wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 12:20 AM EDT

PDB ID	:	5NXH
Title	:	Crystal structure of the carboxy-terminal region of the bacteriophage T4 proximal long tail fibre protein gp34, residues 744-1289 at 2.9 Angstrom resolution
Authors	:	Namura, M.; van Raaij, M.J.; Kanamaru, S.
Deposited on	:	2017-05-10
Resolution	:	2.89 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 (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:

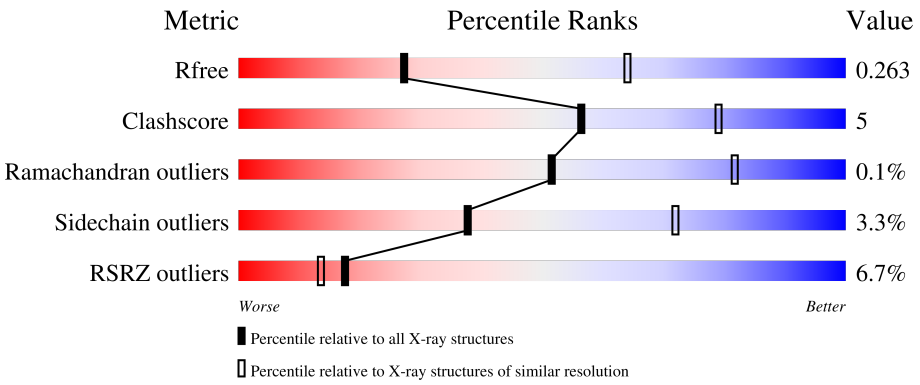
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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% 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	564	8% 84% 13% • •
1	B	564	5% 84% 12% • •
1	C	564	6% 85% 11% •

2 Entry composition (i)

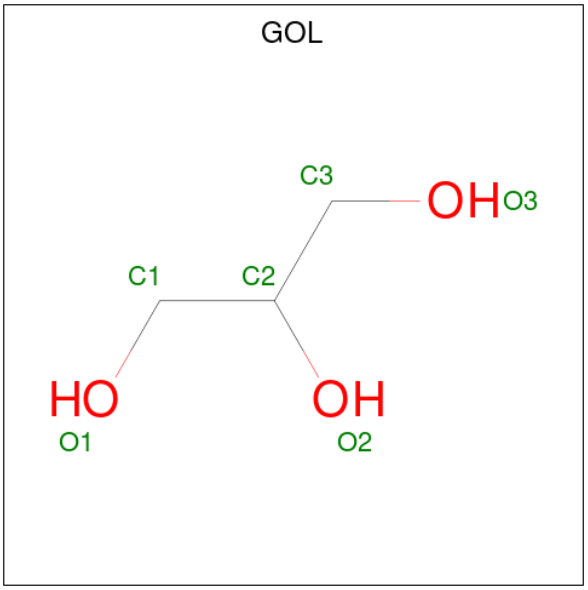
There are 3 unique types of molecules in this entry. The entry contains 12797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Long-tail fiber proximal subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	546	4147	2586	722	834	5	0	0	0
1	B	546	4147	2586	722	834	5	0	0	0
1	C	546	4147	2586	722	834	5	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	6	3	3	0	0

- Molecule 3 is water.

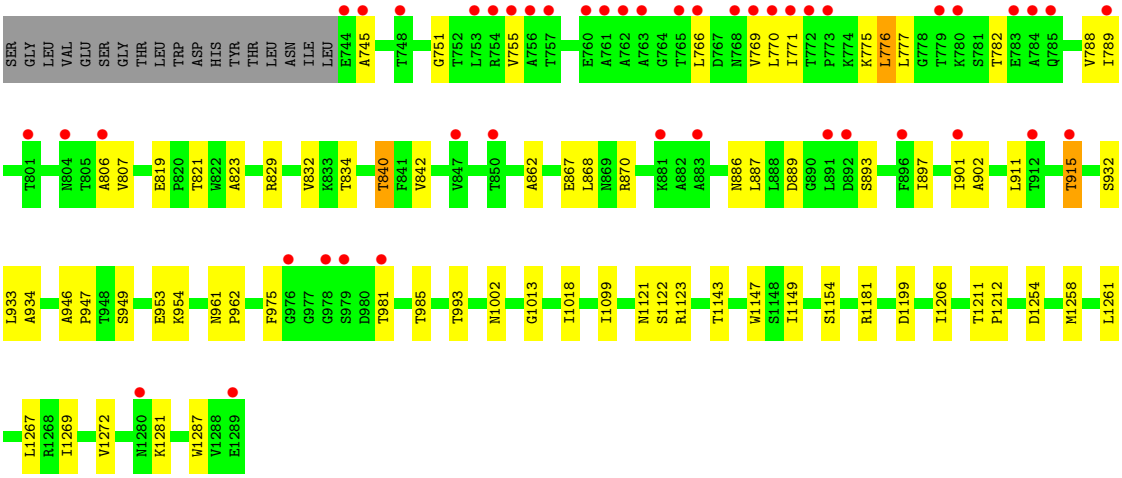
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	105	105	105	0	0
			Total	O		
3	B	126	126	126	0	0
			Total	O		
3	C	119	119	119	0	0

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 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.

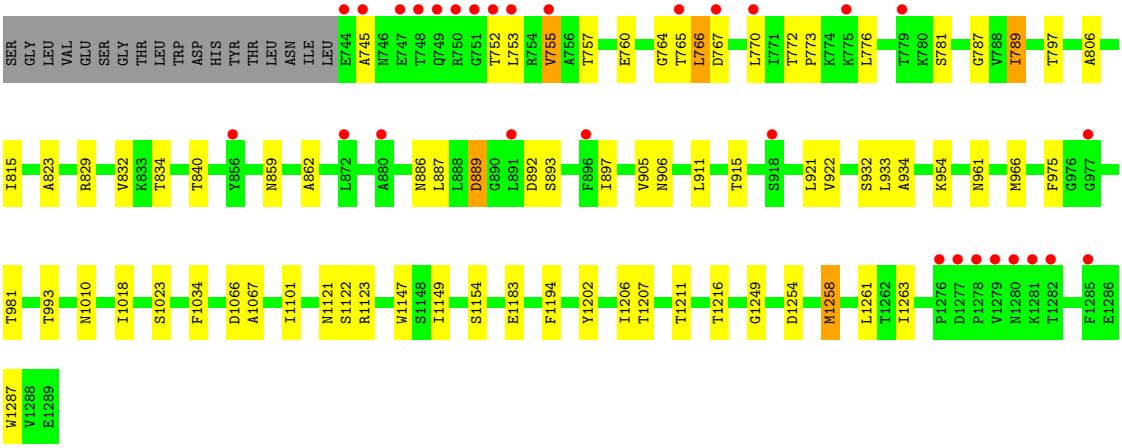
• Molecule 1: Long-tail fiber proximal subunit

Chain A:



• Molecule 1: Long-tail fiber proximal subunit

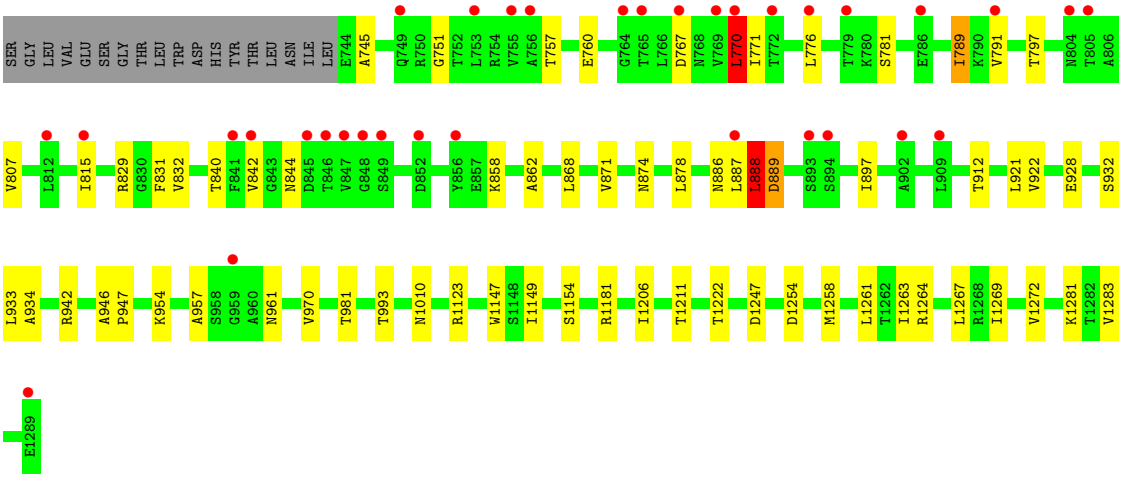
Chain B:



• Molecule 1: Long-tail fiber proximal subunit

Chain C:

6%
85%
11%


SER GLY LEU VAL GLU SER GLY THR LEU TRP ASP HIS TYR THR LEU ASN ILE LEU E744 A745 Q749 R750 G751 T752 L753 R754 V755 A756 T757 E760 G764 T765 L766 D767 N768 V769 L770 I771 T772 L776 T779 K780 S781 E786 I789 K790 V791 T797 N804 T805 A806
V807 L812 I815 R829 G830 F831 V832 T840 F841 V842 G843 N844 D845 T846 V847 G848 S849 D852 Y856 E857 K858 A862 L868 V871 N874 L878 N886 L887 L888 D889 S893 S894 I897 A902 L909 T912 L921 V922 E928 S932
L933 A934 R942 A946 P947 K954 A957 S958 G959 A960 N961 V970 T981 T993 N1010 R1123 W1147 S1148 I1149 S1154 R1181 I1206 T1211 T1222 D1247 D1254 M1258 L1261 T1262 I1263 R1264 L1267 R1268 I1269 V1272 K1281 T1282 V1283
E1289

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.30Å 76.13Å 139.87Å 90.00° 97.62° 90.00°	Depositor
Resolution (Å)	45.18 – 2.89 45.18 – 2.89	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.18-2.89) 96.5 (45.18-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.200 , 0.263 0.206 , 0.263	Depositor DCC
R_{free} test set	1911 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12797	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL

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	0.55	0/4227	0.76	3/5754 (0.1%)
1	B	0.55	0/4227	0.76	1/5754 (0.0%)
1	C	0.54	0/4227	0.76	4/5754 (0.1%)
All	All	0.55	0/12681	0.76	8/17262 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1199	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	1199	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	892	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	888	LEU	CB-CG-CD2	5.57	120.47	111.00
1	C	770	LEU	CA-CB-CG	5.39	127.70	115.30

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	4147	0	4052	59	0
1	B	4147	0	4052	59	0
1	C	4147	0	4052	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	0	0
3	A	105	0	0	4	0
3	B	126	0	0	1	0
3	C	119	0	0	0	0
All	All	12797	0	12164	124	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 5.

The worst 5 of 124 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:B:745:ALA:HB2	1:B:753:LEU:HD21	1.40	1.03
1:B:834:THR:HG21	1:C:858:LYS:O	1.74	0.85
1:A:776:LEU:HD13	1:A:777:LEU:HD23	1.65	0.78
1:B:1207:THR:O	1:B:1216:THR:HG23	1.85	0.77
1:A:789:ILE:CG2	1:B:789:ILE:HD11	2.18	0.72

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	544/564 (96%)	522 (96%)	22 (4%)	0	100 100
1	B	544/564 (96%)	521 (96%)	22 (4%)	1 (0%)	47 78
1	C	544/564 (96%)	519 (95%)	25 (5%)	0	100 100
All	All	1632/1692 (96%)	1562 (96%)	69 (4%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	766	LEU

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	Rotameric	Outliers	Percentiles	
1	A	452/468 (97%)	438 (97%)	14 (3%)	40	74
1	B	452/468 (97%)	437 (97%)	15 (3%)	38	72
1	C	452/468 (97%)	436 (96%)	16 (4%)	36	70
All	All	1356/1404 (97%)	1311 (97%)	45 (3%)	38	72

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1258	MET
1	C	889	ASP
1	C	770	LEU
1	C	842	VAL
1	C	932	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	B	1301	-	5,5,5	0.28	0	5,5,5	0.37	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	GOL	B	1301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	GOL	C1-C2-C3-O3
2	B	1301	GOL	O2-C2-C3-O3
2	B	1301	GOL	O1-C1-C2-O2
2	B	1301	GOL	O1-C1-C2-C3

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	546/564 (96%)	0.43	45 (8%)	11	9	25, 66, 117, 153	0
1	B	546/564 (96%)	0.36	30 (5%)	25	21	20, 62, 117, 176	0
1	C	546/564 (96%)	0.37	34 (6%)	20	16	23, 63, 120, 157	0
All	All	1638/1692 (96%)	0.39	109 (6%)	17	13	20, 64, 118, 176	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	770	LEU	8.6
1	A	769	VAL	5.6
1	A	784	ALA	5.6
1	B	753	LEU	5.4
1	A	779	THR	4.8

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 monosaccharides 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	GOL	B	1301	6/6	0.90	0.33	50,60,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.