



## wwPDB EM Validation Summary Report

Nov 6, 2023 – 11:59 pm GMT

PDB ID : 8BC3  
EMDB ID : EMD-15961  
Title : Cryo-EM Structure of a BmSF-TAL - Sulfofructose Schiff Base Complex  
Authors : Snow, A.J.D.; Sharma, M.; Blaza, J.; Davies, G.J.  
Deposited on : 2022-10-14  
Resolution : 2.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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>.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

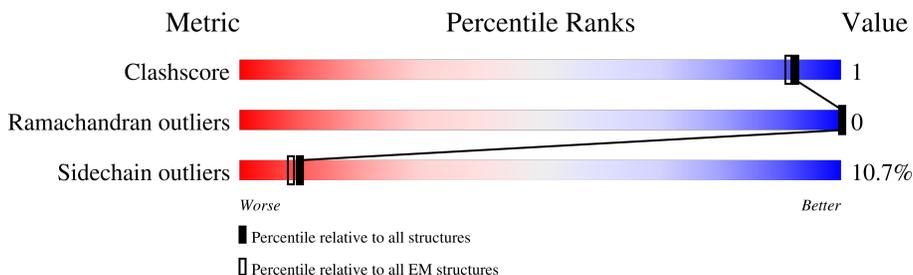
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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
2	QC9	A	301	-	X	-	-
2	QC9	B	301	-	X	-	-
2	QC9	C	301	-	X	-	-
2	QC9	D	301	-	X	-	-
2	QC9	E	301	-	X	-	-
2	QC9	F	301	-	X	-	-
2	QC9	G	301	-	X	-	-
2	QC9	H	301	-	X	-	-
2	QC9	I	301	-	X	-	-
2	QC9	J	301	-	X	-	-

## 2 Entry composition [i](#)

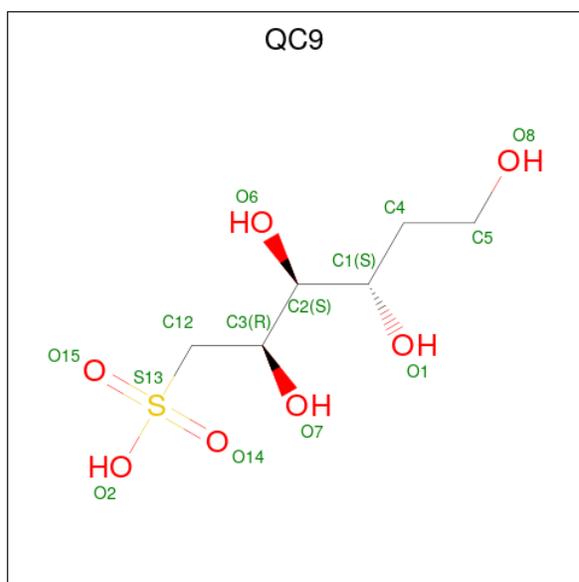
There are 3 unique types of molecules in this entry. The entry contains 16880 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 BmSF-TAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	217	1624	1048	270	302	4	0	0
1	H	217	1624	1048	270	302	4	0	0
1	B	217	1624	1048	270	302	4	0	0
1	C	217	1624	1048	270	302	4	0	0
1	D	217	1624	1048	270	302	4	0	0
1	E	217	1624	1048	270	302	4	0	0
1	F	217	1624	1048	270	302	4	0	0
1	G	217	1624	1048	270	302	4	0	0
1	I	217	1624	1048	270	302	4	0	0
1	J	217	1624	1048	270	302	4	0	0

- Molecule 2 is (2 {R},3 {S},4 {S})-2,3,4,6-tetrakis(oxidanyl)hexane-1-sulfonic acid (three-letter code: QC9) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>7</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
2	A	1	Total	C	O	S	0
			14	6	7	1	
2	H	1	Total	C	O	S	0
			14	6	7	1	
2	B	1	Total	C	O	S	0
			14	6	7	1	
2	C	1	Total	C	O	S	0
			14	6	7	1	
2	D	1	Total	C	O	S	0
			14	6	7	1	
2	E	1	Total	C	O	S	0
			14	6	7	1	
2	F	1	Total	C	O	S	0
			14	6	7	1	
2	G	1	Total	C	O	S	0
			14	6	7	1	
2	I	1	Total	C	O	S	0
			14	6	7	1	
2	J	1	Total	C	O	S	0
			14	6	7	1	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
3	A	50	Total	O	0
			50	50	
3	H	50	Total	O	0
			50	50	

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Mol	Chain	Residues	Atoms	AltConf
3	B	50	Total O 50 50	0
3	C	50	Total O 50 50	0
3	D	50	Total O 50 50	0
3	E	50	Total O 50 50	0
3	F	50	Total O 50 50	0
3	G	50	Total O 50 50	0
3	I	50	Total O 50 50	0
3	J	50	Total O 50 50	0

SEQUENCE-PLOTS INFOmissingINFO

### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	53450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	310000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QC9

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	0.58	0/1664	0.68	0/2274
1	B	0.58	0/1664	0.68	0/2274
1	C	0.58	0/1664	0.68	0/2274
1	D	0.58	0/1664	0.68	0/2274
1	E	0.58	0/1664	0.68	0/2274
1	F	0.58	0/1664	0.68	0/2274
1	G	0.58	0/1664	0.68	0/2274
1	H	0.58	0/1657	0.67	0/2266
1	I	0.58	0/1664	0.68	0/2274
1	J	0.58	0/1664	0.68	0/2274
All	All	0.58	0/16633	0.68	0/22732

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ARG	Sidechain
1	B	126	ARG	Sidechain
1	C	126	ARG	Sidechain
1	D	126	ARG	Sidechain
1	H	126	ARG	Sidechain

## 4.2 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	1624	0	1505	5	0
1	B	1624	0	1505	6	0
1	C	1624	0	1505	3	0
1	D	1624	0	1505	7	0
1	E	1624	0	1505	6	0
1	F	1624	0	1505	7	0
1	G	1624	0	1505	6	0
1	H	1624	0	1505	4	0
1	I	1624	0	1505	5	0
1	J	1624	0	1505	4	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
2	E	14	0	0	0	0
2	F	14	0	0	0	0
2	G	14	0	0	0	0
2	H	14	0	0	0	0
2	I	14	0	0	0	0
2	J	14	0	0	0	0
3	A	50	0	0	0	0
3	B	50	0	0	0	0
3	C	50	0	0	0	0
3	D	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	50	0	0	0	0
3	F	50	0	0	0	0
3	G	50	0	0	0	0
3	H	50	0	0	0	0
3	I	50	0	0	0	0
3	J	50	0	0	0	0
All	All	16880	0	15050	45	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 1.

The worst 5 of 45 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:F:73:VAL:HA	1:F:103:PHE:CZ	2.42	0.55
1:I:73:VAL:HA	1:I:103:PHE:CZ	2.42	0.55
1:G:73:VAL:HA	1:G:103:PHE:CZ	2.42	0.55
1:E:73:VAL:HA	1:E:103:PHE:CZ	2.42	0.55
1:B:73:VAL:HA	1:B:103:PHE:CZ	2.42	0.54

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 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 PDB entries followed by that with respect to all EM entries.

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	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	B	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	C	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	D	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	E	213/226 (94%)	206 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	G	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	H	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	I	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
1	J	213/226 (94%)	206 (97%)	7 (3%)	0	100	100
All	All	2130/2260 (94%)	2060 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 4.3.2 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 PDB entries followed by that with respect to all EM entries.

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	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	B	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	C	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	D	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	E	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	F	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	G	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	H	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	I	159/193 (82%)	142 (89%)	17 (11%)	6	3
1	J	159/193 (82%)	142 (89%)	17 (11%)	6	3
All	All	1590/1930 (82%)	1420 (89%)	170 (11%)	10	3

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	187	VAL
1	I	122	LEU

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Mol	Chain	Res	Type
1	G	9	ILE
1	G	172	ASN
1	I	188	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	172	ASN
1	J	111	ASN
1	E	199	GLN
1	J	85	ASN
1	J	199	GLN

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

#### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 4.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
2	QC9	B	301	1	12,13,13	3.39	8 (66%)	15,18,18	4.93	10 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	QC9	I	301	1	12,13,13	3.37	8 (66%)	15,18,18	4.94	10 (66%)
2	QC9	D	301	1	12,13,13	3.40	8 (66%)	15,18,18	4.79	9 (60%)
2	QC9	G	301	1	12,13,13	3.38	8 (66%)	15,18,18	4.93	10 (66%)
2	QC9	E	301	1	12,13,13	3.41	8 (66%)	15,18,18	4.79	9 (60%)
2	QC9	H	301	1	12,13,13	3.37	8 (66%)	15,18,18	4.93	10 (66%)
2	QC9	C	301	1	12,13,13	3.41	8 (66%)	15,18,18	4.79	9 (60%)
2	QC9	F	301	1	12,13,13	3.40	8 (66%)	15,18,18	4.80	9 (60%)
2	QC9	A	301	1	12,13,13	3.40	8 (66%)	15,18,18	4.79	9 (60%)
2	QC9	J	301	1	12,13,13	3.39	8 (66%)	15,18,18	4.93	10 (66%)

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	QC9	B	301	1	-	8/16/16/16	-
2	QC9	I	301	1	-	8/16/16/16	-
2	QC9	D	301	1	-	8/16/16/16	-
2	QC9	G	301	1	-	8/16/16/16	-
2	QC9	E	301	1	-	8/16/16/16	-
2	QC9	H	301	1	-	8/16/16/16	-
2	QC9	C	301	1	-	8/16/16/16	-
2	QC9	F	301	1	-	8/16/16/16	-
2	QC9	A	301	1	-	8/16/16/16	-
2	QC9	J	301	1	-	8/16/16/16	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	QC9	C1-C2	5.98	1.64	1.53
2	B	301	QC9	C1-C2	5.96	1.64	1.53
2	J	301	QC9	C1-C2	5.95	1.64	1.53
2	G	301	QC9	C1-C2	5.94	1.64	1.53
2	H	301	QC9	C1-C2	5.93	1.64	1.53

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	QC9	C3-C2-C1	11.86	138.02	113.36
2	F	301	QC9	C3-C2-C1	11.85	138.01	113.36
2	I	301	QC9	C3-C2-C1	11.85	138.01	113.36
2	A	301	QC9	C3-C2-C1	11.85	138.00	113.36
2	E	301	QC9	C3-C2-C1	11.84	138.00	113.36

There are no chirality outliers.

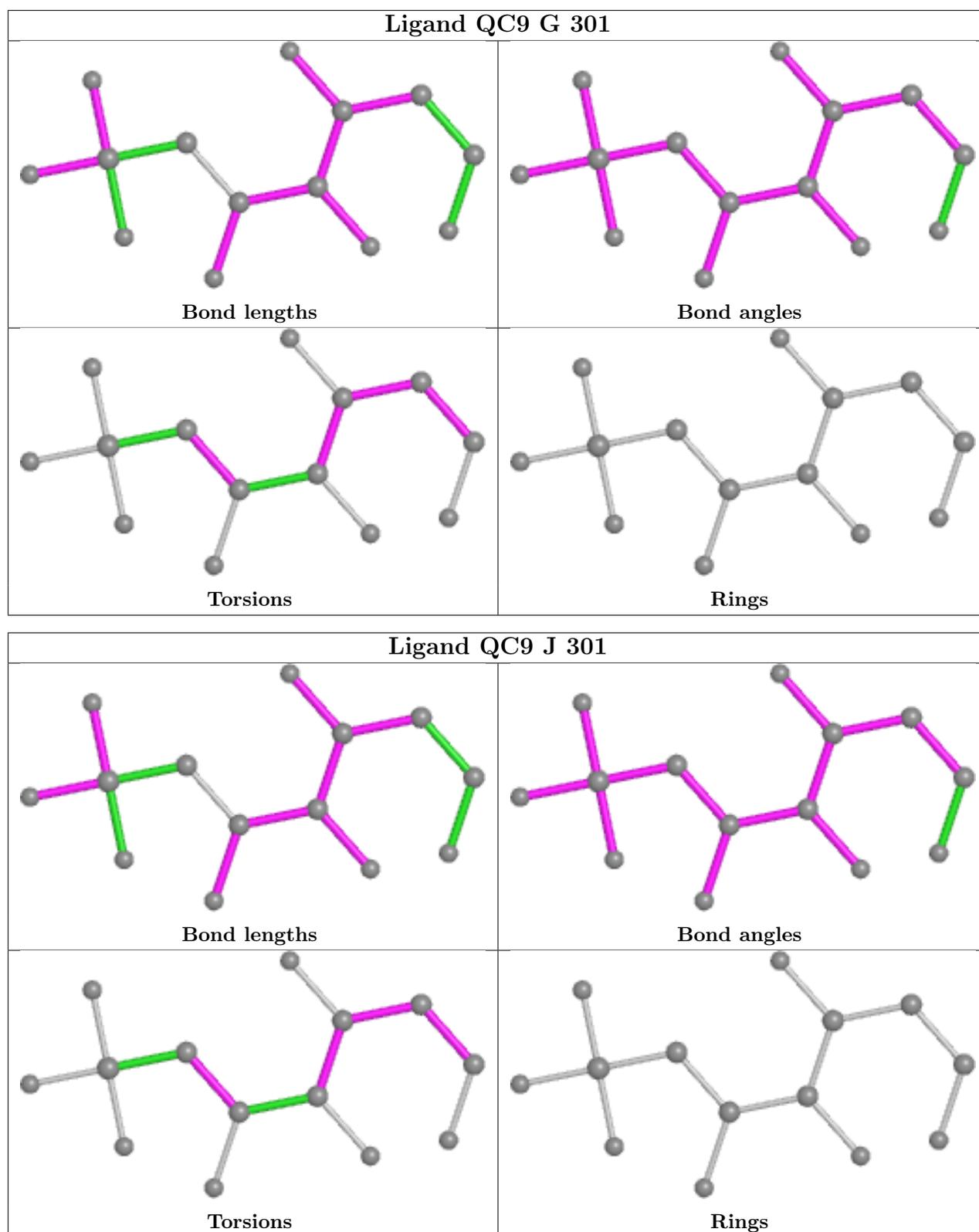
5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	QC9	C4-C1-C2-O6
2	A	301	QC9	O1-C1-C2-C3
2	A	301	QC9	O1-C1-C2-O6
2	A	301	QC9	C2-C1-C4-C5
2	A	301	QC9	S13-C12-C3-O7

There are no ring outliers.

No monomer is involved in short contacts.

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



#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Map visualisation

This section contains visualisations of the EMDB entry EMD-15961. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 5.1 Orthogonal projections

This section was not generated.

### 5.2 Central slices

This section was not generated.

### 5.3 Largest variance slices

This section was not generated.

### 5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 5.5 Orthogonal surface views

This section was not generated.

### 5.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 6 Map analysis

This section contains the results of statistical analysis of the map.

### 6.1 Map-value distribution

This section was not generated.

### 6.2 Volume estimate versus contour level

This section was not generated.

### 6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 7 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 8 Map-model fit

This section was not generated.