



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:12 pm GMT

PDB ID : 1MNC
Title : STRUCTURE OF HUMAN NEUTROPHIL COLLAGENASE REVEALS
LARGE S1' SPECIFICITY POCKET
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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

<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

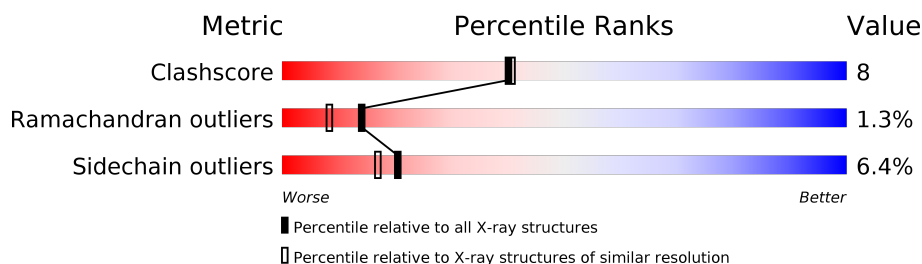
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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 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	163	 65% 26% . . .

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

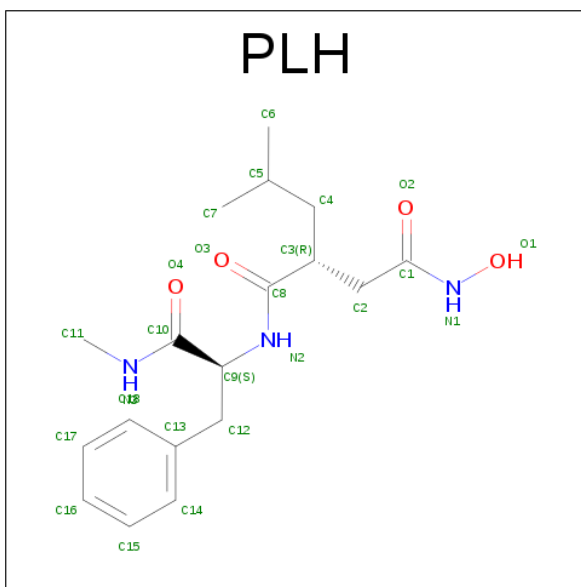
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: 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 (three-letter code: 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		

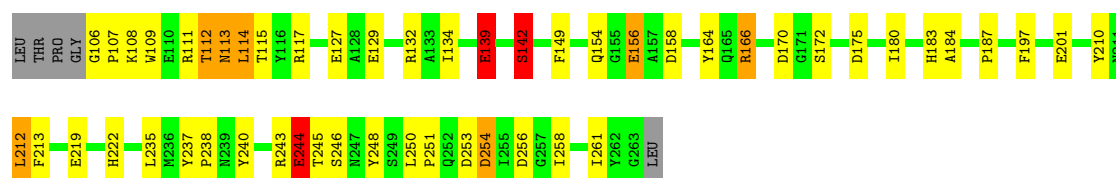
3 Residue-property plots [i](#)

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: NEUTROPHIL 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	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	0.92	1/1270 (0.1%)	2.09	35/1731 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	GLU	CD-OE1	-5.28	1.19	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH2	15.65	128.12	120.30
1	A	256	ASP	CB-CG-OD1	13.74	130.67	118.30
1	A	111	ARG	NE-CZ-NH2	12.52	126.56	120.30
1	A	111	ARG	NE-CZ-NH1	-11.53	114.53	120.30
1	A	253	ASP	CB-CG-OD2	10.55	127.80	118.30
1	A	175	ASP	CB-CG-OD2	9.53	126.88	118.30
1	A	139	GLU	OE1-CD-OE2	-8.27	113.38	123.30
1	A	166	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	A	254	ASP	CB-CG-OD1	-8.07	111.03	118.30
1	A	175	ASP	N-CA-CB	-7.67	96.79	110.60
1	A	243	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	158	ASP	CB-CG-OD2	7.26	124.84	118.30
1	A	114	LEU	CA-CB-CG	7.08	131.58	115.30
1	A	210	TYR	CB-CG-CD1	-7.00	116.80	121.00
1	A	127	GLU	OE1-CD-OE2	6.60	131.22	123.30
1	A	240	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	154	GLN	CB-CG-CD	6.32	128.04	111.60
1	A	212	LEU	CB-CG-CD2	6.13	121.42	111.00
1	A	164	TYR	CB-CG-CD2	6.11	124.67	121.00
1	A	156	GLU	CB-CA-C	-6.08	98.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	OD1-CG-OD2	-6.02	111.86	123.30
1	A	132	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	112	THR	OG1-CB-CG2	5.89	123.55	110.00
1	A	149	PHE	CB-CG-CD1	-5.85	116.71	120.80
1	A	115	THR	CA-CB-OG1	-5.82	96.78	109.00
1	A	112	THR	N-CA-CB	-5.63	99.61	110.30
1	A	197	PHE	O-C-N	5.60	131.66	122.70
1	A	170	ASP	CB-CA-C	5.59	121.58	110.40
1	A	248	TYR	CB-CG-CD1	5.47	124.28	121.00
1	A	201	GLU	CG-CD-OE1	5.43	129.17	118.30
1	A	142	SER	N-CA-CB	-5.42	102.37	110.50
1	A	244	GLU	N-CA-C	-5.35	96.55	111.00
1	A	117	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	134	ILE	O-C-N	-5.06	114.61	122.70
1	A	244	GLU	O-C-N	5.02	130.74	122.70

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:HD13	1:A:180:ILE:HA	1.85	0.41

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	156/163 (96%)	147 (94%)	7 (4%)	2 (1%)	14 8

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%)	117 (94%)	8 (6%)	20	17

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
1	A	209	ASN

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 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	1.75	5 (20%)	29,32,32	1.65	8 (27%)

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	-6.27	1.28	1.39
4	A	280	PLH	C3-C8	-2.55	1.47	1.51
4	A	280	PLH	C2-C1	-2.54	1.46	1.51
4	A	280	PLH	C9-C10	-2.24	1.46	1.52
4	A	280	PLH	C1-N1	2.02	1.34	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	280	PLH	O2-C1-C2	-2.84	117.14	121.42
4	A	280	PLH	C12-C9-C10	-2.21	104.31	110.28
4	A	280	PLH	O3-C8-C3	-2.08	119.45	122.11
4	A	280	PLH	C9-C10-N3	-2.07	113.85	116.99
4	A	280	PLH	O4-C10-N3	2.30	127.02	123.12
4	A	280	PLH	C3-C4-C5	2.39	121.34	115.63
4	A	280	PLH	C3-C8-N2	2.71	120.39	116.16
4	A	280	PLH	O1-N1-C1	3.97	125.76	119.81

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

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.