



wwPDB EM Validation Summary Report ⓘ

Aug 25, 2024 – 12:12 AM JST

PDB ID : 8XUQ
EMDB ID : EMD-38680
Title : Cryo-EM structure of tomato NRC2 tetramer
Authors : Sun, Y.; Ma, S.C.; Chai, J.J.
Deposited on : 2024-01-14
Resolution : 3.17 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

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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

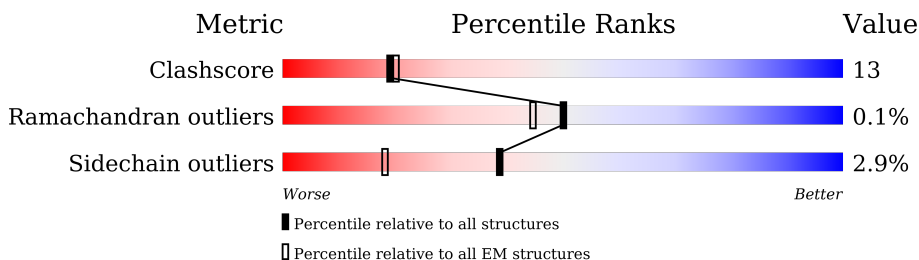
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	885	76%	24%
1	E	885	75%	24%
1	F	885	70%	29%
1	G	885	69%	31%

2 Entry composition [i](#)

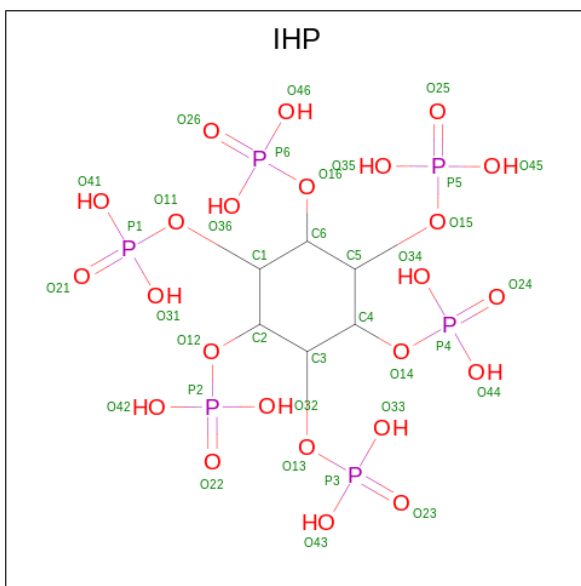
There are 3 unique types of molecules in this entry. The entry contains 28736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NRC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	E	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	F	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	G	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



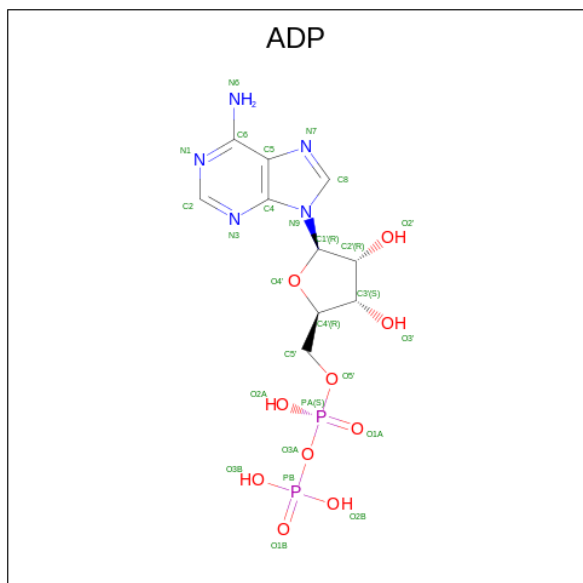
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	Total 36	C 6	O 24	P 6	0
2	E	1	Total 36	C 6	O 24	P 6	0

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Mol	Chain	Residues	Atoms				AltConf
2	F	1	Total	C	O	P	0
			36	6	24	6	
2	G	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

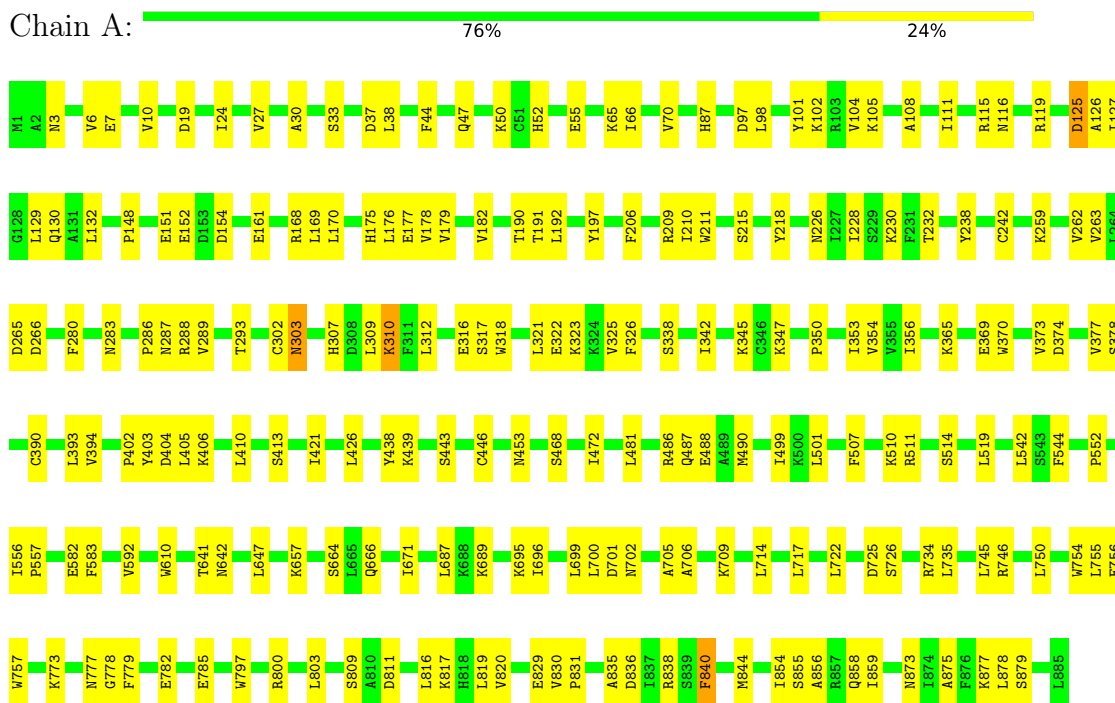


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

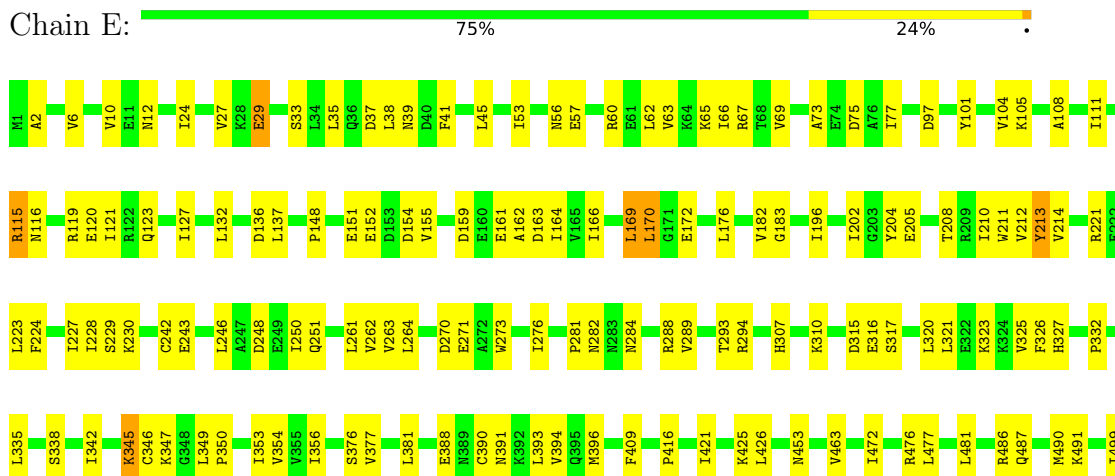
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NRC2



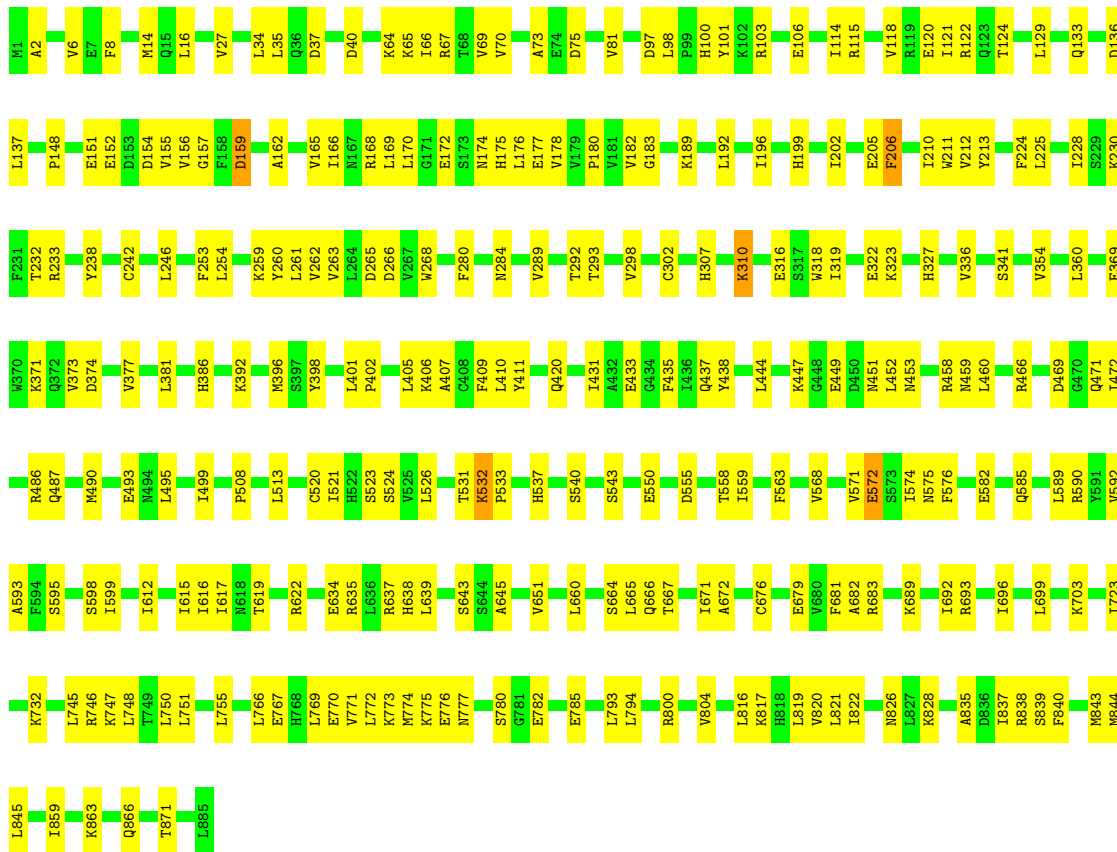
- Molecule 1: NRC2





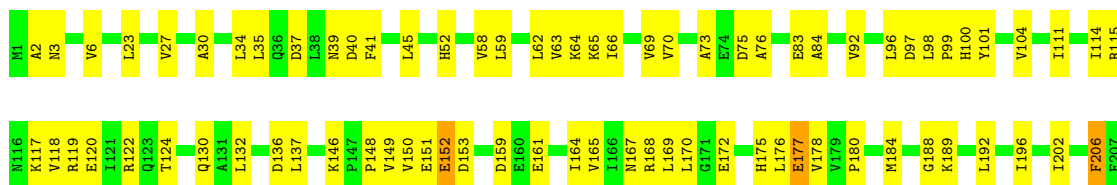
● Molecule 1: NRC2

Chain F: 70% 29%



● Molecule 1: NRC2

Chain G: 69% 31%



N826	L827	K828	E829	V830	P831	A835	M843	M844	L845	T851	A856	R857	Q858	I859	Q866	K877	L878	S879	I880	L885																												
S704	A705	V711	N719	L720	K721	L733	L745	R746	K747	L748	T749	L750	D752	T753	W754	L755	L769	K773	M774	K775	E776	N777	G778	F779	S780	G781	E782	E785	W797	I798	E799	R800	V804	S805	S809	A810	D811	D812	F813	L816	L819	W820	L821	I822	D825			
T558	D570	V571	E572	N575	E582	R590	S595	S596	I599	I612	I615	R622	D625	I626	Q627	M633	L636	A645	L660	V661	N662	Q663	S664	L665	Q666	T667	A672	T677	E678	E679	V680	F681	A682	R683	K689	I692	S697	V698	L699									
F435	E445	L452	L455	I456	V463	M464	E465	R466	D469	C475	M480	L481	H482	E483	F484	C485	R486	A489	M490	Q497	E498	I499	A500	L501	E504	F507	R517	I521	V525	T531	H537	F541	L542	S543	F544	I549	E550	M551	D555									
H307	K310	W318	I319	L320	K323	H327	K328	D329	K330	V336	S341	I342	P350	I353	I356	E369	V373	D374	H380	L381	C390	N391	K392	L393	V394	Q395	M396	S397	Y398	D399	R400	D404	L405	K406	A407	C408	F409	L410	P416	I421	L426							
T208	R209	I210	W211	V212	S215	Q216	S217	Y218	F224	I228	Y238	E244	Q251	E252	F253	L254	Y260	L261	V262	V263	L264	D265	D266	V267	W273	E274	R275	I276	K277	I278	F280	P281	N282	M287	R288	V289	L290	L291	T292	T293	R294	D295	S296	C302	M303	P304	I305	P306

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154084	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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: ADP, IHP

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	0/7260	0.54	0/9803
1	E	0.29	0/7260	0.53	0/9803
1	F	0.28	0/7260	0.53	0/9803
1	G	0.30	0/7260	0.53	0/9803
All	All	0.29	0/29040	0.53	0/39212

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 [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	7121	0	7283	157	0
1	E	7121	0	7283	159	0
1	F	7121	0	7283	196	0
1	G	7121	0	7283	216	0
2	A	36	0	6	1	0
2	E	36	0	6	0	0
2	F	36	0	6	1	0
2	G	36	0	6	0	0
3	A	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	27	0	12	1	0
3	F	27	0	12	1	0
3	G	27	0	12	3	0
All	All	28736	0	29204	725	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 13.

The worst 5 of 725 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:E:169:LEU:HD12	1:E:170:LEU:HG	1.39	1.04
1:G:169:LEU:HD12	1:G:170:LEU:HG	1.38	1.03
1:E:880:ILE:HG22	1:E:882:PRO:HD2	1.59	0.85
1:G:175:HIS:HE1	1:G:177:GLU:HG2	1.42	0.83
1:G:175:HIS:CE1	1:G:177:GLU:HG2	2.15	0.80

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	883/885 (100%)	847 (96%)	36 (4%)	0	100	100
1	E	883/885 (100%)	850 (96%)	32 (4%)	1 (0%)	48	78
1	F	883/885 (100%)	851 (96%)	32 (4%)	0	100	100
1	G	883/885 (100%)	840 (95%)	42 (5%)	1 (0%)	48	78
All	All	3532/3540 (100%)	3388 (96%)	142 (4%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	170	LEU
1	G	148	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	797/797 (100%)	780 (98%)	17 (2%)	48	72
1	E	797/797 (100%)	766 (96%)	31 (4%)	27	57
1	F	797/797 (100%)	776 (97%)	21 (3%)	41	68
1	G	797/797 (100%)	774 (97%)	23 (3%)	37	65
All	All	3188/3188 (100%)	3096 (97%)	92 (3%)	39	65

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	471	GLN
1	G	146	LYS
1	F	532	LYS
1	F	643	SER
1	G	189	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	15	GLN
1	F	174	ASN
1	G	451	ASN
1	G	175	HIS
1	A	818	HIS

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IHP	A	901	-	36,36,36	1.52	6 (16%)	54,60,60	0.95	5 (9%)
2	IHP	G	901	-	36,36,36	1.48	6 (16%)	54,60,60	0.57	0
2	IHP	E	901	-	36,36,36	1.52	6 (16%)	54,60,60	0.93	3 (5%)
3	ADP	F	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.38	3 (10%)
3	ADP	E	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.37	3 (10%)
2	IHP	F	901	-	36,36,36	1.52	6 (16%)	54,60,60	0.91	2 (3%)
3	ADP	A	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.40	5 (17%)
3	ADP	G	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)

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	IHP	A	901	-	-	9/30/54/54	0/1/1/1
2	IHP	G	901	-	-	7/30/54/54	0/1/1/1
2	IHP	E	901	-	-	11/30/54/54	0/1/1/1
3	ADP	F	902	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	E	902	-	-	5/12/32/32	0/3/3/3
2	IHP	F	901	-	-	10/30/54/54	0/1/1/1
3	ADP	A	902	-	-	4/12/32/32	0/3/3/3
3	ADP	G	902	-	-	6/12/32/32	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	IHP	P3-O13	3.50	1.65	1.59
2	F	901	IHP	P5-O15	3.41	1.65	1.59
2	F	901	IHP	P3-O13	3.36	1.65	1.59
2	E	901	IHP	P5-O15	3.35	1.65	1.59
2	A	901	IHP	P5-O15	3.29	1.65	1.59

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	902	ADP	PA-O3A-PB	-3.86	119.57	132.83
2	F	901	IHP	C5-C6-C1	3.78	118.68	110.41
3	G	902	ADP	N3-C2-N1	-3.60	123.05	128.68
3	E	902	ADP	N3-C2-N1	-3.59	123.06	128.68
3	A	902	ADP	N3-C2-N1	-3.57	123.09	128.68

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	IHP	C2-C1-O11-P1
2	A	901	IHP	C6-C1-O11-P1
2	A	901	IHP	C4-C3-O13-P3
2	A	901	IHP	C1-O11-P1-O21
2	A	901	IHP	C6-O16-P6-O26

There are no ring outliers.

6 monomers are involved in 9 short contacts:

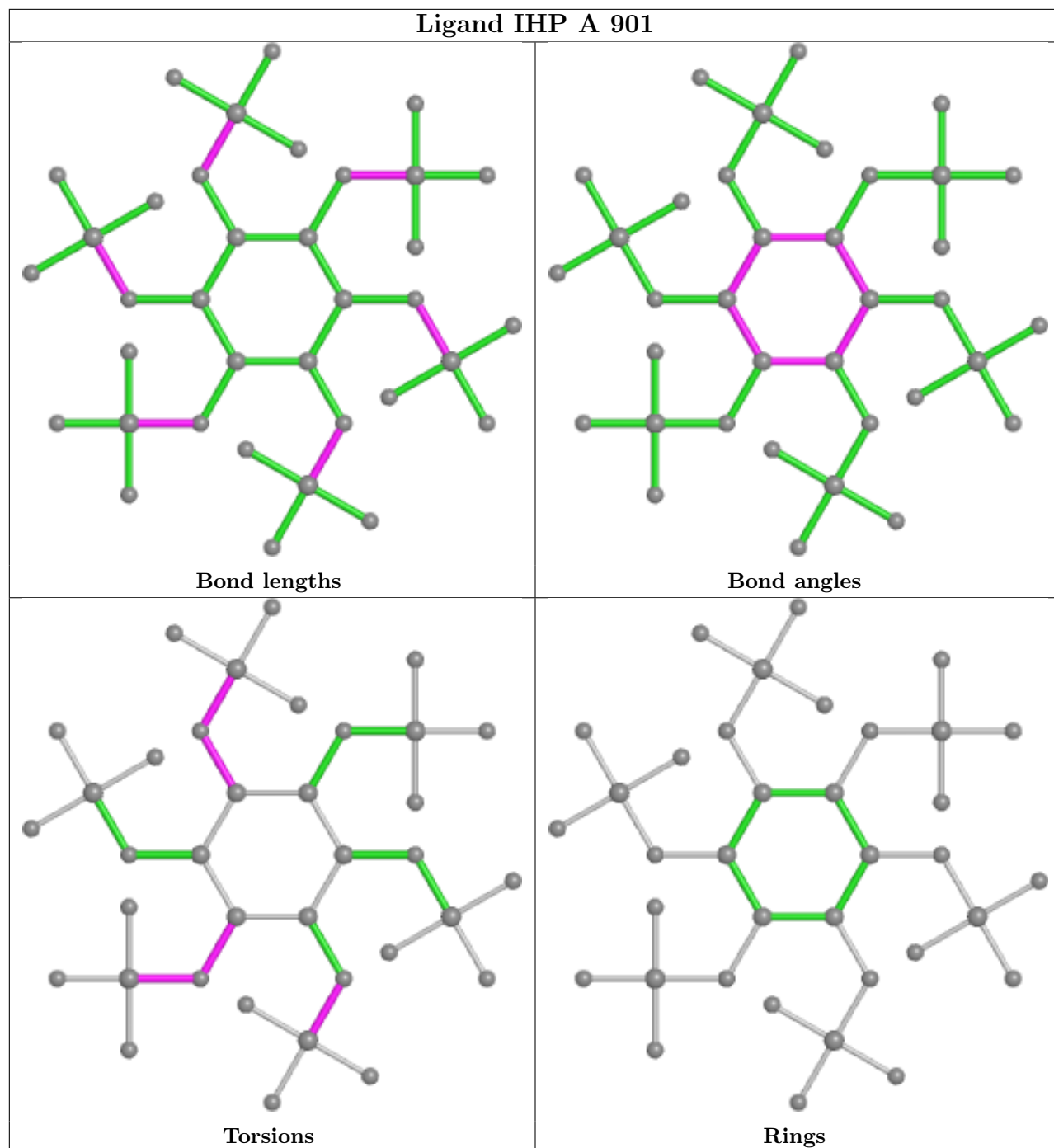
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	IHP	1	0
3	F	902	ADP	1	0
3	E	902	ADP	1	0

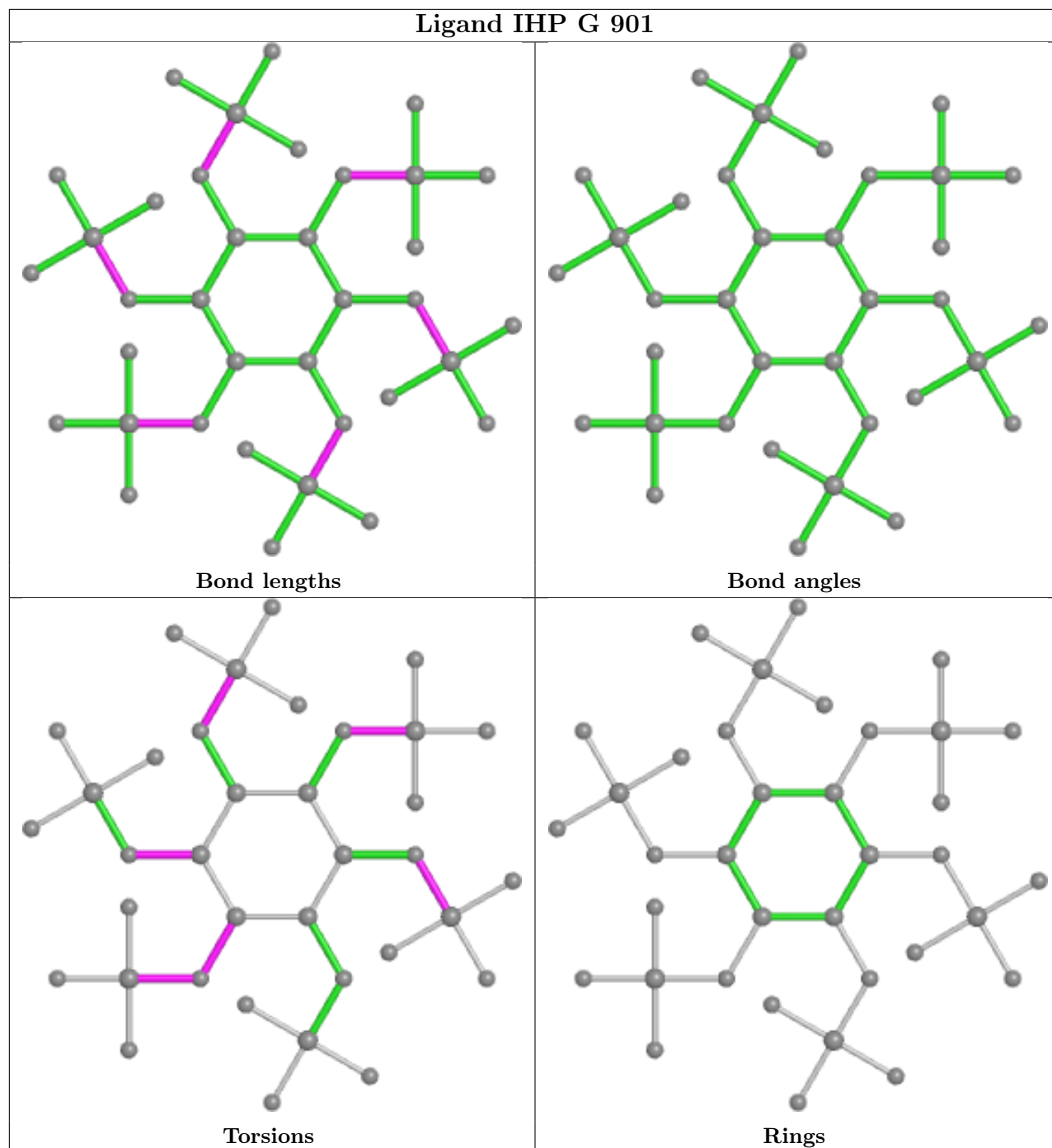
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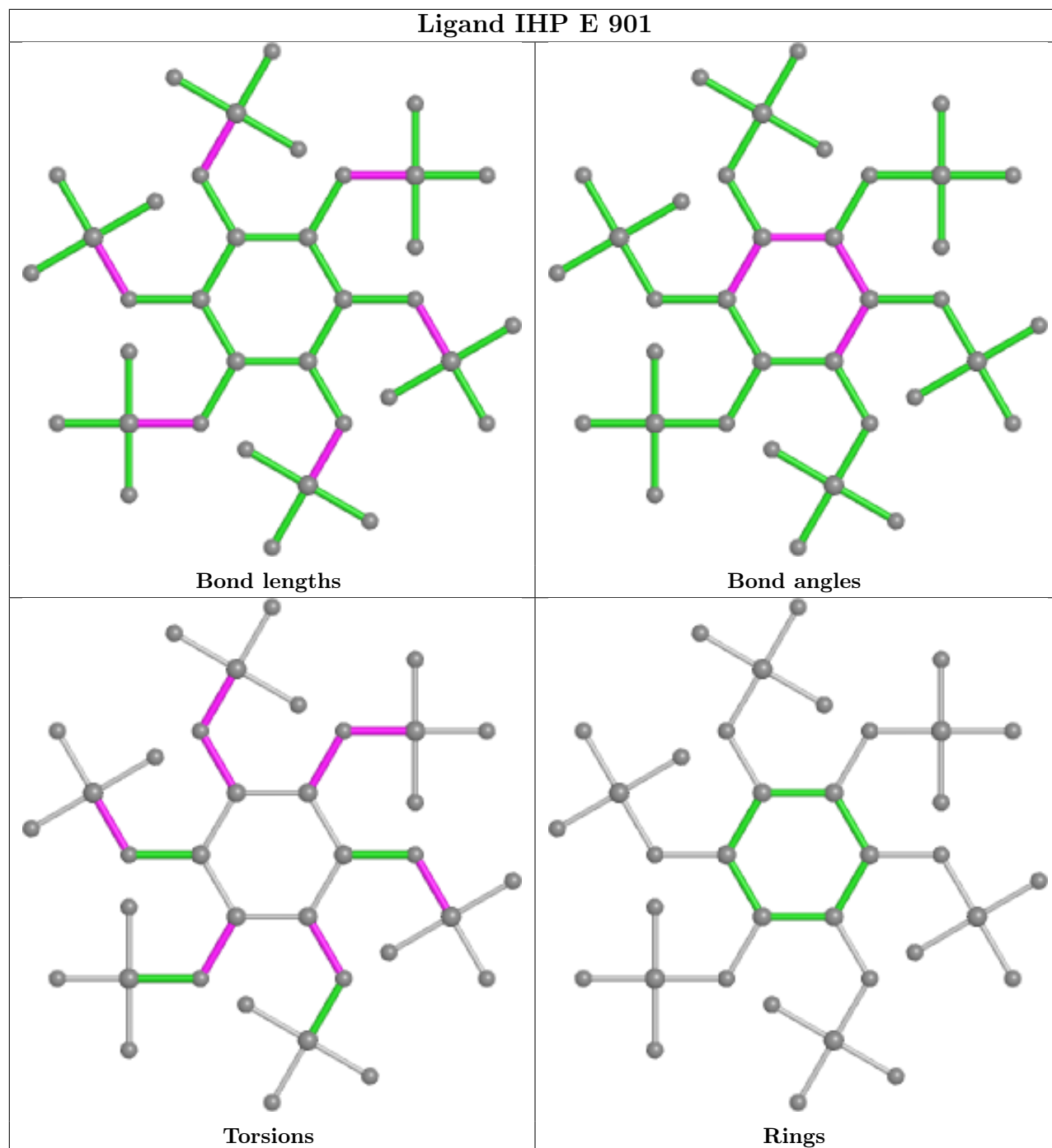
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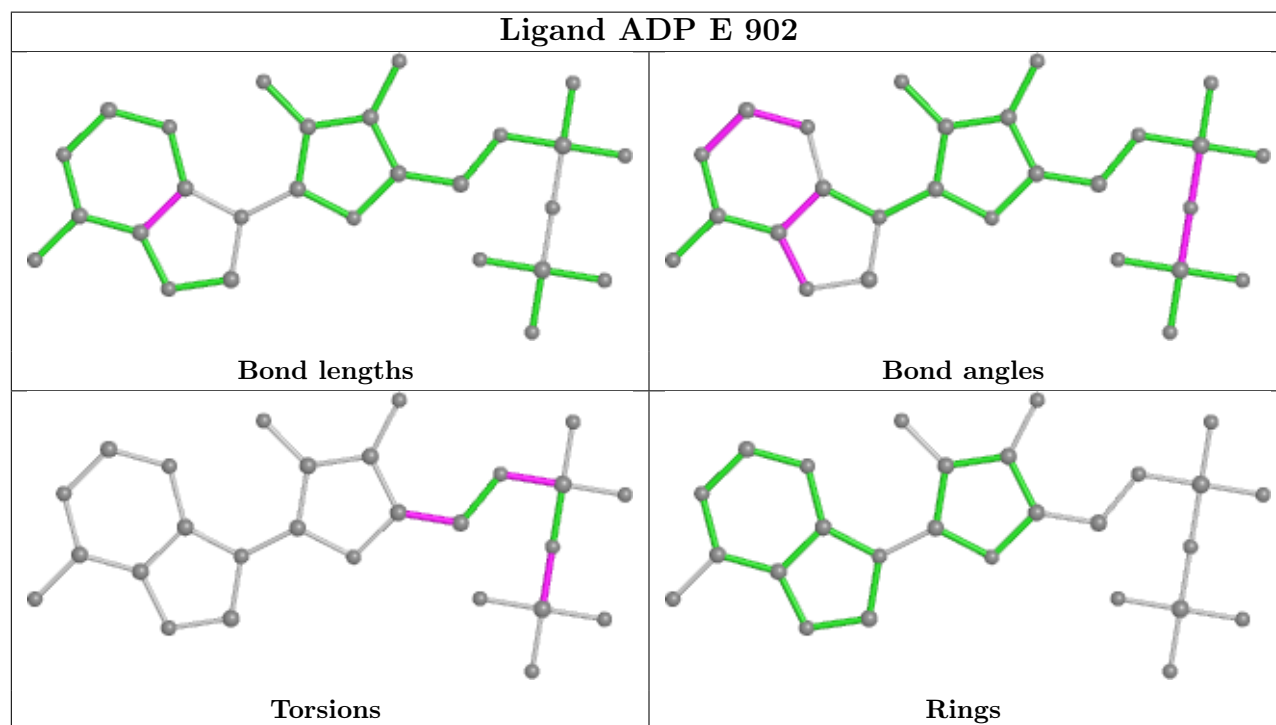
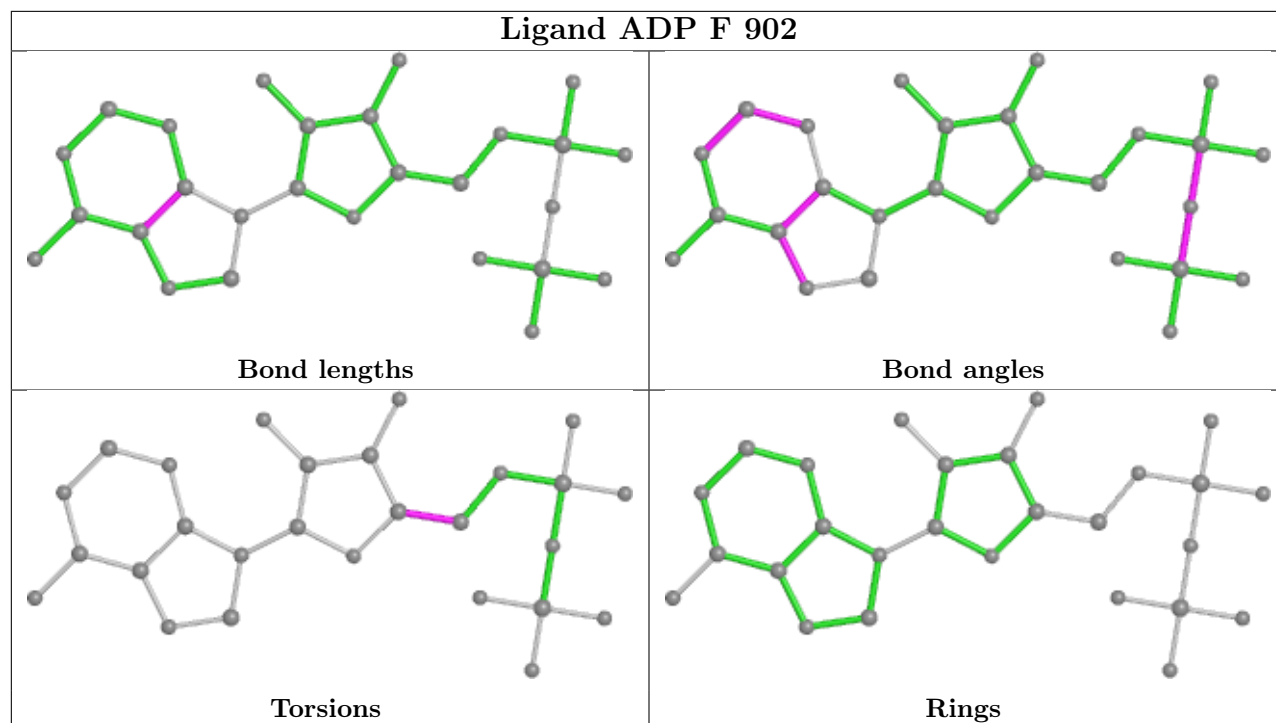
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	IHP	1	0
3	A	902	ADP	2	0
3	G	902	ADP	3	0

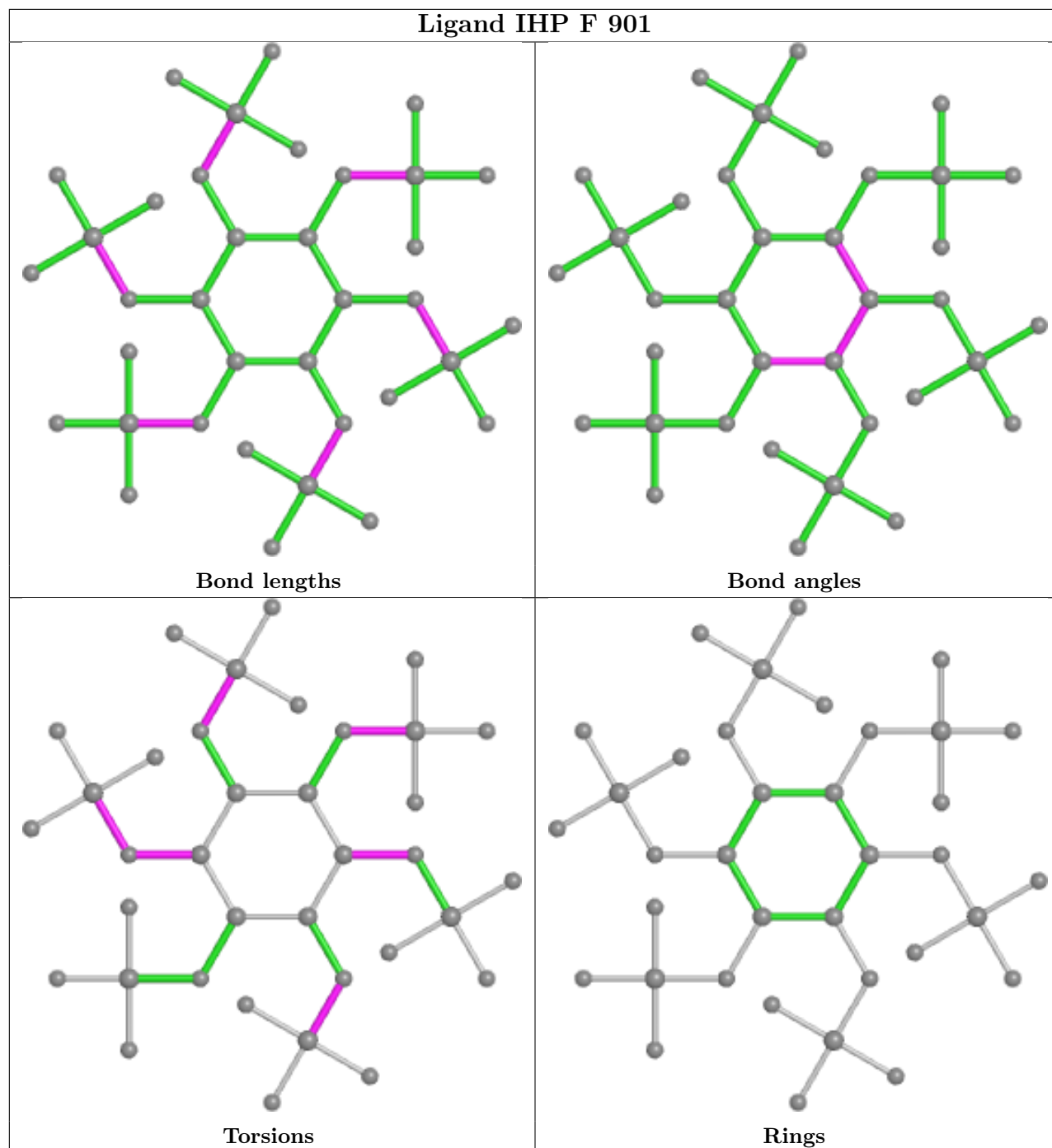
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

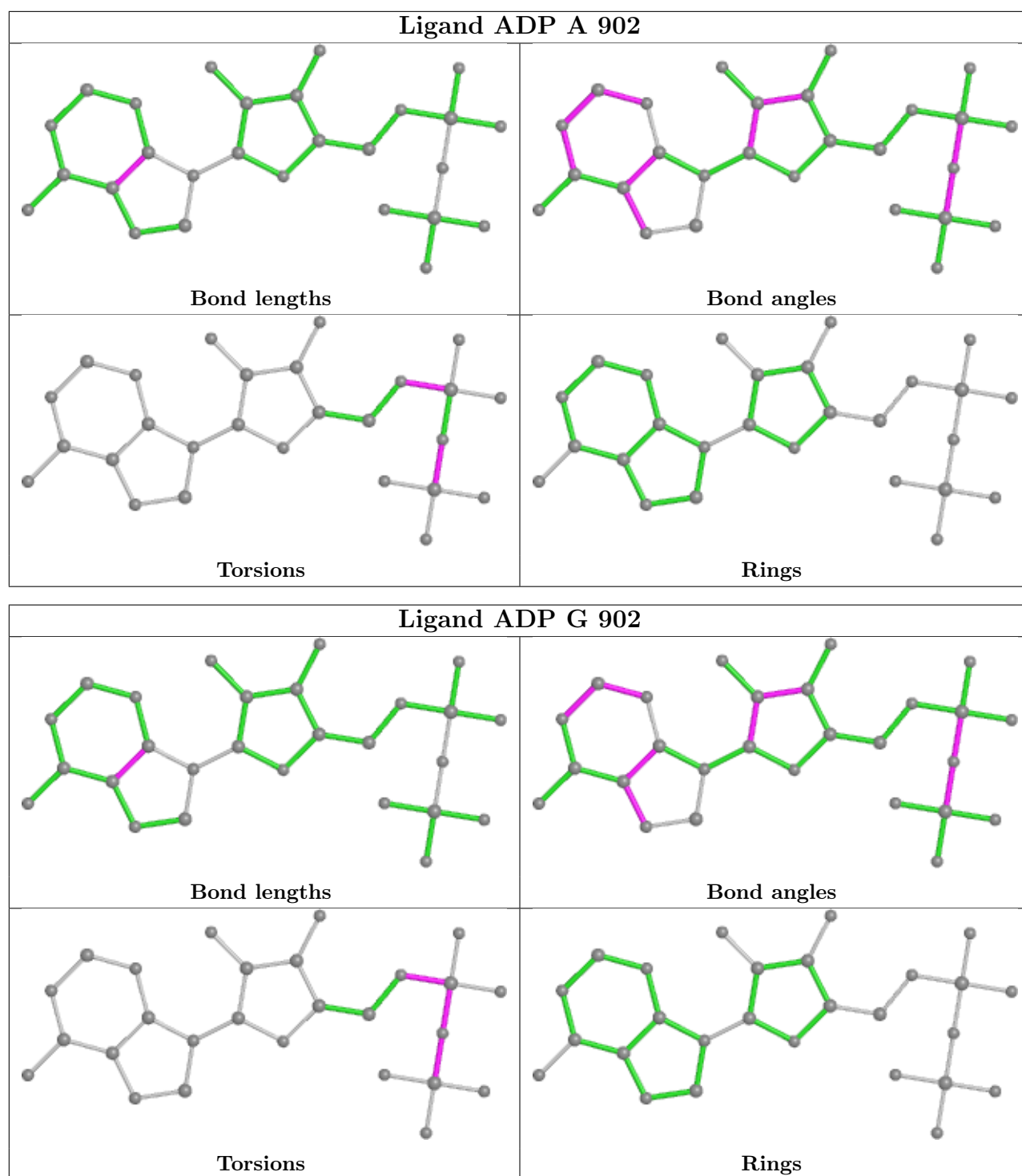












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.