



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:06 PM UTC

PDB ID : 1MNC / pdb_00001mnc
Title : STRUCTURE OF HUMAN NEUTROPHIL COLLAGENASE REVEALS
LARGE S1' SPECIFICITY POCKET
Authors : Stams, T.; Spurlino, J.C.; Smith, D.L.; Rubin, B.
Deposited on : 1994-01-12
Resolution : 2.10 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

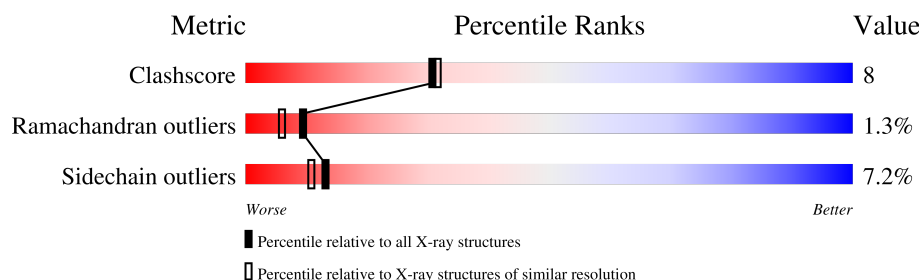
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	163	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1333 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 NEUTROPHIL COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1233	780	209	243	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	ASN	conflict	UNP P22894
A	151	GLY	ARG	conflict	UNP P22894
A	171	GLY	ASN	conflict	UNP P22894

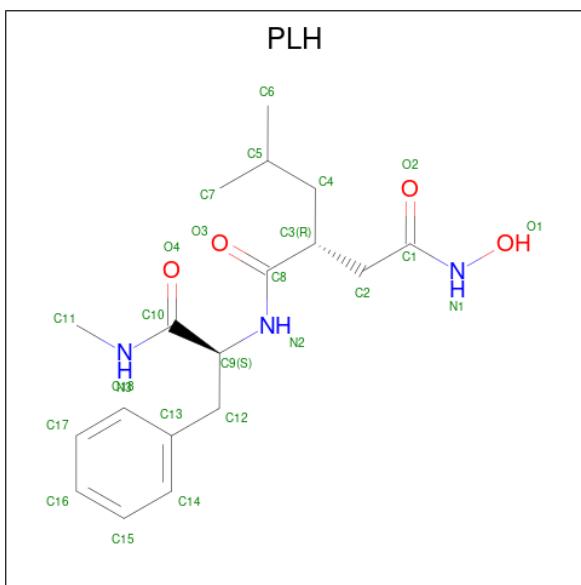
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).



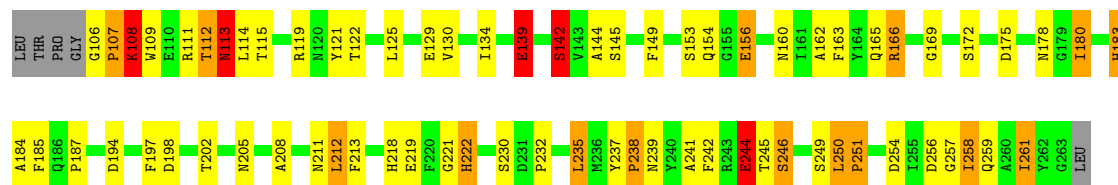
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	3	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		

Note EDS was not executed.

Chain A: 53% 31% 9% 7%



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	34.92Å 61.28Å 68.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1333	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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, CA, PLH

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	1.16	0/1270	2.52	96/1731 (5.5%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	N-CA-CB	-10.17	96.79	111.54
1	A	160	ASN	CA-CB-CG	-10.11	102.50	112.60
1	A	166	ARG	NE-CZ-NH2	9.92	128.12	119.20
1	A	154	GLN	CB-CG-CD	9.08	128.04	112.60
1	A	238	PRO	N-CA-C	9.01	125.01	114.20
1	A	134	ILE	CA-C-N	8.92	132.58	120.44
1	A	134	ILE	C-N-CA	8.92	132.58	120.44
1	A	113	ASN	CA-CB-CG	-8.80	103.80	112.60
1	A	122	THR	N-CA-C	-8.71	99.10	110.07
1	A	115	THR	CA-CB-OG1	-8.55	96.78	109.60
1	A	239	ASN	CA-C-O	8.49	129.52	120.36
1	A	139	GLU	CB-CG-CD	8.33	126.76	112.60
1	A	175	ASP	N-CA-C	8.20	122.88	111.56
1	A	108	LYS	N-CA-C	-8.18	101.42	111.40
1	A	111	ARG	NE-CZ-NH2	8.18	126.56	119.20
1	A	218	HIS	CE1-NE2-CD2	-8.15	100.84	109.00
1	A	162	ALA	CA-C-N	7.79	132.97	122.84
1	A	162	ALA	C-N-CA	7.79	132.97	122.84
1	A	107	PRO	N-CA-C	7.65	122.36	110.80
1	A	185	PHE	CA-CB-CG	-7.63	106.17	113.80
1	A	249	SER	CA-C-O	-7.59	112.83	121.40
1	A	178	ASN	CA-CB-CG	-7.59	105.01	112.60
1	A	134	ILE	O-C-N	-7.49	114.61	121.87
1	A	112	THR	N-CA-CB	-7.43	99.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	PRO	CA-C-O	-7.21	112.81	121.03
1	A	112	THR	OG1-CB-CG2	7.13	123.55	109.30
1	A	156	GLU	CB-CA-C	-7.11	98.25	109.84
1	A	154	GLN	OE1-CD-NE2	-7.11	115.49	122.60
1	A	178	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	A	111	ARG	NE-CZ-NH1	-6.97	114.53	121.50
1	A	251	PRO	CA-C-N	6.94	129.91	120.54
1	A	251	PRO	C-N-CA	6.94	129.91	120.54
1	A	142	SER	O-C-N	-6.89	114.82	122.12
1	A	113	ASN	OD1-CG-ND2	6.87	129.47	122.60
1	A	144	ALA	CA-C-O	-6.79	111.47	119.48
1	A	202	THR	CA-CB-OG1	-6.75	99.47	109.60
1	A	244	GLU	N-CA-C	-6.69	96.55	110.80
1	A	145	SER	O-C-N	6.58	128.89	121.32
1	A	242	PHE	CA-CB-CG	-6.58	107.22	113.80
1	A	197	PHE	O-C-N	6.48	131.66	123.23
1	A	250	LEU	N-CA-C	6.41	118.71	109.48
1	A	250	LEU	O-C-N	6.34	126.94	121.30
1	A	211	ASN	CA-C-O	-6.21	113.38	120.58
1	A	139	GLU	CA-C-N	6.17	128.46	120.44
1	A	139	GLU	C-N-CA	6.17	128.46	120.44
1	A	244	GLU	O-C-N	6.13	130.74	122.59
1	A	241	ALA	O-C-N	-6.09	116.28	123.41
1	A	165	GLN	CG-CD-NE2	6.09	125.54	116.40
1	A	142	SER	CB-CA-C	-6.09	100.69	110.79
1	A	169	GLY	CA-C-O	-6.06	112.28	119.01
1	A	258	ILE	CA-C-N	6.05	128.39	120.28
1	A	258	ILE	C-N-CA	6.05	128.39	120.28
1	A	197	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	163	PHE	CA-C-O	-5.86	114.44	120.54
1	A	183	HIS	CE1-NE2-CD2	-5.82	103.19	109.00
1	A	198	ASP	CB-CA-C	5.79	119.47	110.67
1	A	218	HIS	ND1-CE1-NE2	5.74	114.14	108.40
1	A	112	THR	CB-CA-C	5.73	119.72	109.29
1	A	205	ASN	N-CA-C	-5.71	103.67	111.56
1	A	246	SER	CA-C-O	-5.70	112.36	120.51
1	A	235	LEU	N-CA-CB	-5.61	101.59	110.28
1	A	230	SER	CA-CB-OG	-5.56	99.98	111.10
1	A	261	ILE	CB-CA-C	-5.54	105.19	111.55
1	A	238	PRO	CA-C-N	5.53	130.78	122.99
1	A	238	PRO	C-N-CA	5.53	130.78	122.99
1	A	244	GLU	CA-C-O	-5.51	112.63	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLY	O-C-N	-5.50	116.90	122.18
1	A	183	HIS	CA-CB-CG	5.43	119.23	113.80
1	A	218	HIS	CA-C-N	5.41	127.53	120.28
1	A	218	HIS	C-N-CA	5.41	127.53	120.28
1	A	142	SER	N-CA-C	5.40	117.17	111.28
1	A	257	GLY	CA-C-O	-5.39	114.94	120.66
1	A	197	PHE	CA-C-O	-5.38	114.89	120.70
1	A	232	PRO	CB-CA-C	5.36	119.45	111.62
1	A	218	HIS	CG-CD2-NE2	5.36	112.56	107.20
1	A	180	ILE	CB-CA-C	-5.34	104.21	111.15
1	A	256	ASP	CB-CG-OD1	5.33	130.67	118.40
1	A	121	TYR	N-CA-CB	-5.33	102.28	111.55
1	A	119	ARG	CA-C-O	-5.32	115.24	120.82
1	A	153	SER	CB-CA-C	-5.31	100.80	109.56
1	A	149	PHE	O-C-N	5.31	129.56	123.29
1	A	212	LEU	N-CA-C	5.30	117.06	111.28
1	A	130	VAL	N-CA-CB	5.29	116.74	110.55
1	A	142	SER	N-CA-CB	-5.27	102.37	110.12
1	A	222	HIS	CB-CA-C	-5.25	102.63	110.88
1	A	169	GLY	O-C-N	5.25	128.69	122.50
1	A	166	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	259	GLN	N-CA-CB	5.25	117.83	110.12
1	A	194	ASP	N-CA-C	5.23	117.88	110.50
1	A	221	GLY	N-CA-C	-5.19	106.48	112.50
1	A	185	PHE	O-C-N	5.19	129.70	123.16
1	A	208	ALA	CA-C-O	-5.12	115.98	121.56
1	A	251	PRO	O-C-N	-5.09	116.69	123.01
1	A	202	THR	N-CA-C	-5.06	100.92	108.96
1	A	125	LEU	N-CA-CB	-5.05	103.01	111.20
1	A	165	GLN	O-C-N	-5.01	117.38	123.29

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	1233	0	1127	20	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	25	0	26	1	0
5	A	72	0	0	4	0
All	All	1333	0	1153	20	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 (20) 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:108:LYS:HB3	1:A:187:PRO:HG2	1.43	1.00
1:A:156:GLU:HG3	1:A:156:GLU:O	1.88	0.73
1:A:245:THR:HG21	5:A:60:HOH:O	1.89	0.71
1:A:166:ARG:NH2	5:A:19:HOH:O	2.25	0.64
1:A:106:GLY:O	1:A:261:ILE:HG23	2.00	0.61
1:A:139:GLU:HA	1:A:142:SER:HB2	1.82	0.60
1:A:108:LYS:CB	1:A:187:PRO:HG2	2.25	0.59
1:A:113:ASN:ND2	5:A:66:HOH:O	2.00	0.53
1:A:107:PRO:HB2	1:A:109:TRP:O	2.12	0.50
1:A:108:LYS:HB3	1:A:187:PRO:CG	2.29	0.47
1:A:184:ALA:HB3	1:A:222:HIS:HB2	1.97	0.46
1:A:213:PHE:CD2	1:A:245:THR:HG23	2.51	0.46
1:A:237:TYR:CD1	1:A:238:PRO:HD2	2.52	0.44
1:A:172:SER:O	1:A:183:HIS:HE1	2.00	0.43
1:A:250:LEU:HA	1:A:251:PRO:HD3	1.85	0.43
1:A:251:PRO:HD2	1:A:254:ASP:OD2	2.20	0.42
1:A:244:GLU:HG3	1:A:245:THR:N	2.32	0.42
1:A:129:GLU:O	5:A:59:HOH:O	2.22	0.41
1:A:219:GLU:OE1	4:A:280:PLH:O1	2.39	0.41
1:A:180:ILE:HA	1:A:180:ILE:HD13	1.85	0.41

There are no symmetry-related clashes.

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	156/163 (96%)	147 (94%)	7 (4%)	2 (1%)	9 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	A	246	SER

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	125/129 (97%)	116 (93%)	9 (7%)	13 11

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	112	THR
1	A	113	ASN
1	A	114	LEU
1	A	139	GLU
1	A	142	SER
1	A	212	LEU
1	A	235	LEU
1	A	258	ILE

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	178	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 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	1.56	5 (20%)	30,32,32	1.82	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	280	PLH	O1-N1	-4.61	1.28	1.40
4	A	280	PLH	C2-C1	-2.57	1.46	1.51
4	A	280	PLH	C3-C8	-2.50	1.47	1.51
4	A	280	PLH	C9-C10	-2.43	1.46	1.52
4	A	280	PLH	C1-N1	2.03	1.34	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	280	PLH	C2-C1-N1	4.26	121.59	115.14
4	A	280	PLH	O1-N1-C1	4.04	125.76	119.79
4	A	280	PLH	O2-C1-C2	-3.01	117.14	121.54
4	A	280	PLH	C3-C4-C5	2.76	121.34	115.60
4	A	280	PLH	C3-C8-N2	2.44	120.39	116.19
4	A	280	PLH	C12-C9-C10	-2.34	104.31	110.30
4	A	280	PLH	O4-C10-N3	2.33	127.02	123.13
4	A	280	PLH	C16-C17-C18	-2.23	117.49	120.24
4	A	280	PLH	C9-C10-N3	-2.08	113.85	116.99
4	A	280	PLH	C17-C18-C13	2.05	123.49	120.61

There are no chirality outliers.

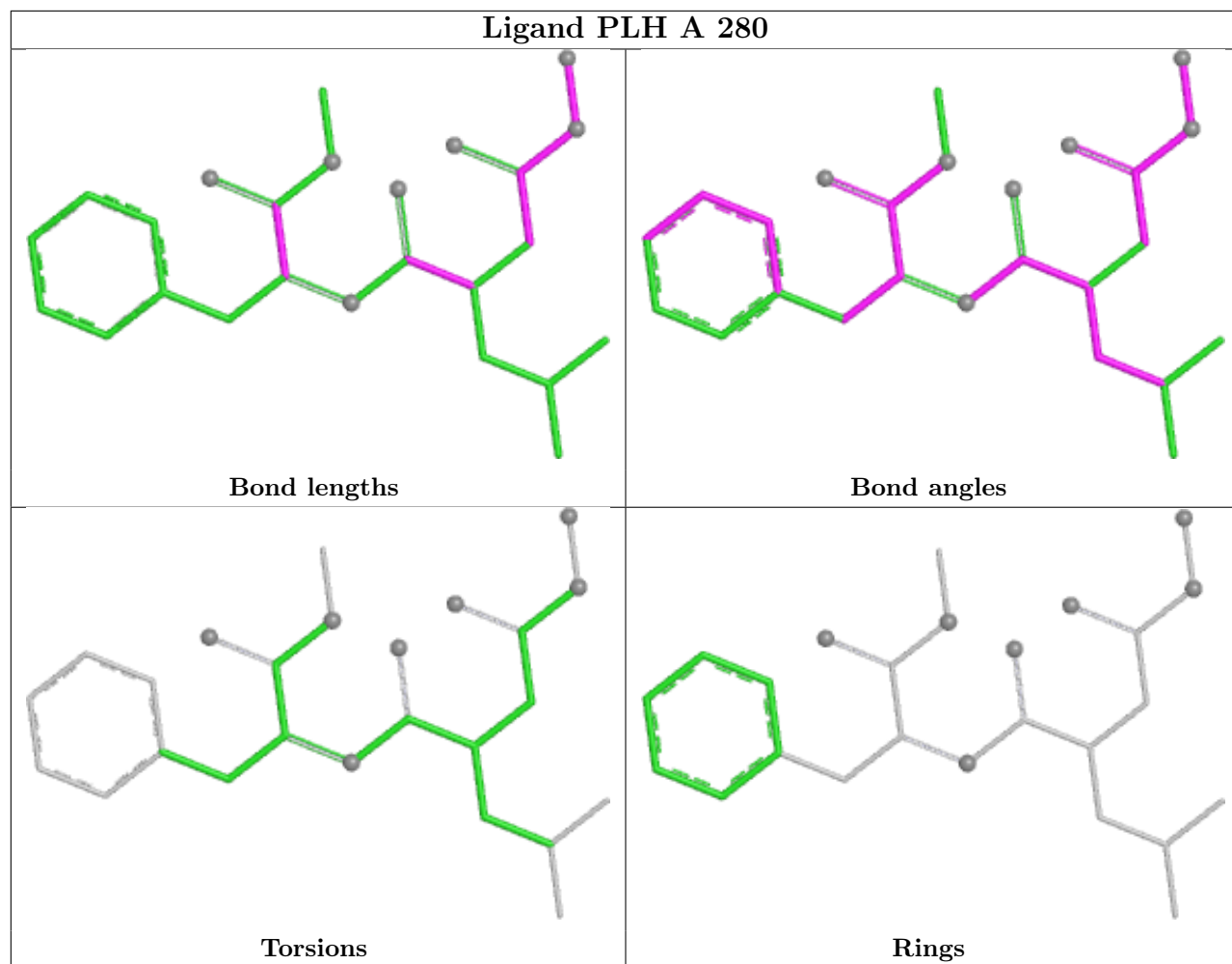
There are no torsion outliers.

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.