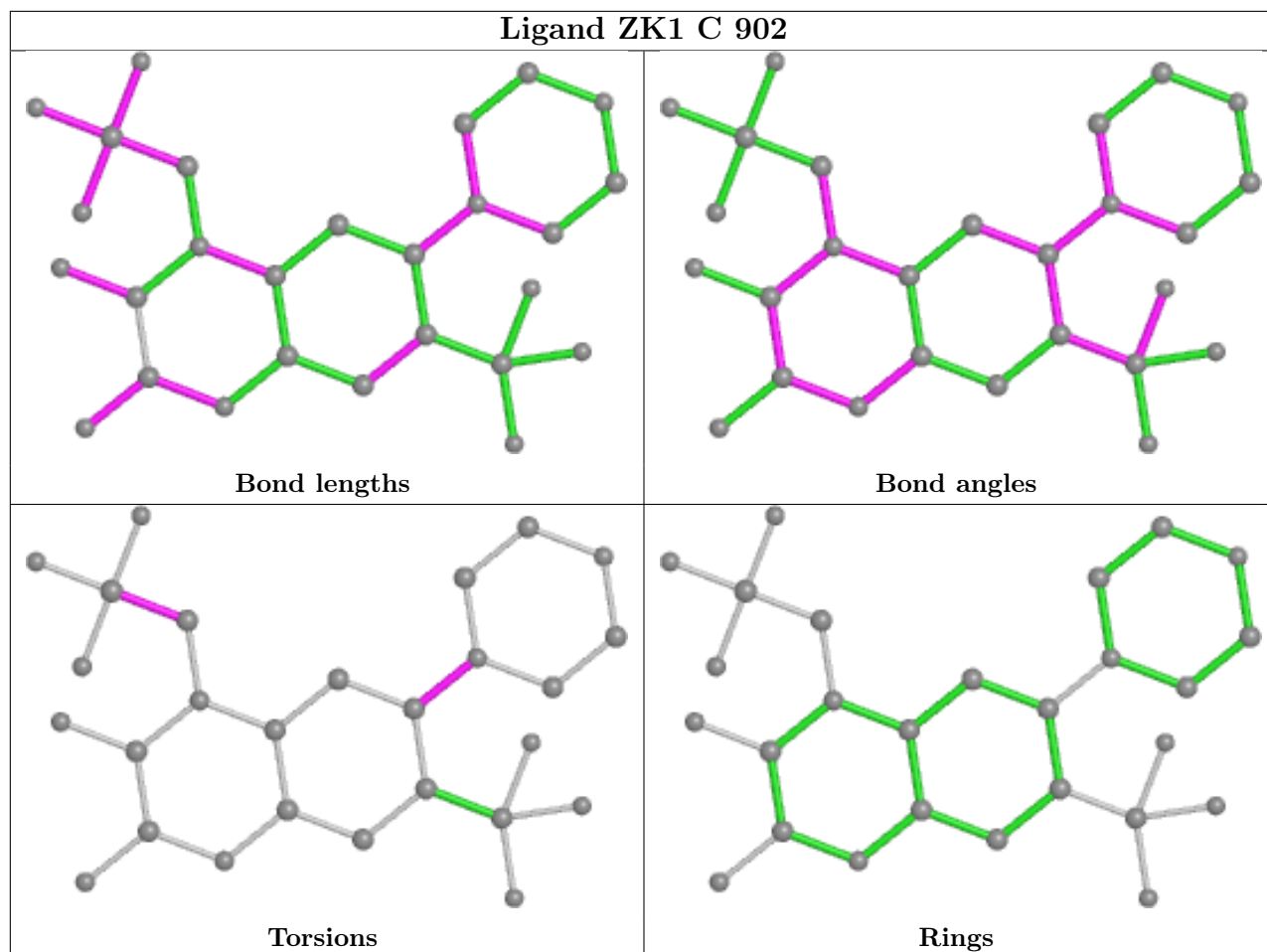
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

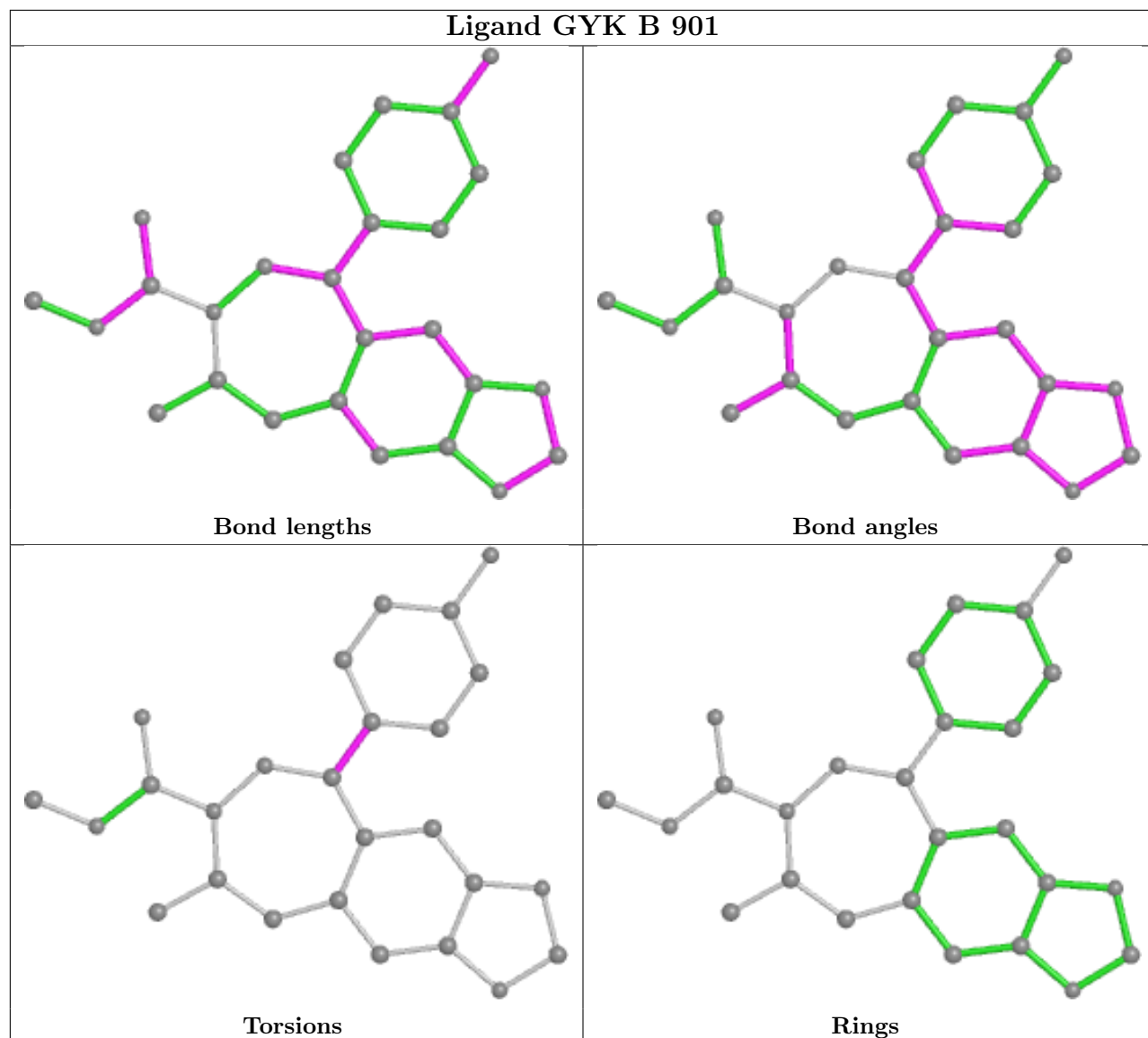


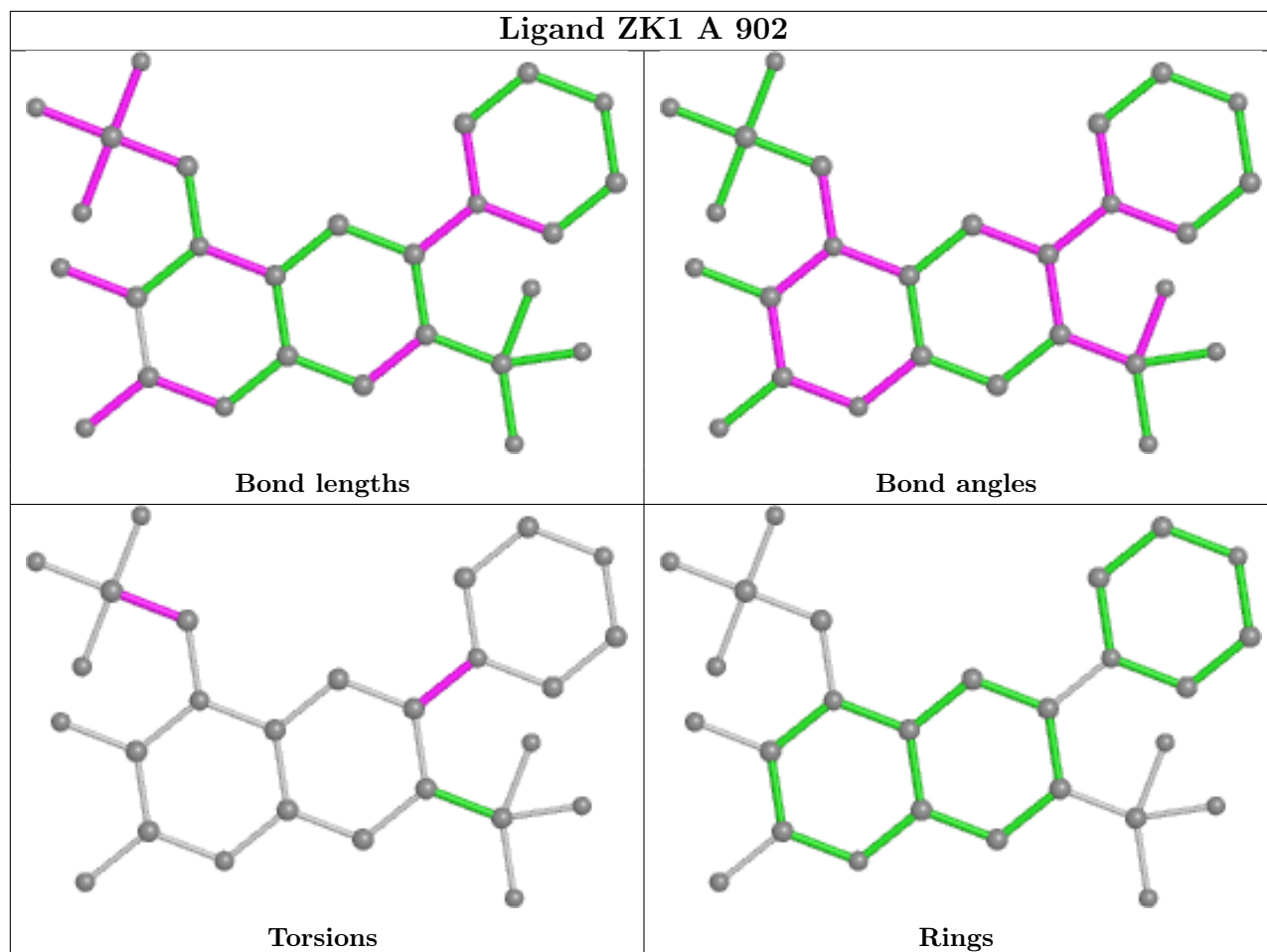


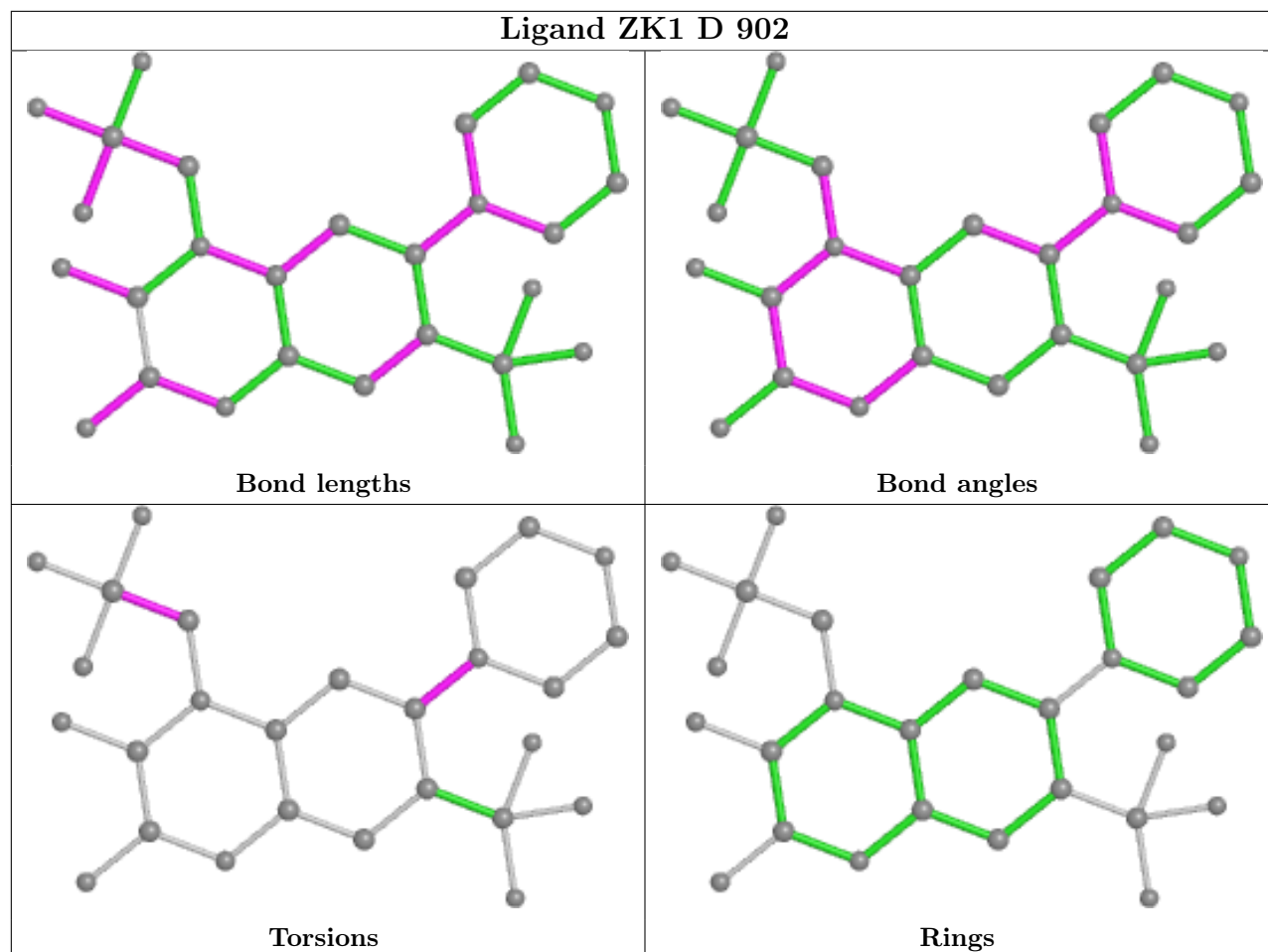












5.7 Other polymers [i](#)

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	784/823 (95%)	0.03	34 (4%) 35 29	126, 201, 264, 306	0
1	B	781/823 (94%)	0.04	29 (3%) 41 33	113, 187, 267, 319	0
1	C	796/823 (96%)	0.39	98 (12%) 4 5	106, 224, 293, 351	0
1	D	786/823 (95%)	0.34	60 (7%) 13 12	142, 219, 290, 354	0
All	All	3147/3292 (95%)	0.20	221 (7%) 16 13	106, 208, 282, 354	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	ALA	7.0
1	D	313	GLY	6.3
1	D	588	GLY	6.2
1	A	512	PRO	6.2
1	C	447	ASP	6.0

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

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

6.3 Carbohydrates [i](#)

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

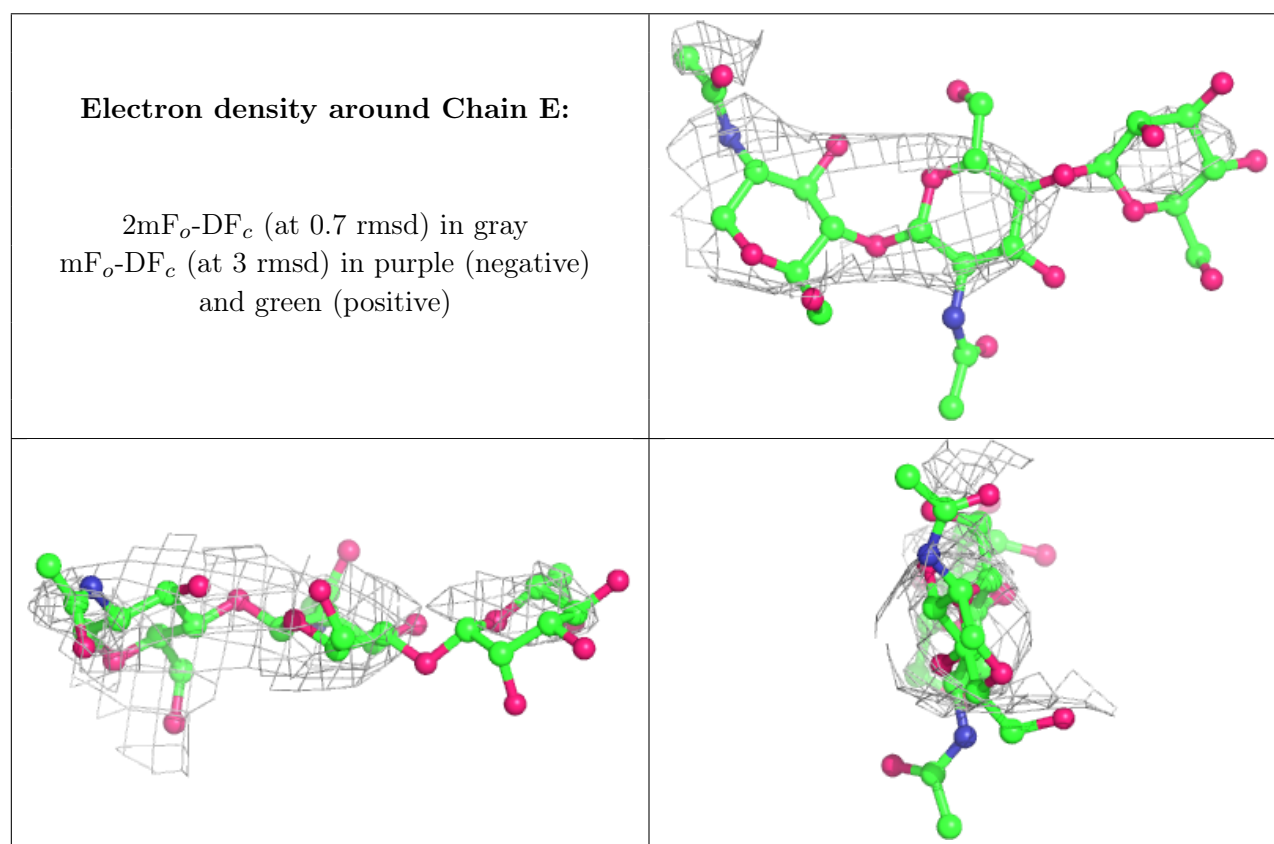
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	F	4	11/12	0.75	0.54	270,299,314,326	0
3	BMA	F	3	11/12	0.81	0.54	280,298,312,316	0

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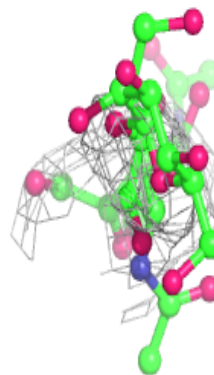
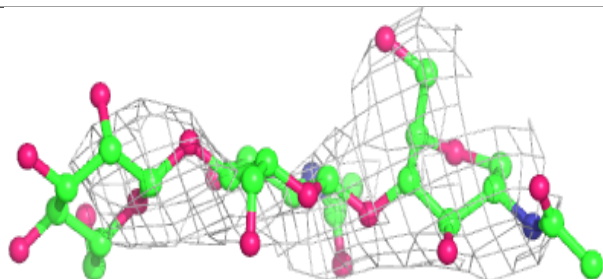
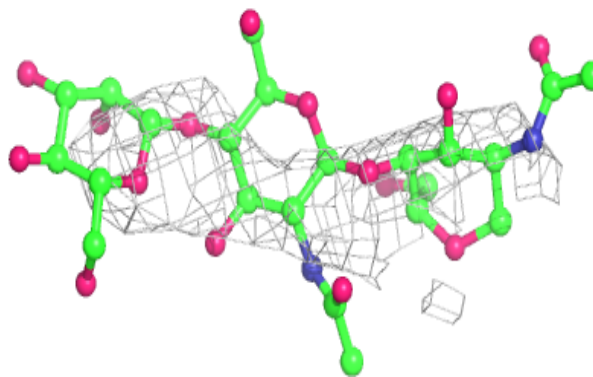
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	1	14/15	0.81	0.35	223,243,260,263	0
2	BMA	E	3	11/12	0.82	0.51	261,282,295,304	0
3	NAG	F	1	14/15	0.82	0.42	225,253,262,279	0
3	NAG	F	2	14/15	0.84	0.37	206,268,284,292	0
2	NAG	E	2	14/15	0.85	0.48	259,283,301,303	0
2	NAG	G	2	14/15	0.85	0.48	229,268,279,281	0
2	NAG	G	1	14/15	0.86	0.34	211,245,258,268	0
2	BMA	G	3	11/12	0.86	0.41	268,290,297,297	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.

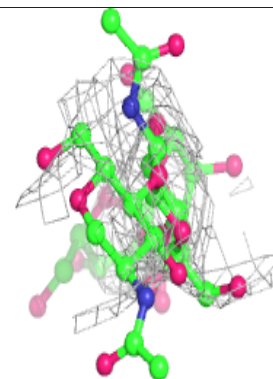
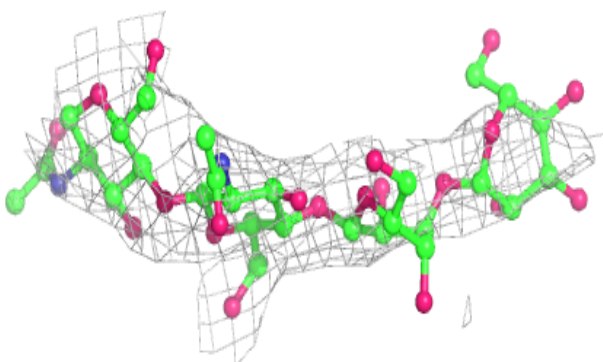
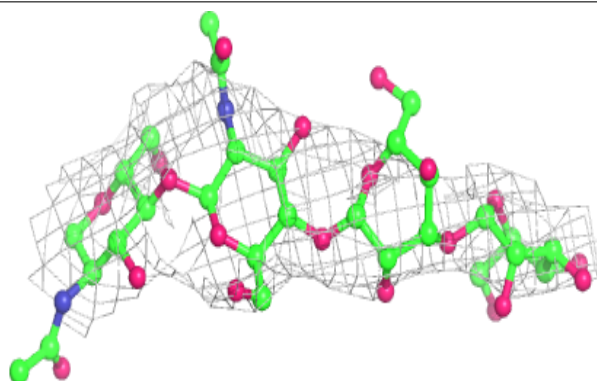


Electron density around Chain G:

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

**Electron density around Chain F:**

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



6.4 Ligands

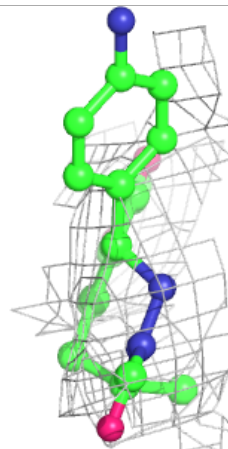
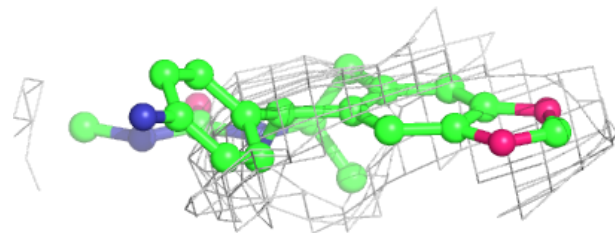
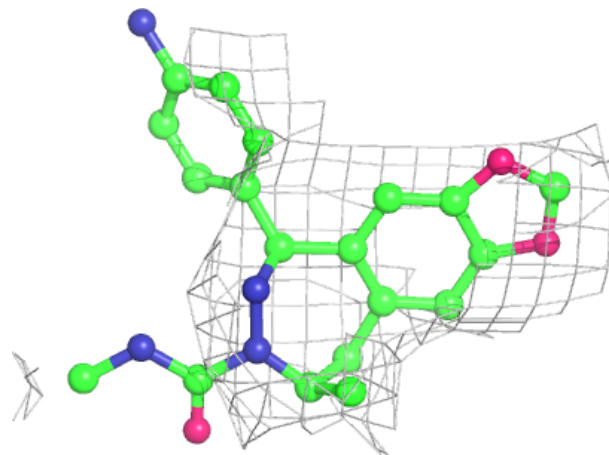
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

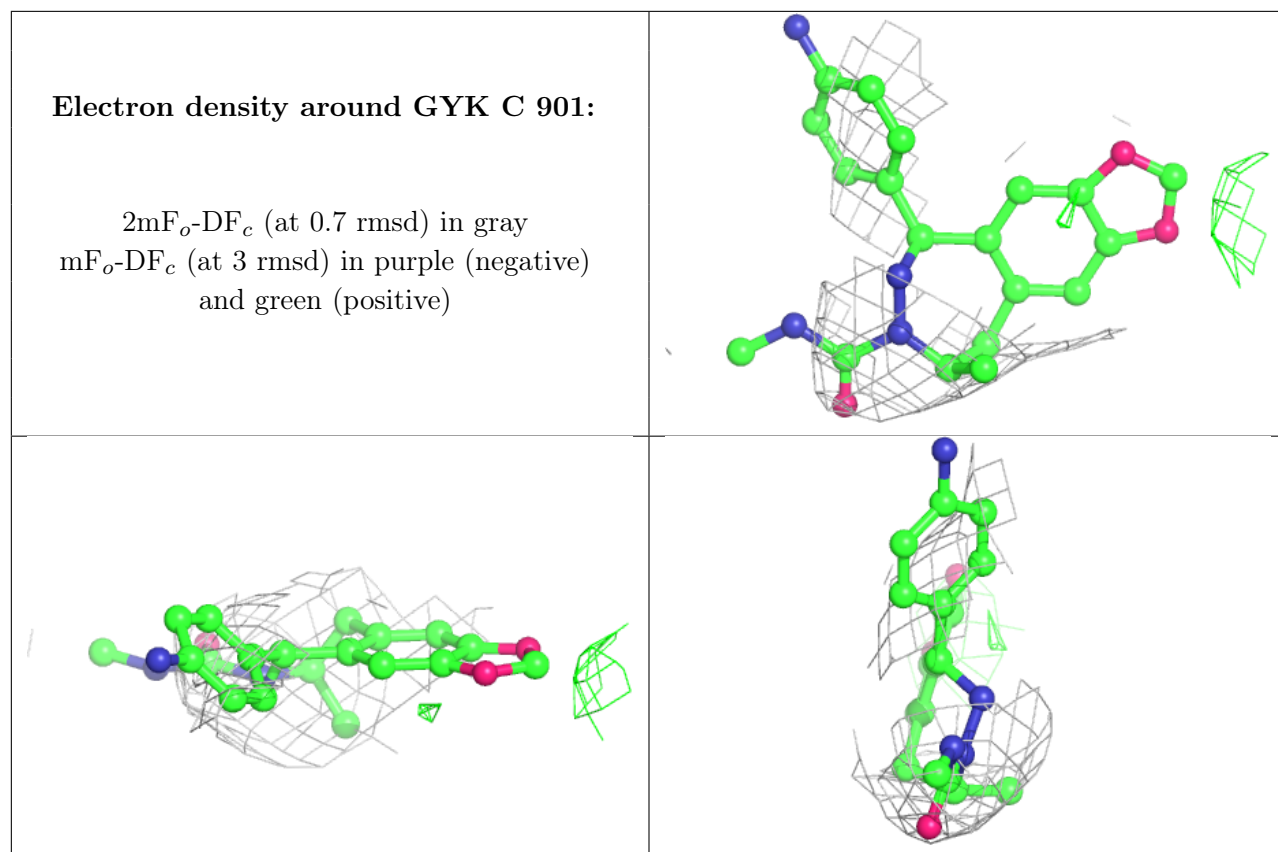
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GYK	B	901	26/26	0.72	0.46	208,225,234,240	0
4	GYK	C	901	26/26	0.74	0.47	205,219,233,237	0
4	GYK	A	901	26/26	0.76	0.60	214,240,251,254	0
5	ZK1	B	902	27/27	0.85	0.33	172,184,201,204	0
5	ZK1	D	902	27/27	0.86	0.35	171,201,216,218	0
5	ZK1	A	902	27/27	0.87	0.26	180,196,223,232	0
5	ZK1	C	902	27/27	0.89	0.41	230,249,268,278	0
4	GYK	D	901	26/26	0.89	0.32	223,244,265,275	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GYK B 901:

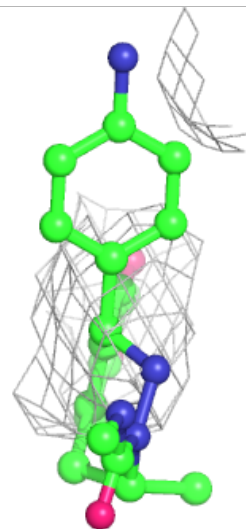
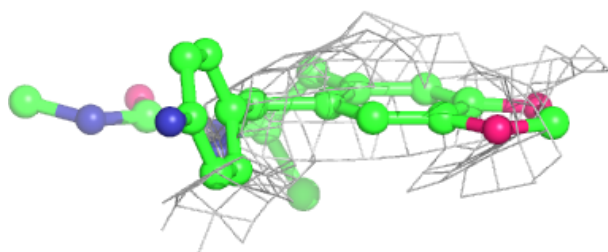
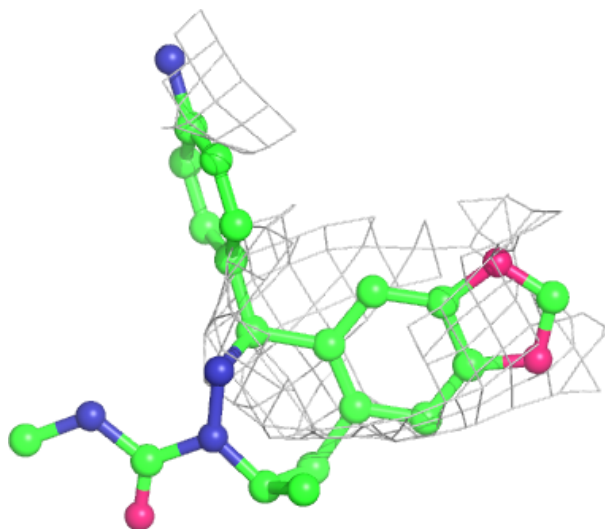
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





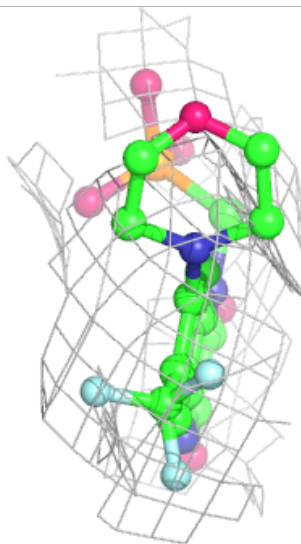
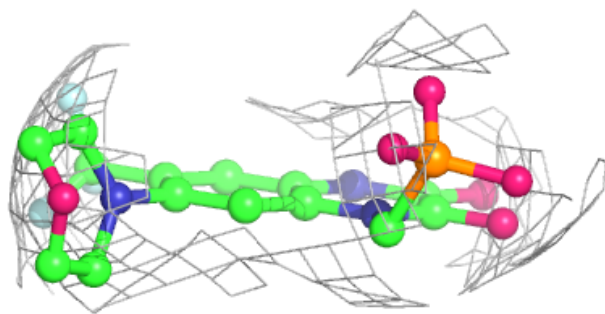
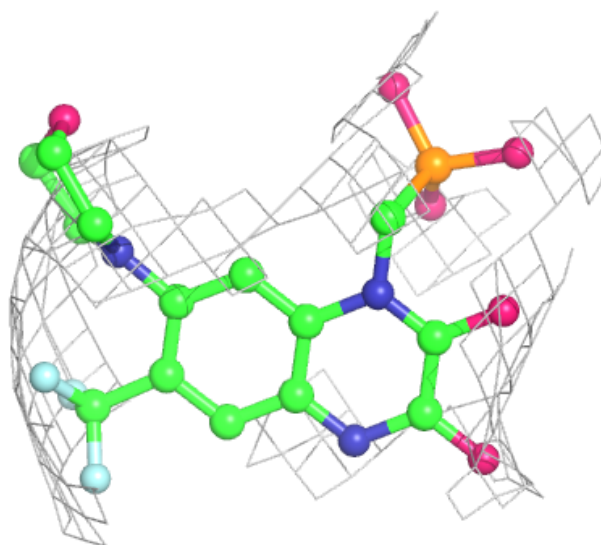
Electron density around GYK A 901:

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



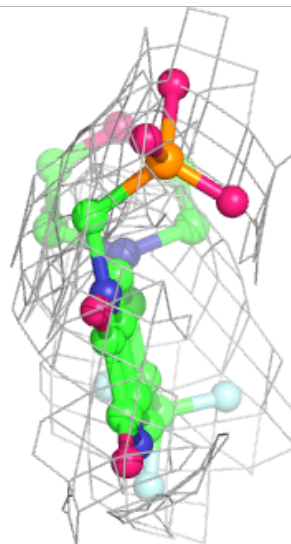
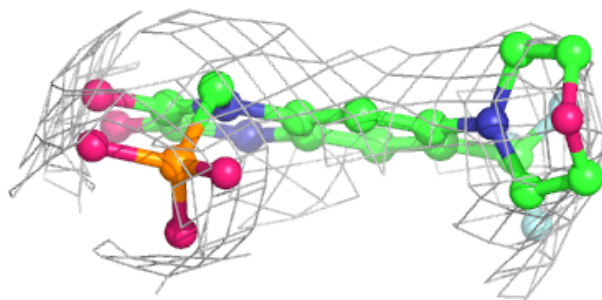
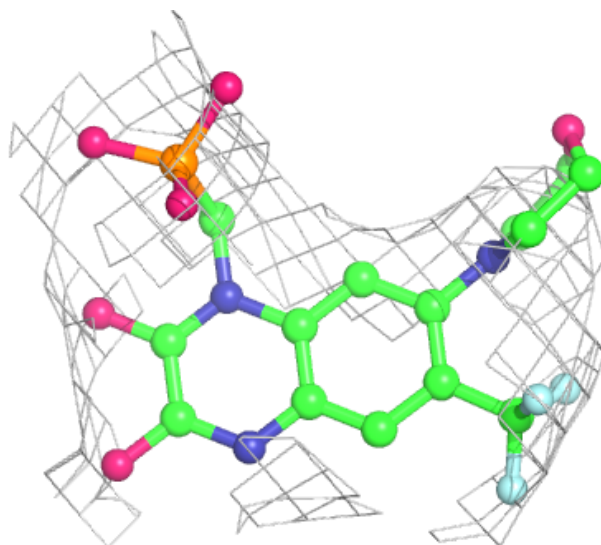
Electron density around ZK1 B 902:

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



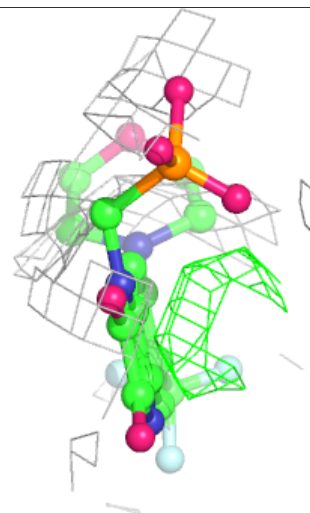
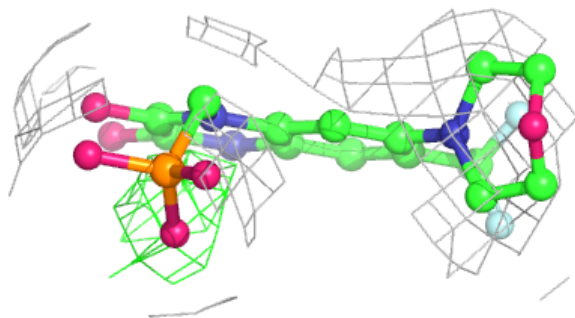
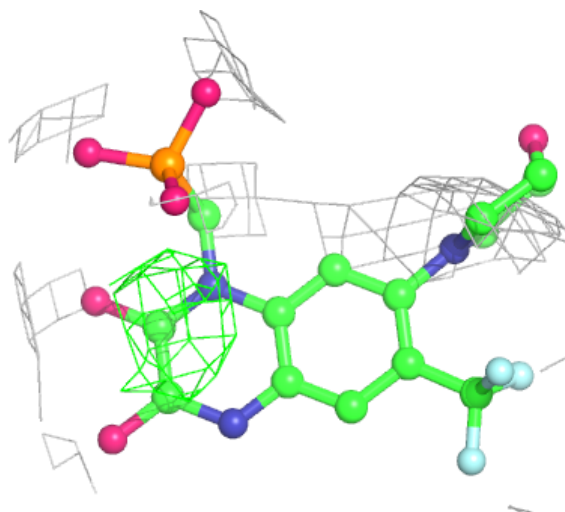
Electron density around ZK1 D 902:

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



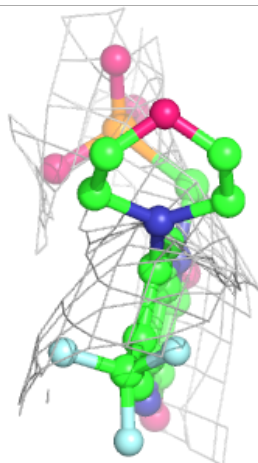
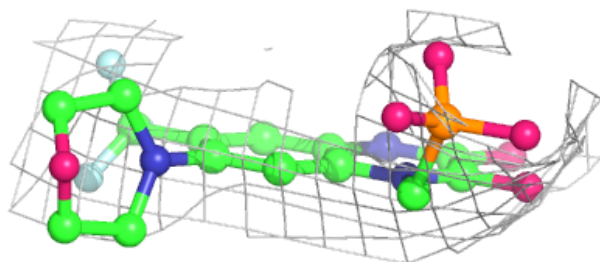
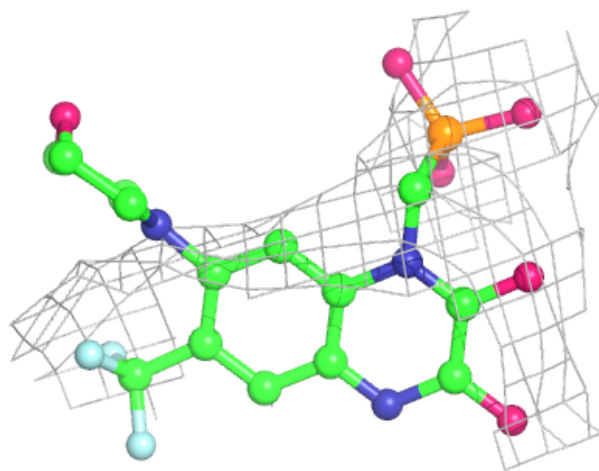
Electron density around ZK1 A 902:

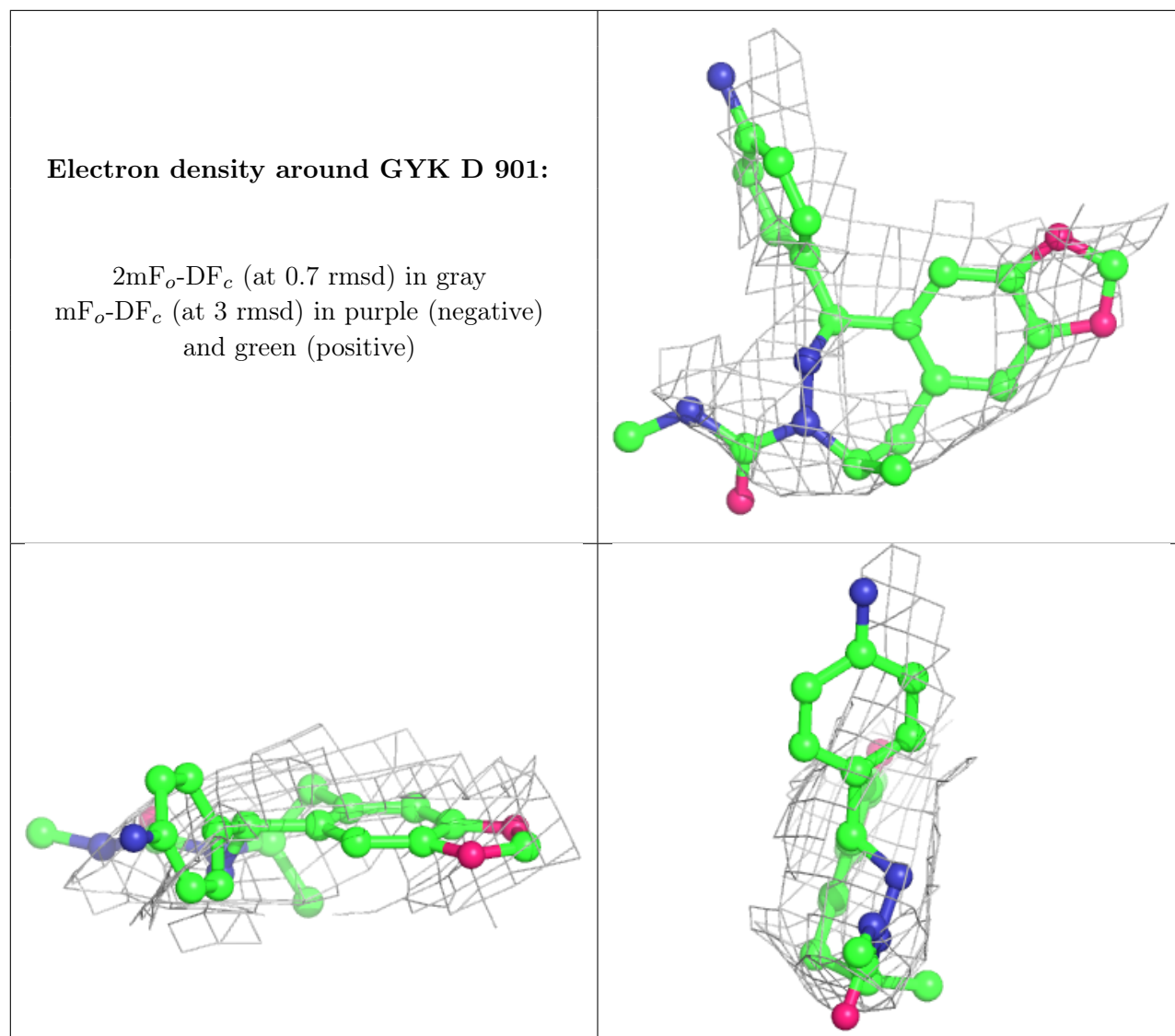
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZK1 C 902:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.