wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 03:36 PM EDT

PDB ID	:	2FS3
Title	:	Bacteriophage HK97 K169Y Head I
Authors	:	Gan, L.; Speir, J.A.; Conway, J.F.; Lander, G.; Cheng, N.; Firek, B.A.; Hendrix, R.W.; Duda, R.L.; Liljas, L.; Johnson, J.E.
Deposited on	:	2006-01-20
Resolution	:	4.20 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:

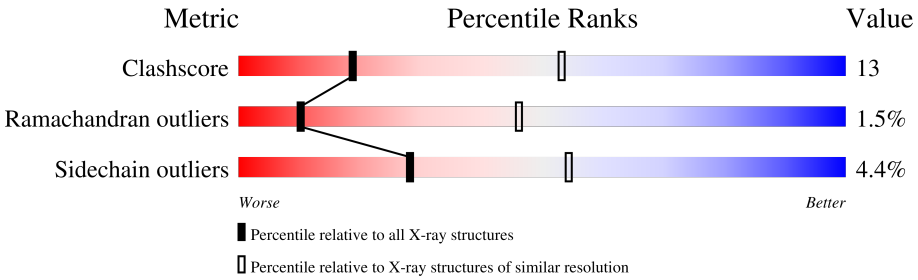
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 4.20 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	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)

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%

Mol	Chain	Length	Quality of chain
1	A	282	71% 26%
1	B	282	73% 24%
1	C	282	68% 27%
1	D	282	70% 28%
1	E	282	74% 23%
1	F	282	64% 25% 9%
1	G	282	59% 24% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14664 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 capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2154	1347	374	423	10			
1	B	280	Total	C	N	O	S	0	0	0
			2154	1347	374	423	10			
1	C	280	Total	C	N	O	S	0	0	0
			2154	1347	374	423	10			
1	D	280	Total	C	N	O	S	0	0	0
			2154	1347	374	423	10			
1	E	280	Total	C	N	O	S	0	0	0
			2154	1347	374	423	10			
1	F	258	Total	C	N	O	S	0	0	0
			2004	1254	350	391	9			
1	G	243	Total	C	N	O	S	0	0	0
			1890	1181	333	368	8			

There are 7 discrepancies between the modelled and reference sequences:

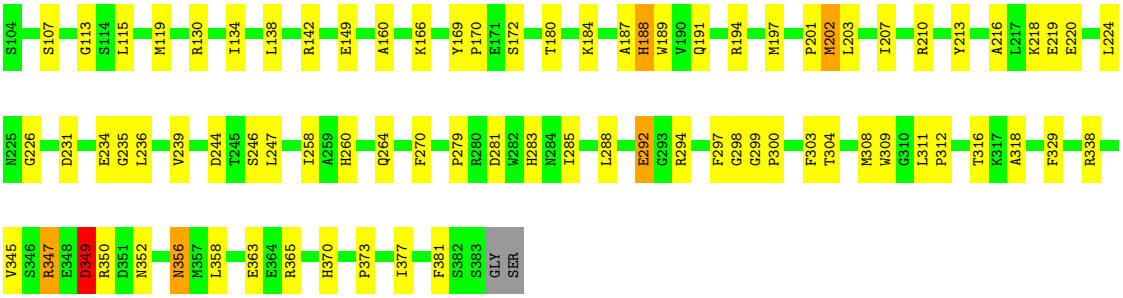
Chain	Residue	Modelled	Actual	Comment	Reference
A	169	TYR	LYS	engineered mutation	UNP P49861
B	169	TYR	LYS	engineered mutation	UNP P49861
C	169	TYR	LYS	engineered mutation	UNP P49861
D	169	TYR	LYS	engineered mutation	UNP P49861
E	169	TYR	LYS	engineered mutation	UNP P49861
F	169	TYR	LYS	engineered mutation	UNP P49861
G	169	TYR	LYS	engineered mutation	UNP P49861

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.

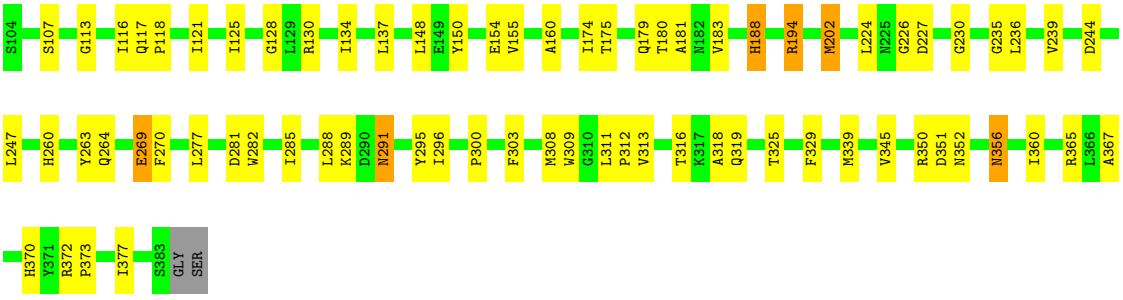
• Molecule 1: Major capsid protein

Chain A:



• Molecule 1: Major capsid protein

Chain B:

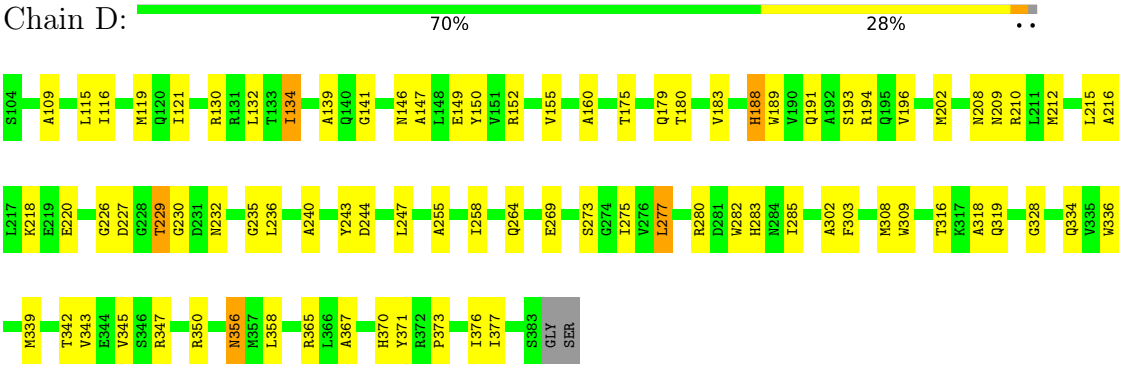


• Molecule 1: Major capsid protein

Chain C:

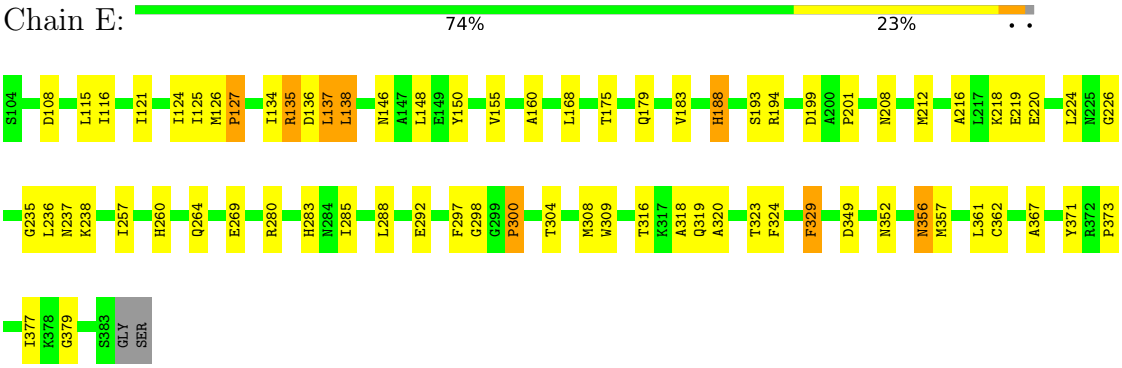
• Molecule 1: Major capsid protein

Chain D:



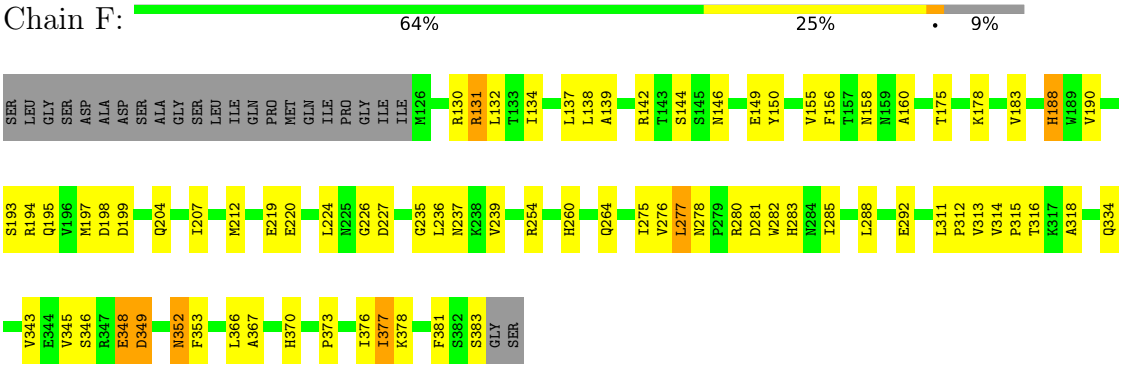
• Molecule 1: Major capsid protein

Chain E:



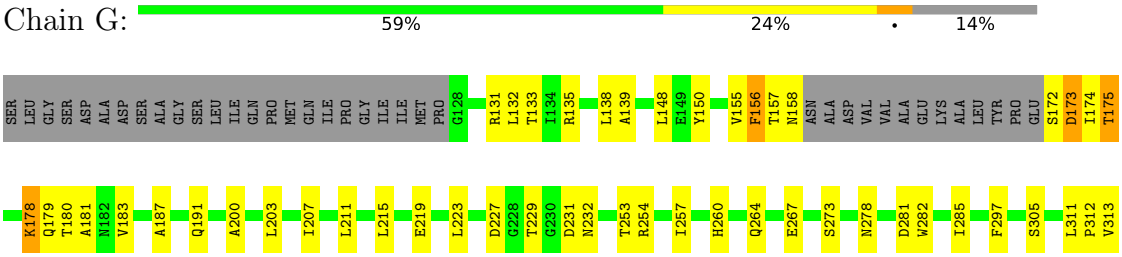
• Molecule 1: Major capsid protein

Chain F:



• Molecule 1: Major capsid protein

Chain G:




T316
K317
A318
V326
G327
G328
F329
A332
S333
Q334
V335
W336
M339
V345
D349
R350
D351
N352
F353
V354
K355
N356
M357
L358
T359
C362
E363
E364
R365
L366
A367
L368
A369
H370
Y371
I376
I377
F381
S382
S383
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	1009.64Å 1009.64Å 729.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.20 29.98 – 4.20	Depositor EDS
% Data completeness (in resolution range)	63.1 (30.00-4.20) 63.1 (29.98-4.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 4.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.384 , (Not available) 0.313 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	2.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 6.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	14664	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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

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	0.25	0/2192	0.48	0/2976
1	B	0.25	0/2192	0.49	0/2976
1	C	0.25	0/2192	0.50	1/2976 (0.0%)
1	D	0.25	0/2192	0.48	0/2976
1	E	0.25	0/2192	0.50	0/2976
1	F	0.26	0/2040	0.49	0/2769
1	G	0.28	0/1922	0.51	0/2605
All	All	0.25	0/14922	0.49	1/20254 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	356	ASN	CB-CA-C	6.05	122.50	110.40

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	2154	0	2115	62	0
1	B	2154	0	2115	54	0
1	C	2154	0	2115	65	0
1	D	2154	0	2115	69	0
1	E	2154	0	2115	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2004	0	1963	58	0
1	G	1890	0	1851	66	0
All	All	14664	0	14389	380	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 13.

The worst 5 of 380 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:F:130:ARG:HD3	1:F:131:ARG:H	1.33	0.92
1:D:264:GLN:HE21	1:D:377:ILE:HD12	1.40	0.85
1:E:297:PHE:HB3	1:E:304:THR:HG21	1.59	0.84
1:G:157:THR:HB	1:G:173:ASP:O	1.76	0.83
1:G:191:GLN:HG3	1:G:359:THR:HG22	1.61	0.83

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	278/282 (99%)	241 (87%)	32 (12%)	5 (2%)	8	42
1	B	278/282 (99%)	239 (86%)	36 (13%)	3 (1%)	14	52
1	C	278/282 (99%)	248 (89%)	27 (10%)	3 (1%)	14	52
1	D	278/282 (99%)	247 (89%)	27 (10%)	4 (1%)	11	47
1	E	278/282 (99%)	244 (88%)	29 (10%)	5 (2%)	8	42
1	F	256/282 (91%)	228 (89%)	24 (9%)	4 (2%)	9	45
1	G	239/282 (85%)	204 (85%)	30 (13%)	5 (2%)	7	39
All	All	1885/1974 (96%)	1651 (88%)	205 (11%)	29 (2%)	10	46

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	PRO
1	E	300	PRO
1	F	352	ASN
1	A	202	MET
1	B	352	ASN

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	230/231 (100%)	220 (96%)	10 (4%)	29	55
1	B	230/231 (100%)	221 (96%)	9 (4%)	32	57
1	C	230/231 (100%)	217 (94%)	13 (6%)	20	48
1	D	230/231 (100%)	224 (97%)	6 (3%)	46	67
1	E	230/231 (100%)	221 (96%)	9 (4%)	32	57
1	F	213/231 (92%)	202 (95%)	11 (5%)	23	50
1	G	201/231 (87%)	190 (94%)	11 (6%)	21	49
All	All	1564/1617 (97%)	1495 (96%)	69 (4%)	28	54

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	377	ILE
1	G	156	PHE
1	G	336	TRP
1	C	224	LEU
1	C	188	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	264	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	204	GLN
1	G	232	ASN
1	D	291	ASN
1	D	356	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.