



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:18 PM UTC

PDB ID : 1HFC / pdb_00001hfc
Title : 1.56 ANGSTROM STRUCTURE OF MATURE TRUNCATED HUMAN FIBROBLAST COLLAGENASE
Authors : Spurlino, J.C.; Smith, D.L.
Deposited on : 1994-09-13
Resolution : 1.50 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

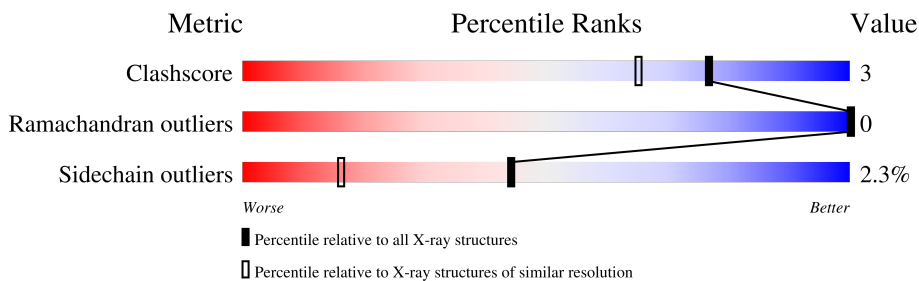
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)

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	169	 52% 37% .. 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1360 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 FIBROBLAST COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1244	779	221	242	2			

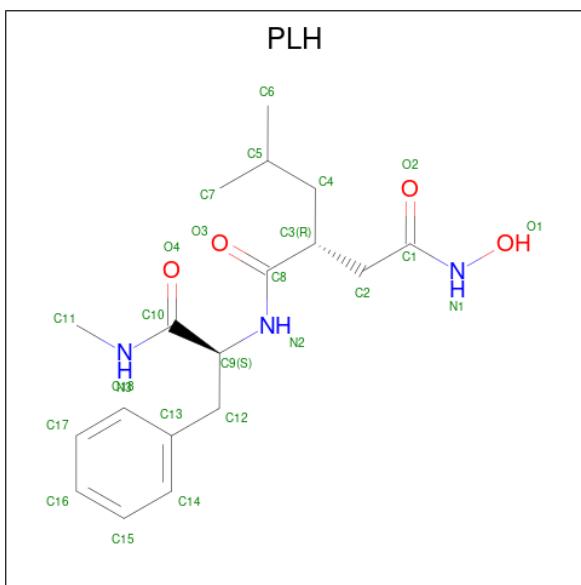
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

- Molecule 4 is METHYLAMINO-PHENYLALANYL-LEUCYL-HYDROXAMIC ACID (CCD ID: PLH) (formula: C₁₈H₂₇N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	3	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		

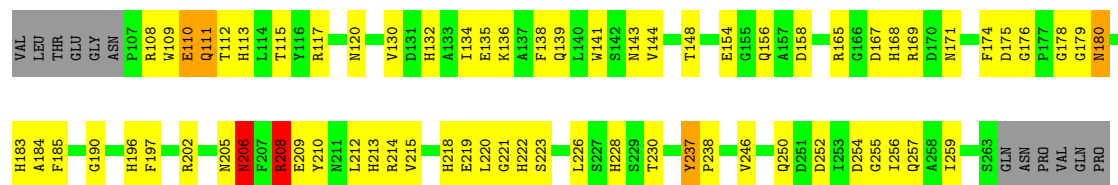
3 Residue-property plots [i](#)

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.

Note EDS was not executed.

• Molecule 1: FIBROBLAST COLLAGENASE

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.21Å 44.57Å 36.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1360	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: CA, PLH, ZN

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	1.52	9/1281 (0.7%)	2.66	102/1743 (5.9%)

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	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	ASN	CG-OD1	6.22	1.35	1.23
1	A	228	HIS	ND1-CE1	5.93	1.38	1.32
1	A	168	HIS	CE1-NE2	5.66	1.38	1.32
1	A	213	HIS	N-CA	5.26	1.52	1.46
1	A	257	GLN	C-N	-5.24	1.26	1.33
1	A	215	VAL	CA-C	5.13	1.59	1.52
1	A	220	LEU	N-CA	5.12	1.52	1.46
1	A	135	GLU	N-CA	5.09	1.52	1.46
1	A	237	TYR	N-CA	5.01	1.52	1.45

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	HIS	CE1-NE2-CD2	-15.39	93.61	109.00
1	A	117	ARG	NE-CZ-NH1	15.14	136.64	121.50
1	A	183	HIS	CG-CD2-NE2	14.43	121.63	107.20
1	A	110	GLU	CB-CG-CD	13.93	136.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	HIS	CE1-NE2-CD2	-13.77	95.23	109.00
1	A	117	ARG	NE-CZ-NH2	-11.92	108.47	119.20
1	A	117	ARG	CD-NE-CZ	11.87	141.02	124.40
1	A	218	HIS	ND1-CE1-NE2	11.85	120.25	108.40
1	A	215	VAL	O-C-N	11.49	133.66	121.83
1	A	183	HIS	ND1-CE1-NE2	10.98	119.38	108.40
1	A	218	HIS	CG-CD2-NE2	10.35	117.55	107.20
1	A	154	GLU	CA-CB-CG	8.90	131.90	114.10
1	A	202	ARG	NE-CZ-NH2	8.88	127.19	119.20
1	A	138	PHE	O-C-N	8.80	131.44	122.12
1	A	144	VAL	O-C-N	8.57	131.43	122.09
1	A	215	VAL	CA-C-O	-8.55	111.78	120.85
1	A	111	GLN	OE1-CD-NE2	8.18	130.78	122.60
1	A	246	VAL	O-C-N	8.17	132.91	122.94
1	A	226	LEU	O-C-N	8.15	132.18	123.06
1	A	223	SER	O-C-N	7.95	132.73	122.39
1	A	117	ARG	O-C-N	7.73	132.68	123.33
1	A	178	GLY	O-C-N	-7.68	115.14	123.05
1	A	256	ILE	CA-C-O	-7.59	112.27	120.47
1	A	176	GLY	O-C-N	-7.42	114.35	121.77
1	A	202	ARG	CA-C-O	7.26	128.12	120.36
1	A	252	ASP	O-C-N	7.25	129.92	122.09
1	A	168	HIS	ND1-CG-CD2	-7.22	98.88	106.10
1	A	113	HIS	CA-CB-CG	-7.07	106.73	113.80
1	A	165	ARG	CD-NE-CZ	7.07	134.30	124.40
1	A	256	ILE	O-C-N	6.97	129.67	121.80
1	A	143	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	144	VAL	CA-C-O	-6.69	113.88	119.97
1	A	202	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	A	196	HIS	CG-CD2-NE2	-6.67	100.53	107.20
1	A	252	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	175	ASP	N-CA-CB	-6.61	100.52	111.49
1	A	168	HIS	ND1-CE1-NE2	-6.61	101.79	108.40
1	A	221	GLY	N-CA-C	-6.57	104.85	112.73
1	A	257	GLN	CA-C-O	-6.53	111.35	119.38
1	A	156	GLN	O-C-N	-6.51	115.80	123.22
1	A	134	ILE	O-C-N	6.38	128.41	121.83
1	A	250	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	A	259	ILE	CB-CA-C	-6.38	105.17	111.30
1	A	115	THR	O-C-N	6.37	131.65	123.11
1	A	202	ARG	CD-NE-CZ	6.36	133.30	124.40
1	A	197	PHE	CA-CB-CG	-6.33	107.47	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	HIS	CG-ND1-CE1	6.33	120.06	109.30
1	A	183	HIS	ND1-CG-CD2	-6.30	99.80	106.10
1	A	132	HIS	CA-CB-CG	-6.29	107.51	113.80
1	A	208	ARG	CG-CD-NE	-6.28	98.19	112.00
1	A	219	GLU	O-C-N	6.19	129.21	122.15
1	A	141	TRP	CA-C-O	-6.18	113.38	120.24
1	A	214	ARG	O-C-N	-6.18	115.71	122.07
1	A	202	ARG	O-C-N	-6.17	116.19	123.22
1	A	167	ASP	CA-C-O	6.16	127.64	120.49
1	A	138	PHE	CA-C-O	-6.12	114.06	120.55
1	A	184	ALA	CA-C-N	-6.12	114.06	122.93
1	A	184	ALA	C-N-CA	-6.12	114.06	122.93
1	A	111	GLN	CA-C-O	-6.11	114.02	121.36
1	A	252	ASP	OD1-CG-OD2	6.11	137.57	122.90
1	A	196	HIS	CE1-NE2-CD2	5.95	114.95	109.00
1	A	143	ASN	CA-C-O	-5.93	112.31	119.49
1	A	230	THR	CA-CB-OG1	-5.89	100.76	109.60
1	A	144	VAL	N-CA-CB	-5.87	104.53	112.16
1	A	110	GLU	CG-CD-OE1	5.84	131.84	118.40
1	A	185	PHE	CA-C-O	-5.81	114.55	120.71
1	A	117	ARG	CA-C-O	-5.79	113.65	120.60
1	A	255	GLY	CA-C-O	-5.79	114.41	120.90
1	A	257	GLN	N-CA-C	-5.77	105.50	112.54
1	A	190	GLY	O-C-N	5.73	131.59	122.36
1	A	218	HIS	CB-CG-CD2	5.72	138.64	131.20
1	A	141	TRP	O-C-N	5.72	129.67	122.23
1	A	228	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
1	A	109	TRP	O-C-N	5.71	129.75	123.01
1	A	222	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	A	219	GLU	CA-C-O	-5.66	114.42	120.42
1	A	205	ASN	CA-C-O	-5.61	113.17	119.95
1	A	180	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	184	ALA	O-C-N	5.50	129.53	123.25
1	A	112	THR	CA-CB-OG1	-5.50	101.35	109.60
1	A	148	THR	N-CA-CB	5.49	120.93	111.00
1	A	108	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	A	158	ASP	CA-C-O	-5.42	114.67	120.42
1	A	221	GLY	O-C-N	-5.42	116.99	122.19
1	A	158	ASP	O-C-N	5.40	128.30	122.15
1	A	212	LEU	O-C-N	5.39	127.62	122.07
1	A	223	SER	CA-C-O	-5.38	112.97	119.49
1	A	174	PHE	N-CA-C	-5.33	103.85	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	VAL	O-C-N	5.31	127.43	121.90
1	A	174	PHE	N-CA-CB	5.16	117.44	110.38
1	A	254	ASP	O-C-N	-5.07	116.75	122.12
1	A	171	ASN	N-CA-CB	-5.06	103.57	110.56
1	A	179	GLY	O-C-N	5.06	128.23	122.62
1	A	176	GLY	CA-C-N	5.05	124.96	119.76
1	A	176	GLY	C-N-CA	5.05	124.96	119.76
1	A	120	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	156	GLN	CA-C-N	5.03	131.78	122.92
1	A	156	GLN	C-N-CA	5.03	131.78	122.92
1	A	171	ASN	CB-CG-ND2	-5.02	108.87	116.40
1	A	202	ARG	N-CA-C	-5.01	100.57	108.73
1	A	228	HIS	CA-CB-CG	-5.01	108.79	113.80
1	A	256	ILE	CA-CB-CG2	5.01	119.02	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ARG	Sidechain

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	1244	0	1141	7	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	25	0	26	1	0
5	A	88	0	0	0	0
All	All	1360	0	1167	7	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 3.

All (7) 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:206:ASN:OD1	1:A:208:ARG:NH1	2.46	0.48
1:A:110:GLU:HG3	1:A:111:GLN:N	2.29	0.48
1:A:237:TYR:CD1	1:A:238:PRO:HD2	2.53	0.43
1:A:169:ARG:N	1:A:169:ARG:HD2	2.34	0.42
1:A:237:TYR:CG	1:A:238:PRO:HD2	2.55	0.41
1:A:180:ASN:HD21	4:A:280:PLH:H22	1.85	0.41
1:A:209:GLU:HA	1:A:210:TYR:HA	1.90	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 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	155/169 (92%)	154 (99%)	1 (1%)	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	130/141 (92%)	127 (98%)	3 (2%)	44	16

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LYS
1	A	139	GLN
1	A	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	113	HIS
1	A	132	HIS
1	A	186	GLN

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 4 ligands modelled in this entry, 3 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	PLH	A	280	2	25,25,25	1.20	3 (12%)	30,32,32	2.67	10 (33%)

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	PLH	A	280	2	-	0/28/28/28	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	280	PLH	C10-N3	2.40	1.36	1.33
4	A	280	PLH	C1-N1	-2.29	1.29	1.32
4	A	280	PLH	C17-C18	2.01	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	280	PLH	O2-C1-C2	-7.64	110.37	121.54
4	A	280	PLH	O2-C1-N1	6.42	131.15	123.27
4	A	280	PLH	O1-N1-C1	-6.02	110.90	119.79
4	A	280	PLH	C2-C3-C8	3.68	114.95	109.71
4	A	280	PLH	O3-C8-C3	-3.29	117.12	122.19
4	A	280	PLH	C17-C16-C15	3.08	124.09	119.87
4	A	280	PLH	O3-C8-N2	2.44	127.33	122.96
4	A	280	PLH	C9-C10-N3	-2.23	113.63	116.99
4	A	280	PLH	C2-C1-N1	2.19	118.45	115.14
4	A	280	PLH	C16-C15-C14	-2.11	117.64	120.24

There are no chirality outliers.

There are no torsion outliers.

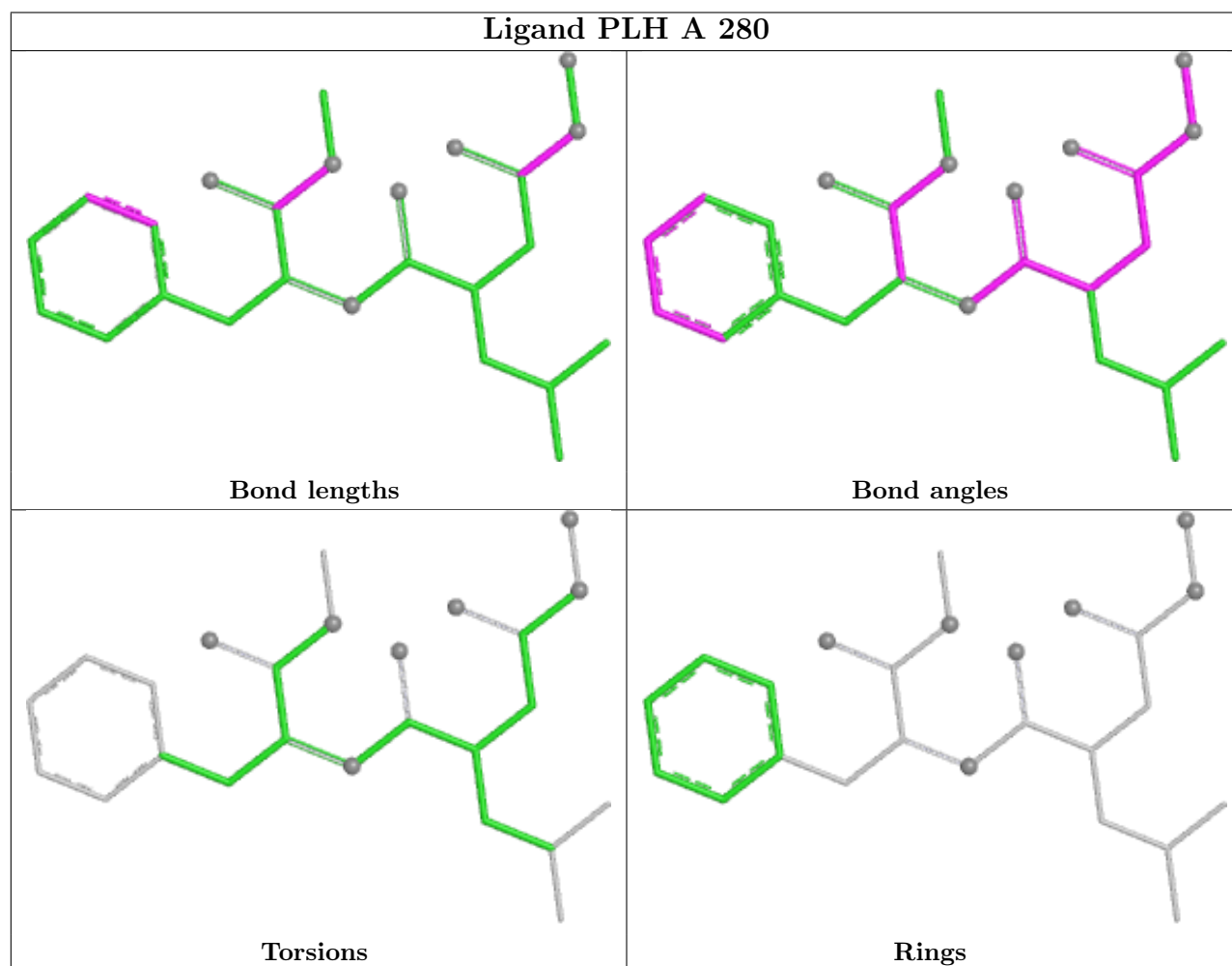
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	280	PLH	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 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](#)

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.