



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:08 PM UTC

PDB ID : 1USN / pdb_00001usn
Title : CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF HUMAN FIBROBLAST STROMELYSIN-1 INHIBITED WITH THIADIAZOLE INHIBITOR PNU-142372
Authors : Finzel, B.C.; Bryant Junior, G.L.; Baldwin, E.T.
Deposited on : 1998-06-09
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

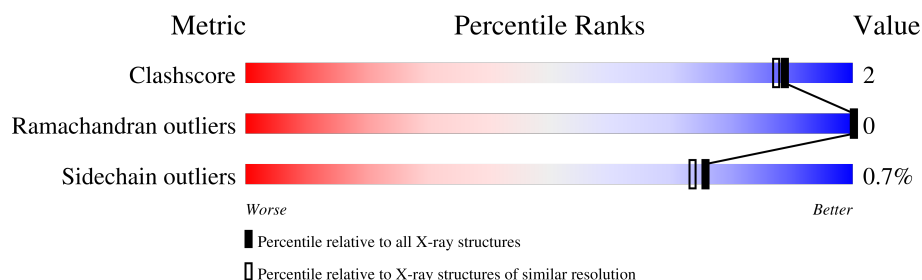
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	165	 65% 32% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1473 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 STROMELYSIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	3	0
			1329	852	219	256	2			

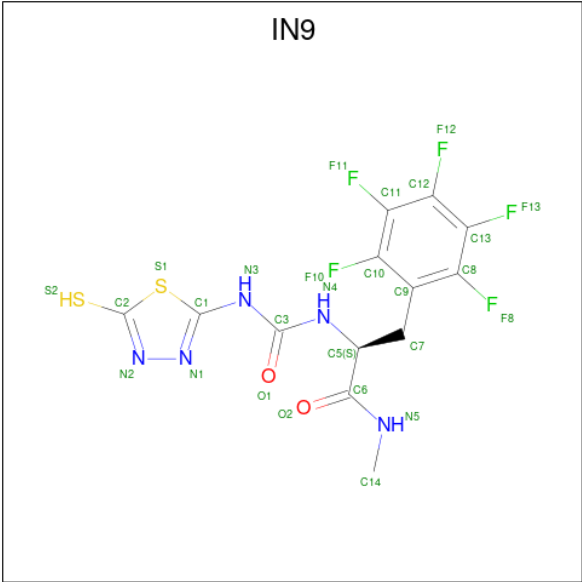
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is 2-[3-(5-MERCAPTO-[1,3,4]THIADIAZOL-2YL)-UREIDO]-N-METHYL-3-P-ENTAFLUOROPHENYL-PROPIONAMIDE (CCD ID: IN9) (formula: C₁₃H₁₀F₅N₅O₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
4	A	1	27	13	5	5	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		

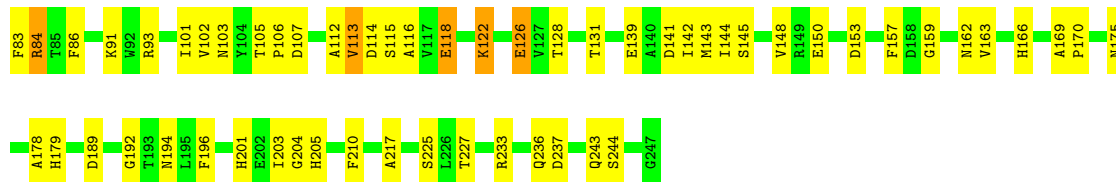
3 Residue-property plots

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: STROMELYSIN-1

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	72.12Å 72.12Å 192.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.0 (10.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1473	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: CA, ZN, IN9

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	1.45	5/1343 (0.4%)	2.20	72/1828 (3.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	GLY	N-CA	7.42	1.51	1.45
1	A	144	ILE	CA-CB	5.51	1.60	1.54
1	A	227	THR	CA-CB	5.25	1.60	1.53
1	A	128	THR	CA-CB	5.20	1.60	1.53
1	A	143	MET	N-CA	5.05	1.52	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	GLU	CB-CG-CD	11.09	131.45	112.60
1	A	107	ASP	CA-CB-CG	10.54	123.14	112.60
1	A	113	VAL	N-CA-CB	9.90	123.24	110.57
1	A	93	ARG	CD-NE-CZ	8.91	136.87	124.40
1	A	122	LYS	CG-CD-CE	8.36	130.53	111.30
1	A	179	HIS	CA-CB-CG	7.61	121.41	113.80
1	A	83	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	102	VAL	N-CA-C	7.27	118.06	110.72
1	A	139	GLU	CB-CG-CD	7.19	124.83	112.60
1	A	113	VAL	CA-CB-CG1	7.16	122.57	110.40
1	A	86	PHE	CA-CB-CG	7.03	120.83	113.80
1	A	116	ALA	CA-C-N	6.99	129.50	120.56
1	A	116	ALA	C-N-CA	6.99	129.50	120.56
1	A	112	ALA	CA-C-N	6.77	129.22	120.56
1	A	112	ALA	C-N-CA	6.77	129.22	120.56
1	A	243	GLN	OE1-CD-NE2	6.75	129.35	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ILE	CA-C-N	6.67	127.35	119.94
1	A	203	ILE	C-N-CA	6.67	127.35	119.94
1	A	115	SER	CA-C-O	-6.60	113.42	120.42
1	A	192	GLY	CA-C-O	-6.53	117.60	122.37
1	A	204	GLY	N-CA-C	-6.50	104.95	112.50
1	A	101	ILE	CA-C-N	6.37	129.47	120.42
1	A	101	ILE	C-N-CA	6.37	129.47	120.42
1	A	196	PHE	CA-C-O	-6.18	114.33	120.82
1	A	106	PRO	CA-C-N	6.14	129.13	120.28
1	A	106	PRO	C-N-CA	6.14	129.13	120.28
1	A	115	SER	CB-CA-C	6.05	121.13	110.85
1	A	217	ALA	N-CA-C	6.00	118.89	110.42
1	A	237	ASP	CA-C-N	5.98	128.22	120.44
1	A	237	ASP	C-N-CA	5.98	128.22	120.44
1	A	153	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	84	ARG	CA-C-O	-5.96	114.15	121.06
1	A	194	ASN	N-CA-CB	-5.94	100.74	109.95
1	A	166	HIS	N-CA-CB	5.89	121.41	110.99
1	A	169	ALA	CA-C-N	5.88	125.88	119.89
1	A	169	ALA	C-N-CA	5.88	125.88	119.89
1	A	243	GLN	CG-CD-NE2	-5.87	107.60	116.40
1	A	145	SER	CA-C-N	5.86	131.39	122.65
1	A	145	SER	C-N-CA	5.86	131.39	122.65
1	A	175	ASN	CB-CA-C	5.85	119.12	109.70
1	A	205	HIS	CA-C-N	5.84	128.69	120.28
1	A	205	HIS	C-N-CA	5.84	128.69	120.28
1	A	225	SER	CA-C-N	5.78	131.92	121.92
1	A	225	SER	C-N-CA	5.78	131.92	121.92
1	A	150	GLU	CB-CG-CD	5.74	122.35	112.60
1	A	163	VAL	CA-C-O	-5.72	114.51	121.04
1	A	107	ASP	N-CA-C	5.71	118.28	111.71
1	A	162	ASN	CB-CA-C	5.69	121.74	110.42
1	A	243	GLN	CA-CB-CG	-5.64	102.81	114.10
1	A	157	PHE	N-CA-CB	5.54	118.28	110.36
1	A	201	HIS	CA-CB-CG	5.50	119.30	113.80
1	A	105	THR	CA-CB-CG2	5.49	119.83	110.50
1	A	113	VAL	CA-CB-CG2	5.46	119.68	110.40
1	A	126	GLU	CG-CD-OE2	-5.46	105.85	118.40
1	A	128	THR	CA-CB-CG2	5.45	119.77	110.50
1	A	189	ASP	O-C-N	5.43	129.16	123.03
1	A	236	GLN	CA-C-N	5.39	127.50	120.28
1	A	236	GLN	C-N-CA	5.39	127.50	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	VAL	CA-C-O	-5.26	115.21	121.05
1	A	159	GLY	CA-C-N	5.26	125.51	119.83
1	A	159	GLY	C-N-CA	5.26	125.51	119.83
1	A	162	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	142	ILE	N-CA-CB	-5.11	105.24	111.67
1	A	233	ARG	CA-CB-CG	5.10	124.29	114.10
1	A	141	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	169	ALA	N-CA-CB	-5.08	102.66	110.03
1	A	148	VAL	CA-CB-CG1	5.06	119.00	110.40
1	A	126	GLU	N-CA-C	5.06	117.53	111.71
1	A	157	PHE	CB-CA-C	5.05	120.03	109.68
1	A	131	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	178	ALA	N-CA-C	5.04	117.11	108.90
1	A	103	ASN	OD1-CG-ND2	-5.02	117.58	122.60

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	1329	0	1241	5	0
2	A	3	0	0	0	0
3	A	3	0	0	0	0
4	A	27	0	9	0	0
5	A	111	0	0	1	1
All	All	1473	0	1250	5	1

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 2.

All (5) 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:91:LYS:HA	1:A:170:PRO:HG2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:O	1:A:126:GLU:HG3	2.11	0.50
1:A:244:SER:HB3	5:A:361:HOH:O	2.13	0.49
1:A:114:ASP:O	1:A:118:GLU:HG3	2.16	0.45
1:A:84:ARG:HH21	1:A:210:PHE:HD2	1.68	0.40

All (1) 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)
5:A:360:HOH:O	5:A:360:HOH:O[11_565]	1.35	0.85

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	166/165 (101%)	160 (96%)	6 (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 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	135/139 (97%)	134 (99%)	1 (1%)	76	73

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	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 7 ligands modelled in this entry, 6 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	IN9	A	300	2	27,28,28	2.67	10 (37%)	38,40,40	1.86	10 (26%)

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
4	IN9	A	300	2	-	0/18/18/18	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	300	IN9	C6-N5	7.61	1.43	1.33
4	A	300	IN9	O1-C3	6.81	1.37	1.23
4	A	300	IN9	C1-N3	5.47	1.46	1.38
4	A	300	IN9	F13-C13	3.04	1.39	1.34
4	A	300	IN9	C3-N4	2.69	1.43	1.35
4	A	300	IN9	C2-S2	2.46	1.81	1.72
4	A	300	IN9	F8-C8	2.28	1.38	1.34
4	A	300	IN9	C2-N2	2.07	1.34	1.30
4	A	300	IN9	C14-N5	2.07	1.49	1.45
4	A	300	IN9	C3-N3	-2.07	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	300	IN9	C14-N5-C6	-4.63	114.13	122.21
4	A	300	IN9	N3-C1-N1	-4.44	116.85	120.81
4	A	300	IN9	C10-C9-C8	4.15	120.79	115.91
4	A	300	IN9	S1-C1-N3	2.98	127.71	123.72
4	A	300	IN9	F8-C8-C9	2.90	123.61	119.36
4	A	300	IN9	S2-C2-N2	-2.73	120.58	127.84
4	A	300	IN9	C9-C8-C13	-2.64	119.34	122.36
4	A	300	IN9	C9-C10-C11	-2.62	119.36	122.36
4	A	300	IN9	S1-C2-N2	-2.26	111.16	114.10
4	A	300	IN9	C6-C5-N4	-2.19	105.18	111.11

There are no chirality outliers.

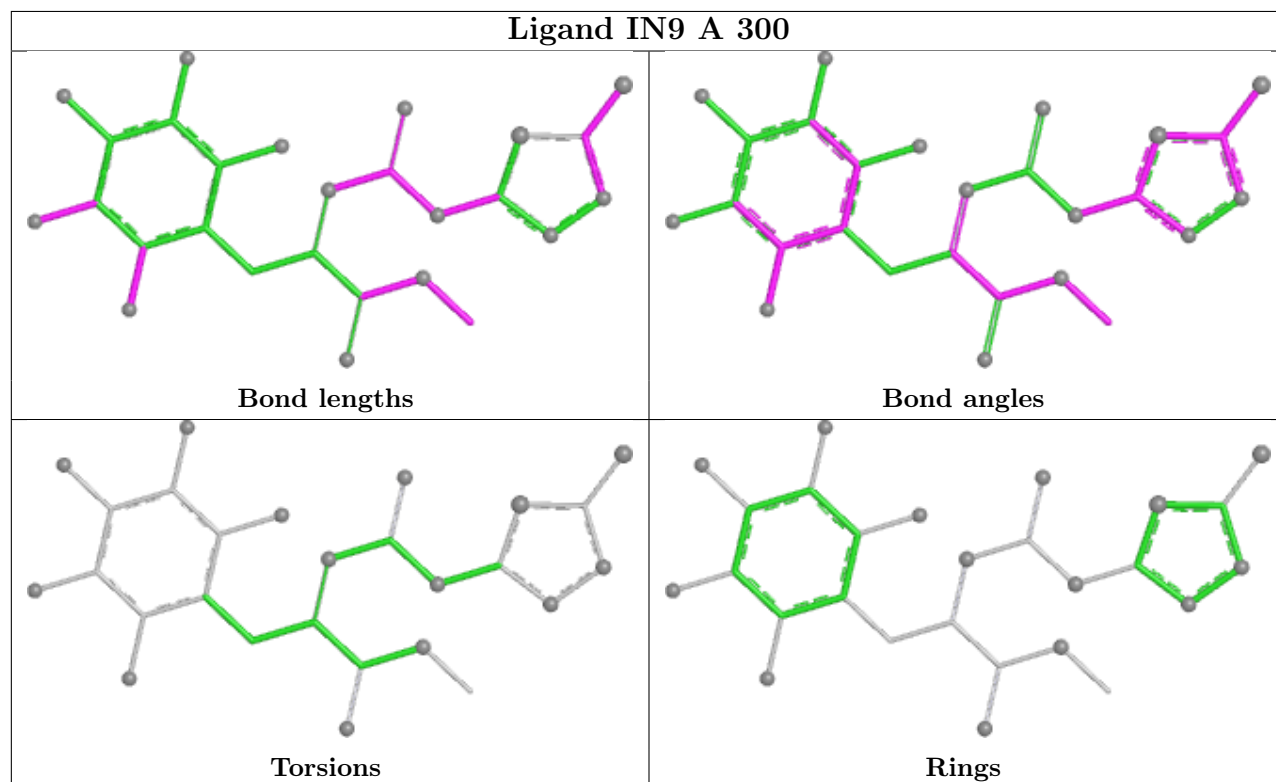
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	216[2]:GLU	C	217:ALA	N	1.17

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.