



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2022 – 12:23 pm GMT

PDB ID : 7ZKN
Title : X-ray structure of the complex between human alpha thrombin and a pseudo-cyclic thrombin binding aptamer (TBA-NNp/DDp) - Crystal form gamma
Authors : Troisi, R.; Sica, F.
Deposited on : 2022-04-13
Resolution : 3.03 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

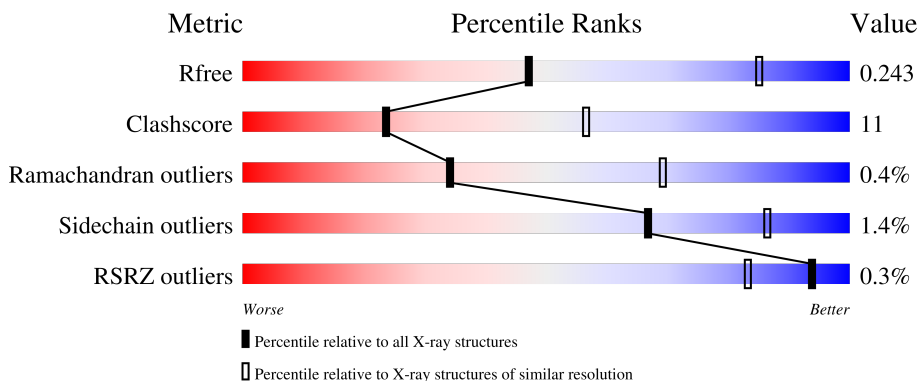
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	36	 61% 11% 28%
1	C	36	 64% 8% 28%
2	B	259	 71% 26% .
2	D	259	 73% 24% ..
3	E	15	 13% 53% 33%

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Mol	Chain	Length	Quality of chain
3	F	15	
3	G	15	
3	I	15	
4	H	2	
4	J	2	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 6100 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	26	Total	C	N	O	S	0	0	0
			214	134	35	44	1			
1	C	26	Total	C	N	O	S	0	0	0
			214	134	35	44	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	Total	C	N	O	S	0	0	0
			2031	1295	359	363	14			
2	D	251	Total	C	N	O	S	0	0	0
			2029	1294	359	362	14			

- Molecule 3 is a DNA chain called TBA-NNp/DDp.

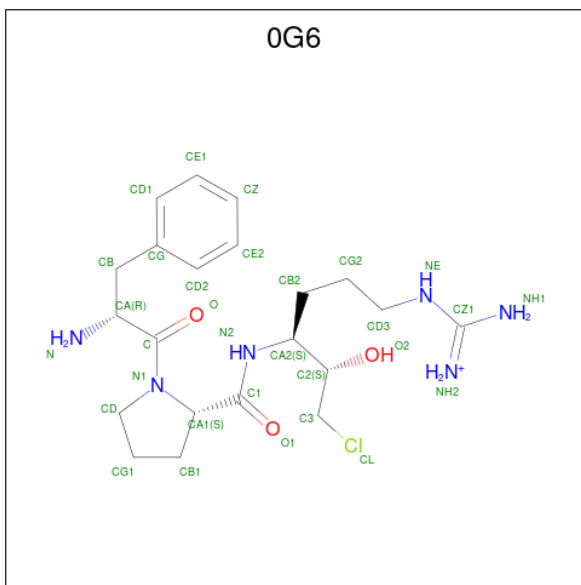
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	15	Total	C	N	O	P	0	0	0
			289	135	48	91	15			
3	F	12	Total	C	N	O	P	0	0	0
			256	120	48	76	12			
3	G	12	Total	C	N	O	P	0	0	0
			256	120	48	76	12			
3	I	12	Total	C	N	O	P	0	0	0
			256	120	48	76	12			

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



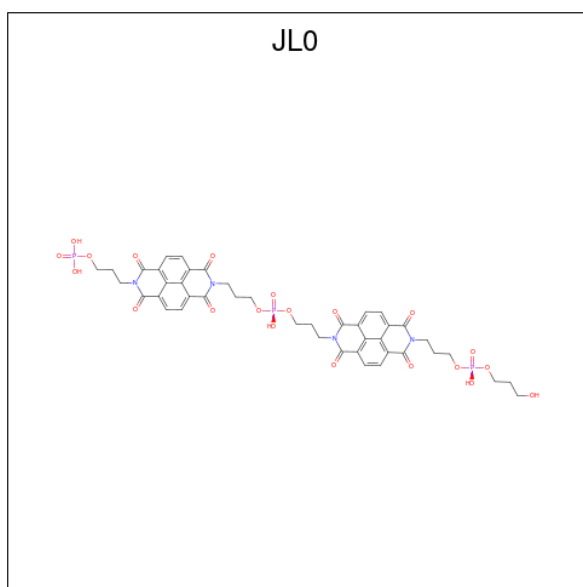
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is D-phenylalanyl-N-[(2S,3S)-6-{{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: C₂₁H₃₄ClN₆O₃).



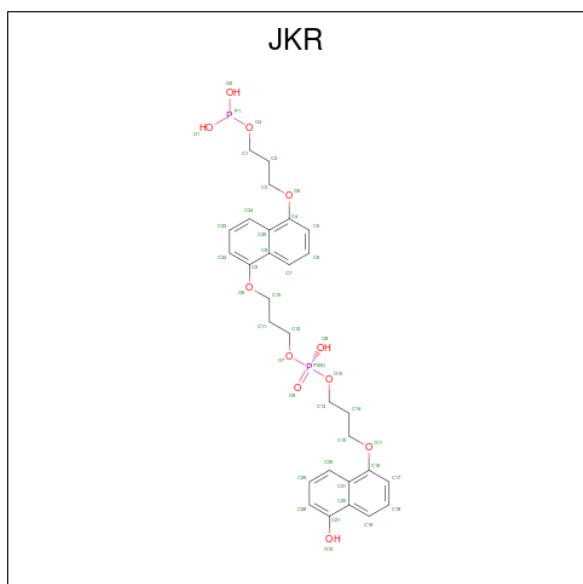
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			30	21	6	3		
5	D	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 6 is 3-[13-methyl-5,7,12,14-tetrakis(oxidanylidene)-6,13-diazatetracyclo[6.6.2.0⁴,16].0^{11,15}]hexadeca-1(15),2,4(16),8,10-pentaen-6-yl]propyl 3-[5,7,12,14-tetrakis(oxidanylidene)-13-(3-oxidanylpropyl)-6,13-diazatetracyclo[6.6.2.0⁴,16].0^{11,15}]hexadeca-1,3,8(16),9,11(15)-pentaen-6-yl]propyl hydrogen phosphate (three-letter code: JL0) (formula: C₄₃H₄₃N₄O₂₁P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	E	1	Total 63	40	4	17	2	0	0
6	F	1	Total 56	38	4	13	1	0	0
6	G	1	Total 63	40	4	17	2	0	0
6	I	1	Total 56	38	4	13	1	0	0

- Molecule 7 is 3-[5-[3-bis(oxidanyl)phosphanyloxypropoxy]naphthalen-1-yl]oxypropyl 3-(5-oxidanylnaphthalen-1-yl)oxypropyl hydrogen phosphate (three-letter code: JKR) (formula: $C_{29}H_{34}O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	O	P	0	0
			42	29	11	2		
7	F	1	Total	C	O	P	0	0
			42	29	11	2		
7	G	1	Total	C	O	P	0	0
			42	29	11	2		
7	I	1	Total	C	O	P	0	0
			42	29	11	2		

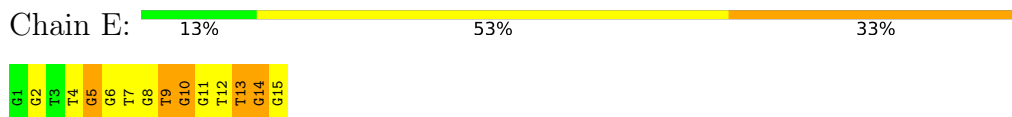
- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	K	0	0
			1	1		
8	F	1	Total	K	0	0
			1	1		
8	G	1	Total	K	0	0
			1	1		
8	I	1	Total	K	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	O	0	0
			1	1		
9	B	16	Total	O	0	0
			16	16		
9	C	2	Total	O	0	0
			2	2		
9	D	8	Total	O	0	0
			8	8		
9	E	1	Total	O	0	0
			1	1		
9	G	1	Total	O	0	0
			1	1		

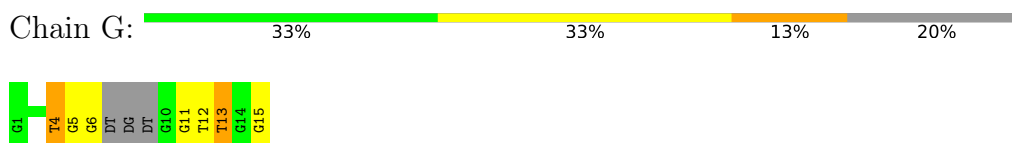
- Molecule 3: TBA-NNp/DDp



- Molecule 3: TBA-NNp/DDp



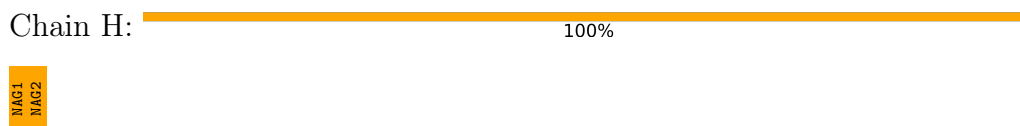
- Molecule 3: TBA-NNp/DDp



- Molecule 3: TBA-NNp/DDp



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.62Å 114.86Å 83.44Å 90.00° 117.25° 90.00°	Depositor
Resolution (Å)	68.13 – 3.03 68.04 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.13-3.03) 99.6 (68.04-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.243 0.201 , 0.243	Depositor DCC
R_{free} test set	1223 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtrriage
Anisotropy	0.223	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.108 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6100	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: JL0, K, 0G6, NAG, JKR

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	0.29	0/216	0.58	0/287
1	C	0.30	0/216	0.59	0/287
2	B	0.28	0/2083	0.58	0/2813
2	D	0.28	0/2081	0.57	0/2811
3	E	0.76	0/323	1.27	8/498 (1.6%)
3	F	0.80	0/286	1.33	6/440 (1.4%)
3	G	0.76	0/286	1.24	3/440 (0.7%)
3	I	0.82	0/286	1.25	6/440 (1.4%)
All	All	0.43	0/5777	0.79	23/8016 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	12	DT	P-O3'-C3'	-8.39	109.63	119.70
3	G	12	DT	P-O3'-C3'	-7.95	110.16	119.70
3	F	12	DT	P-O3'-C3'	-7.33	110.91	119.70
3	E	13	DT	P-O3'-C3'	-7.30	110.94	119.70
3	G	13	DT	P-O3'-C3'	-7.21	111.05	119.70
3	I	2	DG	P-O3'-C3'	-6.98	111.32	119.70
3	E	9	DT	P-O3'-C3'	-6.89	111.43	119.70
3	F	5	DG	P-O3'-C3'	-6.56	111.83	119.70
3	I	3	DT	P-O3'-C3'	-6.55	111.84	119.70
3	F	11	DG	P-O3'-C3'	-6.45	111.96	119.70
3	I	12	DT	P-O3'-C3'	-6.43	111.99	119.70
3	F	13	DT	P-O3'-C3'	-6.35	112.08	119.70
3	E	7	DT	P-O3'-C3'	-6.24	112.21	119.70
3	I	4	DT	P-O3'-C3'	-6.22	112.23	119.70
3	E	10	DG	P-O3'-C3'	-6.15	112.32	119.70
3	F	4	DT	P-O3'-C3'	-6.13	112.34	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	DG	P-O3'-C3'	-6.09	112.39	119.70
3	G	4	DT	P-O3'-C3'	-5.94	112.57	119.70
3	I	5	DG	P-O3'-C3'	-5.75	112.80	119.70
3	E	14	DG	P-O3'-C3'	-5.68	112.89	119.70
3	E	5	DG	P-O3'-C3'	-5.66	112.91	119.70
3	I	11	DG	P-O3'-C3'	-5.21	113.45	119.70
3	F	2	DG	P-O3'-C3'	-5.20	113.46	119.70

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	214	0	214	5	0
1	C	214	0	214	3	0
2	B	2031	0	1998	46	0
2	D	2029	0	2002	45	0
3	E	289	0	154	10	0
3	F	256	0	137	7	0
3	G	256	0	137	6	0
3	I	256	0	137	9	0
4	H	28	0	25	1	0
4	J	28	0	25	0	0
5	B	30	0	31	3	0
5	D	30	0	31	3	0
6	E	63	0	0	1	0
6	F	56	0	0	0	0
6	G	63	0	0	0	0
6	I	56	0	0	0	0
7	E	42	0	0	2	0
7	F	42	0	0	0	0
7	G	42	0	0	4	0
7	I	42	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	1	0	0	0	0
8	I	1	0	0	0	0
9	A	1	0	0	0	0
9	B	16	0	0	0	0
9	C	2	0	0	0	0
9	D	8	0	0	1	0
9	E	1	0	0	0	0
9	G	1	0	0	0	0
All	All	6100	0	5105	122	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 11.

All (122) 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)
7:G:102:JKR:C17	7:G:102:JKR:C14	2.30	1.09
2:D:93:ARG:HD2	3:I:13:DT:O2	1.75	0.86
2:B:18:GLU:HG3	2:B:187:ARG:HG3	1.59	0.83
4:H:1:NAG:H61	4:H:2:NAG:H4	1.66	0.77
2:D:45:SER:HB3	2:D:198:PRO:HG3	1.66	0.77
2:D:77(A):ARG:HG3	3:G:13:DT:O4	1.84	0.77
2:B:146:GLU:HB2	2:B:220:CYS:HB2	1.68	0.75
7:E:102:JKR:C11	7:E:102:JKR:O8	2.33	0.75
2:B:84:MET:HB2	2:B:109:LYS:HG3	1.67	0.74
3:F:5:DG:H2 [?]	3:F:6:DG:C8	2.24	0.72
2:D:144:LEU:HD21	2:D:152:PRO:HB3	1.72	0.72
2:B:77:GLU:HB3	2:B:79:ILE:HB	1.72	0.69
6:E:101:JL0:C11	6:E:101:JL0:O15	2.41	0.68
2:D:77:GLU:HB3	2:D:79:ILE:HB	1.77	0.65
2:B:202:LYS:HE2	2:B:205:ASN:OD1	1.97	0.65
2:D:75:ARG:NH2	3:G:4:DT:O4	2.23	0.63
2:B:66:VAL:CG2	2:B:83:SER:HB2	2.29	0.63
3:E:8:DG:H4 [?]	3:E:9:DT:OP2	1.98	0.62
2:D:132:ALA:HA	2:D:162:ILE:HG22	1.84	0.60
2:D:178:ASP:HB3	2:D:233:ARG:NH1	2.17	0.59
2:B:18:GLU:HB2	2:B:188:GLY:HA2	1.83	0.59
2:B:215:TRP:HA	5:B:301:OG6:HG21	1.85	0.59
1:C:14(E):GLU:OE2	2:D:135:LYS:NZ	2.31	0.58
2:B:36:LYS:O	2:B:38:GLN:HG2	2.04	0.58
2:B:110:LYS:HD2	2:B:111:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:15:DG:H2''	7:E:102:JKR:O4	2.05	0.57
3:G:15:DG:H2''	7:G:102:JKR:O2	2.04	0.57
2:D:60(B):PRO:HB2	2:D:60(C):PRO:HD3	1.86	0.57
2:B:144:LEU:HD21	2:B:152:PRO:HB3	1.86	0.57
2:B:75:ARG:NH2	3:E:4:DT:O4	2.33	0.56
2:B:17:VAL:HG22	2:B:144:LEU:O	2.05	0.56
2:B:77(A):ARG:O	2:B:79:ILE:HD12	2.06	0.56
2:B:67:ARG:HG2	2:B:82:ILE:HG12	1.88	0.56
3:E:14:DG:H2''	3:E:15:DG:C8	2.40	0.55
3:G:5:DG:H2''	3:G:6:DG:C8	2.42	0.54
3:I:5:DG:H2''	3:I:6:DG:C8	2.42	0.54
7:G:102:JKR:O8	7:G:102:JKR:C11	2.56	0.54
3:F:5:DG:H2''	3:F:6:DG:H8	1.72	0.53
2:B:77(A):ARG:HB3	3:E:4:DT:O2	2.08	0.53
2:D:77(A):ARG:O	2:D:79:ILE:HD12	2.08	0.53
2:D:215:TRP:HA	5:D:301:OG6:HG21	1.91	0.53
2:B:50:ARG:NH1	2:B:111:PRO:HD3	2.24	0.53
3:I:14:DG:H2''	3:I:15:DG:C8	2.44	0.53
2:D:103:ILE:HG21	2:D:234:LEU:HD13	1.89	0.53
3:F:5:DG:C2'	3:F:6:DG:C8	2.93	0.51
2:B:35:ARG:HG2	2:B:39:GLU:HG2	1.93	0.51
2:B:79:ILE:HG23	2:B:117:TYR:CD2	2.46	0.50
2:B:103:ILE:HG21	2:B:234:LEU:HD22	1.92	0.50
2:D:79:ILE:HD11	3:G:4:DT:C6	2.46	0.50
2:D:50:ARG:HH21	2:D:107:LYS:HE2	1.77	0.50
2:D:60(A):TYR:H	2:D:60(F):LYS:HB3	1.77	0.49
3:I:14:DG:C6	3:I:15:DG:C6	2.99	0.49
3:F:13:DT:H4'	3:F:14:DG:OP1	2.11	0.49
2:D:146:GLU:OE2	2:D:221:ARG:HD2	2.13	0.49
2:B:129:ALA:O	2:B:130:LEU:HB2	2.12	0.48
2:B:135:LYS:HA	2:B:161:PRO:HA	1.96	0.48
7:G:102:JKR:O8	7:G:102:JKR:C10	2.61	0.48
3:G:11:DG:H2''	3:G:13:DT:H73	1.96	0.48
1:C:6:LEU:HD12	2:D:25:GLY:HA3	1.96	0.48
2:D:215:TRP:CE3	5:D:301:OG6:HD2	2.48	0.48
1:A:5:PRO:CB	2:B:116:ASP:HA	2.44	0.47
2:D:139:THR:HG22	2:D:157:VAL:HG22	1.96	0.47
2:D:48:SER:HB3	2:D:51:TRP:HB2	1.96	0.47
1:A:5:PRO:HB2	2:B:116:ASP:HA	1.96	0.47
2:D:66:VAL:HG12	2:D:68:ILE:HD11	1.97	0.47
3:I:1:DG:H2''	3:I:2:DG:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLU:OE2	2:B:221:ARG:NH1	2.47	0.47
2:B:244:GLN:OE1	3:F:12:DT:H5'	2.15	0.46
2:B:215:TRP:HB2	5:B:301:OG6:O	2.15	0.46
2:D:23:GLU:O	2:D:26:MET:HB2	2.16	0.46
2:B:77(A):ARG:O	2:B:78:ASN:HB2	2.16	0.46
3:I:1:DG:C6	3:I:2:DG:C6	3.03	0.46
2:D:16:ILE:N	9:D:401:HOH:O	2.47	0.46
2:B:125:ASP:O	2:B:126:ARG:C	2.54	0.46
2:D:144:LEU:H	2:D:150:GLY:HA3	1.81	0.45
2:B:66:VAL:HG23	2:B:68:ILE:HD11	1.99	0.45
2:D:182:CYS:HB3	2:D:227:PHE:CE2	2.51	0.45
2:B:182:CYS:HB3	2:B:227:PHE:CE2	2.52	0.45
2:D:54:THR:OG1	2:D:55:ALA:N	2.50	0.45
2:D:119:HIS:CD2	2:D:120:PRO:HD2	2.53	0.44
2:D:31:VAL:CG1	2:D:66:VAL:HG13	2.48	0.44
1:C:1:CYS:C	2:D:122:CYS:SG	2.96	0.44
3:E:5:DG:H2''	3:E:6:DG:C8	2.52	0.44
2:D:79:ILE:HG23	2:D:117:TYR:CD2	2.52	0.44
2:B:137:ARG:HG3	2:B:157:VAL:HG12	2.00	0.43
3:I:5:DG:C5	3:I:6:DG:C6	3.06	0.43
2:D:144:LEU:H	2:D:150:GLY:CA	2.32	0.43
2:B:70:LYS:NZ	2:B:77:GLU:OE1	2.48	0.43
2:B:79:ILE:HD11	3:E:4:DT:C6	2.53	0.43
2:D:59:LEU:HD21	2:D:106:MET:HE3	1.99	0.43
2:B:60(B):PRO:HB2	2:B:60(C):PRO:HD3	2.00	0.42
2:D:164:GLU:OE2	2:D:185:LYS:NZ	2.52	0.42
3:E:13:DT:H2''	3:E:14:DG:N2	2.34	0.42
2:B:124:PRO:O	2:B:235:LYS:HD2	2.18	0.42
5:B:301:OG6:HD3	5:B:301:OG6:CD1	2.49	0.42
2:B:66:VAL:HG22	2:B:83:SER:HB2	2.00	0.42
2:B:211:GLY:HA2	2:B:229:THR:O	2.19	0.42
2:D:131:GLN:O	2:D:134:TYR:HB2	2.19	0.42
2:D:184(A):TYR:CZ	2:D:186(D):LYS:HD3	2.54	0.42
2:D:237:TRP:O	2:D:241:VAL:HG23	2.20	0.42
3:E:5:DG:C2'	3:E:6:DG:C8	3.03	0.42
2:B:103:ILE:HG21	2:B:234:LEU:CD2	2.50	0.42
2:D:77(A):ARG:O	2:D:78:ASN:HB2	2.20	0.42
2:D:186(B):GLU:C	2:D:186(D):LYS:H	2.23	0.42
2:B:60(I):THR:HG22	2:B:62:ASN:H	1.85	0.41
2:B:85:LEU:HD22	2:B:106:MET:HB3	2.02	0.41
2:D:165:ARG:N	2:D:166:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:LEU:HD11	2:B:238:ILE:HG23	2.02	0.41
2:B:128:THR:O	2:B:129(C):LEU:HB2	2.21	0.41
3:E:10:DG:H2''	3:E:11:DG:O5'	2.21	0.41
1:A:14(D):ARG:HD2	2:D:60(D):TRP:CD2	2.56	0.40
2:B:191:CYS:O	2:B:194:ASP:HB2	2.21	0.40
3:I:14:DG:C2'	3:I:15:DG:C8	3.04	0.40
2:B:59:LEU:HD21	2:B:106:MET:HE3	2.03	0.40
2:D:31:VAL:HG13	2:D:66:VAL:HG13	2.04	0.40
2:D:85:LEU:HD22	2:D:106:MET:HB3	2.03	0.40
2:D:215:TRP:HB2	5:D:301:OG6:O	2.22	0.40
1:A:6:LEU:HD12	2:B:25:GLY:HA3	2.03	0.40
1:A:14(D):ARG:HD2	2:D:60(D):TRP:CE2	2.56	0.40
3:F:10:DG:H2''	3:F:11:DG:O5'	2.21	0.40
3:I:10:DG:H2''	3:I:11:DG:O5'	2.21	0.40
3:F:14:DG:C6	3:F:15:DG:C6	3.09	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	24/36 (67%)	22 (92%)	2 (8%)	0	100	100
1	C	24/36 (67%)	21 (88%)	3 (12%)	0	100	100
2	B	248/259 (96%)	228 (92%)	19 (8%)	1 (0%)	34	69
2	D	247/259 (95%)	227 (92%)	19 (8%)	1 (0%)	34	69
All	All	543/590 (92%)	498 (92%)	43 (8%)	2 (0%)	34	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97(A)	GLU
2	D	151	GLN

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	24/31 (77%)	23 (96%)	1 (4%)	30	64
1	C	24/31 (77%)	24 (100%)	0	100	100
2	B	218/225 (97%)	215 (99%)	3 (1%)	67	86
2	D	219/225 (97%)	216 (99%)	3 (1%)	67	86
All	All	485/512 (95%)	478 (99%)	7 (1%)	67	86

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

Mol	Chain	Res	Type
1	A	13	GLU
2	B	77	GLU
2	B	93	ARG
2	B	154	VAL
2	D	60(I)	THR
2	D	77	GLU
2	D	77(A)	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

4 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
4	NAG	H	1	4,2	14,14,15	0.42	0	17,19,21	1.13	1 (5%)
4	NAG	H	2	4	14,14,15	0.60	0	17,19,21	1.43	3 (17%)
4	NAG	J	1	4,2	14,14,15	0.45	0	17,19,21	0.67	0
4	NAG	J	2	4	14,14,15	0.59	0	17,19,21	1.61	4 (23%)

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	NAG	H	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C1-O5-C5	4.45	118.22	112.19
4	H	2	NAG	C1-O5-C5	3.69	117.19	112.19
4	J	2	NAG	C4-C3-C2	2.93	115.31	111.02
4	H	2	NAG	C2-N2-C7	2.89	127.02	122.90
4	J	2	NAG	C3-C4-C5	2.48	114.67	110.24
4	H	2	NAG	O5-C5-C6	2.40	110.97	107.20
4	H	1	NAG	C1-O5-C5	2.21	115.18	112.19
4	J	2	NAG	O5-C1-C2	2.18	114.72	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

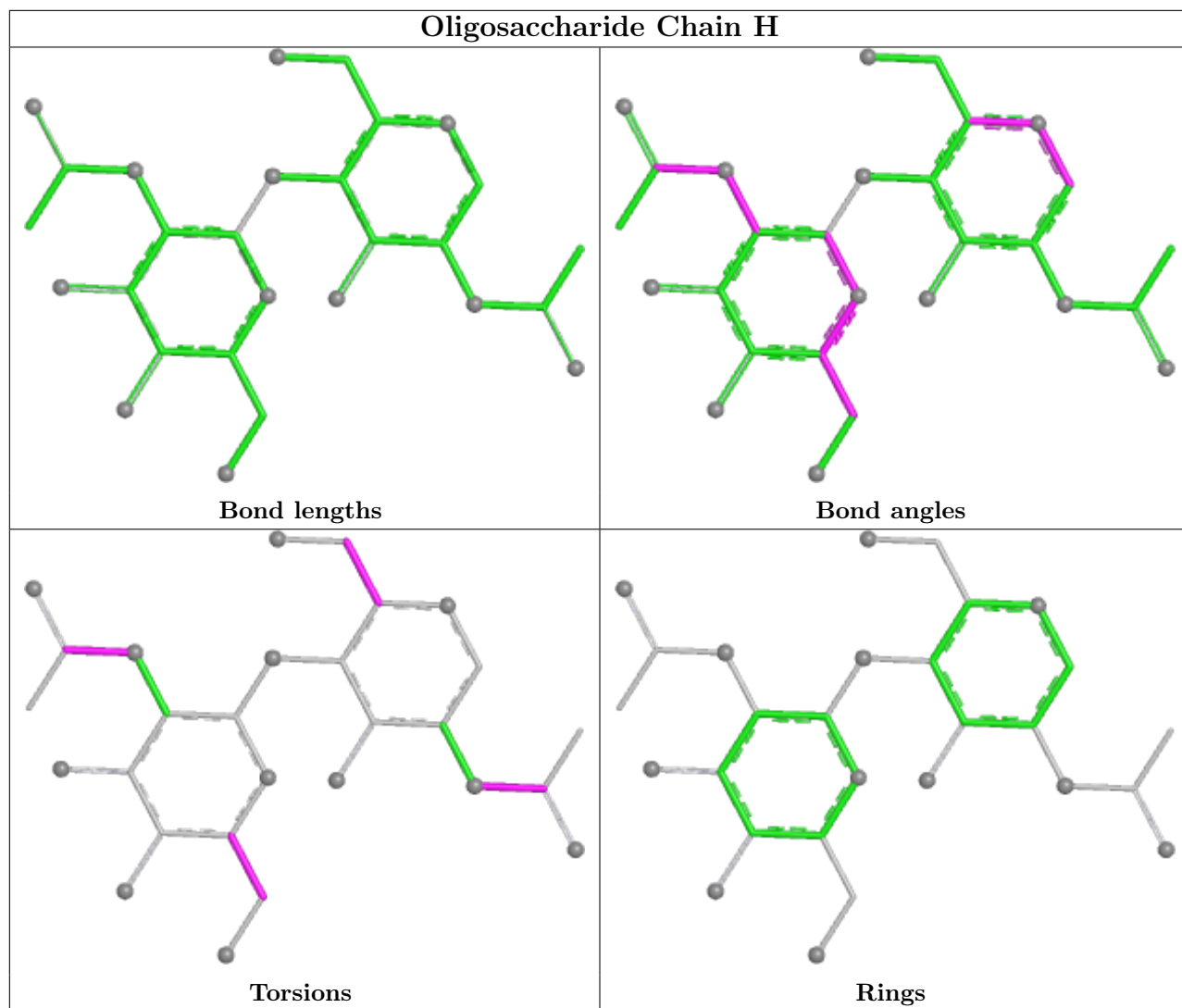
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

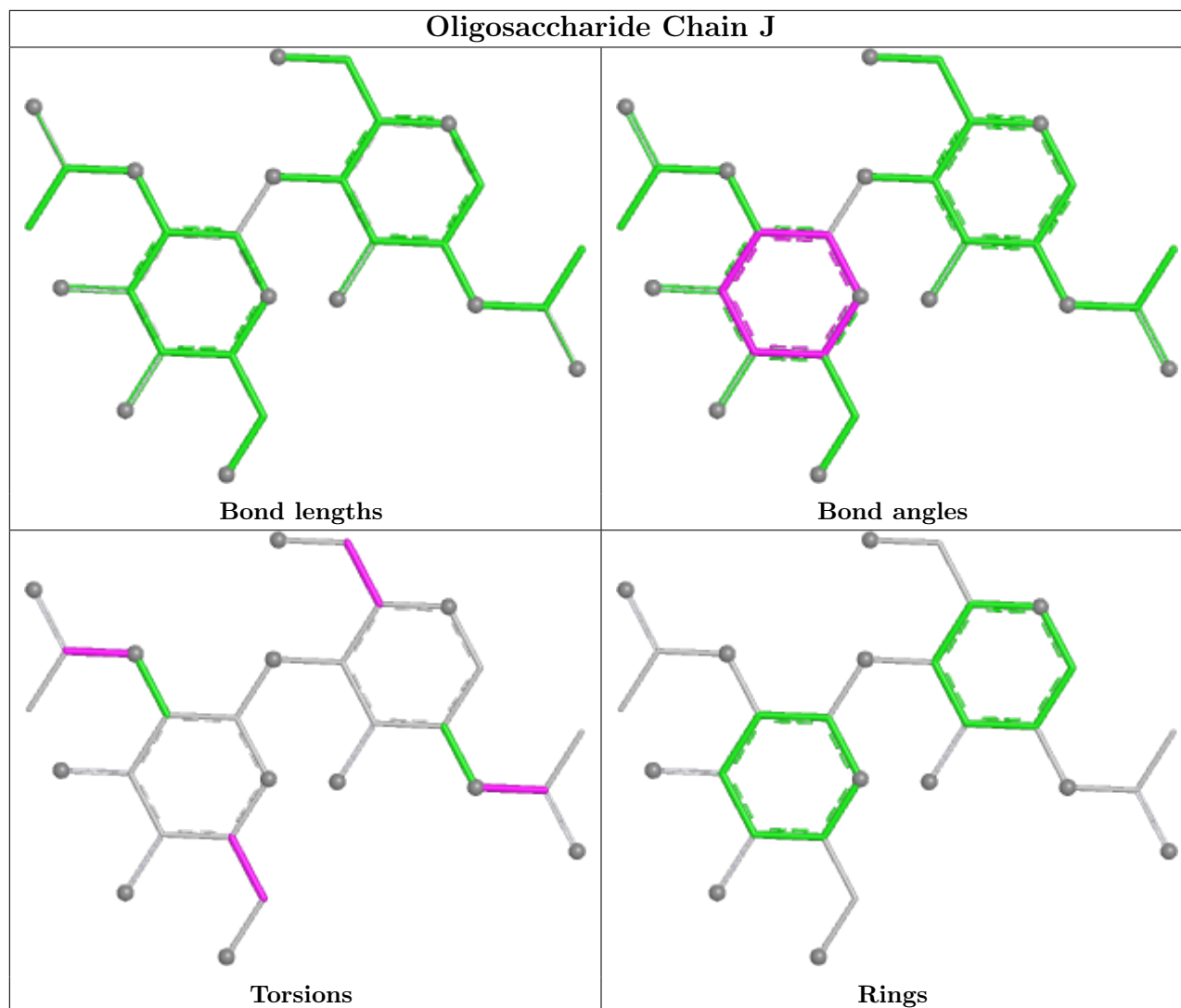
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
4	H	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z > 2$
7	JKR	F	102	7,3	42,45,45	0.45	0	55,60,60	0.44	0
6	JL0	I	101	3	63,63,78	0.43	0	96,97,118	0.33	0
7	JKR	I	102	7,3	42,45,45	0.46	0	55,60,60	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	JKR	E	102	3,7	42,45,45	0.44	0	55,60,60	0.42	0
5	0G6	B	301	2	30,31,32	0.50	0	37,41,42	0.79	0
7	JKR	G	102	3,7	42,45,45	0.61	0	55,60,60	0.58	0
5	0G6	D	301	2	30,31,32	0.49	0	37,41,42	0.82	2 (5%)
6	JL0	F	101	3	63,63,78	0.41	0	96,97,118	0.32	0
6	JL0	E	101	3	70,70,78	0.56	1 (1%)	106,107,118	0.50	1 (0%)
6	JL0	G	101	3	70,70,78	0.57	1 (1%)	106,107,118	0.51	1 (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
7	JKR	F	102	7,3	-	9/24/26/26	0/4/4/4
6	JL0	I	101	3	-	4/20/20/38	0/8/8/8
7	JKR	I	102	7,3	-	8/24/26/26	0/4/4/4
7	JKR	E	102	3,7	-	5/24/26/26	0/4/4/4
5	0G6	B	301	2	-	6/31/41/43	0/2/2/2
7	JKR	G	102	3,7	-	12/24/26/26	0/4/4/4
5	0G6	D	301	2	-	6/31/41/43	0/2/2/2
6	JL0	F	101	3	-	9/20/20/38	0/8/8/8
6	JL0	E	101	3	-	15/28/28/38	0/8/8/8
6	JL0	G	101	3	-	15/28/28/38	0/8/8/8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	101	JL0	P3-O13	3.30	1.61	1.50
6	G	101	JL0	P3-O13	3.30	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	101	JL0	O20-P3-O21	3.17	119.74	107.64
6	G	101	JL0	O20-P3-O21	3.15	119.67	107.64
5	D	301	0G6	CG-CB-CA	-2.66	108.60	114.13
5	D	301	0G6	O1-C1-N2	2.01	126.66	122.93

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	0G6	O2-C2-CA2-CB2
5	D	301	0G6	O2-C2-CA2-CB2
5	D	301	0G6	NH1-CZ1-NE-CD3
5	D	301	0G6	NH2-CZ1-NE-CD3
6	E	101	JL0	C7-C8-C9-O3
6	E	101	JL0	C11-C12-N2-C13
6	E	101	JL0	C11-C12-N2-C30
6	E	101	JL0	N3-C19-C20-C21
6	E	101	JL0	C21-O9-P3-O20
6	F	101	JL0	C9-O3-P1-O5
6	F	101	JL0	C10-O6-P1-O4
6	F	101	JL0	N4-C39-C40-C41
6	G	101	JL0	C11-C10-O6-P1
6	G	101	JL0	C21-O9-P3-O21
6	G	101	JL0	C21-O9-P3-O20
6	G	101	JL0	C21-O9-P3-O13
7	E	102	JKR	C11-C12-O7-P2
7	G	102	JKR	C11-C12-O7-P2
7	G	102	JKR	C13-O10-P2-O8
7	I	102	JKR	C12-O7-P2-O8
7	I	102	JKR	C13-O10-P2-O8
7	I	102	JKR	C13-O10-P2-O9
7	G	102	JKR	C14-C15-O11-C16
6	G	101	JL0	C20-C19-N3-C18
6	E	101	JL0	C20-C19-N3-C18
6	E	101	JL0	C20-C19-N3-C25
7	G	102	JKR	C32-C9-O6-C10
6	G	101	JL0	C20-C19-N3-C25
7	G	102	JKR	C8-C9-O6-C10
5	B	301	0G6	NH2-CZ1-NE-CD3
6	G	101	JL0	C10-C11-C12-N2
6	G	101	JL0	N3-C19-C20-C21
7	G	102	JKR	C13-C14-C15-O11
6	E	101	JL0	C39-C40-C41-O18
6	E	101	JL0	C19-C20-C21-O9
7	F	102	JKR	O4-C1-C2-C3
6	E	101	JL0	C9-O3-P1-O6
6	F	101	JL0	C9-O3-P1-O6
6	F	101	JL0	C10-O6-P1-O3
7	E	102	JKR	C12-O7-P2-O10

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Mol	Chain	Res	Type	Atoms
7	G	102	JKR	C13-O10-P2-O7
7	I	102	JKR	C12-O7-P2-O10
7	I	102	JKR	C13-O10-P2-O7
6	F	101	JL0	O6-C10-C11-C12
6	G	101	JL0	O6-C10-C11-C12
6	G	101	JL0	C19-C20-C21-O9
6	I	101	JL0	C7-C8-C9-O3
7	F	102	JKR	C13-C14-C15-O11
6	I	101	JL0	C9-O3-P1-O6
6	G	101	JL0	N1-C7-C8-C9
6	G	101	JL0	C7-C8-C9-O3
7	I	102	JKR	C2-C3-O5-C4
7	F	102	JKR	C14-C15-O11-C16
5	D	301	0G6	O2-C2-CA2-N2
5	D	301	0G6	C3-C2-CA2-N2
6	E	101	JL0	C10-C11-C12-N2
7	I	102	JKR	O4-C1-C2-C3
7	G	102	JKR	C1-C2-C3-O5
6	I	101	JL0	N1-C7-C8-C9
7	F	102	JKR	C1-C2-C3-O5
6	E	101	JL0	C10-O6-P1-O3
7	E	102	JKR	C11-C10-O6-C9
5	D	301	0G6	C3-C2-CA2-CB2
6	E	101	JL0	C9-O3-P1-O5
6	F	101	JL0	C10-O6-P1-O5
6	I	101	JL0	C9-O3-P1-O5
7	E	102	JKR	C12-O7-P2-O9
7	G	102	JKR	C13-O10-P2-O9
7	F	102	JKR	O10-C13-C14-C15
5	B	301	0G6	NH1-CZ1-NE-CD3
5	B	301	0G6	CA2-CB2-CG2-CD3
6	F	101	JL0	C8-C7-N1-C33
6	E	101	JL0	N1-C7-C8-C9
6	G	101	JL0	C9-O3-P1-O6
7	F	102	JKR	C13-O10-P2-O7
7	G	102	JKR	C12-O7-P2-O10
5	B	301	0G6	CG2-CD3-NE-CZ1
6	G	101	JL0	N4-C39-C40-C41
5	B	301	0G6	C3-C2-CA2-N2
7	F	102	JKR	C10-C11-C12-O7
6	F	101	JL0	C8-C7-N1-C6
7	G	102	JKR	O6-C10-C11-C12

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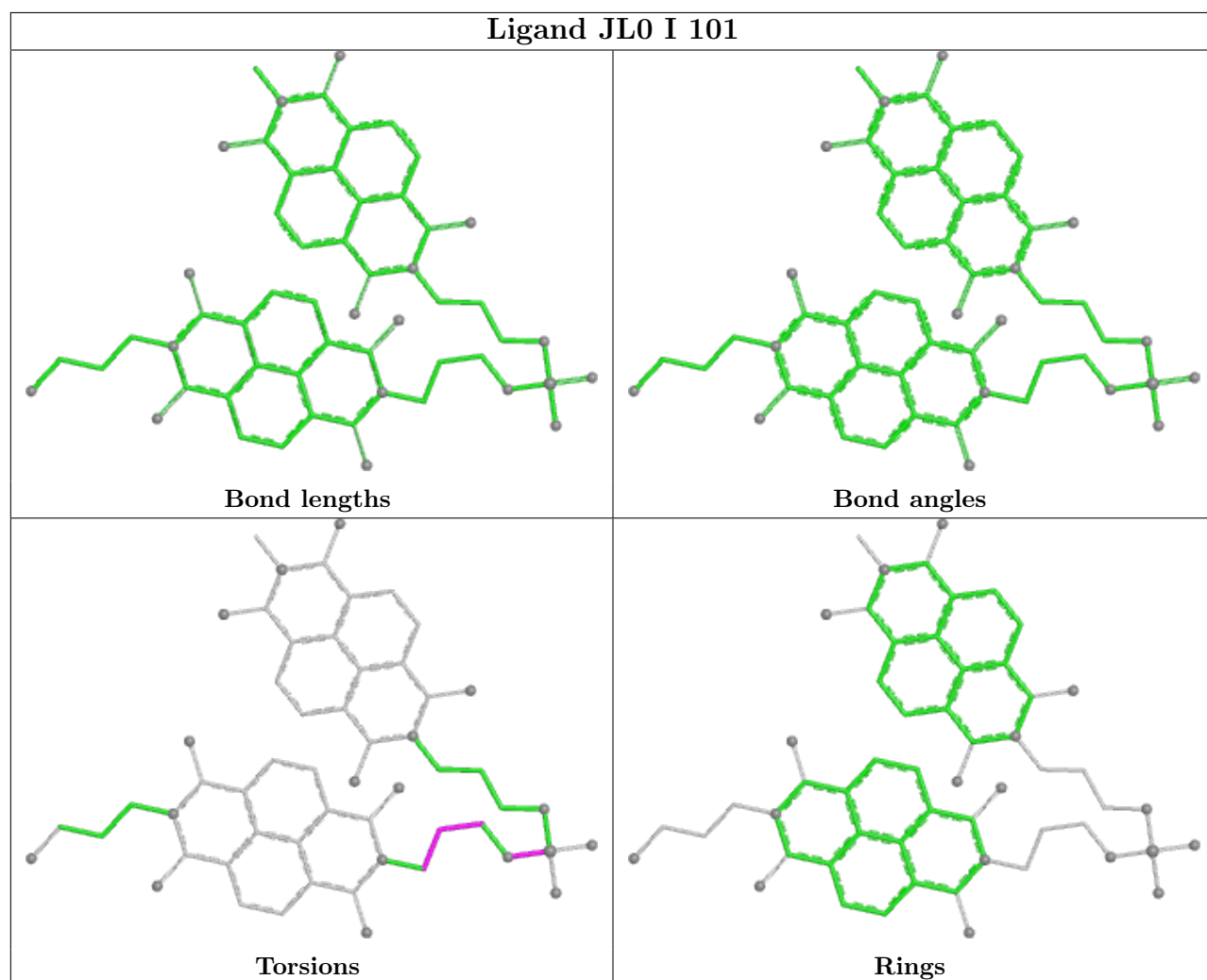
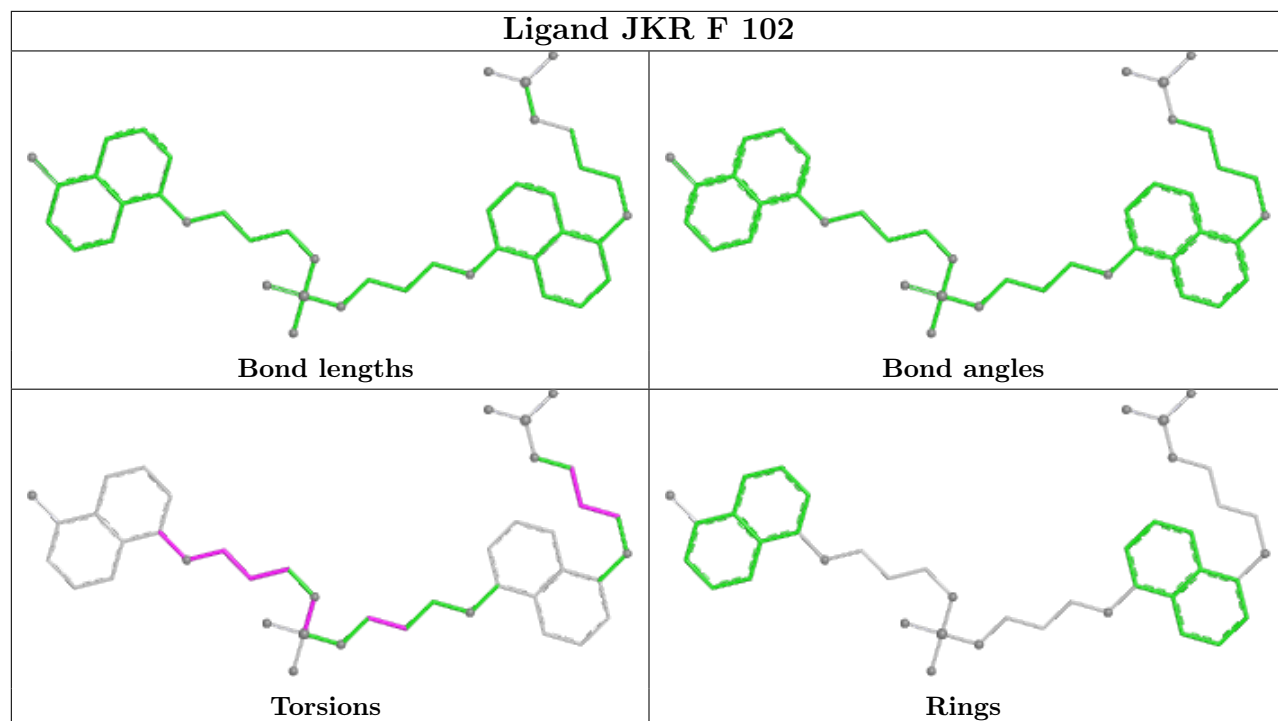
Mol	Chain	Res	Type	Atoms
7	E	102	JKR	C1-C2-C3-O5
7	F	102	JKR	C31-C16-O11-C15
7	I	102	JKR	C2-C1-O4-P1
6	G	101	JL0	C10-O6-P1-O4
7	G	102	JKR	C12-O7-P2-O9
7	F	102	JKR	C17-C16-O11-C15
6	E	101	JL0	C20-C21-O9-P3

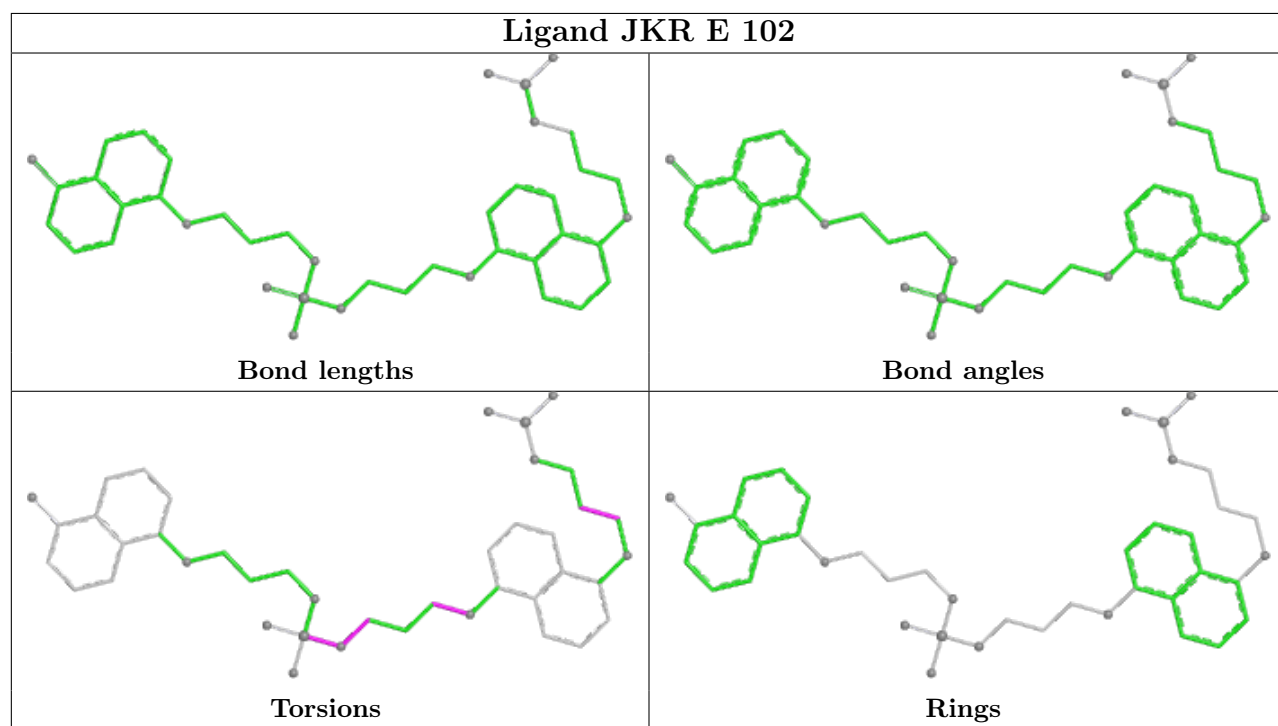
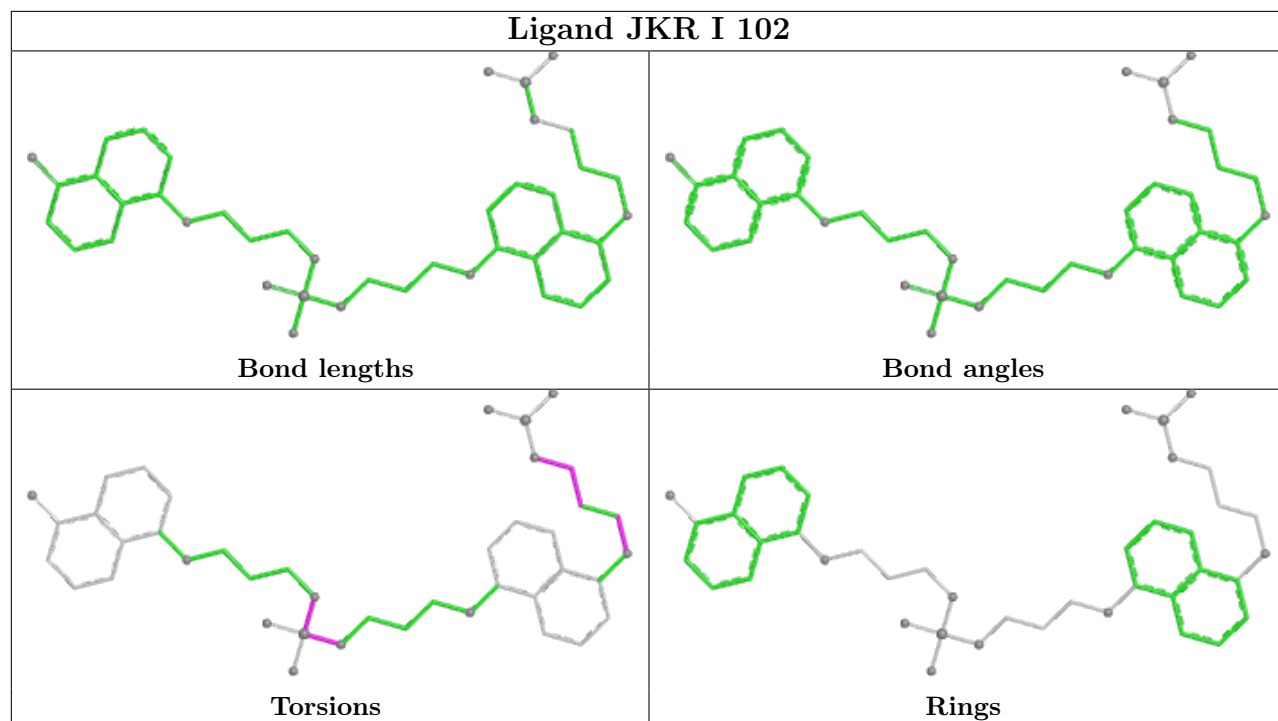
There are no ring outliers.

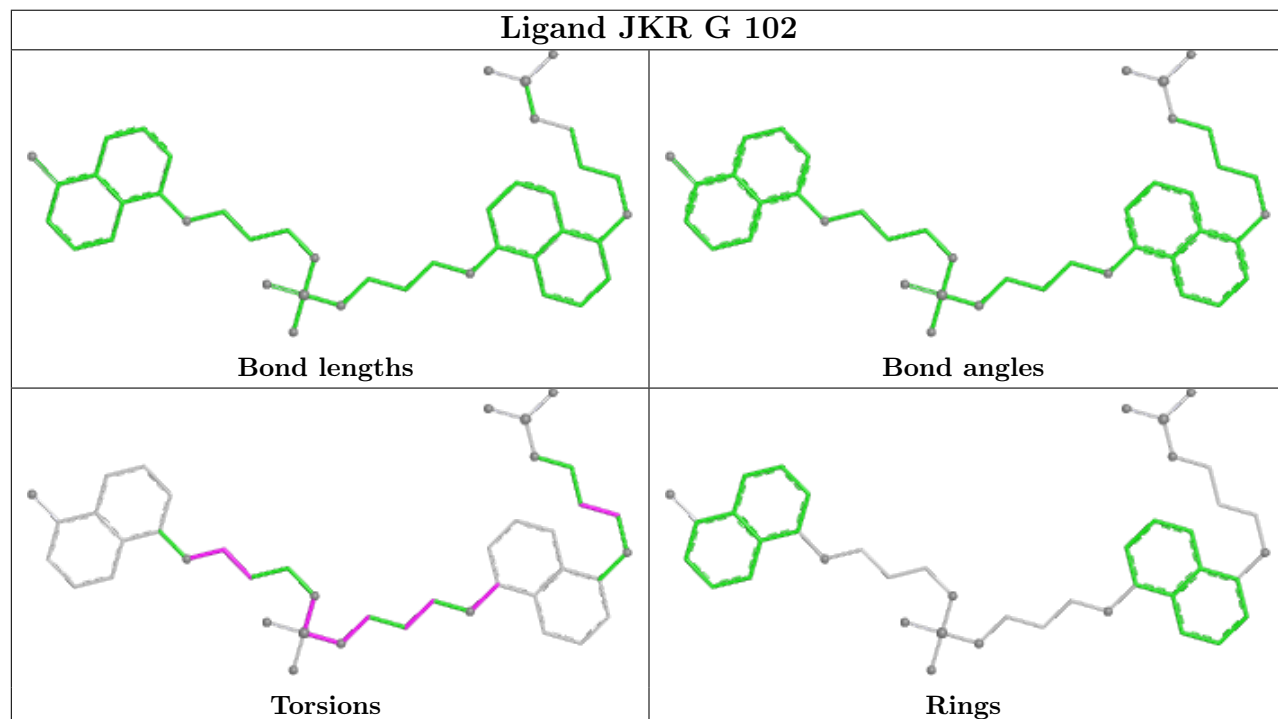
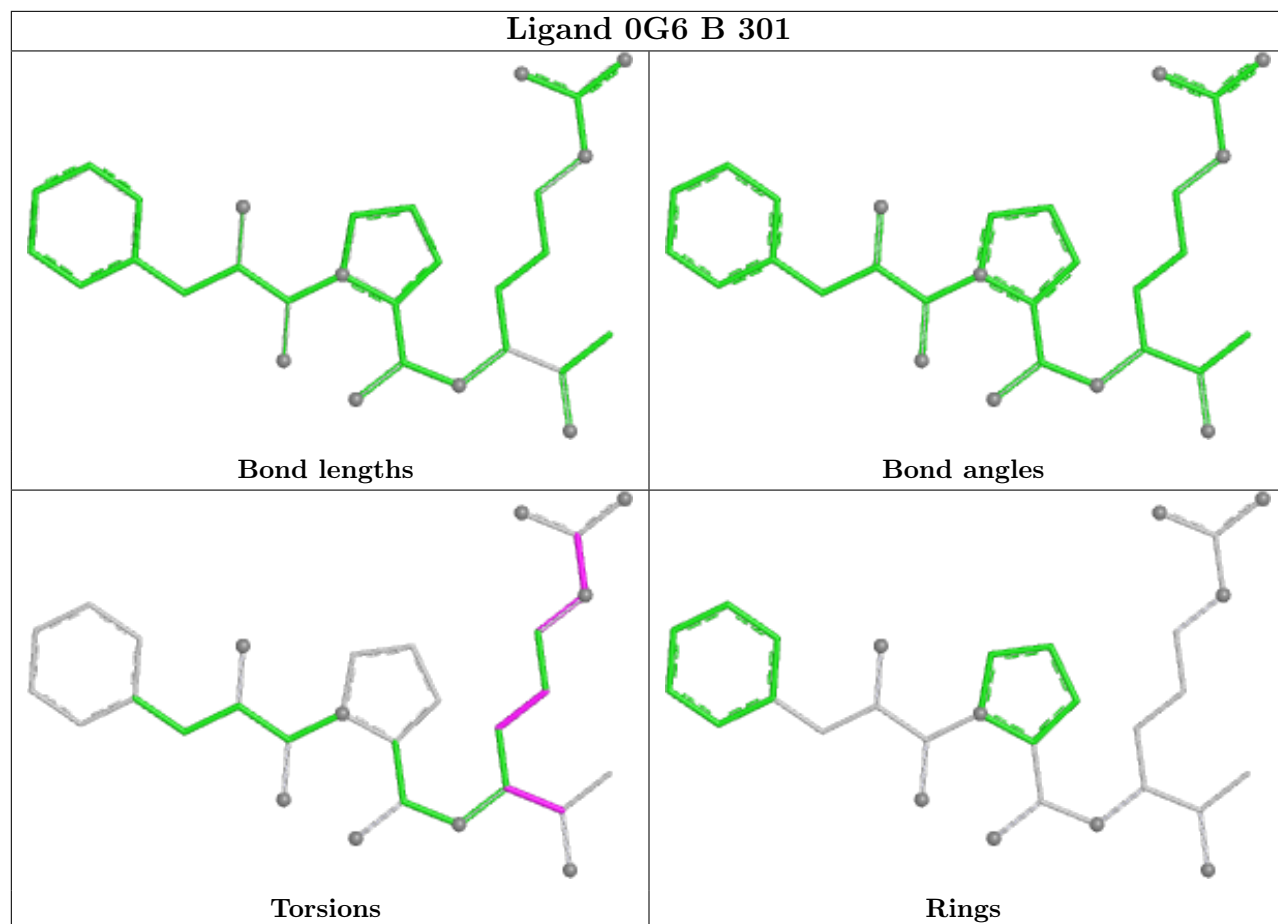
5 monomers are involved in 13 short contacts:

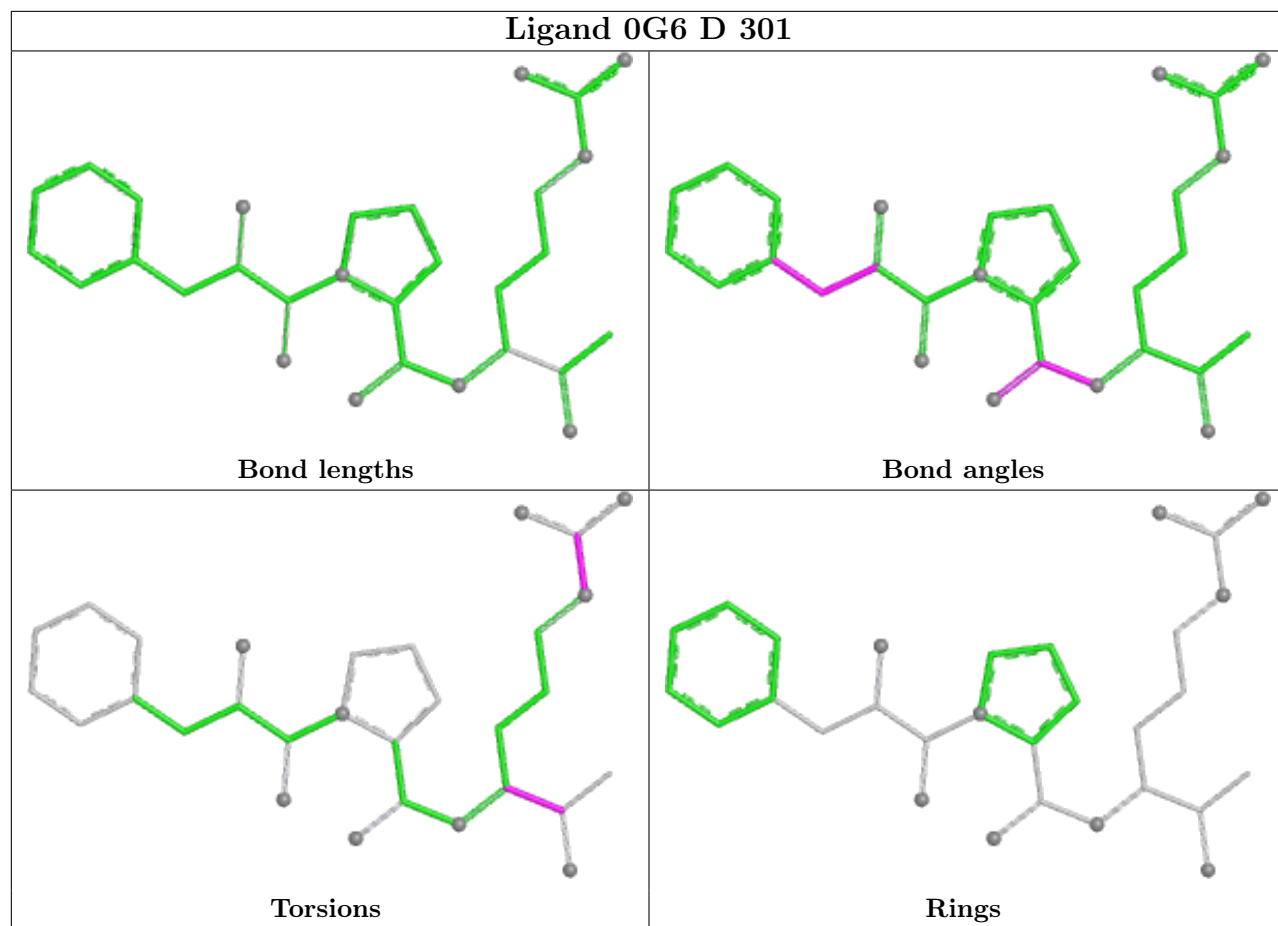
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	102	JKR	2	0
5	B	301	0G6	3	0
7	G	102	JKR	4	0
5	D	301	0G6	3	0
6	E	101	JL0	1	0

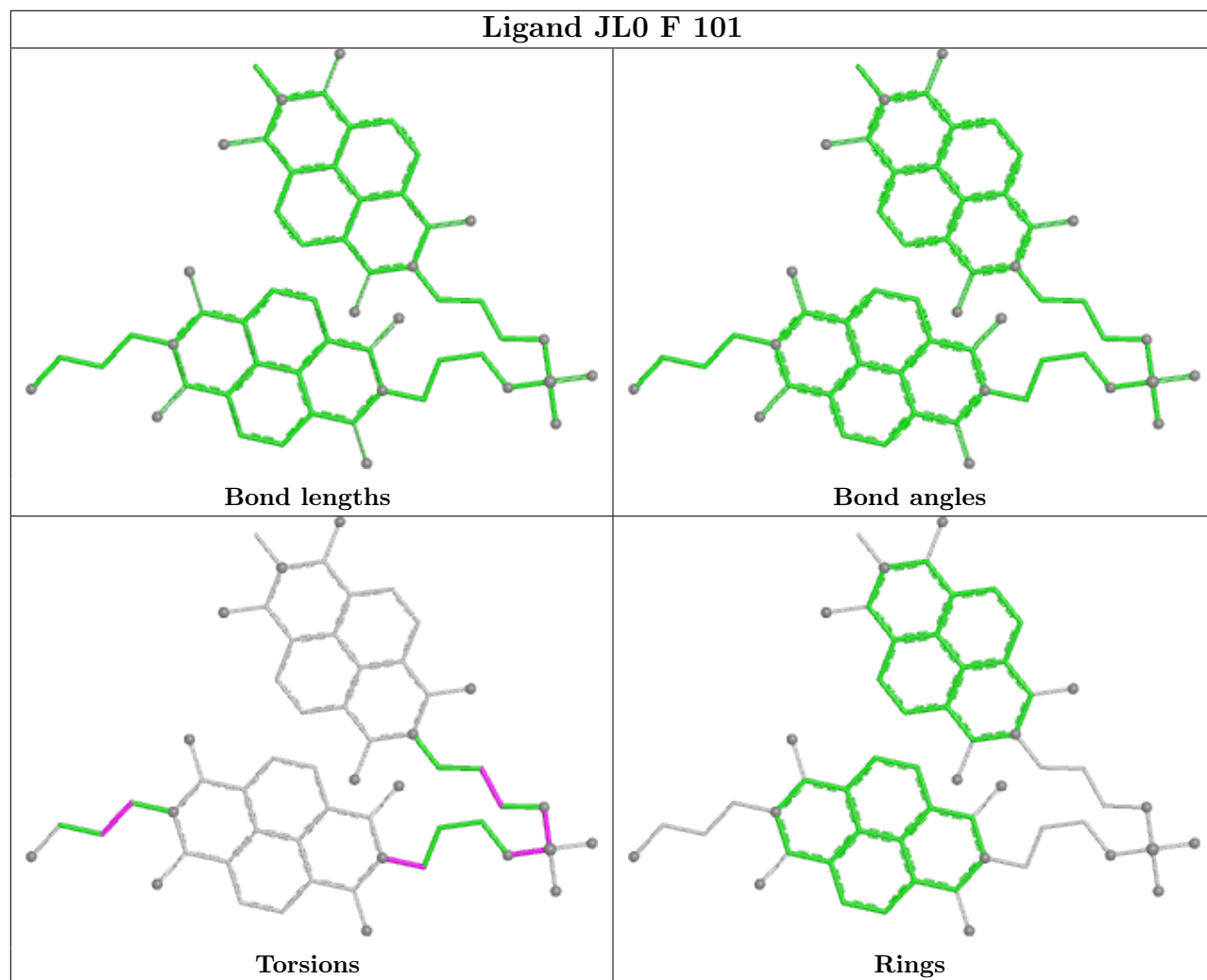
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

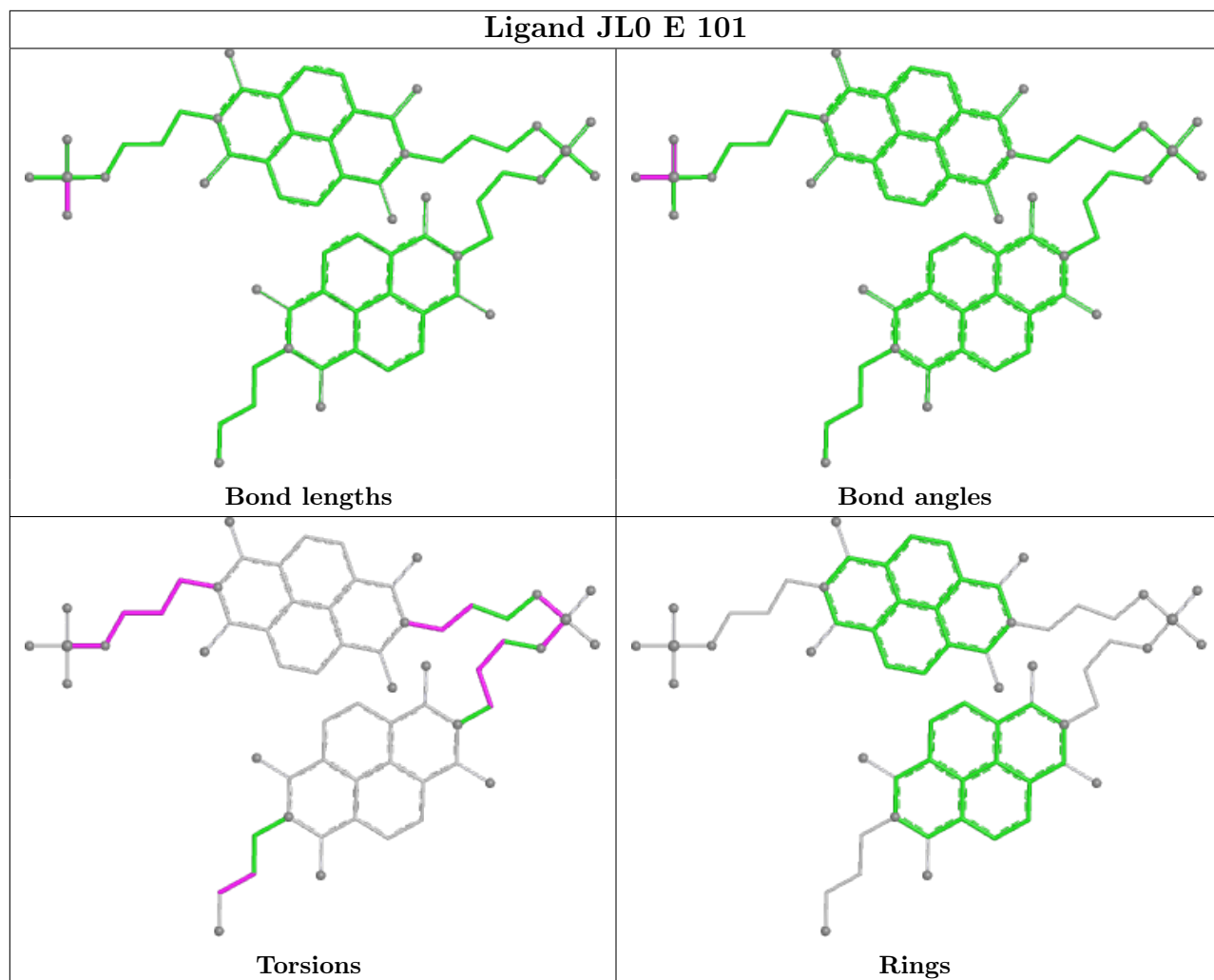


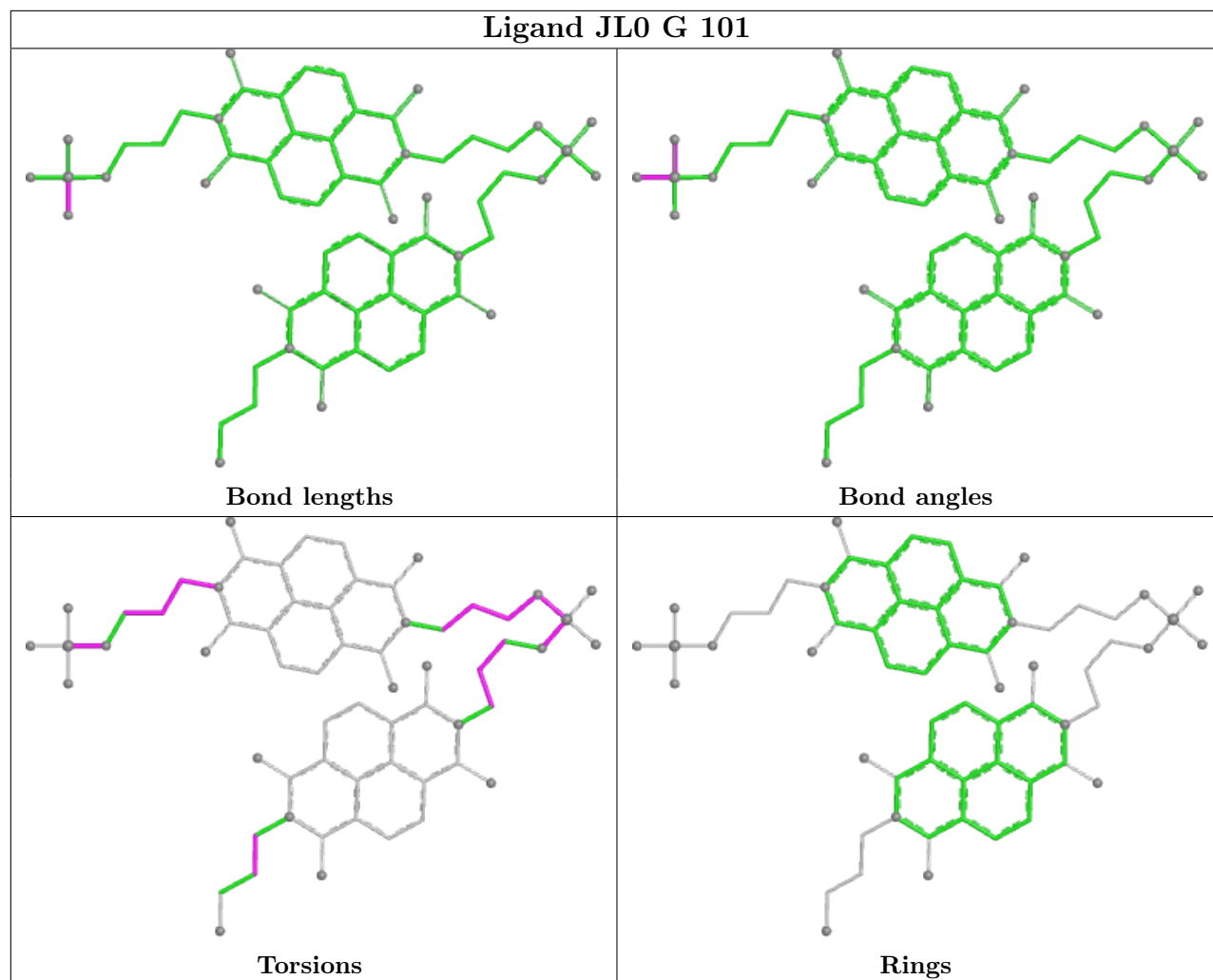












5.7 Other polymers [i](#)

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	26/36 (72%)	0.11	0 100 100	52, 61, 80, 101	0
1	C	26/36 (72%)	-0.17	0 100 100	50, 61, 74, 82	0
2	B	252/259 (97%)	0.02	1 (0%) 92 79	42, 63, 90, 119	0
2	D	251/259 (96%)	0.24	1 (0%) 92 79	42, 63, 88, 114	0
3	E	15/15 (100%)	-0.44	0 100 100	72, 84, 147, 168	0
3	F	12/15 (80%)	-0.35	0 100 100	61, 78, 99, 101	0
3	G	12/15 (80%)	-0.05	0 100 100	60, 72, 92, 94	0
3	I	12/15 (80%)	-0.10	0 100 100	66, 84, 107, 114	0
All	All	606/650 (93%)	0.08	2 (0%) 94 83	42, 64, 94, 168	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	GLU	2.9
2	D	34	PHE	2.4

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

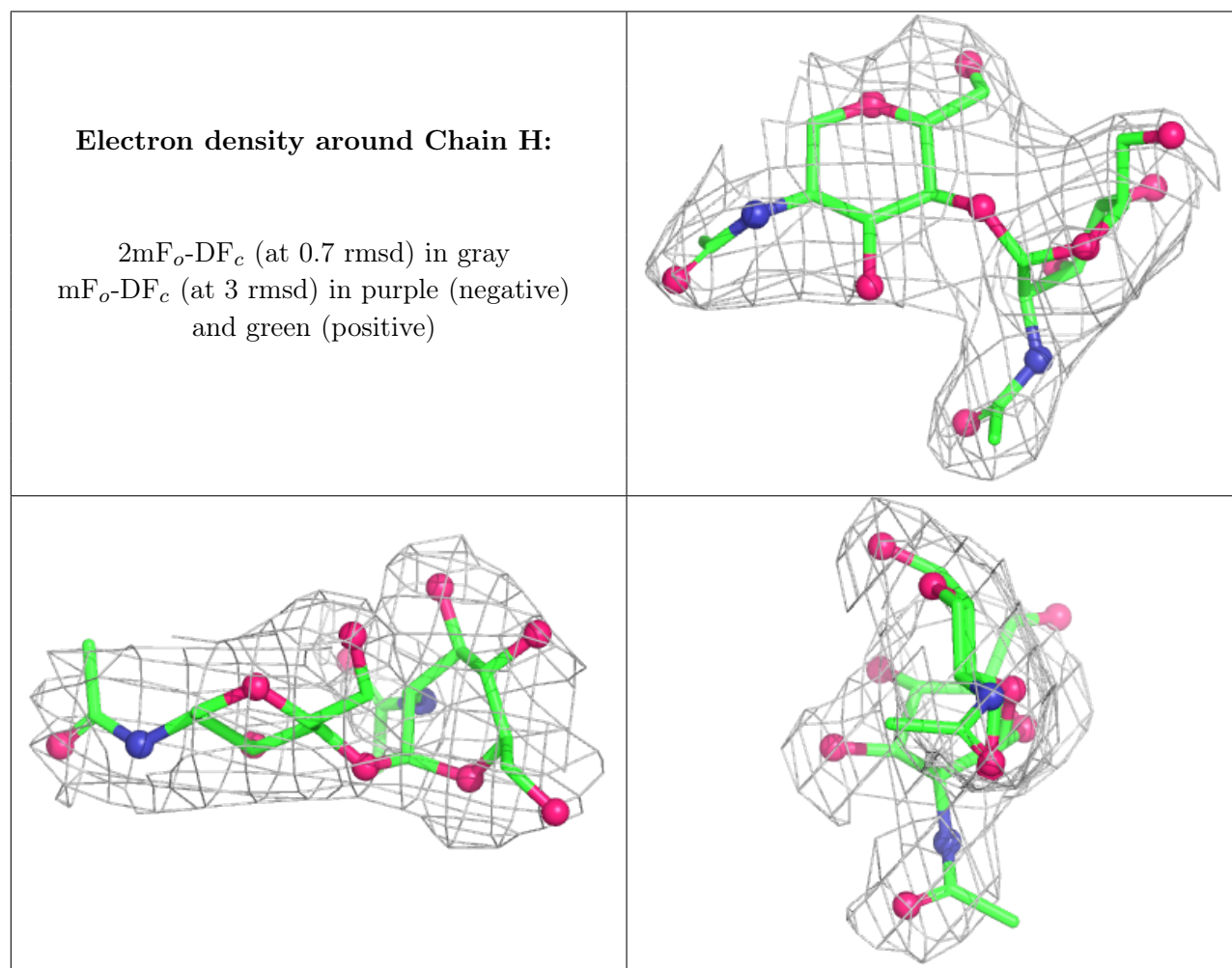
There are no non-standard protein/DNA/RNA residues in this entry.

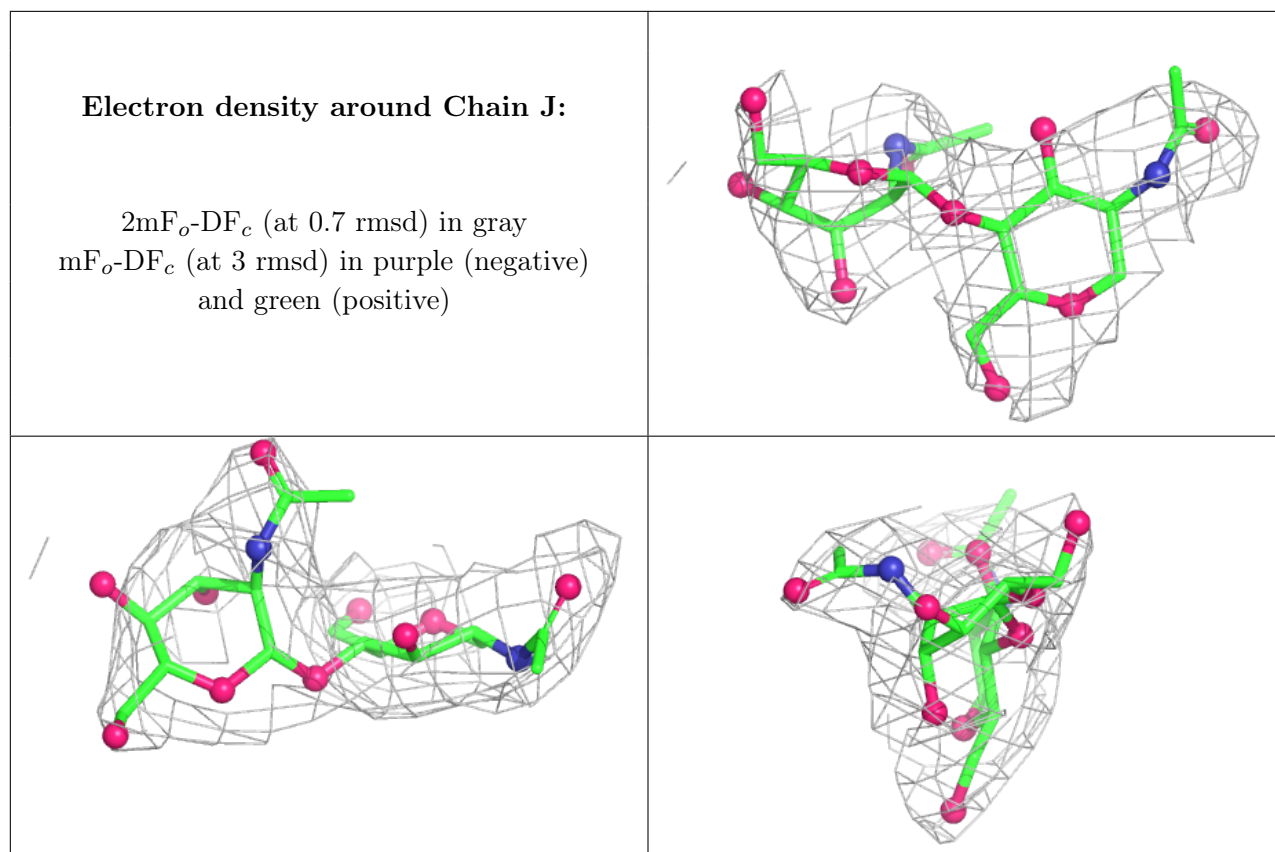
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
4	NAG	J	2	14/15	0.88	0.19	116,123,126,139	0
4	NAG	H	2	14/15	0.90	0.18	103,113,116,122	0
4	NAG	J	1	14/15	0.91	0.21	84,94,112,117	0
4	NAG	H	1	14/15	0.94	0.16	78,88,96,110	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.



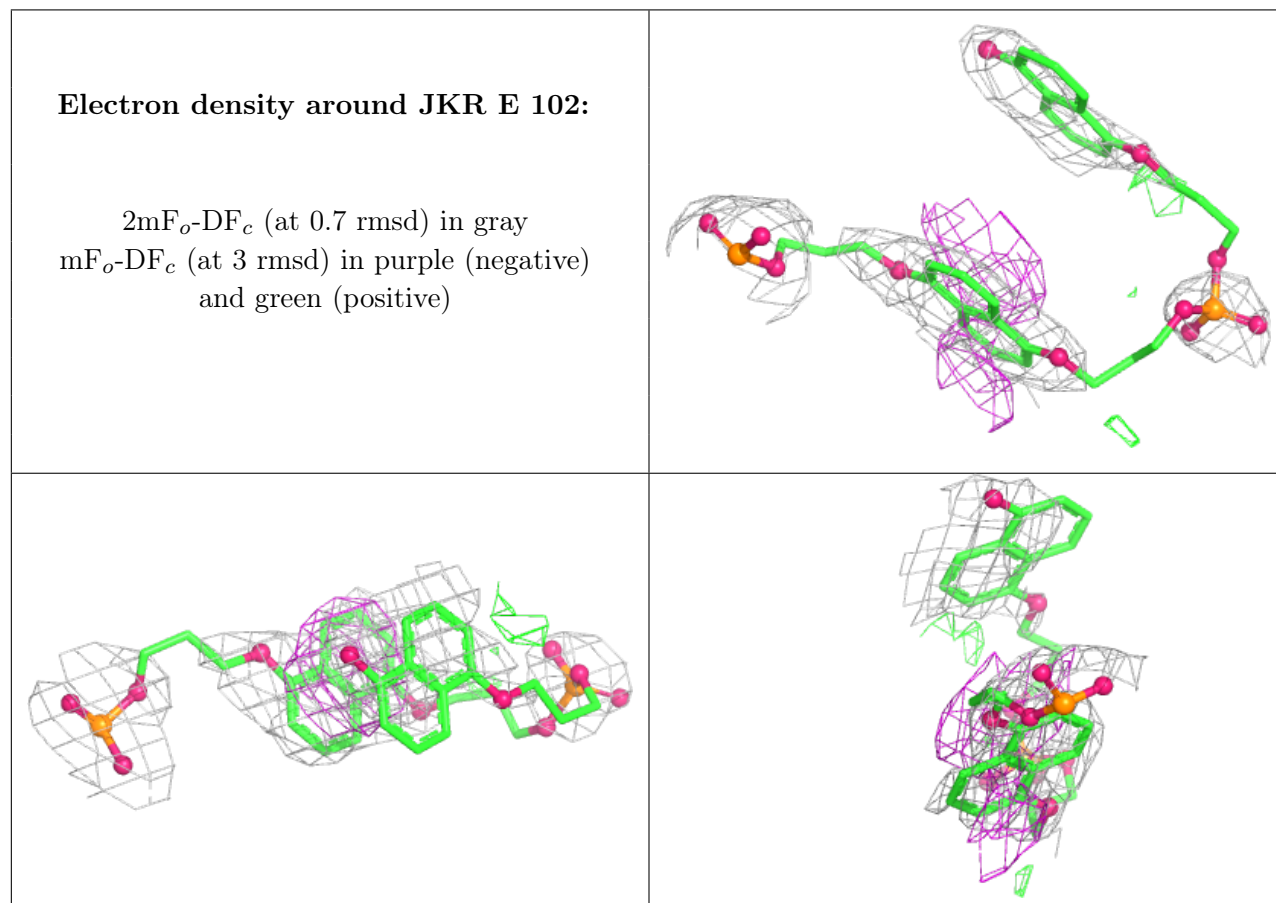


6.4 Ligands [i](#)

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.

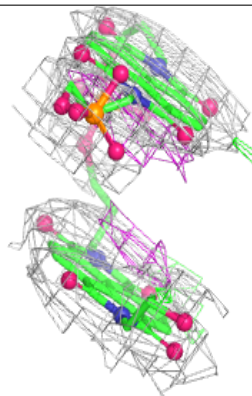
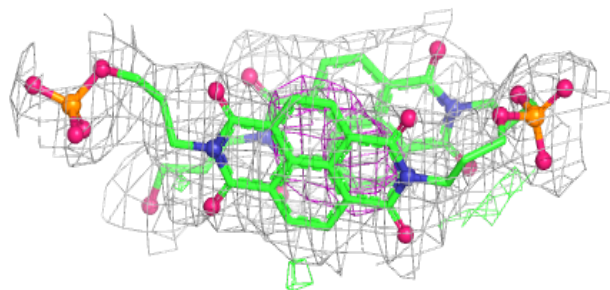
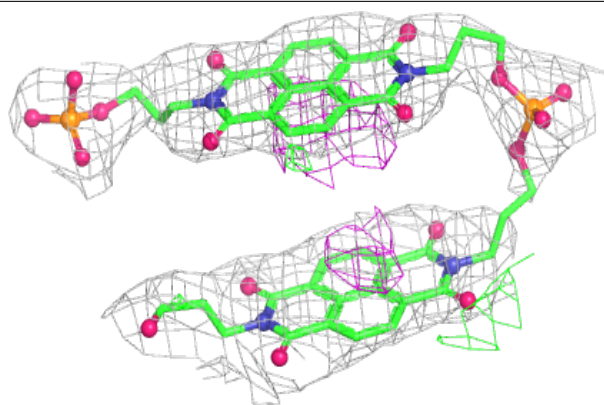
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	K	I	103	1/1	0.63	0.12	91,91,91,91	0
7	JKR	E	102	42/42	0.80	0.46	45,88,109,115	23
6	JL0	E	101	63/71	0.82	0.25	86,94,149,165	0
7	JKR	F	102	42/42	0.83	0.34	40,75,114,128	23
6	JL0	G	101	63/71	0.85	0.28	76,85,143,158	0
6	JL0	F	101	56/71	0.85	0.25	67,78,148,160	0
8	K	F	103	1/1	0.86	0.14	78,78,78,78	0
7	JKR	G	102	42/42	0.87	0.37	38,66,93,99	23
6	JL0	I	101	56/71	0.89	0.24	41,71,129,138	0
7	JKR	I	102	42/42	0.89	0.36	38,60,107,113	23
8	K	G	103	1/1	0.93	0.09	76,76,76,76	0
8	K	E	103	1/1	0.95	0.15	84,84,84,84	0
5	0G6	B	301	30/31	0.95	0.27	56,59,62,69	0
5	0G6	D	301	30/31	0.97	0.27	45,52,54,57	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.

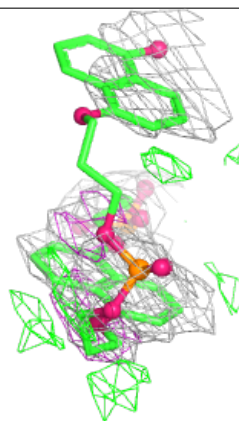
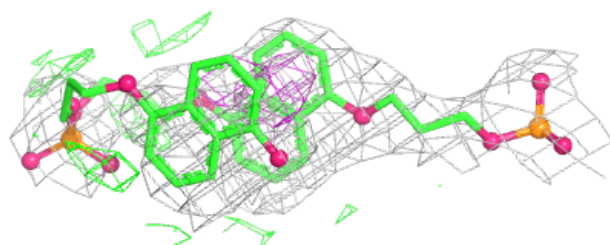
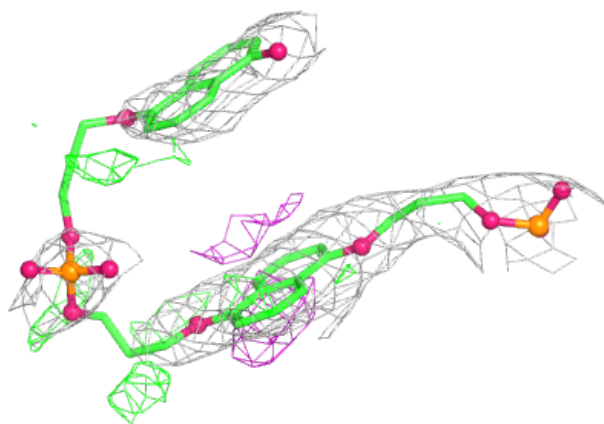


Electron density around JL0 E 101:

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

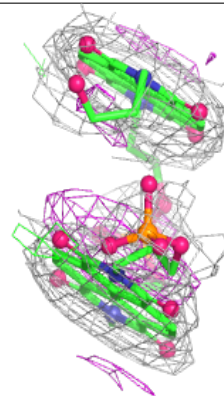
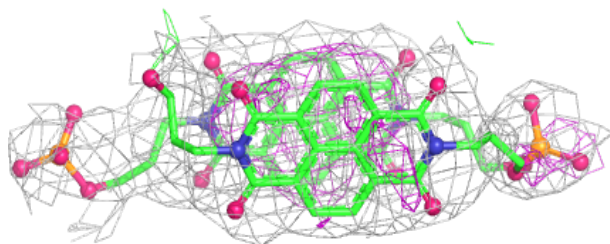
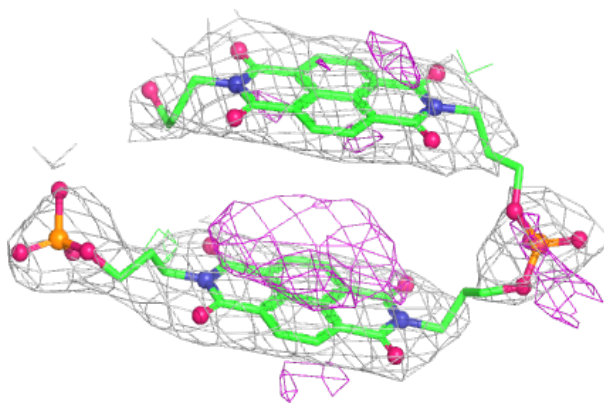
**Electron density around JKR F 102:**

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

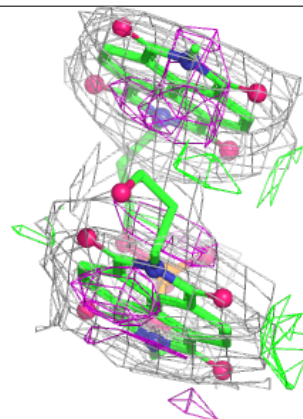
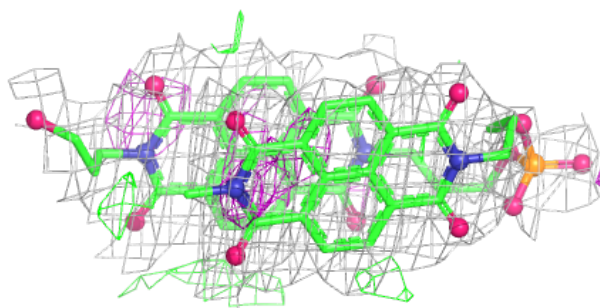
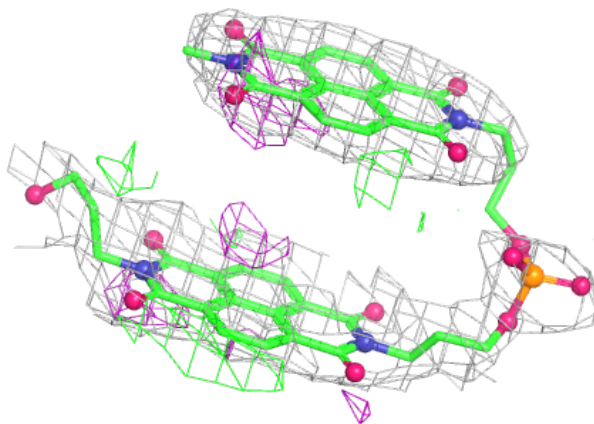


Electron density around JL0 G 101:

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

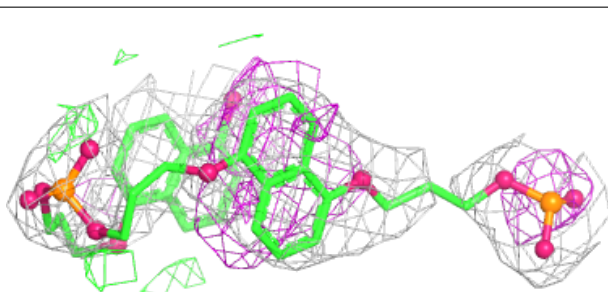
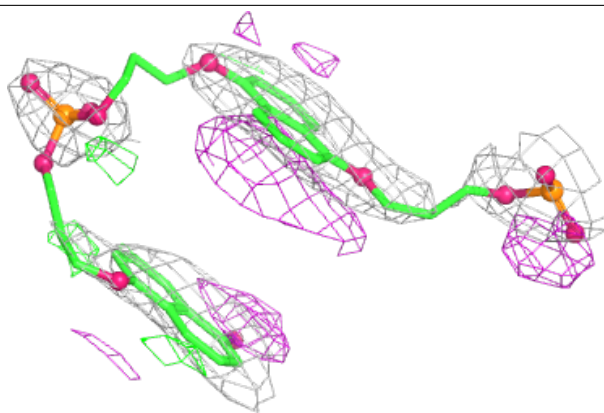
**Electron density around JL0 F 101:**

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

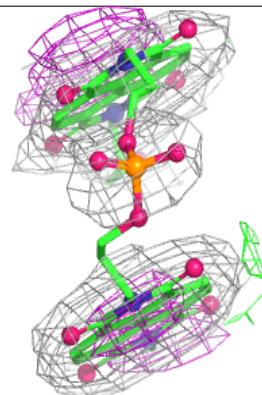
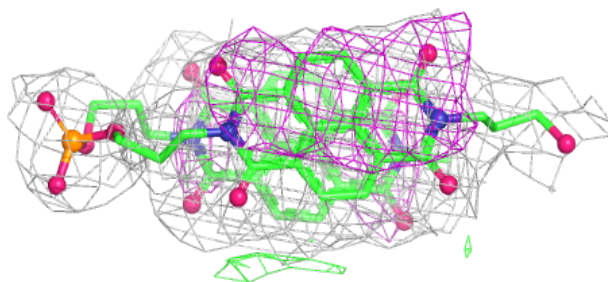
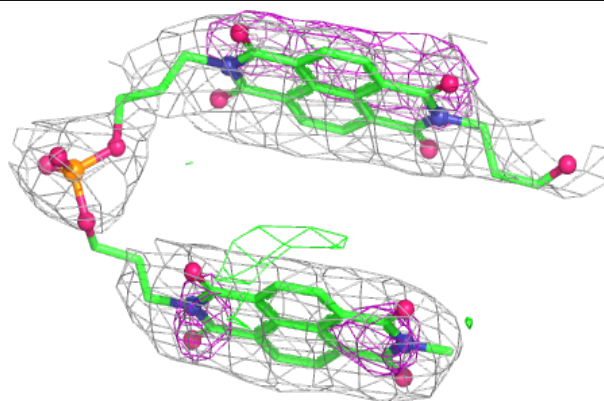


Electron density around JKR G 102:

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

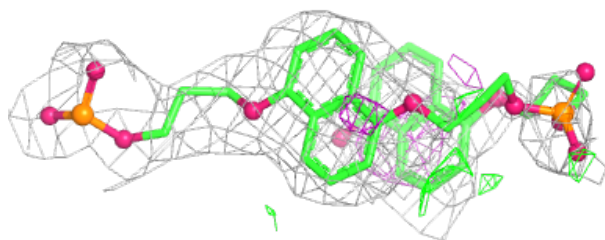
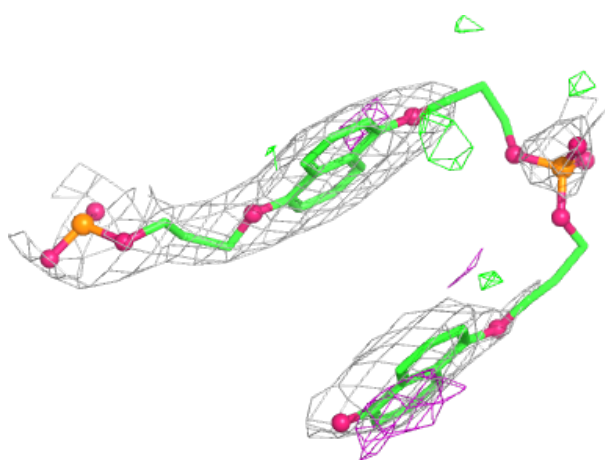
**Electron density around JL0 I 101:**

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



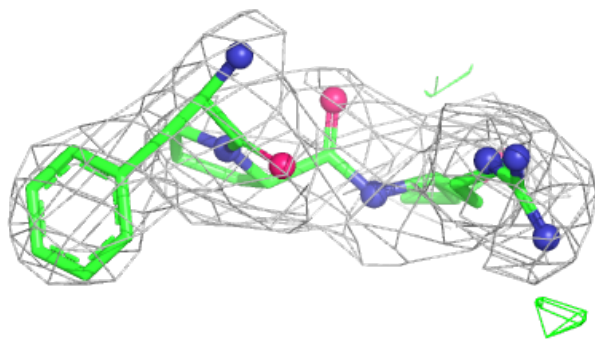
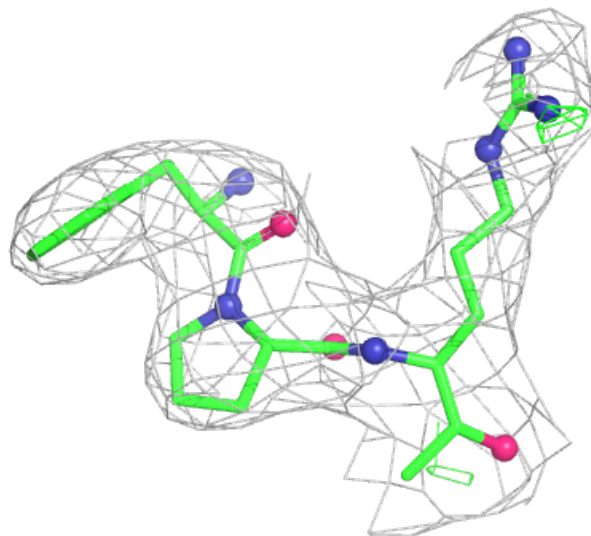
Electron density around JKR I 102:

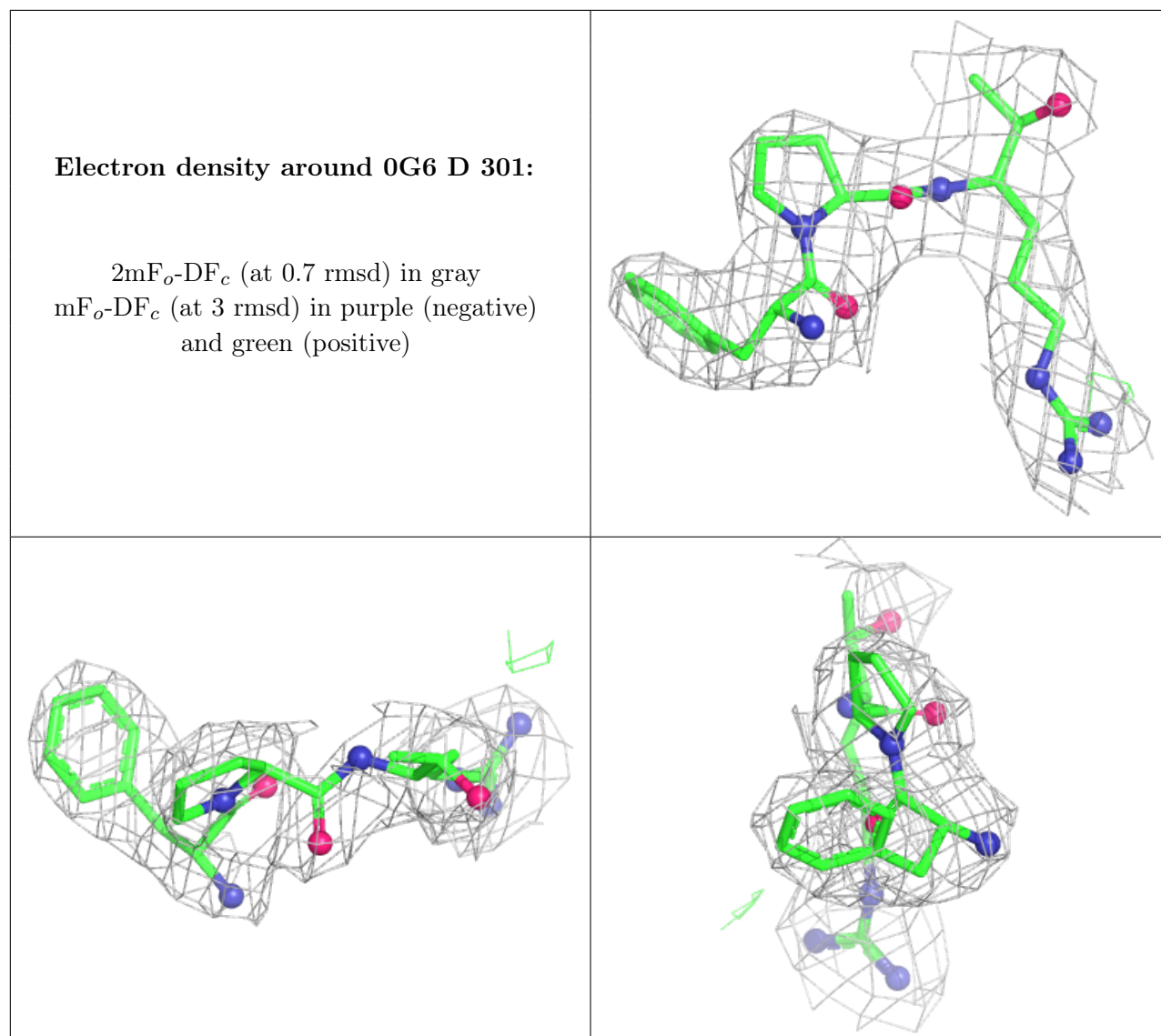
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 0G6 B 301:

$2mF_o-DF_c$ (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.