



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:29 AM UTC

PDB ID : 5TW7 / pdb_00005tw7
Title : Crystal structure of a GMP synthase (glutamine-hydrolyzing) from *Neisseria gonorrhoeae*
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2016-11-11
Resolution : 2.35 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

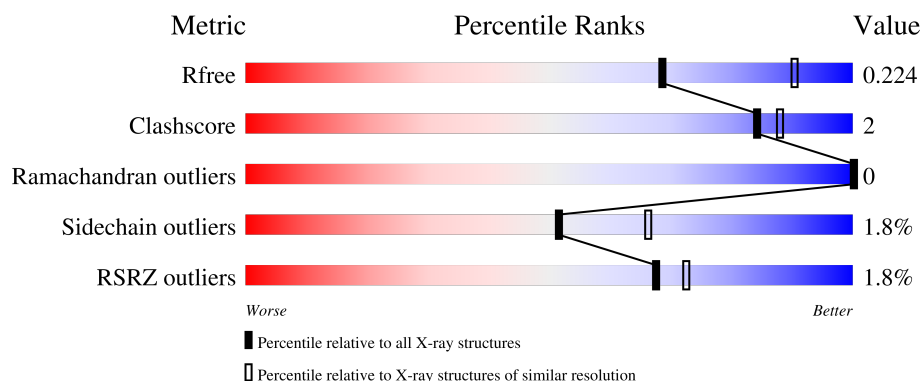
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	529	2% 88% 7%
1	B	529	2% 86% 6% 7%
1	C	529	2% 85% 8% 7%
1	D	529	2% 86% 6% 7%
1	E	529	2% 85% 7% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	529	2% 85% 7% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23028 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 GMP synthase [glutamine-hydrolyzing].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	3	0
			3791	2423	647	704	17			
1	B	490	Total	C	N	O	S	0	5	0
			3807	2431	647	712	17			
1	C	492	Total	C	N	O	S	0	1	0
			3804	2427	646	713	18			
1	D	491	Total	C	N	O	S	0	1	0
			3759	2399	640	703	17			
1	E	489	Total	C	N	O	S	0	0	0
			3757	2398	636	706	17			
1	F	490	Total	C	N	O	S	0	2	0
			3772	2409	639	706	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP B4RJH7
A	-6	ALA	-	expression tag	UNP B4RJH7
A	-5	HIS	-	expression tag	UNP B4RJH7
A	-4	HIS	-	expression tag	UNP B4RJH7
A	-3	HIS	-	expression tag	UNP B4RJH7
A	-2	HIS	-	expression tag	UNP B4RJH7
A	-1	HIS	-	expression tag	UNP B4RJH7
A	0	HIS	-	expression tag	UNP B4RJH7
B	-7	MET	-	expression tag	UNP B4RJH7
B	-6	ALA	-	expression tag	UNP B4RJH7
B	-5	HIS	-	expression tag	UNP B4RJH7
B	-4	HIS	-	expression tag	UNP B4RJH7
B	-3	HIS	-	expression tag	UNP B4RJH7
B	-2	HIS	-	expression tag	UNP B4RJH7
B	-1	HIS	-	expression tag	UNP B4RJH7
B	0	HIS	-	expression tag	UNP B4RJH7
C	-7	MET	-	expression tag	UNP B4RJH7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP B4RJH7
C	-5	HIS	-	expression tag	UNP B4RJH7
C	-4	HIS	-	expression tag	UNP B4RJH7
C	-3	HIS	-	expression tag	UNP B4RJH7
C	-2	HIS	-	expression tag	UNP B4RJH7
C	-1	HIS	-	expression tag	UNP B4RJH7
C	0	HIS	-	expression tag	UNP B4RJH7
D	-7	MET	-	expression tag	UNP B4RJH7
D	-6	ALA	-	expression tag	UNP B4RJH7
D	-5	HIS	-	expression tag	UNP B4RJH7
D	-4	HIS	-	expression tag	UNP B4RJH7
D	-3	HIS	-	expression tag	UNP B4RJH7
D	-2	HIS	-	expression tag	UNP B4RJH7
D	-1	HIS	-	expression tag	UNP B4RJH7
D	0	HIS	-	expression tag	UNP B4RJH7
E	-7	MET	-	expression tag	UNP B4RJH7
E	-6	ALA	-	expression tag	UNP B4RJH7
E	-5	HIS	-	expression tag	UNP B4RJH7
E	-4	HIS	-	expression tag	UNP B4RJH7
E	-3	HIS	-	expression tag	UNP B4RJH7
E	-2	HIS	-	expression tag	UNP B4RJH7
E	-1	HIS	-	expression tag	UNP B4RJH7
E	0	HIS	-	expression tag	UNP B4RJH7
F	-7	MET	-	expression tag	UNP B4RJH7
F	-6	ALA	-	expression tag	UNP B4RJH7
F	-5	HIS	-	expression tag	UNP B4RJH7
F	-4	HIS	-	expression tag	UNP B4RJH7
F	-3	HIS	-	expression tag	UNP B4RJH7
F	-2	HIS	-	expression tag	UNP B4RJH7
F	-1	HIS	-	expression tag	UNP B4RJH7
F	0	HIS	-	expression tag	UNP B4RJH7

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	O 2	0	0
3	D	1	Total 1	O 1	0	0
3	E	147	Total 147	O 147	0	0
3	F	186	Total 186	O 186	0	0

Chain D:

Chain E:

Sequence logo for Chain E. The y-axis represents information content in bits (0.00 to 0.20). The x-axis shows positions 1 to 300. A green bar at the top indicates a 2% overall conservation level. A legend shows 85% for green, 7% for orange, and 8% for grey.

Position	Amino Acid	Information Content (bits)
1	GLY	0.18
2	R460	0.15
3	T473	0.10
4	V507	0.08
5	E521	0.05
6	GLU	0.18
7	SER	0.15
8	ALA	0.10
9	GLY	0.08
10	ALA	0.05
11	LYS	0.10
12	LYS	0.15
13	LYS	0.10
14	ALA	0.08
15	HIS	0.05
16	ALA	0.10
17	ILE	0.05
18	LYS	0.08
19	SER	0.05
20	HIS	0.08
21	HIS	0.10
22	ASN	0.15
23	VAL	0.10
24	GLY	0.08
25	GLY	0.10
26	LEU	0.15
27	PRO	0.05
28	GLU	0.08
29	ASN	0.05
30	LYS	0.10
31	LYS	0.15
32	GLU	0.08
33	PI41	0.05
34	V220	0.08
35	I221	0.05
36	V228	0.08
37	T246	0.05
38	H252	0.10
39	G253	0.08
40	L254	0.05
41	M266	0.10
42	F267	0.08
43	N270	0.15
44	L271	0.08
45	E281	0.05
46	V291	0.08
47	K297	0.05
48	L316	0.15
49	T317	0.10

Chain F:

Amino Acid	Frequency (%)
Y462	2%
T473	7%
W520	7%
E521	7%
W321	85%
L322	85%
A323	85%
T327	85%
T328	85%
P329	85%
D330	85%
V331	85%
T332	85%
GLU	85%
SER	85%
ALA	85%
GLY	85%
ALA	85%
LYS	85%
THR	85%
LYS	85%
LYS	85%
ALA	85%
HIS	85%
ALA	85%
ILE	85%
LYS	85%
SER	85%
HIS	85%
HIS	85%
ASN	85%
VAL	85%
GLY	85%
GLY	85%
LEU	85%
PRO	85%
GLU	85%
ASN	85%
MET	85%
K359	85%
D368	85%
R390	85%
L403	85%
V406	85%
M432	85%
S441	85%
K451	85%
V455	85%
MET	85%
GLY	85%
ASP	85%
GLY	85%
ARG	85%
F461	85%
MET	85%
ALA	85%
HIS	85%
HIS	85%
HIS	85%
HIS	85%
HIS	85%
M1	85%
T2	85%
S34	85%
F35	85%
D36	85%
V59	85%
F86	85%
M87	85%
A88	85%
R101	85%
R117	85%
P141	85%
F144	85%
M160	85%
K163	85%
Q164	85%
F165	85%
V220	85%
I221	85%
L222	85%
G226	85%
H252	85%
G253	85%
L254	85%
L255	85%
E259	85%
R269	85%
N270	85%
K274	85%
Q283	85%
K287	85%
K297	85%
F304	85%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	108.39Å 109.35Å 109.91Å 115.33° 100.00° 108.06°	Depositor
Resolution (Å)	46.12 – 2.35 46.12 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.12-2.35) 98.3 (46.12-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.186 , 0.223 0.187 , 0.224	Depositor DCC
R_{free} test set	7931 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23028	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.36	0/3877	0.54	1/5259 (0.0%)
1	B	0.41	0/3902	0.57	0/5295
1	C	0.36	0/3887	0.53	0/5273
1	D	0.32	0/3842	0.50	0/5221
1	E	0.30	0/3837	0.49	0/5213
1	F	0.31	0/3858	0.49	0/5239
All	All	0.34	0/23203	0.52	1/31500 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ARG	CB-CG-CD	-5.07	99.63	111.30

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	3791	0	3731	12	0
1	B	3807	0	3735	17	0
1	C	3804	0	3728	22	0
1	D	3759	0	3651	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3757	0	3656	22	0
1	F	3772	0	3686	21	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	2	0	0	0	0
3	D	1	0	0	0	0
3	E	147	0	0	0	0
3	F	186	0	0	2	0
All	All	23028	0	22187	105	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 2.

The worst 5 of 105 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:59:VAL:HG21	1:A:86:PHE:HA	1.76	0.66
1:D:59:VAL:HG21	1:D:86:PHE:HA	1.77	0.66
1:E:220:VAL:HG22	1:E:321:TRP:HB2	1.79	0.65
1:D:88:ALA:HA	1:D:141:PRO:HG3	1.80	0.64
1:F:220:VAL:HG22	1:F:321:TRP:HB2	1.84	0.60

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	487/529 (92%)	479 (98%)	8 (2%)	0	100	100
1	B	489/529 (92%)	482 (99%)	7 (1%)	0	100	100
1	C	487/529 (92%)	481 (99%)	6 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	486/529 (92%)	479 (99%)	7 (1%)	0	100	100
1	E	483/529 (91%)	476 (99%)	7 (1%)	0	100	100
1	F	486/529 (92%)	479 (99%)	7 (1%)	0	100	100
All	All	2918/3174 (92%)	2876 (99%)	42 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	397/440 (90%)	393 (99%)	4 (1%)	68	81
1	B	400/440 (91%)	392 (98%)	8 (2%)	48	63
1	C	399/440 (91%)	390 (98%)	9 (2%)	44	58
1	D	389/440 (88%)	380 (98%)	9 (2%)	44	58
1	E	392/440 (89%)	386 (98%)	6 (2%)	57	72
1	F	394/440 (90%)	387 (98%)	7 (2%)	51	66
All	All	2371/2640 (90%)	2328 (98%)	43 (2%)	51	66

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	371	LYS
1	E	473	THR
1	D	386	GLU
1	E	252	HIS
1	F	34	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	GLN
1	E	57	ASN
1	F	427	ASN
1	F	179	GLN
1	F	270	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 2 ligands modelled in this entry, 2 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/529 (92%)	-0.20	6 (1%) 76 81	16, 37, 63, 89	3 (0%)
1	B	490/529 (92%)	-0.30	7 (1%) 73 78	15, 31, 51, 99	5 (1%)
1	C	492/529 (93%)	-0.15	6 (1%) 76 81	21, 38, 61, 94	1 (0%)
1	D	491/529 (92%)	0.10	10 (2%) 65 70	22, 43, 72, 114	1 (0%)
1	E	489/529 (92%)	0.19	13 (2%) 56 63	27, 47, 76, 116	0
1	F	490/529 (92%)	0.11	10 (2%) 65 70	21, 46, 72, 96	2 (0%)
All	All	2942/3174 (92%)	-0.04	52 (1%) 67 72	15, 40, 70, 116	12 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	455	VAL	7.6
1	E	456	MET	5.9
1	E	60	TYR	5.7
1	B	455	VAL	5.7
1	D	2	THR	5.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	E	601	1/1	0.96	0.07	48,48,48,48	0
2	MG	F	601	1/1	0.96	0.06	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.