



wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:33 PM JST

PDB ID : 8JXP
EMDB ID : EMD-36708
Title : Cryo-EM structure of BICHR2 class one
Authors : Zhang, M.F.
Deposited on : 2023-07-01
Resolution : 2.70 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)	: 2.39

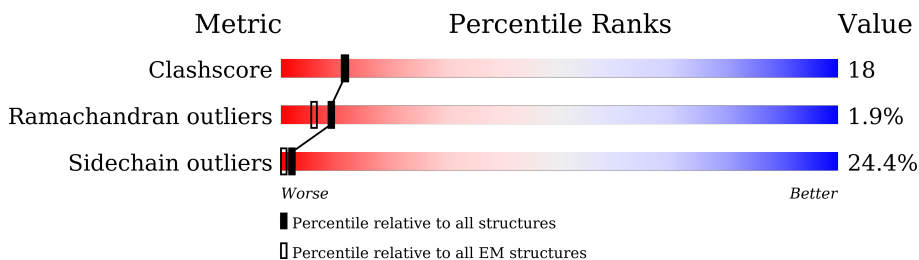
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	391	
1	B	391	
1	C	391	

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
3	RET	A	407	-	-	X	-
3	RET	B	407	-	-	X	-
3	RET	C	407	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6294 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.

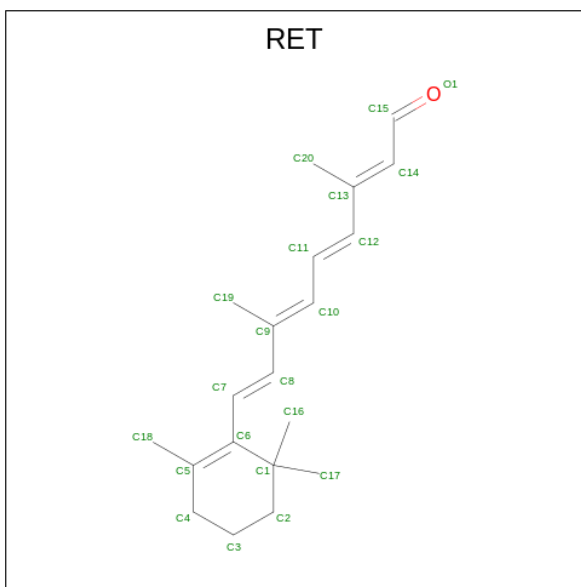
- Molecule 1 is a protein called BICHR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	262	Total	C	N	O	S	0	0
			2069	1372	318	365	14		
1	B	262	Total	C	N	O	S	0	0
			2069	1372	318	365	14		
1	C	262	Total	C	N	O	S	0	0
			2069	1372	318	365	14		

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	6	Total	K	0
			6	6	
2	B	6	Total	K	0
			6	6	
2	C	6	Total	K	0
			6	6	

- Molecule 3 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C 20 20	0
3	B	1	Total C 20 20	0
3	C	1	Total C 20 20	0

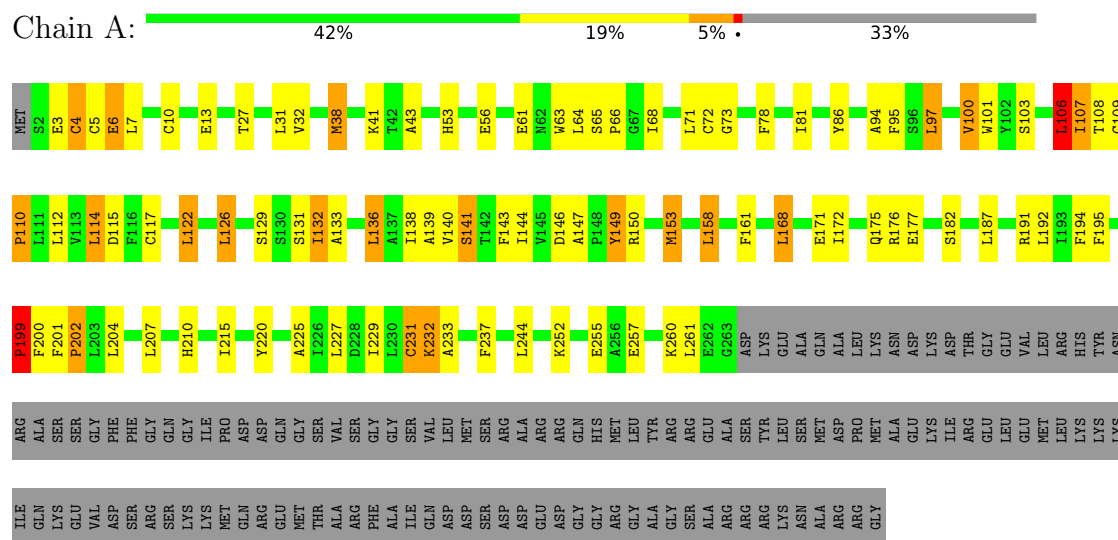
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total O 3 3	0
4	B	3	Total O 3 3	0
4	C	3	Total O 3 3	0

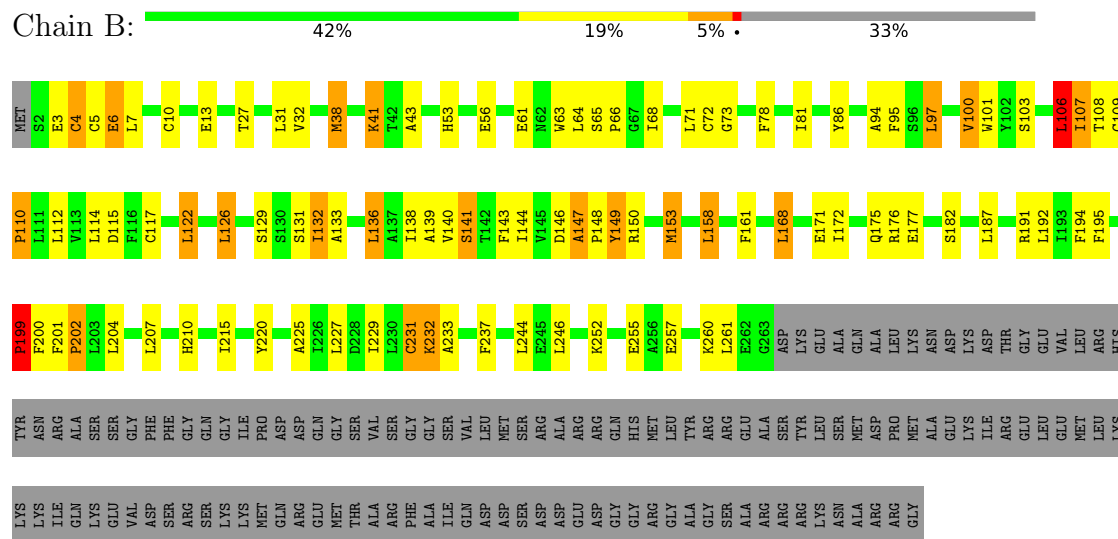
3 Residue-property plots

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: BICHR2



• Molecule 1: BICHR2



• Molecule 1: BICHR2



LYS	ASN	P199	Cl09	Met
ILE	ARG	F200	P110	S2
GLN	ALA	F201	L111	E3
LYS	SER	F202	L112	C4
GLU	SER	P201	V113	C5
VAL	GLY	L293	L114	E6
ASP	PHE	L204	D115	L7
SER	PHE		F116	
ARG	GLY	L207	C117	Cl10
SER	GLN			Q11
LYS	GLY	H210	L122	K12
LYS	ILE			E13
MET	PRO	L215	L126	T27
GLN	ASP			
ARG	ASP	Y220	S129	L31
GLU	GLN		S130	V32
MET	GLY	A225	S131	
THR	SER	L286	L132	K38
ALA	VAL	L227	A133	
ARG	SER	D228		
PHE	GLY	L230	L136	K41
ALA	GLY	L230	A137	T42
ILE	SER	C231	L138	A43
GLN	VAL	K232	A139	
ASP	LEU	A233	V140	H53
ASP	MET		S141	
ASP	SER	F237	L142	E56
ASP	ALA		F143	
ASP	ARG	L244	L144	E61
GLU	ARG		V145	H62
ASP	ARG	K252	D146	M63
GLY	GLN		A147	L64
GLY	HIS	E255	S65	P66
ARG	MET	A256	Y149	
GLY	LEU	E257	R150	G57
ALA	TYR			L68
GLY	ARG	K260	M153	
SER	ARG	L261		L71
ALA	GLU	E262	L158	C72
ARG	ALA	G263		G73
ARG	SER	ASP	F161	
ARG	TYR	LYS		F78
LYS	LEU	GLU	L169	
ASN	SER	ALA		L81
ALA	MET	GLN	E171	
ARG	ASP	ALA	L172	V86
ARG	PRO	LEU		
GLY	MET	LYS	Q175	A94
	ALA	ASN	R176	P95
	GLU	ASP	E177	S96
	LYS	LYS		L97
	ILE	THR	S182	
	ARG	THR		V100
	GLU	GLY	L187	W101
	LEU	GLU		Y102
	GLU	VAL	R191	S103
	MET	LEU	L192	
	LEU	ARG	L193	L106
	LYS	HIS	F194	L107
	TYR	TYR	F195	T109

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40700	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)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: K, RET

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	0.41	0/2135	0.58	3/2915 (0.1%)
1	B	0.41	0/2135	0.58	3/2915 (0.1%)
1	C	0.41	0/2135	0.58	3/2915 (0.1%)
All	All	0.41	0/6405	0.58	9/8745 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	110	PRO	CA-N-CD	-6.51	102.39	111.50
1	A	110	PRO	CA-N-CD	-6.50	102.39	111.50
1	C	110	PRO	CA-N-CD	-6.50	102.40	111.50
1	B	202	PRO	CA-N-CD	-5.95	103.18	111.50
1	C	202	PRO	CA-N-CD	-5.95	103.18	111.50

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	2069	0	2016	89	0
1	B	2069	0	2016	88	0
1	C	2069	0	2016	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	1	0
2	B	6	0	0	1	0
2	C	6	0	0	1	0
3	A	20	0	27	21	0
3	B	20	0	27	20	0
3	C	20	0	27	20	0
4	A	3	0	0	1	0
4	B	3	0	0	1	0
4	C	3	0	0	1	0
All	All	6294	0	6129	218	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 18.

The worst 5 of 218 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:A:81:ILE:HG21	1:B:153:MET:HE3	1.36	1.06
1:B:136:LEU:HD21	3:B:407:RET:H10	1.37	1.05
1:A:153:MET:HE3	1:C:81:ILE:HG21	1.36	1.05
1:B:94:ALA:CB	1:C:144:ILE:HG22	1.87	1.04
1:C:136:LEU:HD21	3:C:407:RET:H10	1.37	1.04

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	260/391 (66%)	237 (91%)	18 (7%)	5 (2%)	6 17
1	B	260/391 (66%)	237 (91%)	18 (7%)	5 (2%)	6 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	260/391 (66%)	237 (91%)	18 (7%)	5 (2%)	6	17
All	All	780/1173 (66%)	711 (91%)	54 (7%)	15 (2%)	9	17

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	LYS
1	B	232	LYS
1	C	232	LYS
1	A	53	HIS
1	A	147	ALA

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	213/319 (67%)	161 (76%)	52 (24%)	0	1
1	B	213/319 (67%)	161 (76%)	52 (24%)	0	1
1	C	213/319 (67%)	161 (76%)	52 (24%)	0	1
All	All	639/957 (67%)	483 (76%)	156 (24%)	2	1

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	SER
1	C	192	LEU
1	C	100	VAL
1	C	141	SER
1	C	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	B	99	GLN
1	C	99	GLN

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](#)

Of 21 ligands modelled in this entry, 18 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	$\# Z > 2$
3	RET	A	407	1	20,20,21	0.73	0	27,27,28	1.98	7 (25%)
3	RET	C	407	1	20,20,21	0.73	0	27,27,28	1.98	7 (25%)
3	RET	B	407	1	20,20,21	0.72	0	27,27,28	1.98	7 (25%)

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
3	RET	A	407	1	-	4/13/30/31	0/1/1/1
3	RET	C	407	1	-	4/13/30/31	0/1/1/1
3	RET	B	407	1	-	4/13/30/31	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	407	RET	C11-C10-C9	-5.05	120.10	127.31
3	B	407	RET	C11-C10-C9	-5.05	120.10	127.31
3	A	407	RET	C11-C10-C9	-5.05	120.11	127.31
3	C	407	RET	C7-C8-C9	-4.79	119.00	126.23
3	B	407	RET	C7-C8-C9	-4.78	119.01	126.23

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	407	RET	C7-C8-C9-C19
3	B	407	RET	C7-C8-C9-C19
3	C	407	RET	C7-C8-C9-C19
3	A	407	RET	C7-C8-C9-C10
3	B	407	RET	C7-C8-C9-C10

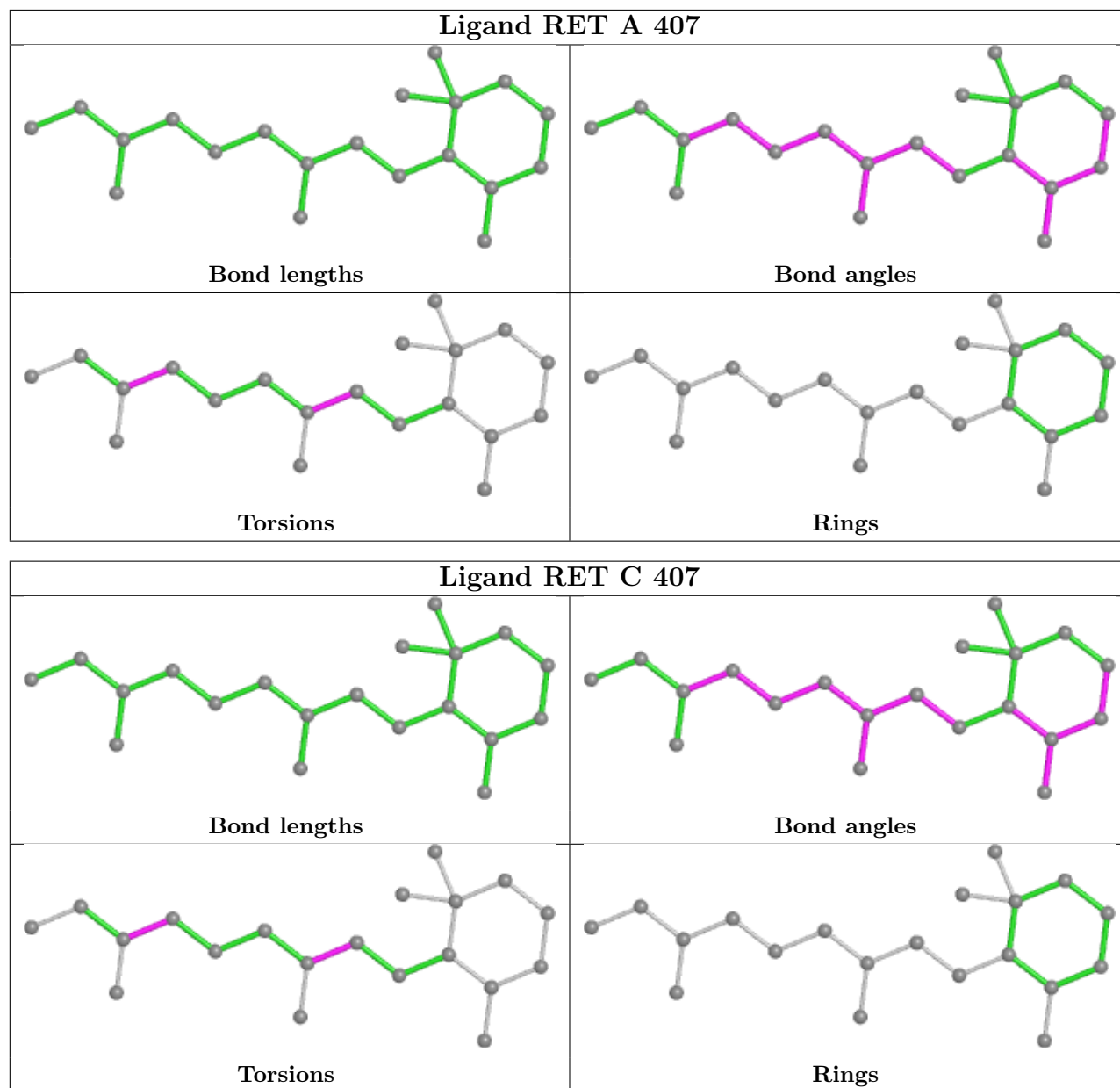
There are no ring outliers.

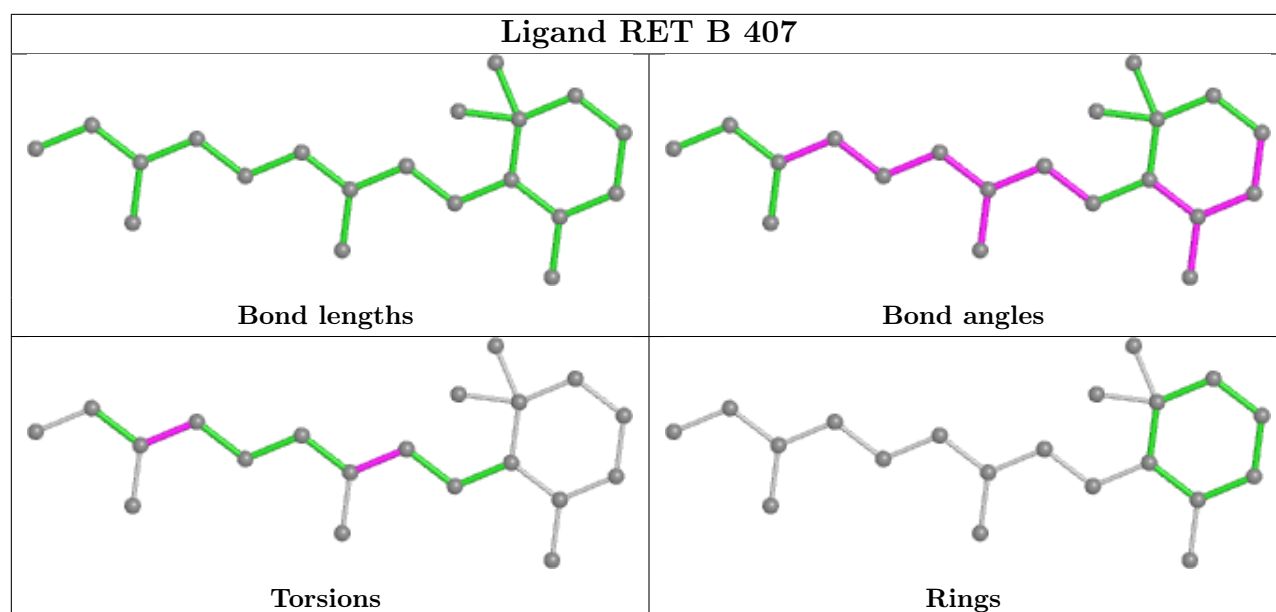
3 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	RET	21	0
3	C	407	RET	20	0
3	B	407	RET	20	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.