W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 12:12 PM EDT

PDB ID	:	1BKC
Title	:	CATALYTIC DOMAIN OF TNF-ALPHA CONVERTING ENZYME (TACE)
Authors	:	Maskos, K.; Fernandez-Catalan, C.; Bode, W.
Deposited on	:	1998-04-23
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

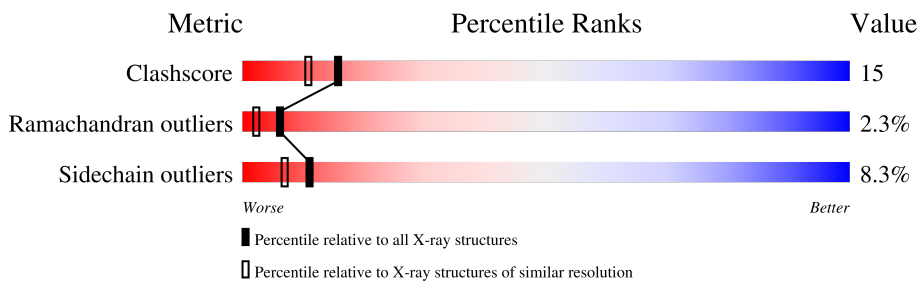|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		2.3%
Sidechain outliers		8.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	68% 25% 5% •
1	C	256	63% 25% 9% • •
2	E	256	69% 26% • •
3	I	256	71% 22% 5% • •

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
5	INN	A	2	X	-	-	-
5	INN	C	2	X	-	-	-
5	INN	E	2	X	-	-	-
5	INN	I	2	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9822 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total 2025	C 1274	N 342	O 396	S 13	9	0	0
1	C	254	Total 2012	C 1265	N 340	O 394	S 13	127	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	engineered mutation	UNP P78536
A	452	GLN	ASN	engineered mutation	UNP P78536
C	266	ALA	SER	engineered mutation	UNP P78536
C	452	GLN	ASN	engineered mutation	UNP P78536

- Molecule 2 is a protein called TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	256	Total 2028	C 1275	N 344	O 396	S 13	18	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	266	ALA	SER	engineered mutation	UNP P78536
E	420	LYS	LEU	conflict	UNP P78536
E	452	GLN	ASN	engineered mutation	UNP P78536

- Molecule 3 is a protein called TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	254	Total 2017	C 1269	N 341	O 394	S 13	48	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	266	ALA	SER	engineered mutation	UNP P78536
I	428	GLU	ASP	conflict	UNP P78536
I	452	GLN	ASN	engineered mutation	UNP P78536

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0
4	E	1	Total 1	Zn 1	0	0
4	I	1	Total 1	Zn 1	0	0

- Molecule 5 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-3-methyl-L-valyl-N-(2-aminoethyl)-L-alaninamide (three-letter code: INN) (formula: $C_{19}H_{37}N_5O_5$).
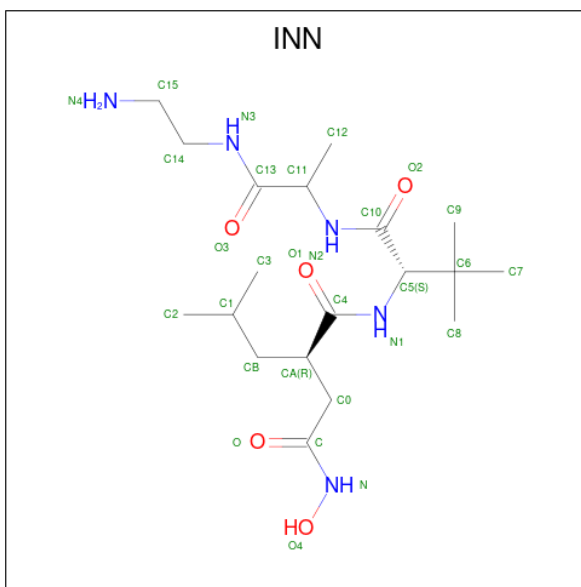
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 29	C 19	N 5	O 5	0	0
5	C	1	Total 29	C 19	N 5	O 5	0	0
5	E	1	Total 29	C 19	N 5	O 5	0	0
5	I	1	Total 29	C 19	N 5	O 5	0	0

• Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	572	Total 572	O 572	0	0
6	C	442	Total 442	O 442	0	0
6	E	368	Total 368	O 368	0	0
6	I	238	Total 238	O 238	0	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.
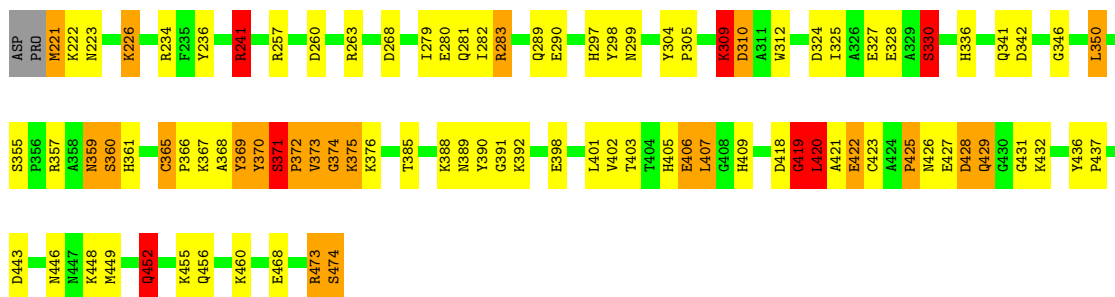
Note EDS was not executed.

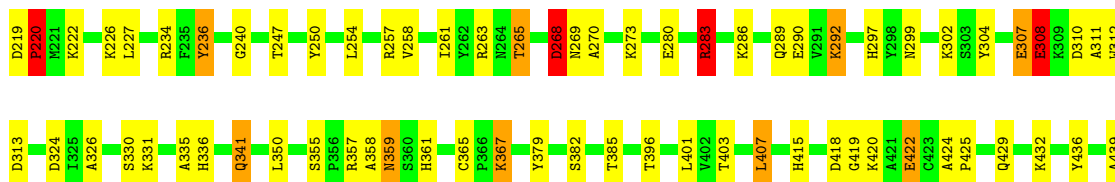- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain A:
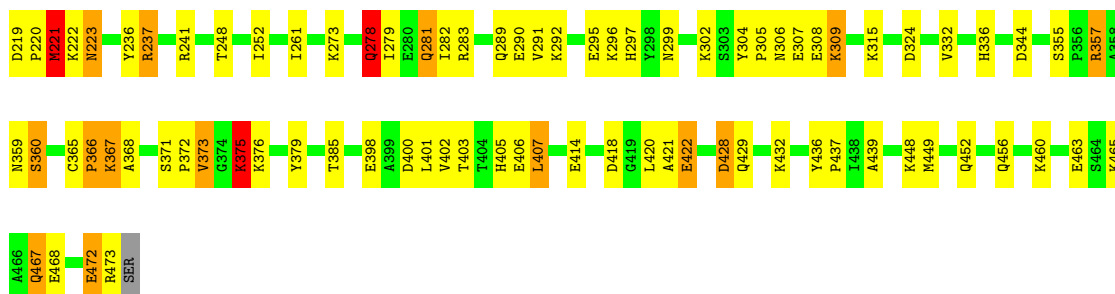
- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain C:

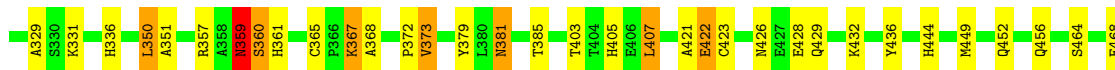- Molecule 2: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain E:

D443 H444 E445 K448 Q452 K455 K465 A466 Q467 E468 C469 F470 S474

• Molecule 3: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain I:

71%   22%   5% ••

ASP PRO M221 K226 L227 H233 R234 F235 Y236 R237 E243 T248 R257 I261 Y262 R263 N264 T265 N269 A270 Q278 I279 E280 Q281 I282 R283 I284 L285 K286 S287 P288 V291 K292 P293 K296 H297 Y298 N299 P305 N306 E307 D310 D313 V314 K315 E319

A329 S330 K331 H336 L350 A351 R357 A358 N359 S360 H361 C365 P366 K367 A368 P372 V373 Y379 L380 N381 T385 T403 T404 H405 E406 L407 A421 E422 C423 N426 E427 E428 Q429 K432 Y436 H444 M449 Q452 Q456 S464 E468

E472 R473 S474

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.38Å 126.27Å 81.27Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	12.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.00)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, INN

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	0.73	1/2071 (0.0%)	1.43	16/2795 (0.6%)
1	C	1.29	13/2056 (0.6%)	2.03	52/2773 (1.9%)
2	E	0.81	2/2074 (0.1%)	1.60	33/2798 (1.2%)
3	I	0.80	4/2062 (0.2%)	1.54	25/2781 (0.9%)
All	All	0.93	20/8263 (0.2%)	1.67	126/11147 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	7
2	E	0	2
3	I	0	3
All	All	0	14

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	420	LEU	C-N	-29.95	0.65	1.34
1	C	376	LYS	C-N	-15.38	0.98	1.34
1	C	452	GLN	C-N	-14.60	1.00	1.34
1	C	374	GLY	N-CA	12.40	1.64	1.46
1	A	376	LYS	C-N	-10.51	1.09	1.34

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	452	GLN	O-C-N	-28.28	77.45	122.70
1	C	419	GLY	O-C-N	-25.11	82.52	122.70
1	C	420	LEU	O-C-N	-22.23	87.13	122.70
1	C	369	TYR	O-C-N	21.44	157.01	122.70
1	C	420	LEU	C-N-CA	21.12	174.51	121.70

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLN	Mainchain
1	A	375	LYS	Mainchain
1	C	371	SER	Peptide,Mainchain
1	C	375	LYS	Peptide
1	C	419	GLY	Mainchain

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	2025	0	1937	67	2
1	C	2012	0	1915	58	4
2	E	2028	0	1937	55	2
3	I	2017	0	1931	50	4
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	29	0	34	1	1
5	C	29	0	35	1	0
5	E	29	0	35	1	1
5	I	29	0	35	0	1
6	A	572	0	0	21	18
6	C	442	0	0	16	8
6	E	368	0	0	9	18
6	I	238	0	0	8	9
All	All	9822	0	7859	231	34

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 15.

The worst 5 of 231 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)
3:I:350:LEU:HG	6:I:1289:HOH:O	1.60	1.00
3:I:281:GLN:HE21	3:I:283:ARG:HE	0.99	0.97
1:C:279:ILE:HG23	6:C:838:HOH:O	1.64	0.95
1:A:219:ASP:N	1:A:467:GLN:HE22	1.67	0.91
1:C:281:GLN:HE21	1:C:283:ARG:NE	1.68	0.91

The worst 5 of 34 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:GLN:CD	6:A:1012:HOH:O[1_655]	1.08	1.12
1:C:452:GLN:CG	6:A:1012:HOH:O[1_655]	1.20	1.00
6:A:920:HOH:O	6:E:606:HOH:O[2_546]	1.55	0.65
6:A:710:HOH:O	6:I:1189:HOH:O[2_656]	1.56	0.64
6:A:600:HOH:O	6:E:628:HOH:O[2_546]	1.66	0.54

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 X-ray entries followed by that with respect to entries of similar resolution.

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	253/256 (99%)	241 (95%)	8 (3%)	4 (2%)	9	4
1	C	250/256 (98%)	228 (91%)	14 (6%)	8 (3%)	4	1
2	E	254/256 (99%)	238 (94%)	11 (4%)	5 (2%)	7	3
3	I	252/256 (98%)	243 (96%)	3 (1%)	6 (2%)	6	2
All	All	1009/1024 (98%)	950 (94%)	36 (4%)	23 (2%)	6	2

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	MET
1	A	373	VAL
1	C	370	TYR
1	C	371	SER
1	C	372	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	218/219 (100%)	198 (91%)	20 (9%)	9	5
1	C	216/219 (99%)	195 (90%)	21 (10%)	8	4
2	E	218/219 (100%)	202 (93%)	16 (7%)	14	9
3	I	217/219 (99%)	202 (93%)	15 (7%)	15	11
All	All	869/876 (99%)	797 (92%)	72 (8%)	11	7

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	263	ARG
3	I	474	SER
3	I	288	PRO
3	I	361	HIS
1	C	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	336	HIS
3	I	381	ASN
1	C	306	ASN
1	C	297	HIS
3	I	429	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
5	INN	C	2	4	28,28,28	3.65	6 (21%)	36,38,38	5.21	22 (61%)
5	INN	I	2	4	28,28,28	3.75	6 (21%)	36,38,38	4.71	19 (52%)
5	INN	E	2	4	28,28,28	3.53	5 (17%)	36,38,38	3.97	15 (41%)
5	INN	A	2	4	28,28,28	3.41	4 (14%)	36,38,38	5.23	22 (61%)

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
5	INN	C	2	4	1/1/9/13	8/40/40/40	-
5	INN	I	2	4	1/1/9/13	8/40/40/40	-
5	INN	E	2	4	1/1/9/13	8/40/40/40	-
5	INN	A	2	4	1/1/9/13	8/40/40/40	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	INN	C4-N1	13.70	1.64	1.34
5	C	2	INN	C4-N1	12.90	1.62	1.34
5	E	2	INN	C4-N1	12.31	1.61	1.34
5	A	2	INN	C4-N1	11.94	1.60	1.34
5	A	2	INN	C11-C13	-9.11	1.29	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	INN	C11-C13-N3	20.02	157.88	116.45
5	A	2	INN	C11-C13-N3	17.58	152.85	116.45
5	I	2	INN	C11-C13-N3	16.82	151.27	116.45
5	C	2	INN	O3-C13-C11	-12.99	91.70	120.52
5	E	2	INN	O3-C13-C11	-12.84	92.04	120.52

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	2	INN	C11
5	C	2	INN	C11
5	E	2	INN	C11
5	I	2	INN	C11

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2	INN	C0-C-N-O4
5	A	2	INN	O-C-N-O4
5	A	2	INN	N3-C14-C15-N4
5	C	2	INN	O-C-N-O4
5	C	2	INN	C13-C11-N2-C10

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	INN	1	0
5	I	2	INN	0	1
5	E	2	INN	1	1
5	A	2	INN	1	1

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 INN C 2

Bond lengths

Bond angles

Torsions

Rings

Ligand INN I 2

Bond lengths

Bond angles

Torsions

Rings

Ligand INN E 2

Bond lengths

Bond angles

Torsions

Rings

Ligand INN A 2

Bond lengths

Bond angles

Torsions

Rings
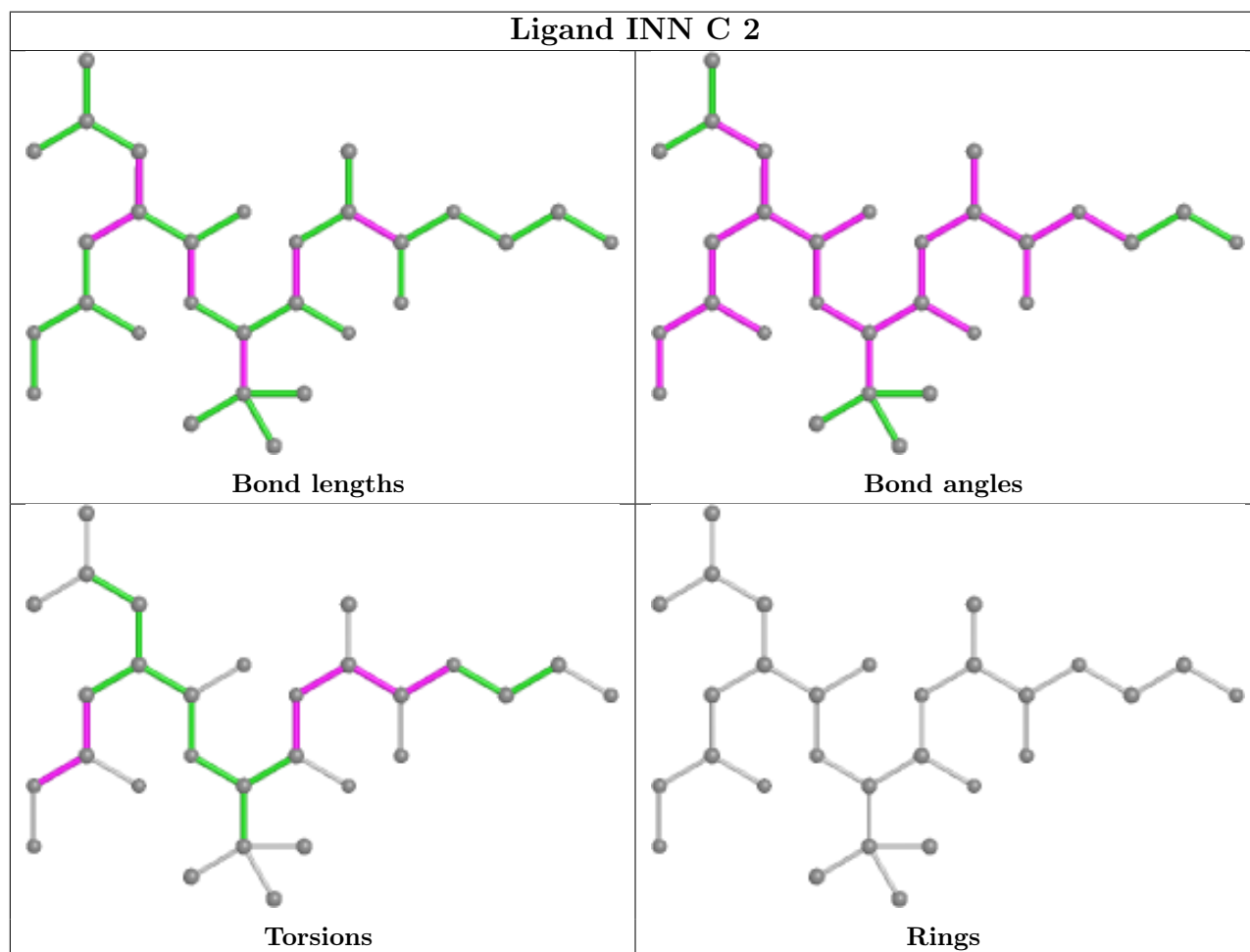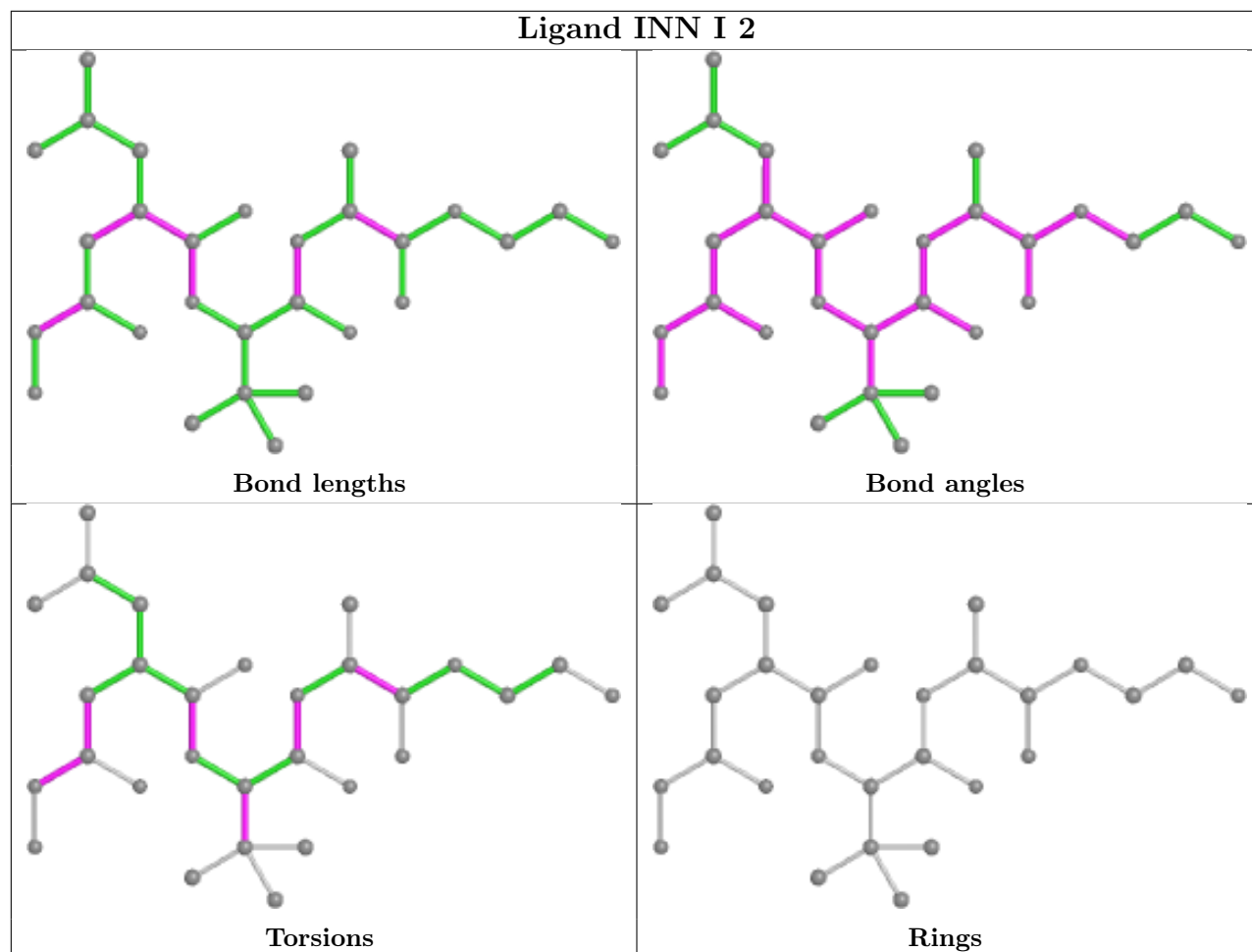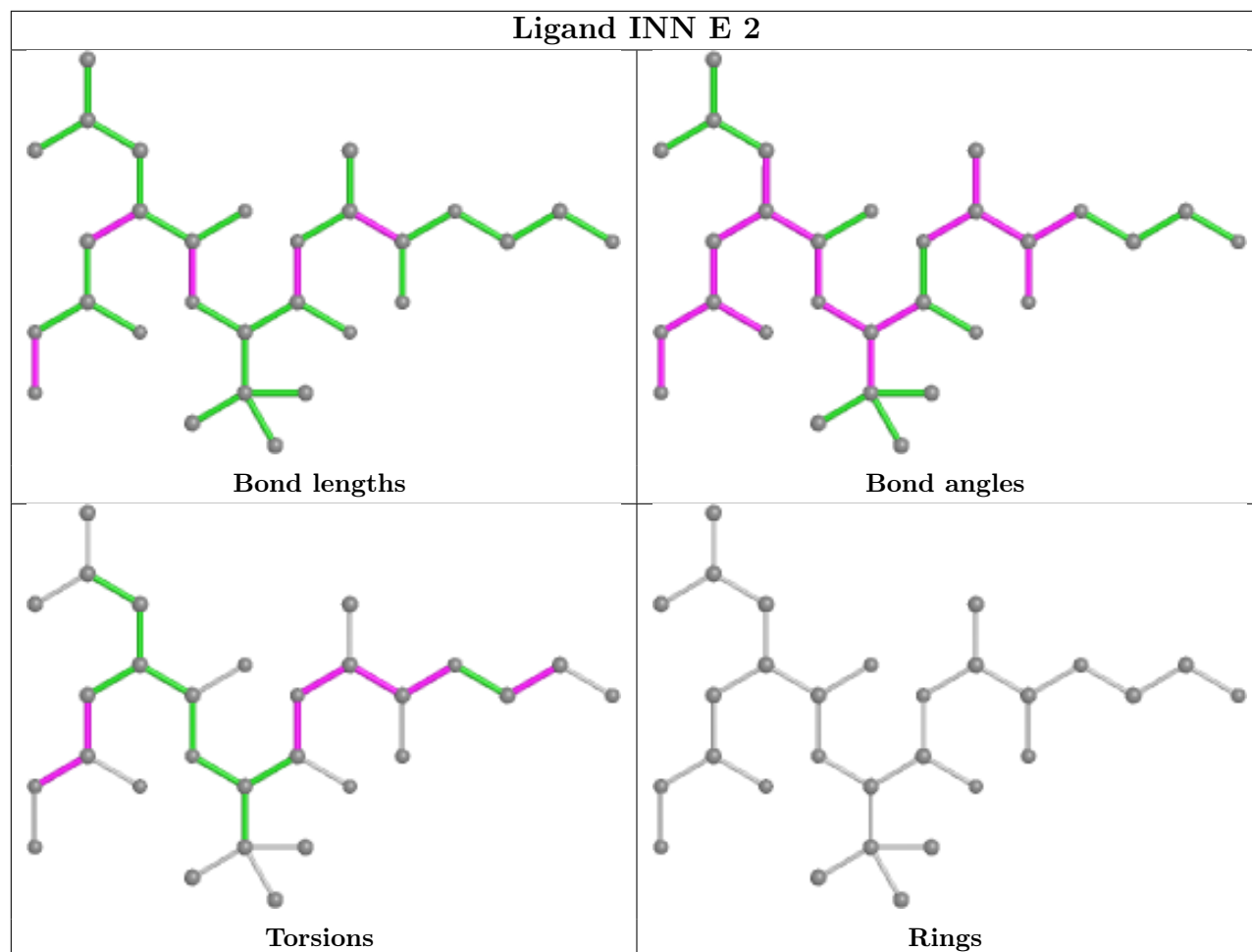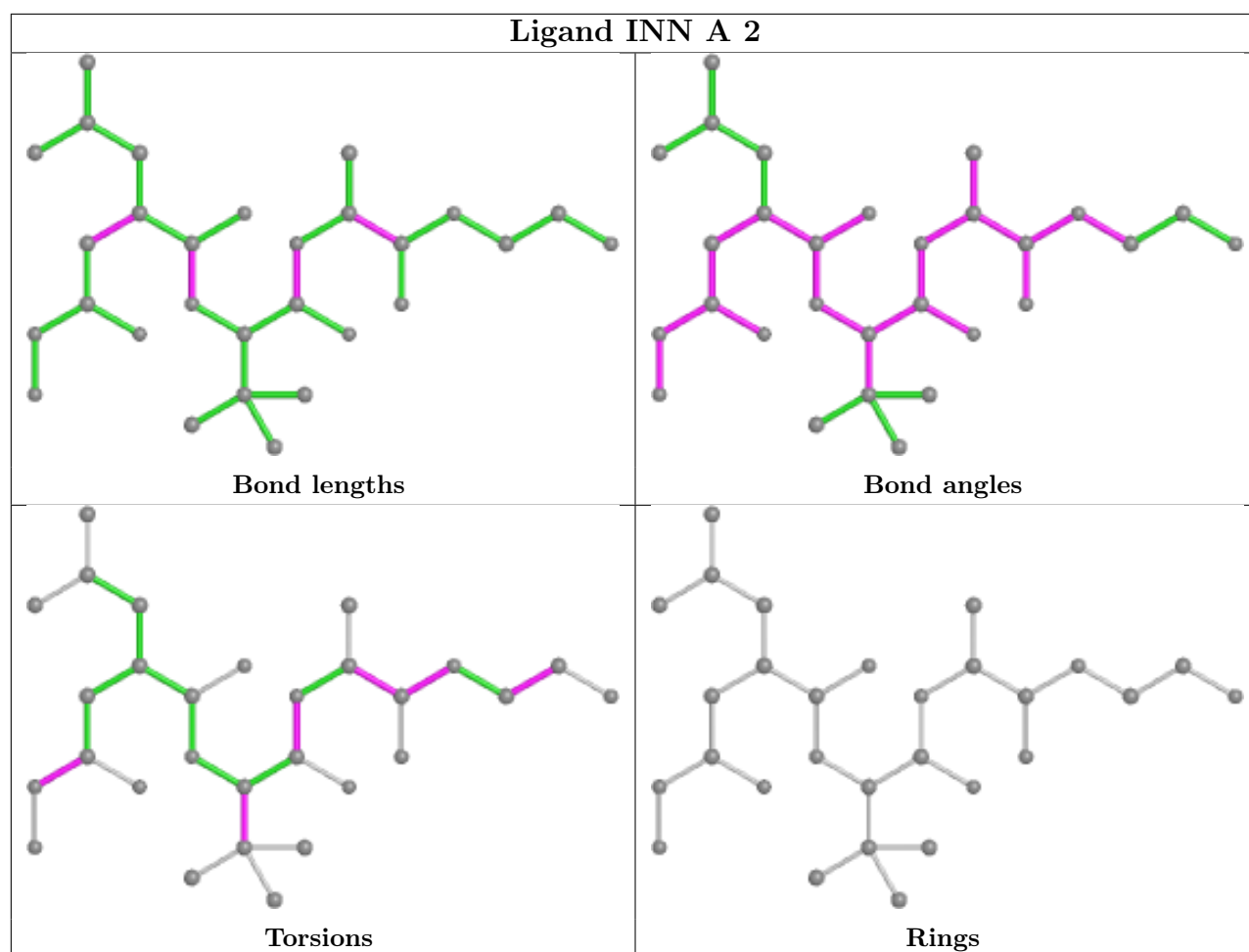
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	6
3	I	3
2	E	2
1	A	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	421:ALA	C	422:GLU	N	2.06

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	422:GLU	C	423:CYS	N	1.20
1	I	444:HIS	C	445:GLU	N	1.20
1	C	426:ASN	C	427:GLU	N	1.18
1	E	455:LYS	C	456:GLN	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.