



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 4BTG
EMDB ID: : EMD-2364
Title : Coordinates of the bacteriophage phi6 capsid subunits (P1A and P1B) fitted into the cryoEM reconstruction of the procapsid at 4.4 Å resolution
Authors : Nemecek, D.; Boura, E.; Wu, W.; Cheng, N.; Plevka, P.; Qiao, J.; Mindich, L.; Heymann, J.B.; Hurley, J.H.; Steven, A.C.
Deposited on : 2013-06-17
Resolution : 4.40 Å (reported)
Based on PDB ID : 4K7H

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

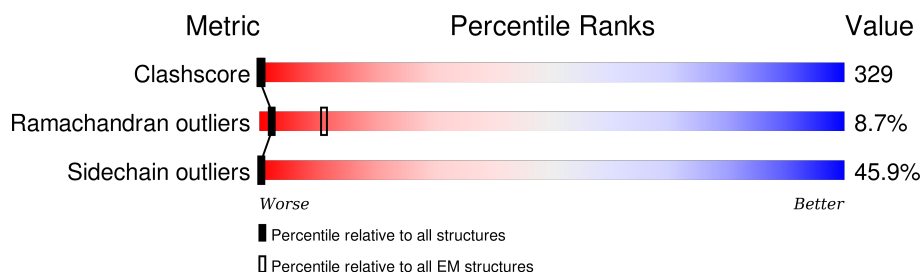
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	761	
1	B	761	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 INNER PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		
1	B	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P11126
B	1	GLY	-	EXPRESSION TAG	UNP P11126

R724
L725
W726
A727
G728
L729
A730
V731
L732
L733
L734
L735
L736
L737
L738
L739
L740
L741
L742
L743
L744
L745
L746
L747
L748
L749
L750
L751
L752
L753
L754
L755
L756
L757
L758
L759
L760
L761

● Molecule 1: MAJOR INNER PROTEIN P1

Chain B: . 48% 38% 10%

H721	L661	R601	H541	R481	Y421	Y361	R301	R241	P181	D121	G1
I722	L662	Y602	T542	S482	E422	E362	G302	G242	N182	A122	F2
I723	L663	Y603	P543	N483	A423	D363	R303	N243	F183	V123	N3
I724	D664	A604	E544	F484	Y424	N364	A304	F244	Y184	G124	L4
I725	G665	E605	P545	F485	A425	Q365	E305	D245	A185	K125	K5
H726	R666	V606	L546	Y486	Q426	F366	V306	A246	L186	V126	V6
A727	L667	R607	E547	Y487	R427	A367	L307	N247	Y187	P127	K7
G728	H668	E608	A548	A488	G428	K368	F308	A248	D188	L128	D8
L729	Q669	F609	L549	A489	T429	R369	S309	V249	C189	T129	L9
L730	L611	E610	A550	V490	V430	L370	D310	V250	V190	L130	N10
L731	L612	L613	Y551	Y491	M431	T371	E311	S251	R191	L131	G11
L732	L614	G615	R552	H492	S432	A372	E312	S252	A192	L132	S12
L733	L615	L616	K553	Y493	M433	F373	L313	V253	S193	E133	A13
L734	L617	G615	P554	A494	G434	T374	S314	T254	D194	Q134	A74
H735	L618	G615	L555	Y495	A435	T375	S315	L255	L195	L135	G15
G736	R676	Q616	Q556	A496	E436	V376	L316	L256	R196	A136	A76
L737	K677	R617	P557	H497	M437	K377	T317	L257	L197	T137	T17
L738	L678	R618	S558	N498	T438	L378	L318	Q258	N198	L138	Q18
S739	E679	E619	E559	P499	L439	A379	P319	R259	L199	A139	A79
R740	H680	R620	V560	E500	G440	N380	M320	L260	T200	P140	F20
S741	L681	V621	P564	V501	F441	T374	F321	M261	A201	S141	A21
E742	G682	R622	Q562	Y502	P442	S382	L322	S262	L202	E142	V82
L743	T683	L623	A563	V503	S443	N383	E323	P263	S203	H143	G23
E744	T684	L624	K564	S504	V444	Q384	A324	S264	S204	E144	E24
A745	G685	R625	V565	E505	V445	K385	M325	T265	V205	L145	L25
L746	L686	P626	L566	H506	E446	F386	S326	P266	D206	F146	V86
T747	G687	T627	D567	Q507	R447	L387	E327	K267	S207	H147	N87
K748	A688	V628	L568	G508	D448	D388	V328	E268	K208	H148	Q88
V749	S689	A629	A569	V509	Y449	V389	S329	L269	M209	I149	F89
L750	A690	H630	N570	A510	A450	E390	P330	D270	L210	T150	T90
S751	H691	A631	H571	A511	D451	G391	F331	P271	Q211	T151	E91
	H692	I632	T572	E512	D452	G392	K332	S272	A212	D152	Y92
N754	L693	L633	T573	Q513	R453	L393	R333	A273	T213	F153	H93
A755	A694	Q634	S574	G514	D454	S394	R334	R274	F214	V154	Q94
L756	G695	M635	L575	S515	P455	D395	P335	L275	K215	C155	S95
G757	S696	R636	H576	L516	M456	R396	L336	R276	A216	H156	T96
M758	R697	Y637	I577	V517	V457	N397	R337	N277	K217	V157	A97
V759	L698	S638	H578	L518	A458	S398	E338	T278	G218	L158	C98
L760	H699	H639	P579	V519	L459	A399	T339	N279	A219	S159	N99
A761	D700	F640	H580	N520	A460	T400	T340	G280	L220	P160	P100
	D701	V641	H581	N521	A461	L401	S341	L281	A221	L161	E101
G762	L702	E642	E582	V522	L462	A402	Y342	D282	P222	G162	L102
	A703	D643	A583	R523	P463	P403	L343	Q283	A223	F163	N103
L704	G704	L644	S584	T524	T464	L404	G344	L284	L224	I164	F43
R705	L705	R645	T585	E525	G465	G405	Q345	R285	L225	L165	S45
G706	L706	T646	E586	L526	L466	N406	T346	S286	S226	P166	A46
L707	L647	F647	F587	R527	V467	T407	S247	N387	Q227	D167	T107
L708	A648	L648	A588	L528	D468	F408	A348	L288	R228	A168	N48
D709	A649	Y589	Y589	P529	E469	A409	L349	A289	L229	A169	Y109
S710	L710	A650	E590	V530	S470	V410	D350	L290	A230	V170	T49
L711	H651	L651	D591	G531	L471	S411	H351	F291	N231	Y171	S50
L712	S712	R652	A592	Y532	E472	A412	M352	L292	A232	Y172	T110
D713	L713	T653	Y593	N533	A473	F413	G353	L293	A233	R173	L52
L714	S654	L654	S594	A534	R474	V414	Q354	Y294	T234	V174	L53
H715	L715	R655	V595	L635	A475	R415	P355	Q295	L235	G175	H54
L716	D656	T596	L596	E536	S476	N416	S356	D296	A236	R176	E55
G717	L717	D657	L597	G537	M477	R417	H357	K297	F237	T177	V57
L718	A658	R598	L598	A538	D478	T418	V358	V298	E238	A178	K58
L719	H659	N599	L599	E539	L479	A419	V359	K299	R239	T179	G59
L720	T660	L660	K600	T540	K480	V620	V260	Q240	N240	A120	N60

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 1	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PARTICLES FROM EACH MICRO-GRAPH	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	46000	Depositor
Image detector	KODAK SO163 FILM	Depositor

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 > 2	RMSZ	# Z > 2
1	A	1.22	32/6038 (0.5%)	1.56	144/8200 (1.8%)
1	B	0.96	27/6039 (0.4%)	1.41	88/8203 (1.1%)
All	All	1.10	59/12077 (0.5%)	1.49	232/16403 (1.4%)

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	A	0	67
1	B	0	45
All	All	0	112

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	ILE	C-N	-36.28	0.50	1.34
1	B	127	PRO	C-N	30.25	1.91	1.34
1	A	437	MET	C-N	11.92	1.61	1.34
1	A	75	GLN	CA-CB	-11.01	1.29	1.53
1	B	124	GLY	C-N	9.05	1.54	1.34

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	PHE	C-N-CD	-46.69	17.89	120.60
1	A	542	THR	C-N-CD	15.13	160.17	128.40
1	A	290	LEU	CB-CG-CD1	-13.07	88.79	111.00
1	A	16	LEU	CB-CG-CD1	-12.81	89.22	111.00
1	A	739	SER	O-C-N	-11.26	104.68	122.70

There are no chirality outliers.

5 of 112 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	GLY	Peptide
1	A	25	LEU	Peptide
1	A	34	LEU	Peptide
1	A	52	LEU	Peptide
1	A	60	ASN	Peptide

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	5920	0	5870	3751	0
1	B	5920	0	5883	4050	0
All	All	11840	0	11753	7764	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 329.

The worst 5 of 7764 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:61:ILE:HG22	1:A:156:HIS:CD2	1.18	1.68
1:A:732:LEU:CD1	1:A:738:LEU:HD22	1.23	1.67
1:B:373:PHE:CD2	1:B:583:ALA:HB1	1.31	1.66
1:B:670:ASN:HD21	1:B:749:VAL:CG1	1.07	1.65
1:B:156:HIS:CD2	1:B:158:LEU:H	1.14	1.65

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 PDB entries followed by that with respect to all EM entries.

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	755/761 (99%)	575 (76%)	109 (14%)	71 (9%)	1	16
1	B	757/761 (100%)	591 (78%)	105 (14%)	61 (8%)	1	18
All	All	1512/1522 (99%)	1166 (77%)	214 (14%)	132 (9%)	2	17

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	61	ILE
1	A	119	LYS
1	A	123	VAL
1	A	144	GLU

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 PDB entries followed by that with respect to all EM entries.

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	629/629 (100%)	341 (54%)	288 (46%)	0	0
1	B	629/629 (100%)	340 (54%)	289 (46%)	0	0
All	All	1258/1258 (100%)	681 (54%)	577 (46%)	0	0

5 of 577 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	698	ILE
1	B	91	GLU
1	B	642	GLU
1	A	714	LEU
1	B	26	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	GLN
1	B	182	ASN
1	B	581	HIS
1	B	75	GLN
1	B	88	GLN

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 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.