



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:10 AM GMT

PDB ID : 2POH
Title : Structure of Phage P22 Tail Needle gp26
Authors : Olia, A.S.; Cingolani, G.
Deposited on : 2007-04-26
Resolution : 2.10 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

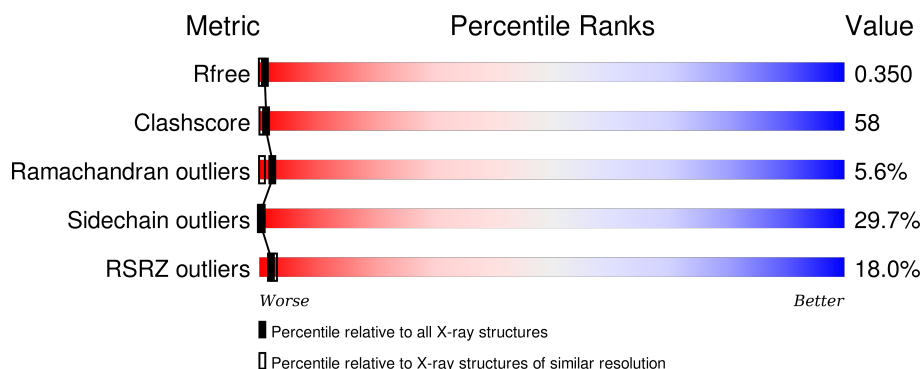
1 Overall quality at a glance ⓘ

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))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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.

Mol	Chain	Length	Quality of chain
1	A	233	<div> <div>15%</div> <div>33%</div> <div>48%</div> <div>17%</div> <div>.</div> </div>
1	B	233	<div> <div>7%</div> <div>31%</div> <div>48%</div> <div>19%</div> <div>.</div> </div>
1	C	233	<div> <div>15%</div> <div>33%</div> <div>47%</div> <div>17%</div> <div>.</div> </div>
1	D	233	<div> <div>26%</div> <div>26%</div> <div>48%</div> <div>22%</div> <div>.</div> </div>
1	E	233	<div> <div>24%</div> <div>33%</div> <div>46%</div> <div>19%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	233	<div><div></div><div>21%</div><div>28%</div><div>48%</div><div>22%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11261 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 Head completion protein.

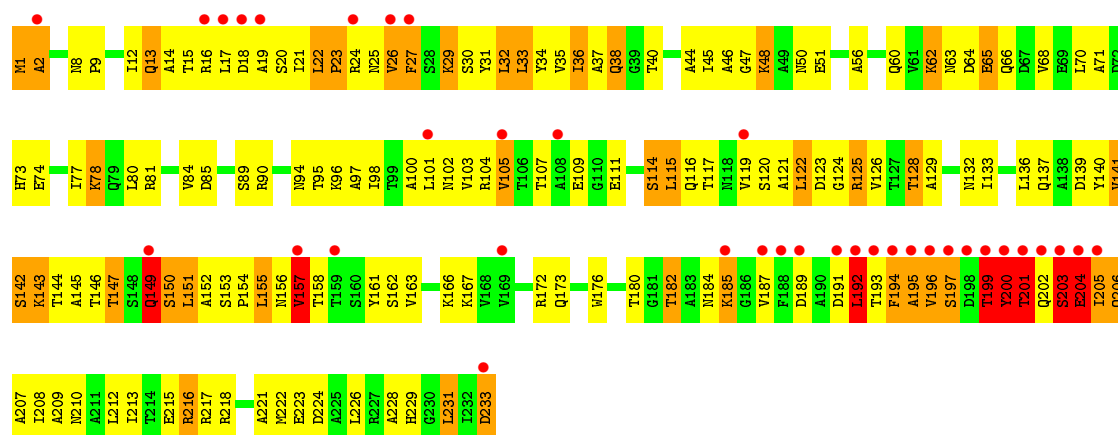
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	B	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	C	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	D	233	Total	C	N	O	Se	0	0	0
			1715	1045	310	358	2			
1	E	233	Total	C	N	O	Se	0	0	0
			1712	1048	308	354	2			
1	F	233	Total	C	N	O	Se	0	0	0
			1734	1062	311	359	2			

There are 12 discrepancies between the modelled and reference sequences:

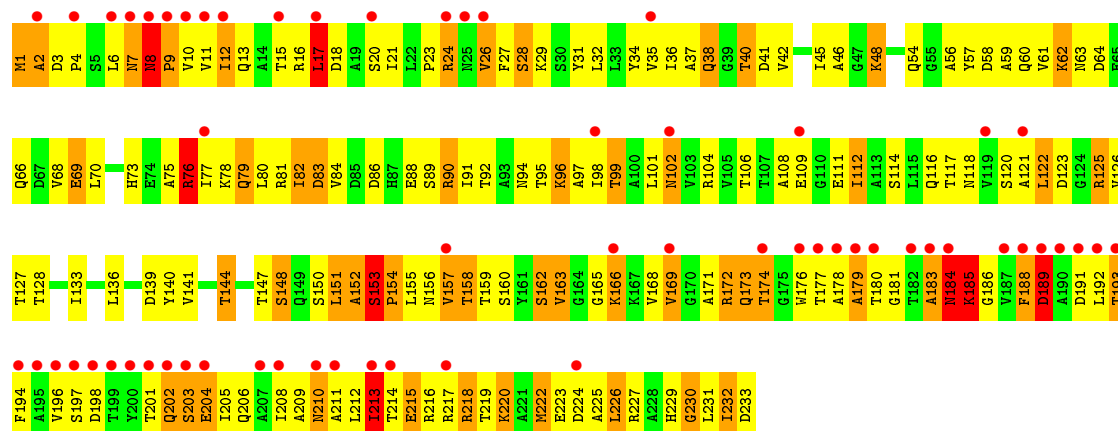
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
A	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
B	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
C	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
D	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
E	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
F	222	MSE	LEU	ENGINEERED	UNP Q8LTG5

- Molecule 2 is water.

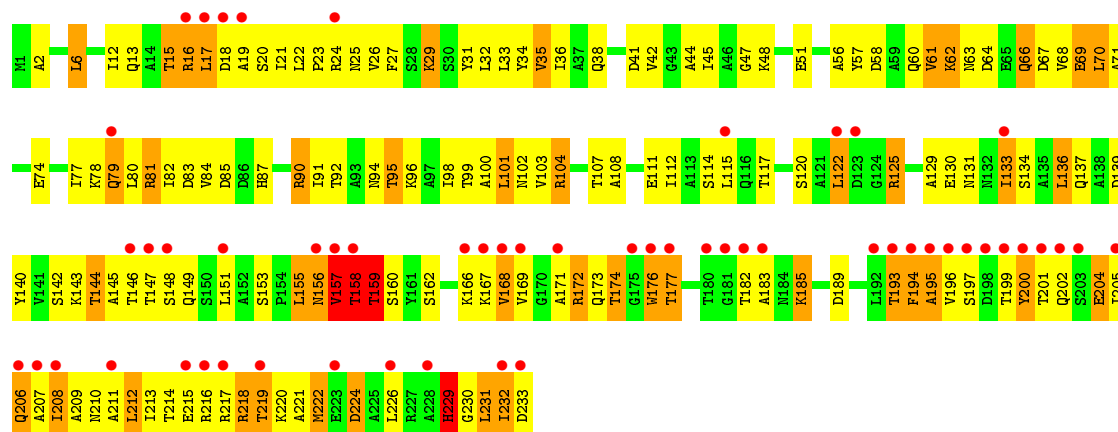
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	155	Total 155	O 155	0	0
2	B	167	Total 167	O 167	0	0
2	C	151	Total 151	O 151	0	0
2	D	124	Total 124	O 124	0	0
2	E	138	Total 138	O 138	0	0
2	F	151	Total 151	O 151	0	0



• Molecule 1: Head completion protein

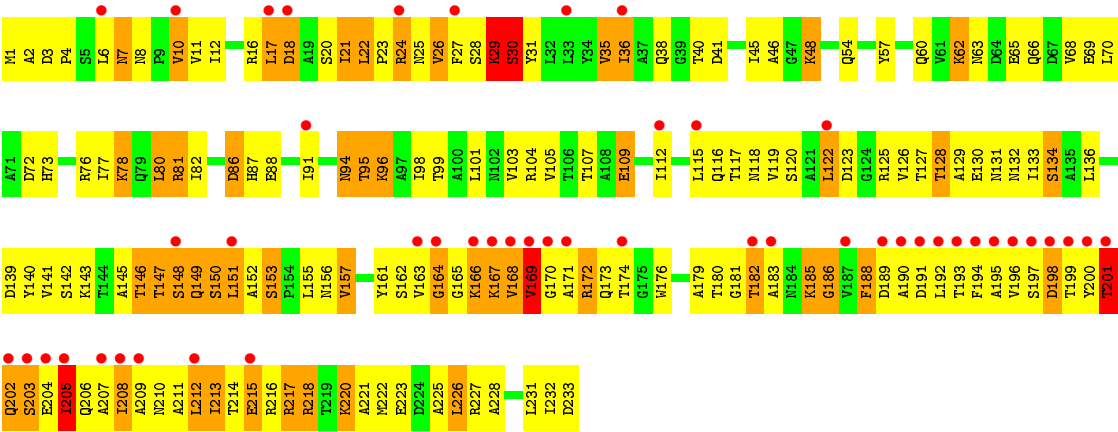


• Molecule 1: Head completion protein



• Molecule 1: Head completion protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.40 Å 114.03 Å 171.92 Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10 39.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 ((Not available)-2.10) 99.0 (39.21-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.00 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.167 , 0.232 0.304 , 0.350	Depositor DCC
R_{free} test set	4967 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.3	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 103960 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11261	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.38	0/1754	1.23	6/2384 (0.3%)
1	B	0.35	0/1754	1.03	2/2384 (0.1%)
1	C	0.46	1/1754 (0.1%)	1.09	7/2384 (0.3%)
1	D	0.33	0/1730	0.96	4/2347 (0.2%)
1	E	0.35	0/1728	0.99	5/2347 (0.2%)
1	F	0.34	0/1750	0.98	1/2377 (0.0%)
All	All	0.37	1/10470 (0.0%)	1.05	25/14223 (0.2%)

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	C	0	3
1	D	0	7
1	E	0	3
1	F	0	2
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	GLN	CD-NE2	11.38	1.61	1.32

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH2	22.31	131.46	120.30
1	A	172	ARG	NE-CZ-NH1	-21.44	109.58	120.30
1	A	172	ARG	CD-NE-CZ	13.99	143.18	123.60
1	E	229	HIS	O-C-N	-8.77	108.28	123.20
1	D	90	ARG	NE-CZ-NH1	8.40	124.50	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	196	VAL	Peptide
1	C	199	THR	Peptide
1	C	203	SER	Peptide
1	D	1	MSE	Peptide
1	D	2	ALA	Peptide

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	1738	0	1731	235	0
1	B	1738	0	1731	210	0
1	C	1738	0	1731	242	0
1	D	1715	0	1677	317	0
1	E	1712	0	1688	270	0
1	F	1734	0	1721	281	0
2	A	155	0	0	34	0
2	B	167	0	0	32	0
2	C	151	0	0	26	0
2	D	124	0	0	34	0
2	E	138	0	0	20	0
2	F	151	0	0	39	0
All	All	11261	0	10279	1200	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 58.

The worst 5 of 1200 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:D:222:MSE:SE	1:E:222:MSE:HE3	1.31	1.75
1:D:222:MSE:SE	1:E:222:MSE:CE	2.22	1.36
1:E:157:VAL:HG23	1:F:164:GLY:CA	1.54	1.35
1:D:153:SER:OG	1:E:158:THR:HB	1.36	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:VAL:CG2	1:E:158:THR:H	1.44	1.23

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	231/233 (99%)	199 (86%)	19 (8%)	13 (6%)	2	0
1	B	231/233 (99%)	211 (91%)	14 (6%)	6 (3%)	7	2
1	C	231/233 (99%)	199 (86%)	18 (8%)	14 (6%)	2	0
1	D	231/233 (99%)	176 (76%)	36 (16%)	19 (8%)	1	0
1	E	231/233 (99%)	204 (88%)	17 (7%)	10 (4%)	3	1
1	F	231/233 (99%)	200 (87%)	16 (7%)	15 (6%)	1	0
All	All	1386/1398 (99%)	1189 (86%)	120 (9%)	77 (6%)	2	0

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	190	ALA
1	A	191	ASP
1	A	194	PHE
1	A	200	TYR

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	184/182 (101%)	136 (74%)	48 (26%)	0	0
1	B	184/182 (101%)	127 (69%)	57 (31%)	0	0
1	C	184/182 (101%)	136 (74%)	48 (26%)	0	0
1	D	177/182 (97%)	121 (68%)	56 (32%)	0	0
1	E	178/182 (98%)	124 (70%)	54 (30%)	0	0
1	F	183/182 (100%)	122 (67%)	61 (33%)	0	0
All	All	1090/1092 (100%)	766 (70%)	324 (30%)	0	0

5 of 324 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	203	SER
1	D	162	SER
1	F	153	SER
1	C	216	ARG
1	D	69	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	ASN
1	D	210	ASN
1	F	131	ASN
1	C	210	ASN
1	D	118	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	231/233 (99%)	1.04	34 (14%) 3 5	2, 14, 36, 48	0
1	B	231/233 (99%)	0.87	17 (7%) 17 24	2, 16, 29, 38	0
1	C	231/233 (99%)	1.41	36 (15%) 3 4	3, 15, 55, 75	0
1	D	231/233 (99%)	1.71	60 (25%) 1 1	5, 21, 56, 75	0
1	E	231/233 (99%)	1.44	55 (23%) 1 1	4, 18, 59, 77	0
1	F	231/233 (99%)	1.41	48 (20%) 1 1	3, 17, 43, 56	0
All	All	1386/1398 (99%)	1.31	250 (18%) 2 2	2, 17, 48, 77	0

The worst 5 of 250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	THR	12.2
1	F	194	PHE	11.5
1	D	196	VAL	11.4
1	D	195	ALA	11.1
1	D	178	ALA	11.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.