Full wwPDB EM Validation Report

Jul 9, 2025 – 12:25 PM JST

PDB ID	:	8IWS / pdb_00008iws
EMDB ID	:	EMD-35778
Title	:	hSPCA1 in the CaE2P state
Authors	:	Liu, Z.M.; Wu, M.Q.; Wu, C.
Deposited on	:	2023-03-31
Resolution	:	3.42 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:

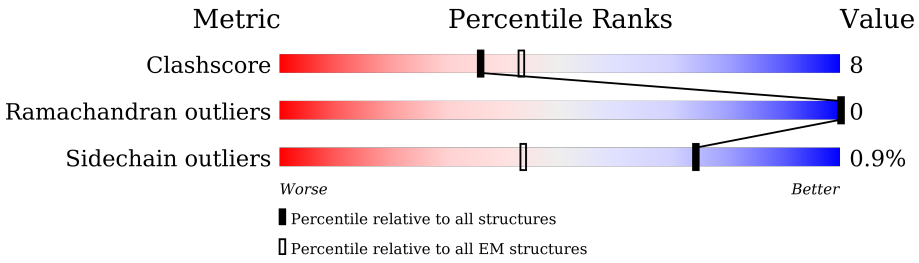
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	919	78% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6809 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 Calcium-transporting ATPase type 2C member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	890	Total	C	N	O	S	0	0
			6803	4336	1137	1278	52		

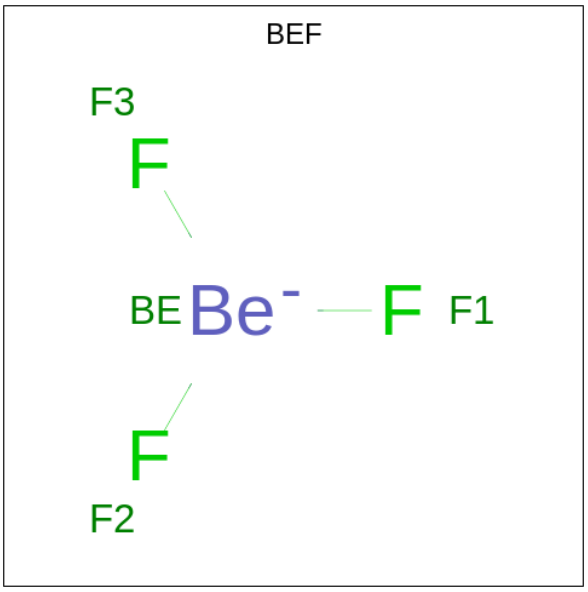
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



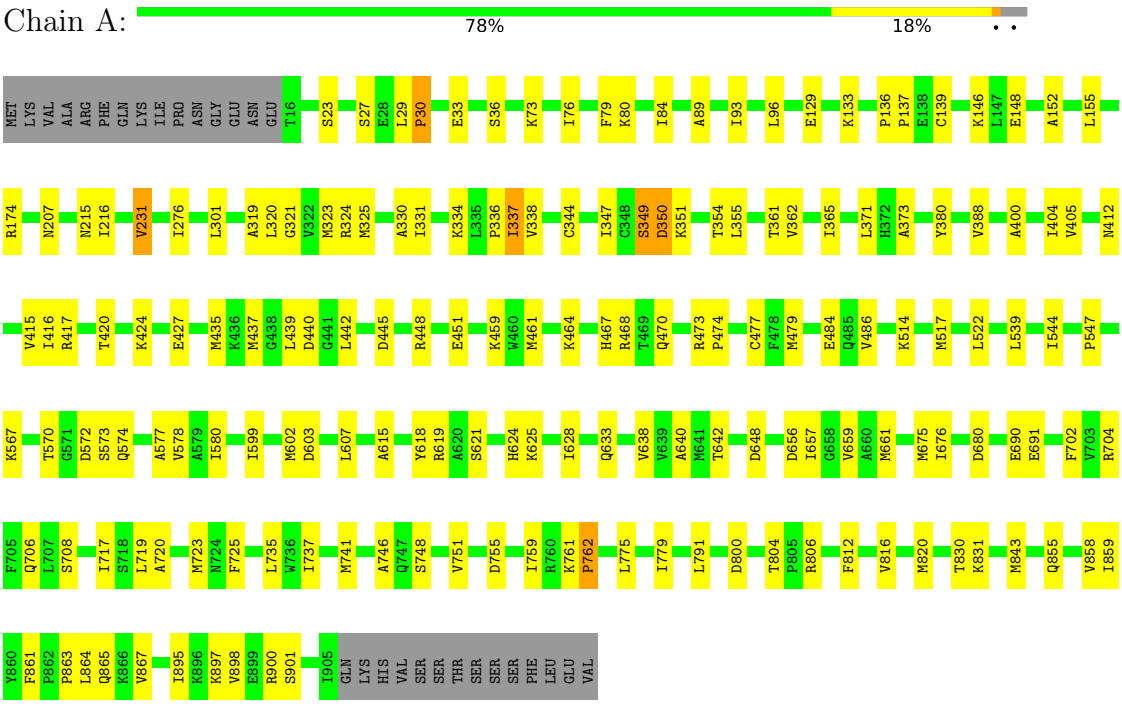
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
4	A	1	4	1	3	0

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: Calcium-transporting ATPase type 2C member 1

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151506	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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: CA, MG, BEF

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	0.20	2/6911 (0.0%)	0.39	7/9359 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ASP	C-O	-7.12	1.15	1.24
1	A	350	ASP	CA-CB	-6.02	1.45	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	ASP	CA-C-N	9.62	133.16	120.28
1	A	350	ASP	C-N-CA	9.62	133.16	120.28
1	A	349	SER	O-C-N	-7.52	114.91	123.48
1	A	762	PRO	CA-C-N	6.31	126.33	119.90
1	A	762	PRO	C-N-CA	6.31	126.33	119.90
1	A	30	PRO	CB-CA-C	-6.17	101.37	111.56
1	A	350	ASP	O-C-N	-5.46	116.85	123.13

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	6803	0	7022	105	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	0	1	0
All	All	6809	0	7022	105	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 8.

All (105) 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:761:LYS:HE3	1:A:762:PRO:HD2	1.66	0.75
1:A:27:SER:HA	1:A:215:ASN:HD21	1.58	0.67
1:A:347:ILE:HG12	1:A:640:ALA:HB3	1.78	0.66
1:A:331:ILE:HB	1:A:676:ILE:HB	1.78	0.66
1:A:633:GLN:NE2	1:A:656:ASP:OD1	2.29	0.65
1:A:334:LYS:HD3	1:A:336:PRO:HD2	1.78	0.64
1:A:830:THR:HG23	1:A:831:LYS:HE2	1.81	0.63
1:A:320:LEU:HD11	1:A:751:VAL:HG23	1.79	0.63
1:A:445:ASP:HA	1:A:468:ARG:HD2	1.80	0.63
1:A:351:LYS:HG3	1:A:580:ILE:HG21	1.79	0.63
1:A:365:ILE:HB	1:A:373:ALA:HB3	1.81	0.61
1:A:602:MET:HE1	1:A:607:LEU:HD12	1.82	0.61
1:A:470:GLN:HG3	1:A:473:ARG:HB2	1.83	0.61
1:A:321:GLY:HA3	1:A:338:VAL:HG11	1.83	0.60
1:A:89:ALA:O	1:A:93:ILE:HG23	2.03	0.58
1:A:816:VAL:O	1:A:820:MET:HG2	2.04	0.57
1:A:464:LYS:HD3	1:A:477:CYS:HB2	1.85	0.57
1:A:861:PHE:HD2	1:A:864:LEU:HD23	1.69	0.57
1:A:621:SER:H	1:A:624:HIS:HB2	1.69	0.56
1:A:804:THR:HG22	1:A:806:ARG:H	1.71	0.55
1:A:859:ILE:O	1:A:865:GLN:NE2	2.38	0.55
1:A:603:ASP:N	1:A:603:ASP:OD1	2.39	0.55
1:A:79:PHE:HA	1:A:84:ILE:HG21	1.88	0.54
1:A:380:TYR:HB3	1:A:416:ILE:HD13	1.89	0.53
1:A:435:MET:HG3	1:A:440:ASP:HB3	1.89	0.53
1:A:350:ASP:OD2	4:A:1003:BEF:F1	2.17	0.53
1:A:706:GLN:NE2	1:A:741:MET:SD	2.81	0.52
1:A:574:GLN:O	1:A:578:VAL:HG22	2.10	0.52
1:A:473:ARG:HG2	1:A:474:PRO:HD2	1.91	0.52
1:A:344:CYS:HA	1:A:638:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:HB2	1:A:427:GLU:HG3	1.91	0.51
1:A:448:ARG:NE	1:A:451:GLU:OE2	2.44	0.51
1:A:567:LYS:HA	1:A:615:ALA:HB1	1.92	0.51
1:A:417:ARG:O	1:A:420:THR:OG1	2.25	0.51
1:A:719:LEU:HD13	1:A:791:LEU:HD11	1.93	0.50
1:A:723:MET:HE3	1:A:725:PHE:HE2	1.75	0.50
1:A:412:ASN:HD21	1:A:427:GLU:HB3	1.76	0.50
1:A:337:ILE:HD12	1:A:657:ILE:HD13	1.92	0.50
1:A:349:SER:HA	1:A:642:THR:HG22	1.93	0.49
1:A:863:PRO:O	1:A:867:VAL:HG12	2.13	0.49
1:A:517:MET:HG2	1:A:522:LEU:HD12	1.94	0.49
1:A:459:LYS:HA	1:A:459:LYS:HE2	1.95	0.49
1:A:800:ASP:OD1	1:A:800:ASP:N	2.44	0.49
1:A:858:VAL:HG22	1:A:864:LEU:HD12	1.95	0.48
1:A:704:ARG:HB2	1:A:775:LEU:HD21	1.95	0.48
1:A:570:THR:HG22	1:A:572:ASP:HB3	1.96	0.48
1:A:404:ILE:HG12	1:A:539:LEU:HB3	1.96	0.47
1:A:29:LEU:HB3	1:A:30:PRO:HD2	1.95	0.47
1:A:337:ILE:HG23	1:A:657:ILE:HD13	1.97	0.47
1:A:146:LYS:NZ	1:A:148:GLU:OE2	2.47	0.47
1:A:861:PHE:HB3	1:A:864:LEU:HB2	1.95	0.47
1:A:324:ARG:HD2	1:A:691:GLU:HG2	1.96	0.47
1:A:325:MET:HA	1:A:325:MET:HE3	1.97	0.47
1:A:690:GLU:HG2	1:A:759:ILE:HG23	1.97	0.47
1:A:412:ASN:ND2	1:A:427:GLU:HB3	2.30	0.47
1:A:599:ILE:HD13	1:A:628:ILE:HD11	1.98	0.46
1:A:301:LEU:HD11	1:A:717:ILE:HG13	1.97	0.46
1:A:73:LYS:HA	1:A:76:ILE:HB	1.97	0.46
1:A:897:LYS:NZ	1:A:900:ARG:HE	2.14	0.46
1:A:133:LYS:HD3	1:A:133:LYS:HA	1.73	0.46
1:A:720:ALA:HA	1:A:725:PHE:CZ	2.51	0.46
1:A:737:ILE:HG13	1:A:812:PHE:HE1	1.81	0.46
1:A:900:ARG:HG3	1:A:901:SER:N	2.30	0.46
1:A:139:CYS:HB3	1:A:152:ALA:HB2	1.97	0.45
1:A:708:SER:HA	1:A:779:ILE:HG23	1.98	0.45
1:A:405:VAL:HG21	1:A:437:MET:HE2	1.99	0.45
1:A:439:LEU:HD13	1:A:442:LEU:HD22	1.98	0.45
1:A:152:ALA:HA	1:A:155:LEU:HG	1.99	0.45
1:A:690:GLU:HB3	1:A:759:ILE:HD12	2.00	0.44
1:A:371:LEU:HD21	1:A:388:VAL:HB	1.99	0.44
1:A:602:MET:SD	1:A:607:LEU:HB2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:THR:HG21	1:A:577:ALA:HB2	2.00	0.44
1:A:33:GLU:HA	1:A:36:SER:OG	2.17	0.44
1:A:319:ALA:O	1:A:323:MET:HG2	2.18	0.43
1:A:479:MET:HE2	1:A:486:VAL:HA	2.00	0.43
1:A:723:MET:HE3	1:A:725:PHE:CE2	2.53	0.43
1:A:129:GLU:HG3	1:A:129:GLU:O	2.19	0.43
1:A:484:GLU:OE1	1:A:514:LYS:NZ	2.52	0.43
1:A:325:MET:HB3	1:A:330:ALA:HB3	2.01	0.43
1:A:27:SER:OG	1:A:207:ASN:ND2	2.40	0.42
1:A:351:LYS:HD2	1:A:580:ILE:HG13	2.00	0.42
1:A:23:SER:HB2	1:A:216:ILE:HG12	2.01	0.42
1:A:735:LEU:HD23	1:A:735:LEU:HA	1.86	0.42
1:A:659:VAL:HG13	1:A:675:MET:HG2	2.01	0.42
1:A:895:ILE:HA	1:A:898:VAL:HG22	2.01	0.42
1:A:361:THR:HB	1:A:547:PRO:HG3	2.01	0.42
1:A:855:GLN:HE21	1:A:859:ILE:HG13	1.84	0.42
1:A:708:SER:HB3	1:A:779:ILE:HG12	2.01	0.42
1:A:216:ILE:HD12	1:A:216:ILE:HA	1.94	0.42
1:A:572:ASP:CG	1:A:573:SER:N	2.78	0.42
1:A:625:LYS:NZ	1:A:648:ASP:OD1	2.39	0.42
1:A:174:ARG:HB3	1:A:231:VAL:HG13	2.01	0.41
1:A:400:ALA:O	1:A:404:ILE:HG13	2.20	0.41
1:A:467:HIS:HB3	1:A:470:GLN:HB3	2.01	0.41
1:A:136:PRO:HA	1:A:137:PRO:HD3	1.90	0.41
1:A:362:VAL:HG22	1:A:544:ILE:HG12	2.02	0.41
1:A:618:TYR:HD2	1:A:619:ARG:HG2	1.84	0.41
1:A:748:SER:O	1:A:751:VAL:HG12	2.21	0.41
1:A:80:LYS:HD3	1:A:80:LYS:HA	1.71	0.41
1:A:661:MET:HE3	1:A:680:ASP:HB3	2.02	0.41
1:A:755:ASP:OD1	1:A:755:ASP:N	2.54	0.41
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.93	0.40
1:A:702:PHE:HE1	1:A:746:ALA:HB1	1.85	0.40
1:A:704:ARG:HA	1:A:779:ILE:HD11	2.03	0.40
1:A:354:THR:OG1	1:A:355:LEU:N	2.53	0.40

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	888/919 (97%)	849 (96%)	39 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	764/792 (96%)	757 (99%)	7 (1%)	75 86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	231	VAL
1	A	276	ILE
1	A	337	ILE
1	A	415	VAL
1	A	461	MET
1	A	843	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	202	GLN
1	A	345	ASN
1	A	470	GLN
1	A	697	ASN

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	BEF	A	1003	1	0,3,3	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

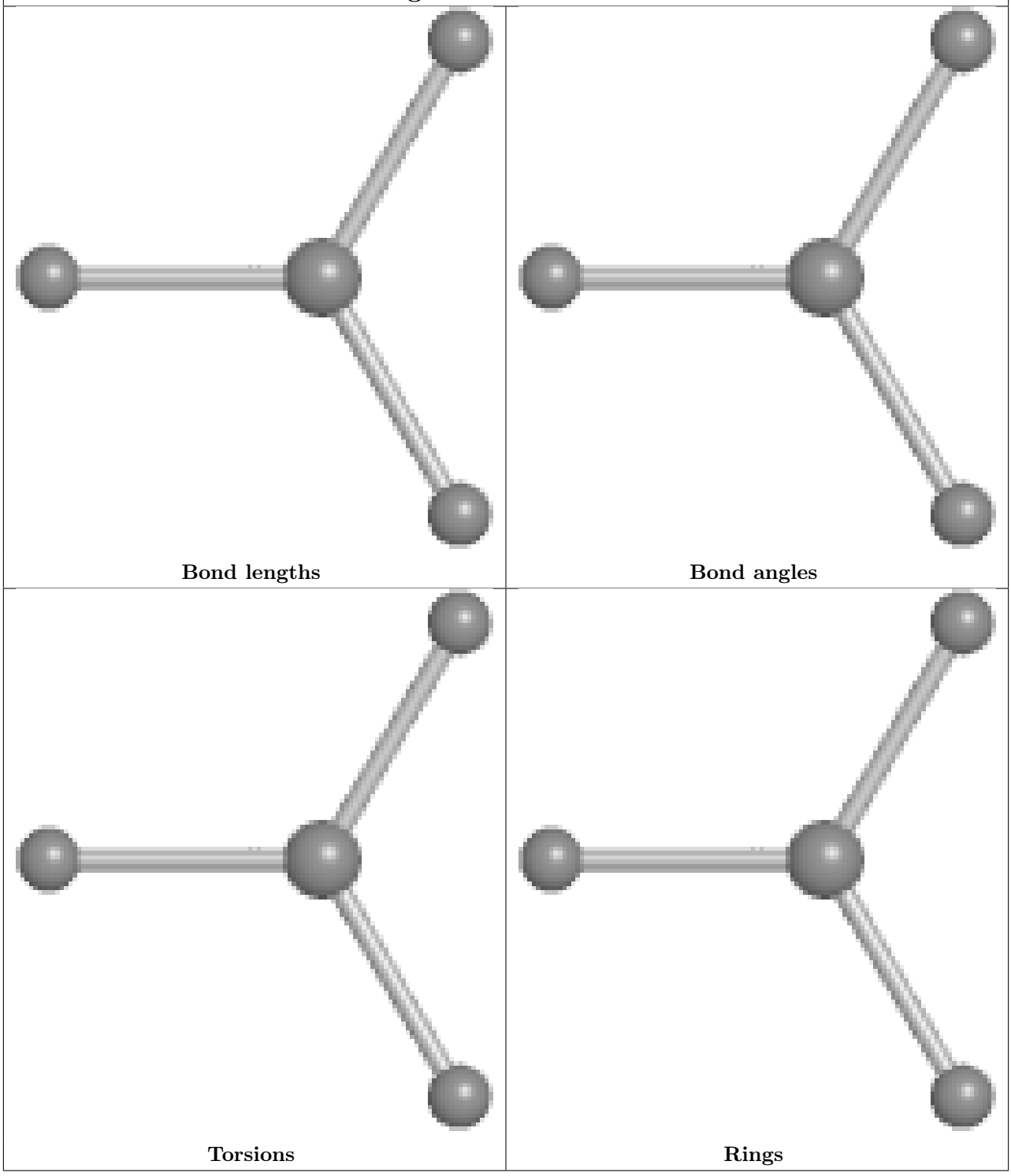
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	BEF	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 BEF A 1003



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.