



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 01:27 AM EST

PDB ID : 6XL9
EMDB ID : EMD-22236
Title : Cryo-EM structure of EcmrR-RNAP-promoter initial transcribing complex with 3-nt RNA transcript (EcmrR-RPitc-3nt)
Authors : Yang, Y.; Liu, C.; Shi, W.; Liu, B.
Deposited on : 2020-06-28
Resolution : 2.50 Å(reported)
Based on initial model : 6OUL

This is a wwPDB EM 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/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>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), 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) : 2.31.2

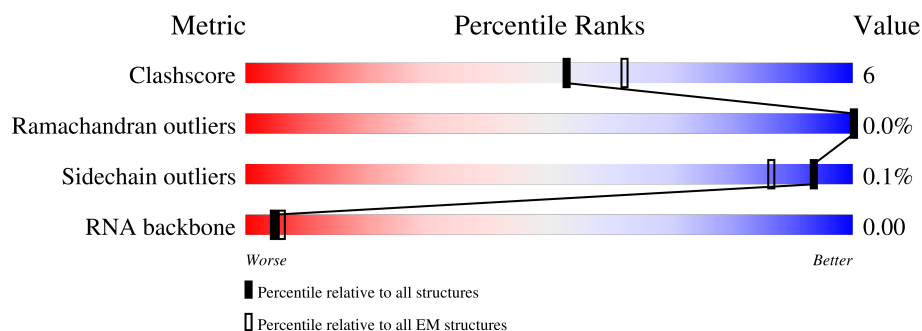
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1407	
4	F	613	
5	N	54	
6	R	3	

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Mol	Chain	Length	Quality of chain
7	T	54	<div><div></div><div>83%</div><div>17%</div></div>
8	G	268	<div><div></div><div>72%</div><div>28%</div></div>
8	H	268	<div><div></div><div>78%</div><div>22%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 35113 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		
1	B	229	Total	C	N	O	S	0	0
			1774	1105	313	350	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1339	Total	C	N	O	S	0	0
			10560	6626	1840	2051	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1338	Total	C	N	O	S	0	0
			10398	6532	1854	1962	50		

- Molecule 4 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	465	Total	C	N	O	S	0	0
			3789	2369	682	715	23		

- Molecule 5 is a DNA chain called synthetic non-template strand DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	54	Total	C	N	O	P	0	0
			1109	526	203	327	53		

- Molecule 6 is a RNA chain called RNA (5'-D*(GTP))-R(P*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	3	Total	C	N	O	P	0	0
			77	30	15	27	5		

- Molecule 7 is a DNA chain called synthetic template strand DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	54	Total	C	N	O	P	0	0
			1104	523	209	319	53		

- Molecule 8 is a protein called MerR family transcriptional regulator EcmrR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	268	Total	C	N	O	S	0	0
			2208	1423	368	404	13		
8	H	268	Total	C	N	O	S	0	0
			2208	1423	368	404	13		

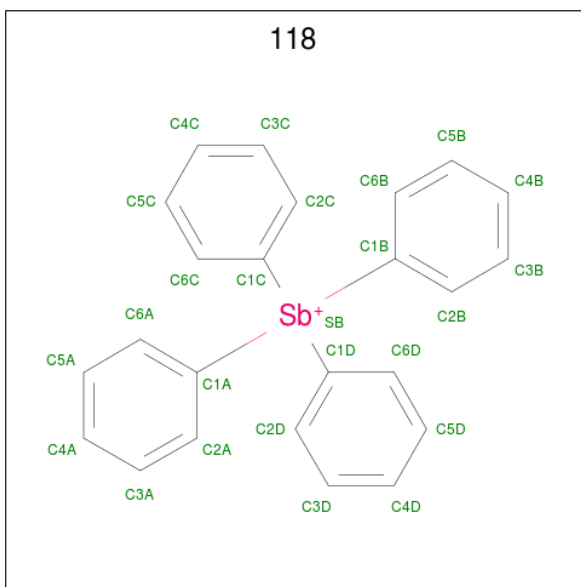
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	
10	R	1	Total	Mg	0
			1	1	

- Molecule 11 is TETRAPHENYLANTIMONIUM ION (three-letter code: 118) (formula: C₂₄H₂₀Sb) (labeled as "Ligand of Interest" by depositor).

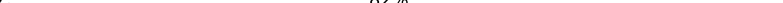


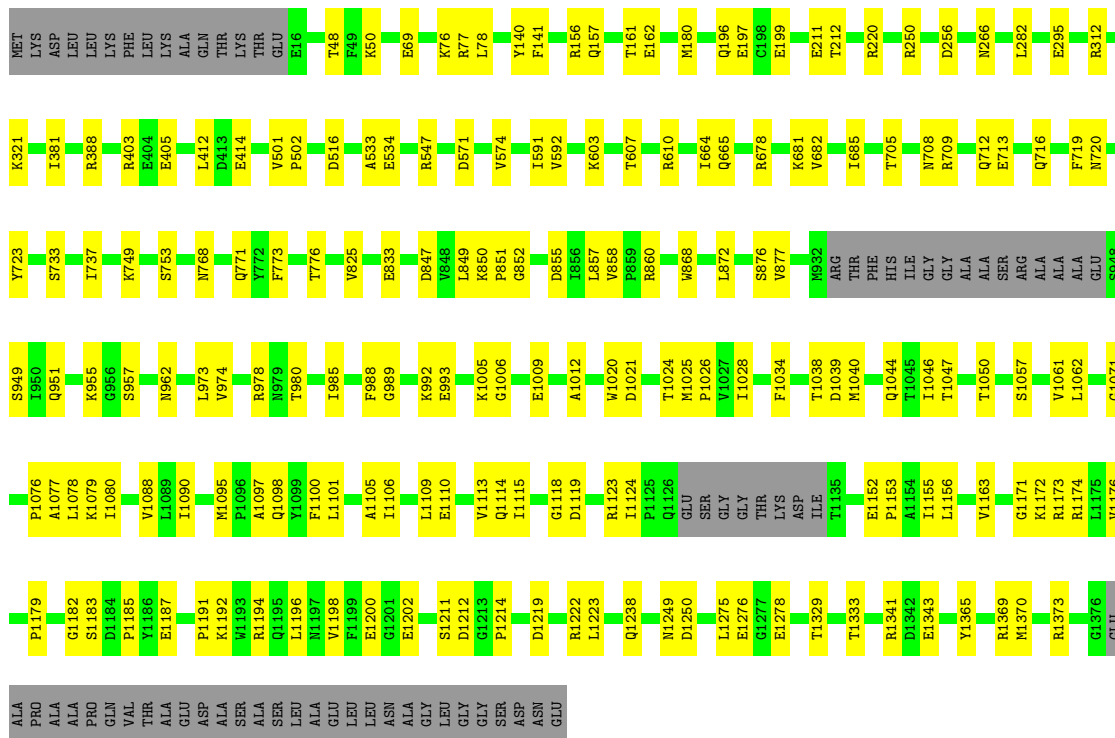
Mol	Chain	Residues	Atoms			AltConf
11	F	1	Total	C	Sb	0
			25	24	1	
11	G	1	Total	C	Sb	0
			25	24	1	
11	H	1	Total	C	Sb	0
			25	24	1	

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	C	8	Total	O	0
			8	8	
12	D	10	Total	O	0
			10	10	
12	T	3	Total	O	0
			3	3	

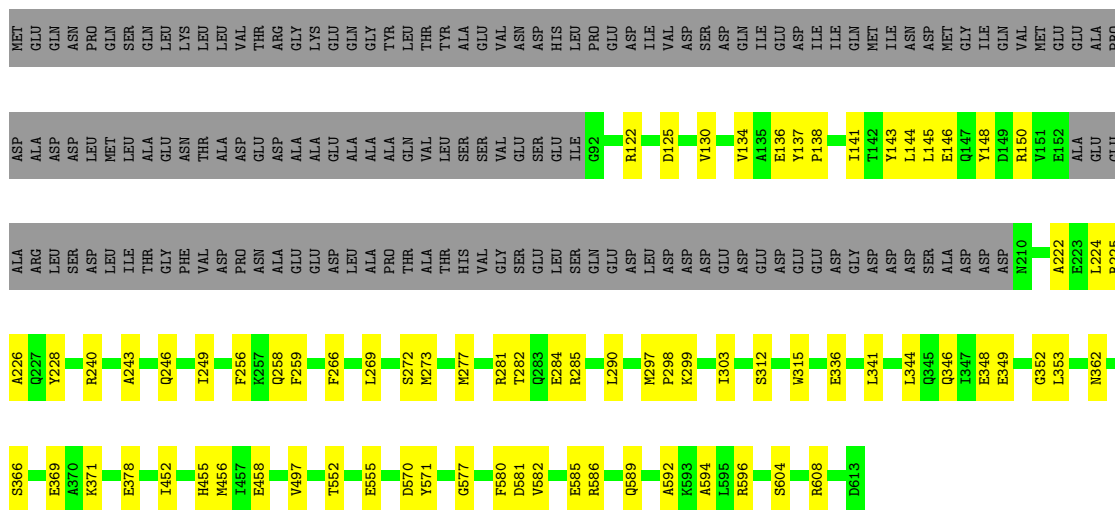
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:  82% 13% 5%



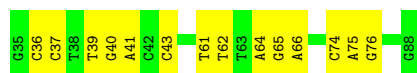
- Molecule 4: RNA polymerase sigma factor RpoD

Chain F:  63% 12% 24%



- Molecule 5: synthetic non-template strand DNA (54-MER)

Chain N:  74% 26%




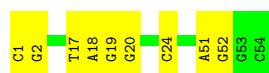
- Molecule 6: RNA (5'-D*(GTP))-R(P*AP*G)-3')

Chain R:  100%

There are no outlier residues recorded for this chain.

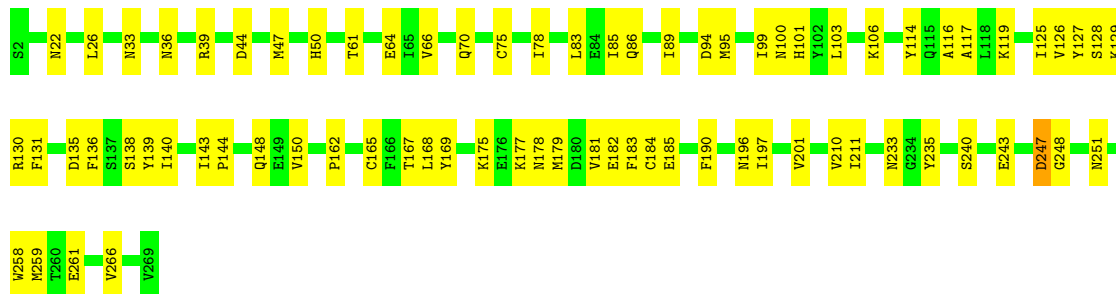
- Molecule 7: synthetic template strand DNA (54-MER)

Chain T:  83% 17%




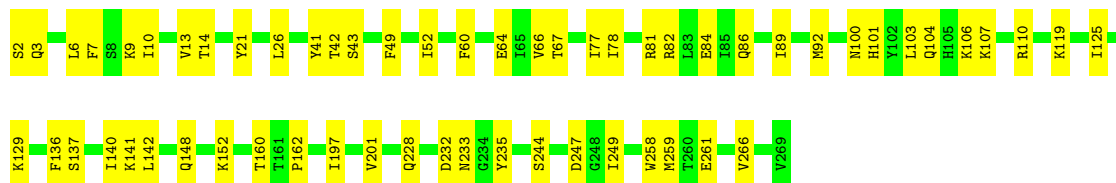
- Molecule 8: MerR family transcriptional regulator EcmrR

Chain G:  72% 28%



- Molecule 8: MerR family transcriptional regulator EcmrR

Chain H:  78% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, 118, ZN

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	0.40	0/1808	0.55	0/2450
1	B	0.33	0/1796	0.51	0/2435
2	C	0.43	0/10729	0.53	0/14477
3	D	0.41	0/10555	0.55	0/14251
4	F	0.32	0/3841	0.54	0/5161
5	N	0.82	0/1243	0.97	0/1919
6	R	1.20	0/50	1.10	0/76
7	T	0.87	0/1239	0.93	0/1910
8	G	0.33	0/2260	0.62	0/3058
8	H	0.33	0/2260	0.66	0/3058
All	All	0.44	0/35781	0.59	0/48795

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1786	0	1813	21	0
1	B	1774	0	1798	14	0
2	C	10560	0	10576	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10398	0	10617	122	0
4	F	3789	0	3860	51	0
5	N	1109	0	609	12	0
6	R	77	0	34	0	0
7	T	1104	0	605	5	0
8	G	2208	0	2209	57	0
8	H	2208	0	2209	45	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
10	R	1	0	0	0	0
11	F	25	0	20	1	0
11	G	25	0	20	3	0
11	H	25	0	20	1	0
12	C	8	0	0	0	0
12	D	10	0	0	0	0
12	T	3	0	0	0	0
All	All	35113	0	34390	389	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 6.

The worst 5 of 389 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)
4:F:580:PHE:HB3	4:F:582:VAL:HG23	1.52	0.92
3:D:1171:GLY:O	3:D:1172:LYS:HG3	1.83	0.78
11:G:301:118:H6A	11:G:301:118:H6C	1.66	0.76
3:D:847:ASP:HA	3:D:858:VAL:HG21	1.69	0.74
3:D:1047:THR:HG23	3:D:1062:LEU:HD21	1.67	0.74

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 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	228/329 (69%)	228 (100%)	0	0	100	100
1	B	227/329 (69%)	224 (99%)	3 (1%)	0	100	100
2	C	1337/1342 (100%)	1319 (99%)	17 (1%)	1 (0%)	51	73
3	D	1332/1407 (95%)	1319 (99%)	12 (1%)	1 (0%)	51	73
4	F	461/613 (75%)	451 (98%)	10 (2%)	0	100	100
8	G	266/268 (99%)	266 (100%)	0	0	100	100
8	H	266/268 (99%)	265 (100%)	1 (0%)	0	100	100
All	All	4117/4556 (90%)	4072 (99%)	43 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	399	ALA
3	D	851	PRO

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 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	198/286 (69%)	198 (100%)	0	100	100
1	B	197/286 (69%)	197 (100%)	0	100	100
2	C	1154/1157 (100%)	1153 (100%)	1 (0%)	93	98
3	D	1120/1168 (96%)	1120 (100%)	0	100	100
4	F	414/540 (77%)	413 (100%)	1 (0%)	93	98
8	G	245/245 (100%)	244 (100%)	1 (0%)	91	97
8	H	245/245 (100%)	245 (100%)	0	100	100
All	All	3573/3927 (91%)	3570 (100%)	3 (0%)	93	98

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

Mol	Chain	Res	Type
2	C	1040	ASP
4	F	148	TYR
8	G	247	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	979	ASN
4	F	461	ASN
3	D	1197	ASN
4	F	362	ASN
4	F	579	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	1/3 (33%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
11	118	G	301	-	28,28,28	0.69	0	24,38,38	0.26	0
11	118	H	301	-	28,28,28	0.68	0	24,38,38	0.27	0
11	118	F	701	-	28,28,28	0.63	0	24,38,38	0.31	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
11	118	G	301	-	-	-	0/4/4/4
11	118	H	301	-	-	-	0/4/4/4
11	118	F	701	-	-	-	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

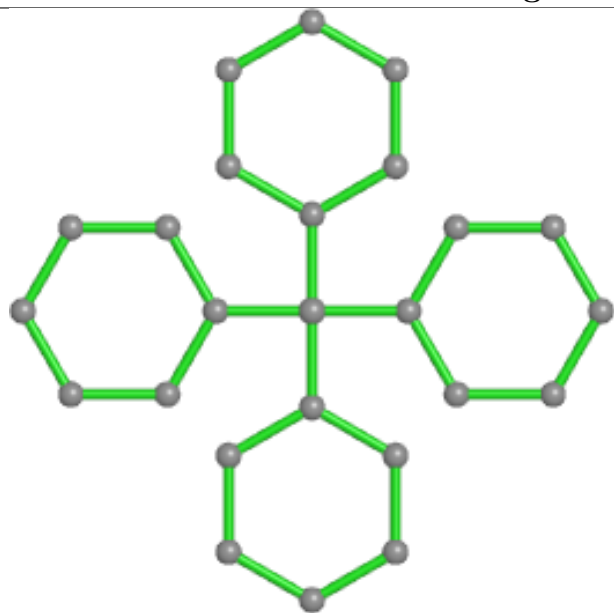
There are no ring outliers.

3 monomers are involved in 5 short contacts:

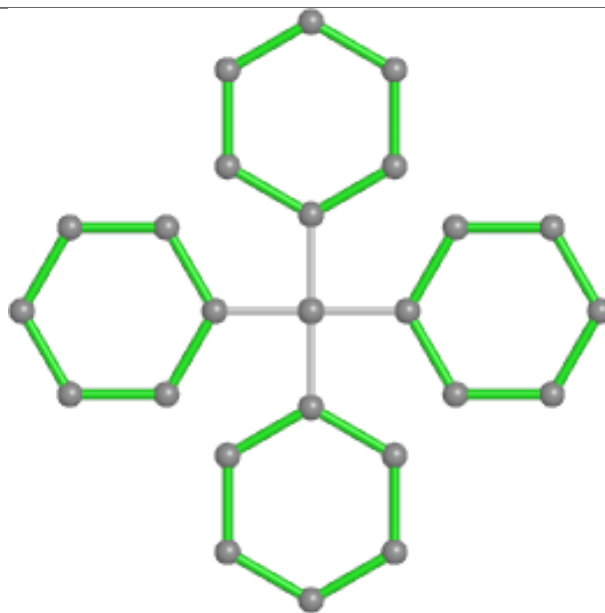
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	301	118	3	0
11	H	301	118	1	0
11	F	701	118	1	0

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.

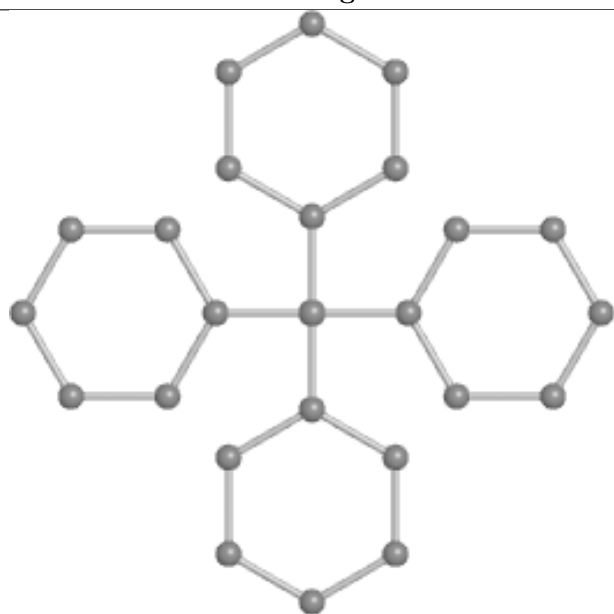
Ligand 118 G 301



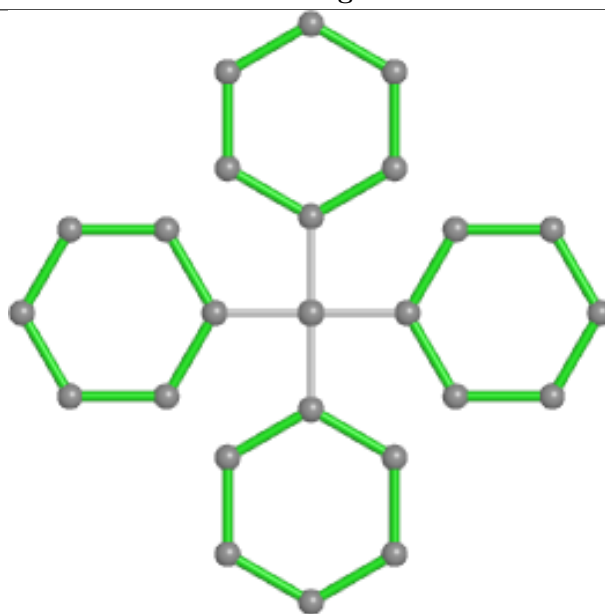
Bond lengths



Bond angles

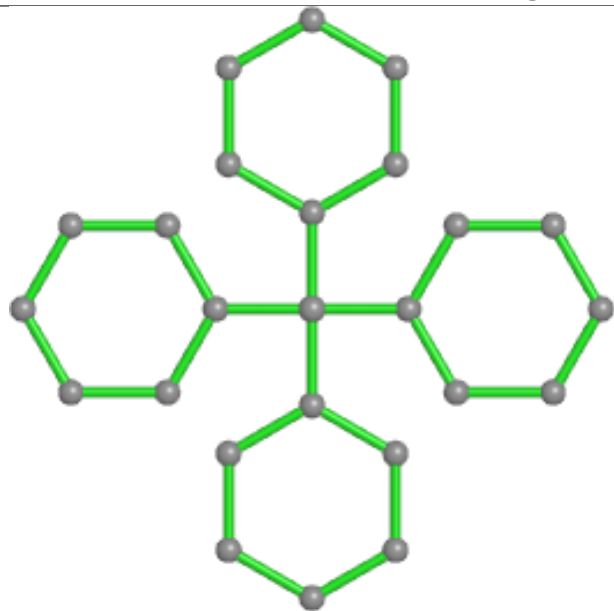


Torsions

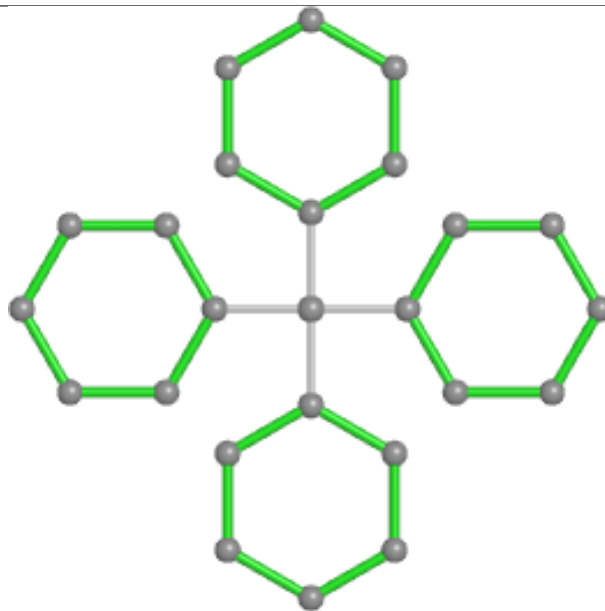


Rings

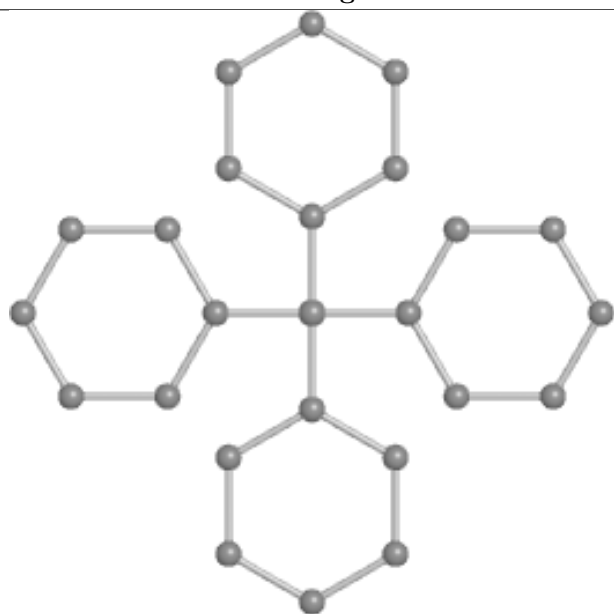
Ligand 118 H 301



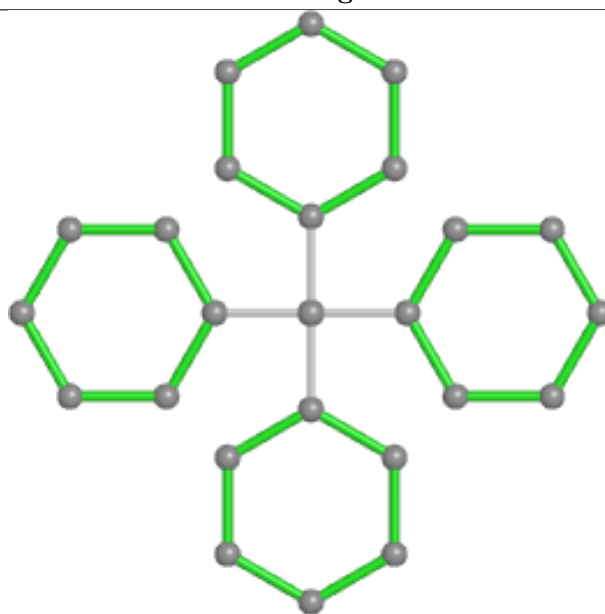
Bond lengths



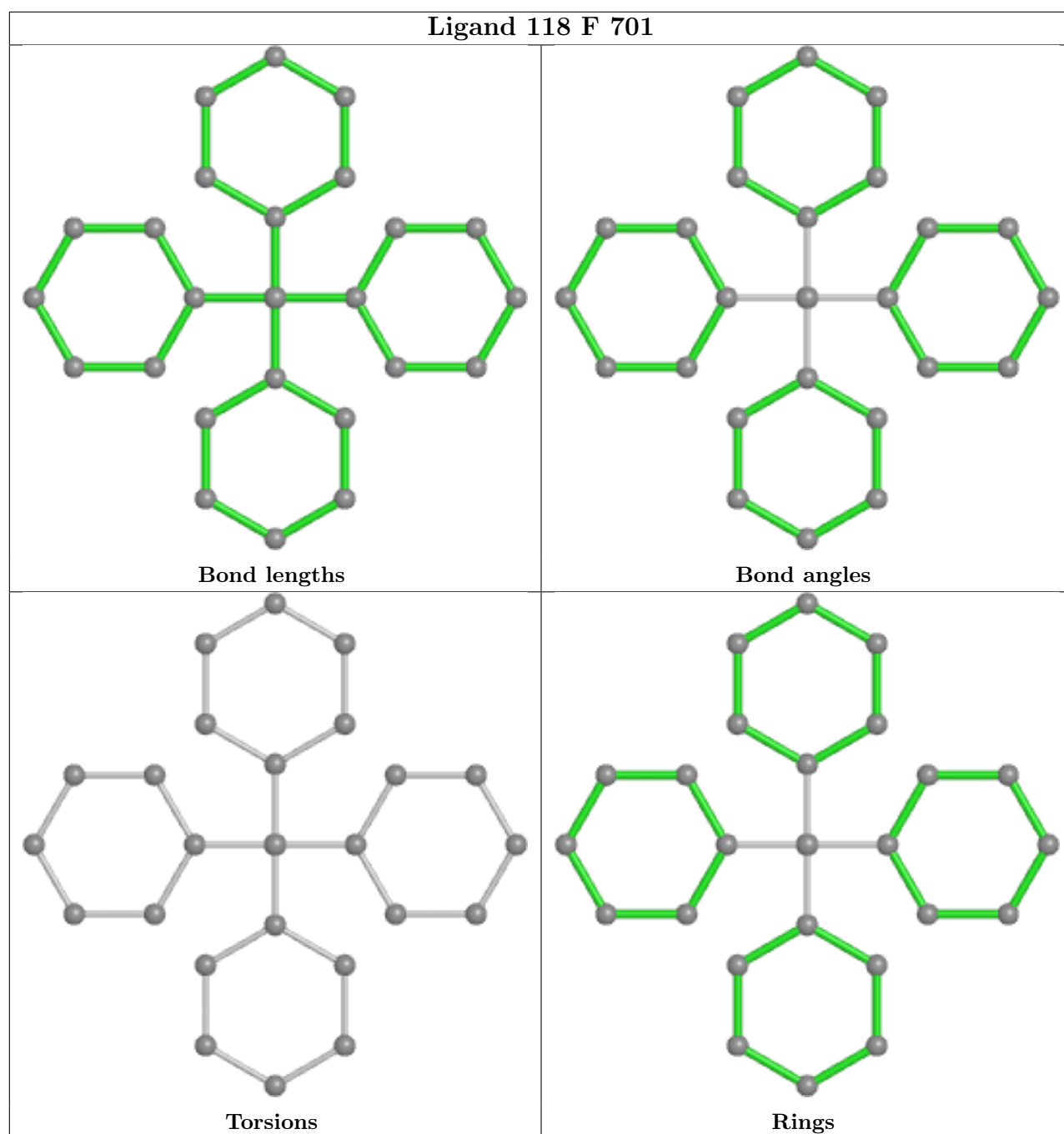
Bond angles



Torsions



Rings



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-22236. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.