



Full wwPDB EM Validation 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 Full wwPDB EM Validation 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

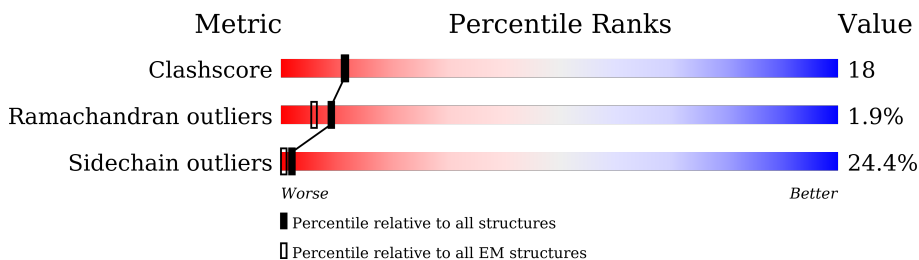
1 Overall quality at a glance

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.

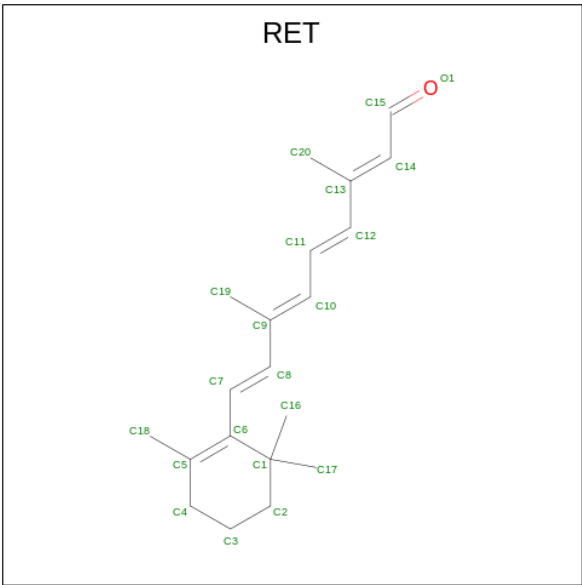
- Molecule 1 is a protein called BICHR2.

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

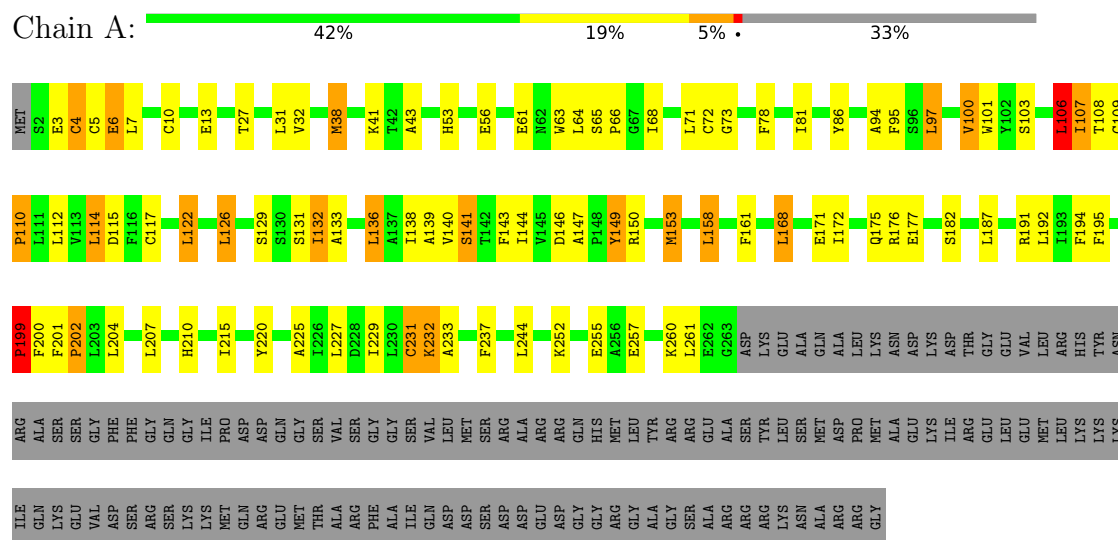
- Molecule 4 is water.

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

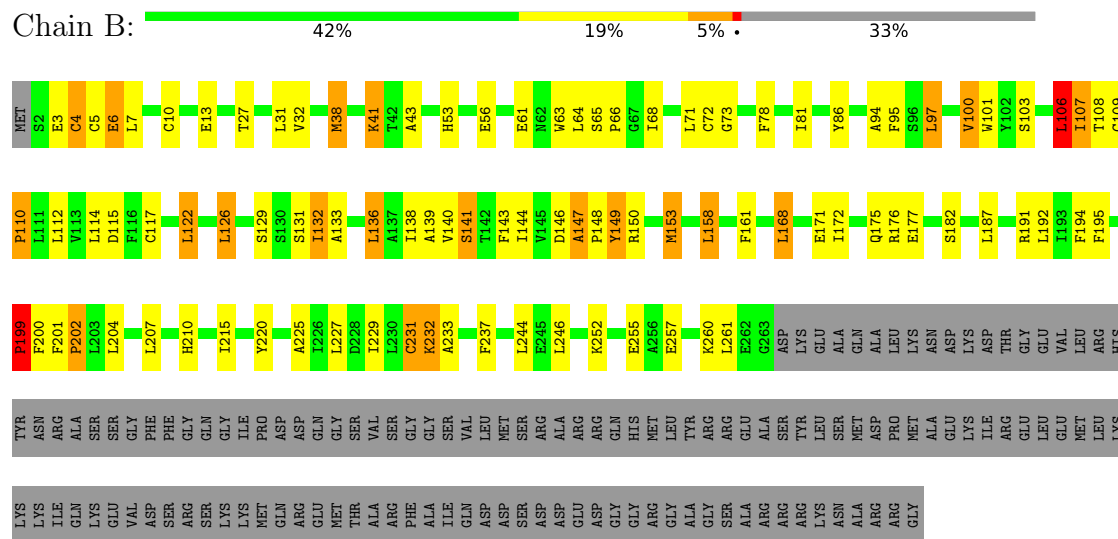
3 Residue-property plots

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	L115	L7
SER	PHE		F116	
ARG	GLY	L207	C117	Cl10
SER	GLN			Q11
LYS	GLY	H210	L122	K12
LYS	ILE			E13
MET	PRO	T215	L126	T27
GLN	ASP	Y220	S129	
ARG	ASP		S130	L31
GLU	GLN	A225	S131	V32
MET	GLY	T286	L132	
THR	SER	L227	A133	M38
ALA	VAL	D228		
ARG	SER	G129	L136	K41
PHE	GLY	L230	A137	T42
ALA	GLY	C231	I138	T42
ILE	SER	K232	A139	A43
GLN	VAL	A233	V140	
ASP	LEU		S141	H53
ASP	MET	F237	T142	
SER	SER		F143	E56
ASP	ALA	L244	I144	E61
ASP	ARG		V145	M62
GLU	ARG	K252	D146	M63
ASP	GLN		A147	L64
GLY	GLY	E255	S65	P66
GLY	HIS	A256	Y149	
ARG	MET	E257	R150	G67
GLY	LEU			L68
ALA	TYR		M153	
GLY	ARG	K260	L158	L71
GLY	SER	L261		C72
SER	GLU	E262	F161	G73
ALA	ARG	G263		
ARG	ALA	ASP		F78
ARG	SER	LYS		
ARG	TYR	GLU	L169	
LYS	LEU	ALA	E171	I81
ASN	SER	ALA	ALA	
ALA	MET	GLN	L172	V86
ARG	ASP	ALA		
ARG	PRO	LEU		
ARG	MET	LYS	Q175	A94
GLY	ALA	ASN	R176	P95
	GLU	ASP	E177	S96
	GLY	LYS		L97
	LYS	ILE	S182	
	ILE	THR		V100
	ARG	GLU	L187	I101
	GLU	GLY		Y102
	LEU	GLU		S103
	LEU	VAL	R191	
	MET	LEU	L192	
	ARG	LEU	K193	L106
	LEU	LYS	F194	I107
	LYS	HIS		T108
	TYR	THR		

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.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	202	PRO	CA-N-CD	-5.93	103.20	111.50
1	A	199	PRO	CA-N-CD	-5.61	103.65	111.50
1	C	199	PRO	CA-N-CD	-5.60	103.66	111.50
1	B	199	PRO	CA-N-CD	-5.59	103.67	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
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.

All (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
1:A:94:ALA:CB	1:B:144:ILE:HG22	1.87	1.04
1:A:136:LEU:HD21	3:A:407:RET:H10	1.37	1.03
1:A:144:ILE:HG22	1:C:94:ALA:CB	1.87	1.03
1:B:81:ILE:HG21	1:C:153:MET:HE3	1.36	1.03
1:A:136:LEU:HD21	3:A:407:RET:C10	1.92	0.99
1:A:110:PRO:HG3	1:A:133:ALA:HB2	1.43	0.99
1:B:136:LEU:HD21	3:B:407:RET:C10	1.92	0.99
1:C:136:LEU:HD21	3:C:407:RET:C10	1.92	0.98
1:C:110:PRO:HG3	1:C:133:ALA:HB2	1.43	0.98
1:B:110:PRO:HG3	1:B:133:ALA:HB2	1.43	0.97
1:A:153:MET:CE	1:C:81:ILE:HG21	2.00	0.90
1:B:81:ILE:HG21	1:C:153:MET:CE	2.00	0.90
1:A:81:ILE:HG21	1:B:153:MET:CE	2.00	0.90
1:A:144:ILE:HG22	1:C:94:ALA:HB1	1.56	0.87
1:A:94:ALA:HB1	1:B:144:ILE:HG22	1.57	0.87
1:C:202:PRO:CD	3:C:407:RET:H7	2.06	0.86
1:B:94:ALA:HB1	1:C:144:ILE:HG22	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PRO:CD	3:B:407:RET:H7	2.06	0.85
1:A:202:PRO:CD	3:A:407:RET:H7	2.06	0.84
1:C:158:LEU:HD23	3:C:407:RET:H162	1.61	0.83
1:A:158:LEU:HD23	3:A:407:RET:H162	1.61	0.83
1:A:78:PHE:CZ	1:B:138:ILE:HG12	2.14	0.83
1:B:158:LEU:HD23	3:B:407:RET:H162	1.61	0.82
1:A:138:ILE:HG12	1:C:78:PHE:CZ	2.14	0.82
1:B:78:PHE:CZ	1:C:138:ILE:HG12	2.14	0.82
1:B:202:PRO:HG3	3:B:407:RET:H7	1.62	0.82
1:A:202:PRO:HG3	3:A:407:RET:H7	1.62	0.81
1:C:202:PRO:HG3	3:C:407:RET:H7	1.62	0.81
1:A:202:PRO:HD3	3:A:407:RET:H7	1.63	0.81
1:B:202:PRO:HD3	3:B:407:RET:H7	1.63	0.81
1:C:202:PRO:HD3	3:C:407:RET:H7	1.63	0.80
1:C:202:PRO:CG	3:C:407:RET:H7	2.11	0.80
1:B:202:PRO:CG	3:B:407:RET:H7	2.11	0.79
1:A:202:PRO:CG	3:A:407:RET:H7	2.12	0.79
1:B:202:PRO:HG3	3:B:407:RET:C16	2.12	0.79
1:A:202:PRO:HG3	3:A:407:RET:C16	2.12	0.79
1:C:202:PRO:HG3	3:C:407:RET:C16	2.12	0.79
1:C:202:PRO:HD3	3:C:407:RET:C7	2.14	0.78
1:B:202:PRO:HD3	3:B:407:RET:C7	2.14	0.78
1:B:94:ALA:HB3	1:C:144:ILE:HG22	1.66	0.77
1:A:202:PRO:HD3	3:A:407:RET:C7	2.14	0.77
1:A:144:ILE:HG22	1:C:94:ALA:HB3	1.65	0.77
1:B:110:PRO:HD3	1:B:132:ILE:HG22	1.67	0.76
1:C:110:PRO:HD3	1:C:132:ILE:HG22	1.67	0.76
1:A:110:PRO:HD3	1:A:132:ILE:HG22	1.67	0.75
1:A:94:ALA:HB3	1:B:144:ILE:HG22	1.65	0.75
1:C:72:CYS:SG	2:C:404:K:K	2.39	0.74
1:A:72:CYS:SG	2:A:404:K:K	2.39	0.74
1:B:72:CYS:SG	2:B:404:K:K	2.39	0.74
1:A:78:PHE:HZ	1:B:138:ILE:HG12	1.53	0.73
1:B:78:PHE:HZ	1:C:138:ILE:HG12	1.53	0.72
1:B:94:ALA:HB1	1:C:144:ILE:CG2	2.20	0.72
1:A:138:ILE:HG12	1:C:78:PHE:HZ	1.53	0.72
1:A:144:ILE:CG2	1:C:94:ALA:HB1	2.20	0.71
1:A:94:ALA:HB1	1:B:144:ILE:CG2	2.20	0.71
1:C:202:PRO:HG3	3:C:407:RET:H161	1.73	0.69
1:B:202:PRO:HG3	3:B:407:RET:H161	1.73	0.69
1:A:202:PRO:HG3	3:A:407:RET:H161	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:O	4:B:501:HOH:O	2.11	0.69
1:C:97:LEU:O	4:C:501:HOH:O	2.11	0.68
1:C:158:LEU:HD23	3:C:407:RET:C16	2.24	0.68
1:A:97:LEU:O	4:A:501:HOH:O	2.11	0.68
1:B:81:ILE:CG2	1:C:153:MET:CE	2.72	0.67
1:B:143:PHE:CE1	1:B:210:HIS:NE2	2.63	0.67
1:B:27:THR:HG21	1:B:225:ALA:HB1	1.77	0.66
1:A:158:LEU:HD23	3:A:407:RET:C16	2.24	0.66
1:A:81:ILE:CG2	1:B:153:MET:CE	2.72	0.66
1:B:158:LEU:HD23	3:B:407:RET:C16	2.24	0.66
1:A:143:PHE:CE1	1:A:210:HIS:NE2	2.63	0.66
1:C:143:PHE:CE1	1:C:210:HIS:NE2	2.63	0.66
1:A:153:MET:CE	1:C:81:ILE:CG2	2.72	0.65
1:C:27:THR:HG21	1:C:225:ALA:HB1	1.77	0.65
1:A:27:THR:HG21	1:A:225:ALA:HB1	1.77	0.64
1:B:81:ILE:CG2	1:C:149:TYR:HB3	2.30	0.62
1:A:81:ILE:CG2	1:B:149:TYR:HB3	2.30	0.62
1:B:231:CYS:O	1:B:232:LYS:C	2.38	0.62
1:A:231:CYS:O	1:A:232:LYS:C	2.38	0.62
1:A:149:TYR:HB3	1:C:81:ILE:CG2	2.30	0.62
1:A:202:PRO:HG3	3:A:407:RET:C7	2.30	0.62
1:B:78:PHE:CE2	1:C:138:ILE:HG12	2.36	0.61
1:B:202:PRO:HG3	3:B:407:RET:C7	2.30	0.61
1:A:138:ILE:HG12	1:C:78:PHE:CE2	2.36	0.60
1:A:112:LEU:HD11	1:A:232:LYS:HD3	1.84	0.60
1:A:139:ALA:CB	3:A:407:RET:H42	2.32	0.60
1:C:231:CYS:O	1:C:232:LYS:C	2.38	0.60
1:C:139:ALA:CB	3:C:407:RET:H42	2.32	0.60
1:A:78:PHE:CE2	1:B:138:ILE:HG12	2.36	0.60
1:B:139:ALA:CB	3:B:407:RET:H42	2.32	0.60
1:C:202:PRO:HG3	3:C:407:RET:C7	2.30	0.59
1:A:27:THR:HG22	1:A:229:ILE:HD11	1.83	0.59
1:B:27:THR:HG22	1:B:229:ILE:HD11	1.83	0.59
1:C:27:THR:HG22	1:C:229:ILE:HD11	1.83	0.59
1:B:108:THR:HB	1:B:232:LYS:HD2	1.85	0.59
1:B:4:CYS:HB3	1:B:10:CYS:HB2	1.84	0.59
1:C:108:THR:HB	1:C:232:LYS:HD2	1.85	0.59
1:C:4:CYS:HB3	1:C:10:CYS:HB2	1.84	0.59
1:C:38:MET:HB3	1:C:66:PRO:HG3	1.85	0.58
1:A:4:CYS:HB3	1:A:10:CYS:HB2	1.84	0.58
1:A:108:THR:HB	1:A:232:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:HD11	1:C:232:LYS:HD3	1.84	0.58
1:B:38:MET:HB3	1:B:66:PRO:HG3	1.85	0.58
1:B:112:LEU:HD11	1:B:232:LYS:HD3	1.84	0.58
1:A:38:MET:HB3	1:A:66:PRO:HG3	1.85	0.58
1:A:94:ALA:CB	1:B:144:ILE:CG2	2.73	0.57
1:A:106:LEU:O	1:A:110:PRO:HD2	2.06	0.56
1:C:106:LEU:O	1:C:110:PRO:HD2	2.06	0.55
1:B:106:LEU:O	1:B:110:PRO:HD2	2.06	0.55
1:B:143:PHE:CD1	1:B:210:HIS:NE2	2.75	0.55
1:C:143:PHE:CD1	1:C:210:HIS:NE2	2.75	0.55
1:A:143:PHE:CD1	1:A:210:HIS:NE2	2.75	0.55
1:C:32:VAL:HG23	1:C:73:GLY:HA3	1.90	0.54
1:B:202:PRO:HG3	3:B:407:RET:H163	1.87	0.53
1:B:32:VAL:HG23	1:B:73:GLY:HA3	1.90	0.53
1:A:32:VAL:HG23	1:A:73:GLY:HA3	1.90	0.53
1:C:202:PRO:HG3	3:C:407:RET:H163	1.87	0.53
1:A:144:ILE:CG2	1:C:94:ALA:CB	2.73	0.52
1:B:94:ALA:CB	1:C:144:ILE:CG2	2.73	0.52
1:C:202:PRO:HD2	3:C:407:RET:H193	1.92	0.52
1:A:202:PRO:HG3	3:A:407:RET:H163	1.88	0.52
1:B:202:PRO:HD2	3:B:407:RET:H193	1.92	0.52
1:B:139:ALA:HA	3:B:407:RET:H42	1.93	0.51
1:A:202:PRO:HD2	3:A:407:RET:H193	1.92	0.51
1:A:139:ALA:HA	3:A:407:RET:H42	1.93	0.51
1:B:95:PHE:CD2	1:C:141:SER:HB2	2.46	0.51
1:A:141:SER:HB2	1:C:95:PHE:CD2	2.46	0.50
1:C:68:ILE:HG22	1:C:232:LYS:HG3	1.94	0.50
1:B:109:CYS:HB3	1:B:132:ILE:CG2	2.42	0.50
1:A:95:PHE:CD2	1:B:141:SER:HB2	2.46	0.50
1:B:68:ILE:HG22	1:B:232:LYS:HG3	1.94	0.50
1:C:139:ALA:HA	3:C:407:RET:H42	1.93	0.50
1:C:109:CYS:HB3	1:C:132:ILE:CG2	2.42	0.49
1:A:109:CYS:HB3	1:A:132:ILE:CG2	2.42	0.49
1:A:68:ILE:HG22	1:A:232:LYS:HG3	1.94	0.48
1:A:107:ILE:H	1:A:107:ILE:HG13	1.41	0.48
1:B:201:PHE:CZ	1:B:227:LEU:HB3	2.49	0.48
1:A:78:PHE:CE1	1:B:153:MET:HG2	2.49	0.48
1:C:110:PRO:HG3	1:C:133:ALA:CB	2.30	0.48
1:A:149:TYR:HB3	1:C:81:ILE:HG23	1.96	0.48
1:A:153:MET:HG2	1:C:78:PHE:CE1	2.49	0.47
1:A:81:ILE:HG23	1:B:149:TYR:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:TRP:O	1:C:140:VAL:HG13	2.15	0.47
1:B:81:ILE:HG23	1:C:149:TYR:HB3	1.96	0.47
1:B:101:TRP:O	1:B:140:VAL:HG13	2.15	0.47
1:C:201:PHE:CZ	1:C:227:LEU:HB3	2.49	0.47
1:A:201:PHE:CZ	1:A:227:LEU:HB3	2.49	0.47
1:B:78:PHE:CE1	1:C:153:MET:HG2	2.49	0.47
1:B:161:PHE:CE2	1:B:199:PRO:HD3	2.50	0.47
1:C:187:LEU:HA	1:C:187:LEU:HD12	1.65	0.47
1:A:31:LEU:HD23	1:A:233:ALA:HB2	1.97	0.47
1:B:31:LEU:HD23	1:B:233:ALA:HB2	1.97	0.46
1:A:110:PRO:HG3	1:A:133:ALA:CB	2.30	0.46
1:B:110:PRO:HG3	1:B:133:ALA:CB	2.30	0.46
1:C:31:LEU:HD23	1:C:233:ALA:HB2	1.97	0.46
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.78	0.46
1:A:161:PHE:CE2	1:A:199:PRO:HD3	2.50	0.46
1:C:161:PHE:CE2	1:C:199:PRO:HD3	2.50	0.46
1:A:101:TRP:O	1:A:140:VAL:HG13	2.15	0.46
1:B:126:LEU:HD13	1:B:126:LEU:HA	1.74	0.46
1:B:97:LEU:HD12	1:B:97:LEU:HA	1.84	0.45
1:A:202:PRO:HD3	3:A:407:RET:H181	1.98	0.45
1:B:107:ILE:H	1:B:107:ILE:HG13	1.41	0.45
1:C:136:LEU:CD2	3:C:407:RET:H10	2.27	0.45
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.78	0.45
1:B:136:LEU:CD2	3:B:407:RET:H10	2.28	0.45
1:A:97:LEU:HD12	1:A:97:LEU:HA	1.84	0.44
1:A:195:PHE:O	1:A:199:PRO:HG2	2.17	0.44
1:B:195:PHE:O	1:B:199:PRO:HG2	2.17	0.44
1:A:6:GLU:H	1:A:6:GLU:HG3	1.38	0.44
1:B:187:LEU:HA	1:B:187:LEU:HD12	1.65	0.44
1:C:195:PHE:O	1:C:199:PRO:HG2	2.17	0.44
1:B:202:PRO:HD3	3:B:407:RET:H181	1.98	0.44
3:C:407:RET:H191	3:C:407:RET:H11	1.72	0.44
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.90	0.44
1:C:6:GLU:H	1:C:6:GLU:HG3	1.38	0.44
1:C:202:PRO:HD3	3:C:407:RET:H181	1.98	0.43
1:C:126:LEU:HD13	1:C:126:LEU:HA	1.74	0.43
1:C:12:LYS:HB3	1:C:12:LYS:HE2	1.78	0.42
1:A:43:ALA:HB2	1:A:63:TRP:HH2	1.84	0.42
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.79	0.42
1:A:204:LEU:HB3	1:A:220:TYR:HE1	1.83	0.42
1:B:139:ALA:CA	3:B:407:RET:H42	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ALA:HB2	1:C:63:TRP:HH2	1.84	0.42
1:C:117:CYS:HA	1:C:122:LEU:HB2	2.01	0.42
1:C:139:ALA:CA	3:C:407:RET:H42	2.50	0.42
1:A:126:LEU:HD13	1:A:126:LEU:HA	1.74	0.42
1:A:136:LEU:CD2	3:A:407:RET:H10	2.28	0.42
1:B:204:LEU:HB3	1:B:220:TYR:HE1	1.83	0.42
1:A:117:CYS:HA	1:A:122:LEU:HB2	2.01	0.42
1:A:143:PHE:HE1	1:A:210:HIS:HE2	1.58	0.42
1:C:204:LEU:HB3	1:C:220:TYR:HE1	1.83	0.42
1:C:106:LEU:O	1:C:110:PRO:CD	2.68	0.42
1:A:139:ALA:CA	3:A:407:RET:H42	2.50	0.41
1:A:106:LEU:O	1:A:110:PRO:CD	2.68	0.41
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.65	0.41
1:B:6:GLU:H	1:B:6:GLU:HG3	1.38	0.41
1:B:100:VAL:HB	1:B:103:SER:HB3	2.03	0.41
1:C:168:LEU:HD13	1:C:172:ILE:HD11	2.02	0.41
3:A:407:RET:H191	3:A:407:RET:H11	1.72	0.41
1:B:106:LEU:O	1:B:110:PRO:CD	2.68	0.41
1:B:168:LEU:HD13	1:B:172:ILE:HD11	2.02	0.41
1:B:43:ALA:HB2	1:B:63:TRP:HH2	1.84	0.41
1:A:168:LEU:HD13	1:A:172:ILE:HD11	2.02	0.41
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.90	0.41
1:B:117:CYS:HA	1:B:122:LEU:HB2	2.01	0.41
1:A:100:VAL:HB	1:A:103:SER:HB3	2.03	0.41
1:B:202:PRO:CD	3:B:407:RET:H193	2.51	0.41
1:C:100:VAL:HB	1:C:103:SER:HB3	2.03	0.40
1:B:147:ALA:HB3	1:B:148:PRO:HD3	2.03	0.40
1:C:147:ALA:HB3	1:C:148:PRO:HD3	2.04	0.40
1:A:202:PRO:CD	3:A:407:RET:H193	2.51	0.40
1:B:41:LYS:HD3	1:B:41:LYS:HA	1.98	0.40
1:B:246:LEU:HD23	1:B:246:LEU:HA	1.91	0.40
1:A:161:PHE:CZ	1:A:199:PRO:HD3	2.57	0.40

There are no symmetry-related clashes.

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 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
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

All (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
1	A	231	CYS
1	B	53	HIS
1	B	147	ALA
1	B	231	CYS
1	C	53	HIS
1	C	147	ALA
1	C	231	CYS
1	A	106	LEU
1	B	106	LEU
1	C	106	LEU

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	639/957 (67%)	483 (76%)	156 (24%)	2 1

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	CYS
1	A	5	CYS
1	A	6	GLU
1	A	7	LEU
1	A	13	GLU
1	A	38	MET
1	A	41	LYS
1	A	56	GLU
1	A	61	GLU
1	A	64	LEU
1	A	65	SER
1	A	71	LEU
1	A	86	TYR
1	A	97	LEU
1	A	100	VAL
1	A	106	LEU
1	A	107	ILE
1	A	114	LEU
1	A	115	ASP
1	A	122	LEU
1	A	126	LEU
1	A	129	SER
1	A	131	SER
1	A	132	ILE
1	A	136	LEU
1	A	141	SER
1	A	146	ASP
1	A	149	TYR
1	A	150	ARG
1	A	153	MET
1	A	158	LEU
1	A	168	LEU
1	A	171	GLU
1	A	175	GLN
1	A	176	ARG
1	A	177	GLU

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Mol	Chain	Res	Type
1	A	182	SER
1	A	191	ARG
1	A	192	LEU
1	A	194	PHE
1	A	199	PRO
1	A	200	PHE
1	A	207	LEU
1	A	215	ILE
1	A	237	PHE
1	A	244	LEU
1	A	252	LYS
1	A	255	GLU
1	A	257	GLU
1	A	260	LYS
1	A	261	LEU
1	B	3	GLU
1	B	4	CYS
1	B	5	CYS
1	B	6	GLU
1	B	7	LEU
1	B	13	GLU
1	B	38	MET
1	B	41	LYS
1	B	56	GLU
1	B	61	GLU
1	B	64	LEU
1	B	65	SER
1	B	71	LEU
1	B	86	TYR
1	B	97	LEU
1	B	100	VAL
1	B	106	LEU
1	B	107	ILE
1	B	114	LEU
1	B	115	ASP
1	B	122	LEU
1	B	126	LEU
1	B	129	SER
1	B	131	SER
1	B	132	ILE
1	B	136	LEU
1	B	141	SER

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Mol	Chain	Res	Type
1	B	146	ASP
1	B	149	TYR
1	B	150	ARG
1	B	153	MET
1	B	158	LEU
1	B	168	LEU
1	B	171	GLU
1	B	175	GLN
1	B	176	ARG
1	B	177	GLU
1	B	182	SER
1	B	191	ARG
1	B	192	LEU
1	B	194	PHE
1	B	199	PRO
1	B	200	PHE
1	B	207	LEU
1	B	215	ILE
1	B	237	PHE
1	B	244	LEU
1	B	252	LYS
1	B	255	GLU
1	B	257	GLU
1	B	260	LYS
1	B	261	LEU
1	C	3	GLU
1	C	4	CYS
1	C	5	CYS
1	C	6	GLU
1	C	7	LEU
1	C	13	GLU
1	C	38	MET
1	C	41	LYS
1	C	56	GLU
1	C	61	GLU
1	C	64	LEU
1	C	65	SER
1	C	71	LEU
1	C	86	TYR
1	C	97	LEU
1	C	100	VAL
1	C	106	LEU

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Mol	Chain	Res	Type
1	C	107	ILE
1	C	114	LEU
1	C	115	ASP
1	C	122	LEU
1	C	126	LEU
1	C	129	SER
1	C	131	SER
1	C	132	ILE
1	C	136	LEU
1	C	141	SER
1	C	146	ASP
1	C	149	TYR
1	C	150	ARG
1	C	153	MET
1	C	158	LEU
1	C	168	LEU
1	C	171	GLU
1	C	175	GLN
1	C	176	ARG
1	C	177	GLU
1	C	182	SER
1	C	191	ARG
1	C	192	LEU
1	C	194	PHE
1	C	199	PRO
1	C	200	PHE
1	C	207	LEU
1	C	215	ILE
1	C	237	PHE
1	C	244	LEU
1	C	252	LYS
1	C	255	GLU
1	C	257	GLU
1	C	260	LYS
1	C	261	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 ⓘ

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

All (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
3	A	407	RET	C7-C8-C9	-4.78	119.02	126.23
3	B	407	RET	C18-C5-C6	-3.72	120.35	124.53
3	A	407	RET	C18-C5-C6	-3.71	120.36	124.53
3	C	407	RET	C18-C5-C6	-3.71	120.37	124.53
3	B	407	RET	C18-C5-C4	2.80	118.99	113.62
3	A	407	RET	C18-C5-C4	2.80	118.99	113.62
3	C	407	RET	C18-C5-C4	2.79	118.98	113.62
3	A	407	RET	C19-C9-C10	-2.12	119.96	122.92
3	B	407	RET	C19-C9-C10	-2.12	119.96	122.92
3	C	407	RET	C19-C9-C10	-2.11	119.96	122.92
3	B	407	RET	C11-C12-C13	-2.07	120.60	126.42
3	A	407	RET	C11-C12-C13	-2.07	120.61	126.42
3	C	407	RET	C11-C12-C13	-2.06	120.63	126.42
3	B	407	RET	C3-C4-C5	-2.02	110.48	114.08
3	A	407	RET	C3-C4-C5	-2.01	110.48	114.08
3	C	407	RET	C3-C4-C5	-2.01	110.49	114.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

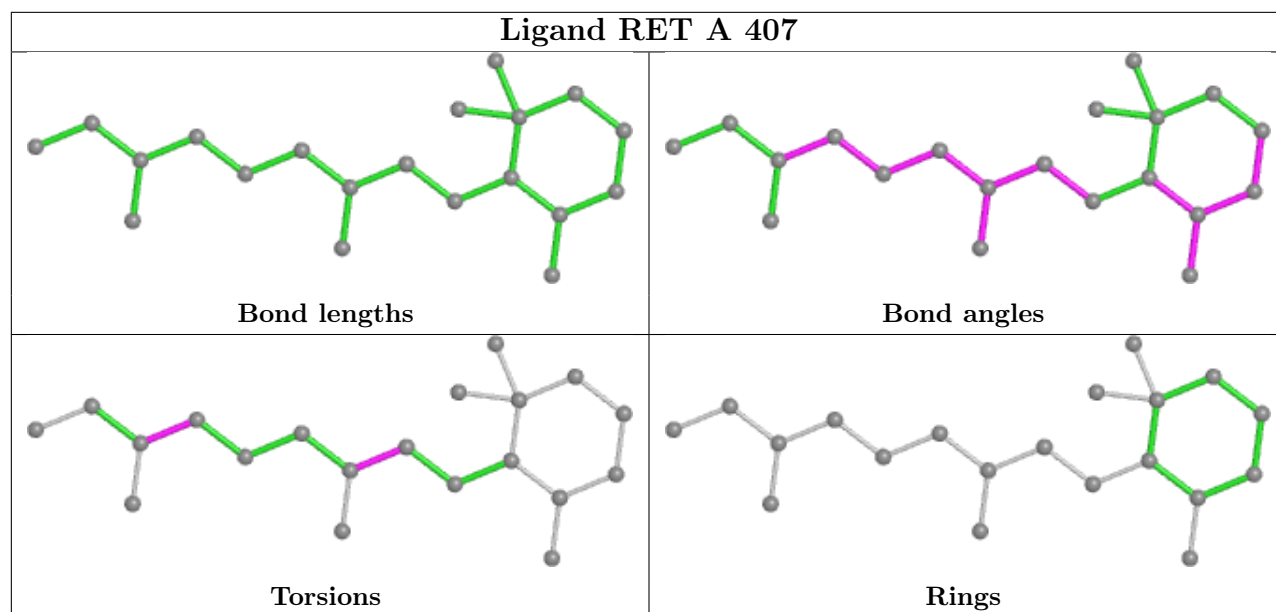
Mol	Chain	Res	Type	Atoms
3	A	407	RET	C7-C8-C9-C19
3	B	407	RET	C7-C8-C9-C19
3	C	407	RET	C7-C8-C9-C19
3	A	407	RET	C7-C8-C9-C10
3	B	407	RET	C7-C8-C9-C10
3	C	407	RET	C7-C8-C9-C10
3	A	407	RET	C11-C12-C13-C20
3	B	407	RET	C11-C12-C13-C20
3	C	407	RET	C11-C12-C13-C20
3	A	407	RET	C11-C12-C13-C14
3	B	407	RET	C11-C12-C13-C14
3	C	407	RET	C11-C12-C13-C14

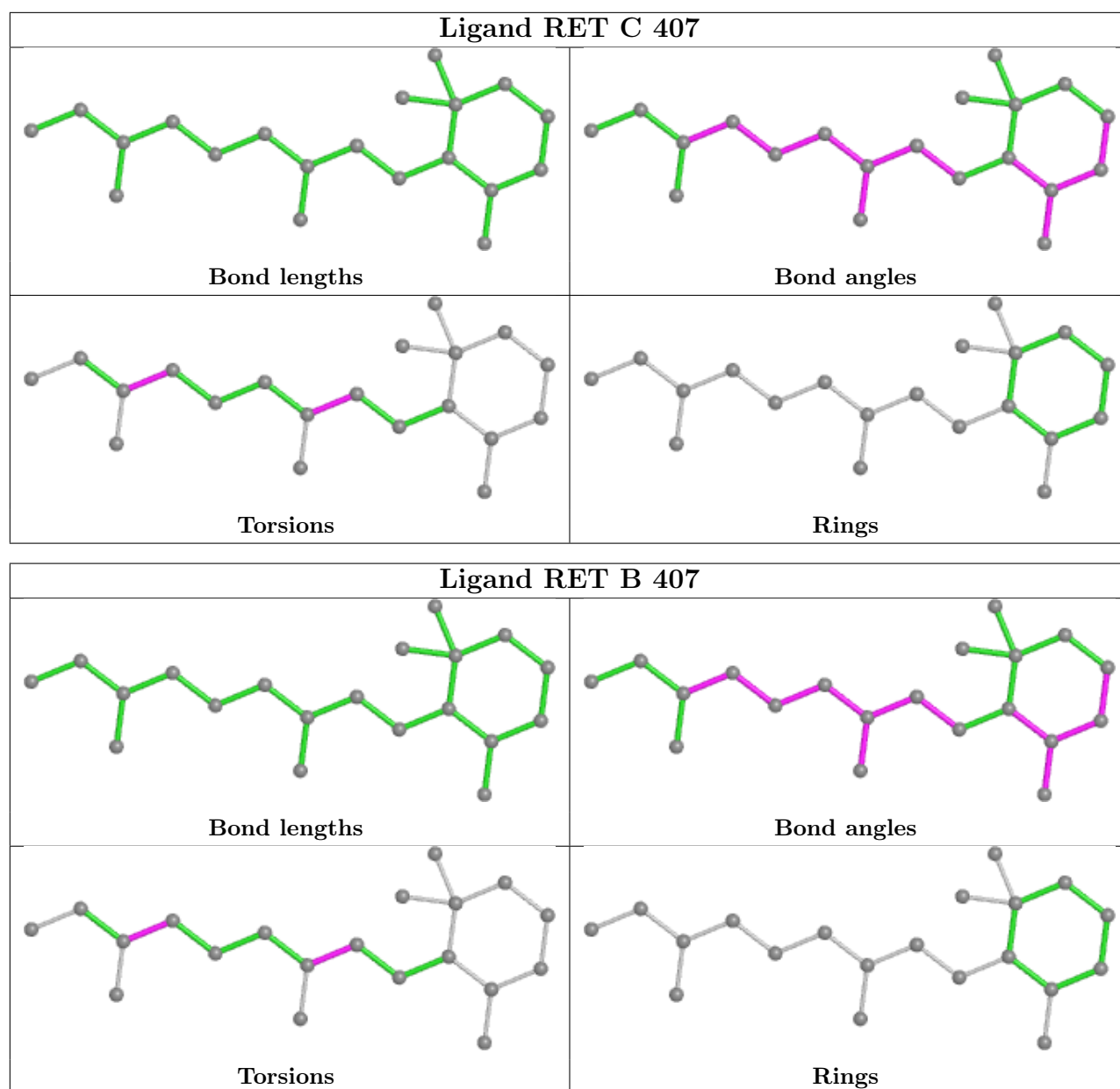
There are no ring outliers.

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.