



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3H3Y
EMDB ID: : EMD-1086
Title : Fitting of the gp6 crystal structure into 3D cryo-EM reconstruction of bacteriophage T4 star-shaped baseplate
Authors : Aksyuk, A.A.; Leiman, P.G.; Shneider, M.M.; Mesyanzhinov, V.V.; Rossmann, M.G.
Deposited on : 2009-04-17
Resolution : 16.00 Å(reported)

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

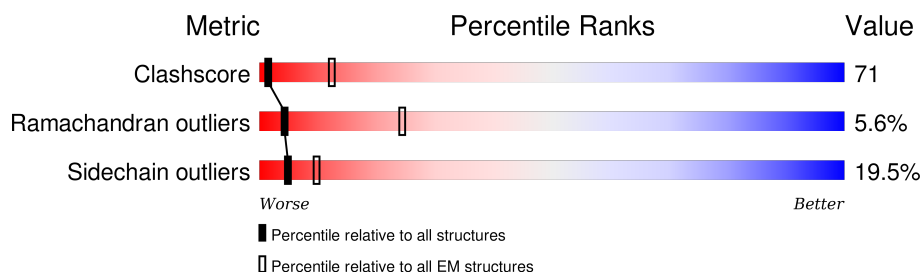
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 16.00 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	335	35% 48% 13% ..
1	B	335	34% 45% 16% ..
1	C	335	34% 48% 14% ..
1	D	335	33% 45% 16% ..
1	E	335	35% 48% 13% ..
1	F	335	34% 45% 16% ..
1	G	335	34% 48% 14% ..
1	H	335	35% 44% 16% ..
1	I	335	34% 48% 14% ..

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Mol	Chain	Length	Quality of chain
1	J	335	<div><div></div><div>34%44%16%<div><div></div><div></div></div></div></div>
1	K	335	<div><div></div><div>36%47%14%<div><div></div><div></div></div></div></div>
1	L	335	<div><div></div><div>34%45%16%<div><div></div><div></div></div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31380 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 Baseplate structural protein Gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	326	Total	C	N	O	S	0	0
			2622	1667	424	528	3		
1	B	324	Total	C	N	O	S	0	0
			2608	1658	422	525	3		
1	C	326	Total	C	N	O	S	0	0
			2622	1667	424	528	3		
1	D	324	Total	C	N	O	S	0	0
			2608	1658	422	525	3		
1	E	326	Total	C	N	O	S	0	0
			2622	1667	424	528	3		
1	F	324	Total	C	N	O	S	0	0
			2608	1658	422	525	3		
1	G	326	Total	C	N	O	S	0	0
			2622	1667	424	528	3		
1	H	324	Total	C	N	O	S	0	0
			2608	1658	422	525	3		
1	I	326	Total	C	N	O	S	0	0
			2622	1667	424	528	3		
1	J	324	Total	C	N	O	S	0	0
			2608	1658	422	525	3		
1	K	326	Total	C	N	O	S	0	0
			2622	1667	424	528	3		
1	L	324	Total	C	N	O	S	0	0
			2608	1658	422	525	3		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	661	LEU	-	EXPRESSION TAG	UNP P19060
A	662	GLU	-	EXPRESSION TAG	UNP P19060
A	663	HIS	-	EXPRESSION TAG	UNP P19060
A	664	HIS	-	EXPRESSION TAG	UNP P19060
A	665	HIS	-	EXPRESSION TAG	UNP P19060
A	666	HIS	-	EXPRESSION TAG	UNP P19060

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Chain	Residue	Modelled	Actual	Comment	Reference
A	667	HIS	-	EXPRESSION TAG	UNP P19060
A	668	HIS	-	EXPRESSION TAG	UNP P19060
B	661	LEU	-	EXPRESSION TAG	UNP P19060
B	662	GLU	-	EXPRESSION TAG	UNP P19060
B	663	HIS	-	EXPRESSION TAG	UNP P19060
B	664	HIS	-	EXPRESSION TAG	UNP P19060
B	665	HIS	-	EXPRESSION TAG	UNP P19060
B	666	HIS	-	EXPRESSION TAG	UNP P19060
B	667	HIS	-	EXPRESSION TAG	UNP P19060
B	668	HIS	-	EXPRESSION TAG	UNP P19060
C	661	LEU	-	EXPRESSION TAG	UNP P19060
C	662	GLU	-	EXPRESSION TAG	UNP P19060
C	663	HIS	-	EXPRESSION TAG	UNP P19060
C	664	HIS	-	EXPRESSION TAG	UNP P19060
C	665	HIS	-	EXPRESSION TAG	UNP P19060
C	666	HIS	-	EXPRESSION TAG	UNP P19060
C	667	HIS	-	EXPRESSION TAG	UNP P19060
C	668	HIS	-	EXPRESSION TAG	UNP P19060
D	661	LEU	-	EXPRESSION TAG	UNP P19060
D	662	GLU	-	EXPRESSION TAG	UNP P19060
D	663	HIS	-	EXPRESSION TAG	UNP P19060
D	664	HIS	-	EXPRESSION TAG	UNP P19060
D	665	HIS	-	EXPRESSION TAG	UNP P19060
D	666	HIS	-	EXPRESSION TAG	UNP P19060
D	667	HIS	-	EXPRESSION TAG	UNP P19060
D	668	HIS	-	EXPRESSION TAG	UNP P19060
E	661	LEU	-	EXPRESSION TAG	UNP P19060
E	662	GLU	-	EXPRESSION TAG	UNP P19060
E	663	HIS	-	EXPRESSION TAG	UNP P19060
E	664	HIS	-	EXPRESSION TAG	UNP P19060
E	665	HIS	-	EXPRESSION TAG	UNP P19060
E	666	HIS	-	EXPRESSION TAG	UNP P19060
E	667	HIS	-	EXPRESSION TAG	UNP P19060
E	668	HIS	-	EXPRESSION TAG	UNP P19060
F	661	LEU	-	EXPRESSION TAG	UNP P19060
F	662	GLU	-	EXPRESSION TAG	UNP P19060
F	663	HIS	-	EXPRESSION TAG	UNP P19060
F	664	HIS	-	EXPRESSION TAG	UNP P19060
F	665	HIS	-	EXPRESSION TAG	UNP P19060
F	666	HIS	-	EXPRESSION TAG	UNP P19060
F	667	HIS	-	EXPRESSION TAG	UNP P19060
F	668	HIS	-	EXPRESSION TAG	UNP P19060

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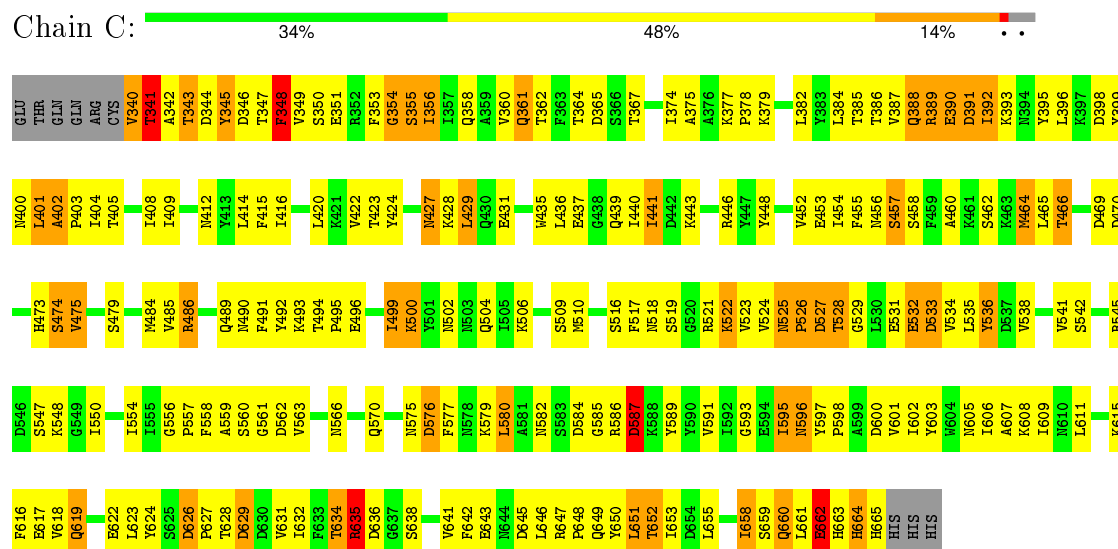
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Chain	Residue	Modelled	Actual	Comment	Reference
G	661	LEU	-	EXPRESSION TAG	UNP P19060
G	662	GLU	-	EXPRESSION TAG	UNP P19060
G	663	HIS	-	EXPRESSION TAG	UNP P19060
G	664	HIS	-	EXPRESSION TAG	UNP P19060
G	665	HIS	-	EXPRESSION TAG	UNP P19060
G	666	HIS	-	EXPRESSION TAG	UNP P19060
G	667	HIS	-	EXPRESSION TAG	UNP P19060
G	668	HIS	-	EXPRESSION TAG	UNP P19060
H	661	LEU	-	EXPRESSION TAG	UNP P19060
H	662	GLU	-	EXPRESSION TAG	UNP P19060
H	663	HIS	-	EXPRESSION TAG	UNP P19060
H	664	HIS	-	EXPRESSION TAG	UNP P19060
H	665	HIS	-	EXPRESSION TAG	UNP P19060
H	666	HIS	-	EXPRESSION TAG	UNP P19060
H	667	HIS	-	EXPRESSION TAG	UNP P19060
H	668	HIS	-	EXPRESSION TAG	UNP P19060
I	661	LEU	-	EXPRESSION TAG	UNP P19060
I	662	GLU	-	EXPRESSION TAG	UNP P19060
I	663	HIS	-	EXPRESSION TAG	UNP P19060
I	664	HIS	-	EXPRESSION TAG	UNP P19060
I	665	HIS	-	EXPRESSION TAG	UNP P19060
I	666	HIS	-	EXPRESSION TAG	UNP P19060
I	667	HIS	-	EXPRESSION TAG	UNP P19060
I	668	HIS	-	EXPRESSION TAG	UNP P19060
J	661	LEU	-	EXPRESSION TAG	UNP P19060
J	662	GLU	-	EXPRESSION TAG	UNP P19060
J	663	HIS	-	EXPRESSION TAG	UNP P19060
J	664	HIS	-	EXPRESSION TAG	UNP P19060
J	665	HIS	-	EXPRESSION TAG	UNP P19060
J	666	HIS	-	EXPRESSION TAG	UNP P19060
J	667	HIS	-	EXPRESSION TAG	UNP P19060
J	668	HIS	-	EXPRESSION TAG	UNP P19060
K	661	LEU	-	EXPRESSION TAG	UNP P19060
K	662	GLU	-	EXPRESSION TAG	UNP P19060
K	663	HIS	-	EXPRESSION TAG	UNP P19060
K	664	HIS	-	EXPRESSION TAG	UNP P19060
K	665	HIS	-	EXPRESSION TAG	UNP P19060
K	666	HIS	-	EXPRESSION TAG	UNP P19060
K	667	HIS	-	EXPRESSION TAG	UNP P19060
K	668	HIS	-	EXPRESSION TAG	UNP P19060
L	661	LEU	-	EXPRESSION TAG	UNP P19060
L	662	GLU	-	EXPRESSION TAG	UNP P19060

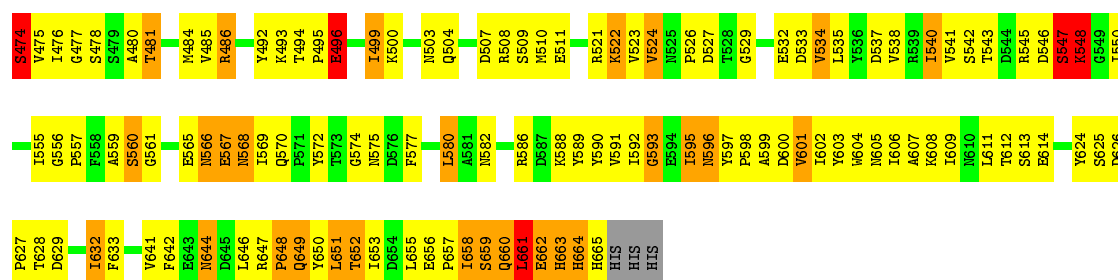
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Chain	Residue	Modelled	Actual	Comment	Reference
L	663	HIS	-	EXPRESSION TAG	UNP P19060
L	664	HIS	-	EXPRESSION TAG	UNP P19060
L	665	HIS	-	EXPRESSION TAG	UNP P19060
L	666	HIS	-	EXPRESSION TAG	UNP P19060
L	667	HIS	-	EXPRESSION TAG	UNP P19060
L	668	HIS	-	EXPRESSION TAG	UNP P19060

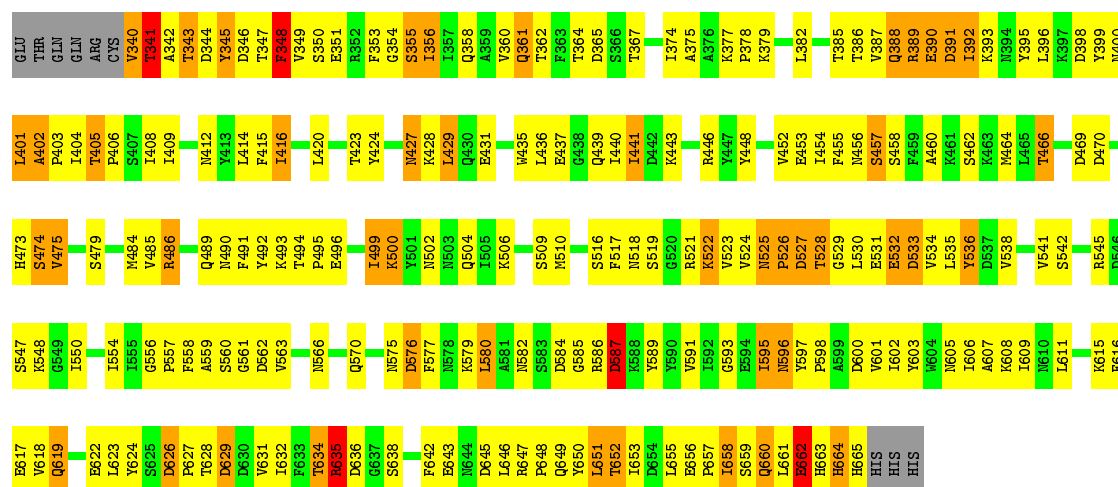


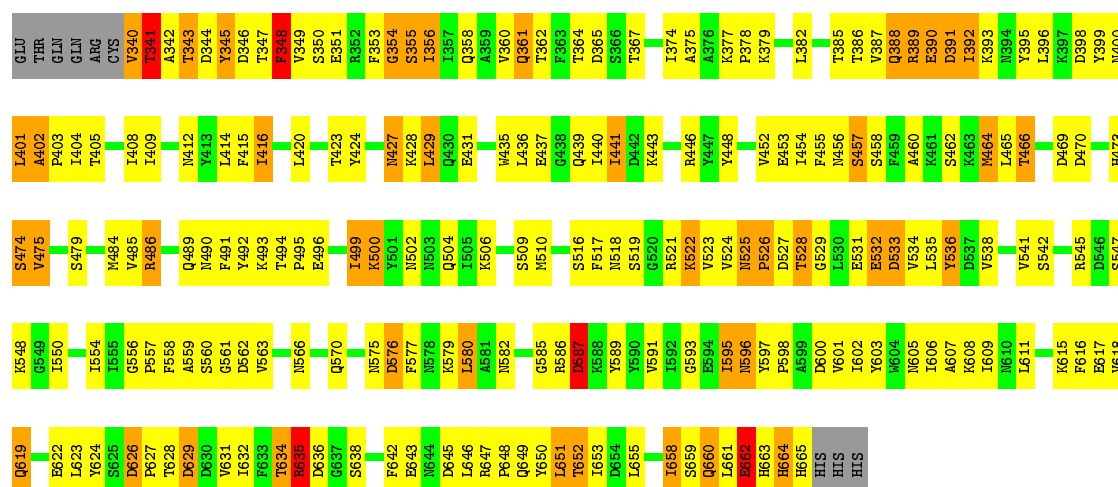




• Molecule 1: Baseplate structural protein Gp6

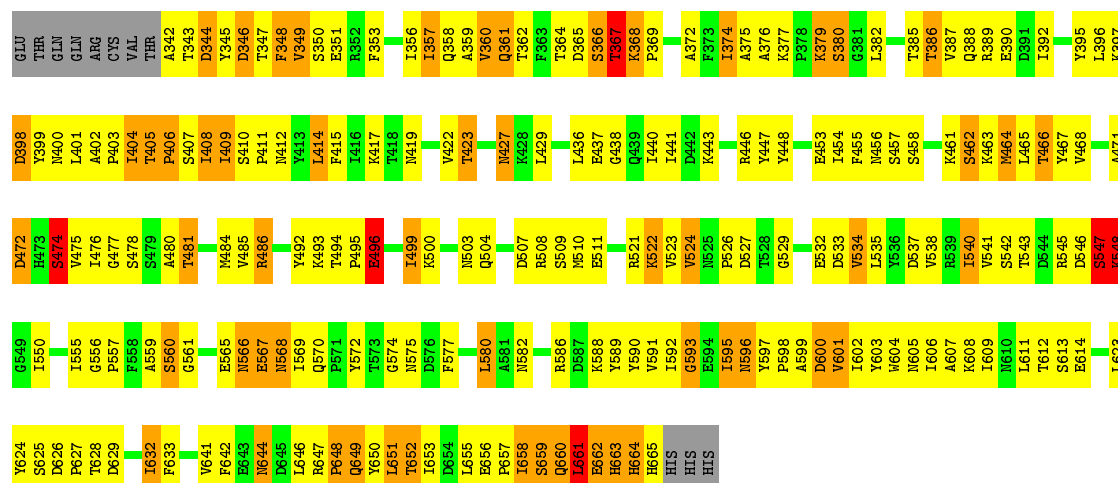
Chain I: 34% 48% 14% . .





• Molecule 1: Baseplate structural protein Gp6

Chain L: 34% 45% 16%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of images	1965	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each particle	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	45000	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	0.50	0/2677	0.80	7/3637 (0.2%)
1	B	0.51	0/2663	0.96	11/3617 (0.3%)
1	C	0.50	0/2677	0.80	7/3637 (0.2%)
1	D	0.51	0/2663	0.96	11/3617 (0.3%)
1	E	0.50	0/2677	0.80	7/3637 (0.2%)
1	F	0.51	0/2663	0.96	11/3617 (0.3%)
1	G	0.50	0/2677	0.80	7/3637 (0.2%)
1	H	0.51	0/2663	0.96	11/3617 (0.3%)
1	I	0.50	0/2677	0.80	7/3637 (0.2%)
1	J	0.51	0/2663	0.96	11/3617 (0.3%)
1	K	0.50	0/2677	0.80	7/3637 (0.2%)
1	L	0.51	0/2663	0.96	11/3617 (0.3%)
All	All	0.51	0/32040	0.88	108/43524 (0.2%)

There are no bond length outliers.

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	405	THR	C-N-CD	-29.03	56.74	120.60
1	B	405	THR	C-N-CD	-29.02	56.75	120.60
1	J	405	THR	C-N-CD	-29.01	56.78	120.60
1	D	405	THR	C-N-CD	-29.01	56.78	120.60
1	F	405	THR	C-N-CD	-29.01	56.78	120.60

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	2622	0	2544	408	0
1	B	2608	0	2529	374	0
1	C	2622	0	2544	405	0
1	D	2608	0	2529	392	0
1	E	2622	0	2544	420	0
1	F	2608	0	2529	396	0
1	G	2622	0	2544	421	0
1	H	2608	0	2529	380	0
1	I	2622	0	2544	404	0
1	J	2608	0	2529	387	0
1	K	2622	0	2544	415	0
1	L	2608	0	2529	380	0
All	All	31380	0	30438	4384	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 71.

The worst 5 of 4384 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:401:LEU:HD11	1:C:403:PRO:CD	1.24	1.68
1:B:401:LEU:CD1	1:C:403:PRO:HD2	1.27	1.64
1:J:403:PRO:CG	1:K:403:PRO:HG2	1.35	1.53
1:D:401:LEU:CD1	1:E:403:PRO:HD2	1.11	1.53
1:D:401:LEU:HD11	1:E:403:PRO:CD	1.05	1.53

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	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	30
1	B	322/335 (96%)	261 (81%)	42 (13%)	19 (6%)	2	27
1	C	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	30
1	D	322/335 (96%)	261 (81%)	42 (13%)	19 (6%)	2	27
1	E	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	30
1	F	322/335 (96%)	262 (81%)	41 (13%)	19 (6%)	2	27
1	G	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	30
1	H	322/335 (96%)	261 (81%)	42 (13%)	19 (6%)	2	27
1	I	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	30
1	J	322/335 (96%)	261 (81%)	42 (13%)	19 (6%)	2	27
1	K	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	30
1	L	322/335 (96%)	262 (81%)	41 (13%)	19 (6%)	2	27
All	All	3876/4020 (96%)	3128 (81%)	532 (14%)	216 (6%)	4	28

5 of 216 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PHE
1	A	354	GLY
1	A	389	ARG
1	A	390	GLU
1	A	526	PRO

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	295/304 (97%)	240 (81%)	55 (19%)	2	14
1	B	293/304 (96%)	234 (80%)	59 (20%)	1	11
1	C	295/304 (97%)	240 (81%)	55 (19%)	2	14
1	D	293/304 (96%)	234 (80%)	59 (20%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	295/304 (97%)	239 (81%)	56 (19%)	2	13
1	F	293/304 (96%)	234 (80%)	59 (20%)	1	11
1	G	295/304 (97%)	239 (81%)	56 (19%)	2	13
1	H	293/304 (96%)	234 (80%)	59 (20%)	1	11
1	I	295/304 (97%)	239 (81%)	56 (19%)	2	13
1	J	293/304 (96%)	234 (80%)	59 (20%)	1	11
1	K	295/304 (97%)	239 (81%)	56 (19%)	2	13
1	L	293/304 (96%)	234 (80%)	59 (20%)	1	11
All	All	3528/3648 (97%)	2840 (80%)	688 (20%)	5	12

5 of 688 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	466	THR
1	G	619	GLN
1	L	366	SER
1	F	535	LEU
1	G	356	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	575	ASN
1	H	358	GLN
1	L	427	ASN
1	F	582	ASN
1	G	473	HIS

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.