



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 09:18 AM EST

PDB ID : 6W19
EMDB ID : EMD-21504
Title : Structures of Capsid and Capsid-Associated Tegument Complex inside the Epstein-Barr Virus
Authors : Liu, W.; Cui, Y.X.; Wang, C.Y.; Li, Z.H.; Gong, D.Y.; Dai, X.H.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2020-03-03
Resolution : 5.50 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 : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

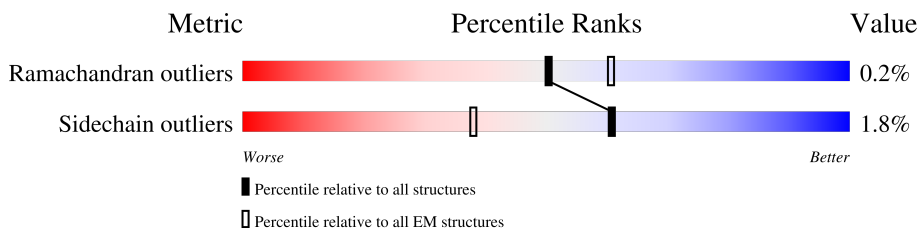
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



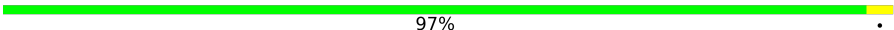
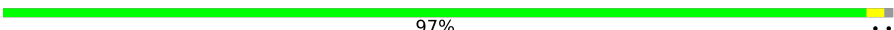
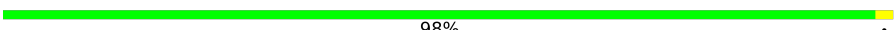
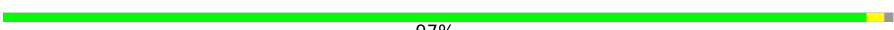
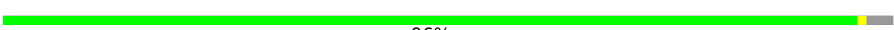





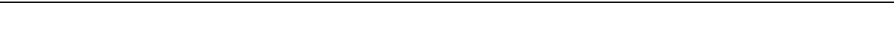

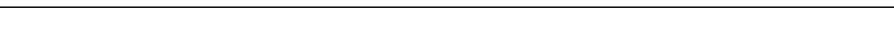
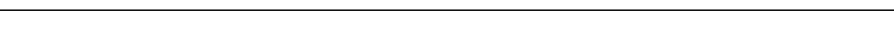











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1381	99% .
1	B	1381	98% ..
1	C	1381	97% ..
1	D	1381	99% .
1	E	1381	99% .
1	F	1381	97% ..
1	G	1381	98% .
1	H	1381	99% .
1	I	1381	97% ..
1	J	1381	96% ..





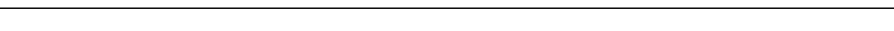
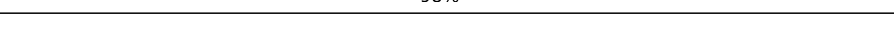
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Mol	Chain	Length	Quality of chain	
1	K	1381		97%
1	L	1381		97%
1	M	1381		98%
1	N	1381		97%
1	O	1381		96%
1	P	1381		91%
2	Q	176		44%
2	R	176		43%
2	S	176		43%
2	T	176		44%
2	U	176		43%
2	V	176		44%
2	W	176		43%
2	X	176		44%
2	Y	176		44%
2	Z	176		44%
2	a	176		42%
2	b	176		43%
2	c	176		42%
2	d	176		42%
2	e	176		43%
2	u	176		36%
3	1	364		92%
3	f	364		82%
3	g	364		90%

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Mol	Chain	Length	Quality of chain
3	h	364	 91% 8%
3	i	364	 91% 8%
3	j	364	 90% 8%
4	2	301	 98% ..
4	3	301	 99% .
4	k	301	 97% ..
4	l	301	 97% ..
4	m	301	 98% ..
4	n	301	 98% ..
4	o	301	 98% ..
4	p	301	 98% ..
4	q	301	 96% ..
4	r	301	 96% ...
4	s	301	 98% ..
4	t	301	 98% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 225047 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	B	1364	Total	C	N	O	S	0	0
			10701	6788	1859	1993	61		
1	C	1363	Total	C	N	O	S	0	0
			10690	6782	1855	1992	61		
1	D	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	E	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	F	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	G	1381	Total	C	N	O	S	0	0
			10831	6868	1884	2017	62		
1	H	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	I	1364	Total	C	N	O	S	0	0
			10702	6787	1860	1994	61		
1	J	1348	Total	C	N	O	S	0	0
			10601	6730	1844	1966	61		
1	K	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	L	1365	Total	C	N	O	S	0	0
			10705	6790	1860	1994	61		
1	M	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	N	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	O	1335	Total	C	N	O	S	0	0
			10473	6647	1819	1947	60		
1	P	1292	Total	C	N	O	S	0	0
			10173	6466	1764	1884	59		

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	R	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	S	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	T	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	U	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	V	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	W	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	X	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	Y	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	Z	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	a	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	b	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	c	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	d	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	e	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	u	63	Total	C	N	O	S	0	0
			528	339	90	98	1		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	315	Total	C	N	O	S	0	0
			2474	1586	436	444	8		
3	g	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		
3	h	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		
3	i	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	j	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		
3	1	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	l	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	n	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	o	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	2	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	q	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	s	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	t	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	3	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Major capsid protein

Chain A:  99%



- Molecule 1: Major capsid protein

Chain B:  98%



- Molecule 1: Major capsid protein

Chain C:  97%



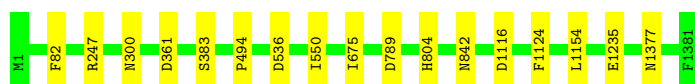
- Molecule 1: Major capsid protein

Chain D:  99%



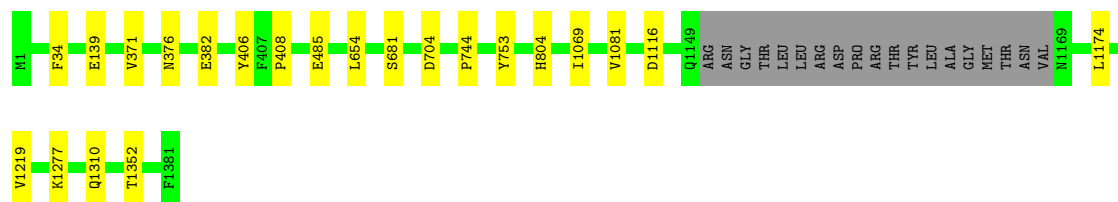
- Molecule 1: Major capsid protein

Chain E:  99%



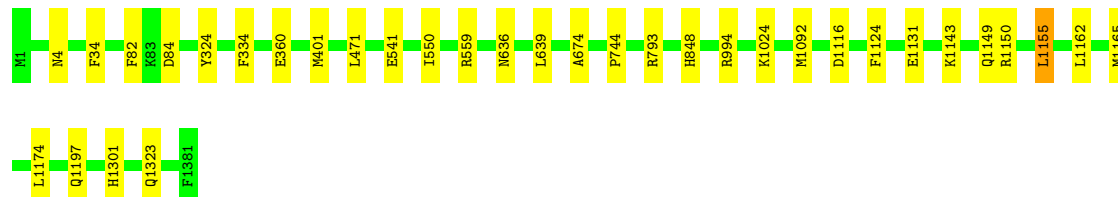
- Molecule 1: Major capsid protein

Chain F:  97%



- Molecule 1: Major capsid protein

Chain G: 98%



- Molecule 1: Major capsid protein

Chain H: 99%



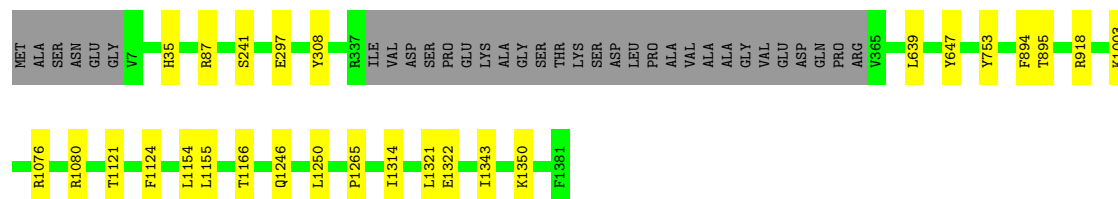
- Molecule 1: Major capsid protein

Chain I: 97%



- Molecule 1: Major capsid protein

Chain J: 96%



- Molecule 1: Major capsid protein

Chain K: 97%





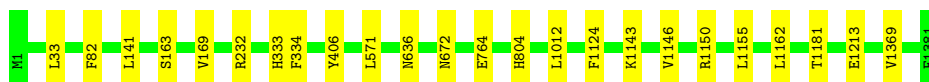
- Molecule 1: Major capsid protein

Chain L: 97%



- Molecule 1: Major capsid protein

Chain M: 98%



- Molecule 1: Major capsid protein

Chain N: 97%



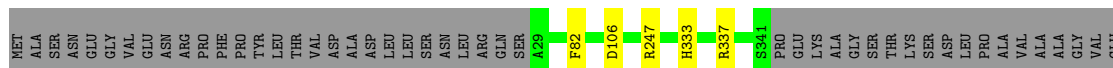
- Molecule 1: Major capsid protein

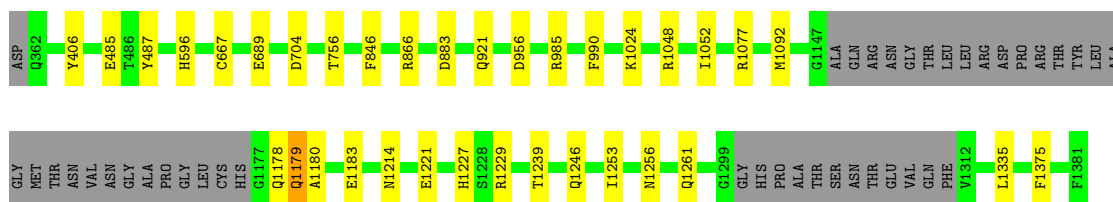
Chain O: 96%



- Molecule 1: Major capsid protein

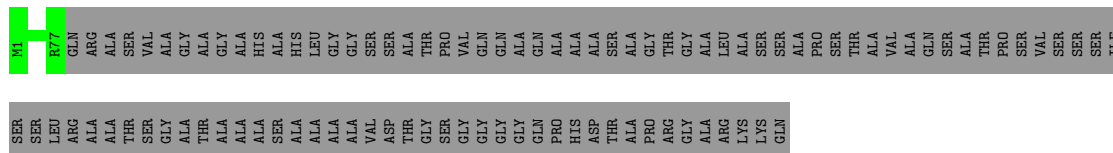
Chain P: 91% 6%





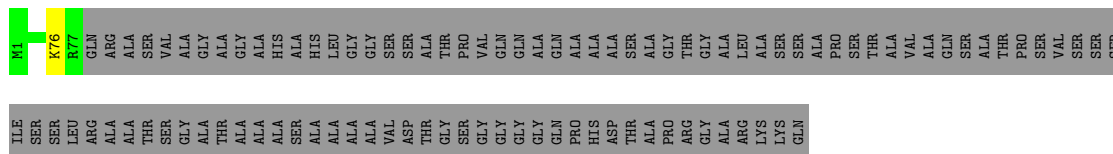
- Molecule 2: Small capsomere-interacting protein

Chain Q: 44% 56%



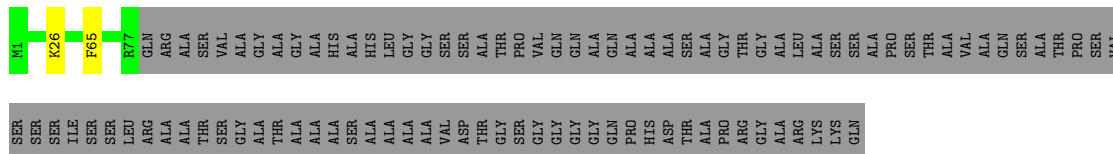
- Molecule 2: Small capsomere-interacting protein

Chain R: 43% 56%



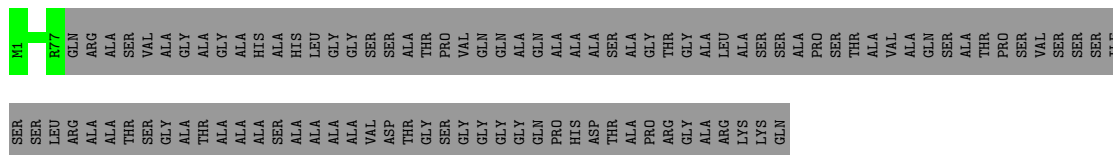
- Molecule 2: Small capsomere-interacting protein

Chain S: 43% 56%



- Molecule 2: Small capsomere-interacting protein

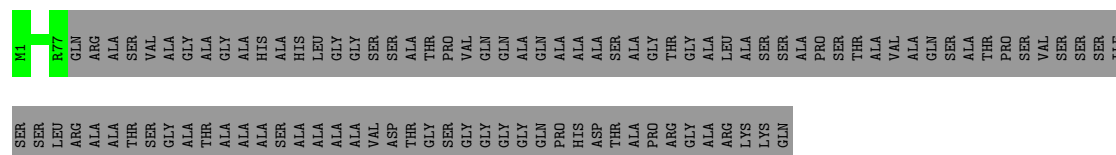
Chain T: 44% 56%



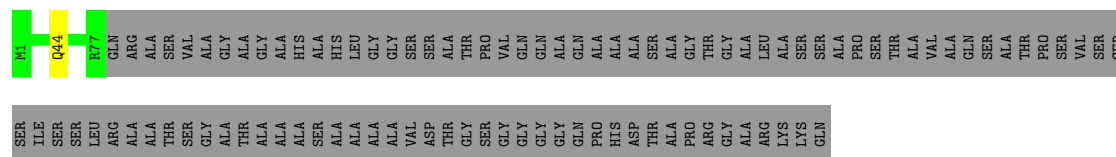
- Molecule 2: Small capsomere-interacting protein

Chain U: 43% 56%

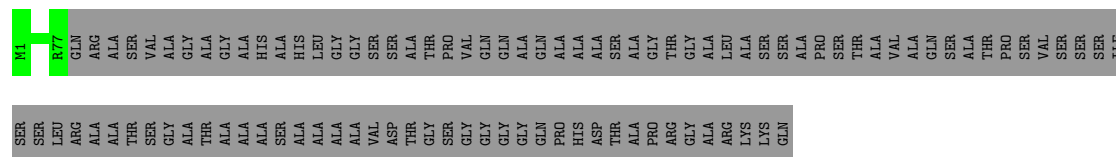
- Molecule 2: Small capsomere-interacting protein



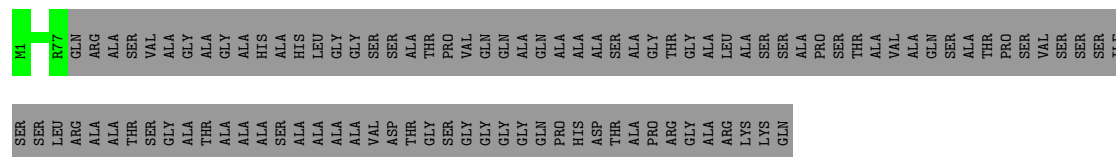
- Molecule 2: Small capsomere-interacting protein



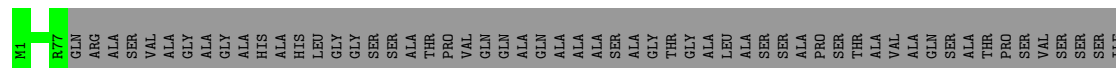
- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein



SER SER LEU ARG ALA THR SER GLY THR ALA ALA SER ALA ALA ALA VAL ASP THR GLY SER GLY GLY GLY GLN PRO HIS ASP THR ALA PRO ARG GLY ALA ARG LYS GLN

- Molecule 2: Small capsomere-interacting protein

Chain a:  42% 56%

W1 R13 L14 R69 R77 GLN ARG ALA THR VAL ALA GLY THR ALA ALA HIS VAL HIS LEU GLY SER SER ALA THR PRO GLN GLN THR ALA PRO ALA ARG GLY THR GLY ALA LEU ALA SER SER SER SER THR VAL ALA THR SER

VAL SER SER ILE SER LEU ARG ALA THR SER GLY THR ALA ALA ALA ALA SER ALA THR VAL ASP THR GLY THR SER GLY GLY GLN GLN THR ALA PRO HIS THR ALA ARG LYS GLN

- Molecule 2: Small capsomere-interacting protein

Chain b:  43% 56%

W1 K76 R77 GLN ARG ALA VAL SER VAL GLY ALA GLY HIS ALA HIS LEU GLY THR PRO VAL GLN GLN ALA ALA SER THR GLY LEU ALA SER SER THR VAL ALA GLN ALA THR PRO VAL SER SER

ILE SER SER LEU ARG ALA THR SER GLY THR ALA ALA ALA SER ALA ALA ALA VAL THR GLY THR VAL ASP THR GLY THR SER GLY GLN GLN PRO HIS THR ALA ARG GLY ALA ARG LYS GLN

- Molecule 2: Small capsomere-interacting protein

Chain c:  42% 56%

W1 Q32 N33 N37 R77 GLN ARG ALA THR VAL ALA GLY THR ALA ALA HIS ALA HIS LEU GLY THR PRO VAL GLN GLN ALA ALA SER THR GLY LEU ALA SER SER THR VAL ALA GLN ALA THR PRO VAL SER SER

VAL SER SER ILE SER SER ARG ALA THR SER GLY THR ALA ALA ALA ALA SER ALA THR VAL ASP THR GLY THR SER GLY GLN GLN PRO HIS THR ALA ARG LYS GLN

- Molecule 2: Small capsomere-interacting protein

Chain d:  42% 56%

W1 A2 P19 L24 R77 GLN ARG ALA THR VAL ALA GLY THR ALA ALA HIS ALA HIS LEU GLY THR PRO VAL GLN GLN ALA ALA SER THR GLY LEU ALA SER SER THR VAL ALA GLN ALA THR PRO VAL SER SER

VAL SER SER ILE SER SER ARG ALA THR SER GLY THR ALA ALA ALA ALA SER ALA THR VAL ASP THR GLY THR SER GLY GLN GLN PRO HIS THR ALA ARG LYS GLN

- Molecule 2: Small capsomere-interacting protein

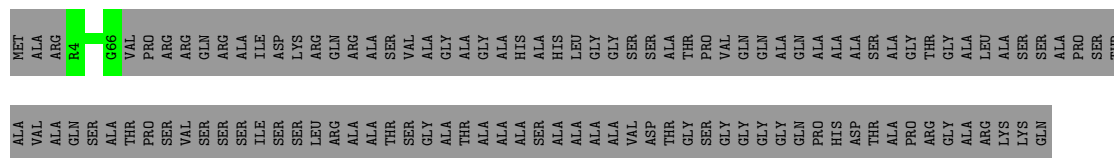
Chain e:  43% 56%

W1 N31 R77 GLN ARG ALA THR VAL ALA GLY THR ALA ALA HIS ALA HIS LEU GLY THR PRO VAL GLN GLN ALA ALA SER THR GLY LEU ALA SER SER THR VAL ALA GLN ALA THR PRO VAL SER SER


SER ILE SER SER LEU ARG ALA THR SER GLY THR ALA ALA ALA SER ALA THR VAL ASP THR GLY THR SER GLY GLN GLN PRO HIS THR ALA ARG LYS GLN

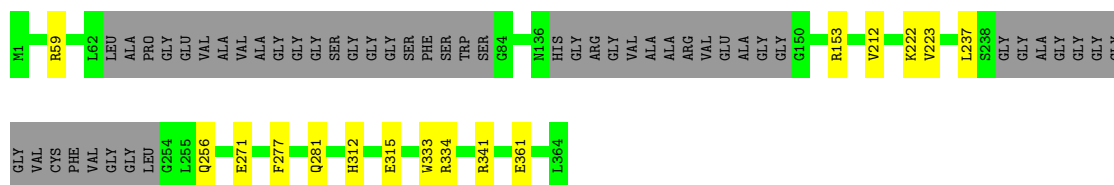
- Molecule 2: Small capsomere-interacting protein

Chain u:  36% 64%

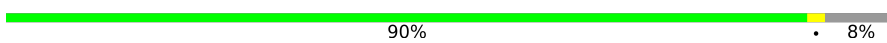


- Molecule 3: Triplex capsid protein 1

Chain f:  82% 13%



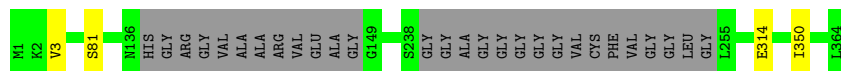
- Molecule 3: Triplex capsid protein 1

Chain g:  90% 8%

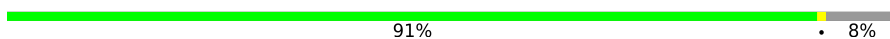


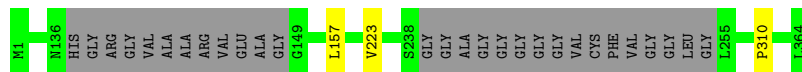
- Molecule 3: Triplex capsid protein 1

Chain h:  91% 8%




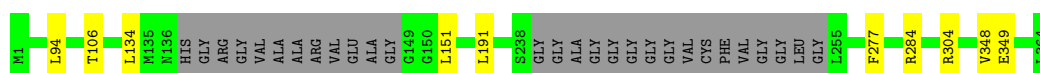
- Molecule 3: Triplex capsid protein 1

Chain i:  91% 8%




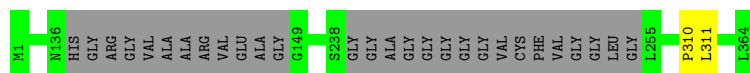
- Molecule 3: Triplex capsid protein 1

Chain j:  90% 8%



- Molecule 3: Triplex capsid protein 1

Chain 1:  92% 8%



- Molecule 4: Triplex capsid protein 2

Chain k:  97%



- Molecule 4: Triplex capsid protein 2

Chain l:  97%



- Molecule 4: Triplex capsid protein 2

Chain m:  98%



- Molecule 4: Triplex capsid protein 2

Chain n:  98%



- Molecule 4: Triplex capsid protein 2

Chain o:  98%



- Molecule 4: Triplex capsid protein 2

Chain 2:  98%



- Molecule 4: Triplex capsid protein 2

Chain p:  98% ..



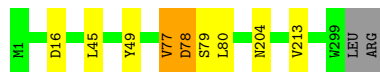
- Molecule 4: Triplex capsid protein 2

Chain q:  96% ..



- Molecule 4: Triplex capsid protein 2

Chain r:  96% ..



- Molecule 4: Triplex capsid protein 2

Chain s:  98% ..



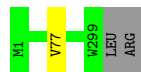
- Molecule 4: Triplex capsid protein 2

Chain t:  98% ..



- Molecule 4: Triplex capsid protein 2

Chain 3:  99% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2048	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/11085	0.49	1/15066 (0.0%)
1	B	0.42	0/10951	0.50	0/14882
1	C	0.42	0/10940	0.50	0/14868
1	D	0.42	0/11085	0.51	0/15066
1	E	0.41	0/11085	0.49	0/15066
1	F	0.40	0/10933	0.50	0/14858
1	G	0.38	0/11084	0.50	1/15065 (0.0%)
1	H	0.37	0/11085	0.46	0/15066
1	I	0.38	0/10952	0.48	0/14883
1	J	0.54	0/10850	0.55	0/14745
1	K	0.53	0/11085	0.53	0/15066
1	L	0.35	0/10955	0.46	0/14887
1	M	0.35	0/11085	0.46	0/15066
1	N	0.37	0/10933	0.49	0/14858
1	O	0.40	0/10719	0.50	0/14565
1	P	0.46	0/10410	0.54	0/14140
2	Q	0.32	0/664	0.44	0/896
2	R	0.35	0/664	0.50	0/896
2	S	0.41	0/664	0.51	0/896
2	T	0.33	0/664	0.43	0/896
2	U	0.36	0/664	0.44	0/896
2	V	0.33	0/664	0.41	0/896
2	W	0.30	0/664	0.43	0/896
2	X	0.32	0/664	0.41	0/896
2	Y	0.31	0/664	0.43	0/896
2	Z	0.39	0/664	0.44	0/896
2	a	0.38	0/664	0.50	0/896
2	b	0.28	0/664	0.41	0/896
2	c	0.30	0/664	0.44	0/896
2	d	0.28	0/664	0.45	0/896
2	e	0.32	0/664	0.47	0/896
2	u	0.32	0/542	0.45	0/735
3	l	0.33	0/2672	0.48	0/3635
3	f	0.43	0/2537	0.50	0/3450

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	g	0.35	0/2672	0.46	0/3635
3	h	0.37	0/2672	0.48	0/3635
3	i	0.37	0/2672	0.48	0/3635
3	j	0.35	0/2672	0.48	0/3635
4	2	0.37	0/2388	0.53	1/3254 (0.0%)
4	3	0.34	0/2388	0.49	0/3254
4	k	0.34	0/2388	0.50	0/3254
4	l	0.36	0/2388	0.48	0/3254
4	m	0.33	0/2388	0.51	0/3254
4	n	0.37	0/2388	0.54	0/3254
4	o	0.34	0/2388	0.47	0/3254
4	p	0.32	0/2388	0.51	0/3254
4	q	0.35	0/2388	0.48	0/3254
4	r	0.36	0/2388	0.50	0/3254
4	s	0.37	0/2388	0.51	0/3254
4	t	0.35	0/2388	0.47	0/3254
All	All	0.40	0/230292	0.50	3/312995 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	182	LEU	CA-CB-CG	5.74	128.49	115.30
1	G	1155	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	1264	VAL	C-N-CD	5.22	139.36	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1379/1381 (100%)	1297 (94%)	78 (6%)	4 (0%)	41	76
1	B	1360/1381 (98%)	1287 (95%)	72 (5%)	1 (0%)	51	85
1	C	1359/1381 (98%)	1277 (94%)	80 (6%)	2 (0%)	51	85
1	D	1379/1381 (100%)	1301 (94%)	78 (6%)	0	100	100
1	E	1379/1381 (100%)	1286 (93%)	91 (7%)	2 (0%)	51	85
1	F	1358/1381 (98%)	1272 (94%)	84 (6%)	2 (0%)	51	85
1	G	1379/1381 (100%)	1296 (94%)	80 (6%)	3 (0%)	47	81
1	H	1379/1381 (100%)	1301 (94%)	75 (5%)	3 (0%)	47	81
1	I	1360/1381 (98%)	1288 (95%)	70 (5%)	2 (0%)	51	85
1	J	1344/1381 (97%)	1238 (92%)	104 (8%)	2 (0%)	51	85
1	K	1379/1381 (100%)	1268 (92%)	110 (8%)	1 (0%)	51	85
1	L	1361/1381 (99%)	1299 (95%)	60 (4%)	2 (0%)	51	85
1	M	1379/1381 (100%)	1299 (94%)	79 (6%)	1 (0%)	51	85
1	N	1358/1381 (98%)	1312 (97%)	42 (3%)	4 (0%)	41	76
1	O	1331/1381 (96%)	1274 (96%)	52 (4%)	5 (0%)	34	72
1	P	1284/1381 (93%)	1183 (92%)	97 (8%)	4 (0%)	41	76
2	Q	75/176 (43%)	68 (91%)	7 (9%)	0	100	100
2	R	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	S	75/176 (43%)	68 (91%)	6 (8%)	1 (1%)	12	47
2	T	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	U	75/176 (43%)	69 (92%)	6 (8%)	0	100	100
2	V	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	W	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	X	75/176 (43%)	73 (97%)	2 (3%)	0	100	100
2	Y	75/176 (43%)	72 (96%)	3 (4%)	0	100	100
2	Z	75/176 (43%)	69 (92%)	6 (8%)	0	100	100
2	a	75/176 (43%)	70 (93%)	5 (7%)	0	100	100
2	b	75/176 (43%)	69 (92%)	6 (8%)	0	100	100
2	c	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	d	75/176 (43%)	71 (95%)	2 (3%)	2 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	75/176 (43%)	75 (100%)	0	0	100	100
2	u	61/176 (35%)	56 (92%)	5 (8%)	0	100	100
3	1	330/364 (91%)	303 (92%)	25 (8%)	2 (1%)	25	65
3	f	307/364 (84%)	280 (91%)	27 (9%)	0	100	100
3	g	330/364 (91%)	308 (93%)	22 (7%)	0	100	100
3	h	330/364 (91%)	318 (96%)	10 (3%)	2 (1%)	25	65
3	i	330/364 (91%)	306 (93%)	23 (7%)	1 (0%)	41	76
3	j	330/364 (91%)	299 (91%)	31 (9%)	0	100	100
4	2	297/301 (99%)	253 (85%)	42 (14%)	2 (1%)	22	62
4	3	297/301 (99%)	279 (94%)	17 (6%)	1 (0%)	41	76
4	k	297/301 (99%)	284 (96%)	12 (4%)	1 (0%)	41	76
4	l	297/301 (99%)	286 (96%)	11 (4%)	0	100	100
4	m	297/301 (99%)	287 (97%)	10 (3%)	0	100	100
4	n	297/301 (99%)	277 (93%)	20 (7%)	0	100	100
4	o	297/301 (99%)	275 (93%)	22 (7%)	0	100	100
4	p	297/301 (99%)	293 (99%)	3 (1%)	1 (0%)	41	76
4	q	297/301 (99%)	283 (95%)	14 (5%)	0	100	100
4	r	297/301 (99%)	279 (94%)	15 (5%)	3 (1%)	15	53
4	s	297/301 (99%)	283 (95%)	12 (4%)	2 (1%)	22	62
4	t	297/301 (99%)	284 (96%)	12 (4%)	1 (0%)	41	76
All	All	28475/30708 (93%)	26770 (94%)	1648 (6%)	57 (0%)	50	81

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	978	ARG
1	K	1011	SER
1	O	1284	ASN
1	P	1179	GLN
2	d	19	PRO
3	h	81	SER
3	l	311	LEU
4	r	77	VAL
4	r	78	ASP
1	A	803	GLY

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Mol	Chain	Res	Type
1	J	894	PHE
1	N	703	SER
1	O	977	GLN
4	s	77	VAL
4	t	201	LEU
4	3	77	VAL
1	A	744	PRO
1	A	1172	PRO
1	G	674	ALA
1	H	949	PRO
1	M	1213	GLU
1	N	262	LYS
1	N	744	PRO
1	P	1180	ALA
3	i	310	PRO
4	2	161	MET
4	s	192	GLU
1	C	744	PRO
1	F	408	PRO
1	J	1265	PRO
1	L	952	MET
1	O	331	PHE
1	P	106	ASP
2	S	65	PHE
3	h	3	VAL
3	1	310	PRO
4	2	279	ASN
1	E	300	ASN
1	G	4	ASN
1	H	1118	GLY
1	I	805	ALA
1	P	337	ARG
4	p	196	PRO
1	H	1119	ILE
1	O	670	LEU
2	d	2	ALA
4	k	194	PRO
4	r	80	LEU
1	I	478	PRO
1	F	744	PRO
1	G	744	PRO
1	C	1204	GLY

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Mol	Chain	Res	Type
1	E	494	PRO
1	N	110	PRO
1	O	744	PRO
1	A	1265	PRO
1	L	744	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1171/1171 (100%)	1160 (99%)	11 (1%)	78	88
1	B	1157/1171 (99%)	1142 (99%)	15 (1%)	69	82
1	C	1156/1171 (99%)	1140 (99%)	16 (1%)	67	80
1	D	1171/1171 (100%)	1155 (99%)	16 (1%)	67	80
1	E	1171/1171 (100%)	1156 (99%)	15 (1%)	69	82
1	F	1155/1171 (99%)	1135 (98%)	20 (2%)	60	78
1	G	1170/1171 (100%)	1139 (97%)	31 (3%)	46	67
1	H	1171/1171 (100%)	1154 (98%)	17 (2%)	65	80
1	I	1157/1171 (99%)	1141 (99%)	16 (1%)	67	80
1	J	1146/1171 (98%)	1121 (98%)	25 (2%)	52	71
1	K	1171/1171 (100%)	1126 (96%)	45 (4%)	33	57
1	L	1157/1171 (99%)	1138 (98%)	19 (2%)	62	79
1	M	1171/1171 (100%)	1148 (98%)	23 (2%)	55	73
1	N	1155/1171 (99%)	1136 (98%)	19 (2%)	62	79
1	O	1131/1171 (97%)	1120 (99%)	11 (1%)	76	86
1	P	1100/1171 (94%)	1063 (97%)	37 (3%)	37	60
2	Q	71/128 (56%)	71 (100%)	0	100	100
2	R	71/128 (56%)	70 (99%)	1 (1%)	67	80
2	S	71/128 (56%)	70 (99%)	1 (1%)	67	80
2	T	71/128 (56%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	71/128 (56%)	70 (99%)	1 (1%)	67	80
2	V	71/128 (56%)	71 (100%)	0	100	100
2	W	71/128 (56%)	70 (99%)	1 (1%)	67	80
2	X	71/128 (56%)	71 (100%)	0	100	100
2	Y	71/128 (56%)	71 (100%)	0	100	100
2	Z	71/128 (56%)	71 (100%)	0	100	100
2	a	71/128 (56%)	68 (96%)	3 (4%)	30	54
2	b	71/128 (56%)	70 (99%)	1 (1%)	67	80
2	c	71/128 (56%)	68 (96%)	3 (4%)	30	54
2	d	71/128 (56%)	70 (99%)	1 (1%)	67	80
2	e	71/128 (56%)	70 (99%)	1 (1%)	67	80
2	u	59/128 (46%)	59 (100%)	0	100	100
3	1	278/289 (96%)	278 (100%)	0	100	100
3	f	267/289 (92%)	251 (94%)	16 (6%)	19	46
3	g	278/289 (96%)	270 (97%)	8 (3%)	42	64
3	h	278/289 (96%)	276 (99%)	2 (1%)	84	90
3	i	278/289 (96%)	276 (99%)	2 (1%)	84	90
3	j	278/289 (96%)	268 (96%)	10 (4%)	35	59
4	2	265/267 (99%)	263 (99%)	2 (1%)	81	89
4	3	265/267 (99%)	265 (100%)	0	100	100
4	k	265/267 (99%)	258 (97%)	7 (3%)	46	67
4	l	265/267 (99%)	257 (97%)	8 (3%)	41	63
4	m	265/267 (99%)	260 (98%)	5 (2%)	57	75
4	n	265/267 (99%)	261 (98%)	4 (2%)	65	80
4	o	265/267 (99%)	260 (98%)	5 (2%)	57	75
4	p	265/267 (99%)	261 (98%)	4 (2%)	65	80
4	q	265/267 (99%)	255 (96%)	10 (4%)	33	57
4	r	265/267 (99%)	257 (97%)	8 (3%)	41	63
4	s	265/267 (99%)	262 (99%)	3 (1%)	73	84
4	t	265/267 (99%)	262 (99%)	3 (1%)	73	84
All	All	24471/25722 (95%)	24025 (98%)	446 (2%)	61	77

All (446) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	141	LEU
1	A	172	LEU
1	A	247	ARG
1	A	700	LEU
1	A	1116	ASP
1	A	1209	VAL
1	A	1240	VAL
1	A	1283	ASN
1	A	1323	GLN
1	A	1372	ILE
1	B	20	ASP
1	B	93	ILE
1	B	155	VAL
1	B	223	LEU
1	B	297	GLU
1	B	409	VAL
1	B	678	GLU
1	B	746	ILE
1	B	753	TYR
1	B	903	ASP
1	B	942	GLN
1	B	1012	LEU
1	B	1116	ASP
1	B	1216	ASN
1	B	1298	LEU
1	C	176	LEU
1	C	224	LEU
1	C	265	SER
1	C	351	ASP
1	C	352	LEU
1	C	385	GLN
1	C	474	LEU
1	C	602	VAL
1	C	791	ASP
1	C	887	SER
1	C	928	LEU
1	C	1031	ILE
1	C	1092	MET
1	C	1116	ASP
1	C	1124	PHE
1	C	1192	ASP

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Mol	Chain	Res	Type
1	D	82	PHE
1	D	194	LEU
1	D	355	VAL
1	D	415	ASN
1	D	542	LEU
1	D	647	TYR
1	D	884	LEU
1	D	903	ASP
1	D	994	ARG
1	D	1071	THR
1	D	1081	VAL
1	D	1116	ASP
1	D	1124	PHE
1	D	1174	LEU
1	D	1211	SER
1	D	1335	LEU
1	E	82	PHE
1	E	247	ARG
1	E	361	ASP
1	E	383	SER
1	E	536	ASP
1	E	550	ILE
1	E	675	ILE
1	E	789	ASP
1	E	804	HIS
1	E	842	ASN
1	E	1116	ASP
1	E	1124	PHE
1	E	1154	LEU
1	E	1235	GLU
1	E	1377	ASN
1	F	34	PHE
1	F	139	GLU
1	F	371	VAL
1	F	376	ASN
1	F	382	GLU
1	F	406	TYR
1	F	485	GLU
1	F	654	LEU
1	F	681	SER
1	F	704	ASP
1	F	753	TYR

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Mol	Chain	Res	Type
1	F	804	HIS
1	F	1069	ILE
1	F	1081	VAL
1	F	1116	ASP
1	F	1174	LEU
1	F	1219	VAL
1	F	1277	LYS
1	F	1310	GLN
1	F	1352	THR
1	G	34	PHE
1	G	82	PHE
1	G	84	ASP
1	G	324	TYR
1	G	334	PHE
1	G	360	GLU
1	G	401	MET
1	G	471	LEU
1	G	541	GLU
1	G	550	ILE
1	G	559	ARG
1	G	636	ASN
1	G	639	LEU
1	G	793	ARG
1	G	848	HIS
1	G	994	ARG
1	G	1024	LYS
1	G	1092	MET
1	G	1116	ASP
1	G	1124	PHE
1	G	1131	GLU
1	G	1143	LYS
1	G	1149	GLN
1	G	1150	ARG
1	G	1155	LEU
1	G	1162	LEU
1	G	1165	MET
1	G	1174	LEU
1	G	1197	GLN
1	G	1301	HIS
1	G	1323	GLN
1	H	54	VAL
1	H	324	TYR

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Mol	Chain	Res	Type
1	H	406	TYR
1	H	542	LEU
1	H	557	ARG
1	H	742	ARG
1	H	804	HIS
1	H	825	MET
1	H	834	HIS
1	H	921	GLN
1	H	981	GLU
1	H	1056	ASN
1	H	1124	PHE
1	H	1174	LEU
1	H	1301	HIS
1	H	1327	PHE
1	H	1343	ILE
1	I	82	PHE
1	I	243	TYR
1	I	291	LEU
1	I	382	GLU
1	I	411	LEU
1	I	582	GLU
1	I	768	ASN
1	I	861	GLU
1	I	895	THR
1	I	899	ARG
1	I	942	GLN
1	I	992	GLU
1	I	1012	LEU
1	I	1267	LEU
1	I	1298	LEU
1	I	1323	GLN
1	J	35	HIS
1	J	87	ARG
1	J	241	SER
1	J	297	GLU
1	J	308	TYR
1	J	639	LEU
1	J	647	TYR
1	J	753	TYR
1	J	895	THR
1	J	918	ARG
1	J	1003	LYS

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Mol	Chain	Res	Type
1	J	1076	ARG
1	J	1080	ARG
1	J	1121	THR
1	J	1124	PHE
1	J	1154	LEU
1	J	1155	LEU
1	J	1166	THR
1	J	1246	GLN
1	J	1250	LEU
1	J	1314	ILE
1	J	1321	LEU
1	J	1322	GLU
1	J	1343	ILE
1	J	1350	LYS
1	K	113	GLN
1	K	136	LEU
1	K	238	SER
1	K	318	LEU
1	K	399	ARG
1	K	440	ILE
1	K	550	ILE
1	K	629	PHE
1	K	713	GLN
1	K	874	LEU
1	K	884	LEU
1	K	896	ARG
1	K	921	GLN
1	K	946	HIS
1	K	966	ASP
1	K	981	GLU
1	K	994	ARG
1	K	1056	ASN
1	K	1122	GLN
1	K	1131	GLU
1	K	1154	LEU
1	K	1155	LEU
1	K	1157	ASP
1	K	1159	ARG
1	K	1190	THR
1	K	1211	SER
1	K	1241	ASN
1	K	1245	SER

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Mol	Chain	Res	Type
1	K	1246	GLN
1	K	1252	ASP
1	K	1253	ILE
1	K	1272	ARG
1	K	1277	LYS
1	K	1283	ASN
1	K	1287	LEU
1	K	1292	ASN
1	K	1304	THR
1	K	1307	THR
1	K	1310	GLN
1	K	1313	VAL
1	K	1321	LEU
1	K	1327	PHE
1	K	1335	LEU
1	K	1364	GLU
1	K	1371	ARG
1	L	34	PHE
1	L	46	ARG
1	L	63	ILE
1	L	82	PHE
1	L	113	GLN
1	L	377	HIS
1	L	447	LEU
1	L	509	ASN
1	L	636	ASN
1	L	700	LEU
1	L	847	SER
1	L	956	ASP
1	L	976	GLN
1	L	981	GLU
1	L	994	ARG
1	L	1082	ASP
1	L	1092	MET
1	L	1116	ASP
1	L	1250	LEU
1	M	33	LEU
1	M	82	PHE
1	M	141	LEU
1	M	163	SER
1	M	169	VAL
1	M	232	ARG

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Mol	Chain	Res	Type
1	M	333	HIS
1	M	334	PHE
1	M	406	TYR
1	M	571	LEU
1	M	636	ASN
1	M	672	ASN
1	M	764	GLU
1	M	804	HIS
1	M	1012	LEU
1	M	1124	PHE
1	M	1143	LYS
1	M	1146	VAL
1	M	1150	ARG
1	M	1155	LEU
1	M	1162	LEU
1	M	1181	THR
1	M	1369	VAL
1	N	34	PHE
1	N	37	PHE
1	N	82	PHE
1	N	327	VAL
1	N	672	ASN
1	N	673	ASN
1	N	846	PHE
1	N	891	CYS
1	N	928	LEU
1	N	942	GLN
1	N	998	ARG
1	N	1012	LEU
1	N	1028	MET
1	N	1095	ILE
1	N	1209	VAL
1	N	1218	GLU
1	N	1272	ARG
1	N	1295	SER
1	N	1298	LEU
1	O	27	GLN
1	O	339	VAL
1	O	382	GLU
1	O	489	LEU
1	O	567	MET
1	O	787	ASP

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Mol	Chain	Res	Type
1	O	937	THR
1	O	1008	CYS
1	O	1174	LEU
1	O	1205	ARG
1	O	1239	THR
1	P	82	PHE
1	P	247	ARG
1	P	333	HIS
1	P	406	TYR
1	P	485	GLU
1	P	487	TYR
1	P	596	HIS
1	P	667	CYS
1	P	689	GLU
1	P	704	ASP
1	P	756	THR
1	P	846	PHE
1	P	866	ARG
1	P	883	ASP
1	P	921	GLN
1	P	956	ASP
1	P	985	ARG
1	P	990	PHE
1	P	1024	LYS
1	P	1048	ARG
1	P	1052	ILE
1	P	1077	ARG
1	P	1092	MET
1	P	1178	GLN
1	P	1179	GLN
1	P	1183	GLU
1	P	1214	ASN
1	P	1221	GLU
1	P	1227	HIS
1	P	1229	ARG
1	P	1239	THR
1	P	1246	GLN
1	P	1253	ILE
1	P	1256	ASN
1	P	1261	GLN
1	P	1335	LEU
1	P	1375	PHE

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Mol	Chain	Res	Type
2	R	76	LYS
2	S	26	LYS
2	U	65	PHE
2	W	44	GLN
2	a	13	ARG
2	a	14	LEU
2	a	69	ARG
2	b	76	LYS
2	c	32	GLN
2	c	33	ASN
2	c	37	ASN
2	d	24	LEU
2	e	31	ASN
3	f	59	ARG
3	f	153	ARG
3	f	212	VAL
3	f	222	LYS
3	f	223	VAL
3	f	237	LEU
3	f	256	GLN
3	f	271	GLU
3	f	277	PHE
3	f	281	GLN
3	f	312	HIS
3	f	315	GLU
3	f	333	TRP
3	f	334	ARG
3	f	341	ARG
3	f	361	GLU
3	g	25	ARG
3	g	50	SER
3	g	110	LEU
3	g	117	ASP
3	g	212	VAL
3	g	277	PHE
3	g	305	TYR
3	g	347	VAL
3	h	314	GLU
3	h	350	ILE
3	i	157	LEU
3	i	223	VAL
3	j	94	LEU

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Mol	Chain	Res	Type
3	j	106	THR
3	j	134	LEU
3	j	151	LEU
3	j	191	LEU
3	j	277	PHE
3	j	284	ARG
3	j	304	ARG
3	j	348	VAL
3	j	349	GLU
4	k	25	ILE
4	k	48	VAL
4	k	147	LEU
4	k	170	LEU
4	k	190	LEU
4	k	215	LEU
4	k	252	LEU
4	l	49	TYR
4	l	98	GLN
4	l	112	MET
4	l	137	VAL
4	l	168	ASP
4	l	171	ASP
4	l	215	LEU
4	l	277	LEU
4	m	48	VAL
4	m	49	TYR
4	m	66	ASP
4	m	155	VAL
4	m	162	GLN
4	n	13	LEU
4	n	132	ILE
4	n	182	LEU
4	n	203	ASP
4	o	4	LYS
4	o	12	ARG
4	o	49	TYR
4	o	83	THR
4	o	137	VAL
4	2	131	ASP
4	2	276	SER
4	p	45	LEU
4	p	49	TYR

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Mol	Chain	Res	Type
4	p	170	LEU
4	p	203	ASP
4	q	31	LEU
4	q	49	TYR
4	q	109	LEU
4	q	118	ARG
4	q	126	GLU
4	q	128	ASN
4	q	158	ARG
4	q	261	LEU
4	q	267	MET
4	q	277	LEU
4	r	16	ASP
4	r	45	LEU
4	r	49	TYR
4	r	77	VAL
4	r	78	ASP
4	r	79	SER
4	r	204	ASN
4	r	213	VAL
4	s	49	TYR
4	s	204	ASN
4	s	214	THR
4	t	49	TYR
4	t	222	ARG
4	t	252	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (608) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	104	HIS
1	A	142	HIS
1	A	178	ASN
1	A	222	HIS
1	A	333	HIS
1	A	433	GLN
1	A	445	ASN
1	A	465	HIS
1	A	543	HIS
1	A	564	HIS
1	A	596	HIS

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Mol	Chain	Res	Type
1	A	775	GLN
1	A	785	ASN
1	A	788	HIS
1	A	790	HIS
1	A	908	GLN
1	A	909	GLN
1	A	951	HIS
1	A	964	HIS
1	A	997	HIS
1	A	1022	HIS
1	A	1149	GLN
1	A	1216	ASN
1	A	1246	GLN
1	A	1261	GLN
1	A	1289	ASN
1	A	1301	HIS
1	A	1357	HIS
1	A	1377	ASN
1	B	94	GLN
1	B	113	GLN
1	B	178	ASN
1	B	317	ASN
1	B	362	GLN
1	B	433	GLN
1	B	442	ASN
1	B	496	HIS
1	B	543	HIS
1	B	564	HIS
1	B	587	GLN
1	B	627	HIS
1	B	645	ASN
1	B	785	ASN
1	B	804	HIS
1	B	824	HIS
1	B	837	GLN
1	B	849	HIS
1	B	859	ASN
1	B	909	GLN
1	B	913	ASN
1	B	926	ASN
1	B	942	GLN
1	B	964	HIS

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Mol	Chain	Res	Type
1	B	965	GLN
1	B	974	ASN
1	B	977	GLN
1	B	1022	HIS
1	B	1089	HIS
1	B	1176	HIS
1	B	1261	GLN
1	B	1284	ASN
1	B	1296	GLN
1	B	1351	GLN
1	B	1353	HIS
1	B	1357	HIS
1	C	4	ASN
1	C	27	GLN
1	C	64	GLN
1	C	142	HIS
1	C	187	HIS
1	C	226	HIS
1	C	433	GLN
1	C	531	HIS
1	C	543	HIS
1	C	564	HIS
1	C	600	GLN
1	C	735	HIS
1	C	761	GLN
1	C	790	HIS
1	C	795	HIS
1	C	824	HIS
1	C	909	GLN
1	C	913	ASN
1	C	921	GLN
1	C	926	ASN
1	C	964	HIS
1	C	976	GLN
1	C	984	ASN
1	C	1022	HIS
1	C	1089	HIS
1	C	1149	GLN
1	C	1176	HIS
1	C	1217	GLN
1	C	1284	ASN
1	C	1289	ASN

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Mol	Chain	Res	Type
1	C	1301	HIS
1	C	1353	HIS
1	C	1357	HIS
1	D	4	ASN
1	D	126	HIS
1	D	142	HIS
1	D	222	HIS
1	D	317	ASN
1	D	333	HIS
1	D	433	GLN
1	D	442	ASN
1	D	461	HIS
1	D	531	HIS
1	D	543	HIS
1	D	564	HIS
1	D	581	GLN
1	D	596	HIS
1	D	600	GLN
1	D	636	ASN
1	D	761	GLN
1	D	790	HIS
1	D	804	HIS
1	D	824	HIS
1	D	833	GLN
1	D	862	ASN
1	D	908	GLN
1	D	909	GLN
1	D	926	ASN
1	D	951	HIS
1	D	964	HIS
1	D	1022	HIS
1	D	1073	ASN
1	D	1137	GLN
1	D	1176	HIS
1	D	1261	GLN
1	D	1357	HIS
1	E	9	ASN
1	E	27	GLN
1	E	79	ASN
1	E	104	HIS
1	E	289	GLN
1	E	317	ASN

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Mol	Chain	Res	Type
1	E	392	GLN
1	E	429	ASN
1	E	433	GLN
1	E	442	ASN
1	E	491	HIS
1	E	531	HIS
1	E	543	HIS
1	E	560	HIS
1	E	564	HIS
1	E	596	HIS
1	E	658	ASN
1	E	695	GLN
1	E	790	HIS
1	E	804	HIS
1	E	824	HIS
1	E	908	GLN
1	E	909	GLN
1	E	965	GLN
1	E	974	ASN
1	E	1022	HIS
1	E	1073	ASN
1	E	1169	ASN
1	E	1176	HIS
1	E	1179	GLN
1	E	1284	ASN
1	E	1301	HIS
1	E	1306	ASN
1	E	1323	GLN
1	E	1353	HIS
1	E	1357	HIS
1	E	1377	ASN
1	F	4	ASN
1	F	24	ASN
1	F	126	HIS
1	F	362	GLN
1	F	402	GLN
1	F	429	ASN
1	F	433	GLN
1	F	442	ASN
1	F	496	HIS
1	F	543	HIS
1	F	695	GLN

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Mol	Chain	Res	Type
1	F	775	GLN
1	F	788	HIS
1	F	804	HIS
1	F	824	HIS
1	F	833	GLN
1	F	848	HIS
1	F	909	GLN
1	F	921	GLN
1	F	942	GLN
1	F	951	HIS
1	F	964	HIS
1	F	988	GLN
1	F	1022	HIS
1	F	1090	HIS
1	F	1169	ASN
1	F	1197	GLN
1	F	1246	GLN
1	F	1310	GLN
1	F	1357	HIS
1	G	64	GLN
1	G	166	GLN
1	G	317	ASN
1	G	333	HIS
1	G	433	GLN
1	G	442	ASN
1	G	465	HIS
1	G	531	HIS
1	G	534	ASN
1	G	543	HIS
1	G	564	HIS
1	G	596	HIS
1	G	735	HIS
1	G	768	ASN
1	G	788	HIS
1	G	849	HIS
1	G	908	GLN
1	G	909	GLN
1	G	926	ASN
1	G	965	GLN
1	G	1022	HIS
1	G	1089	HIS
1	G	1122	GLN

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Mol	Chain	Res	Type
1	G	1137	GLN
1	G	1139	ASN
1	G	1149	GLN
1	G	1176	HIS
1	G	1178	GLN
1	G	1179	GLN
1	G	1216	ASN
1	G	1276	ASN
1	G	1283	ASN
1	G	1306	ASN
1	G	1357	HIS
1	H	166	GLN
1	H	226	HIS
1	H	433	GLN
1	H	442	ASN
1	H	531	HIS
1	H	543	HIS
1	H	564	HIS
1	H	596	HIS
1	H	669	HIS
1	H	824	HIS
1	H	849	HIS
1	H	908	GLN
1	H	909	GLN
1	H	942	GLN
1	H	964	HIS
1	H	1022	HIS
1	H	1073	ASN
1	H	1176	HIS
1	H	1178	GLN
1	H	1197	GLN
1	H	1216	ASN
1	H	1289	ASN
1	H	1323	GLN
1	H	1329	GLN
1	H	1351	GLN
1	H	1353	HIS
1	H	1357	HIS
1	I	24	ASN
1	I	35	HIS
1	I	166	GLN
1	I	178	ASN

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Mol	Chain	Res	Type
1	I	402	GLN
1	I	433	GLN
1	I	444	ASN
1	I	461	HIS
1	I	465	HIS
1	I	531	HIS
1	I	534	ASN
1	I	596	HIS
1	I	695	GLN
1	I	824	HIS
1	I	837	GLN
1	I	909	GLN
1	I	964	HIS
1	I	997	HIS
1	I	1022	HIS
1	I	1284	ASN
1	I	1357	HIS
1	J	35	HIS
1	J	121	ASN
1	J	126	HIS
1	J	195	GLN
1	J	285	ASN
1	J	301	GLN
1	J	376	ASN
1	J	392	GLN
1	J	454	ASN
1	J	465	HIS
1	J	531	HIS
1	J	560	HIS
1	J	564	HIS
1	J	581	GLN
1	J	596	HIS
1	J	722	ASN
1	J	745	GLN
1	J	785	ASN
1	J	788	HIS
1	J	837	GLN
1	J	849	HIS
1	J	859	ASN
1	J	908	GLN
1	J	951	HIS
1	J	976	GLN

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Mol	Chain	Res	Type
1	J	997	HIS
1	J	1056	ASN
1	J	1073	ASN
1	J	1136	GLN
1	J	1216	ASN
1	J	1276	ASN
1	J	1284	ASN
1	J	1357	HIS
1	K	4	ASN
1	K	27	GLN
1	K	79	ASN
1	K	104	HIS
1	K	113	GLN
1	K	142	HIS
1	K	195	GLN
1	K	389	ASN
1	K	392	GLN
1	K	433	GLN
1	K	454	ASN
1	K	465	HIS
1	K	498	ASN
1	K	543	HIS
1	K	570	ASN
1	K	750	ASN
1	K	790	HIS
1	K	834	HIS
1	K	909	GLN
1	K	964	HIS
1	K	965	GLN
1	K	977	GLN
1	K	997	HIS
1	K	1176	HIS
1	K	1197	GLN
1	K	1256	ASN
1	K	1283	ASN
1	K	1289	ASN
1	K	1329	GLN
1	L	113	GLN
1	L	142	HIS
1	L	195	GLN
1	L	333	HIS
1	L	377	HIS

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Mol	Chain	Res	Type
1	L	433	GLN
1	L	465	HIS
1	L	543	HIS
1	L	564	HIS
1	L	587	GLN
1	L	596	HIS
1	L	658	ASN
1	L	672	ASN
1	L	695	GLN
1	L	722	ASN
1	L	735	HIS
1	L	790	HIS
1	L	833	GLN
1	L	842	ASN
1	L	859	ASN
1	L	909	GLN
1	L	942	GLN
1	L	997	HIS
1	L	1022	HIS
1	L	1090	HIS
1	L	1136	GLN
1	L	1176	HIS
1	L	1179	GLN
1	L	1216	ASN
1	L	1296	GLN
1	L	1310	GLN
1	L	1357	HIS
1	M	113	GLN
1	M	178	ASN
1	M	317	ASN
1	M	333	HIS
1	M	402	GLN
1	M	433	GLN
1	M	444	ASN
1	M	454	ASN
1	M	496	HIS
1	M	498	ASN
1	M	531	HIS
1	M	543	HIS
1	M	564	HIS
1	M	735	HIS
1	M	848	HIS

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Mol	Chain	Res	Type
1	M	849	HIS
1	M	913	ASN
1	M	964	HIS
1	M	977	GLN
1	M	997	HIS
1	M	1022	HIS
1	M	1149	GLN
1	M	1296	GLN
1	M	1351	GLN
1	M	1353	HIS
1	N	35	HIS
1	N	113	GLN
1	N	126	HIS
1	N	289	GLN
1	N	301	GLN
1	N	333	HIS
1	N	402	GLN
1	N	433	GLN
1	N	453	GLN
1	N	531	HIS
1	N	543	HIS
1	N	560	HIS
1	N	564	HIS
1	N	587	GLN
1	N	596	HIS
1	N	636	ASN
1	N	669	HIS
1	N	672	ASN
1	N	673	ASN
1	N	745	GLN
1	N	804	HIS
1	N	833	GLN
1	N	964	HIS
1	N	965	GLN
1	N	976	GLN
1	N	1022	HIS
1	N	1056	ASN
1	N	1120	HIS
1	N	1176	HIS
1	N	1179	GLN
1	N	1246	GLN
1	N	1310	GLN

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Mol	Chain	Res	Type
1	N	1351	GLN
1	O	64	GLN
1	O	166	GLN
1	O	222	HIS
1	O	301	GLN
1	O	317	ASN
1	O	389	ASN
1	O	432	GLN
1	O	454	ASN
1	O	465	HIS
1	O	490	GLN
1	O	491	HIS
1	O	496	HIS
1	O	531	HIS
1	O	534	ASN
1	O	560	HIS
1	O	581	GLN
1	O	587	GLN
1	O	596	HIS
1	O	695	GLN
1	O	713	GLN
1	O	722	ASN
1	O	775	GLN
1	O	822	ASN
1	O	824	HIS
1	O	842	ASN
1	O	862	ASN
1	O	942	GLN
1	O	964	HIS
1	O	977	GLN
1	O	997	HIS
1	O	1056	ASN
1	O	1120	HIS
1	O	1176	HIS
1	O	1261	GLN
1	O	1284	ASN
1	O	1310	GLN
1	O	1351	GLN
1	O	1357	HIS
1	P	94	GLN
1	P	123	HIS
1	P	178	ASN

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Mol	Chain	Res	Type
1	P	222	HIS
1	P	317	ASN
1	P	454	ASN
1	P	461	HIS
1	P	531	HIS
1	P	564	HIS
1	P	586	GLN
1	P	587	GLN
1	P	636	ASN
1	P	695	GLN
1	P	735	HIS
1	P	788	HIS
1	P	824	HIS
1	P	842	ASN
1	P	921	GLN
1	P	942	GLN
1	P	946	HIS
1	P	964	HIS
1	P	965	GLN
1	P	977	GLN
1	P	984	ASN
1	P	1033	GLN
1	P	1137	GLN
1	P	1178	GLN
1	P	1246	GLN
1	P	1261	GLN
2	Q	34	ASN
2	Q	71	GLN
2	R	28	GLN
2	R	71	GLN
2	S	34	ASN
2	T	62	GLN
2	U	44	GLN
2	V	11	GLN
2	W	11	GLN
2	W	44	GLN
2	W	54	GLN
2	Y	44	GLN
2	Y	71	GLN
2	Z	31	ASN
2	Z	44	GLN
2	Z	54	GLN

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Mol	Chain	Res	Type
2	a	32	GLN
2	a	34	ASN
2	a	37	ASN
2	b	33	ASN
2	b	44	GLN
2	b	71	GLN
2	c	44	GLN
2	d	32	GLN
2	d	44	GLN
2	d	54	GLN
2	d	71	GLN
2	e	31	ASN
2	e	33	ASN
2	e	37	ASN
2	e	54	GLN
3	f	46	HIS
3	f	48	GLN
3	f	156	ASN
3	g	227	GLN
3	g	312	HIS
3	h	4	GLN
3	h	13	GLN
3	h	136	ASN
3	h	156	ASN
3	h	227	GLN
3	h	312	HIS
3	i	136	ASN
3	i	309	GLN
3	i	312	HIS
3	j	46	HIS
3	j	256	GLN
3	j	288	GLN
3	l	136	ASN
3	l	182	HIS
4	k	35	HIS
4	k	120	HIS
4	k	128	ASN
4	k	148	GLN
4	k	184	HIS
4	k	291	GLN
4	l	39	ASN
4	l	291	GLN

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Mol	Chain	Res	Type
4	m	35	HIS
4	m	128	ASN
4	m	173	HIS
4	m	291	GLN
4	n	41	GLN
4	n	102	GLN
4	n	104	HIS
4	n	279	ASN
4	o	98	GLN
4	o	102	GLN
4	o	120	HIS
4	o	128	ASN
4	o	230	HIS
4	o	291	GLN
4	2	35	HIS
4	2	38	GLN
4	2	47	GLN
4	2	204	ASN
4	2	279	ASN
4	p	120	HIS
4	p	128	ASN
4	p	154	ASN
4	p	184	HIS
4	p	230	HIS
4	p	233	HIS
4	p	272	GLN
4	q	23	GLN
4	q	35	HIS
4	q	62	ASN
4	q	233	HIS
4	r	38	GLN
4	r	154	ASN
4	r	204	ASN
4	r	233	HIS
4	r	272	GLN
4	s	23	GLN
4	s	35	HIS
4	s	89	GLN
4	s	154	ASN
4	s	175	HIS
4	s	204	ASN
4	s	233	HIS

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Mol	Chain	Res	Type
4	s	240	GLN
4	s	272	GLN
4	t	35	HIS
4	t	162	GLN
4	t	230	HIS
4	t	233	HIS
4	3	154	ASN
4	3	233	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.