



Full wwPDB EM Validation Report ⓘ

Jun 30, 2026 – 06:51 PM EDT

PDB ID : 9MKB / pdb_00009mkb
EMDB ID : EMD-48324
Title : Structure of the bacteriophage T4 portal-neck-tail complex
Authors : Fokine, A.; Zhu, J.; Klose, T.; Vago, F.; Arnaud, C.; Wang, Z.; Khare, B.;
Rossmann, M.G.; Chen, Z.; Sun, L.; Fang, Q.; Kuhn, R.; Rao, V.B.
Deposited on : 2024-12-17
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
MolProbity : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

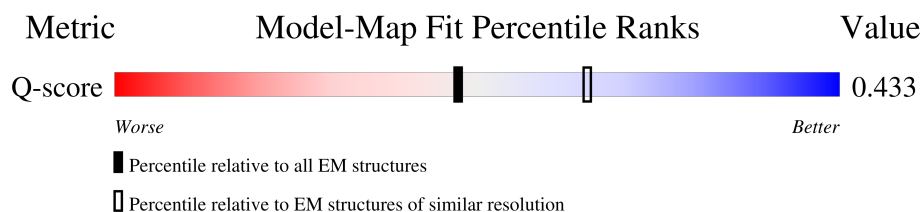
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	10198 (3.30 - 4.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 1533268 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 gp14, neck protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	k	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	l	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	m	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	n	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	p	244	Total 1993	C 1279	N 323	O 387	S 4	0	0

- Molecule 2 is a protein called gp18, tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	2	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	3	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	4	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	5	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	AD	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	AK	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	AL	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	AM	655	Total 5000	C 3152	N 841	O 996	S 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AN	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	AO	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	AP	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	B1	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	B2	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	B3	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	B4	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	B5	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	B6	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	B7	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bp	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bq	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Br	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bs	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bt	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bu	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bv	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bw	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bx	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	By	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Bz	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K0	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K1	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K2	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K3	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K4	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K5	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K6	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K7	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K8	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	K9	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L0	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L1	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L2	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L3	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L4	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L5	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L6	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L7	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L8	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	L9	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	LS	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	LU	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	LV	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	LW	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	LX	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	LY	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	LZ	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	La	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Lb	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Lc	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Ld	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Le	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Lx	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Lz	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M0	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M1	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M2	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M3	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M4	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M5	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M6	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M7	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M8	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	M9	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	MS	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	MU	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	MV	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	MW	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	MX	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	MY	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	MZ	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Ma	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Mb	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Mc	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Md	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Me	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Mx	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Mz	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	NX	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	NZ	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Na	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Nb	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Nc	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Nd	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Ne	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Nf	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Ng	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Nh	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Ni	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Nj	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Nx	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	Nz	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b0	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b3	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b4	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b5	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b6	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b7	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b8	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	b9	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	bN	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	bO	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	bP	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	bQ	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	bR	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	bY	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cA	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cB	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cC	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cD	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cE	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cF	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cG	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cH	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cI	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cJ	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cK	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cL	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cM	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cN	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cO	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	cP	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
2	dS	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
2	dT	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
2	dU	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	dV	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
2	dW	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
2	dZ	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		

There are 414 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	109	ASN	SER	conflict	UNP A0A7S9SVW9
1	301	GLY	GLU	conflict	UNP A0A7S9SVW9
1	399	VAL	ALA	conflict	UNP A0A7S9SVW9
2	109	ASN	SER	conflict	UNP A0A7S9SVW9
2	301	GLY	GLU	conflict	UNP A0A7S9SVW9
2	399	VAL	ALA	conflict	UNP A0A7S9SVW9
3	109	ASN	SER	conflict	UNP A0A7S9SVW9
3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
4	109	ASN	SER	conflict	UNP A0A7S9SVW9
4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
5	109	ASN	SER	conflict	UNP A0A7S9SVW9
5	301	GLY	GLU	conflict	UNP A0A7S9SVW9
5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AD	109	ASN	SER	conflict	UNP A0A7S9SVW9
AD	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AD	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AK	109	ASN	SER	conflict	UNP A0A7S9SVW9
AK	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AK	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AL	109	ASN	SER	conflict	UNP A0A7S9SVW9
AL	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AL	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AM	109	ASN	SER	conflict	UNP A0A7S9SVW9
AM	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AM	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AN	109	ASN	SER	conflict	UNP A0A7S9SVW9
AN	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AN	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AO	109	ASN	SER	conflict	UNP A0A7S9SVW9
AO	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AO	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AP	109	ASN	SER	conflict	UNP A0A7S9SVW9
AP	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AP	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B1	109	ASN	SER	conflict	UNP A0A7S9SVW9
B1	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B1	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B2	109	ASN	SER	conflict	UNP A0A7S9SVW9
B2	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B2	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B3	109	ASN	SER	conflict	UNP A0A7S9SVW9
B3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B4	109	ASN	SER	conflict	UNP A0A7S9SVW9
B4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B5	109	ASN	SER	conflict	UNP A0A7S9SVW9
B5	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B6	109	ASN	SER	conflict	UNP A0A7S9SVW9
B6	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B6	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B7	109	ASN	SER	conflict	UNP A0A7S9SVW9
B7	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B7	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bp	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bp	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bp	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bq	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bq	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bq	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Br	109	ASN	SER	conflict	UNP A0A7S9SVW9
Br	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Br	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bs	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bs	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bs	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bt	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bt	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bt	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bu	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bu	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bu	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bv	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bv	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bv	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bw	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bw	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bw	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bx	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bx	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bx	399	VAL	ALA	conflict	UNP A0A7S9SVW9
By	109	ASN	SER	conflict	UNP A0A7S9SVW9
By	301	GLY	GLU	conflict	UNP A0A7S9SVW9
By	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bz	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bz	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bz	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K0	109	ASN	SER	conflict	UNP A0A7S9SVW9
K0	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K0	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K1	109	ASN	SER	conflict	UNP A0A7S9SVW9
K1	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K1	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K2	109	ASN	SER	conflict	UNP A0A7S9SVW9
K2	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K2	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K3	109	ASN	SER	conflict	UNP A0A7S9SVW9
K3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K4	109	ASN	SER	conflict	UNP A0A7S9SVW9
K4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K5	109	ASN	SER	conflict	UNP A0A7S9SVW9
K5	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K6	109	ASN	SER	conflict	UNP A0A7S9SVW9
K6	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K6	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K7	109	ASN	SER	conflict	UNP A0A7S9SVW9
K7	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K7	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K8	109	ASN	SER	conflict	UNP A0A7S9SVW9
K8	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K8	399	VAL	ALA	conflict	UNP A0A7S9SVW9
K9	109	ASN	SER	conflict	UNP A0A7S9SVW9
K9	301	GLY	GLU	conflict	UNP A0A7S9SVW9
K9	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L0	109	ASN	SER	conflict	UNP A0A7S9SVW9
L0	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L0	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L1	109	ASN	SER	conflict	UNP A0A7S9SVW9
L1	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L1	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L2	109	ASN	SER	conflict	UNP A0A7S9SVW9
L2	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L2	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L3	109	ASN	SER	conflict	UNP A0A7S9SVW9
L3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L4	109	ASN	SER	conflict	UNP A0A7S9SVW9
L4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L5	109	ASN	SER	conflict	UNP A0A7S9SVW9
L5	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L6	109	ASN	SER	conflict	UNP A0A7S9SVW9
L6	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L6	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L7	109	ASN	SER	conflict	UNP A0A7S9SVW9
L7	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L7	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L8	109	ASN	SER	conflict	UNP A0A7S9SVW9
L8	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L8	399	VAL	ALA	conflict	UNP A0A7S9SVW9
L9	109	ASN	SER	conflict	UNP A0A7S9SVW9
L9	301	GLY	GLU	conflict	UNP A0A7S9SVW9
L9	399	VAL	ALA	conflict	UNP A0A7S9SVW9
LS	109	ASN	SER	conflict	UNP A0A7S9SVW9
LS	301	GLY	GLU	conflict	UNP A0A7S9SVW9
LS	399	VAL	ALA	conflict	UNP A0A7S9SVW9
LU	109	ASN	SER	conflict	UNP A0A7S9SVW9
LU	301	GLY	GLU	conflict	UNP A0A7S9SVW9
LU	399	VAL	ALA	conflict	UNP A0A7S9SVW9
LV	109	ASN	SER	conflict	UNP A0A7S9SVW9
LV	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LV	399	VAL	ALA	conflict	UNP A0A7S9SVW9
LW	109	ASN	SER	conflict	UNP A0A7S9SVW9
LW	301	GLY	GLU	conflict	UNP A0A7S9SVW9
LW	399	VAL	ALA	conflict	UNP A0A7S9SVW9
LX	109	ASN	SER	conflict	UNP A0A7S9SVW9
LX	301	GLY	GLU	conflict	UNP A0A7S9SVW9
LX	399	VAL	ALA	conflict	UNP A0A7S9SVW9
LY	109	ASN	SER	conflict	UNP A0A7S9SVW9
LY	301	GLY	GLU	conflict	UNP A0A7S9SVW9
LY	399	VAL	ALA	conflict	UNP A0A7S9SVW9
LZ	109	ASN	SER	conflict	UNP A0A7S9SVW9
LZ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
LZ	399	VAL	ALA	conflict	UNP A0A7S9SVW9
La	109	ASN	SER	conflict	UNP A0A7S9SVW9
La	301	GLY	GLU	conflict	UNP A0A7S9SVW9
La	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Lb	109	ASN	SER	conflict	UNP A0A7S9SVW9
Lb	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Lb	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Lc	109	ASN	SER	conflict	UNP A0A7S9SVW9
Lc	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Lc	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Ld	109	ASN	SER	conflict	UNP A0A7S9SVW9
Ld	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Ld	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Le	109	ASN	SER	conflict	UNP A0A7S9SVW9
Le	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Le	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Lx	109	ASN	SER	conflict	UNP A0A7S9SVW9
Lx	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Lx	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Lz	109	ASN	SER	conflict	UNP A0A7S9SVW9
Lz	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Lz	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M0	109	ASN	SER	conflict	UNP A0A7S9SVW9
M0	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M0	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M1	109	ASN	SER	conflict	UNP A0A7S9SVW9
M1	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M1	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M2	109	ASN	SER	conflict	UNP A0A7S9SVW9
M2	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M2	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M3	109	ASN	SER	conflict	UNP A0A7S9SVW9
M3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M4	109	ASN	SER	conflict	UNP A0A7S9SVW9
M4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M5	109	ASN	SER	conflict	UNP A0A7S9SVW9
M5	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M6	109	ASN	SER	conflict	UNP A0A7S9SVW9
M6	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M6	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M7	109	ASN	SER	conflict	UNP A0A7S9SVW9
M7	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M7	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M8	109	ASN	SER	conflict	UNP A0A7S9SVW9
M8	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M8	399	VAL	ALA	conflict	UNP A0A7S9SVW9
M9	109	ASN	SER	conflict	UNP A0A7S9SVW9
M9	301	GLY	GLU	conflict	UNP A0A7S9SVW9
M9	399	VAL	ALA	conflict	UNP A0A7S9SVW9
MS	109	ASN	SER	conflict	UNP A0A7S9SVW9
MS	301	GLY	GLU	conflict	UNP A0A7S9SVW9
MS	399	VAL	ALA	conflict	UNP A0A7S9SVW9
MU	109	ASN	SER	conflict	UNP A0A7S9SVW9
MU	301	GLY	GLU	conflict	UNP A0A7S9SVW9
MU	399	VAL	ALA	conflict	UNP A0A7S9SVW9
MV	109	ASN	SER	conflict	UNP A0A7S9SVW9
MV	301	GLY	GLU	conflict	UNP A0A7S9SVW9
MV	399	VAL	ALA	conflict	UNP A0A7S9SVW9
MW	109	ASN	SER	conflict	UNP A0A7S9SVW9
MW	301	GLY	GLU	conflict	UNP A0A7S9SVW9
MW	399	VAL	ALA	conflict	UNP A0A7S9SVW9
MX	109	ASN	SER	conflict	UNP A0A7S9SVW9
MX	301	GLY	GLU	conflict	UNP A0A7S9SVW9
MX	399	VAL	ALA	conflict	UNP A0A7S9SVW9
MY	109	ASN	SER	conflict	UNP A0A7S9SVW9
MY	301	GLY	GLU	conflict	UNP A0A7S9SVW9
MY	399	VAL	ALA	conflict	UNP A0A7S9SVW9
MZ	109	ASN	SER	conflict	UNP A0A7S9SVW9
MZ	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
MZ	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Ma	109	ASN	SER	conflict	UNP A0A7S9SVW9
Ma	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Ma	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Mb	109	ASN	SER	conflict	UNP A0A7S9SVW9
Mb	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Mb	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Mc	109	ASN	SER	conflict	UNP A0A7S9SVW9
Mc	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Mc	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Md	109	ASN	SER	conflict	UNP A0A7S9SVW9
Md	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Md	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Me	109	ASN	SER	conflict	UNP A0A7S9SVW9
Me	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Me	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Mx	109	ASN	SER	conflict	UNP A0A7S9SVW9
Mx	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Mx	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Mz	109	ASN	SER	conflict	UNP A0A7S9SVW9
Mz	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Mz	399	VAL	ALA	conflict	UNP A0A7S9SVW9
NX	109	ASN	SER	conflict	UNP A0A7S9SVW9
NX	301	GLY	GLU	conflict	UNP A0A7S9SVW9
NX	399	VAL	ALA	conflict	UNP A0A7S9SVW9
NZ	109	ASN	SER	conflict	UNP A0A7S9SVW9
NZ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
NZ	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Na	109	ASN	SER	conflict	UNP A0A7S9SVW9
Na	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Na	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nb	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nb	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nb	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nc	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nc	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nc	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nd	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nd	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nd	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Ne	109	ASN	SER	conflict	UNP A0A7S9SVW9
Ne	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Ne	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nf	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nf	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nf	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Ng	109	ASN	SER	conflict	UNP A0A7S9SVW9
Ng	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Ng	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nh	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nh	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nh	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Ni	109	ASN	SER	conflict	UNP A0A7S9SVW9
Ni	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Ni	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nj	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nj	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nj	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nx	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nx	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nx	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Nz	109	ASN	SER	conflict	UNP A0A7S9SVW9
Nz	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Nz	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b0	109	ASN	SER	conflict	UNP A0A7S9SVW9
b0	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b0	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b3	109	ASN	SER	conflict	UNP A0A7S9SVW9
b3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b4	109	ASN	SER	conflict	UNP A0A7S9SVW9
b4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b5	109	ASN	SER	conflict	UNP A0A7S9SVW9
b5	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b6	109	ASN	SER	conflict	UNP A0A7S9SVW9
b6	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b6	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b7	109	ASN	SER	conflict	UNP A0A7S9SVW9
b7	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b7	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b8	109	ASN	SER	conflict	UNP A0A7S9SVW9
b8	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b8	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b9	109	ASN	SER	conflict	UNP A0A7S9SVW9
b9	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b9	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bN	109	ASN	SER	conflict	UNP A0A7S9SVW9
bN	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bN	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bO	109	ASN	SER	conflict	UNP A0A7S9SVW9
bO	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bO	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bP	109	ASN	SER	conflict	UNP A0A7S9SVW9
bP	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bP	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bQ	109	ASN	SER	conflict	UNP A0A7S9SVW9
bQ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bQ	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bR	109	ASN	SER	conflict	UNP A0A7S9SVW9
bR	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bR	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bY	109	ASN	SER	conflict	UNP A0A7S9SVW9
bY	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bY	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cA	109	ASN	SER	conflict	UNP A0A7S9SVW9
cA	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cA	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cB	109	ASN	SER	conflict	UNP A0A7S9SVW9
cB	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cB	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cC	109	ASN	SER	conflict	UNP A0A7S9SVW9
cC	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cC	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cD	109	ASN	SER	conflict	UNP A0A7S9SVW9
cD	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cD	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cE	109	ASN	SER	conflict	UNP A0A7S9SVW9
cE	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cE	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cF	109	ASN	SER	conflict	UNP A0A7S9SVW9
cF	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cF	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cG	109	ASN	SER	conflict	UNP A0A7S9SVW9
cG	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
cG	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cH	109	ASN	SER	conflict	UNP A0A7S9SVW9
cH	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cH	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cI	109	ASN	SER	conflict	UNP A0A7S9SVW9
cI	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cI	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cJ	109	ASN	SER	conflict	UNP A0A7S9SVW9
cJ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cJ	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cK	109	ASN	SER	conflict	UNP A0A7S9SVW9
cK	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cK	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cL	109	ASN	SER	conflict	UNP A0A7S9SVW9
cL	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cL	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cM	109	ASN	SER	conflict	UNP A0A7S9SVW9
cM	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cM	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cN	109	ASN	SER	conflict	UNP A0A7S9SVW9
cN	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cN	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cO	109	ASN	SER	conflict	UNP A0A7S9SVW9
cO	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cO	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cP	109	ASN	SER	conflict	UNP A0A7S9SVW9
cP	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cP	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dS	109	ASN	SER	conflict	UNP A0A7S9SVW9
dS	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dS	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dT	109	ASN	SER	conflict	UNP A0A7S9SVW9
dT	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dT	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dU	109	ASN	SER	conflict	UNP A0A7S9SVW9
dU	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dU	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dV	109	ASN	SER	conflict	UNP A0A7S9SVW9
dV	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dV	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dW	109	ASN	SER	conflict	UNP A0A7S9SVW9
dW	301	GLY	GLU	conflict	UNP A0A7S9SVW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
dW	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dZ	109	ASN	SER	conflict	UNP A0A7S9SVW9
dZ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dZ	399	VAL	ALA	conflict	UNP A0A7S9SVW9

- Molecule 3 is a protein called gp19, tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	7	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	8	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	9	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	AA	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	AE	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AF	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AG	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AH	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AI	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AJ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	BX	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	BY	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	BZ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Ba	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bb	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bc	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Bd	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Be	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bf	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bg	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bh	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bi	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bj	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bk	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bl	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bm	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bn	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bo	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OE	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OF	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OG	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OH	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OI	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OJ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OK	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OL	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OM	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	ON	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	OO	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Oj	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Ok	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Ol	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Om	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	On	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Oo	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Op	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Oq	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Or	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Os	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Ot	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PE	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PF	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PG	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PH	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PI	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PJ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PK	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PL	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	PM	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PN	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	PO	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pj	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pk	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pl	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pm	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pn	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Po	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pp	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pq	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pr	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Ps	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Pt	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RE	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RF	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RG	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RH	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RI	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RJ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RK	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	RL	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RM	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RN	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RO	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	RT	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rk	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rl	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rm	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rn	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Ro	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rp	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rq	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rr	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rs	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Rt	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	h1	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	h2	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hI	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hJ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hK	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hL	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	hM	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hX	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	he	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hf	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hg	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hh	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hi	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hj	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hk	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hl	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hm	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hn	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	ho	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hp	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hq	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hr	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hs	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	ht	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hu	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hv	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hw	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	hx	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hy	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	hz	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	o	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		

- Molecule 4 is a protein called gpwac, fibrinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	B	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	C	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	D	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	E	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	F	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	G	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	H	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	I	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	J	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	K	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	L	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	M	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	N	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	O	79	Total	C	N	O	S	0	0
			601	373	102	125	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	Q	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	R	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	S	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	T	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	U	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	V	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	W	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	X	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	Y	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	Z	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	a	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	b	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	c	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	d	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	e	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	f	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	g	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	h	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	i	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	j	79	Total 601	C 373	N 102	O 125	S 1	0	0

- Molecule 5 is a protein called gp20, portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A0	507	Total	C	N	O	S	0	0
			4140	2611	717	790	22		
5	A1	507	Total	C	N	O	S	0	0
			4140	2611	717	790	22		
5	A2	506	Total	C	N	O	S	0	0
			4132	2607	715	788	22		
5	A3	506	Total	C	N	O	S	0	0
			4132	2607	715	788	22		
5	Av	506	Total	C	N	O	S	0	0
			4132	2607	715	788	22		
5	Ax	506	Total	C	N	O	S	0	0
			4132	2607	715	788	22		
5	BA	500	Total	C	N	O	S	0	0
			4074	2571	707	776	20		
5	BB	488	Total	C	N	O	S	0	0
			3995	2517	695	761	22		
5	BD	506	Total	C	N	O	S	0	0
			4132	2607	715	788	22		
5	BF	506	Total	C	N	O	S	0	0
			4132	2607	715	788	22		
5	BG	497	Total	C	N	O	S	0	0
			4039	2549	702	768	20		
5	BH	506	Total	C	N	O	S	0	0
			4091	2582	710	779	20		

- Molecule 6 is a protein called gp23, major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A4	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	A5	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	A7	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	A8	440	Total	C	N	O	S	0	0
			3311	2099	564	633	15		
6	A9	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	AV	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	AW	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AX	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	AZ	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ac	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ad	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ae	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Af	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ag	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ah	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ai	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Aj	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ak	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Am	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	An	440	Total	C	N	O	S	0	0
			3311	2099	564	633	15		
6	Ao	437	Total	C	N	O	S	0	0
			3291	2088	560	628	15		
6	Ap	440	Total	C	N	O	S	0	0
			3311	2099	564	633	15		
6	Au	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Aw	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ay	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Az	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	BI	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	BJ	437	Total	C	N	O	S	0	0
			3291	2088	560	628	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BK	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	BM	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

- Molecule 7 is a protein called gp13, neck protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	AY	308	Total	C	N	O	S	0	0
			2435	1550	412	460	13		
7	Aa	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	Ab	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	Al	308	Total	C	N	O	S	0	0
			2435	1550	412	460	13		
7	Aq	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	Ar	290	Total	C	N	O	S	0	0
			2310	1473	389	437	11		
7	As	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	At	298	Total	C	N	O	S	0	0
			2371	1512	402	445	12		
7	BC	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	BE	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	BL	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		

- Molecule 8 is a protein called gp15, tail terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AB	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	q	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	r	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	s	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	t	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	u	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		

- Molecule 9 is a protein called gp3, tube terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AC	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	v	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	w	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	x	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	y	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	z	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		

- Molecule 10 is a protein called Hoc, highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AQ	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AR	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AS	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AT	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AU	96	Total	C	N	O	S	0	0
			805	519	129	152	5		

- Molecule 11 is a protein called Soc, small outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	BN	79	Total	C	N	O	0	0
			636	405	106	125		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
11	BO	79	Total 636	C 405	N 106	O 125	0	0
11	BP	79	Total 636	C 405	N 106	O 125	0	0
11	BQ	79	Total 636	C 405	N 106	O 125	0	0
11	BR	79	Total 636	C 405	N 106	O 125	0	0
11	BS	79	Total 636	C 405	N 106	O 125	0	0
11	BT	79	Total 636	C 405	N 106	O 125	0	0
11	BU	79	Total 636	C 405	N 106	O 125	0	0
11	BV	79	Total 636	C 405	N 106	O 125	0	0
11	BW	79	Total 636	C 405	N 106	O 125	0	0

- Molecule 12 is a protein called gp12, short tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S0	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S1	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S2	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S3	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S4	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S5	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S6	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S7	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	S8	526	Total 3945	C 2429	N 702	O 803	S 11	0	0
12	SA	526	Total 3945	C 2429	N 702	O 803	S 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SO	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
12	SP	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
12	SQ	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
12	Sv	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
12	Sw	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
12	Sx	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
12	Sy	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
12	Sz	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		

- Molecule 13 is a protein called gp9, baseplate wedge tail fiber connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T1	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T2	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T3	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T4	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T5	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T6	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T7	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T8	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	T9	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	TF	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	TG	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
13	TH	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	Td	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	Te	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	Tf	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	Tg	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	Th	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
13	Ti	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

- Molecule 14 is a protein called gp11, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UL	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	UM	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	UN	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Up	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Uq	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Ur	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Us	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Ut	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Uu	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	VL	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	VM	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	VN	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Vp	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Vq	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Vr	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Vs	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Vt	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
14	Vu	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

- Molecule 15 is a protein called gp10, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	WI	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	WJ	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	WK	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Wj	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Wk	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Wl	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Wm	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Wn	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Wo	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	XI	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	XJ	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	XK	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Xj	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Xk	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Xl	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Xm	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Xn	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
15	Xo	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		

- Molecule 16 is a protein called gp7, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	YC	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
16	YX	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
16	YY	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
16	Yc	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
16	Yx	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
16	Yy	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		

- Molecule 17 is a protein called gp8, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	ZD	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
17	ZE	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
17	ZZ	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
17	Za	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
17	Zb	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
17	Zc	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	aD	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
17	aE	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
17	aZ	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
17	aa	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
17	ab	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
17	ac	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		

- Molecule 18 is a protein called gp6, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	eB	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
18	eU	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
18	eW	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
18	f9	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
18	fA	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
18	fB	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
18	fR	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
18	fS	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
18	fU	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
18	fW	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
18	fr	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
18	fs	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		

- Molecule 19 is a protein called gp5, baseplate central spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	gE	559	Total	C	N	O	S	0	0
			4321	2681	761	856	23		
19	gG	559	Total	C	N	O	S	0	0
			4321	2681	761	856	23		
19	gH	559	Total	C	N	O	S	0	0
			4321	2681	761	856	23		

- Molecule 20 is a protein called gp5.4, tip of the central spike.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	gd	96	Total	C	N	O	S	0	0
			709	447	120	139	3		

- Molecule 21 is a protein called gp27, baseplate hub protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	iC	375	Total	C	N	O	S	0	0
			3000	1916	491	575	18		
21	iD	375	Total	C	N	O	S	0	0
			3000	1916	491	575	18		
21	iF	375	Total	C	N	O	S	0	0
			3000	1916	491	575	18		

- Molecule 22 is a protein called gp29, tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	ja	20	Total	C	N	O	S	0	0
			137	84	22	30	1		
22	jb	20	Total	C	N	O	S	0	0
			137	84	22	30	1		
22	jc	20	Total	C	N	O	S	0	0
			137	84	22	30	1		

- Molecule 23 is a protein called gp53, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	k3	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
23	k4	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
23	k7	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
23	k8	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
23	kV	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
23	lV	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		

- Molecule 24 is a protein called gp25, baseplate protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	m1	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
24	m2	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
24	m5	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
24	m6	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
24	mT	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
24	nT	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		

- Molecule 25 is a protein called gp48, baseplate protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	o0	358	Total	C	N	O	S	0	0
			2749	1714	467	559	9		
25	o1	314	Total	C	N	O	S	0	0
			2436	1523	414	491	8		
25	o2	314	Total	C	N	O	S	0	0
			2436	1523	414	491	8		
25	o6	314	Total	C	N	O	S	0	0
			2436	1523	414	491	8		
25	pA	358	Total	C	N	O	S	0	0
			2749	1714	467	559	9		
25	pB	358	Total	C	N	O	S	0	0
			2749	1714	467	559	9		

- Molecule 26 is a protein called gp54, baseplate protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	q3	207	Total	C	N	O	S	0	0
			1650	1037	280	321	12		
26	q4	207	Total	C	N	O	S	0	0
			1650	1037	280	321	12		
26	q5	213	Total	C	N	O	S	0	0
			1693	1064	287	330	12		
26	q7	213	Total	C	N	O	S	0	0
			1693	1064	287	330	12		
26	q8	207	Total	C	N	O	S	0	0
			1650	1037	280	321	12		
26	q9	213	Total	C	N	O	S	0	0
			1693	1064	287	330	12		

- Molecule 27 is a protein called unassigned peptide A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	rc	25	Total	C	N	O	0	0
			125	75	25	25		
27	rd	25	Total	C	N	O	0	0
			125	75	25	25		
27	re	25	Total	C	N	O	0	0
			125	75	25	25		
27	rf	25	Total	C	N	O	0	0
			125	75	25	25		
27	rg	25	Total	C	N	O	0	0
			125	75	25	25		
27	rh	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 28 is a protein called unassigned peptide B.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	sQ	18	Total	C	N	O	0	0
			90	54	18	18		
28	sT	18	Total	C	N	O	0	0
			90	54	18	18		
28	sU	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 29 is a protein called unassigned peptide C.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	tS	10	Total	C	N	O	0	0
			50	30	10	10		
29	tX	10	Total	C	N	O	0	0
			50	30	10	10		
29	tY	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 30 is a protein called unassigned peptide D.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	uR	7	Total	C	N	O	0	0
			35	21	7	7		
30	uV	7	Total	C	N	O	0	0
			35	21	7	7		
30	uW	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 31 is a protein called unassigned peptide E.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	vZ	9	Total	C	N	O	0	0
			45	27	9	9		
31	va	9	Total	C	N	O	0	0
			45	27	9	9		
31	vb	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	S0	1	Total	Zn	0
			1	1	
32	S1	1	Total	Zn	0
			1	1	
32	S4	1	Total	Zn	0
			1	1	
32	SA	1	Total	Zn	0
			1	1	
32	SQ	1	Total	Zn	0
			1	1	
32	Sv	1	Total	Zn	0
			1	1	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	659.328, 657.71204, 1664.4801	wwPDB
Map dimensions	408, 407, 1030	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.616, 1.616, 1.616	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

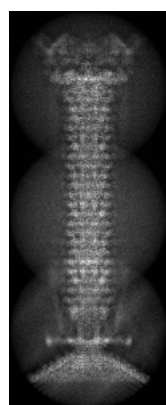
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48324. These allow visual inspection of the internal detail of the map and identification of artifacts.

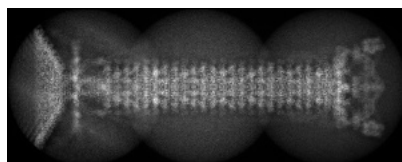
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

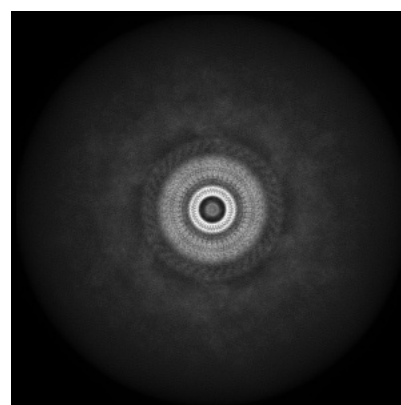
5.1.1 Primary map



X



Y



Z

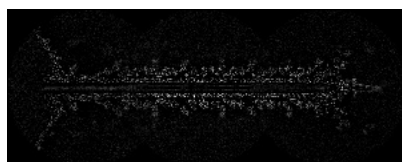
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

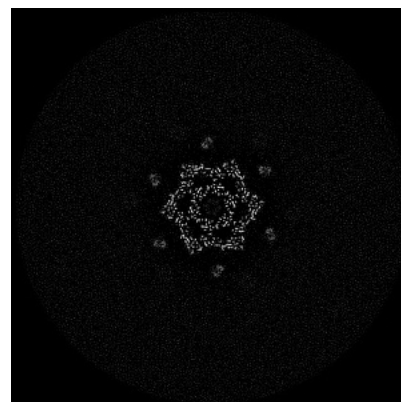
5.2.1 Primary map



X Index: 204



Y Index: 203

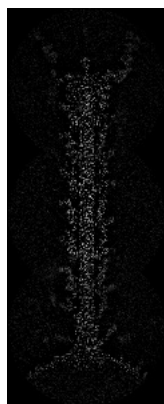


Z Index: 515

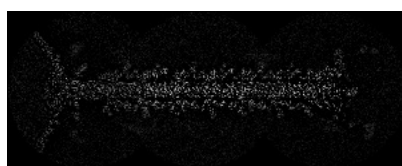
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

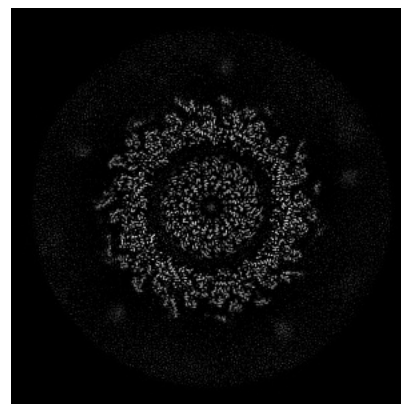
5.3.1 Primary map



X Index: 220



Y Index: 219

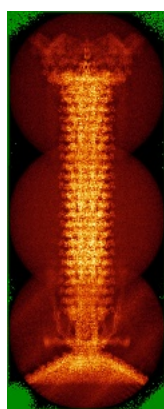


Z Index: 118

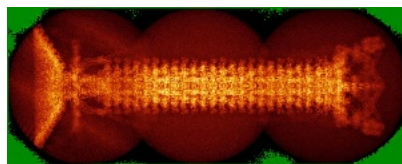
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

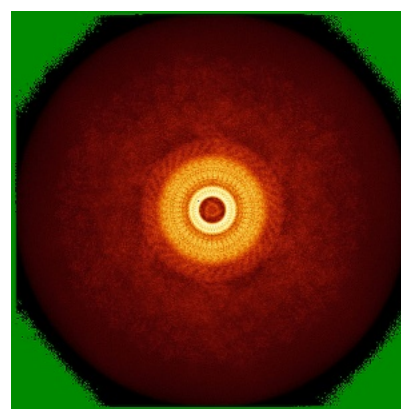
5.4.1 Primary map



X



Y

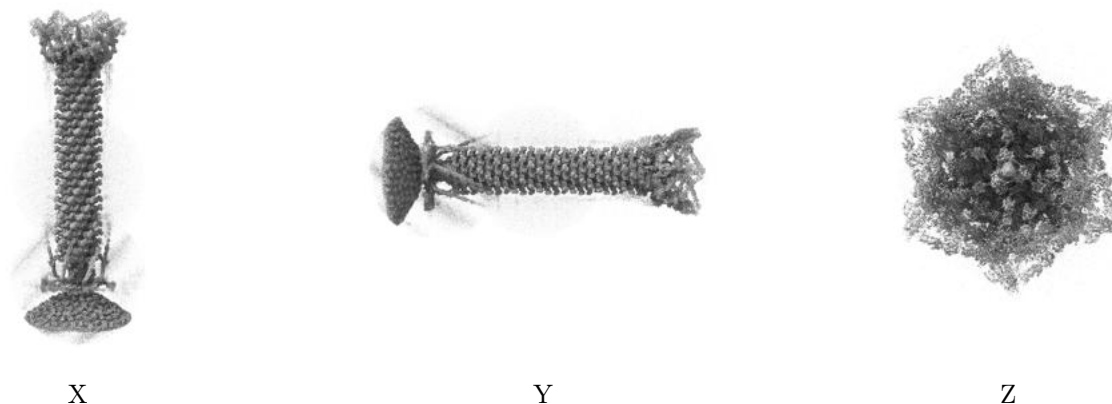


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

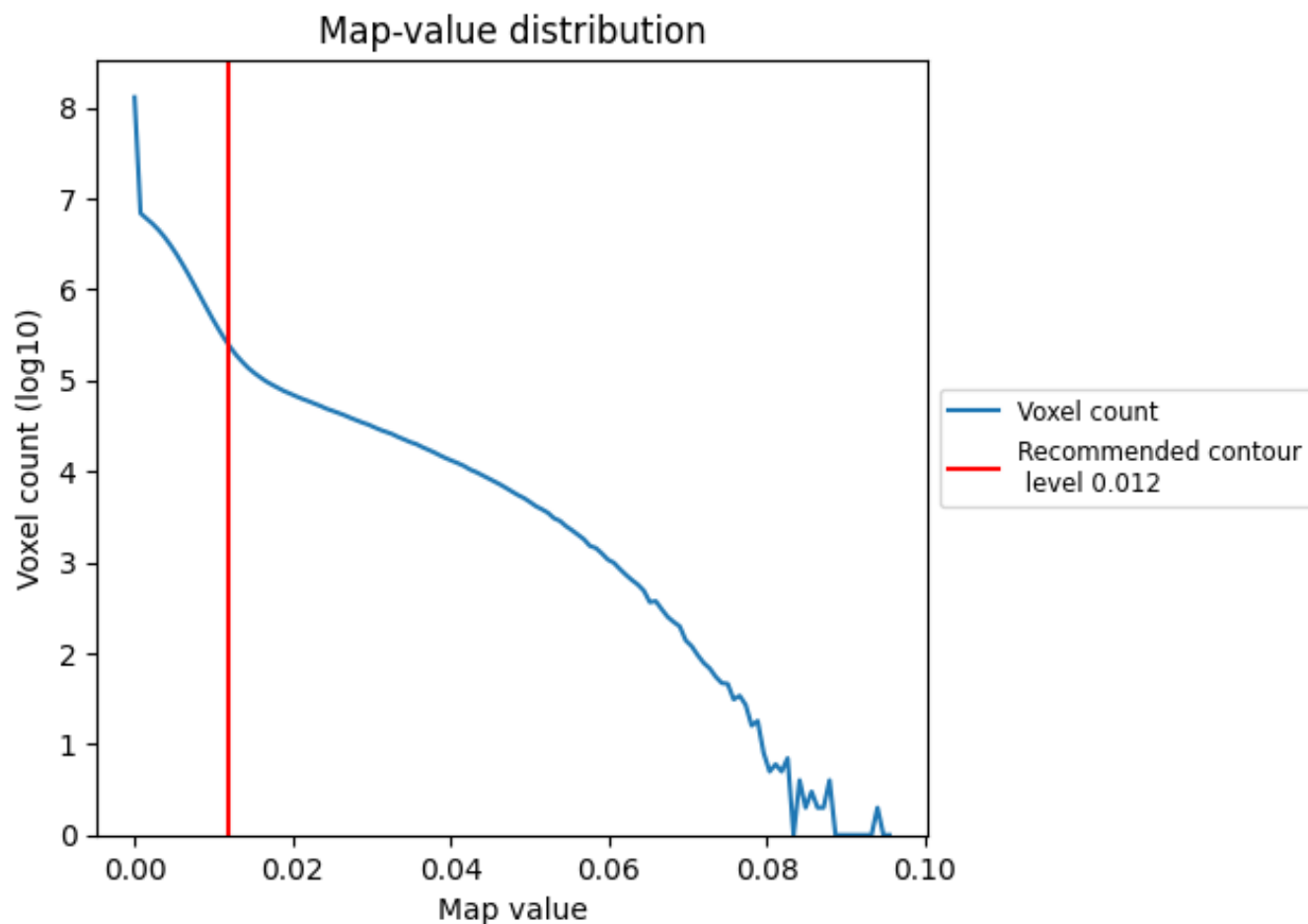
5.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

6 Map analysis [i](#)

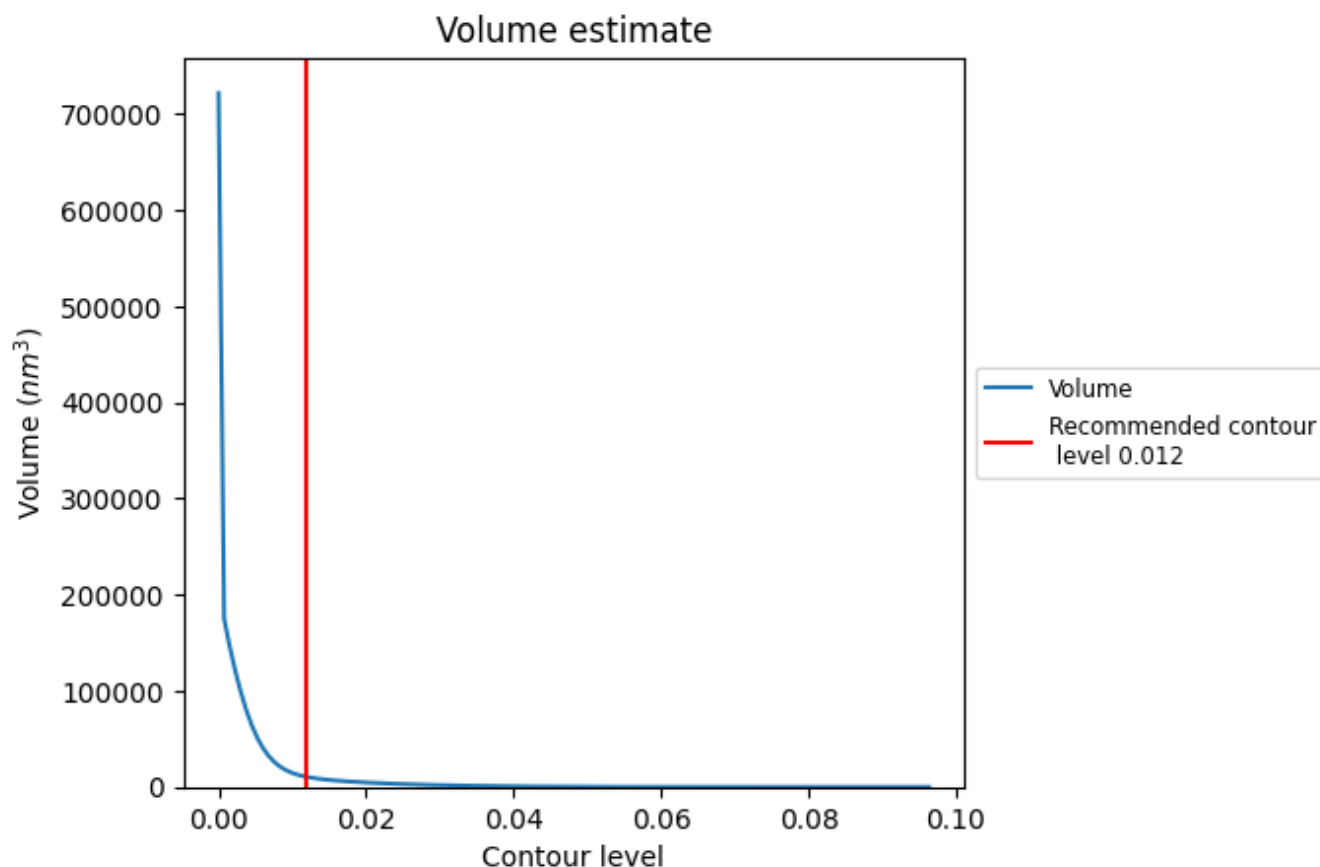
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

6.2 Volume estimate [i](#)



The volume at the recommended contour level is 10391 nm^3 ; this corresponds to an approximate mass of 9387 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

6.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

7 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

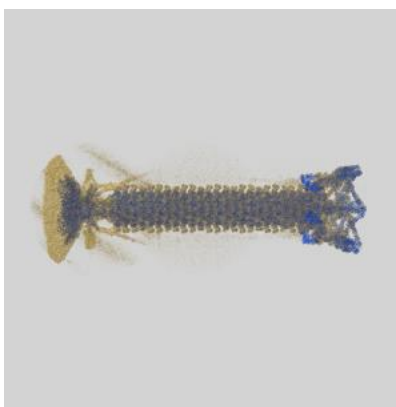
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48324 and PDB model 9MKB. Per-residue inclusion information can be found in section ?? on page ??.

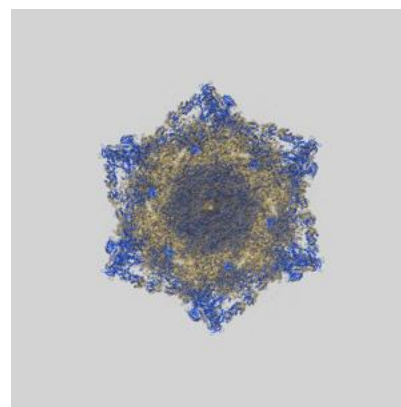
8.1 Map-model overlay [i](#)



X



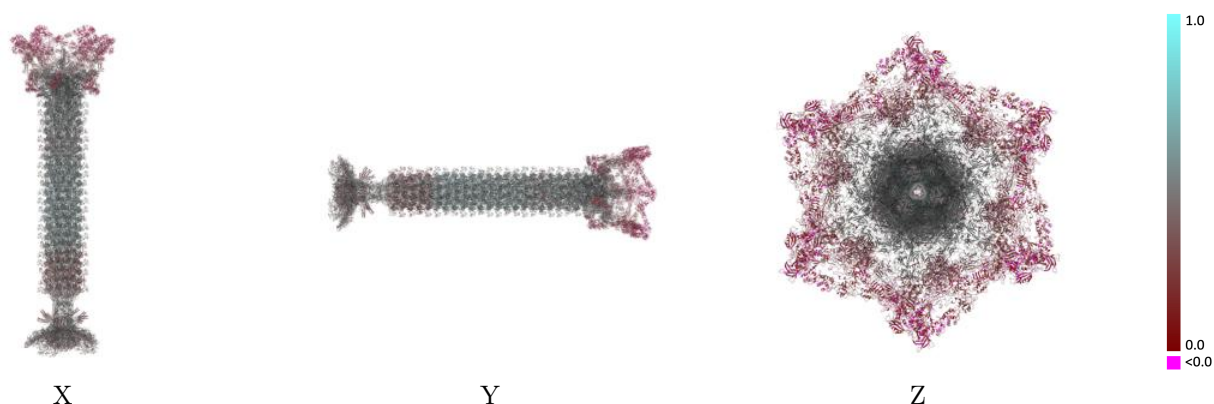
Y



Z

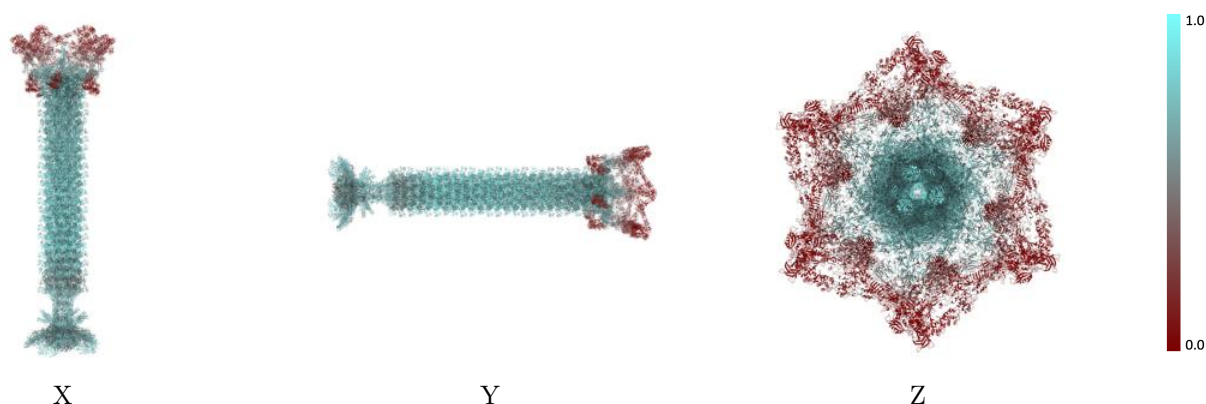
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

8.2 Q-score mapped to coordinate model [i](#)



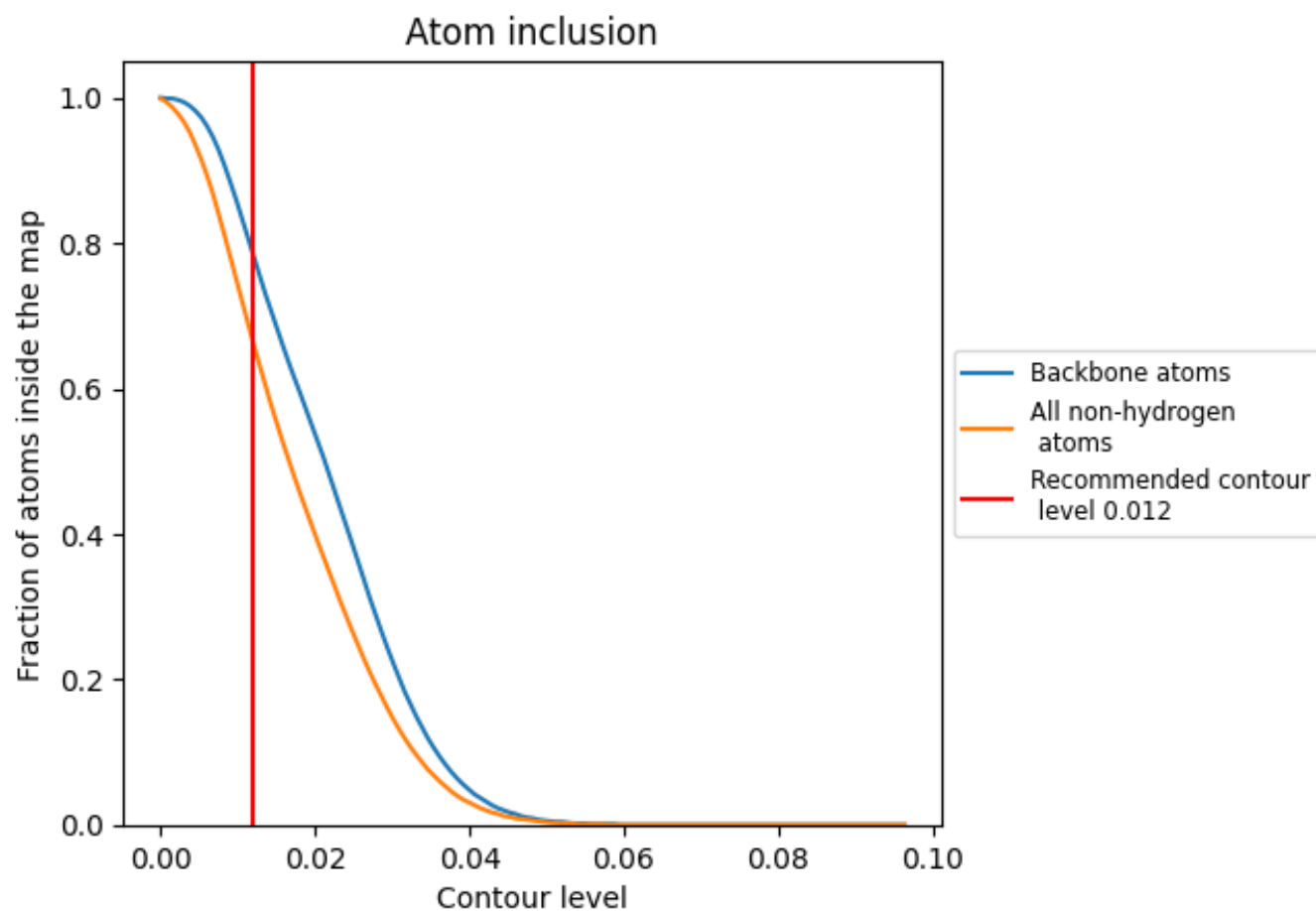
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

8.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.4330
0	 0.7580	 0.4680
1	 0.6620	 0.3990
2	 0.6610	 0.4030
3	 0.7210	 0.4150
4	 0.7010	 0.4100
5	 0.6770	 0.4050
6	 0.6710	 0.4490
7	 0.6910	 0.4510
8	 0.7240	 0.4560
9	 0.7110	 0.4610
A	 0.7030	 0.4060
A0	 0.4950	 0.4000
A1	 0.5470	 0.4180
A2	 0.5010	 0.3970
A3	 0.5180	 0.4040
A4	 0.6630	 0.4340
A5	 0.6800	 0.4360
A6	 0.6370	 0.4310
A7	 0.6930	 0.4480
A8	 0.6350	 0.4380
A9	 0.6410	 0.4390
AA	 0.6970	 0.4660
AB	 0.7720	 0.4590
AC	 0.7170	 0.4610
AD	 0.6610	 0.3980
AE	 0.7150	 0.4560
AF	 0.6770	 0.4480
AG	 0.6780	 0.4450
AH	 0.6740	 0.4490
AI	 0.6820	 0.4500
AJ	 0.7130	 0.4530
AK	 0.6410	 0.3990
AL	 0.5990	 0.3870
AM	 0.6130	 0.3910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AN	 0.5800	 0.3850
AO	 0.6060	 0.3830
AP	 0.6480	 0.3950
AQ	 0.3550	 0.3300
AR	 0.2820	 0.3390
AS	 0.3920	 0.3590
AT	 0.3380	 0.3430
AU	 0.3400	 0.3590
AV	 0.7250	 0.4600
AW	 0.6930	 0.4330
AX	 0.7430	 0.4650
AY	 0.6790	 0.4510
AZ	 0.7460	 0.4680
Aa	 0.6510	 0.4390
Ab	 0.6550	 0.4380
Ac	 0.6220	 0.4320
Ad	 0.7540	 0.4600
Ae	 0.6880	 0.4460
Af	 0.6440	 0.4310
Ag	 0.6480	 0.4320
Ah	 0.7410	 0.4550
Ai	 0.6820	 0.4350
Aj	 0.6730	 0.4380
Ak	 0.6880	 0.4500
Al	 0.6320	 0.4330
Am	 0.6970	 0.4490
An	 0.7210	 0.4540
Ao	 0.6960	 0.4520
Ap	 0.6850	 0.4430
Aq	 0.6710	 0.4470
Ar	 0.6890	 0.4490
As	 0.6560	 0.4430
At	 0.6630	 0.4420
Au	 0.6850	 0.4520
Av	 0.5020	 0.4040
Aw	 0.6240	 0.4340
Ax	 0.4930	 0.4080
Ay	 0.6740	 0.4540
Az	 0.6940	 0.4460
B	 0.7300	 0.4250
B1	 0.7980	 0.3990
B2	 0.6690	 0.3760

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B3	 0.7570	 0.3990
B4	 0.7860	 0.3990
B5	 0.7090	 0.3880
B6	 0.7680	 0.4000
B7	 0.7930	 0.4040
BA	 0.4890	 0.3960
BB	 0.5500	 0.4200
BC	 0.6950	 0.4520
BD	 0.5380	 0.4120
BE	 0.6700	 0.4480
BF	 0.5020	 0.3960
BG	 0.5170	 0.4050
BH	 0.4830	 0.3970
BI	 0.6970	 0.4500
BJ	 0.7200	 0.4520
BK	 0.7640	 0.4670
BL	 0.6250	 0.4350
BM	 0.6680	 0.4480
BN	 0.7570	 0.4730
BO	 0.6500	 0.4350
BP	 0.7090	 0.4470
BQ	 0.7070	 0.4480
BR	 0.7440	 0.4680
BS	 0.6820	 0.4390
BT	 0.7170	 0.4530
BU	 0.7070	 0.4360
BV	 0.6580	 0.4400
BW	 0.6610	 0.4400
BX	 0.7140	 0.4420
BY	 0.7680	 0.4310
BZ	 0.8130	 0.4360
Ba	 0.7140	 0.4370
Bb	 0.7640	 0.4370
Bc	 0.8060	 0.4350
Bd	 0.7200	 0.4340
Be	 0.7630	 0.4310
Bf	 0.8060	 0.4240
Bg	 0.7200	 0.4430
Bh	 0.7830	 0.4470
Bi	 0.8030	 0.4390
Bj	 0.7360	 0.4500
Bk	 0.7710	 0.4480

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bl	 0.8130	 0.4260
Bm	 0.7210	 0.4460
Bn	 0.7740	 0.4370
Bo	 0.8090	 0.4310
Bp	 0.7120	 0.3870
Bq	 0.7560	 0.3950
Br	 0.7890	 0.4050
Bs	 0.6750	 0.3760
Bt	 0.7390	 0.3870
Bu	 0.7880	 0.4040
Bv	 0.6740	 0.3770
Bw	 0.7500	 0.3900
Bx	 0.7880	 0.3920
By	 0.6930	 0.3800
Bz	 0.7580	 0.3980
C	 0.7790	 0.4450
D	 0.7590	 0.4200
E	 0.7290	 0.4070
F	 0.7390	 0.4060
G	 0.7660	 0.4080
H	 0.8010	 0.4310
I	 0.7570	 0.4070
J	 0.7230	 0.4110
K	 0.7490	 0.4120
K0	 0.8020	 0.4720
K1	 0.8530	 0.5210
K2	 0.8490	 0.5240
K3	 0.8460	 0.5200
K4	 0.8450	 0.5200
K5	 0.8460	 0.5230
K6	 0.8440	 0.5180
K7	 0.8440	 0.5170
K8	 0.8230	 0.5120
K9	 0.7990	 0.4980
L	 0.6930	 0.4080
L0	 0.8060	 0.4700
L1	 0.8530	 0.5220
L2	 0.8450	 0.5190
L3	 0.8470	 0.5230
L4	 0.8450	 0.5170
L5	 0.8460	 0.5220
L6	 0.8410	 0.5190

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L7	 0.8450	 0.5190
L8	 0.8220	 0.5100
L9	 0.7990	 0.4960
LS	 0.8790	 0.4940
LU	 0.8520	 0.5130
LV	 0.8530	 0.5250
LW	 0.8540	 0.5240
LX	 0.8480	 0.5200
LY	 0.8530	 0.5190
LZ	 0.8470	 0.5220
La	 0.8440	 0.5180
Lb	 0.8350	 0.5190
Lc	 0.8270	 0.5140
Ld	 0.7990	 0.4940
Le	 0.7970	 0.4680
Lx	 0.8820	 0.4940
Lz	 0.8530	 0.5140
M	 0.6860	 0.3670
M0	 0.8040	 0.4710
M1	 0.8480	 0.5220
M2	 0.8430	 0.5250
M3	 0.8480	 0.5220
M4	 0.8410	 0.5180
M5	 0.8490	 0.5220
M6	 0.8420	 0.5190
M7	 0.8400	 0.5150
M8	 0.8270	 0.5090
M9	 0.7950	 0.4950
MS	 0.8780	 0.4980
MU	 0.8540	 0.5150
MV	 0.8530	 0.5210
MW	 0.8500	 0.5230
MX	 0.8500	 0.5220
MY	 0.8490	 0.5170
MZ	 0.8520	 0.5220
Ma	 0.8440	 0.5170
Mb	 0.8410	 0.5170
Mc	 0.8210	 0.5140
Md	 0.7960	 0.4960
Me	 0.8030	 0.4680
Mx	 0.8820	 0.4960
Mz	 0.8570	 0.5150

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
N	 0.6860	 0.3760
NX	 0.8810	 0.4930
NZ	 0.8540	 0.5130
Na	 0.8570	 0.5260
Nb	 0.8490	 0.5230
Nc	 0.8510	 0.5220
Nd	 0.8460	 0.5170
Ne	 0.8510	 0.5230
Nf	 0.8410	 0.5170
Ng	 0.8360	 0.5190
Nh	 0.8290	 0.5130
Ni	 0.8010	 0.4950
Nj	 0.8060	 0.4680
Nx	 0.8820	 0.4920
Nz	 0.8500	 0.5150
O	 0.6880	 0.3940
OE	 0.9030	 0.5370
OF	 0.8790	 0.5420
OG	 0.8730	 0.5400
OH	 0.8700	 0.5450
OI	 0.8700	 0.5380
OJ	 0.8610	 0.5380
OK	 0.8590	 0.5460
OL	 0.8670	 0.5380
OM	 0.8560	 0.5360
ON	 0.8560	 0.5390
OO	 0.8350	 0.5230
Oj	 0.8920	 0.5350
Ok	 0.8760	 0.5410
Ol	 0.8760	 0.5430
Om	 0.8580	 0.5390
On	 0.8700	 0.5420
Oo	 0.8560	 0.5360
Op	 0.8580	 0.5420
Oq	 0.8720	 0.5440
Or	 0.8630	 0.5370
Os	 0.8460	 0.5450
Ot	 0.8310	 0.5180
P	 0.7270	 0.3900
PE	 0.8940	 0.5320
PF	 0.8750	 0.5450
PG	 0.8770	 0.5480

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PH	 0.8730	 0.5490
PI	 0.8700	 0.5410
PJ	 0.8560	 0.5300
PK	 0.8580	 0.5400
PL	 0.8670	 0.5440
PM	 0.8590	 0.5380
PN	 0.8580	 0.5370
PO	 0.8280	 0.5150
Pj	 0.8910	 0.5340
Pk	 0.8780	 0.5390
Pl	 0.8770	 0.5430
Pm	 0.8660	 0.5440
Pn	 0.8650	 0.5430
Po	 0.8550	 0.5420
Pp	 0.8600	 0.5440
Pq	 0.8560	 0.5390
Pr	 0.8560	 0.5380
Ps	 0.8570	 0.5420
Pt	 0.8420	 0.5210
Q	 0.7030	 0.4040
R	 0.7180	 0.4050
RE	 0.8950	 0.5340
RF	 0.8840	 0.5460
RG	 0.8780	 0.5410
RH	 0.8720	 0.5490
RI	 0.8660	 0.5370
RJ	 0.8560	 0.5330
RK	 0.8550	 0.5430
RL	 0.8750	 0.5430
RM	 0.8560	 0.5440
RN	 0.8560	 0.5400
RO	 0.8240	 0.5130
RT	 0.8870	 0.5290
Rk	 0.8810	 0.5460
Rl	 0.8770	 0.5460
Rm	 0.8700	 0.5420
Rn	 0.8630	 0.5420
Ro	 0.8580	 0.5330
Rp	 0.8630	 0.5420
Rq	 0.8720	 0.5430
Rr	 0.8490	 0.5370
Rs	 0.8560	 0.5390

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Rt	 0.8270	 0.5160
S	 0.7640	 0.4210
S0	 0.0940	 0.1860
S1	 0.1110	 0.2010
S2	 0.1130	 0.1800
S3	 0.1010	 0.1970
S4	 0.1190	 0.1970
S5	 0.1140	 0.1900
S6	 0.1210	 0.1860
S7	 0.1090	 0.1840
S8	 0.1110	 0.1920
SA	 0.1150	 0.1900
SO	 0.1160	 0.1880
SP	 0.1160	 0.1840
SQ	 0.1010	 0.1970
Sv	 0.1200	 0.1980
Sw	 0.1230	 0.1910
Sx	 0.1200	 0.1780
Sy	 0.1280	 0.1780
Sz	 0.1130	 0.1920
T	 0.7370	 0.4110
T1	 0.0230	 0.2310
T2	 0.0330	 0.2410
T3	 0.0360	 0.2440
T4	 0.0200	 0.2320
T5	 0.0260	 0.2260
T6	 0.0210	 0.2480
T7	 0.0330	 0.2460
T8	 0.0230	 0.2520
T9	 0.0310	 0.2610
TF	 0.0300	 0.2370
TG	 0.0390	 0.2410
TH	 0.0410	 0.2630
Td	 0.0250	 0.2210
Te	 0.0280	 0.2300
Tf	 0.0370	 0.2390
Tg	 0.0440	 0.2440
Th	 0.0320	 0.2430
Ti	 0.0440	 0.2640
U	 0.7030	 0.4030
UL	 0.0530	 0.1790
UM	 0.0570	 0.1650

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
UN	0.0720	0.1620
Up	0.0430	0.1810
Uq	0.0470	0.1720
Ur	0.0580	0.1530
Us	0.0470	0.1630
Ut	0.0670	0.1550
Uu	0.0590	0.1570
V	0.7230	0.4000
VL	0.0350	0.1680
VM	0.0410	0.1580
VN	0.0580	0.1700
Vp	0.0390	0.1750
Vq	0.0430	0.1730
Vr	0.0460	0.1640
Vs	0.0350	0.1700
Vt	0.0630	0.1600
Vu	0.0550	0.1610
W	0.7320	0.3970
WI	0.2280	0.2430
WJ	0.2620	0.2460
WK	0.2650	0.2570
Wj	0.2270	0.2510
Wk	0.2070	0.2420
Wl	0.2560	0.2550
Wm	0.2530	0.2420
Wn	0.2570	0.2500
Wo	0.2460	0.2540
X	0.7370	0.3800
XI	0.2100	0.2360
XJ	0.2410	0.2520
XK	0.2400	0.2490
Xj	0.2070	0.2490
Xk	0.2110	0.2450
Xl	0.2370	0.2570
Xm	0.2440	0.2460
Xn	0.2390	0.2550
Xo	0.2430	0.2490
Y	0.6660	0.3900
YC	0.5930	0.4000
YX	0.5980	0.4010
YY	0.5890	0.3970
Yc	0.5970	0.4030

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Yx	 0.5790	 0.4000
Yy	 0.5890	 0.3990
Z	 0.7250	 0.4000
ZD	 0.6040	 0.4090
ZE	 0.6740	 0.4570
ZZ	 0.6090	 0.4120
Za	 0.5970	 0.4000
Zb	 0.6750	 0.4560
Zc	 0.6750	 0.4540
a	 0.6930	 0.3770
aD	 0.6040	 0.4090
aE	 0.6580	 0.4480
aZ	 0.5960	 0.4100
aa	 0.6020	 0.4100
ab	 0.6610	 0.4550
ac	 0.6540	 0.4520
b	 0.7470	 0.3970
b0	 0.7680	 0.4790
b3	 0.7870	 0.4560
b4	 0.7890	 0.4540
b5	 0.7990	 0.4610
b6	 0.7910	 0.4540
b7	 0.7960	 0.4610
b8	 0.7560	 0.4790
b9	 0.7710	 0.4770
bN	 0.7620	 0.4930
bO	 0.7640	 0.4930
bP	 0.7690	 0.4950
bQ	 0.7650	 0.4900
bR	 0.7660	 0.4910
bY	 0.7560	 0.4900
c	 0.7080	 0.3670
cA	 0.7700	 0.4760
cB	 0.7640	 0.4780
cC	 0.7650	 0.4850
cD	 0.7670	 0.4830
cE	 0.7890	 0.4540
cF	 0.7680	 0.4750
cG	 0.7580	 0.4830
cH	 0.7450	 0.4790
cI	 0.7750	 0.4840
cJ	 0.7670	 0.4900

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
cK	 0.7720	 0.4830
cL	 0.7520	 0.4770
cM	 0.7590	 0.4800
cN	 0.7550	 0.4790
cO	 0.7580	 0.4810
cP	 0.7650	 0.4780
d	 0.6460	 0.3670
dS	 0.7670	 0.4930
dT	 0.7590	 0.4890
dU	 0.7740	 0.4940
dV	 0.7600	 0.4890
dW	 0.7650	 0.4920
dZ	 0.7430	 0.4840
e	 0.6930	 0.3750
eB	 0.7430	 0.4760
eU	 0.7390	 0.4800
eW	 0.7430	 0.4740
f	 0.6640	 0.3940
f9	 0.7430	 0.4780
fA	 0.7390	 0.4720
fB	 0.7260	 0.4720
fR	 0.7500	 0.4760
fS	 0.7330	 0.4760
fU	 0.7320	 0.4760
fW	 0.7230	 0.4680
fr	 0.7310	 0.4760
fs	 0.7350	 0.4770
g	 0.7070	 0.3950
gE	 0.8050	 0.4990
gG	 0.8070	 0.4970
gH	 0.8180	 0.5010
gd	 0.6220	 0.3140
h	 0.7220	 0.4140
h1	 0.8030	 0.5060
h2	 0.8020	 0.5060
hI	 0.7990	 0.5130
hJ	 0.7970	 0.5060
hK	 0.8040	 0.5130
hL	 0.7980	 0.5090
hM	 0.8050	 0.5100
hX	 0.7990	 0.5100
he	 0.7990	 0.4940

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
hf	 0.8020	 0.5020
hg	 0.8000	 0.4920
hh	 0.7970	 0.4980
hi	 0.8120	 0.4930
hj	 0.8240	 0.5010
hk	 0.8260	 0.4990
hl	 0.8250	 0.5030
hm	 0.8280	 0.4980
hn	 0.8280	 0.4990
ho	 0.8090	 0.5120
hp	 0.8090	 0.5110
hq	 0.8170	 0.5150
hr	 0.8240	 0.5150
hs	 0.8060	 0.5080
ht	 0.8020	 0.4970
hu	 0.8220	 0.4960
hv	 0.8120	 0.5130
hw	 0.8030	 0.5070
hx	 0.8090	 0.5150
hy	 0.8030	 0.5070
hz	 0.8150	 0.5120
i	 0.6420	 0.3840
iC	 0.7800	 0.5100
iD	 0.7800	 0.5130
iF	 0.7840	 0.5110
j	 0.6680	 0.3870
ja	 0.7080	 0.4900
jb	 0.6790	 0.4830
jc	 0.6710	 0.4680
k	 0.7430	 0.4550
k3	 0.7530	 0.4940
k4	 0.7640	 0.4900
k7	 0.7770	 0.4990
k8	 0.7800	 0.4970
kV	 0.7820	 0.4980
l	 0.7210	 0.4480
lV	 0.7730	 0.5020
m	 0.7230	 0.4550
m1	 0.6980	 0.4700
m2	 0.6360	 0.4610
m5	 0.7260	 0.4790
m6	 0.6380	 0.4600

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
mT	 0.6400	 0.4660
n	 0.7230	 0.4520
nT	 0.7230	 0.4790
o	 0.6850	 0.4580
o0	 0.6930	 0.4940
o1	 0.6390	 0.4710
o2	 0.6380	 0.4700
o6	 0.6470	 0.4720
p	 0.7470	 0.4530
pA	 0.6990	 0.4970
pB	 0.6860	 0.4930
q	 0.7330	 0.4540
q3	 0.7870	 0.5050
q4	 0.7850	 0.5030
q5	 0.7870	 0.5120
q7	 0.7840	 0.5030
q8	 0.7870	 0.5060
q9	 0.7840	 0.5100
r	 0.7240	 0.4490
rc	 0.8480	 0.5240
rd	 0.8720	 0.5270
re	 0.8480	 0.5270
rf	 0.8400	 0.5390
rg	 0.8400	 0.5140
rh	 0.8480	 0.5160
s	 0.7330	 0.4550
sQ	 0.7220	 0.5320
sT	 0.6890	 0.5100
sU	 0.6220	 0.5000
t	 0.7340	 0.4550
tS	 0.8200	 0.5070
tX	 0.8000	 0.4840
tY	 0.7400	 0.4870
u	 0.7440	 0.4520
uR	 0.6000	 0.5020
uV	 0.6860	 0.5050
uW	 0.7430	 0.5190
v	 0.7030	 0.4570
vZ	 0.8890	 0.5880
va	 0.8440	 0.5840
vb	 0.8220	 0.5790
w	 0.7030	 0.4540

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
x	 0.7290	 0.4610
y	 0.7390	 0.4630
z	 0.7120	 0.4560