



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:05 PM UTC

PDB ID : 1KBW / pdb_00001kbw
Title : CRYSTAL STRUCTURE OF THE SOLUBLE DOMAIN OF ANIA FROM
NEISSERIA GONORRHOEAE
Authors : Boulanger, M.J.; Murphy, M.E.P.
Deposited on : 2001-11-06
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

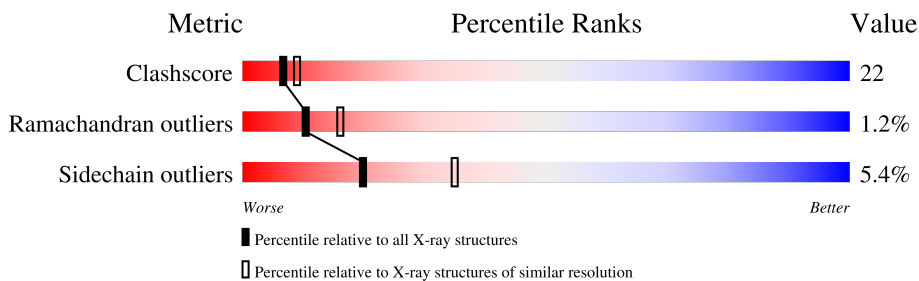
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	327	
1	B	327	
1	C	327	
1	D	327	
1	E	327	
1	F	327	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14902 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 Major outer membrane protein PAN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	B	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	C	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	D	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	E	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	F	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02219
A	209	ALA	SER	SEE REMARK 999	UNP Q02219
A	210	LEU	ILE	SEE REMARK 999	UNP Q02219
A	211	THR	ALA	SEE REMARK 999	UNP Q02219
A	283	ASN	SER	SEE REMARK 999	UNP Q02219
A	325	VAL	-	cloning artifact	UNP Q02219
A	326	PRO	-	cloning artifact	UNP Q02219
A	327	ARG	-	cloning artifact	UNP Q02219
B	1	MET	-	initiating methionine	UNP Q02219
B	209	ALA	SER	SEE REMARK 999	UNP Q02219
B	210	LEU	ILE	SEE REMARK 999	UNP Q02219
B	211	THR	ALA	SEE REMARK 999	UNP Q02219
B	283	ASN	SER	SEE REMARK 999	UNP Q02219
B	325	VAL	-	cloning artifact	UNP Q02219
B	326	PRO	-	cloning artifact	UNP Q02219
B	327	ARG	-	cloning artifact	UNP Q02219
C	1	MET	-	initiating methionine	UNP Q02219

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Chain	Residue	Modelled	Actual	Comment	Reference
C	209	ALA	SER	SEE REMARK 999	UNP Q02219
C	210	LEU	ILE	SEE REMARK 999	UNP Q02219
C	211	THR	ALA	SEE REMARK 999	UNP Q02219
C	283	ASN	SER	SEE REMARK 999	UNP Q02219
C	325	VAL	-	cloning artifact	UNP Q02219
C	326	PRO	-	cloning artifact	UNP Q02219
C	327	ARG	-	cloning artifact	UNP Q02219
D	1	MET	-	initiating methionine	UNP Q02219
D	209	ALA	SER	SEE REMARK 999	UNP Q02219
D	210	LEU	ILE	SEE REMARK 999	UNP Q02219
D	211	THR	ALA	SEE REMARK 999	UNP Q02219
D	283	ASN	SER	SEE REMARK 999	UNP Q02219
D	325	VAL	-	cloning artifact	UNP Q02219
D	326	PRO	-	cloning artifact	UNP Q02219
D	327	ARG	-	cloning artifact	UNP Q02219
E	1	MET	-	initiating methionine	UNP Q02219
E	209	ALA	SER	SEE REMARK 999	UNP Q02219
E	210	LEU	ILE	SEE REMARK 999	UNP Q02219
E	211	THR	ALA	SEE REMARK 999	UNP Q02219
E	283	ASN	SER	SEE REMARK 999	UNP Q02219
E	325	VAL	-	cloning artifact	UNP Q02219
E	326	PRO	-	cloning artifact	UNP Q02219
E	327	ARG	-	cloning artifact	UNP Q02219
F	1	MET	-	initiating methionine	UNP Q02219
F	209	ALA	SER	SEE REMARK 999	UNP Q02219
F	210	LEU	ILE	SEE REMARK 999	UNP Q02219
F	211	THR	ALA	SEE REMARK 999	UNP Q02219
F	283	ASN	SER	SEE REMARK 999	UNP Q02219
F	325	VAL	-	cloning artifact	UNP Q02219
F	326	PRO	-	cloning artifact	UNP Q02219
F	327	ARG	-	cloning artifact	UNP Q02219

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Cu	0	0
			2	2		
2	F	2	Total	Cu	0	0
			2	2		

- Molecule 3 is water.

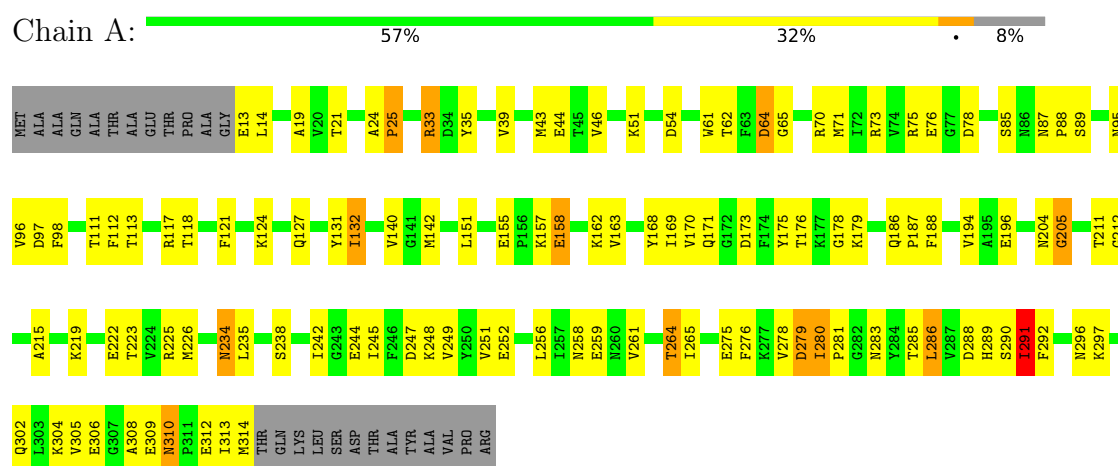
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	183	Total	O	0	0
			183	183		
3	C	182	Total	O	0	0
			182	182		
3	D	210	Total	O	0	0
			210	210		
3	E	192	Total	O	0	0
			192	192		
3	F	156	Total	O	0	0
			156	156		

3 Residue-property plots

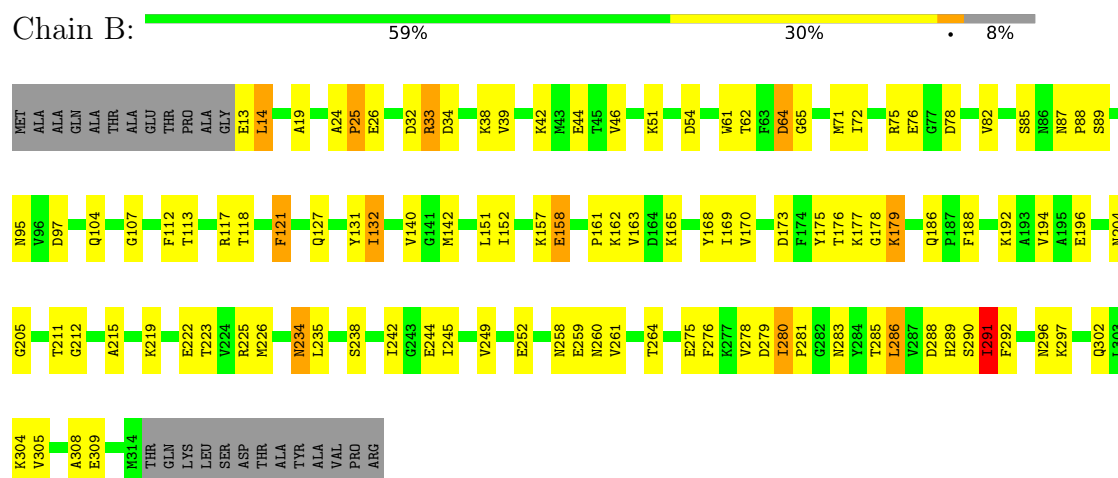
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Major outer membrane protein PAN 1

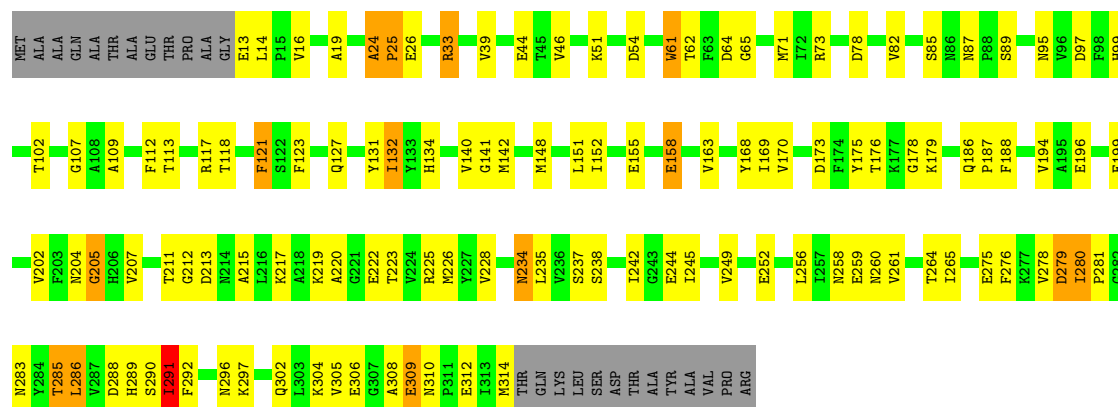


• Molecule 1: Major outer membrane protein PAN 1



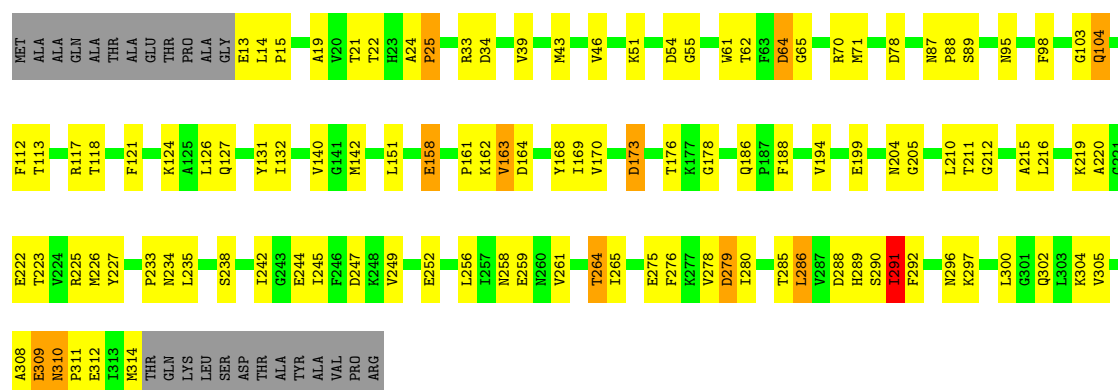
• Molecule 1: Major outer membrane protein PAN 1





- Molecule 1: Major outer membrane protein PAN 1

Chain D: 58% 31% 8%



- Molecule 1: Major outer membrane protein PAN 1

Chain E: 57% 31% 8%



- Molecule 1: Major outer membrane protein PAN 1

Chain F: 57% 31% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.23Å 99.55Å 103.71Å 83.55° 73.70° 73.01°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	80.7 (50.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14902	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: CU

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	0.48	0/2346	1.62	23/3185 (0.7%)
1	B	0.47	0/2346	1.62	22/3185 (0.7%)
1	C	0.48	0/2346	1.65	27/3185 (0.8%)
1	D	0.45	0/2346	1.66	26/3185 (0.8%)
1	E	0.48	0/2346	1.20	21/3185 (0.7%)
1	F	0.46	0/2346	1.66	25/3185 (0.8%)
All	All	0.47	0/14076	1.58	144/19110 (0.8%)

There are no bond length outliers.

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	24	ALA	CA-C-N	47.90	179.72	119.84
1	F	24	ALA	C-N-CA	47.90	179.72	119.84
1	D	24	ALA	CA-C-N	47.61	179.35	119.84
1	D	24	ALA	C-N-CA	47.61	179.35	119.84
1	C	24	ALA	CA-C-N	46.96	178.54	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2291	0	2234	113	0
1	B	2291	0	2234	100	0
1	C	2291	0	2234	109	0
1	D	2291	0	2234	102	0
1	E	2291	0	2234	103	0
1	F	2291	0	2234	111	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	221	0	0	28	0
3	B	183	0	0	28	0
3	C	182	0	0	19	0
3	D	210	0	0	17	0
3	E	192	0	0	21	0
3	F	156	0	0	24	0
All	All	14902	0	13404	585	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 22.

The worst 5 of 585 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:C:278:VAL:HG11	1:C:305:VAL:HG21	1.24	1.17
1:E:201:VAL:HB	3:E:679:HOH:O	1.46	1.14
1:D:264:THR:HG22	1:F:252:GLU:OE1	1.50	1.12
1:A:264:THR:HG22	1:C:252:GLU:OE1	1.48	1.12
1:A:278:VAL:HG11	1:A:305:VAL:HG21	1.37	1.05

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	300/327 (92%)	289 (96%)	7 (2%)	4 (1%)	9	14
1	B	300/327 (92%)	289 (96%)	7 (2%)	4 (1%)	9	14
1	C	300/327 (92%)	289 (96%)	7 (2%)	4 (1%)	9	14
1	D	300/327 (92%)	288 (96%)	9 (3%)	3 (1%)	12	20
1	E	300/327 (92%)	286 (95%)	11 (4%)	3 (1%)	12	20
1	F	300/327 (92%)	286 (95%)	10 (3%)	4 (1%)	9	14
All	All	1800/1962 (92%)	1727 (96%)	51 (3%)	22 (1%)	10	16

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	B	14	LEU
1	B	25	PRO
1	C	25	PRO
1	D	25	PRO

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	239/259 (92%)	226 (95%)	13 (5%)	20	35
1	B	239/259 (92%)	227 (95%)	12 (5%)	22	38
1	C	239/259 (92%)	227 (95%)	12 (5%)	22	38
1	D	239/259 (92%)	226 (95%)	13 (5%)	20	35
1	E	239/259 (92%)	226 (95%)	13 (5%)	20	35
1	F	239/259 (92%)	225 (94%)	14 (6%)	18	31
All	All	1434/1554 (92%)	1357 (95%)	77 (5%)	20	35

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	264	THR
1	F	279	ASP
1	E	280	ILE
1	F	132	ILE
1	F	290	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	197	GLN
1	F	204	ASN
1	C	127	GLN
1	C	87	ASN
1	F	258	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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.