



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:36 AM UTC

PDB ID : 7QTV / pdb_00007qtv
Title : Beryllium fluoride form of the Na⁺,K⁺-ATPase (E2-BeFx)
Authors : Fruergaard, M.U.; Dach, I.; Andersen, J.L.; Ozol, M.; Shahsavar, A.; Quistgaard, E.M.; Poulsen, H.; Fedosova, N.U.; Nissen, P.
Deposited on : 2022-01-16
Resolution : 4.05 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:

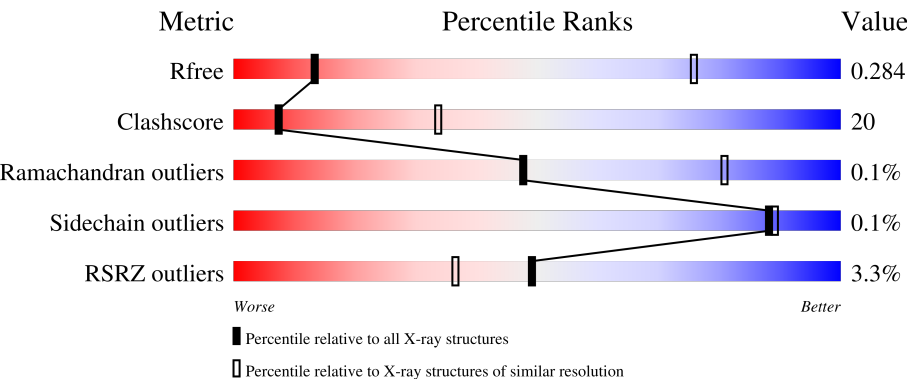
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1183 (4.32-3.80)
Clashscore	190562	1231 (4.32-3.80)
Ramachandran outliers	187476	1154 (4.32-3.80)
Sidechain outliers	187428	1144 (4.32-3.80)
RSRZ outliers	180081	1182 (4.32-3.80)

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	1021	4% 64% 33%
1	C	1021	3% 62% 35%
2	B	303	5% 50% 45%
2	D	303	% 60% 35%
3	E	65	38% 11% 51%

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Mol	Chain	Length	Quality of chain
3	G	65	
4	F	2	

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
5	BEF	C	1101	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21017 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	S	0	0	0
			7726	4922	1301	1456	47			
1	C	996	Total	C	N	O	S	0	0	0
			7726	4922	1301	1456	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			
2	D	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			

- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

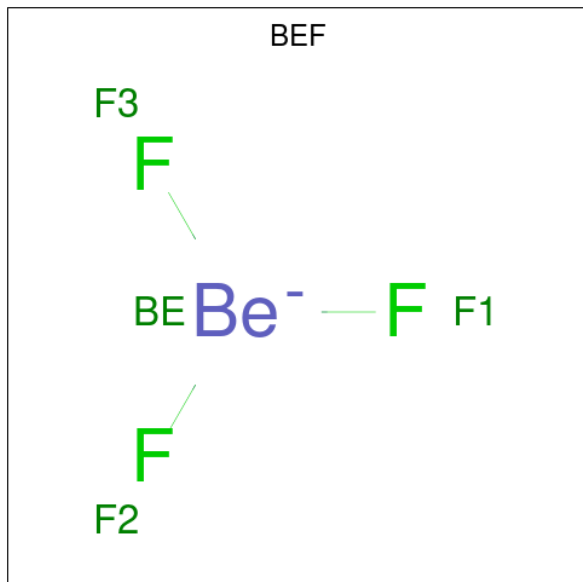
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

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



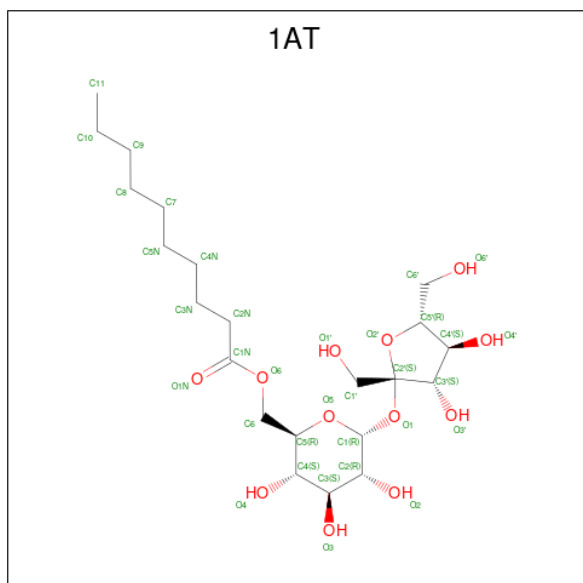
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			30	16	2	12			

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



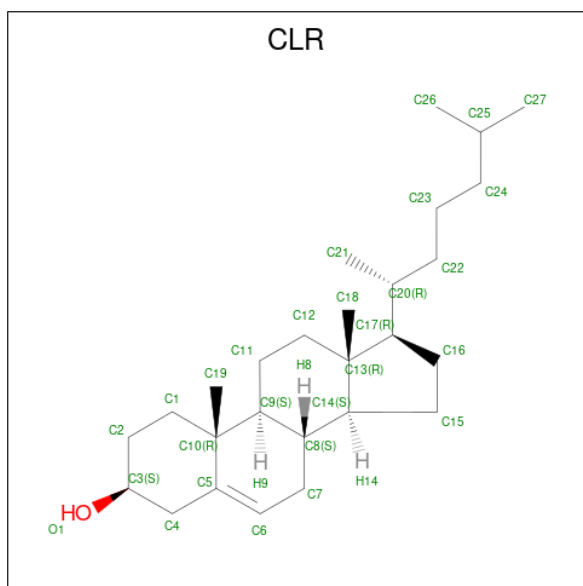
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		
5	C	1	Total	Be	F	0	0
			4	1	3		

- Molecule 6 is beta-D-fructofuranosyl 6-O-decanoyl-alpha-D-glucopyranoside (CCD ID: 1AT) (formula: $\text{C}_{22}\text{H}_{40}\text{O}_{12}$).



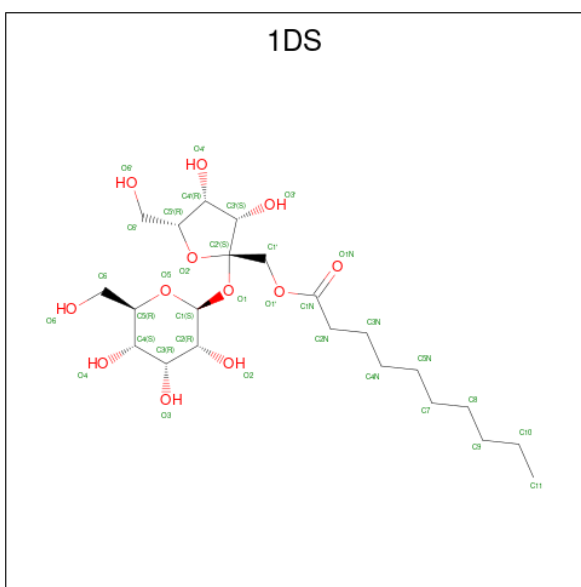
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			29	17	12		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		
7	G	1	Total	C	O	0	0
			28	27	1		
7	C	1	Total	C	O	0	0
			28	27	1		
7	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 8 is 1-O-decanoyl-beta-D-tagatofuranosyl beta-D-allopyranoside (CCD ID: 1DS) (formula: $C_{22}H_{40}O_{12}$).

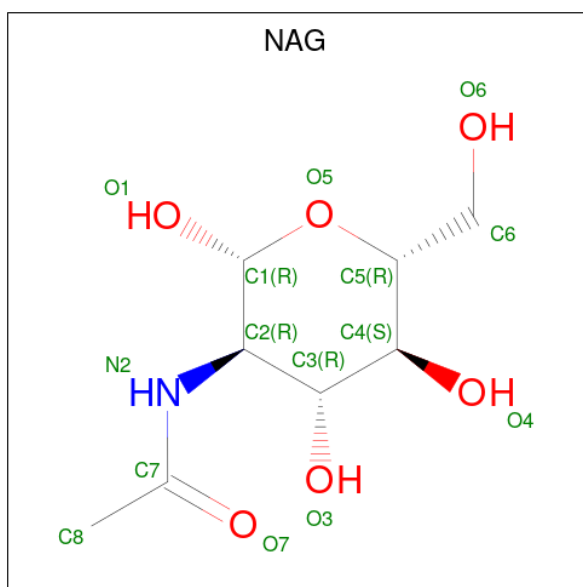


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			29	17	12		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	Mg	0	0
			3	3		
9	C	3	Total	Mg	0	0
			3	3		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



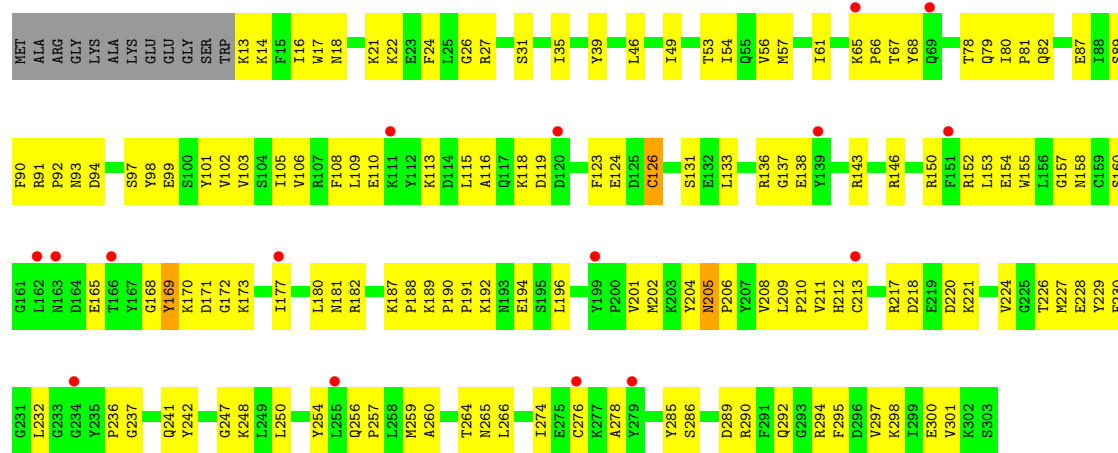
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			15	8	1	6		
10	B	1	Total	C	N	O	0	0
			15	8	1	6		
10	D	1	Total	C	N	O	0	0
			15	8	1	6		
10	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 11 is water.

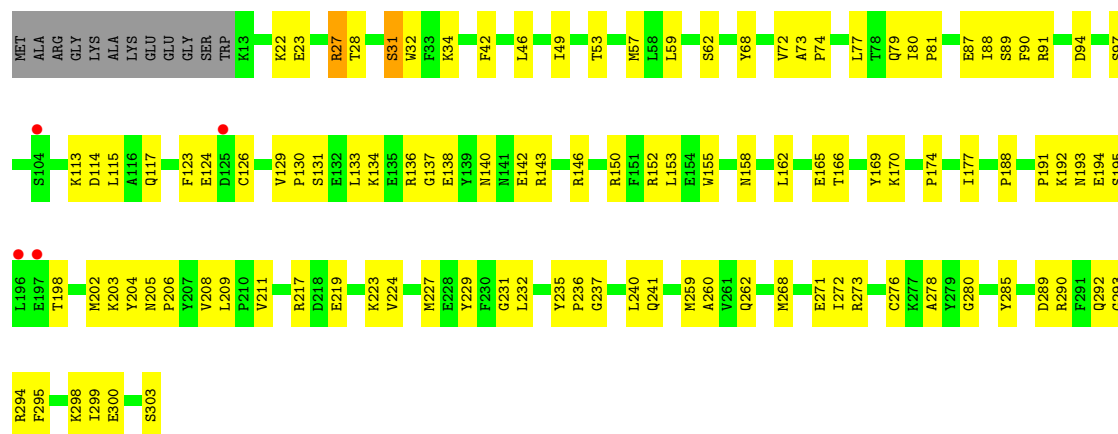
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	O	0	0
			5	5		
11	C	4	Total	O	0	0
			4	4		

Chain C: 3% 62% 35%

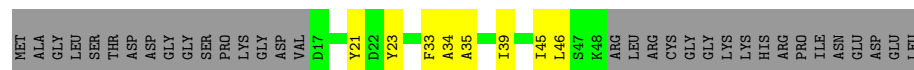
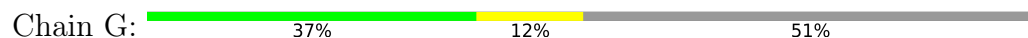




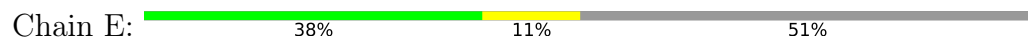
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: FXYP domain-containing ion transport regulator



• Molecule 3: FXYP domain-containing ion transport regulator



• 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.47Å 118.08Å 494.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 4.05 29.67 – 4.05	Depositor EDS
% Data completeness (in resolution range)	68.9 (29.67-4.05) 68.6 (29.67-4.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 4.11Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.246 , 0.281 0.250 , 0.284	Depositor DCC
R_{free} test set	1928 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	147.7	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 104.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21017	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: MG, NAG, 1AT, CLR, 1DS, BEF

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	0.23	0/7876	0.57	1/10688 (0.0%)
1	C	0.24	0/7876	0.60	2/10688 (0.0%)
2	B	0.27	0/2449	0.66	0/3301
2	D	0.26	0/2449	0.67	2/3301 (0.1%)
3	E	0.15	0/261	0.46	0/354
3	G	0.21	0/261	0.45	0/354
All	All	0.24	0/21172	0.60	5/28686 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	ARG	N-CA-C	-7.03	103.62	111.28
1	C	566	THR	OG1-CB-CG2	-6.92	95.46	109.30
1	A	487	LYS	CA-CB-CG	5.66	125.42	114.10
2	D	27	ARG	CA-CB-CG	5.24	124.59	114.10
2	D	31	SER	CB-CA-C	5.12	119.29	110.79

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	7726	0	7776	312	1
1	C	7726	0	7776	294	0
2	B	2386	0	2360	144	0
2	D	2386	0	2363	115	0
3	E	255	0	259	7	0
3	G	255	0	259	8	0
4	F	30	0	29	1	0
5	A	4	0	0	1	0
5	C	4	0	0	4	0
6	A	29	0	25	6	0
7	A	28	0	46	8	0
7	C	28	0	46	4	0
7	E	28	0	46	4	0
7	G	28	0	46	6	0
8	A	29	0	27	10	0
9	A	3	0	0	0	0
9	C	3	0	0	0	0
10	B	30	0	29	3	0
10	D	30	0	28	4	0
11	A	5	0	0	2	0
11	C	4	0	0	3	0
All	All	21017	0	21115	858	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 858 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:ASN:ND2	10:D:401:NAG:O3	1.87	1.08
1:C:845:MET:SD	1:C:998:ARG:NH1	2.31	1.03
1:A:487:LYS:NZ	1:A:494:PRO:O	1.92	1.01
2:B:208:VAL:HG22	2:B:237:GLY:HA3	1.40	0.99
2:B:80:ILE:HG13	2:B:81:PRO:HD3	1.45	0.98

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:SER:OG	1:A:640:ARG:O[4_445]	1.85	0.35

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	994/1021 (97%)	935 (94%)	59 (6%)	0	100	100
1	C	994/1021 (97%)	936 (94%)	58 (6%)	0	100	100
2	B	289/303 (95%)	267 (92%)	20 (7%)	2 (1%)	18	55
2	D	289/303 (95%)	272 (94%)	17 (6%)	0	100	100
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	27 (90%)	3 (10%)	0	100	100
All	All	2626/2778 (94%)	2465 (94%)	159 (6%)	2 (0%)	48	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	169	TYR
2	B	205	ASN

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	847/865 (98%)	847 (100%)	0	100	100
1	C	847/865 (98%)	847 (100%)	0	100	100
2	B	261/269 (97%)	260 (100%)	1 (0%)	84	83
2	D	261/269 (97%)	259 (99%)	2 (1%)	73	78
3	E	26/52 (50%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	26/52 (50%)	26 (100%)	0	100	100
All	All	2268/2372 (96%)	2265 (100%)	3 (0%)	88	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	126	CYS
2	D	126	CYS
2	D	158	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	262	GLN
1	C	399	GLN
2	D	292	GLN
1	C	156	ASN
1	C	488	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 ⓘ

2 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	F	1	4,2	15,15,15	1.36	2 (13%)	21,21,21	1.58	4 (19%)
4	NAG	F	2	4	15,15,15	1.08	1 (6%)	21,21,21	0.94	2 (9%)

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	F	1	4,2	-	0/6/26/26	0/1/1/1
4	NAG	F	2	4	-	1/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-4.80	1.31	1.42
4	F	2	NAG	C1-C2	-3.57	1.48	1.52
4	F	1	NAG	C1-C2	-2.02	1.50	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	O1-C1-O5	-4.63	96.67	110.41
4	F	1	NAG	C4-C3-C2	2.97	114.72	110.40
4	F	1	NAG	O1-C1-C2	-2.63	103.76	109.22
4	F	2	NAG	C1-C2-C3	-2.50	107.14	110.54
4	F	1	NAG	C3-C4-C5	2.41	114.61	110.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

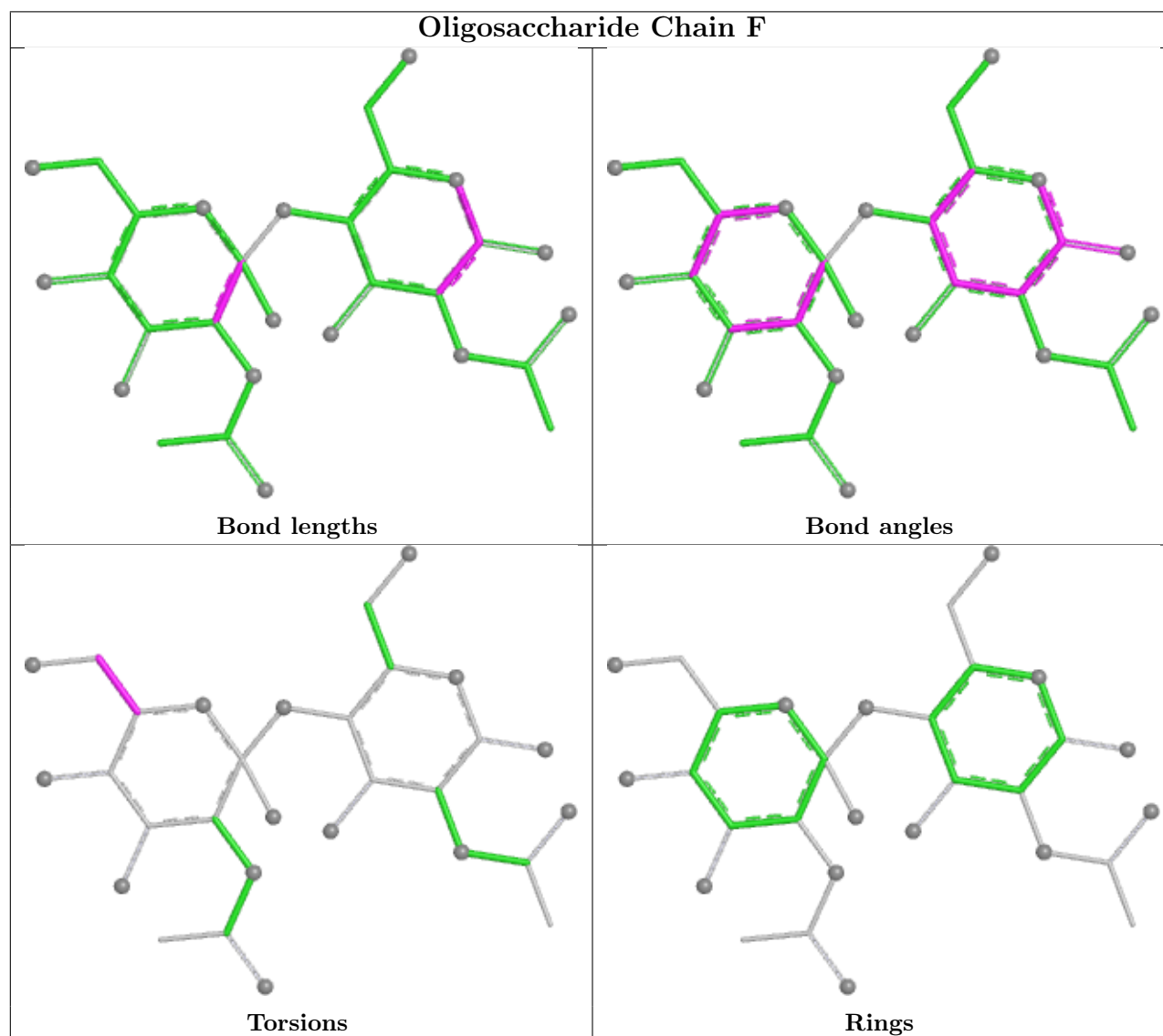
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
8	1DS	A	1104	-	30,30,35	1.34	5 (16%)	42,43,48	2.89	18 (42%)
10	NAG	D	402	2	15,15,15	0.90	1 (6%)	21,21,21	0.71	0
7	CLR	C	1102	-	31,31,31	0.75	1 (3%)	48,48,48	1.41	8 (16%)
5	BEF	C	1101	-	0,3,3	-	-	-	-	-
10	NAG	B	402	2	15,15,15	0.87	1 (6%)	21,21,21	1.47	2 (9%)
6	1AT	A	1102	-	30,30,35	1.49	3 (10%)	43,43,48	2.51	15 (34%)
7	CLR	A	1103	-	31,31,31	0.71	0	48,48,48	1.63	8 (16%)
7	CLR	E	101	-	31,31,31	0.77	1 (3%)	48,48,48	1.25	6 (12%)
7	CLR	G	101	-	31,31,31	0.73	1 (3%)	48,48,48	1.33	9 (18%)
5	BEF	A	1101	1	0,3,3	-	-	-	-	-
10	NAG	B	401	2	15,15,15	0.43	0	21,21,21	0.60	1 (4%)
10	NAG	D	401	-	15,15,15	0.25	0	21,21,21	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	1DS	A	1104	-	-	7/19/58/63	0/2/2/2
10	NAG	D	402	2	-	2/6/26/26	0/1/1/1
7	CLR	C	1102	-	-	4/10/68/68	0/4/4/4
10	NAG	B	402	2	-	0/6/26/26	0/1/1/1
6	1AT	A	1102	-	-	10/19/58/63	0/2/2/2
7	CLR	E	101	-	-	6/10/68/68	0/4/4/4
7	CLR	A	1103	-	-	9/10/68/68	0/4/4/4
7	CLR	G	101	-	-	2/10/68/68	0/4/4/4
10	NAG	B	401	2	-	2/6/26/26	0/1/1/1
10	NAG	D	401	-	-	2/6/26/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1102	1AT	O6-C1N	4.66	1.46	1.33
8	A	1104	1DS	O1'-C1N	3.01	1.42	1.33
10	B	402	NAG	O5-C1	-2.91	1.35	1.42
10	D	402	NAG	C1-C2	2.85	1.56	1.52
6	A	1102	1AT	C4'-C5'	-2.75	1.46	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1104	1DS	C1'-O1'-C1N	6.82	128.87	116.71
6	A	1102	1AT	O2-C2-C3	-6.79	94.36	110.38
6	A	1102	1AT	O1-C1-C2	6.23	125.76	108.42
8	A	1104	1DS	O2-C2-C3	6.09	124.72	110.38
8	A	1104	1DS	O1-C2'-C3'	6.01	126.47	108.20

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1102	1AT	O1'-C1'-C2'-O1
6	A	1102	1AT	O1'-C1'-C2'-C3'
8	A	1104	1DS	O1'-C1'-C2'-O1
8	A	1104	1DS	O1'-C1'-C2'-C3'
8	A	1104	1DS	O1'-C1'-C2'-O2'

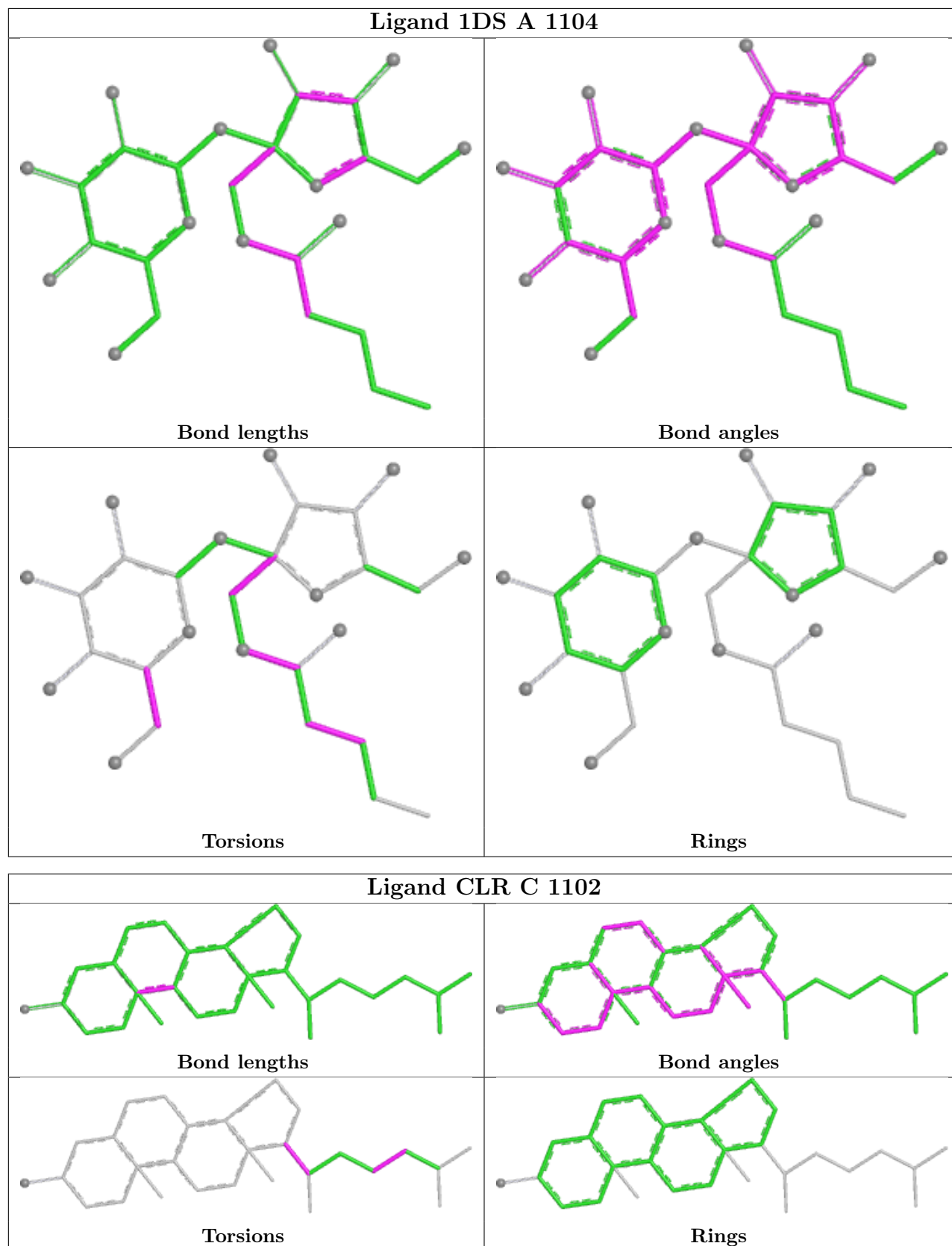
There are no ring outliers.

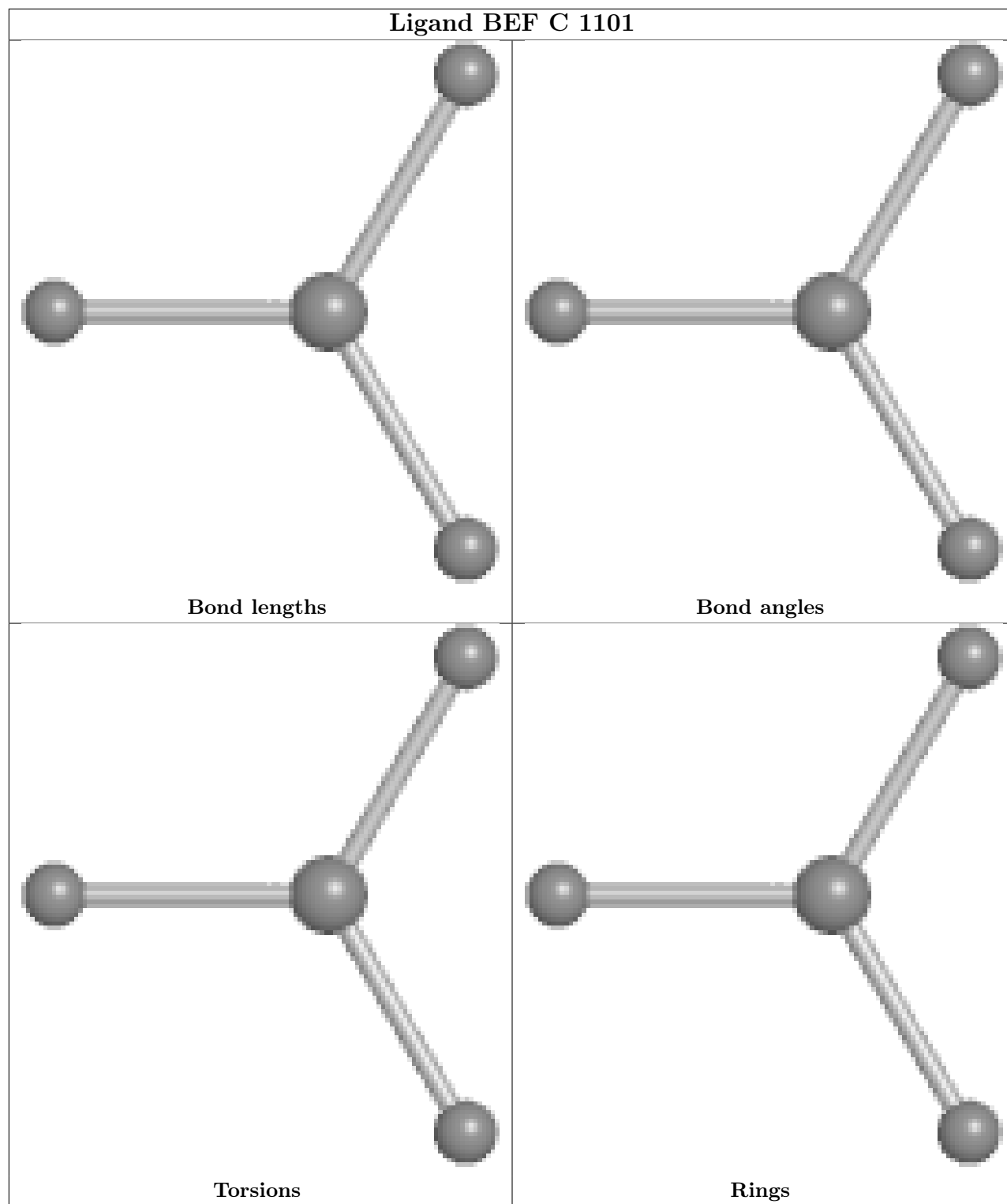
11 monomers are involved in 50 short contacts:

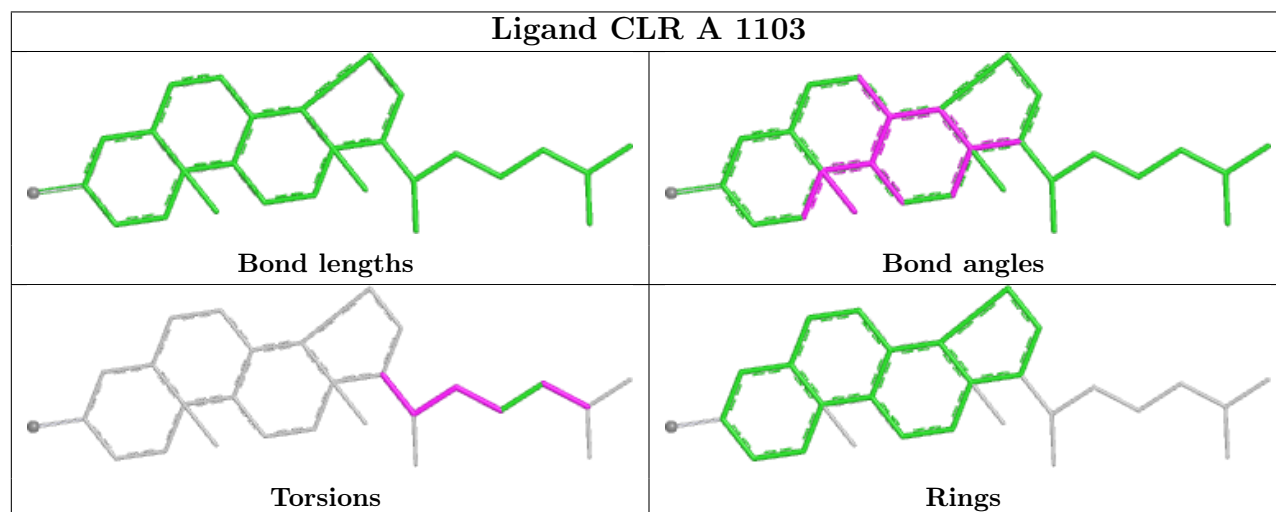
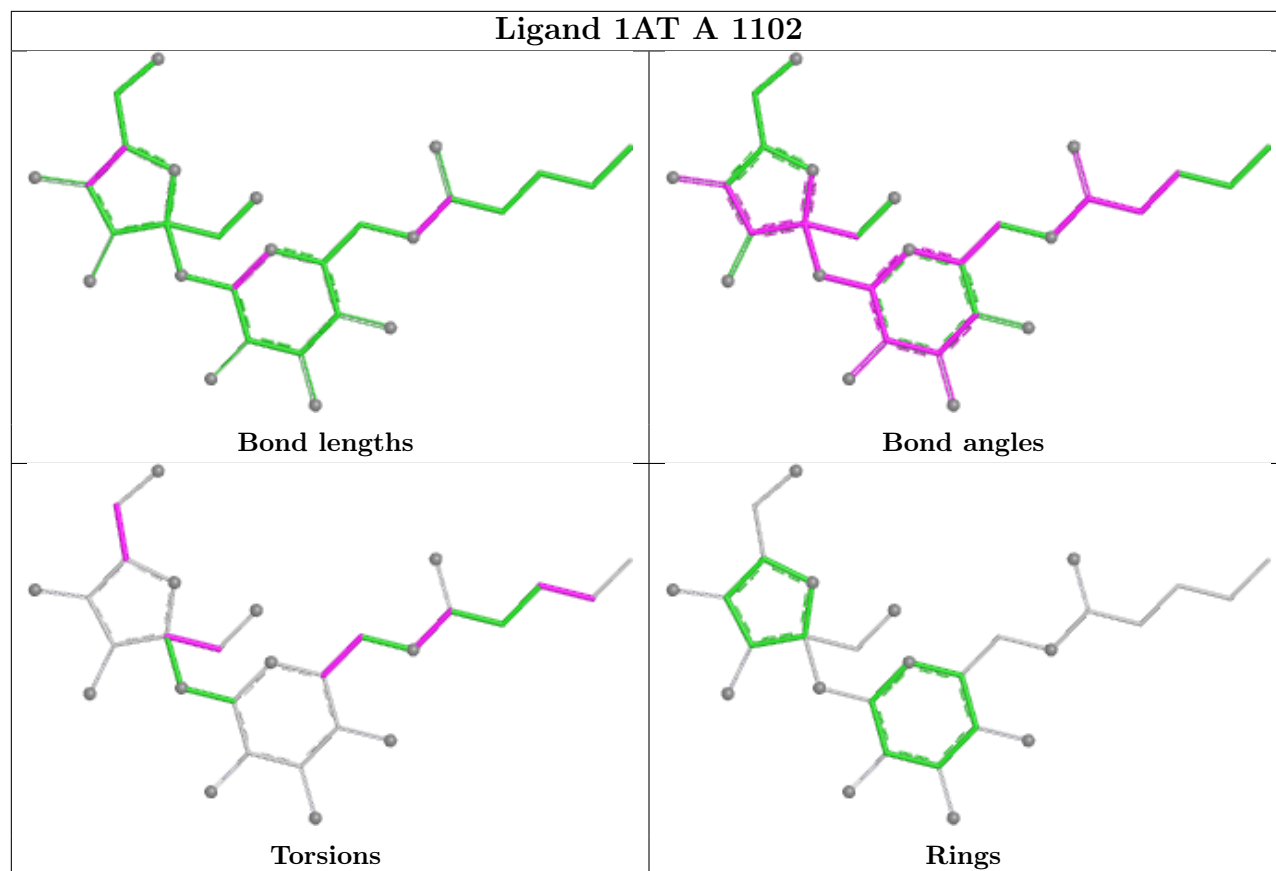
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1104	1DS	10	0
7	C	1102	CLR	4	0
5	C	1101	BEF	4	0
10	B	402	NAG	1	0
6	A	1102	1AT	6	0
7	A	1103	CLR	8	0
7	E	101	CLR	4	0
7	G	101	CLR	6	0
5	A	1101	BEF	1	0
10	B	401	NAG	2	0
10	D	401	NAG	4	0

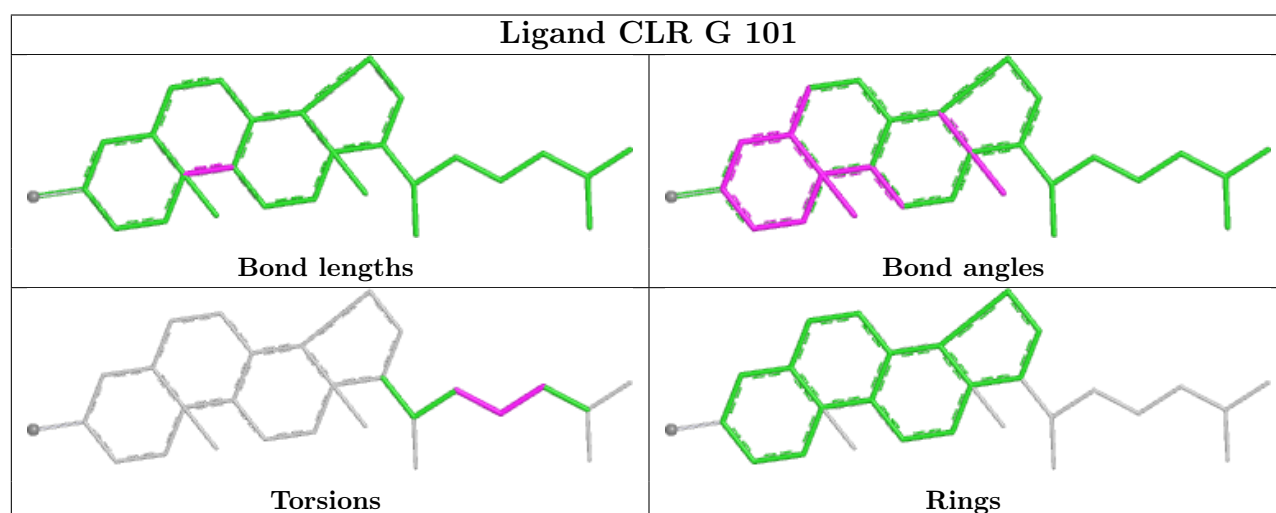
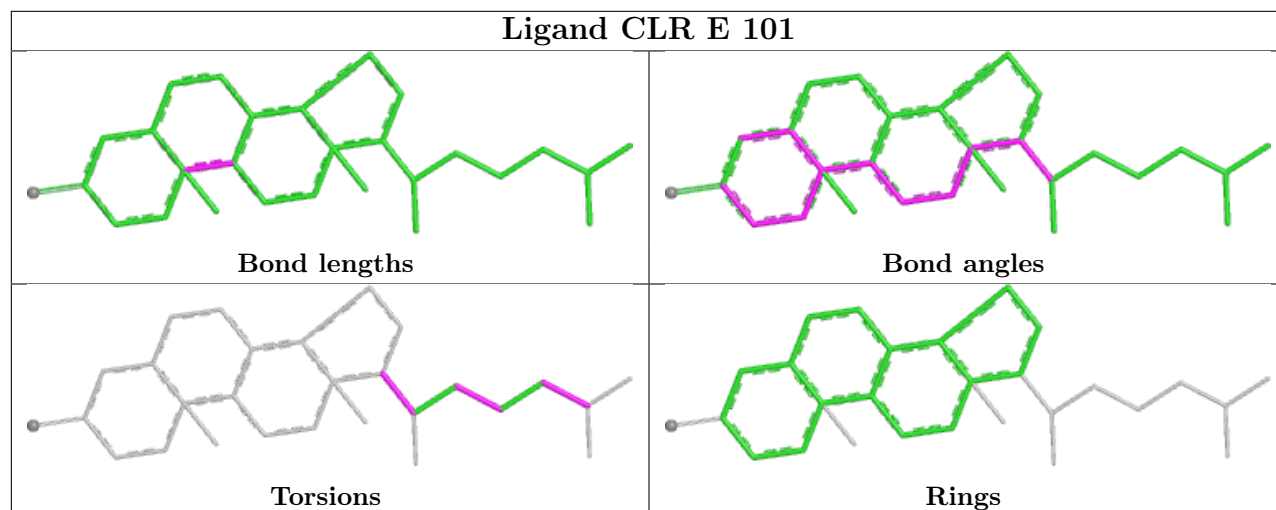
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

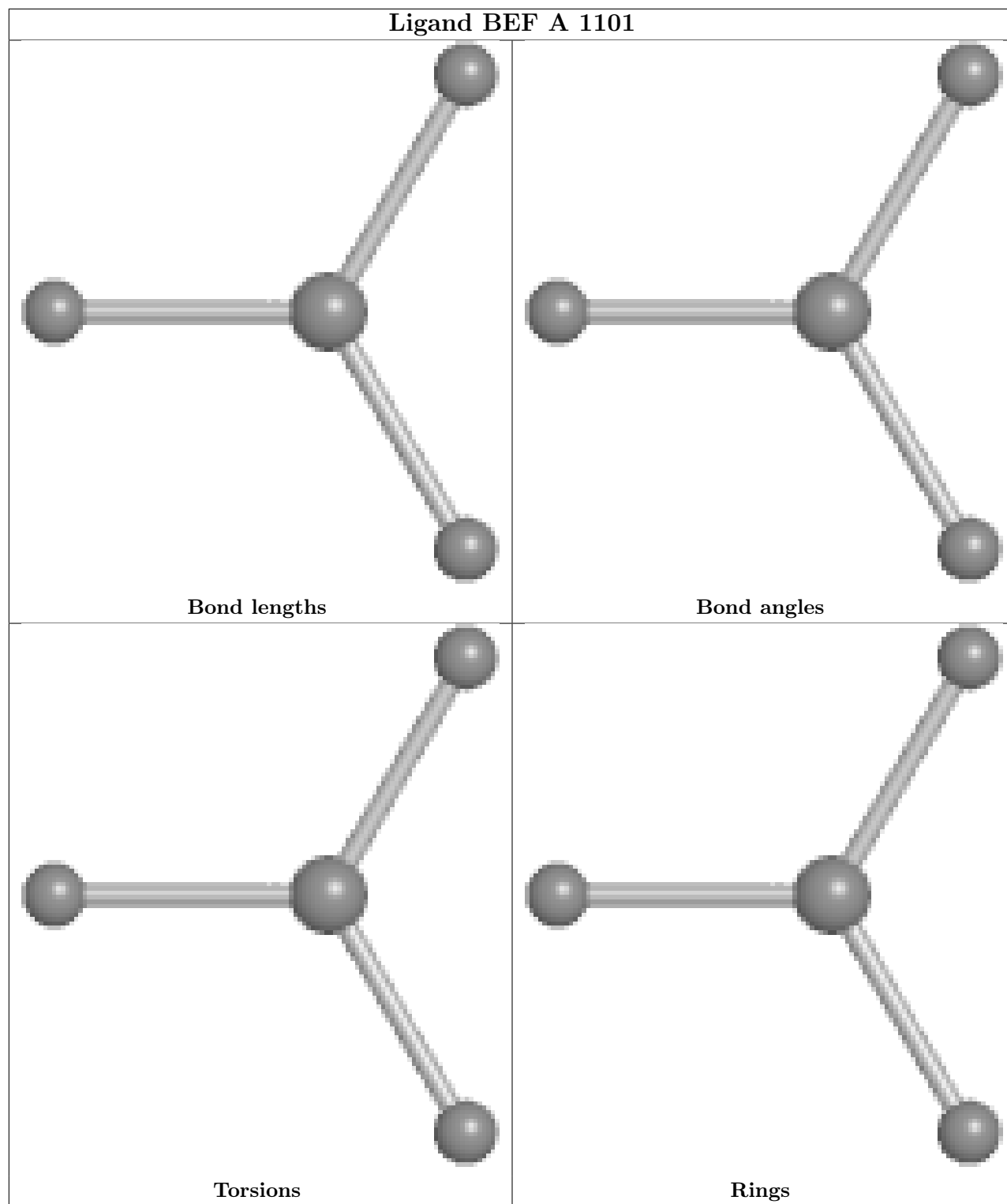
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	996/1021 (97%)	0.25	36 (3%) 46 35	86, 151, 281, 440	0
1	C	996/1021 (97%)	0.30	32 (3%) 50 38	90, 179, 337, 502	0
2	B	291/303 (96%)	0.48	16 (5%) 30 26	101, 221, 315, 407	0
2	D	291/303 (96%)	0.28	4 (1%) 73 55	116, 196, 292, 362	0
3	E	32/65 (49%)	-0.20	0 100 100	106, 139, 202, 243	0
3	G	32/65 (49%)	-0.15	0 100 100	90, 124, 195, 213	0
All	All	2638/2778 (94%)	0.29	88 (3%) 49 36	86, 174, 307, 502	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	PRO	4.1
1	C	527	LEU	4.1
1	C	573	LEU	3.8
2	B	166	THR	3.7
2	B	151	PHE	3.7

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

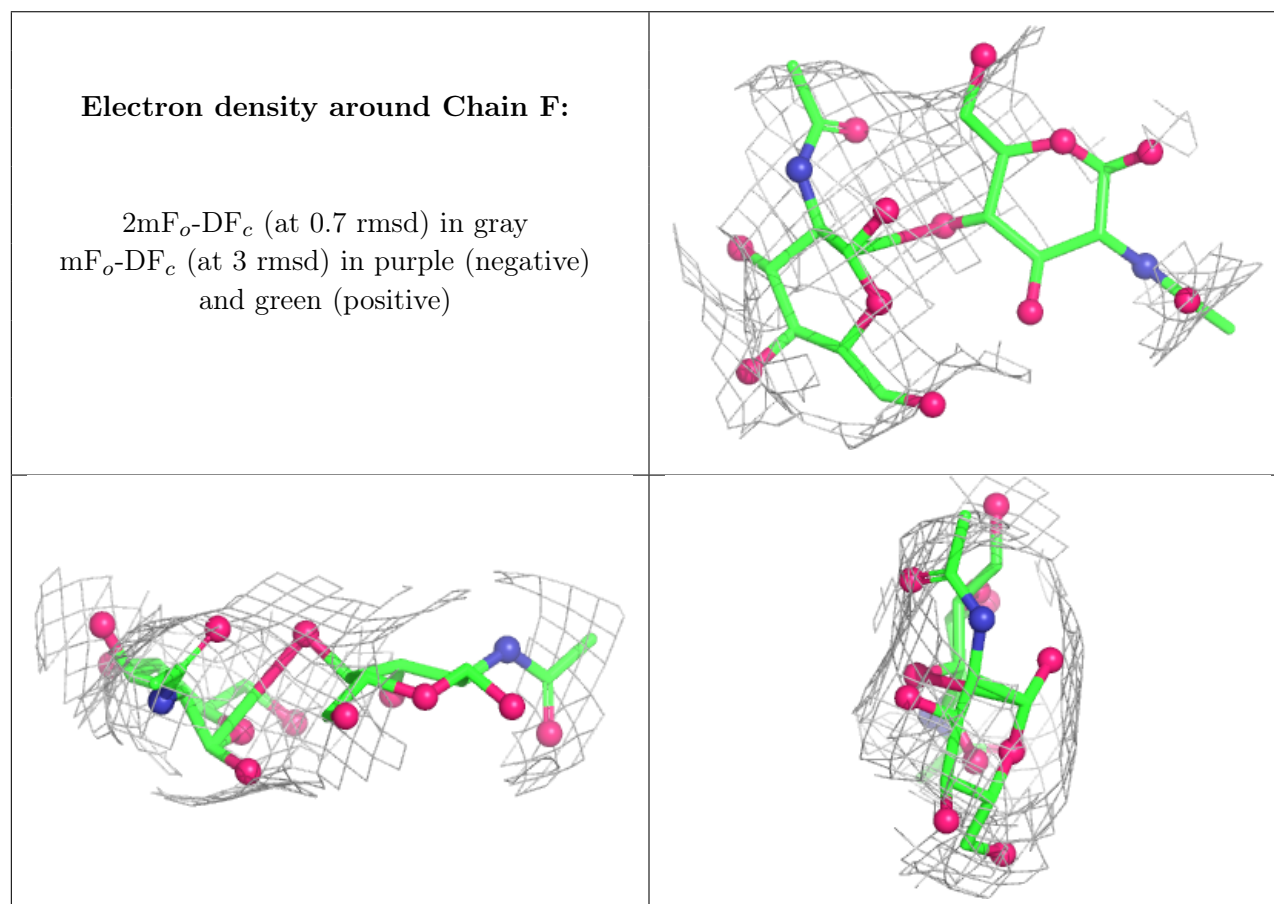
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	F	1	15/15	-	-	267,281,291,294	0
4	NAG	F	2	15/15	-	-	251,274,291,304	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.

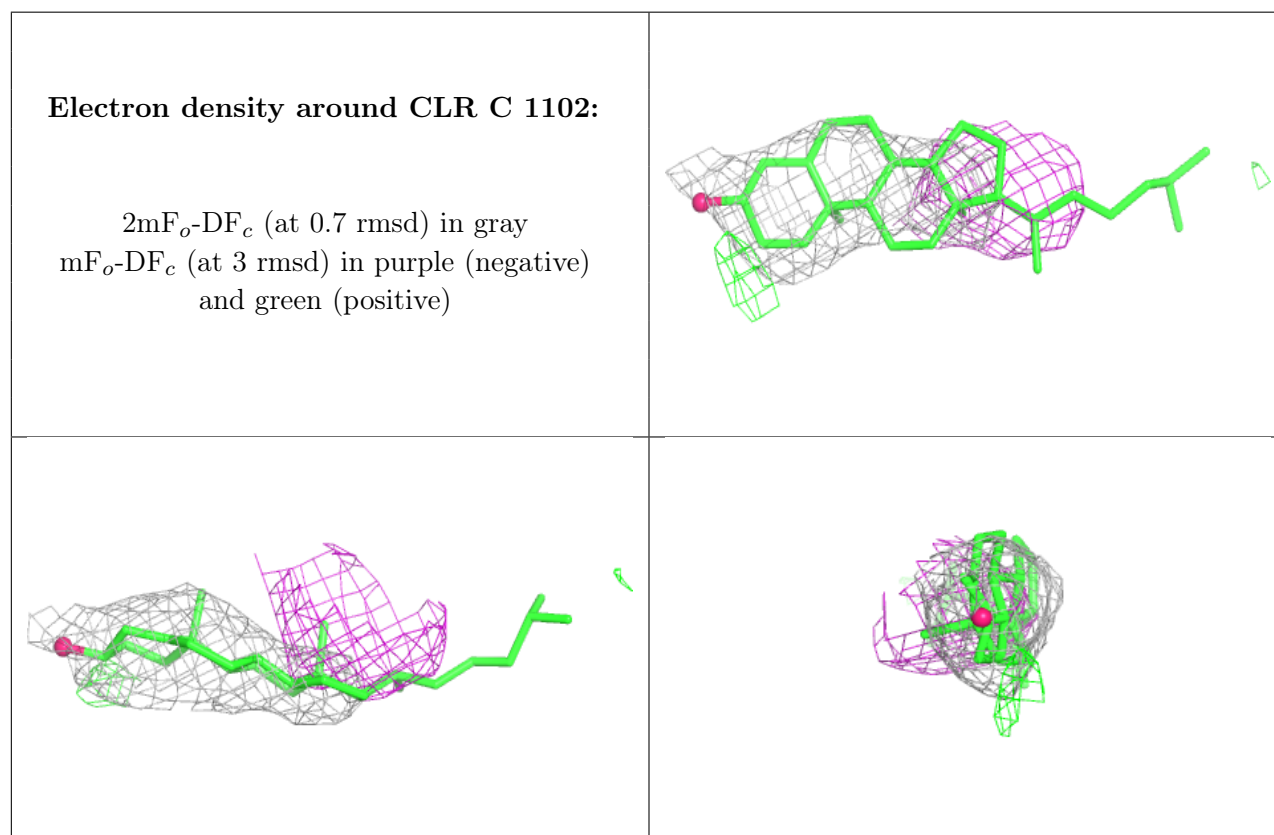
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	B	401	15/15	0.44	0.14	241,261,267,272	0
10	NAG	B	402	15/15	0.48	0.18	212,263,275,278	0
10	NAG	D	402	15/15	0.59	0.16	214,253,263,266	0
10	NAG	D	401	15/15	0.74	0.13	227,246,255,256	0
7	CLR	C	1102	28/28	0.79	0.28	115,161,175,179	0
7	CLR	A	1103	28/28	0.81	0.21	107,129,146,151	0

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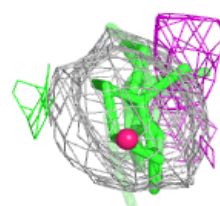
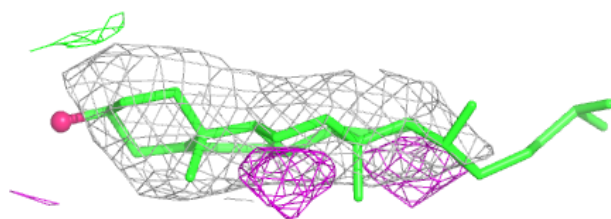
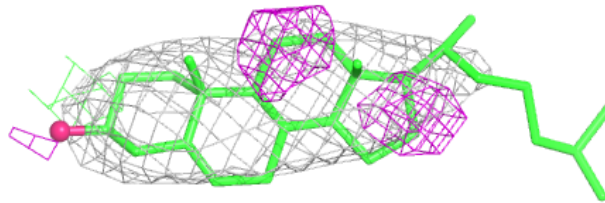
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	1DS	A	1104	29/34	0.82	0.18	107,154,164,164	0
6	1AT	A	1102	29/34	0.84	0.16	97,139,165,182	0
5	BEF	C	1101	4/4	0.91	0.13	155,165,173,175	0
7	CLR	E	101	28/28	0.92	0.12	65,90,109,132	0
7	CLR	G	101	28/28	0.94	0.12	88,103,121,128	0
5	BEF	A	1101	4/4	0.95	0.08	191,192,197,207	0
9	MG	C	1104	1/1	0.95	0.11	144,144,144,144	0
9	MG	A	1105	1/1	0.97	0.08	160,160,160,160	0
9	MG	C	1103	1/1	0.98	0.03	187,187,187,187	0
9	MG	A	1107	1/1	0.98	0.06	115,115,115,115	0
9	MG	A	1106	1/1	0.99	0.09	145,145,145,145	0
9	MG	C	1105	1/1	0.99	0.04	163,163,163,163	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.



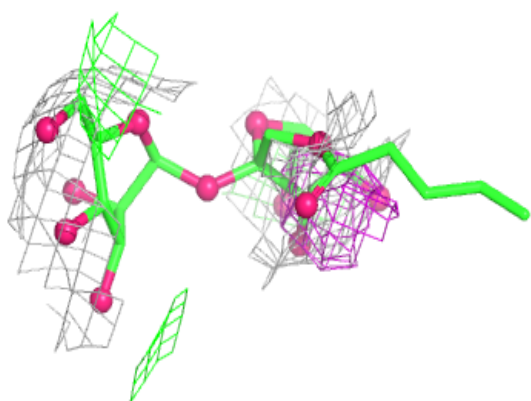
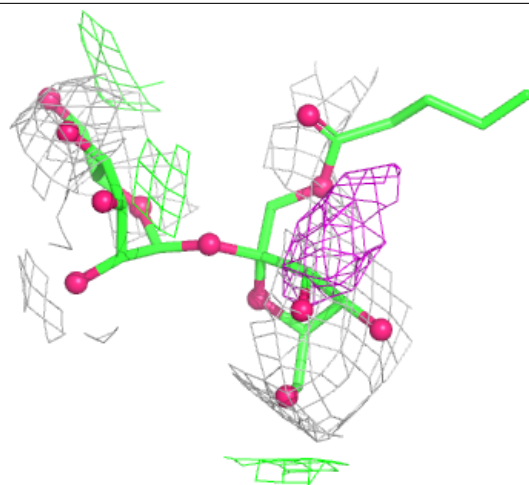
Electron density around CLR A 1103:

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



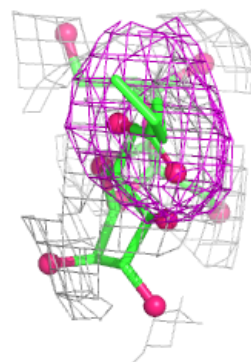
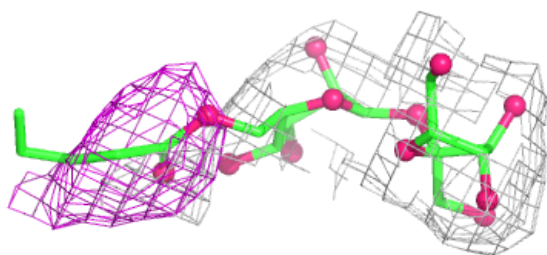
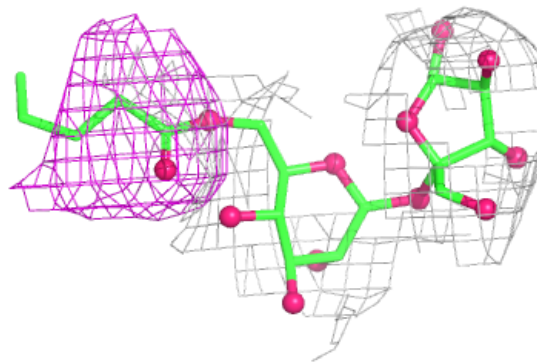
Electron density around 1DS A 1104:

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



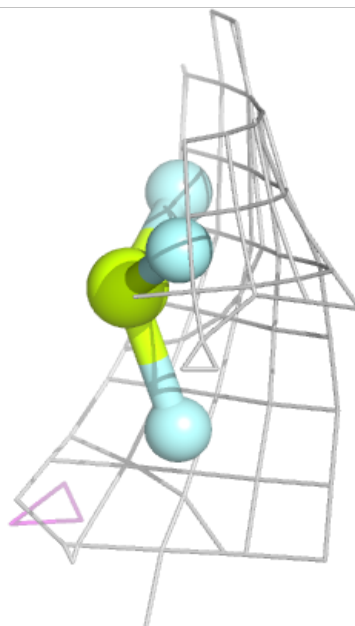
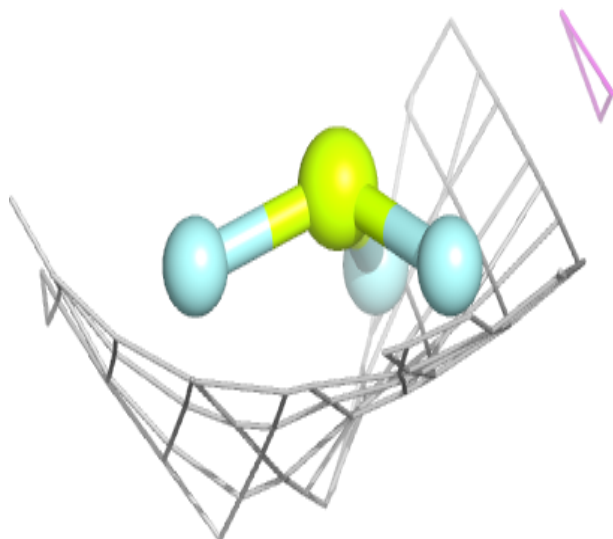
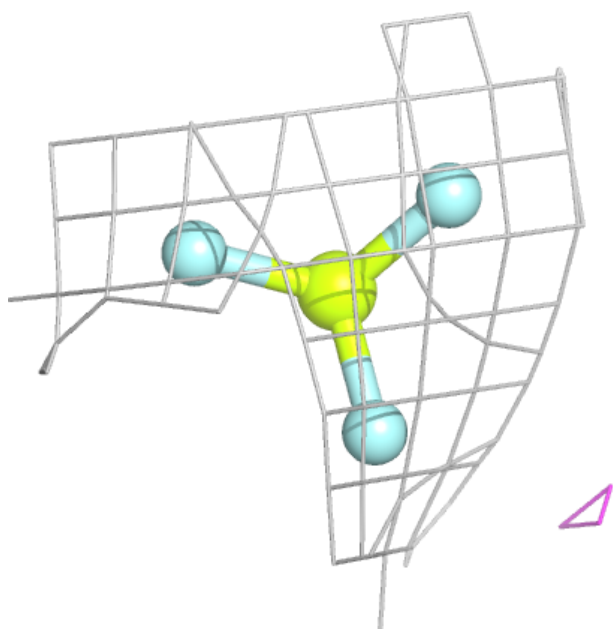
Electron density around 1AT A 1102:

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



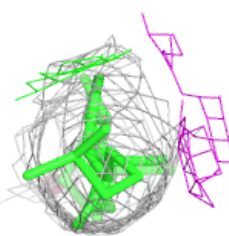
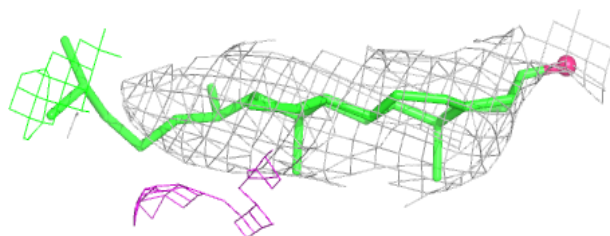
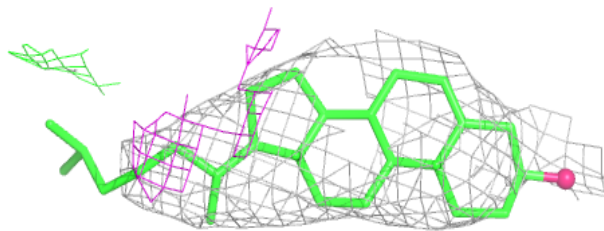
Electron density around BEF C 1101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

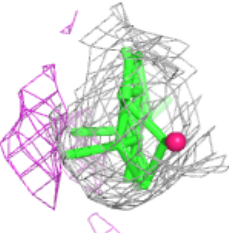
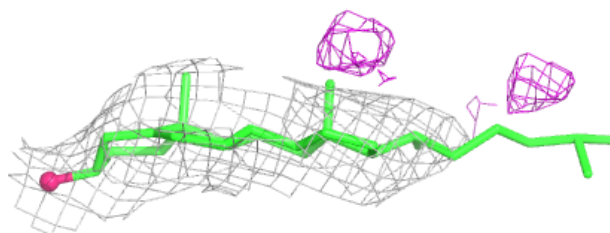
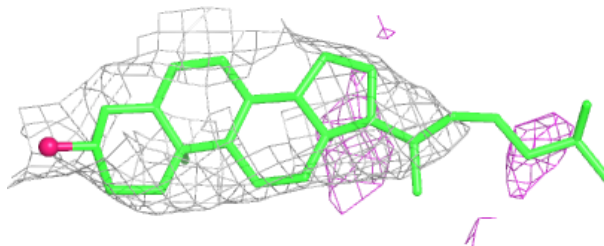


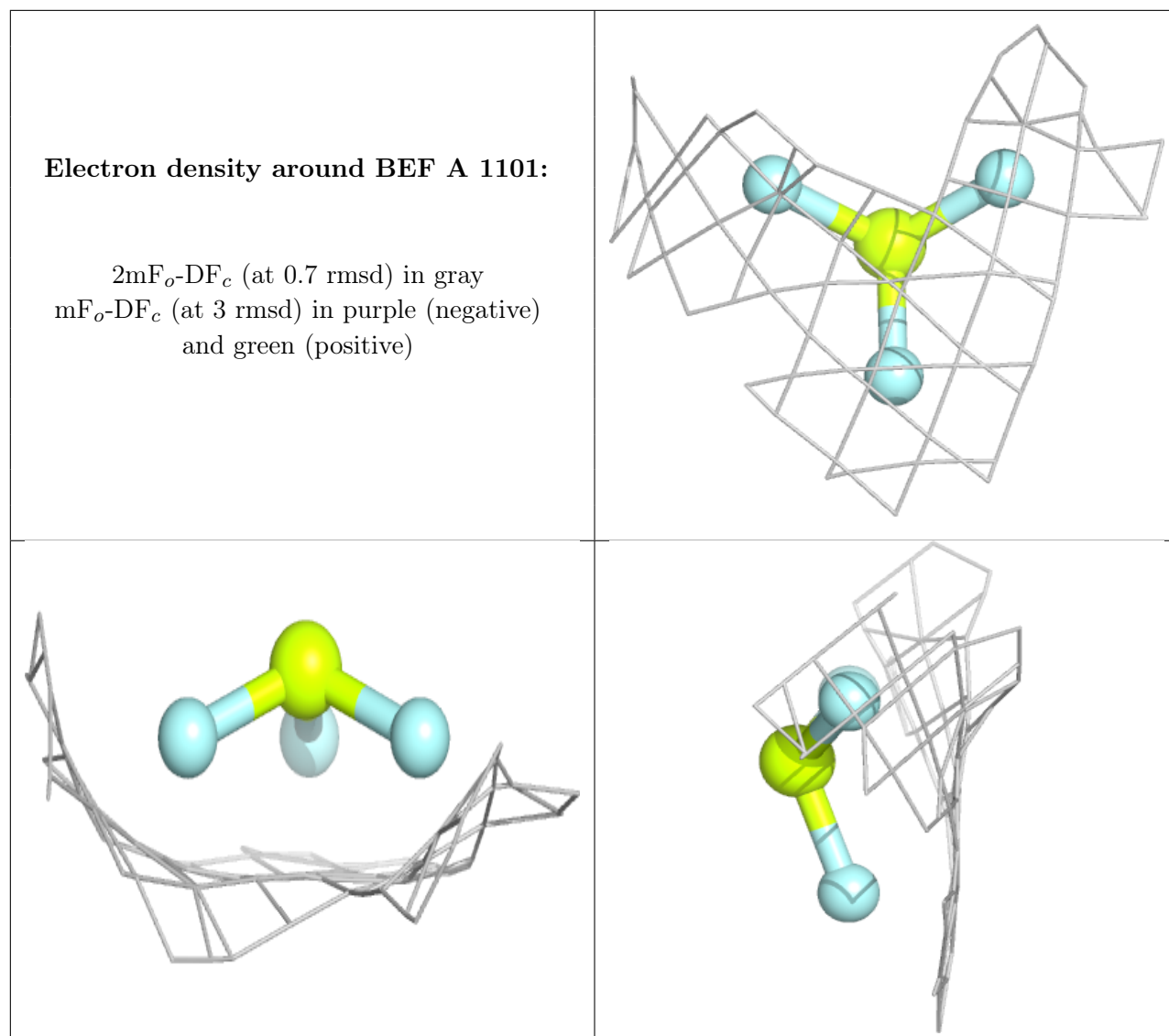
Electron density around CLR E 101:

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

**Electron density around CLR 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.