



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:09 pm GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

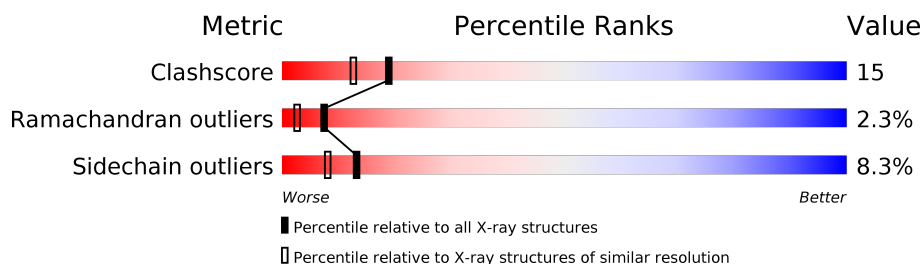
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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	C	N	O	S	9	0	0
			2025	1274	342	396	13			
1	C	254	Total	C	N	O	S	127	0	0
			2012	1265	340	394	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	ENGINEERED	UNP P78536
A	452	GLN	ASN	ENGINEERED	UNP P78536
C	266	ALA	SER	ENGINEERED	UNP P78536
C	452	GLN	ASN	ENGINEERED	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	C	N	O	S	18	0	0
			2028	1275	344	396	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	266	ALA	SER	ENGINEERED	UNP P78536
E	420	LYS	LEU	CONFLICT	UNP P78536
E	452	GLN	ASN	ENGINEERED	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	C	N	O	S	48	0	0
			2017	1269	341	394	13			

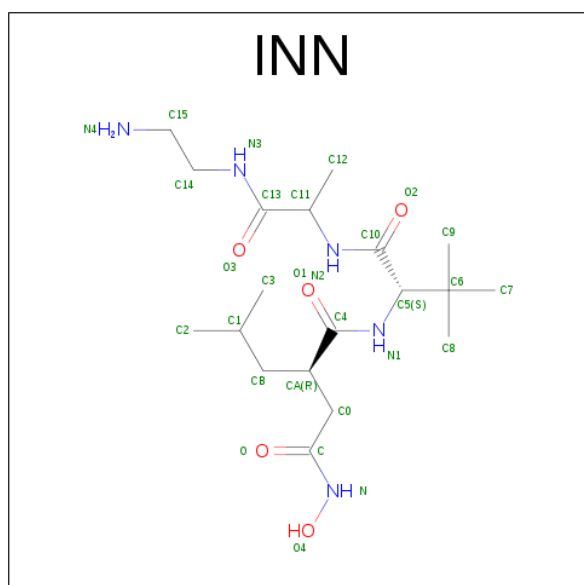
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	266	ALA	SER	ENGINEERED	UNP P78536
I	428	GLU	ASP	CONFLICT	UNP P78536
I	452	GLN	ASN	ENGINEERED	UNP P78536

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

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

- 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: C₁₉H₃₇N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			29	19	5	5		
5	C	1	Total	C	N	O	0	0
			29	19	5	5		
5	E	1	Total	C	N	O	0	0
			29	19	5	5		
5	I	1	Total	C	N	O	0	0
			29	19	5	5		

- Molecule 6 is water.

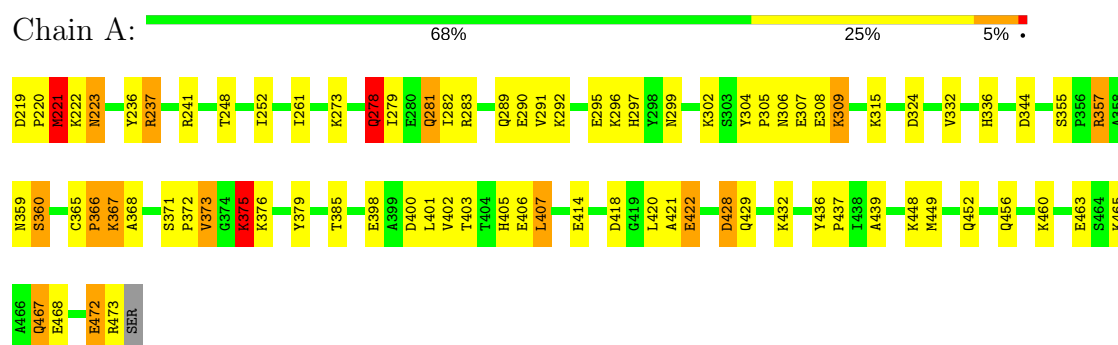
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	572	Total	O	0	0
			572	572		
6	C	442	Total	O	0	0
			442	442		
6	E	368	Total	O	0	0
			368	368		
6	I	238	Total	O	0	0
			238	238		

3 Residue-property plots [i](#)

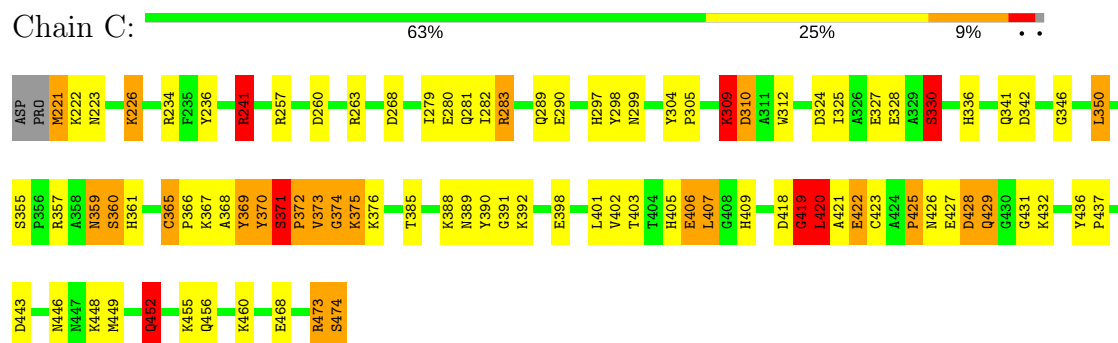
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

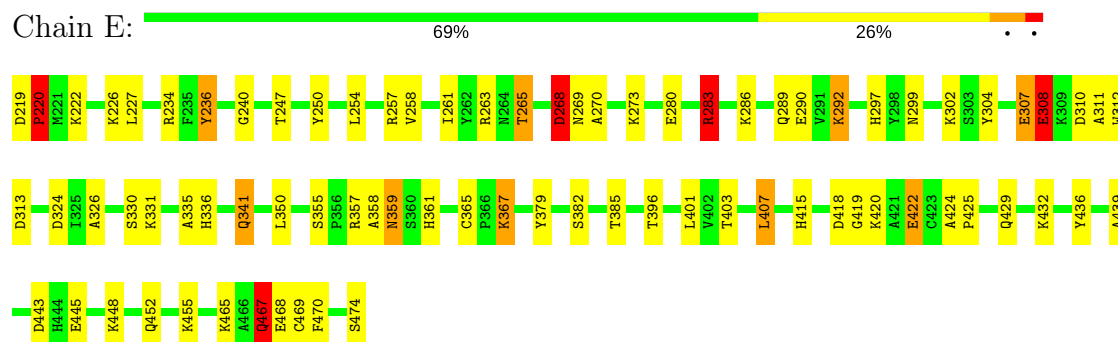
• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME



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

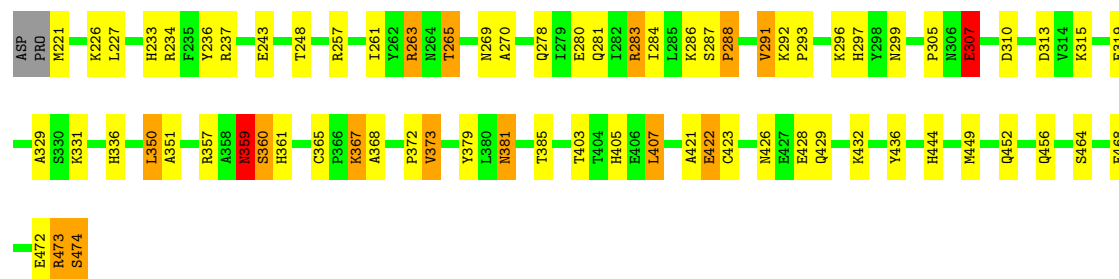


• Molecule 2: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME



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

Chain I:



4 Data and refinement statistics

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 [i](#)

5.1 Standard geometry [i](#)

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

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 [i](#)

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%)	11	6
1	C	216/219 (99%)	195 (90%)	21 (10%)	9	5
2	E	218/219 (100%)	202 (93%)	16 (7%)	16	11
3	I	217/219 (99%)	202 (93%)	15 (7%)	18	12
All	All	869/876 (99%)	797 (92%)	72 (8%)	13	8

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

Mol	Chain	Res	Type
1	C	375	LYS
1	C	474	SER
3	I	367	LYS
1	C	407	LEU
1	C	427	GLU

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

Mol	Chain	Res	Type
1	C	341	GLN
1	C	429	GLN
3	I	381	ASN
1	C	389	ASN
1	C	456	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 carbohydrates 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	A	2	4	28,28,28	3.36	5 (17%)	35,38,38	5.16	20 (57%)
5	INN	C	2	4	28,28,28	3.58	6 (21%)	35,38,38	5.16	20 (57%)
5	INN	E	2	4	28,28,28	3.48	5 (17%)	35,38,38	3.77	13 (37%)
5	INN	I	2	4	28,28,28	3.68	6 (21%)	35,38,38	4.64	18 (51%)

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	A	2	4	1/1/9/13	0/40/40/40	0/0/0/0
5	INN	C	2	4	1/1/9/13	0/40/40/40	0/0/0/0
5	INN	E	2	4	1/1/9/13	0/40/40/40	0/0/0/0
5	INN	I	2	4	1/1/9/13	0/40/40/40	0/0/0/0

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2	INN	C11-C13	-8.88	1.29	1.52
5	C	2	INN	C11-C13	-8.62	1.29	1.52
5	C	2	INN	C10-N2	-8.56	1.14	1.34
5	E	2	INN	C11-C13	-8.42	1.30	1.52
5	I	2	INN	C11-C13	-8.31	1.30	1.52

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	INN	O3-C13-C11	-12.69	91.70	120.48
5	E	2	INN	O3-C13-C11	-12.54	92.04	120.48
5	A	2	INN	O3-C13-C11	-12.10	93.04	120.48
5	I	2	INN	O3-C13-C11	-11.73	93.88	120.48
5	A	2	INN	C5-N1-C4	-8.25	104.55	122.02

All (4) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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.