



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:12 am GMT

PDB ID : 4GQH
Title : The Conformations and Interactions of the Four-Layer Aggregate Revealed by X-ray Crystallography Diffraction Implied the Importance of Peptides at Opposite Ends in Their Assemblies
Authors : Li, X.Y.; Song, B.A.; Hu, D.Y.; Chen, X.; Wang, Z.C.; Zeng, M.J.; Yu, D.D.; Chen, Z.; Jin, L.H.; Yang, S.
Deposited on : 2012-08-23
Resolution : 3.06 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

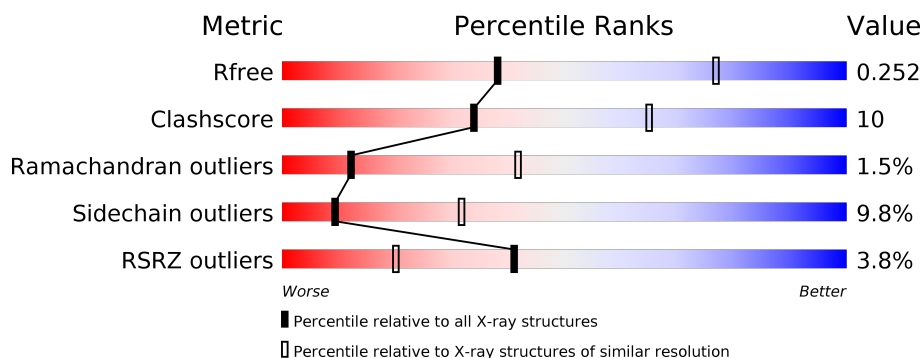
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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}	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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	174	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>24%</div> <div>• •</div> <div>18%</div> </div> </div>
1	B	174	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>27%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	174	<div> <div>6%</div> <div> <div></div> <div>55%</div> <div>25%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	174	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>28%</div> <div>•</div> <div>18%</div> </div> </div>
1	E	174	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>19%</div> <div>6%</div> <div>20%</div> </div> </div>
1	F	174	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>26%</div> <div>5%</div> <div>18%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	174	
1	H	174	
1	I	174	
1	J	174	
1	K	174	
1	L	174	
1	M	174	
1	N	174	
1	O	174	
1	P	174	
1	Q	174	
1	R	174	
1	S	174	
1	T	174	
1	U	174	
1	V	174	
1	W	174	
1	X	174	
1	Y	174	
1	Z	174	
1	a	174	
1	b	174	
1	c	174	
1	d	174	
1	e	174	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	f	174	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>70%</div><div>7%</div><div>23%</div></div></div>
1	h	174	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>68%</div><div>9%</div><div>23%</div></div></div>
1	i	174	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>70%</div><div>7%</div><div>23%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 36918 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1115	703	195	216	1			
1	B	139	Total	C	N	O	S	0	0	0
			1096	691	192	212	1			
1	C	144	Total	C	N	O	S	0	0	0
			1132	713	197	221	1			
1	D	143	Total	C	N	O	S	0	0	0
			1126	709	199	217	1			
1	E	140	Total	C	N	O	S	0	0	0
			1100	693	193	213	1			
1	F	143	Total	C	N	O	S	0	0	0
			1131	712	199	219	1			
1	G	143	Total	C	N	O	S	0	0	0
			1131	715	199	216	1			
1	H	144	Total	C	N	O	S	0	0	0
			1135	714	200	220	1			
1	I	141	Total	C	N	O	S	0	0	0
			1111	701	194	215	1			
1	J	145	Total	C	N	O	S	0	0	0
			1143	719	201	222	1			
1	K	143	Total	C	N	O	S	0	0	0
			1131	712	199	219	1			
1	L	141	Total	C	N	O	S	0	0	0
			1111	701	194	215	1			
1	M	142	Total	C	N	O	S	0	0	0
			1122	707	198	216	1			
1	N	142	Total	C	N	O	S	0	0	0
			1122	707	198	216	1			
1	O	140	Total	C	N	O	S	0	0	0
			1100	693	193	213	1			
1	P	147	Total	C	N	O	S	0	0	0
			1157	728	203	225	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	146	Total	C	N	O	S	0	0	0
			1150	723	202	224	1			
1	R	133	Total	C	N	O	S	0	0	0
			1046	664	179	202	1			
1	S	133	Total	C	N	O	S	0	0	0
			1046	664	179	202	1			
1	T	132	Total	C	N	O	S	0	0	0
			1039	659	178	201	1			
1	U	133	Total	C	N	O	S	0	0	0
			1046	664	179	202	1			
1	V	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	W	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	X	131	Total	C	N	O	S	0	0	0
			1028	653	174	200	1			
1	Y	132	Total	C	N	O	S	0	0	0
			1035	658	175	201	1			
1	Z	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	a	131	Total	C	N	O	S	0	0	0
			1029	655	174	199	1			
1	b	132	Total	C	N	O	S	0	0	0
			1035	658	175	201	1			
1	c	136	Total	C	N	O	S	0	0	0
			1069	676	186	206	1			
1	d	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	e	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	f	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	h	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	i	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			

There are 680 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P69687
A	-18	GLY	-	EXPRESSION TAG	UNP P69687
A	-17	SER	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	SER	-	EXPRESSION TAG	UNP P69687
A	-15	HIS	-	EXPRESSION TAG	UNP P69687
A	-14	HIS	-	EXPRESSION TAG	UNP P69687
A	-13	HIS	-	EXPRESSION TAG	UNP P69687
A	-12	HIS	-	EXPRESSION TAG	UNP P69687
A	-11	HIS	-	EXPRESSION TAG	UNP P69687
A	-10	HIS	-	EXPRESSION TAG	UNP P69687
A	-9	SER	-	EXPRESSION TAG	UNP P69687
A	-8	SER	-	EXPRESSION TAG	UNP P69687
A	-7	GLY	-	EXPRESSION TAG	UNP P69687
A	-6	LEU	-	EXPRESSION TAG	UNP P69687
A	-5	VAL	-	EXPRESSION TAG	UNP P69687
A	-4	PRO	-	EXPRESSION TAG	UNP P69687
A	-3	ARG	-	EXPRESSION TAG	UNP P69687
A	-2	GLY	-	EXPRESSION TAG	UNP P69687
A	-1	SER	-	EXPRESSION TAG	UNP P69687
A	0	HIS	-	EXPRESSION TAG	UNP P69687
B	-19	MET	-	EXPRESSION TAG	UNP P69687
B	-18	GLY	-	EXPRESSION TAG	UNP P69687
B	-17	SER	-	EXPRESSION TAG	UNP P69687
B	-16	SER	-	EXPRESSION TAG	UNP P69687
B	-15	HIS	-	EXPRESSION TAG	UNP P69687
B	-14	HIS	-	EXPRESSION TAG	UNP P69687
B	-13	HIS	-	EXPRESSION TAG	UNP P69687
B	-12	HIS	-	EXPRESSION TAG	UNP P69687
B	-11	HIS	-	EXPRESSION TAG	UNP P69687
B	-10	HIS	-	EXPRESSION TAG	UNP P69687
B	-9	SER	-	EXPRESSION TAG	UNP P69687
B	-8	SER	-	EXPRESSION TAG	UNP P69687
B	-7	GLY	-	EXPRESSION TAG	UNP P69687
B	-6	LEU	-	EXPRESSION TAG	UNP P69687
B	-5	VAL	-	EXPRESSION TAG	UNP P69687
B	-4	PRO	-	EXPRESSION TAG	UNP P69687
B	-3	ARG	-	EXPRESSION TAG	UNP P69687
B	-2	GLY	-	EXPRESSION TAG	UNP P69687
B	-1	SER	-	EXPRESSION TAG	UNP P69687
B	0	HIS	-	EXPRESSION TAG	UNP P69687
C	-19	MET	-	EXPRESSION TAG	UNP P69687
C	-18	GLY	-	EXPRESSION TAG	UNP P69687
C	-17	SER	-	EXPRESSION TAG	UNP P69687
C	-16	SER	-	EXPRESSION TAG	UNP P69687
C	-15	HIS	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	EXPRESSION TAG	UNP P69687
C	-13	HIS	-	EXPRESSION TAG	UNP P69687
C	-12	HIS	-	EXPRESSION TAG	UNP P69687
C	-11	HIS	-	EXPRESSION TAG	UNP P69687
C	-10	HIS	-	EXPRESSION TAG	UNP P69687
C	-9	SER	-	EXPRESSION TAG	UNP P69687
C	-8	SER	-	EXPRESSION TAG	UNP P69687
C	-7	GLY	-	EXPRESSION TAG	UNP P69687
C	-6	LEU	-	EXPRESSION TAG	UNP P69687
C	-5	VAL	-	EXPRESSION TAG	UNP P69687
C	-4	PRO	-	EXPRESSION TAG	UNP P69687
C	-3	ARG	-	EXPRESSION TAG	UNP P69687
C	-2	GLY	-	EXPRESSION TAG	UNP P69687
C	-1	SER	-	EXPRESSION TAG	UNP P69687
C	0	HIS	-	EXPRESSION TAG	UNP P69687
D	-19	MET	-	EXPRESSION TAG	UNP P69687
D	-18	GLY	-	EXPRESSION TAG	UNP P69687
D	-17	SER	-	EXPRESSION TAG	UNP P69687
D	-16	SER	-	EXPRESSION TAG	UNP P69687
D	-15	HIS	-	EXPRESSION TAG	UNP P69687
D	-14	HIS	-	EXPRESSION TAG	UNP P69687
D	-13	HIS	-	EXPRESSION TAG	UNP P69687
D	-12	HIS	-	EXPRESSION TAG	UNP P69687
D	-11	HIS	-	EXPRESSION TAG	UNP P69687
D	-10	HIS	-	EXPRESSION TAG	UNP P69687
D	-9	SER	-	EXPRESSION TAG	UNP P69687
D	-8	SER	-	EXPRESSION TAG	UNP P69687
D	-7	GLY	-	EXPRESSION TAG	UNP P69687
D	-6	LEU	-	EXPRESSION TAG	UNP P69687
D	-5	VAL	-	EXPRESSION TAG	UNP P69687
D	-4	PRO	-	EXPRESSION TAG	UNP P69687
D	-3	ARG	-	EXPRESSION TAG	UNP P69687
D	-2	GLY	-	EXPRESSION TAG	UNP P69687
D	-1	SER	-	EXPRESSION TAG	UNP P69687
D	0	HIS	-	EXPRESSION TAG	UNP P69687
E	-19	MET	-	EXPRESSION TAG	UNP P69687
E	-18	GLY	-	EXPRESSION TAG	UNP P69687
E	-17	SER	-	EXPRESSION TAG	UNP P69687
E	-16	SER	-	EXPRESSION TAG	UNP P69687
E	-15	HIS	-	EXPRESSION TAG	UNP P69687
E	-14	HIS	-	EXPRESSION TAG	UNP P69687
E	-13	HIS	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	EXPRESSION TAG	UNP P69687
E	-11	HIS	-	EXPRESSION TAG	UNP P69687
E	-10	HIS	-	EXPRESSION TAG	UNP P69687
E	-9	SER	-	EXPRESSION TAG	UNP P69687
E	-8	SER	-	EXPRESSION TAG	UNP P69687
E	-7	GLY	-	EXPRESSION TAG	UNP P69687
E	-6	LEU	-	EXPRESSION TAG	UNP P69687
E	-5	VAL	-	EXPRESSION TAG	UNP P69687
E	-4	PRO	-	EXPRESSION TAG	UNP P69687
E	-3	ARG	-	EXPRESSION TAG	UNP P69687
E	-2	GLY	-	EXPRESSION TAG	UNP P69687
E	-1	SER	-	EXPRESSION TAG	UNP P69687
E	0	HIS	-	EXPRESSION TAG	UNP P69687
F	-19	MET	-	EXPRESSION TAG	UNP P69687
F	-18	GLY	-	EXPRESSION TAG	UNP P69687
F	-17	SER	-	EXPRESSION TAG	UNP P69687
F	-16	SER	-	EXPRESSION TAG	UNP P69687
F	-15	HIS	-	EXPRESSION TAG	UNP P69687
F	-14	HIS	-	EXPRESSION TAG	UNP P69687
F	-13	HIS	-	EXPRESSION TAG	UNP P69687
F	-12	HIS	-	EXPRESSION TAG	UNP P69687
F	-11	HIS	-	EXPRESSION TAG	UNP P69687
F	-10	HIS	-	EXPRESSION TAG	UNP P69687
F	-9	SER	-	EXPRESSION TAG	UNP P69687
F	-8	SER	-	EXPRESSION TAG	UNP P69687
F	-7	GLY	-	EXPRESSION TAG	UNP P69687
F	-6	LEU	-	EXPRESSION TAG	UNP P69687
F	-5	VAL	-	EXPRESSION TAG	UNP P69687
F	-4	PRO	-	EXPRESSION TAG	UNP P69687
F	-3	ARG	-	EXPRESSION TAG	UNP P69687
F	-2	GLY	-	EXPRESSION TAG	UNP P69687
F	-1	SER	-	EXPRESSION TAG	UNP P69687
F	0	HIS	-	EXPRESSION TAG	UNP P69687
G	-19	MET	-	EXPRESSION TAG	UNP P69687
G	-18	GLY	-	EXPRESSION TAG	UNP P69687
G	-17	SER	-	EXPRESSION TAG	UNP P69687
G	-16	SER	-	EXPRESSION TAG	UNP P69687
G	-15	HIS	-	EXPRESSION TAG	UNP P69687
G	-14	HIS	-	EXPRESSION TAG	UNP P69687
G	-13	HIS	-	EXPRESSION TAG	UNP P69687
G	-12	HIS	-	EXPRESSION TAG	UNP P69687
G	-11	HIS	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	HIS	-	EXPRESSION TAG	UNP P69687
G	-9	SER	-	EXPRESSION TAG	UNP P69687
G	-8	SER	-	EXPRESSION TAG	UNP P69687
G	-7	GLY	-	EXPRESSION TAG	UNP P69687
G	-6	LEU	-	EXPRESSION TAG	UNP P69687
G	-5	VAL	-	EXPRESSION TAG	UNP P69687
G	-4	PRO	-	EXPRESSION TAG	UNP P69687
G	-3	ARG	-	EXPRESSION TAG	UNP P69687
G	-2	GLY	-	EXPRESSION TAG	UNP P69687
G	-1	SER	-	EXPRESSION TAG	UNP P69687
G	0	HIS	-	EXPRESSION TAG	UNP P69687
H	-19	MET	-	EXPRESSION TAG	UNP P69687
H	-18	GLY	-	EXPRESSION TAG	UNP P69687
H	-17	SER	-	EXPRESSION TAG	UNP P69687
H	-16	SER	-	EXPRESSION TAG	UNP P69687
H	-15	HIS	-	EXPRESSION TAG	UNP P69687
H	-14	HIS	-	EXPRESSION TAG	UNP P69687
H	-13	HIS	-	EXPRESSION TAG	UNP P69687
H	-12	HIS	-	EXPRESSION TAG	UNP P69687
H	-11	HIS	-	EXPRESSION TAG	UNP P69687
H	-10	HIS	-	EXPRESSION TAG	UNP P69687
H	-9	SER	-	EXPRESSION TAG	UNP P69687
H	-8	SER	-	EXPRESSION TAG	UNP P69687
H	-7	GLY	-	EXPRESSION TAG	UNP P69687
H	-6	LEU	-	EXPRESSION TAG	UNP P69687
H	-5	VAL	-	EXPRESSION TAG	UNP P69687
H	-4	PRO	-	EXPRESSION TAG	UNP P69687
H	-3	ARG	-	EXPRESSION TAG	UNP P69687
H	-2	GLY	-	EXPRESSION TAG	UNP P69687
H	-1	SER	-	EXPRESSION TAG	UNP P69687
H	0	HIS	-	EXPRESSION TAG	UNP P69687
I	-19	MET	-	EXPRESSION TAG	UNP P69687
I	-18	GLY	-	EXPRESSION TAG	UNP P69687
I	-17	SER	-	EXPRESSION TAG	UNP P69687
I	-16	SER	-	EXPRESSION TAG	UNP P69687
I	-15	HIS	-	EXPRESSION TAG	UNP P69687
I	-14	HIS	-	EXPRESSION TAG	UNP P69687
I	-13	HIS	-	EXPRESSION TAG	UNP P69687
I	-12	HIS	-	EXPRESSION TAG	UNP P69687
I	-11	HIS	-	EXPRESSION TAG	UNP P69687
I	-10	HIS	-	EXPRESSION TAG	UNP P69687
I	-9	SER	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	SER	-	EXPRESSION TAG	UNP P69687
I	-7	GLY	-	EXPRESSION TAG	UNP P69687
I	-6	LEU	-	EXPRESSION TAG	UNP P69687
I	-5	VAL	-	EXPRESSION TAG	UNP P69687
I	-4	PRO	-	EXPRESSION TAG	UNP P69687
I	-3	ARG	-	EXPRESSION TAG	UNP P69687
I	-2	GLY	-	EXPRESSION TAG	UNP P69687
I	-1	SER	-	EXPRESSION TAG	UNP P69687
I	0	HIS	-	EXPRESSION TAG	UNP P69687
J	-19	MET	-	EXPRESSION TAG	UNP P69687
J	-18	GLY	-	EXPRESSION TAG	UNP P69687
J	-17	SER	-	EXPRESSION TAG	UNP P69687
J	-16	SER	-	EXPRESSION TAG	UNP P69687
J	-15	HIS	-	EXPRESSION TAG	UNP P69687
J	-14	HIS	-	EXPRESSION TAG	UNP P69687
J	-13	HIS	-	EXPRESSION TAG	UNP P69687
J	-12	HIS	-	EXPRESSION TAG	UNP P69687
J	-11	HIS	-	EXPRESSION TAG	UNP P69687
J	-10	HIS	-	EXPRESSION TAG	UNP P69687
J	-9	SER	-	EXPRESSION TAG	UNP P69687
J	-8	SER	-	EXPRESSION TAG	UNP P69687
J	-7	GLY	-	EXPRESSION TAG	UNP P69687
J	-6	LEU	-	EXPRESSION TAG	UNP P69687
J	-5	VAL	-	EXPRESSION TAG	UNP P69687
J	-4	PRO	-	EXPRESSION TAG	UNP P69687
J	-3	ARG	-	EXPRESSION TAG	UNP P69687
J	-2	GLY	-	EXPRESSION TAG	UNP P69687
J	-1	SER	-	EXPRESSION TAG	UNP P69687
J	0	HIS	-	EXPRESSION TAG	UNP P69687
K	-19	MET	-	EXPRESSION TAG	UNP P69687
K	-18	GLY	-	EXPRESSION TAG	UNP P69687
K	-17	SER	-	EXPRESSION TAG	UNP P69687
K	-16	SER	-	EXPRESSION TAG	UNP P69687
K	-15	HIS	-	EXPRESSION TAG	UNP P69687
K	-14	HIS	-	EXPRESSION TAG	UNP P69687
K	-13	HIS	-	EXPRESSION TAG	UNP P69687
K	-12	HIS	-	EXPRESSION TAG	UNP P69687
K	-11	HIS	-	EXPRESSION TAG	UNP P69687
K	-10	HIS	-	EXPRESSION TAG	UNP P69687
K	-9	SER	-	EXPRESSION TAG	UNP P69687
K	-8	SER	-	EXPRESSION TAG	UNP P69687
K	-7	GLY	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	LEU	-	EXPRESSION TAG	UNP P69687
K	-5	VAL	-	EXPRESSION TAG	UNP P69687
K	-4	PRO	-	EXPRESSION TAG	UNP P69687
K	-3	ARG	-	EXPRESSION TAG	UNP P69687
K	-2	GLY	-	EXPRESSION TAG	UNP P69687
K	-1	SER	-	EXPRESSION TAG	UNP P69687
K	0	HIS	-	EXPRESSION TAG	UNP P69687
L	-19	MET	-	EXPRESSION TAG	UNP P69687
L	-18	GLY	-	EXPRESSION TAG	UNP P69687
L	-17	SER	-	EXPRESSION TAG	UNP P69687
L	-16	SER	-	EXPRESSION TAG	UNP P69687
L	-15	HIS	-	EXPRESSION TAG	UNP P69687
L	-14	HIS	-	EXPRESSION TAG	UNP P69687
L	-13	HIS	-	EXPRESSION TAG	UNP P69687
L	-12	HIS	-	EXPRESSION TAG	UNP P69687
L	-11	HIS	-	EXPRESSION TAG	UNP P69687
L	-10	HIS	-	EXPRESSION TAG	UNP P69687
L	-9	SER	-	EXPRESSION TAG	UNP P69687
L	-8	SER	-	EXPRESSION TAG	UNP P69687
L	-7	GLY	-	EXPRESSION TAG	UNP P69687
L	-6	LEU	-	EXPRESSION TAG	UNP P69687
L	-5	VAL	-	EXPRESSION TAG	UNP P69687
L	-4	PRO	-	EXPRESSION TAG	UNP P69687
L	-3	ARG	-	EXPRESSION TAG	UNP P69687
L	-2	GLY	-	EXPRESSION TAG	UNP P69687
L	-1	SER	-	EXPRESSION TAG	UNP P69687
L	0	HIS	-	EXPRESSION TAG	UNP P69687
M	-19	MET	-	EXPRESSION TAG	UNP P69687
M	-18	GLY	-	EXPRESSION TAG	UNP P69687
M	-17	SER	-	EXPRESSION TAG	UNP P69687
M	-16	SER	-	EXPRESSION TAG	UNP P69687
M	-15	HIS	-	EXPRESSION TAG	UNP P69687
M	-14	HIS	-	EXPRESSION TAG	UNP P69687
M	-13	HIS	-	EXPRESSION TAG	UNP P69687
M	-12	HIS	-	EXPRESSION TAG	UNP P69687
M	-11	HIS	-	EXPRESSION TAG	UNP P69687
M	-10	HIS	-	EXPRESSION TAG	UNP P69687
M	-9	SER	-	EXPRESSION TAG	UNP P69687
M	-8	SER	-	EXPRESSION TAG	UNP P69687
M	-7	GLY	-	EXPRESSION TAG	UNP P69687
M	-6	LEU	-	EXPRESSION TAG	UNP P69687
M	-5	VAL	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	-4	PRO	-	EXPRESSION TAG	UNP P69687
M	-3	ARG	-	EXPRESSION TAG	UNP P69687
M	-2	GLY	-	EXPRESSION TAG	UNP P69687
M	-1	SER	-	EXPRESSION TAG	UNP P69687
M	0	HIS	-	EXPRESSION TAG	UNP P69687
N	-19	MET	-	EXPRESSION TAG	UNP P69687
N	-18	GLY	-	EXPRESSION TAG	UNP P69687
N	-17	SER	-	EXPRESSION TAG	UNP P69687
N	-16	SER	-	EXPRESSION TAG	UNP P69687
N	-15	HIS	-	EXPRESSION TAG	UNP P69687
N	-14	HIS	-	EXPRESSION TAG	UNP P69687
N	-13	HIS	-	EXPRESSION TAG	UNP P69687
N	-12	HIS	-	EXPRESSION TAG	UNP P69687
N	-11	HIS	-	EXPRESSION TAG	UNP P69687
N	-10	HIS	-	EXPRESSION TAG	UNP P69687
N	-9	SER	-	EXPRESSION TAG	UNP P69687
N	-8	SER	-	EXPRESSION TAG	UNP P69687
N	-7	GLY	-	EXPRESSION TAG	UNP P69687
N	-6	LEU	-	EXPRESSION TAG	UNP P69687
N	-5	VAL	-	EXPRESSION TAG	UNP P69687
N	-4	PRO	-	EXPRESSION TAG	UNP P69687
N	-3	ARG	-	EXPRESSION TAG	UNP P69687
N	-2	GLY	-	EXPRESSION TAG	UNP P69687
N	-1	SER	-	EXPRESSION TAG	UNP P69687
N	0	HIS	-	EXPRESSION TAG	UNP P69687
O	-19	MET	-	EXPRESSION TAG	UNP P69687
O	-18	GLY	-	EXPRESSION TAG	UNP P69687
O	-17	SER	-	EXPRESSION TAG	UNP P69687
O	-16	SER	-	EXPRESSION TAG	UNP P69687
O	-15	HIS	-	EXPRESSION TAG	UNP P69687
O	-14	HIS	-	EXPRESSION TAG	UNP P69687
O	-13	HIS	-	EXPRESSION TAG	UNP P69687
O	-12	HIS	-	EXPRESSION TAG	UNP P69687
O	-11	HIS	-	EXPRESSION TAG	UNP P69687
O	-10	HIS	-	EXPRESSION TAG	UNP P69687
O	-9	SER	-	EXPRESSION TAG	UNP P69687
O	-8	SER	-	EXPRESSION TAG	UNP P69687
O	-7	GLY	-	EXPRESSION TAG	UNP P69687
O	-6	LEU	-	EXPRESSION TAG	UNP P69687
O	-5	VAL	-	EXPRESSION TAG	UNP P69687
O	-4	PRO	-	EXPRESSION TAG	UNP P69687
O	-3	ARG	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	EXPRESSION TAG	UNP P69687
O	-1	SER	-	EXPRESSION TAG	UNP P69687
O	0	HIS	-	EXPRESSION TAG	UNP P69687
P	-19	MET	-	EXPRESSION TAG	UNP P69687
P	-18	GLY	-	EXPRESSION TAG	UNP P69687
P	-17	SER	-	EXPRESSION TAG	UNP P69687
P	-16	SER	-	EXPRESSION TAG	UNP P69687
P	-15	HIS	-	EXPRESSION TAG	UNP P69687
P	-14	HIS	-	EXPRESSION TAG	UNP P69687
P	-13	HIS	-	EXPRESSION TAG	UNP P69687
P	-12	HIS	-	EXPRESSION TAG	UNP P69687
P	-11	HIS	-	EXPRESSION TAG	UNP P69687
P	-10	HIS	-	EXPRESSION TAG	UNP P69687
P	-9	SER	-	EXPRESSION TAG	UNP P69687
P	-8	SER	-	EXPRESSION TAG	UNP P69687
P	-7	GLY	-	EXPRESSION TAG	UNP P69687
P	-6	LEU	-	EXPRESSION TAG	UNP P69687
P	-5	VAL	-	EXPRESSION TAG	UNP P69687
P	-4	PRO	-	EXPRESSION TAG	UNP P69687
P	-3	ARG	-	EXPRESSION TAG	UNP P69687
P	-2	GLY	-	EXPRESSION TAG	UNP P69687
P	-1	SER	-	EXPRESSION TAG	UNP P69687
P	0	HIS	-	EXPRESSION TAG	UNP P69687
Q	-19	MET	-	EXPRESSION TAG	UNP P69687
Q	-18	GLY	-	EXPRESSION TAG	UNP P69687
Q	-17	SER	-	EXPRESSION TAG	UNP P69687
Q	-16	SER	-	EXPRESSION TAG	UNP P69687
Q	-15	HIS	-	EXPRESSION TAG	UNP P69687
Q	-14	HIS	-	EXPRESSION TAG	UNP P69687
Q	-13	HIS	-	EXPRESSION TAG	UNP P69687
Q	-12	HIS	-	EXPRESSION TAG	UNP P69687
Q	-11	HIS	-	EXPRESSION TAG	UNP P69687
Q	-10	HIS	-	EXPRESSION TAG	UNP P69687
Q	-9	SER	-	EXPRESSION TAG	UNP P69687
Q	-8	SER	-	EXPRESSION TAG	UNP P69687
Q	-7	GLY	-	EXPRESSION TAG	UNP P69687
Q	-6	LEU	-	EXPRESSION TAG	UNP P69687
Q	-5	VAL	-	EXPRESSION TAG	UNP P69687
Q	-4	PRO	-	EXPRESSION TAG	UNP P69687
Q	-3	ARG	-	EXPRESSION TAG	UNP P69687
Q	-2	GLY	-	EXPRESSION TAG	UNP P69687
Q	-1	SER	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	HIS	-	EXPRESSION TAG	UNP P69687
R	-19	MET	-	EXPRESSION TAG	UNP P69687
R	-18	GLY	-	EXPRESSION TAG	UNP P69687
R	-17	SER	-	EXPRESSION TAG	UNP P69687
R	-16	SER	-	EXPRESSION TAG	UNP P69687
R	-15	HIS	-	EXPRESSION TAG	UNP P69687
R	-14	HIS	-	EXPRESSION TAG	UNP P69687
R	-13	HIS	-	EXPRESSION TAG	UNP P69687
R	-12	HIS	-	EXPRESSION TAG	UNP P69687
R	-11	HIS	-	EXPRESSION TAG	UNP P69687
R	-10	HIS	-	EXPRESSION TAG	UNP P69687
R	-9	SER	-	EXPRESSION TAG	UNP P69687
R	-8	SER	-	EXPRESSION TAG	UNP P69687
R	-7	GLY	-	EXPRESSION TAG	UNP P69687
R	-6	LEU	-	EXPRESSION TAG	UNP P69687
R	-5	VAL	-	EXPRESSION TAG	UNP P69687
R	-4	PRO	-	EXPRESSION TAG	UNP P69687
R	-3	ARG	-	EXPRESSION TAG	UNP P69687
R	-2	GLY	-	EXPRESSION TAG	UNP P69687
R	-1	SER	-	EXPRESSION TAG	UNP P69687
R	0	HIS	-	EXPRESSION TAG	UNP P69687
S	-19	MET	-	EXPRESSION TAG	UNP P69687
S	-18	GLY	-	EXPRESSION TAG	UNP P69687
S	-17	SER	-	EXPRESSION TAG	UNP P69687
S	-16	SER	-	EXPRESSION TAG	UNP P69687
S	-15	HIS	-	EXPRESSION TAG	UNP P69687
S	-14	HIS	-	EXPRESSION TAG	UNP P69687
S	-13	HIS	-	EXPRESSION TAG	UNP P69687
S	-12	HIS	-	EXPRESSION TAG	UNP P69687
S	-11	HIS	-	EXPRESSION TAG	UNP P69687
S	-10	HIS	-	EXPRESSION TAG	UNP P69687
S	-9	SER	-	EXPRESSION TAG	UNP P69687
S	-8	SER	-	EXPRESSION TAG	UNP P69687
S	-7	GLY	-	EXPRESSION TAG	UNP P69687
S	-6	LEU	-	EXPRESSION TAG	UNP P69687
S	-5	VAL	-	EXPRESSION TAG	UNP P69687
S	-4	PRO	-	EXPRESSION TAG	UNP P69687
S	-3	ARG	-	EXPRESSION TAG	UNP P69687
S	-2	GLY	-	EXPRESSION TAG	UNP P69687
S	-1	SER	-	EXPRESSION TAG	UNP P69687
S	0	HIS	-	EXPRESSION TAG	UNP P69687
T	-19	MET	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	-18	GLY	-	EXPRESSION TAG	UNP P69687
T	-17	SER	-	EXPRESSION TAG	UNP P69687
T	-16	SER	-	EXPRESSION TAG	UNP P69687
T	-15	HIS	-	EXPRESSION TAG	UNP P69687
T	-14	HIS	-	EXPRESSION TAG	UNP P69687
T	-13	HIS	-	EXPRESSION TAG	UNP P69687
T	-12	HIS	-	EXPRESSION TAG	UNP P69687
T	-11	HIS	-	EXPRESSION TAG	UNP P69687
T	-10	HIS	-	EXPRESSION TAG	UNP P69687
T	-9	SER	-	EXPRESSION TAG	UNP P69687
T	-8	SER	-	EXPRESSION TAG	UNP P69687
T	-7	GLY	-	EXPRESSION TAG	UNP P69687
T	-6	LEU	-	EXPRESSION TAG	UNP P69687
T	-5	VAL	-	EXPRESSION TAG	UNP P69687
T	-4	PRO	-	EXPRESSION TAG	UNP P69687
T	-3	ARG	-	EXPRESSION TAG	UNP P69687
T	-2	GLY	-	EXPRESSION TAG	UNP P69687
T	-1	SER	-	EXPRESSION TAG	UNP P69687
T	0	HIS	-	EXPRESSION TAG	UNP P69687
U	-19	MET	-	EXPRESSION TAG	UNP P69687
U	-18	GLY	-	EXPRESSION TAG	UNP P69687
U	-17	SER	-	EXPRESSION TAG	UNP P69687
U	-16	SER	-	EXPRESSION TAG	UNP P69687
U	-15	HIS	-	EXPRESSION TAG	UNP P69687
U	-14	HIS	-	EXPRESSION TAG	UNP P69687
U	-13	HIS	-	EXPRESSION TAG	UNP P69687
U	-12	HIS	-	EXPRESSION TAG	UNP P69687
U	-11	HIS	-	EXPRESSION TAG	UNP P69687
U	-10	HIS	-	EXPRESSION TAG	UNP P69687
U	-9	SER	-	EXPRESSION TAG	UNP P69687
U	-8	SER	-	EXPRESSION TAG	UNP P69687
U	-7	GLY	-	EXPRESSION TAG	UNP P69687
U	-6	LEU	-	EXPRESSION TAG	UNP P69687
U	-5	VAL	-	EXPRESSION TAG	UNP P69687
U	-4	PRO	-	EXPRESSION TAG	UNP P69687
U	-3	ARG	-	EXPRESSION TAG	UNP P69687
U	-2	GLY	-	EXPRESSION TAG	UNP P69687
U	-1	SER	-	EXPRESSION TAG	UNP P69687
U	0	HIS	-	EXPRESSION TAG	UNP P69687
V	-19	MET	-	EXPRESSION TAG	UNP P69687
V	-18	GLY	-	EXPRESSION TAG	UNP P69687
V	-17	SER	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	-16	SER	-	EXPRESSION TAG	UNP P69687
V	-15	HIS	-	EXPRESSION TAG	UNP P69687
V	-14	HIS	-	EXPRESSION TAG	UNP P69687
V	-13	HIS	-	EXPRESSION TAG	UNP P69687
V	-12	HIS	-	EXPRESSION TAG	UNP P69687
V	-11	HIS	-	EXPRESSION TAG	UNP P69687
V	-10	HIS	-	EXPRESSION TAG	UNP P69687
V	-9	SER	-	EXPRESSION TAG	UNP P69687
V	-8	SER	-	EXPRESSION TAG	UNP P69687
V	-7	GLY	-	EXPRESSION TAG	UNP P69687
V	-6	LEU	-	EXPRESSION TAG	UNP P69687
V	-5	VAL	-	EXPRESSION TAG	UNP P69687
V	-4	PRO	-	EXPRESSION TAG	UNP P69687
V	-3	ARG	-	EXPRESSION TAG	UNP P69687
V	-2	GLY	-	EXPRESSION TAG	UNP P69687
V	-1	SER	-	EXPRESSION TAG	UNP P69687
V	0	HIS	-	EXPRESSION TAG	UNP P69687
W	-19	MET	-	EXPRESSION TAG	UNP P69687
W	-18	GLY	-	EXPRESSION TAG	UNP P69687
W	-17	SER	-	EXPRESSION TAG	UNP P69687
W	-16	SER	-	EXPRESSION TAG	UNP P69687
W	-15	HIS	-	EXPRESSION TAG	UNP P69687
W	-14	HIS	-	EXPRESSION TAG	UNP P69687
W	-13	HIS	-	EXPRESSION TAG	UNP P69687
W	-12	HIS	-	EXPRESSION TAG	UNP P69687
W	-11	HIS	-	EXPRESSION TAG	UNP P69687
W	-10	HIS	-	EXPRESSION TAG	UNP P69687
W	-9	SER	-	EXPRESSION TAG	UNP P69687
W	-8	SER	-	EXPRESSION TAG	UNP P69687
W	-7	GLY	-	EXPRESSION TAG	UNP P69687
W	-6	LEU	-	EXPRESSION TAG	UNP P69687
W	-5	VAL	-	EXPRESSION TAG	UNP P69687
W	-4	PRO	-	EXPRESSION TAG	UNP P69687
W	-3	ARG	-	EXPRESSION TAG	UNP P69687
W	-2	GLY	-	EXPRESSION TAG	UNP P69687
W	-1	SER	-	EXPRESSION TAG	UNP P69687
W	0	HIS	-	EXPRESSION TAG	UNP P69687
X	-19	MET	-	EXPRESSION TAG	UNP P69687
X	-18	GLY	-	EXPRESSION TAG	UNP P69687
X	-17	SER	-	EXPRESSION TAG	UNP P69687
X	-16	SER	-	EXPRESSION TAG	UNP P69687
X	-15	HIS	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	-14	HIS	-	EXPRESSION TAG	UNP P69687
X	-13	HIS	-	EXPRESSION TAG	UNP P69687
X	-12	HIS	-	EXPRESSION TAG	UNP P69687
X	-11	HIS	-	EXPRESSION TAG	UNP P69687
X	-10	HIS	-	EXPRESSION TAG	UNP P69687
X	-9	SER	-	EXPRESSION TAG	UNP P69687
X	-8	SER	-	EXPRESSION TAG	UNP P69687
X	-7	GLY	-	EXPRESSION TAG	UNP P69687
X	-6	LEU	-	EXPRESSION TAG	UNP P69687
X	-5	VAL	-	EXPRESSION TAG	UNP P69687
X	-4	PRO	-	EXPRESSION TAG	UNP P69687
X	-3	ARG	-	EXPRESSION TAG	UNP P69687
X	-2	GLY	-	EXPRESSION TAG	UNP P69687
X	-1	SER	-	EXPRESSION TAG	UNP P69687
X	0	HIS	-	EXPRESSION TAG	UNP P69687
Y	-19	MET	-	EXPRESSION TAG	UNP P69687
Y	-18	GLY	-	EXPRESSION TAG	UNP P69687
Y	-17	SER	-	EXPRESSION TAG	UNP P69687
Y	-16	SER	-	EXPRESSION TAG	UNP P69687
Y	-15	HIS	-	EXPRESSION TAG	UNP P69687
Y	-14	HIS	-	EXPRESSION TAG	UNP P69687
Y	-13	HIS	-	EXPRESSION TAG	UNP P69687
Y	-12	HIS	-	EXPRESSION TAG	UNP P69687
Y	-11	HIS	-	EXPRESSION TAG	UNP P69687
Y	-10	HIS	-	EXPRESSION TAG	UNP P69687
Y	-9	SER	-	EXPRESSION TAG	UNP P69687
Y	-8	SER	-	EXPRESSION TAG	UNP P69687
Y	-7	GLY	-	EXPRESSION TAG	UNP P69687
Y	-6	LEU	-	EXPRESSION TAG	UNP P69687
Y	-5	VAL	-	EXPRESSION TAG	UNP P69687
Y	-4	PRO	-	EXPRESSION TAG	UNP P69687
Y	-3	ARG	-	EXPRESSION TAG	UNP P69687
Y	-2	GLY	-	EXPRESSION TAG	UNP P69687
Y	-1	SER	-	EXPRESSION TAG	UNP P69687
Y	0	HIS	-	EXPRESSION TAG	UNP P69687
Z	-19	MET	-	EXPRESSION TAG	UNP P69687
Z	-18	GLY	-	EXPRESSION TAG	UNP P69687
Z	-17	SER	-	EXPRESSION TAG	UNP P69687
Z	-16	SER	-	EXPRESSION TAG	UNP P69687
Z	-15	HIS	-	EXPRESSION TAG	UNP P69687
Z	-14	HIS	-	EXPRESSION TAG	UNP P69687
Z	-13	HIS	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Z	-12	HIS	-	EXPRESSION TAG	UNP P69687
Z	-11	HIS	-	EXPRESSION TAG	UNP P69687
Z	-10	HIS	-	EXPRESSION TAG	UNP P69687
Z	-9	SER	-	EXPRESSION TAG	UNP P69687
Z	-8	SER	-	EXPRESSION TAG	UNP P69687
Z	-7	GLY	-	EXPRESSION TAG	UNP P69687
Z	-6	LEU	-	EXPRESSION TAG	UNP P69687
Z	-5	VAL	-	EXPRESSION TAG	UNP P69687
Z	-4	PRO	-	EXPRESSION TAG	UNP P69687
Z	-3	ARG	-	EXPRESSION TAG	UNP P69687
Z	-2	GLY	-	EXPRESSION TAG	UNP P69687
Z	-1	SER	-	EXPRESSION TAG	UNP P69687
Z	0	HIS	-	EXPRESSION TAG	UNP P69687
a	-19	MET	-	EXPRESSION TAG	UNP P69687
a	-18	GLY	-	EXPRESSION TAG	UNP P69687
a	-17	SER	-	EXPRESSION TAG	UNP P69687
a	-16	SER	-	EXPRESSION TAG	UNP P69687
a	-15	HIS	-	EXPRESSION TAG	UNP P69687
a	-14	HIS	-	EXPRESSION TAG	UNP P69687
a	-13	HIS	-	EXPRESSION TAG	UNP P69687
a	-12	HIS	-	EXPRESSION TAG	UNP P69687
a	-11	HIS	-	EXPRESSION TAG	UNP P69687
a	-10	HIS	-	EXPRESSION TAG	UNP P69687
a	-9	SER	-	EXPRESSION TAG	UNP P69687
a	-8	SER	-	EXPRESSION TAG	UNP P69687
a	-7	GLY	-	EXPRESSION TAG	UNP P69687
a	-6	LEU	-	EXPRESSION TAG	UNP P69687
a	-5	VAL	-	EXPRESSION TAG	UNP P69687
a	-4	PRO	-	EXPRESSION TAG	UNP P69687
a	-3	ARG	-	EXPRESSION TAG	UNP P69687
a	-2	GLY	-	EXPRESSION TAG	UNP P69687
a	-1	SER	-	EXPRESSION TAG	UNP P69687
a	0	HIS	-	EXPRESSION TAG	UNP P69687
b	-19	MET	-	EXPRESSION TAG	UNP P69687
b	-18	GLY	-	EXPRESSION TAG	UNP P69687
b	-17	SER	-	EXPRESSION TAG	UNP P69687
b	-16	SER	-	EXPRESSION TAG	UNP P69687
b	-15	HIS	-	EXPRESSION TAG	UNP P69687
b	-14	HIS	-	EXPRESSION TAG	UNP P69687
b	-13	HIS	-	EXPRESSION TAG	UNP P69687
b	-12	HIS	-	EXPRESSION TAG	UNP P69687
b	-11	HIS	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	-10	HIS	-	EXPRESSION TAG	UNP P69687
b	-9	SER	-	EXPRESSION TAG	UNP P69687
b	-8	SER	-	EXPRESSION TAG	UNP P69687
b	-7	GLY	-	EXPRESSION TAG	UNP P69687
b	-6	LEU	-	EXPRESSION TAG	UNP P69687
b	-5	VAL	-	EXPRESSION TAG	UNP P69687
b	-4	PRO	-	EXPRESSION TAG	UNP P69687
b	-3	ARG	-	EXPRESSION TAG	UNP P69687
b	-2	GLY	-	EXPRESSION TAG	UNP P69687
b	-1	SER	-	EXPRESSION TAG	UNP P69687
b	0	HIS	-	EXPRESSION TAG	UNP P69687
c	-19	MET	-	EXPRESSION TAG	UNP P69687
c	-18	GLY	-	EXPRESSION TAG	UNP P69687
c	-17	SER	-	EXPRESSION TAG	UNP P69687
c	-16	SER	-	EXPRESSION TAG	UNP P69687
c	-15	HIS	-	EXPRESSION TAG	UNP P69687
c	-14	HIS	-	EXPRESSION TAG	UNP P69687
c	-13	HIS	-	EXPRESSION TAG	UNP P69687
c	-12	HIS	-	EXPRESSION TAG	UNP P69687
c	-11	HIS	-	EXPRESSION TAG	UNP P69687
c	-10	HIS	-	EXPRESSION TAG	UNP P69687
c	-9	SER	-	EXPRESSION TAG	UNP P69687
c	-8	SER	-	EXPRESSION TAG	UNP P69687
c	-7	GLY	-	EXPRESSION TAG	UNP P69687
c	-6	LEU	-	EXPRESSION TAG	UNP P69687
c	-5	VAL	-	EXPRESSION TAG	UNP P69687
c	-4	PRO	-	EXPRESSION TAG	UNP P69687
c	-3	ARG	-	EXPRESSION TAG	UNP P69687
c	-2	GLY	-	EXPRESSION TAG	UNP P69687
c	-1	SER	-	EXPRESSION TAG	UNP P69687
c	0	HIS	-	EXPRESSION TAG	UNP P69687
d	-19	MET	-	EXPRESSION TAG	UNP P69687
d	-18	GLY	-	EXPRESSION TAG	UNP P69687
d	-17	SER	-	EXPRESSION TAG	UNP P69687
d	-16	SER	-	EXPRESSION TAG	UNP P69687
d	-15	HIS	-	EXPRESSION TAG	UNP P69687
d	-14	HIS	-	EXPRESSION TAG	UNP P69687
d	-13	HIS	-	EXPRESSION TAG	UNP P69687
d	-12	HIS	-	EXPRESSION TAG	UNP P69687
d	-11	HIS	-	EXPRESSION TAG	UNP P69687
d	-10	HIS	-	EXPRESSION TAG	UNP P69687
d	-9	SER	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
d	-8	SER	-	EXPRESSION TAG	UNP P69687
d	-7	GLY	-	EXPRESSION TAG	UNP P69687
d	-6	LEU	-	EXPRESSION TAG	UNP P69687
d	-5	VAL	-	EXPRESSION TAG	UNP P69687
d	-4	PRO	-	EXPRESSION TAG	UNP P69687
d	-3	ARG	-	EXPRESSION TAG	UNP P69687
d	-2	GLY	-	EXPRESSION TAG	UNP P69687
d	-1	SER	-	EXPRESSION TAG	UNP P69687
d	0	HIS	-	EXPRESSION TAG	UNP P69687
e	-19	MET	-	EXPRESSION TAG	UNP P69687
e	-18	GLY	-	EXPRESSION TAG	UNP P69687
e	-17	SER	-	EXPRESSION TAG	UNP P69687
e	-16	SER	-	EXPRESSION TAG	UNP P69687
e	-15	HIS	-	EXPRESSION TAG	UNP P69687
e	-14	HIS	-	EXPRESSION TAG	UNP P69687
e	-13	HIS	-	EXPRESSION TAG	UNP P69687
e	-12	HIS	-	EXPRESSION TAG	UNP P69687
e	-11	HIS	-	EXPRESSION TAG	UNP P69687
e	-10	HIS	-	EXPRESSION TAG	UNP P69687
e	-9	SER	-	EXPRESSION TAG	UNP P69687
e	-8	SER	-	EXPRESSION TAG	UNP P69687
e	-7	GLY	-	EXPRESSION TAG	UNP P69687
e	-6	LEU	-	EXPRESSION TAG	UNP P69687
e	-5	VAL	-	EXPRESSION TAG	UNP P69687
e	-4	PRO	-	EXPRESSION TAG	UNP P69687
e	-3	ARG	-	EXPRESSION TAG	UNP P69687
e	-2	GLY	-	EXPRESSION TAG	UNP P69687
e	-1	SER	-	EXPRESSION TAG	UNP P69687
e	0	HIS	-	EXPRESSION TAG	UNP P69687
f	-19	MET	-	EXPRESSION TAG	UNP P69687
f	-18	GLY	-	EXPRESSION TAG	UNP P69687
f	-17	SER	-	EXPRESSION TAG	UNP P69687
f	-16	SER	-	EXPRESSION TAG	UNP P69687
f	-15	HIS	-	EXPRESSION TAG	UNP P69687
f	-14	HIS	-	EXPRESSION TAG	UNP P69687
f	-13	HIS	-	EXPRESSION TAG	UNP P69687
f	-12	HIS	-	EXPRESSION TAG	UNP P69687
f	-11	HIS	-	EXPRESSION TAG	UNP P69687
f	-10	HIS	-	EXPRESSION TAG	UNP P69687
f	-9	SER	-	EXPRESSION TAG	UNP P69687
f	-8	SER	-	EXPRESSION TAG	UNP P69687
f	-7	GLY	-	EXPRESSION TAG	UNP P69687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
f	-6	LEU	-	EXPRESSION TAG	UNP P69687
f	-5	VAL	-	EXPRESSION TAG	UNP P69687
f	-4	PRO	-	EXPRESSION TAG	UNP P69687
f	-3	ARG	-	EXPRESSION TAG	UNP P69687
f	-2	GLY	-	EXPRESSION TAG	UNP P69687
f	-1	SER	-	EXPRESSION TAG	UNP P69687
f	0	HIS	-	EXPRESSION TAG	UNP P69687
h	-19	MET	-	EXPRESSION TAG	UNP P69687
h	-18	GLY	-	EXPRESSION TAG	UNP P69687
h	-17	SER	-	EXPRESSION TAG	UNP P69687
h	-16	SER	-	EXPRESSION TAG	UNP P69687
h	-15	HIS	-	EXPRESSION TAG	UNP P69687
h	-14	HIS	-	EXPRESSION TAG	UNP P69687
h	-13	HIS	-	EXPRESSION TAG	UNP P69687
h	-12	HIS	-	EXPRESSION TAG	UNP P69687
h	-11	HIS	-	EXPRESSION TAG	UNP P69687
h	-10	HIS	-	EXPRESSION TAG	UNP P69687
h	-9	SER	-	EXPRESSION TAG	UNP P69687
h	-8	SER	-	EXPRESSION TAG	UNP P69687
h	-7	GLY	-	EXPRESSION TAG	UNP P69687
h	-6	LEU	-	EXPRESSION TAG	UNP P69687
h	-5	VAL	-	EXPRESSION TAG	UNP P69687
h	-4	PRO	-	EXPRESSION TAG	UNP P69687
h	-3	ARG	-	EXPRESSION TAG	UNP P69687
h	-2	GLY	-	EXPRESSION TAG	UNP P69687
h	-1	SER	-	EXPRESSION TAG	UNP P69687
h	0	HIS	-	EXPRESSION TAG	UNP P69687
i	-19	MET	-	EXPRESSION TAG	UNP P69687
i	-18	GLY	-	EXPRESSION TAG	UNP P69687
i	-17	SER	-	EXPRESSION TAG	UNP P69687
i	-16	SER	-	EXPRESSION TAG	UNP P69687
i	-15	HIS	-	EXPRESSION TAG	UNP P69687
i	-14	HIS	-	EXPRESSION TAG	UNP P69687
i	-13	HIS	-	EXPRESSION TAG	UNP P69687
i	-12	HIS	-	EXPRESSION TAG	UNP P69687
i	-11	HIS	-	EXPRESSION TAG	UNP P69687
i	-10	HIS	-	EXPRESSION TAG	UNP P69687
i	-9	SER	-	EXPRESSION TAG	UNP P69687
i	-8	SER	-	EXPRESSION TAG	UNP P69687
i	-7	GLY	-	EXPRESSION TAG	UNP P69687
i	-6	LEU	-	EXPRESSION TAG	UNP P69687
i	-5	VAL	-	EXPRESSION TAG	UNP P69687

Continued on next page...

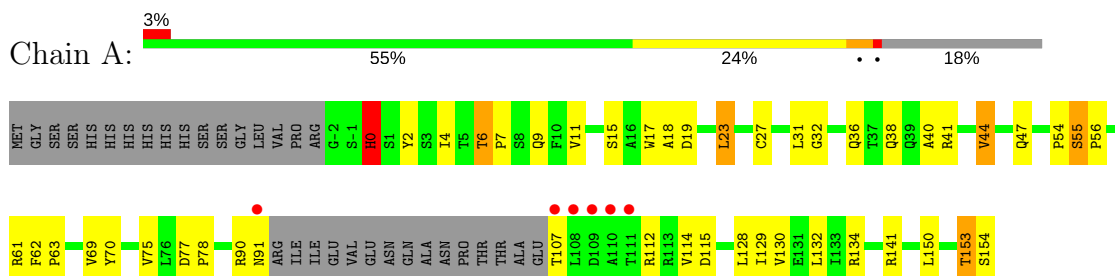
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
i	-4	PRO	-	EXPRESSION TAG	UNP P69687
i	-3	ARG	-	EXPRESSION TAG	UNP P69687
i	-2	GLY	-	EXPRESSION TAG	UNP P69687
i	-1	SER	-	EXPRESSION TAG	UNP P69687
i	0	HIS	-	EXPRESSION TAG	UNP P69687

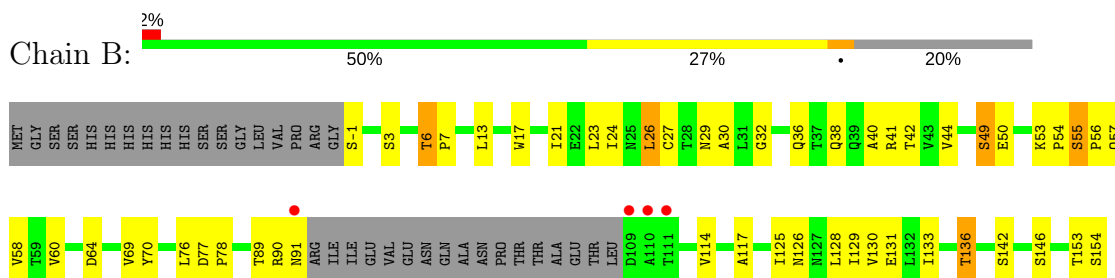
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

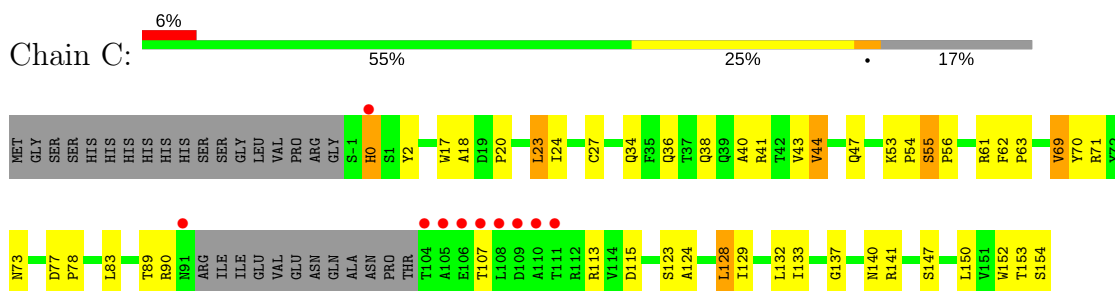
- Molecule 1: Capsid protein



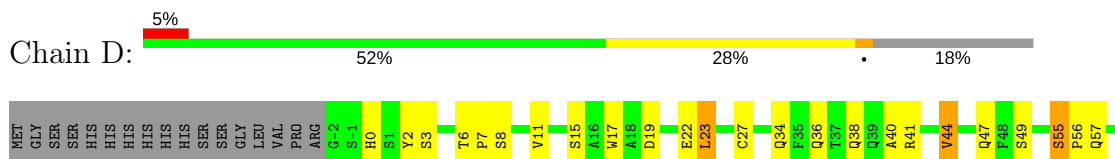
- Molecule 1: Capsid protein



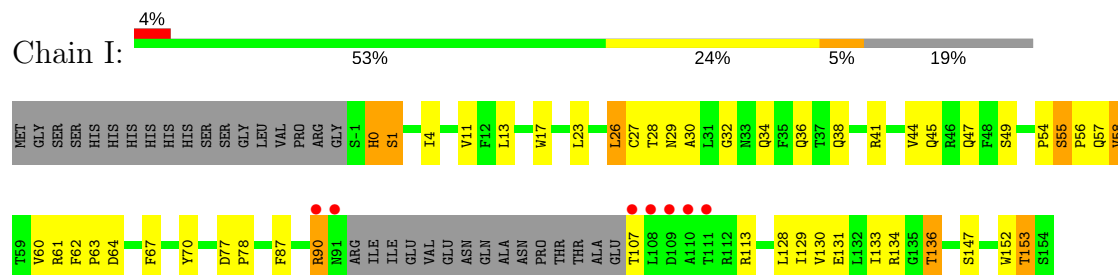
- Molecule 1: Capsid protein



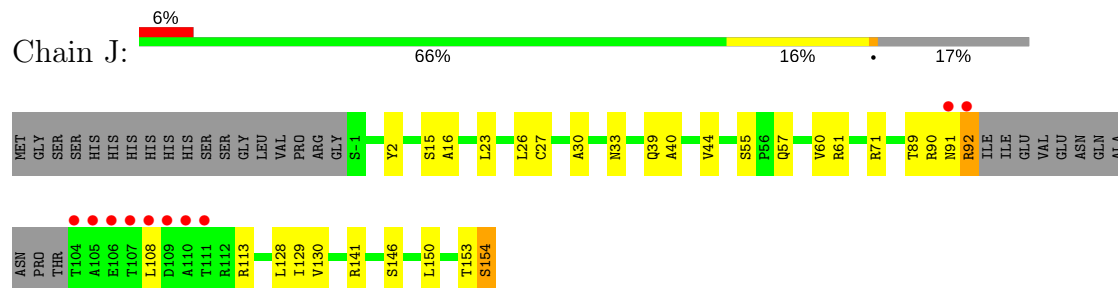
- Molecule 1: Capsid protein



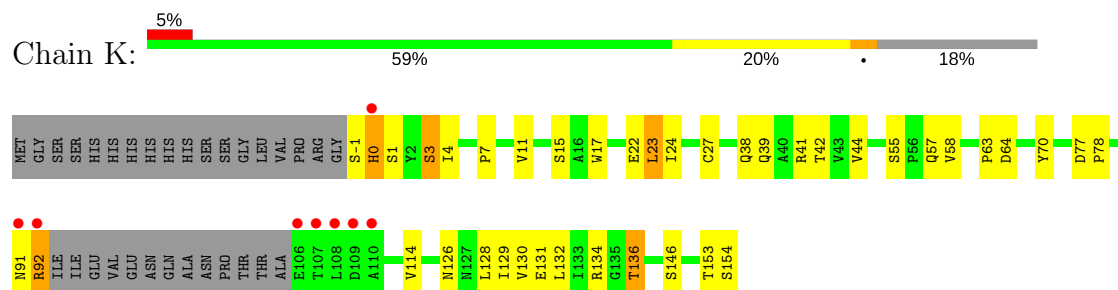
- Molecule 1: Capsid protein



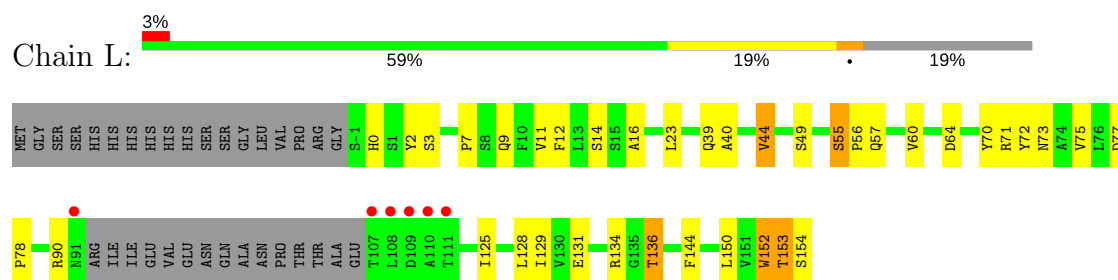
- Molecule 1: Capsid protein



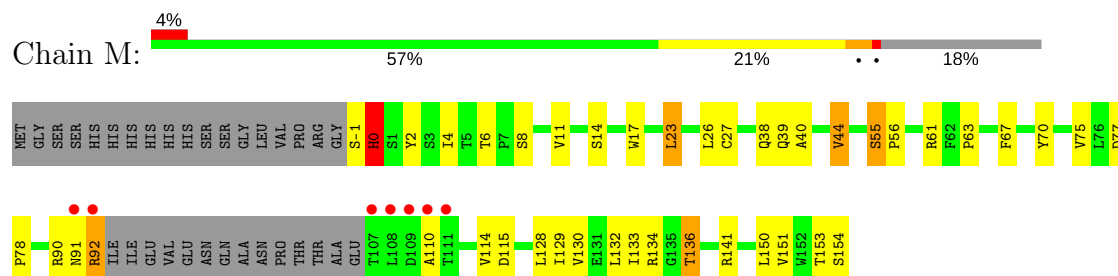
- Molecule 1: Capsid protein



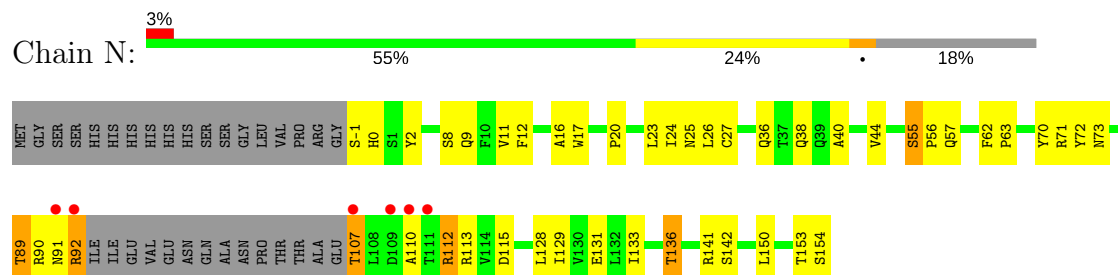
- Molecule 1: Capsid protein



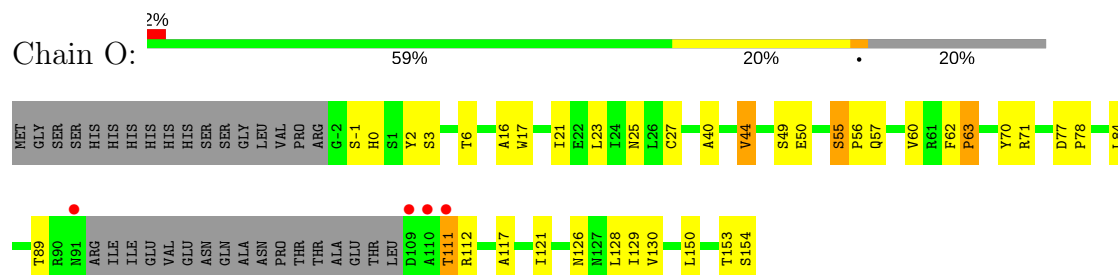
- Molecule 1: Capsid protein



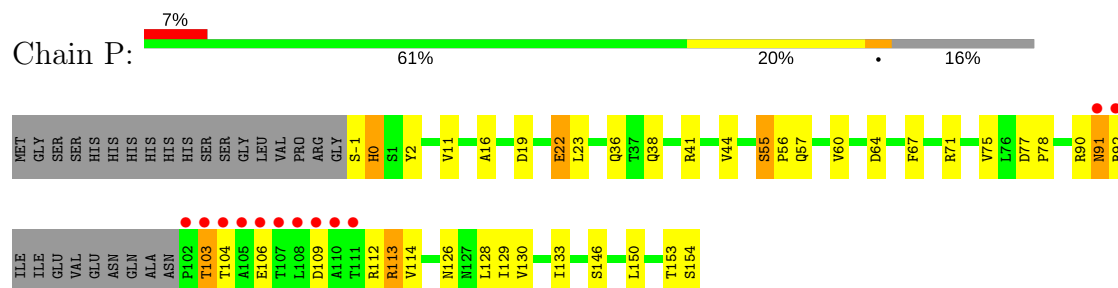
● Molecule 1: Capsid protein



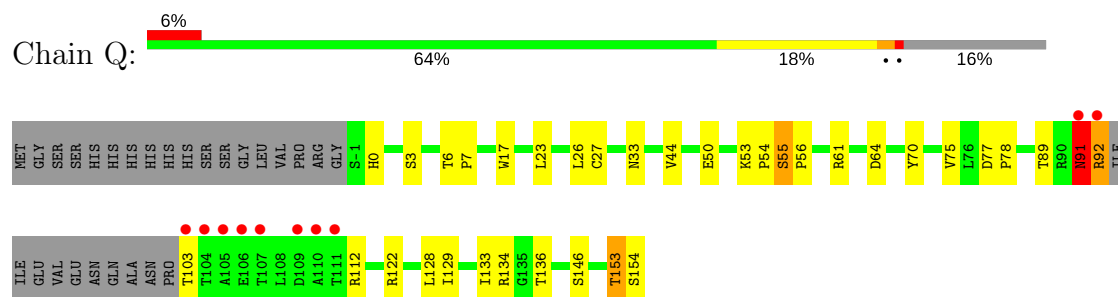
● Molecule 1: Capsid protein



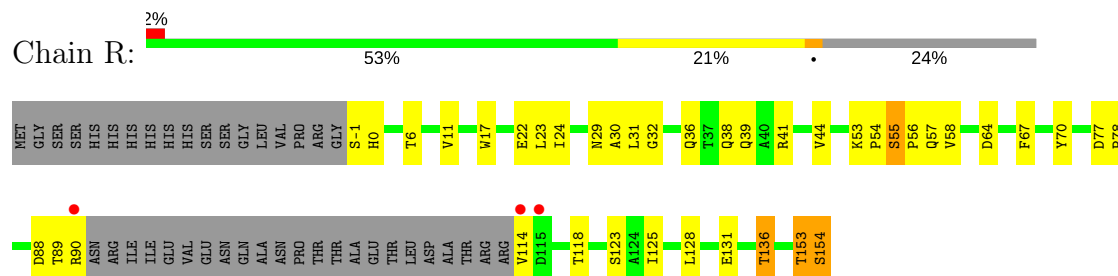
● Molecule 1: Capsid protein



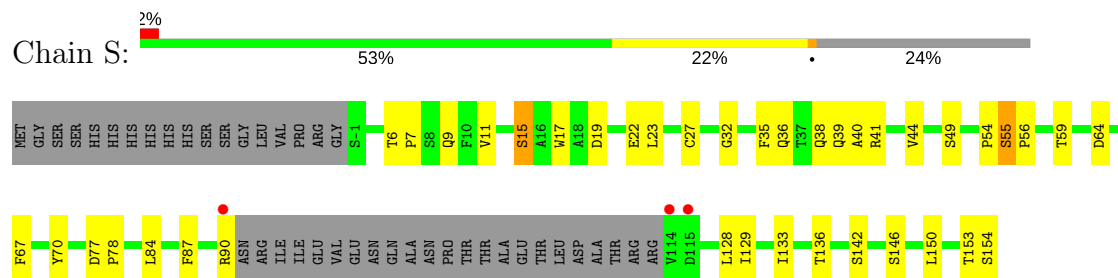
● Molecule 1: Capsid protein



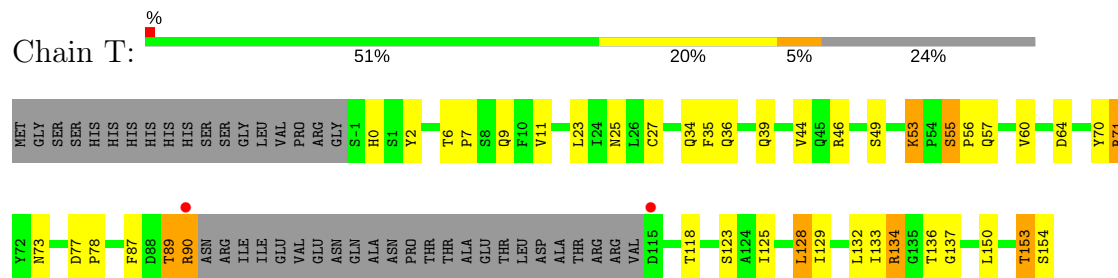
● Molecule 1: Capsid protein



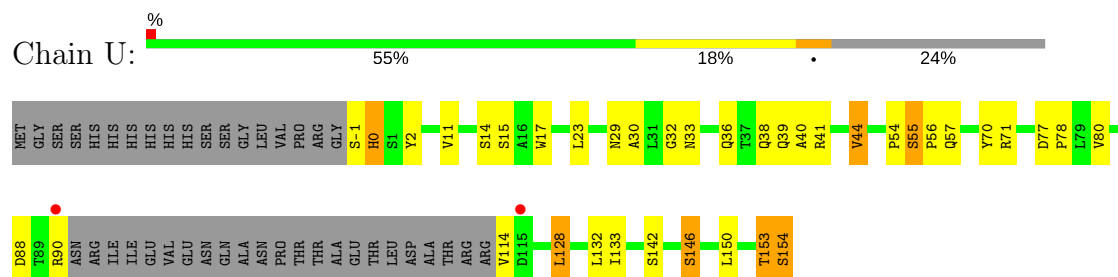
- Molecule 1: Capsid protein



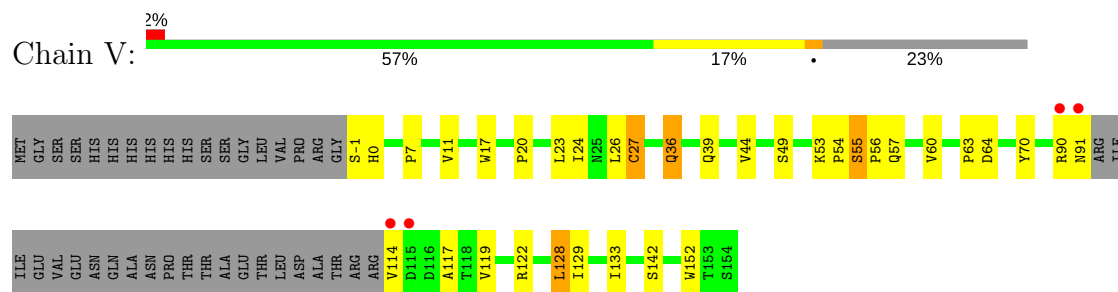
- Molecule 1: Capsid protein



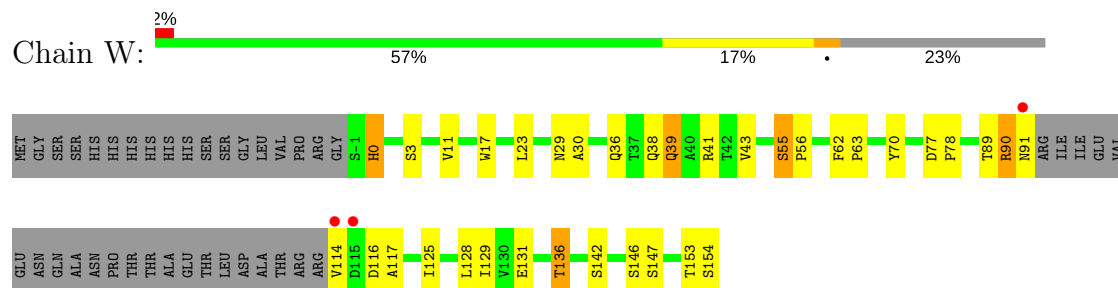
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



ILE	ILE	GLU	VAL	GLU	ASN	GLN	ALA	ASN	PRO	THR	THR	ALA	GLU	THR	LEU	ASP	ALA	THR	ARG	ARG	VAL	D115	I126	M126	M127	I128	I129	S146	I150	V151	M152	T153	S154															
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	ASN	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	S-1	H0	S1	Y2	P7	V11	W17	A18	D19	E22	L23	G32	Q36	T37	Q38	Q39	A40	R41	S49	K53	P54	S55	P56	Y70	D77	P78	D88	T89	ASN	ARG	ASP

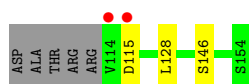
ASN	PRO	THR	THR	ALA	GLU	THR	LEU	ASP	ALA	THR	ARG	ARG	V114	D115	S123	L128	I133	S138	R141	S142	S143	S146	S147	T153	S154																					
GLY	SER	SER	ALA	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	S-1	H0	T6	L23	L26	N29	A30	L31	G32	Q36	Q39	V44	S49	P54	S55	P56	D64	F87	D88	T89	ASN	ASN	ARG	ILE	ILE	GLU	VAL	GLU	ASN	GLN	ALA

[illegible]

Metabolite	Pathway	Value
MET		
GLY		
SER		
HIS		
HIS		
HIS		
HIS		
HIS		
SER		
SER		
GLY		
LEU		
VAL		
PRO		
ARG		
GLY		
SER		
HO		
T6		
\$15		
L23		
L26		
Q39		
V44		
E50		
\$85		
D64		
L76		
T89		
ARG		
ASN		
ARG		
ILE		
ILE		
GLU		
VAL		
ASN		
GLN		
ALA		
ASN		
PRO		
THR		
THR		
ALA		
GLU		
THR		

Metabolite	Pathway	Value
LEU		
ASP		
ALA		
THR		
ARG		
ARG		
V114		
D115		
D116		
L128		
\$154		

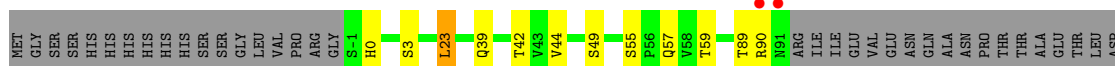
MET	GLY	SER	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	ARG	PRO	GLY	S-1	H0	S14	L23	Q36	Q39	V44	S49	S55	V58	T59	D64	T69	ARG	ASN	ARG	ARG	ILE	ILE	GLU	GLU	VAL	GLU	GLU	ASN	GLN	GLN	ALA	ALA	ASN	PRO	THR	THR	ALA	GLU	THR	THR	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



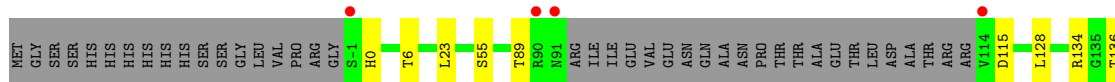
● Molecule 1: Capsid protein



● Molecule 1: Capsid protein



● Molecule 1: Capsid protein

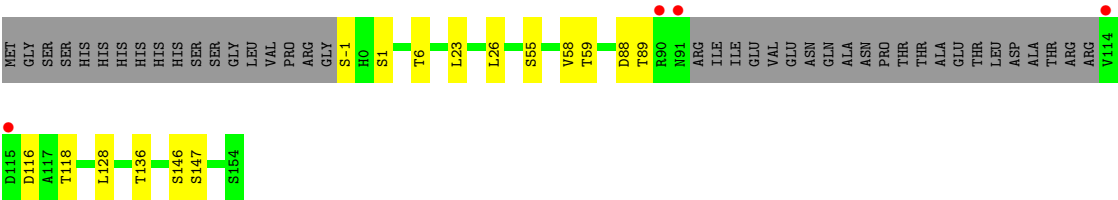


● Molecule 1: Capsid protein

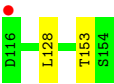


● Molecule 1: Capsid protein





● Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.07Å 221.68Å 225.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.06 49.91 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.06) 99.7 (49.91-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.255 0.202 , 0.252	Depositor DCC
R_{free} test set	8195 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 17.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	36918	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.64	0/1138	0.72	0/1552
1	B	0.62	0/1119	0.70	0/1526
1	C	0.67	0/1155	0.74	0/1576
1	D	0.65	0/1149	0.74	0/1566
1	E	0.64	0/1123	0.75	0/1531
1	F	0.63	0/1154	0.69	0/1573
1	G	0.63	0/1154	0.73	0/1573
1	H	0.61	0/1158	0.71	0/1578
1	I	0.58	0/1134	0.71	0/1547
1	J	0.61	0/1166	0.69	0/1590
1	K	0.66	0/1154	0.73	0/1573
1	L	0.62	0/1134	0.76	1/1547 (0.1%)
1	M	0.65	0/1145	0.71	0/1561
1	N	0.59	0/1145	0.70	0/1561
1	O	0.64	1/1123 (0.1%)	0.70	0/1531
1	P	0.65	0/1181	0.69	0/1611
1	Q	0.65	1/1173 (0.1%)	0.72	1/1600 (0.1%)
1	R	0.67	0/1069	0.73	0/1459
1	S	0.65	0/1069	0.74	0/1459
1	T	0.64	0/1062	0.73	1/1449 (0.1%)
1	U	0.61	0/1069	0.67	0/1459
1	V	0.69	1/1077 (0.1%)	0.78	1/1470 (0.1%)
1	W	0.65	0/1077	0.72	0/1470
1	X	0.63	0/1051	0.71	0/1435
1	Y	0.66	0/1058	0.72	0/1445
1	Z	0.64	0/1077	0.72	0/1470
1	a	0.61	0/1052	0.69	0/1437
1	b	0.63	0/1058	0.73	0/1445
1	c	0.67	1/1092 (0.1%)	0.73	0/1489
1	d	0.70	0/1077	0.79	1/1470 (0.1%)
1	e	0.65	0/1077	0.73	0/1470
1	f	0.66	0/1077	0.75	0/1470
1	h	0.61	0/1077	0.75	0/1470
1	i	0.68	0/1077	0.74	0/1470

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.64	4/37701 (0.0%)	0.72	5/51433 (0.0%)

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	L	0	1
1	d	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	27	CYS	CB-SG	-6.52	1.71	1.82
1	Q	103	THR	CB-OG1	5.65	1.54	1.43
1	O	50	GLU	CG-CD	5.38	1.60	1.51
1	c	27	CYS	CB-SG	-5.08	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	71	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	d	23	LEU	CA-CB-CG	5.63	128.24	115.30
1	L	152	TRP	C-N-CA	5.45	135.32	121.70
1	V	128	LEU	CA-CB-CG	5.28	127.45	115.30
1	Q	61	ARG	NE-CZ-NH1	-5.17	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	152	TRP	Peptide
1	d	153	THR	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	1115	0	1092	32	0
1	B	1096	0	1071	45	0
1	C	1132	0	1107	43	0
1	D	1126	0	1105	41	0
1	E	1100	0	1074	46	0
1	F	1131	0	1108	39	0
1	G	1131	0	1117	30	0
1	H	1135	0	1111	52	0
1	I	1111	0	1089	39	0
1	J	1143	0	1120	19	0
1	K	1131	0	1108	27	0
1	L	1111	0	1089	25	0
1	M	1122	0	1102	27	0
1	N	1122	0	1102	33	0
1	O	1100	0	1074	21	0
1	P	1157	0	1135	29	0
1	Q	1150	0	1127	17	0
1	R	1046	0	1023	27	0
1	S	1046	0	1023	31	0
1	T	1039	0	1014	35	0
1	U	1046	0	1023	33	0
1	V	1054	0	1029	28	0
1	W	1054	0	1029	24	0
1	X	1028	0	1001	23	0
1	Y	1035	0	1010	16	0
1	Z	1054	0	1029	39	0
1	a	1029	0	1005	0	0
1	b	1035	0	1010	0	0
1	c	1069	0	1045	0	0
1	d	1054	0	1029	0	0
1	e	1054	0	1029	0	0
1	f	1054	0	1029	0	0
1	h	1054	0	1029	0	0
1	i	1054	0	1029	0	0
All	All	36918	0	36117	697	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 10.

The worst 5 of 697 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:Q:27:CYS:HB3	1:Q:129:ILE:HD11	1.27	1.15
1:E:27:CYS:HB3	1:E:129:ILE:HD11	1.19	1.14
1:H:27:CYS:HB3	1:H:129:ILE:HD11	1.31	1.12
1:E:0:HIS:HB3	1:E:153:THR:O	4.61	1.11
1:T:36:GLN:HB2	1:U:90:ARG:HD2	1.32	1.09

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	138/174 (79%)	129 (94%)	7 (5%)	2 (1%)	13	43
1	B	135/174 (78%)	129 (96%)	5 (4%)	1 (1%)	25	61
1	C	140/174 (80%)	130 (93%)	9 (6%)	1 (1%)	25	61
1	D	139/174 (80%)	128 (92%)	10 (7%)	1 (1%)	25	61
1	E	136/174 (78%)	126 (93%)	7 (5%)	3 (2%)	8	31
1	F	139/174 (80%)	127 (91%)	10 (7%)	2 (1%)	13	43
1	G	139/174 (80%)	129 (93%)	8 (6%)	2 (1%)	13	43
1	H	140/174 (80%)	126 (90%)	10 (7%)	4 (3%)	5	25
1	I	137/174 (79%)	121 (88%)	11 (8%)	5 (4%)	4	20
1	J	141/174 (81%)	129 (92%)	11 (8%)	1 (1%)	25	61
1	K	139/174 (80%)	128 (92%)	9 (6%)	2 (1%)	13	43
1	L	137/174 (79%)	128 (93%)	7 (5%)	2 (2%)	12	42
1	M	138/174 (79%)	131 (95%)	4 (3%)	3 (2%)	8	31
1	N	138/174 (79%)	129 (94%)	8 (6%)	1 (1%)	25	61
1	O	136/174 (78%)	127 (93%)	7 (5%)	2 (2%)	12	42
1	P	143/174 (82%)	131 (92%)	8 (6%)	4 (3%)	6	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	142/174 (82%)	132 (93%)	7 (5%)	3 (2%)	8	32
1	R	129/174 (74%)	122 (95%)	5 (4%)	2 (2%)	11	40
1	S	129/174 (74%)	121 (94%)	6 (5%)	2 (2%)	11	40
1	T	128/174 (74%)	122 (95%)	5 (4%)	1 (1%)	22	58
1	U	129/174 (74%)	118 (92%)	9 (7%)	2 (2%)	11	40
1	V	130/174 (75%)	122 (94%)	6 (5%)	2 (2%)	12	42
1	W	130/174 (75%)	119 (92%)	10 (8%)	1 (1%)	22	58
1	X	127/174 (73%)	117 (92%)	9 (7%)	1 (1%)	22	58
1	Y	128/174 (74%)	118 (92%)	9 (7%)	1 (1%)	22	58
1	Z	130/174 (75%)	123 (95%)	6 (5%)	1 (1%)	22	58
1	a	127/174 (73%)	117 (92%)	8 (6%)	2 (2%)	11	40
1	b	128/174 (74%)	115 (90%)	10 (8%)	3 (2%)	7	30
1	c	132/174 (76%)	120 (91%)	9 (7%)	3 (2%)	7	30
1	d	130/174 (75%)	119 (92%)	10 (8%)	1 (1%)	22	58
1	e	130/174 (75%)	116 (89%)	13 (10%)	1 (1%)	22	58
1	f	130/174 (75%)	121 (93%)	8 (6%)	1 (1%)	22	58
1	h	130/174 (75%)	122 (94%)	6 (5%)	2 (2%)	12	42
1	i	130/174 (75%)	116 (89%)	11 (8%)	3 (2%)	7	30
All	All	4554/5916 (77%)	4208 (92%)	278 (6%)	68 (2%)	12	42

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	G	55	SER
1	I	1	SER
1	L	153	THR
1	M	0	HIS

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 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	125/153 (82%)	115 (92%)	10 (8%)	14	44
1	B	123/153 (80%)	111 (90%)	12 (10%)	9	32
1	C	127/153 (83%)	118 (93%)	9 (7%)	17	49
1	D	126/153 (82%)	112 (89%)	14 (11%)	7	26
1	E	123/153 (80%)	109 (89%)	14 (11%)	7	24
1	F	127/153 (83%)	114 (90%)	13 (10%)	8	29
1	G	127/153 (83%)	110 (87%)	17 (13%)	4	17
1	H	127/153 (83%)	108 (85%)	19 (15%)	3	13
1	I	125/153 (82%)	111 (89%)	14 (11%)	7	26
1	J	128/153 (84%)	118 (92%)	10 (8%)	15	45
1	K	127/153 (83%)	113 (89%)	14 (11%)	7	27
1	L	125/153 (82%)	114 (91%)	11 (9%)	12	39
1	M	126/153 (82%)	114 (90%)	12 (10%)	10	34
1	N	126/153 (82%)	115 (91%)	11 (9%)	12	40
1	O	123/153 (80%)	113 (92%)	10 (8%)	14	42
1	P	130/153 (85%)	120 (92%)	10 (8%)	15	45
1	Q	129/153 (84%)	116 (90%)	13 (10%)	9	30
1	R	118/153 (77%)	103 (87%)	15 (13%)	5	19
1	S	118/153 (77%)	110 (93%)	8 (7%)	18	50
1	T	117/153 (76%)	102 (87%)	15 (13%)	5	19
1	U	118/153 (77%)	109 (92%)	9 (8%)	15	46
1	V	119/153 (78%)	110 (92%)	9 (8%)	15	46
1	W	119/153 (78%)	110 (92%)	9 (8%)	15	46
1	X	116/153 (76%)	108 (93%)	8 (7%)	18	50
1	Y	117/153 (76%)	103 (88%)	14 (12%)	6	21
1	Z	119/153 (78%)	105 (88%)	14 (12%)	6	22
1	a	116/153 (76%)	105 (90%)	11 (10%)	10	34
1	b	117/153 (76%)	106 (91%)	11 (9%)	10	35
1	c	120/153 (78%)	110 (92%)	10 (8%)	13	42
1	d	119/153 (78%)	102 (86%)	17 (14%)	4	15
1	e	119/153 (78%)	109 (92%)	10 (8%)	13	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	119/153 (78%)	107 (90%)	12 (10%)	9	30
1	h	119/153 (78%)	105 (88%)	14 (12%)	6	22
1	i	119/153 (78%)	110 (92%)	9 (8%)	15	46
All	All	4153/5202 (80%)	3745 (90%)	408 (10%)	9	32

5 of 408 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	44	VAL
1	S	6	THR
1	f	39	GLN
1	O	153	THR
1	Q	91	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	38	GLN
1	U	34	GLN
1	h	0	HIS
1	P	126	ASN
1	R	38	GLN

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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	142/174 (81%)	-0.29	6 (4%) 37 18	35, 41, 84, 113	0
1	B	139/174 (79%)	-0.36	4 (2%) 52 27	34, 41, 76, 107	0
1	C	144/174 (82%)	-0.18	10 (6%) 18 7	33, 41, 105, 128	0
1	D	143/174 (82%)	-0.23	8 (5%) 25 11	31, 40, 87, 111	0
1	E	140/174 (80%)	-0.30	5 (3%) 43 21	33, 40, 80, 108	0
1	F	143/174 (82%)	-0.20	8 (5%) 25 11	35, 44, 92, 121	0
1	G	143/174 (82%)	-0.20	10 (6%) 17 6	36, 42, 101, 117	0
1	H	144/174 (82%)	-0.23	7 (4%) 30 14	35, 45, 93, 116	0
1	I	141/174 (81%)	-0.32	7 (4%) 30 13	35, 44, 88, 114	0
1	J	145/174 (83%)	-0.15	10 (6%) 18 7	34, 44, 105, 124	0
1	K	143/174 (82%)	-0.22	8 (5%) 25 11	32, 40, 90, 116	0
1	L	141/174 (81%)	-0.26	6 (4%) 36 17	35, 43, 84, 112	0
1	M	142/174 (81%)	-0.30	7 (4%) 30 14	34, 43, 90, 112	0
1	N	142/174 (81%)	-0.24	6 (4%) 37 18	35, 44, 88, 106	0
1	O	140/174 (80%)	-0.33	4 (2%) 52 27	37, 45, 79, 107	0
1	P	147/174 (84%)	-0.13	12 (8%) 12 5	36, 45, 114, 130	0
1	Q	146/174 (83%)	-0.16	10 (6%) 18 7	36, 44, 110, 129	0
1	R	133/174 (76%)	-0.47	3 (2%) 61 37	32, 40, 65, 86	0
1	S	133/174 (76%)	-0.47	3 (2%) 61 37	33, 42, 63, 87	0
1	T	132/174 (75%)	-0.36	2 (1%) 74 52	36, 44, 62, 83	0
1	U	133/174 (76%)	-0.35	2 (1%) 74 52	36, 47, 69, 89	0
1	V	134/174 (77%)	-0.39	4 (2%) 51 26	29, 40, 65, 86	0
1	W	134/174 (77%)	-0.37	3 (2%) 62 39	35, 42, 67, 88	0
1	X	131/174 (75%)	-0.40	2 (1%) 74 52	36, 44, 59, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	132/174 (75%)	-0.40	2 (1%) 74 52	33, 43, 61, 85	0
1	Z	134/174 (77%)	-0.46	3 (2%) 62 39	34, 42, 69, 87	0
1	a	131/174 (75%)	-0.38	2 (1%) 74 52	37, 47, 64, 89	0
1	b	132/174 (75%)	-0.38	3 (2%) 61 37	37, 47, 67, 83	0
1	c	136/174 (78%)	-0.36	4 (2%) 52 27	36, 45, 76, 95	0
1	d	134/174 (77%)	-0.44	3 (2%) 62 39	30, 41, 68, 85	0
1	e	134/174 (77%)	-0.33	4 (2%) 51 26	37, 46, 68, 88	0
1	f	134/174 (77%)	-0.45	3 (2%) 62 39	30, 41, 65, 84	0
1	h	134/174 (77%)	-0.43	4 (2%) 51 26	35, 45, 69, 89	0
1	i	134/174 (77%)	-0.33	3 (2%) 62 39	34, 43, 68, 86	0
All	All	4690/5916 (79%)	-0.32	178 (3%) 41 20	29, 43, 82, 130	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	109	ASP	7.5
1	L	107	THR	7.4
1	Q	104	THR	6.9
1	A	107	THR	6.5
1	N	107	THR	6.3

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.