wwPDB EM Validation Summary Report

May 21, 2024 – 10:14 AM JST

PDB ID	:	8J1F
EMDB ID	:	EMD-35921
Title	:	GSK101 bound state of mTRPV4
Authors	:	Zhen, W.X.; Yang, F.
Deposited on	:	2023-04-12
Resolution	:	3.62 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:

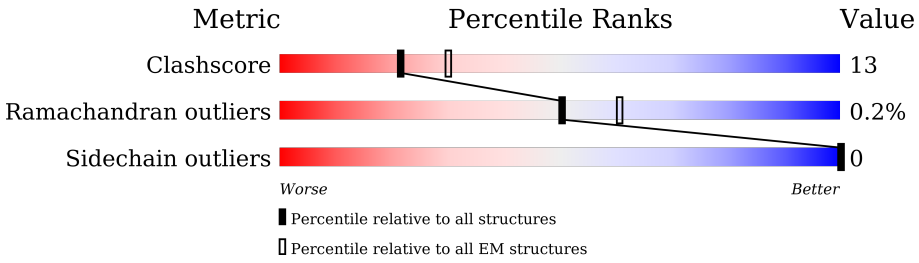
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.62 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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	700	60% 24% 16%
1	B	700	60% 24% 16%
1	C	700	60% 24% 16%
1	D	700	60% 24% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 38524 atoms, of which 19408 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 Transient receptor potential cation channel subfamily V member 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	587	Total	C	H	N	O	S	0	0
			9557	3084	4820	786	843	24		
1	B	587	Total	C	H	N	O	S	0	0
			9557	3084	4820	786	843	24		
1	C	587	Total	C	H	N	O	S	0	0
			9557	3084	4820	786	843	24		
1	D	587	Total	C	H	N	O	S	0	0
			9557	3084	4820	786	843	24		

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ASP	-	expression tag	UNP Q9EPK8
A	103	TYR	-	expression tag	UNP Q9EPK8
A	104	LYS	-	expression tag	UNP Q9EPK8
A	105	ASP	-	expression tag	UNP Q9EPK8
A	106	ASP	-	expression tag	UNP Q9EPK8
A	107	ASP	-	expression tag	UNP Q9EPK8
A	108	ASP	-	expression tag	UNP Q9EPK8
A	109	LYS	-	expression tag	UNP Q9EPK8
A	110	TRP	-	expression tag	UNP Q9EPK8
A	111	SER	-	expression tag	UNP Q9EPK8
A	112	HIS	-	expression tag	UNP Q9EPK8
A	113	PRO	-	expression tag	UNP Q9EPK8
A	114	GLN	-	expression tag	UNP Q9EPK8
A	115	PHE	-	expression tag	UNP Q9EPK8
A	116	GLU	-	expression tag	UNP Q9EPK8
A	117	LYS	-	expression tag	UNP Q9EPK8
A	118	GLY	-	expression tag	UNP Q9EPK8
A	119	GLY	-	expression tag	UNP Q9EPK8
A	120	GLY	-	expression tag	UNP Q9EPK8
A	121	GLY	-	expression tag	UNP Q9EPK8
A	122	SER	-	expression tag	UNP Q9EPK8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q9EPK8
A	124	GLY	-	expression tag	UNP Q9EPK8
A	125	SER	-	expression tag	UNP Q9EPK8
A	126	ALA	-	expression tag	UNP Q9EPK8
A	127	TRP	-	expression tag	UNP Q9EPK8
A	128	SER	-	expression tag	UNP Q9EPK8
A	129	HIS	-	expression tag	UNP Q9EPK8
A	130	PRO	-	expression tag	UNP Q9EPK8
A	131	GLN	-	expression tag	UNP Q9EPK8
A	132	PHE	-	expression tag	UNP Q9EPK8
A	133	GLU	-	expression tag	UNP Q9EPK8
A	134	LYS	-	expression tag	UNP Q9EPK8
A	135	GLU	-	expression tag	UNP Q9EPK8
A	136	PHE	-	expression tag	UNP Q9EPK8
B	102	ASP	-	expression tag	UNP Q9EPK8
B	103	TYR	-	expression tag	UNP Q9EPK8
B	104	LYS	-	expression tag	UNP Q9EPK8
B	105	ASP	-	expression tag	UNP Q9EPK8
B	106	ASP	-	expression tag	UNP Q9EPK8
B	107	ASP	-	expression tag	UNP Q9EPK8
B	108	ASP	-	expression tag	UNP Q9EPK8
B	109	LYS	-	expression tag	UNP Q9EPK8
B	110	TRP	-	expression tag	UNP Q9EPK8
B	111	SER	-	expression tag	UNP Q9EPK8
B	112	HIS	-	expression tag	UNP Q9EPK8
B	113	PRO	-	expression tag	UNP Q9EPK8
B	114	GLN	-	expression tag	UNP Q9EPK8
B	115	PHE	-	expression tag	UNP Q9EPK8
B	116	GLU	-	expression tag	UNP Q9EPK8
B	117	LYS	-	expression tag	UNP Q9EPK8
B	118	GLY	-	expression tag	UNP Q9EPK8
B	119	GLY	-	expression tag	UNP Q9EPK8
B	120	GLY	-	expression tag	UNP Q9EPK8
B	121	GLY	-	expression tag	UNP Q9EPK8
B	122	SER	-	expression tag	UNP Q9EPK8
B	123	GLY	-	expression tag	UNP Q9EPK8
B	124	GLY	-	expression tag	UNP Q9EPK8
B	125	SER	-	expression tag	UNP Q9EPK8
B	126	ALA	-	expression tag	UNP Q9EPK8
B	127	TRP	-	expression tag	UNP Q9EPK8
B	128	SER	-	expression tag	UNP Q9EPK8
B	129	HIS	-	expression tag	UNP Q9EPK8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	130	PRO	-	expression tag	UNP Q9EPK8
B	131	GLN	-	expression tag	UNP Q9EPK8
B	132	PHE	-	expression tag	UNP Q9EPK8
B	133	GLU	-	expression tag	UNP Q9EPK8
B	134	LYS	-	expression tag	UNP Q9EPK8
B	135	GLU	-	expression tag	UNP Q9EPK8
B	136	PHE	-	expression tag	UNP Q9EPK8
C	102	ASP	-	expression tag	UNP Q9EPK8
C	103	TYR	-	expression tag	UNP Q9EPK8
C	104	LYS	-	expression tag	UNP Q9EPK8
C	105	ASP	-	expression tag	UNP Q9EPK8
C	106	ASP	-	expression tag	UNP Q9EPK8
C	107	ASP	-	expression tag	UNP Q9EPK8
C	108	ASP	-	expression tag	UNP Q9EPK8
C	109	LYS	-	expression tag	UNP Q9EPK8
C	110	TRP	-	expression tag	UNP Q9EPK8
C	111	SER	-	expression tag	UNP Q9EPK8
C	112	HIS	-	expression tag	UNP Q9EPK8
C	113	PRO	-	expression tag	UNP Q9EPK8
C	114	GLN	-	expression tag	UNP Q9EPK8
C	115	PHE	-	expression tag	UNP Q9EPK8
C	116	GLU	-	expression tag	UNP Q9EPK8
C	117	LYS	-	expression tag	UNP Q9EPK8
C	118	GLY	-	expression tag	UNP Q9EPK8
C	119	GLY	-	expression tag	UNP Q9EPK8
C	120	GLY	-	expression tag	UNP Q9EPK8
C	121	GLY	-	expression tag	UNP Q9EPK8
C	122	SER	-	expression tag	UNP Q9EPK8
C	123	GLY	-	expression tag	UNP Q9EPK8
C	124	GLY	-	expression tag	UNP Q9EPK8
C	125	SER	-	expression tag	UNP Q9EPK8
C	126	ALA	-	expression tag	UNP Q9EPK8
C	127	TRP	-	expression tag	UNP Q9EPK8
C	128	SER	-	expression tag	UNP Q9EPK8
C	129	HIS	-	expression tag	UNP Q9EPK8
C	130	PRO	-	expression tag	UNP Q9EPK8
C	131	GLN	-	expression tag	UNP Q9EPK8
C	132	PHE	-	expression tag	UNP Q9EPK8
C	133	GLU	-	expression tag	UNP Q9EPK8
C	134	LYS	-	expression tag	UNP Q9EPK8
C	135	GLU	-	expression tag	UNP Q9EPK8
C	136	PHE	-	expression tag	UNP Q9EPK8

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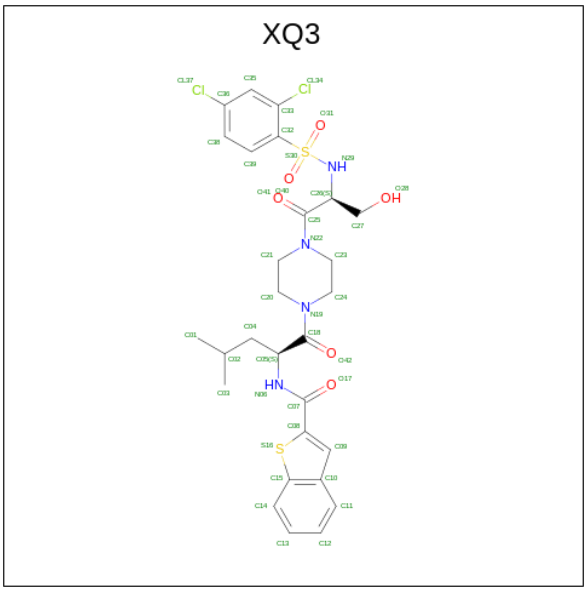
Chain	Residue	Modelled	Actual	Comment	Reference
D	102	ASP	-	expression tag	UNP Q9EPK8
D	103	TYR	-	expression tag	UNP Q9EPK8
D	104	LYS	-	expression tag	UNP Q9EPK8
D	105	ASP	-	expression tag	UNP Q9EPK8
D	106	ASP	-	expression tag	UNP Q9EPK8
D	107	ASP	-	expression tag	UNP Q9EPK8
D	108	ASP	-	expression tag	UNP Q9EPK8
D	109	LYS	-	expression tag	UNP Q9EPK8
D	110	TRP	-	expression tag	UNP Q9EPK8
D	111	SER	-	expression tag	UNP Q9EPK8
D	112	HIS	-	expression tag	UNP Q9EPK8
D	113	PRO	-	expression tag	UNP Q9EPK8
D	114	GLN	-	expression tag	UNP Q9EPK8
D	115	PHE	-	expression tag	UNP Q9EPK8
D	116	GLU	-	expression tag	UNP Q9EPK8
D	117	LYS	-	expression tag	UNP Q9EPK8
D	118	GLY	-	expression tag	UNP Q9EPK8
D	119	GLY	-	expression tag	UNP Q9EPK8
D	120	GLY	-	expression tag	UNP Q9EPK8
D	121	GLY	-	expression tag	UNP Q9EPK8
D	122	SER	-	expression tag	UNP Q9EPK8
D	123	GLY	-	expression tag	UNP Q9EPK8
D	124	GLY	-	expression tag	UNP Q9EPK8
D	125	SER	-	expression tag	UNP Q9EPK8
D	126	ALA	-	expression tag	UNP Q9EPK8
D	127	TRP	-	expression tag	UNP Q9EPK8
D	128	SER	-	expression tag	UNP Q9EPK8
D	129	HIS	-	expression tag	UNP Q9EPK8
D	130	PRO	-	expression tag	UNP Q9EPK8
D	131	GLN	-	expression tag	UNP Q9EPK8
D	132	PHE	-	expression tag	UNP Q9EPK8
D	133	GLU	-	expression tag	UNP Q9EPK8
D	134	LYS	-	expression tag	UNP Q9EPK8
D	135	GLU	-	expression tag	UNP Q9EPK8
D	136	PHE	-	expression tag	UNP Q9EPK8

- Molecule 2 is N-[(2S)-1-{4-[N-(2,4-dichlorobenzene-1-sulfonyl)-L-seryl]piperazin-1-yl}-4-methyl-1-oxopentan-2-yl]-1-benzothiophene-2-carboxamide (three-letter code: XQ3) (formula: $C_{28}H_{32}Cl_2N_4O_6S_2$).



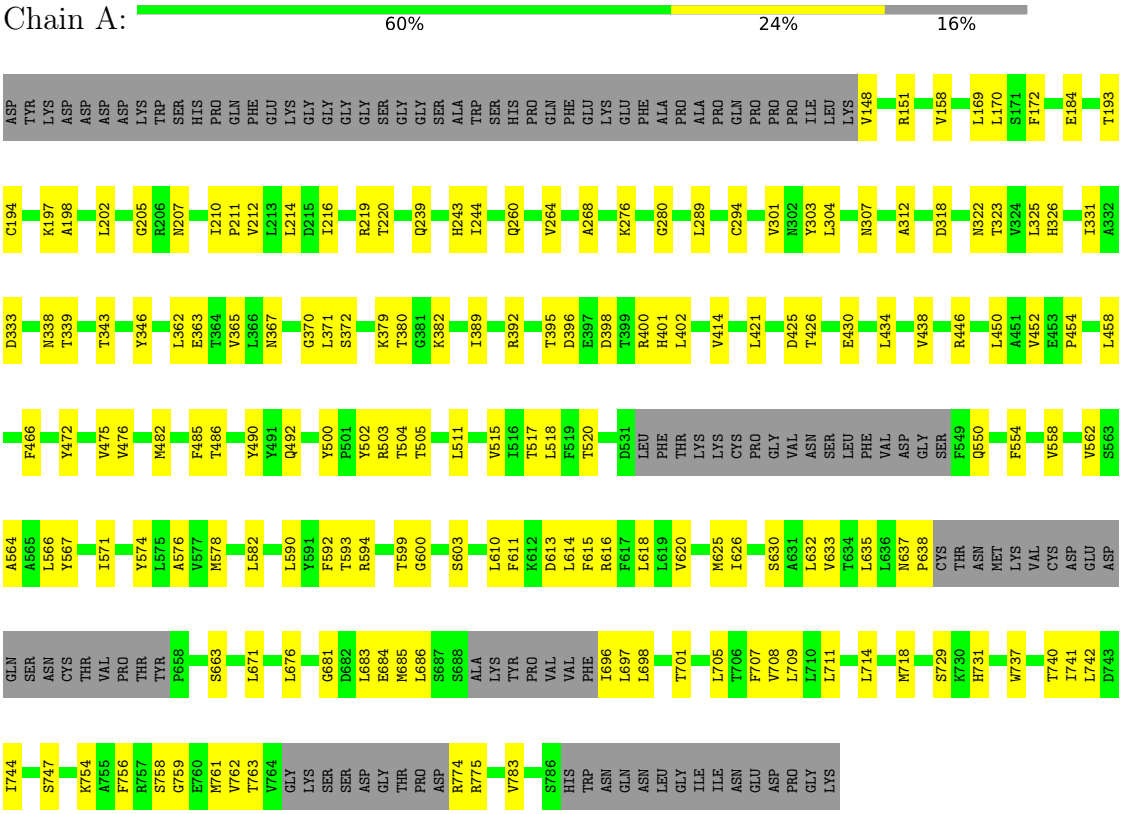
Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total	C	Cl	H	N	O	S	0
			74	28	2	32	4	6	2	
2	B	1	Total	C	Cl	H	N	O	S	0
			74	28	2	32	4	6	2	
2	C	1	Total	C	Cl	H	N	O	S	0
			74	28	2	32	4	6	2	
2	D	1	Total	C	Cl	H	N	O	S	0
			74	28	2	32	4	6	2	

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.

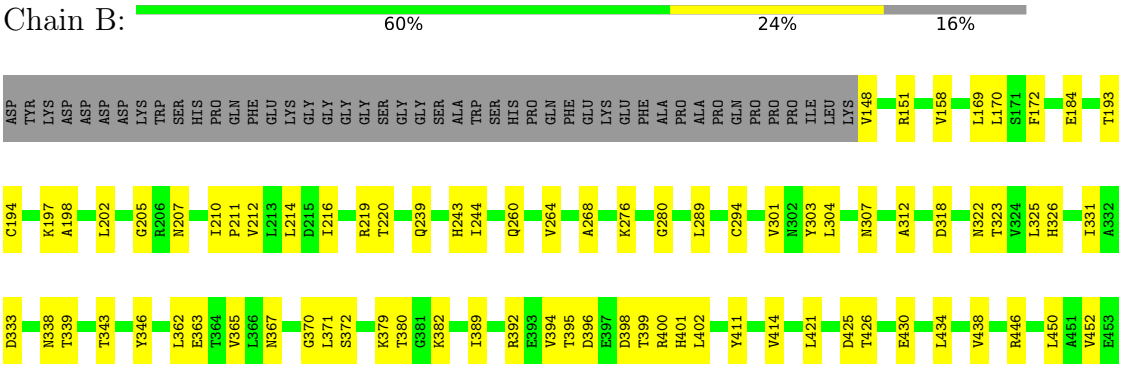
• Molecule 1: Transient receptor potential cation channel subfamily V member 4

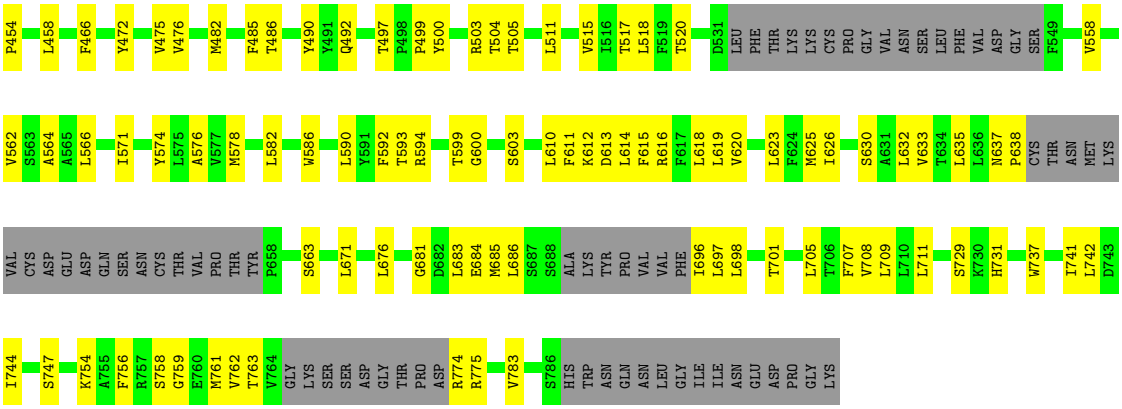
Chain A:



• Molecule 1: Transient receptor potential cation channel subfamily V member 4

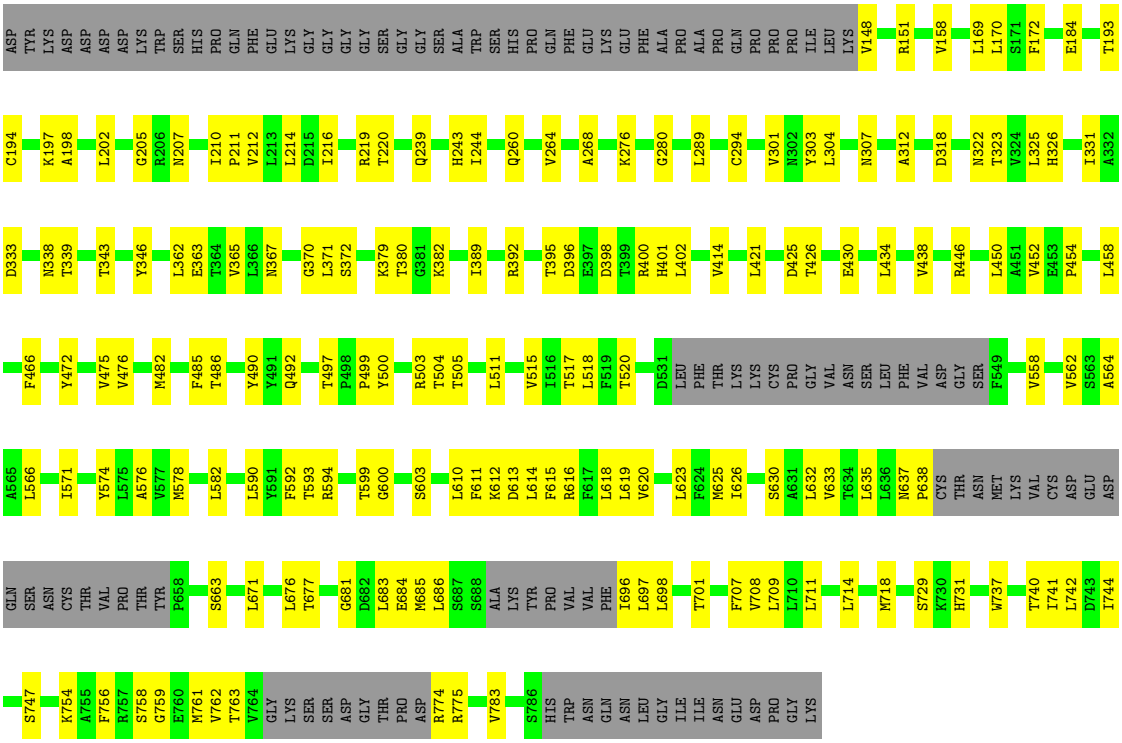
Chain B:





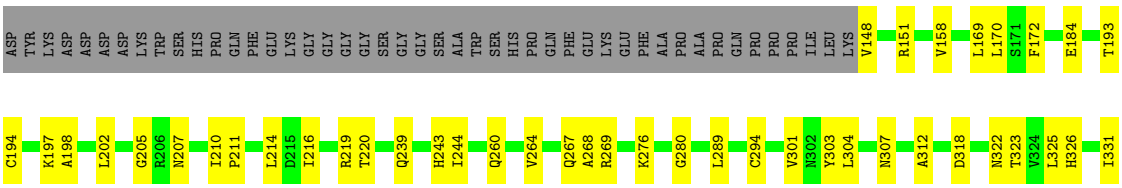
• Molecule 1: Transient receptor potential cation channel subfamily V member 4

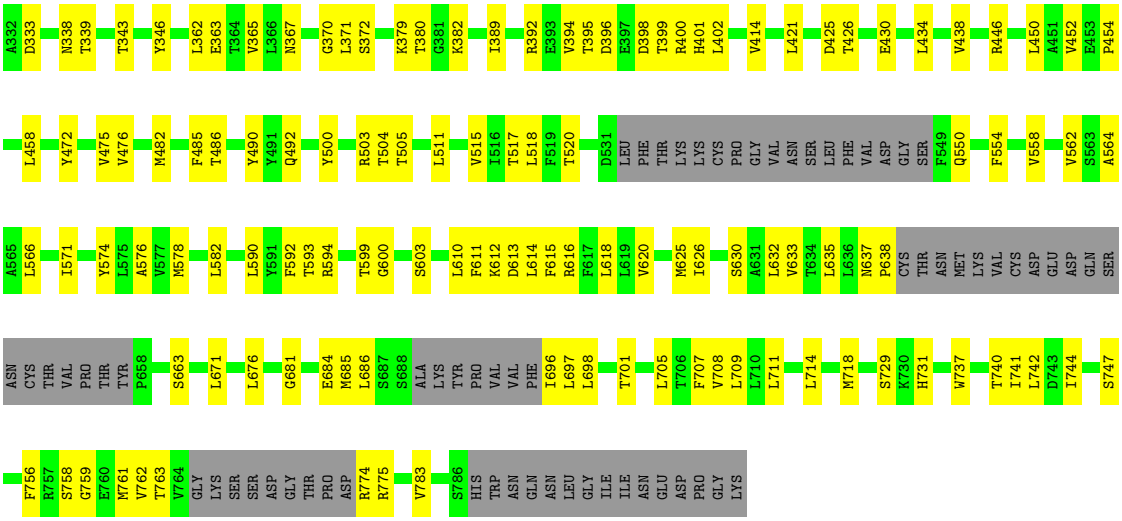
Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 4

Chain D:




A332 D333 N338 T339 T343 Y346 L362 E363 T364 V365 L366 N367 G370 L371 S372 K379 T380 G381 K382 I389 R392 E393 V394 T395 D396 E397 D398 T399 R400 H401 L402 V414 L421 D425 T426 E430 L434 V438 R446 L450 A451 V452 E453 P454
L458 Y472 V475 V476 M482 F485 T486 Y490 Y491 Q492 Y500 R503 T504 T505 L511 V515 I516 T517 L518 F519 T520 D531 LEU PHE THR LYS LYS CYS PRO GLY VAL ASN SER LEU PHE VAL ASP GLY SER F549 Q550 F554 V558 V562 S563 A564
A565 L566 I571 Y574 L575 A576 V577 M578 L582 L590 Y591 F592 T593 R594 T599 G600 S603 L610 F611 K612 D613 L614 F615 R616 F617 L618 L619 V620 M625 I626 S630 A631 L632 V633 T634 L635 L636 N637 P638 CYS THR ASN MET LYS VAL CYS ASP GLU ASP GLN SER
ASN CYS THR VAL PRO THR TYR P658 S663 L671 L676 G681 E684 M685 L686 S687 S688 ALA LYS TYR PRO VAL VAL PHE I696 L697 L698 T701 L705 T706 F707 V708 L709 L710 L711 L714 M718 S729 K730 H731 W737 T740 I741 L742 D743 I744 S747
F756 R757 S758 G759 E760 M761 V762 T763 V764 GLY LYS SER SER ASP GLY THR PRO ASP R774 R775 V783 S786 HIS TRP ASN GLN ASN LEU GLY ILE ILE ASN GLU ASP PRO GLY LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	452263	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	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: XQ3

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	0.25	0/4841	0.49	0/6557
1	B	0.25	0/4841	0.49	0/6557
1	C	0.25	0/4841	0.49	0/6557
1	D	0.25	0/4841	0.49	0/6557
All	All	0.25	0/19364	0.49	0/26228

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	4737	4820	4815	128	0
1	B	4737	4820	4815	129	0
1	C	4737	4820	4815	129	0
1	D	4737	4820	4815	125	0
2	A	42	32	0	1	0
2	B	42	32	0	1	0
2	C	42	32	0	1	0
2	D	42	32	0	1	0
All	All	19116	19408	19260	497	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 497 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:C:761:MET:O	1:C:774:ARG:N	2.04	0.90
1:A:761:MET:O	1:A:774:ARG:N	2.04	0.90
1:D:761:MET:O	1:D:774:ARG:N	2.04	0.90
1:B:761:MET:O	1:B:774:ARG:N	2.04	0.89
1:A:744:ILE:O	1:A:747:SER:OG	1.91	0.88

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	577/700 (82%)	539 (93%)	37 (6%)	1 (0%)	47 79
1	B	577/700 (82%)	539 (93%)	37 (6%)	1 (0%)	47 79
1	C	577/700 (82%)	539 (93%)	37 (6%)	1 (0%)	47 79
1	D	577/700 (82%)	539 (93%)	37 (6%)	1 (0%)	47 79
All	All	2308/2800 (82%)	2156 (93%)	148 (6%)	4 (0%)	50 79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	SER
1	B	663	SER
1	C	663	SER
1	D	663	SER

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	520/617 (84%)	520 (100%)	0	100	100
1	B	520/617 (84%)	520 (100%)	0	100	100
1	C	520/617 (84%)	520 (100%)	0	100	100
1	D	520/617 (84%)	520 (100%)	0	100	100
All	All	2080/2468 (84%)	2080 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	XQ3	A	901	-	41,45,45	2.52	10 (24%)	54,65,65	2.53	14 (25%)
2	XQ3	D	901	-	41,45,45	2.52	10 (24%)	54,65,65	2.53	14 (25%)
2	XQ3	C	901	-	41,45,45	2.52	10 (24%)	54,65,65	2.53	14 (25%)
2	XQ3	B	901	-	41,45,45	2.52	10 (24%)	54,65,65	2.53	14 (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
2	XQ3	A	901	-	-	9/39/51/51	0/4/4/4
2	XQ3	D	901	-	-	9/39/51/51	0/4/4/4
2	XQ3	C	901	-	-	9/39/51/51	0/4/4/4
2	XQ3	B	901	-	-	9/39/51/51	0/4/4/4

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	XQ3	C18-N19	8.03	1.46	1.34
2	B	901	XQ3	C18-N19	8.03	1.46	1.34
2	C	901	XQ3	C18-N19	8.03	1.46	1.34
2	D	901	XQ3	C18-N19	8.03	1.46	1.34
2	A	901	XQ3	C25-N22	7.71	1.46	1.34

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	XQ3	O40-S30-O31	-14.64	101.55	119.55
2	C	901	XQ3	O40-S30-O31	-14.64	101.55	119.55
2	B	901	XQ3	O40-S30-O31	-14.64	101.55	119.55
2	D	901	XQ3	O40-S30-O31	-14.64	101.55	119.55
2	D	901	XQ3	C33-C32-S30	-4.32	120.43	123.25

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	XQ3	C25-C26-N29-S30
2	A	901	XQ3	C27-C26-N29-S30
2	A	901	XQ3	C02-C04-C05-N06
2	A	901	XQ3	C18-C05-N06-C07
2	B	901	XQ3	C25-C26-N29-S30

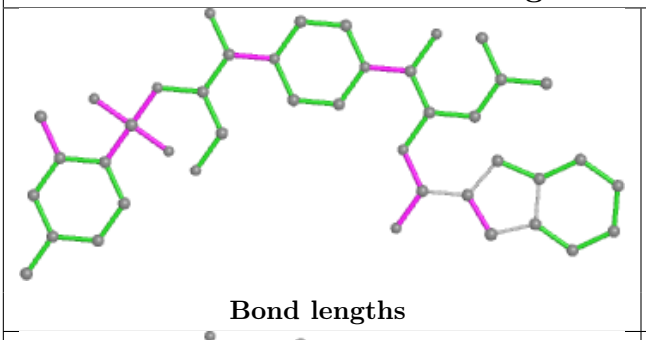
There are no ring outliers.

4 monomers are involved in 4 short contacts:

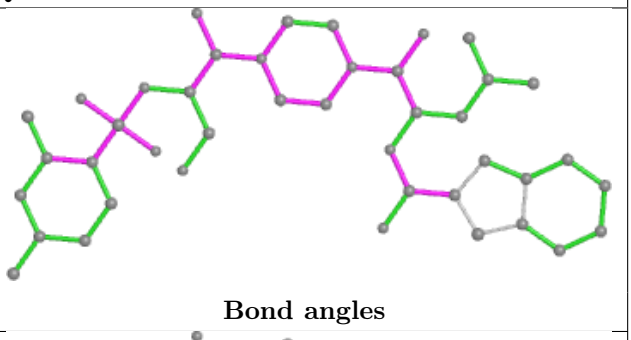
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	XQ3	1	0
2	D	901	XQ3	1	0
2	C	901	XQ3	1	0
2	B	901	XQ3	1	0

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 then 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.

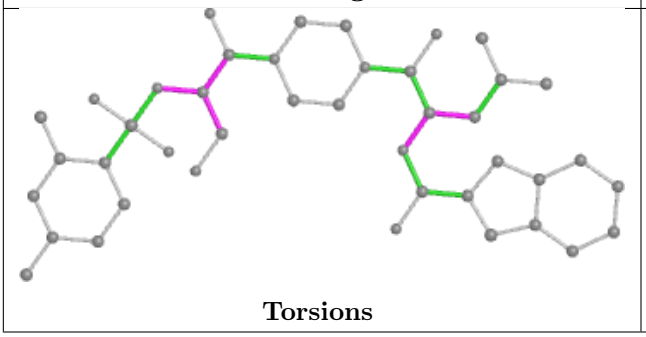
Ligand XQ3 A 901



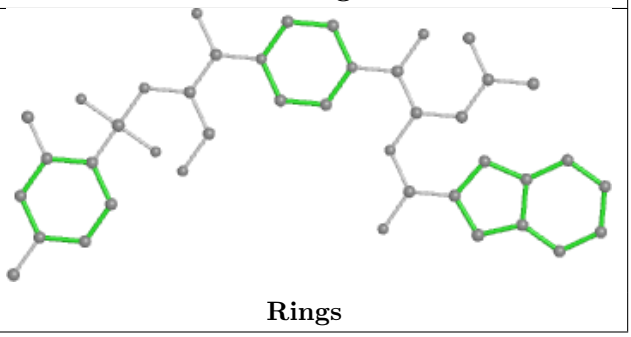
Bond lengths



Bond angles

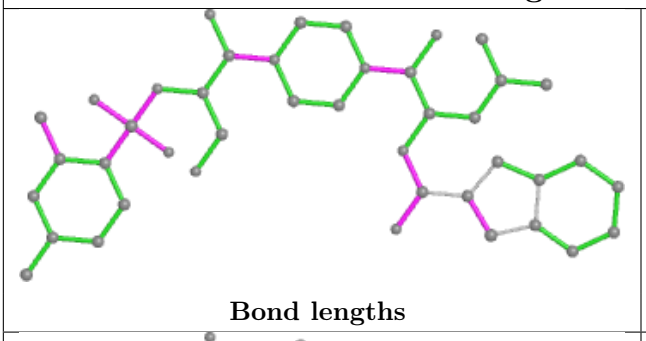


Torsions

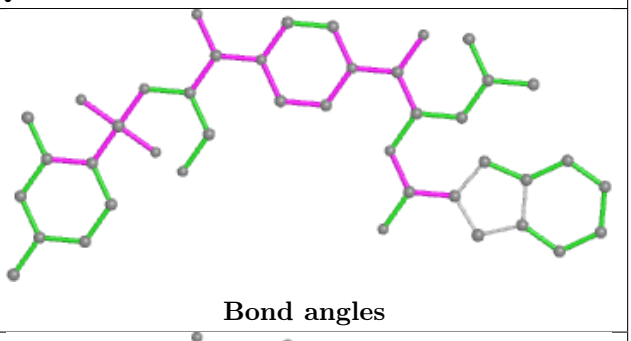


Rings

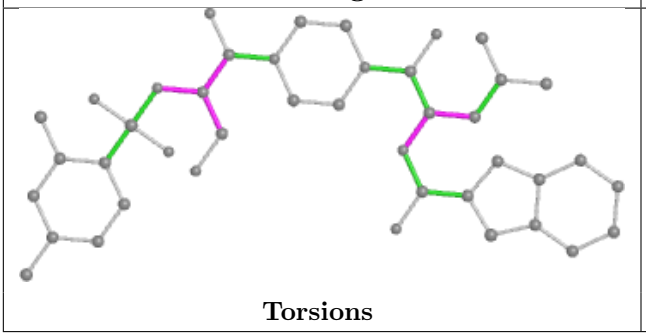
Ligand XQ3 D 901



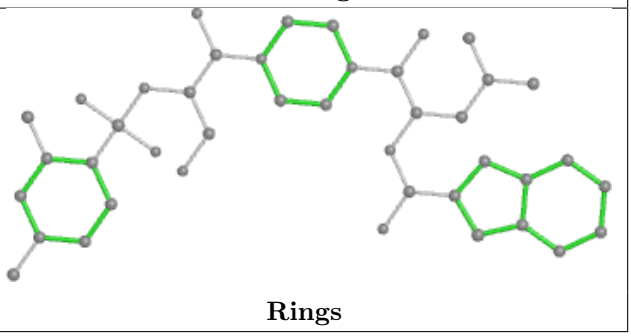
Bond lengths



Bond angles

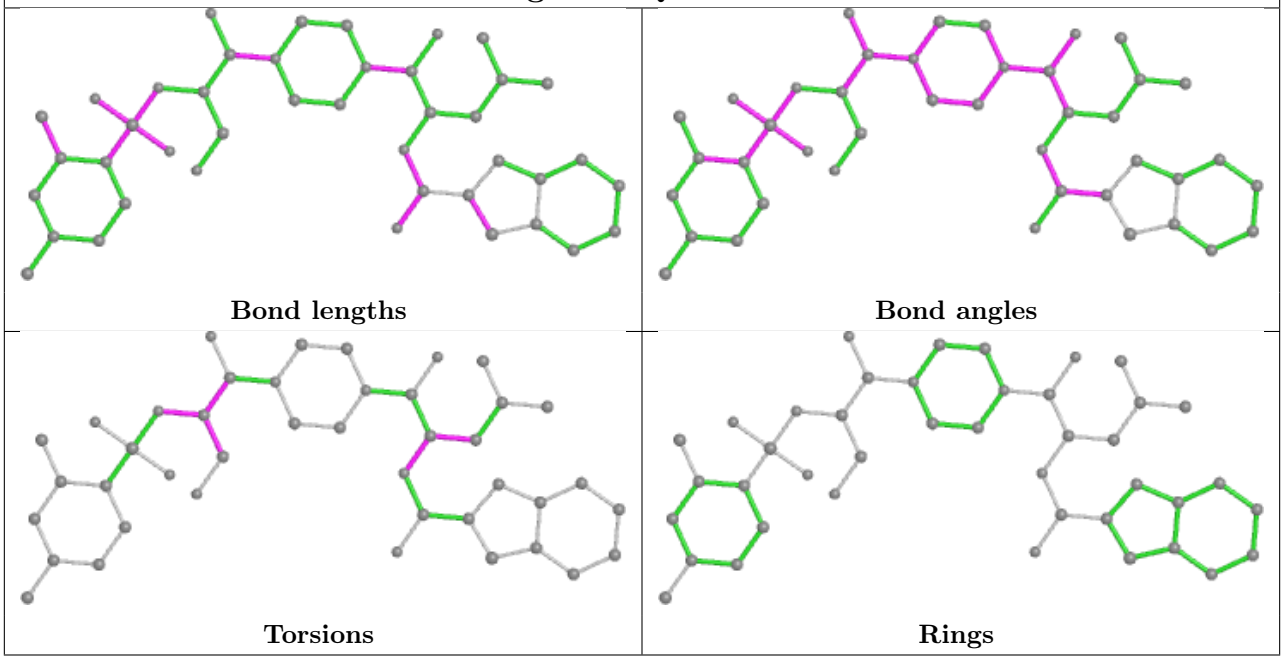


Torsions



Rings

Ligand XQ3 C 901



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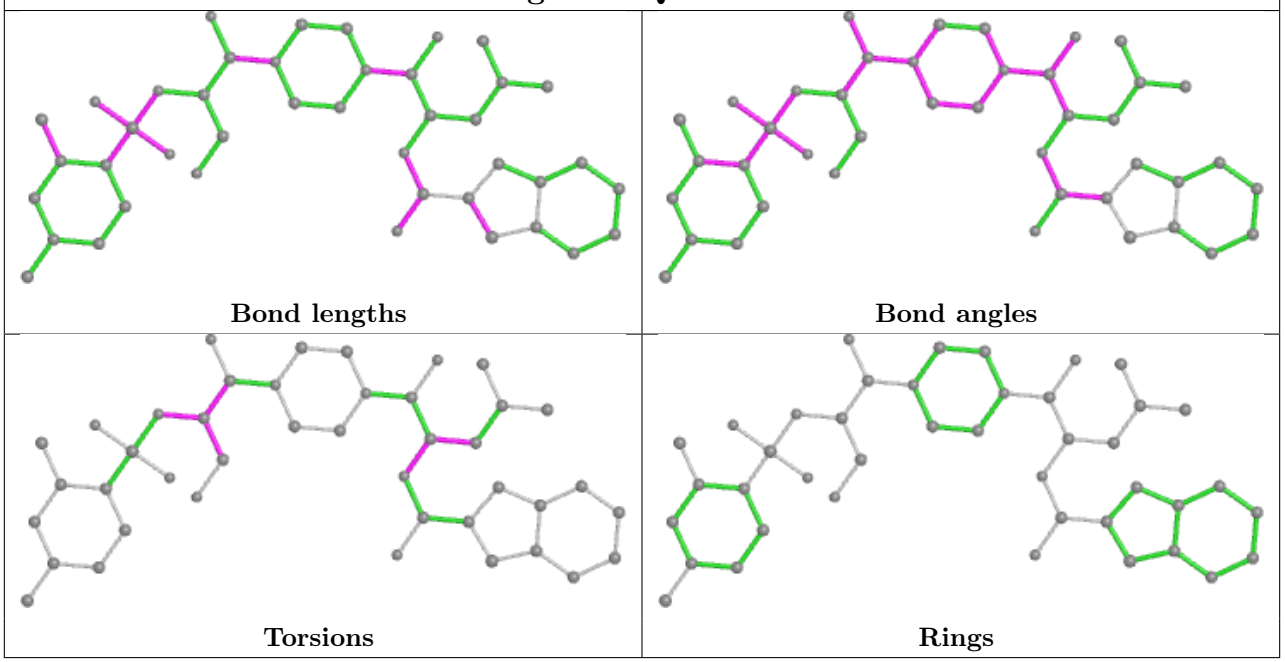

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.