

Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 05:03 AM EDT

PDB ID : 1G86

Title : CHARCOT-LEYDEN CRYSTAL PROTEIN/N-ETHYLMALEIMIDE COM-

PLEX

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Deposited on : 2000-11-16

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 (i) 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

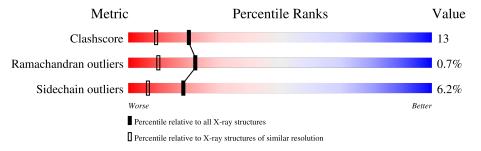
Validation Pipeline (wwPDB-VP) : 2.34

1 Overall quality at a glance (i)

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	Similar resolution	
Metric	$(\# \mathrm{Entries})$	$(\# \text{Entries, resolution range}(\mathring{A}))$	
Clashscore	141614	6793 (1.80-1.80)	
Ramachandran outliers	138981	6697 (1.80-1.80)	
Sidechain outliers	138945	6696 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain			
1	A	142	77%	20%		



2 Entry composition (i)

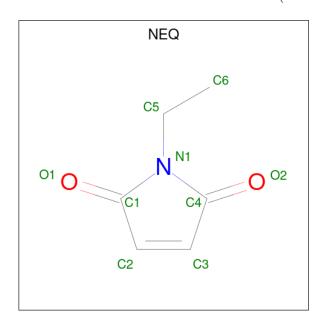
There are 3 unique types of molecules in this entry. The entry contains 1245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHARCOT-LEYDEN CRYSTAL PROTEIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	141	Total	С	N	О	S	0	0	0
1	11	141	1145	734	190	214	7			U

• Molecule 2 is N-ETHYLMALEIMIDE (three-letter code: NEQ) (formula: C₆H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 9		N 1		0	0
2	A	1	Total 9	C 6	N 1	O 2	0	0

• Molecule 3 is water.

\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0

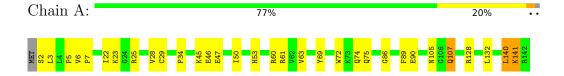


3 Residue-property plots (i)

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: CHARCOT-LEYDEN CRYSTAL PROTEIN





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 65 2 2	Depositor	
Cell constants	49.71Å 49.71Å 264.86Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	20.00 - 1.80	Depositor	
% Data completeness	93.3 (20.00-1.80)	Depositor	
(in resolution range)	30.9 (20.00 1.00)		
R_{merge}	0.13	Depositor	
R_{sym}	0.05	Depositor	
Refinement program	X-PLOR 3.851	Depositor	
R, R_{free}	0.203 , 0.242	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1245	wwPDB-VP	
Average B, all atoms (Å ²)	24.0	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: NEQ

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.48	0/1173	0.72	0/1586	

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	TYR	Sidechain

5.2 Too-close contacts (i)

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	1145	0	1123	29	0
2	A	18	0	14	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	82	0	0	5	1
All	All	1245	0	1137	29	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 13.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	$-$ overlap (\AA)
1:A:53:HIS:NE2	2:A:153:NEQ:H21	1.71	1.03
1:A:140:LEU:HD22	1:A:141:LYS:NZ	1.93	0.84
1:A:140:LEU:HD12	1:A:140:LEU:H	1.43	0.81
1:A:53:HIS:CE1	2:A:153:NEQ:H21	2.23	0.74
1:A:140:LEU:HD12	1:A:140:LEU:N	2.10	0.66
1:A:140:LEU:HD22	1:A:141:LYS:CE	2.32	0.59
1:A:63:VAL:HG13	1:A:75:GLN:HG3	1.85	0.58
1:A:90:GLU:H	1:A:105:ASN:ND2	2.03	0.57
1:A:5:PRO:HA	3:A:181:HOH:O	2.04	0.57
1:A:140:LEU:HD22	1:A:141:LYS:HZ1	1.70	0.56
1:A:107:GLN:NE2	3:A:155:HOH:O	2.37	0.56
1:A:29:CYS:SG	2:A:143:NEQ:H21	2.50	0.51
1:A:2:SER:N	3:A:167:HOH:O	2.44	0.50
1:A:140:LEU:HD22	1:A:141:LYS:HE3	1.94	0.49
1:A:46:GLU:HG2	3:A:177:HOH:O	2.12	0.49
1:A:140:LEU:HD22	1:A:141:LYS:HZ2	1.76	0.48
1:A:45:LYS:HD3	1:A:47:GLU:OE1	2.13	0.47
1:A:140:LEU:CD1	1:A:141:LYS:H	2.28	0.47
1:A:86:GLY:HA2	3:A:214:HOH:O	2.14	0.47
1:A:89:PHE:HA	1:A:105:ASN:HD21	1.80	0.46
1:A:140:LEU:HD13	1:A:141:LYS:H	1.80	0.46
1:A:29:CYS:SG	2:A:143:NEQ:C2	3.05	0.45
1:A:50:ILE:HG21	1:A:53:HIS:HB2	2.00	0.44
1:A:23:LYS:HE2	1:A:90:GLU:OE2	2.19	0.43
1:A:72:TRP:CG	2:A:153:NEQ:H62	2.54	0.43
1:A:22:ILE:HG23	1:A:132:LEU:HD11	2.01	0.42
1:A:140:LEU:N	1:A:140:LEU:CD1	2.80	0.42
1:A:28:VAL:HG22	1:A:34:PRO:HB3	2.02	0.41
1:A:6:VAL:HA	1:A:7:PRO:C	2.40	0.41

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	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	Clash overlap (Å)
3:A:169:HOH:O	3:A:169:HOH:O[11_555]	2.03	0.17

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	139/142 (98%)	135 (97%)	3 (2%)	1 (1%)	22 10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ARG

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	Analysed Rotameric Outliers		Percentiles
1	A	130/132 (98%)	122 (94%)	8 (6%)	18 6

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

Mol	Chain	Res	Type
1	A	3	LEU
1	A	25	ARG
1	A	60	ARG
1	A	61	ARG
1	A	74	GLN

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Mol	Chain	Res	Type
1	A	107	GLN
1	A	140	LEU
1	A	141	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	105	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	Trme	Chain	$oxed{\operatorname{Res}} oxed{\operatorname{Link}}$		B	ond leng	gths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NEQ	A	143	-	9,9,9	1.31	1 (11%)	12,12,12	0.67	0
2	NEQ	A	153	-	9,9,9	1.08	0	12,12,12	0.79	0



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
2	NEQ	A	143	-	-	0/2/15/15	0/1/1/1
2	NEQ	A	153	-	-	2/2/15/15	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	A	143	NEQ	C4-N1	2.27	1.44	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	153	NEQ	C6-C5-N1-C4
2	A	153	NEQ	C6-C5-N1-C1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	143	NEQ	2	0
2	A	153	NEQ	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

