Full wwPDB X-ray Structure Validation Report (i)

Sep 15, 2023 – 12:55 AM EDT

PDB ID	:	4V4M
Title	:	1.45 Angstrom Structure of STNV coat protein
Authors	:	Lane, S.W.; Dennis, C.A.; Lane, C.L.; Trinh, C.H.; Rizkallah, P.J.; Stockley, P.G.; Phillips, S.E.V.
Deposited on	:	2011-04-28
Resolution	:	1.45 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

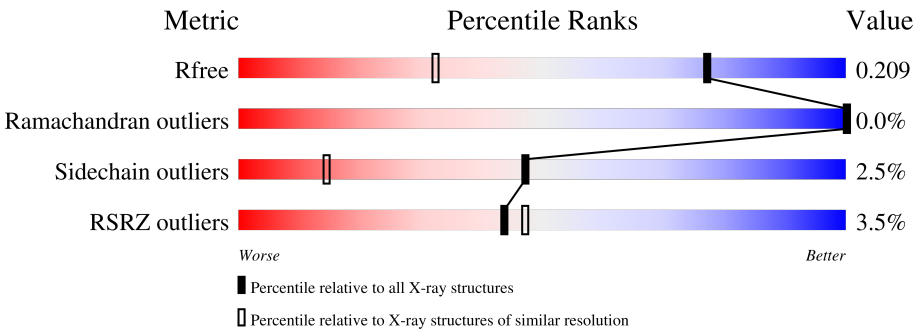
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	196	4% 93% • 6%
1	1	196	3% 92% • 6%
1	2	196	3% 91% • 6%
1	3	196	4% 92% • 6%
1	4	196	4% 92% • 6%
1	5	196	5% 92% • 6%

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Mol	Chain	Length	Quality of chain
1	6	196	5% 93% 6%
1	7	196	3% 92% 6%
1	A	196	4% 92% 6%
1	B	196	3% 92% 6%
1	C	196	4% 90% 6%
1	D	196	4% 91% 6%
1	E	196	3% 92% 6%
1	F	196	3% 92% 6%
1	G	196	3% 91% 6%
1	H	196	4% 91% 6%
1	I	196	4% 93% 6%
1	J	196	4% 91% 6%
1	K	196	4% 91% 6%
1	L	196	3% 91% 6%
1	M	196	4% 91% 6%
1	N	196	3% 92% 6%
1	O	196	3% 91% 6%
1	P	196	4% 92% 6%
1	Q	196	4% 92% 6%
1	R	196	3% 91% 6%
1	S	196	3% 92% 6%
1	T	196	3% 91% 6%
1	U	196	4% 92% 6%
1	V	196	3% 92% 6%
1	W	196	4% 92% 6%

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Mol	Chain	Length	Quality of chain
1	X	196	3% 92% 6%
1	Y	196	4% 92% 6%
1	Z	196	3% 92% 6%
1	a	196	3% 93% 6%
1	b	196	3% 91% 6%
1	c	196	5% 91% 6%
1	d	196	3% 92% 6%
1	e	196	3% 92% 6%
1	f	196	3% 91% 6%
1	g	196	3% 92% 6%
1	h	196	3% 92% 6%
1	i	196	4% 92% 6%
1	j	196	4% 93% 6%
1	k	196	4% 92% 6%
1	l	196	4% 92% 6%
1	m	196	3% 92% 6%
1	n	196	3% 92% 6%
1	o	196	4% 92% 6%
1	p	196	4% 92% 6%
1	q	196	3% 92% 6%
1	r	196	3% 90% 6%
1	s	196	5% 92% 6%
1	t	196	3% 91% 6%
1	u	196	4% 91% 6%
1	v	196	4% 92% 6%

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Mol	Chain	Length	Quality of chain
1	w	196	3% 93% • 6%
1	x	196	4% 92% • 6%
1	y	196	4% 92% • 6%
1	z	196	3% 92% • • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 102135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	e	184	1439	898	261	273	7	0	2	0
1	f	184	1450	908	263	272	7	0	4	0
1	g	184	1437	898	260	272	7	0	2	0
1	h	184	1451	906	265	274	6	0	4	0
1	i	184	1448	902	265	274	7	0	3	0
1	j	184	1441	898	264	273	6	0	2	0
1	k	184	1440	897	264	273	6	0	2	0
1	l	184	1432	893	260	272	7	0	1	0
1	m	184	1440	898	263	272	7	0	2	0
1	n	184	1450	906	264	273	7	0	4	0
1	o	184	1433	893	261	273	6	0	1	0
1	p	184	1432	893	260	272	7	0	1	0
1	q	184	1432	893	260	272	7	0	1	0
1	r	184	1448	903	266	272	7	0	3	0
1	s	184	1436	897	260	272	7	0	2	0
1	t	184	1472	919	272	274	7	0	7	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	u	184	1440	898	263	272	7	0	2	0
			Total	C	N	O	S			
1	v	184	1440	898	263	272	7	0	2	0
			Total	C	N	O	S			
1	w	184	1444	902	263	272	7	0	3	0
			Total	C	N	O	S			
1	x	184	1445	901	264	273	7	0	3	0
			Total	C	N	O	S			
1	y	184	1436	897	260	272	7	0	2	0
			Total	C	N	O	S			
1	z	184	1451	907	264	273	7	0	4	0
			Total	C	N	O	S			
1	0	184	1440	898	263	272	7	0	2	0
			Total	C	N	O	S			
1	1	184	1446	902	264	273	7	0	3	0
			Total	C	N	O	S			
1	2	184	1452	906	266	273	7	0	4	0
			Total	C	N	O	S			
1	3	184	1454	907	267	273	7	0	4	0
			Total	C	N	O	S			
1	4	184	1443	900	262	274	7	0	3	0
			Total	C	N	O	S			
1	5	184	1432	892	261	273	6	0	1	0
			Total	C	N	O	S			
1	6	184	1448	903	266	272	7	0	3	0
			Total	C	N	O	S			
1	7	184	1438	897	261	273	7	0	2	0
			Total	C	N	O	S			
1	A	184	1460	913	265	275	7	0	6	0
			Total	C	N	O	S			
1	B	184	1464	917	267	273	7	0	6	0
			Total	C	N	O	S			
1	C	184	1454	906	265	276	7	0	4	0
			Total	C	N	O	S			
1	D	184	1445	905	260	273	7	0	4	0
			Total	C	N	O	S			
1	E	184	1437	898	260	272	7	0	2	0
			Total	C	N	O	S			
1	F	184	1438	897	261	273	7	0	2	0
			Total	C	N	O	S			
1	G	184	1450	906	264	273	7	0	4	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	184	1440	898	263	272	7	0	2	0
			Total	C	N	O	S			
1	I	184	1443	902	260	274	7	0	3	0
			Total	C	N	O	S			
1	J	184	1440	898	263	272	7	0	2	0
			Total	C	N	O	S			
1	K	184	1470	919	269	275	7	0	7	0
			Total	C	N	O	S			
1	L	184	1458	913	266	272	7	0	5	0
			Total	C	N	O	S			
1	M	184	1442	901	261	273	7	0	3	0
			Total	C	N	O	S			
1	N	184	1445	901	264	273	7	0	3	0
			Total	C	N	O	S			
1	O	184	1440	898	263	272	7	0	2	0
			Total	C	N	O	S			
1	P	184	1465	917	268	273	7	0	6	0
			Total	C	N	O	S			
1	Q	184	1437	896	261	273	7	0	2	0
			Total	C	N	O	S			
1	R	184	1442	903	260	272	7	0	3	0
			Total	C	N	O	S			
1	S	184	1465	916	268	274	7	0	6	0
			Total	C	N	O	S			
1	T	184	1440	900	260	273	7	0	3	0
			Total	C	N	O	S			
1	U	184	1451	905	265	274	7	0	4	0
			Total	C	N	O	S			
1	V	184	1443	902	260	274	7	0	3	0
			Total	C	N	O	S			
1	W	184	1432	893	260	272	7	0	1	0
			Total	C	N	O	S			
1	X	184	1437	898	260	272	7	0	2	0
			Total	C	N	O	S			
1	Y	184	1445	901	264	273	7	0	3	0
			Total	C	N	O	S			
1	Z	184	1448	903	266	272	7	0	3	0
			Total	C	N	O	S			
1	a	184	1456	910	265	274	7	0	5	0
			Total	C	N	O	S			
1	b	184	1432	893	260	272	7	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	c	184	1448	903	266	272	7	0	3	0
			Total	C	N	O	S			
1	d	184	1439	898	261	273	7	0	2	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	e	1	1	1	0	0
			Total	Ca		
2	f	1	1	1	0	0
			Total	Ca		
2	g	1	1	1	0	0
			Total	Ca		
2	h	1	1	1	0	0
			Total	Ca		
2	i	2	2	2	0	0
			Total	Ca		
2	j	2	2	2	0	0
			Total	Ca		
2	k	1	1	1	0	0
			Total	Ca		
2	l	1	1	1	0	0
			Total	Ca		
2	m	1	1	1	0	0
			Total	Ca		
2	n	2	2	2	0	0
			Total	Ca		
2	o	2	2	2	0	0
			Total	Ca		
2	p	1	1	1	0	0
			Total	Ca		
2	q	2	2	2	0	0
			Total	Ca		
2	r	1	1	1	0	0
			Total	Ca		
2	s	1	1	1	0	0
			Total	Ca		
2	t	1	1	1	0	0
			Total	Ca		
2	u	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	v	1	1	1	0	0
2	w	1	1	1	0	0
2	x	1	1	1	0	0
2	y	1	1	1	0	0
2	z	1	1	1	0	0
2	0	2	2	2	0	0
2	1	3	3	3	0	0
2	2	2	2	2	0	0
2	3	2	2	2	0	0
2	4	2	2	2	0	0
2	5	2	2	2	0	0
2	6	2	2	2	0	0
2	7	1	1	1	0	0
2	A	2	2	2	0	0
2	B	3	3	3	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	3	3	3	0	0
2	F	1	1	1	0	0
2	G	3	3	3	0	0
2	H	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	I	2	2	2	0	0
2	J	1	1	1	0	0
2	K	2	2	2	0	0
2	L	1	1	1	0	0
2	M	1	1	1	0	0
2	N	2	2	2	0	0
2	O	1	1	1	0	0
2	P	1	1	1	0	0
2	Q	2	2	2	0	0
2	R	2	2	2	0	0
2	S	2	2	2	0	0
2	T	2	2	2	0	0
2	U	3	3	3	0	0
2	V	2	2	2	0	0
2	W	1	1	1	0	0
2	X	1	1	1	0	0
2	Y	1	1	1	0	0
2	Z	1	1	1	0	0
2	a	1	1	1	0	0
2	b	2	2	2	0	0
2	c	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	d	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	e	258	258	258	0	0
3	f	231	231	231	0	0
3	g	260	260	260	0	0
3	h	281	281	281	0	0
3	i	282	282	282	0	0
3	j	267	267	267	0	0
3	k	256	256	256	0	0
3	l	257	257	257	0	0
3	m	252	252	252	0	0
3	n	251	251	251	0	0
3	o	262	262	262	0	0
3	p	238	238	238	0	0
3	q	258	258	258	0	0
3	r	287	287	287	0	0
3	s	226	226	226	0	0
3	t	236	236	236	0	0
3	u	240	240	240	0	0
3	v	249	249	249	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	w	279	Total O 279 279	0	0
3	x	260	Total O 260 260	0	0
3	y	294	Total O 294 294	0	0
3	z	264	Total O 264 264	0	0
3	0	242	Total O 242 242	0	0
3	1	256	Total O 256 256	0	0
3	2	259	Total O 259 259	0	0
3	3	245	Total O 245 245	0	0
3	4	278	Total O 278 278	0	0
3	5	247	Total O 247 247	0	0
3	6	264	Total O 264 264	0	0
3	7	249	Total O 249 249	0	0
3	A	246	Total O 246 246	0	0
3	B	235	Total O 235 235	0	0
3	C	250	Total O 250 250	0	0
3	D	255	Total O 255 255	0	0
3	E	229	Total O 229 229	0	0
3	F	217	Total O 217 217	0	0
3	G	253	Total O 253 253	0	0
3	H	248	Total O 248 248	0	0
3	I	240	Total O 240 240	0	0

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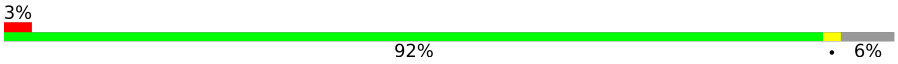
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	245	Total O 245 245	0	0
3	K	273	Total O 273 273	0	0
3	L	239	Total O 239 239	0	0
3	M	253	Total O 253 253	0	0
3	N	256	Total O 256 256	0	0
3	O	250	Total O 250 250	0	0
3	P	250	Total O 250 250	0	0
3	Q	255	Total O 255 255	0	0
3	R	286	Total O 286 286	0	0
3	S	237	Total O 237 237	0	0
3	T	295	Total O 295 295	0	0
3	U	266	Total O 266 266	0	0
3	V	258	Total O 258 258	0	0
3	W	256	Total O 256 256	0	0
3	X	256	Total O 256 256	0	0
3	Y	262	Total O 262 262	0	0
3	Z	285	Total O 285 285	0	0
3	a	257	Total O 257 257	0	0
3	b	254	Total O 254 254	0	0
3	c	269	Total O 269 269	0	0
3	d	244	Total O 244 244	0	0

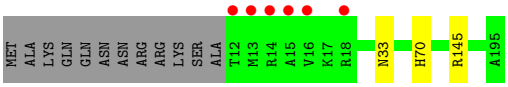
3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Coat protein

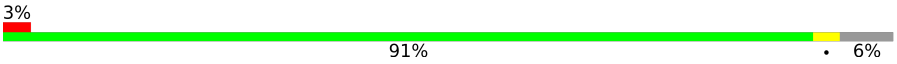
Chain e:

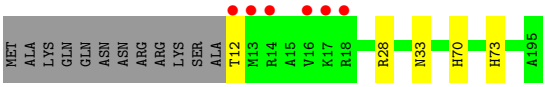




- Molecule 1: Coat protein

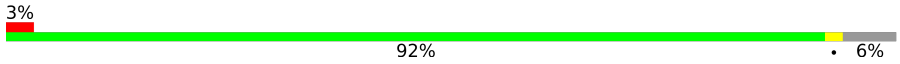
Chain f:

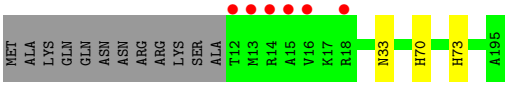




- Molecule 1: Coat protein

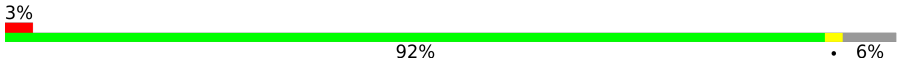
Chain g:

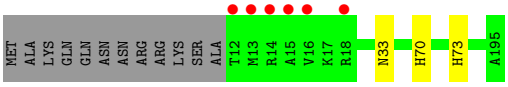




- Molecule 1: Coat protein

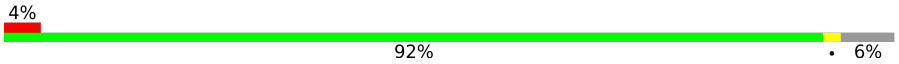
Chain h:

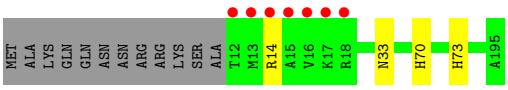




- Molecule 1: Coat protein

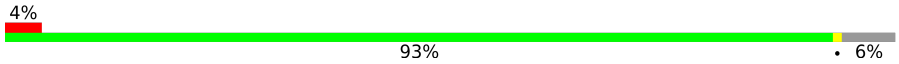
Chain i:

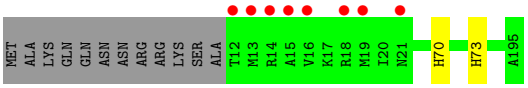




- Molecule 1: Coat protein

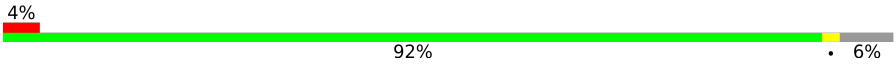
Chain j:

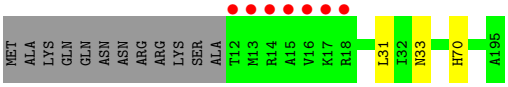




• Molecule 1: Coat protein

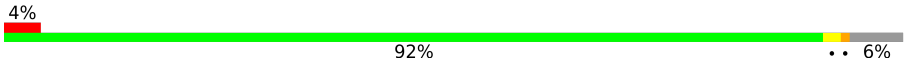
Chain k:

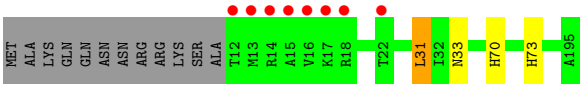




• Molecule 1: Coat protein

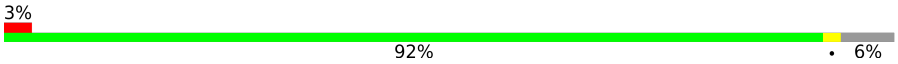
Chain l:

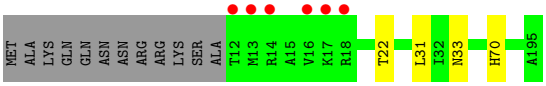




• Molecule 1: Coat protein

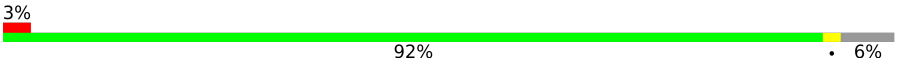
Chain m:

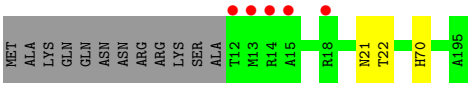




• Molecule 1: Coat protein

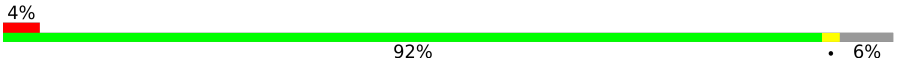
Chain n:

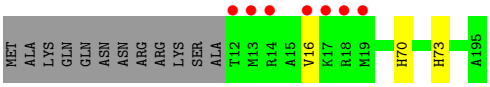




• Molecule 1: Coat protein

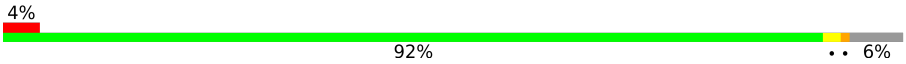
Chain o:

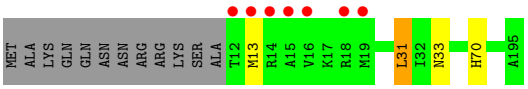




• Molecule 1: Coat protein

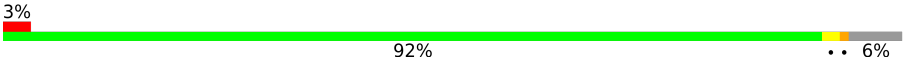
Chain p:

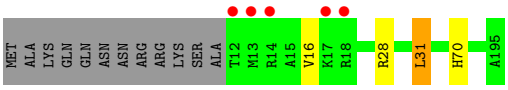




- Molecule 1: Coat protein

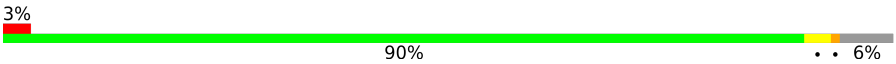
Chain q:

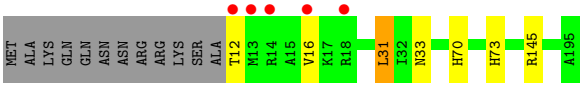




- Molecule 1: Coat protein

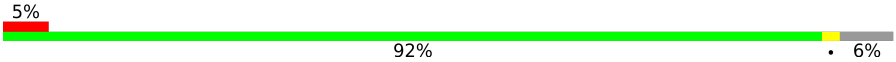
Chain r:

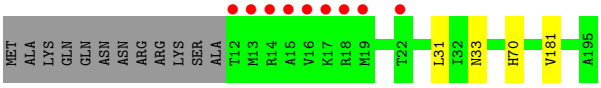




- Molecule 1: Coat protein

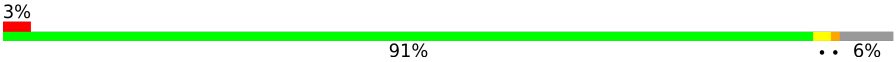
Chain s:

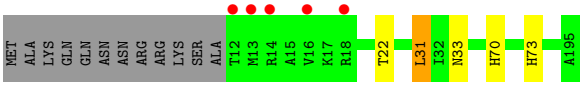




- Molecule 1: Coat protein

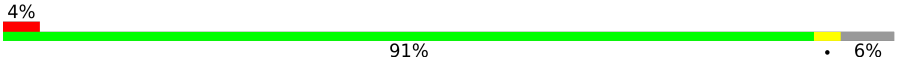
Chain t:

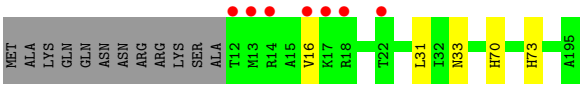




- Molecule 1: Coat protein

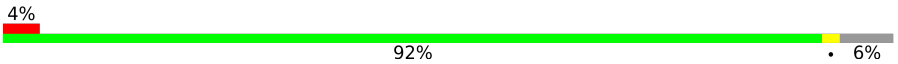
Chain u:

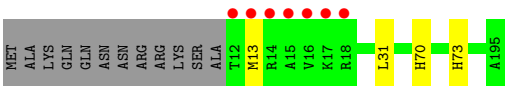




- Molecule 1: Coat protein

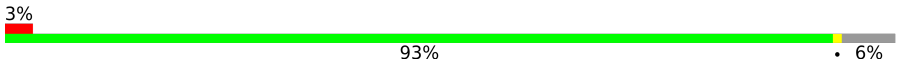
Chain v:

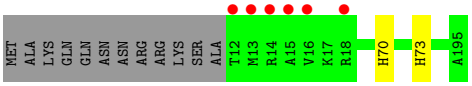




- Molecule 1: Coat protein

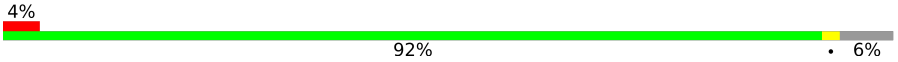
Chain w:

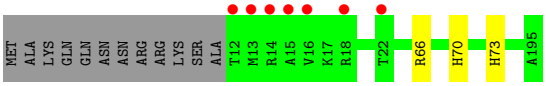




• Molecule 1: Coat protein

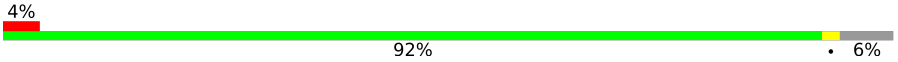
Chain x:

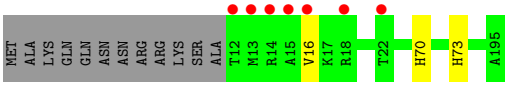




• Molecule 1: Coat protein

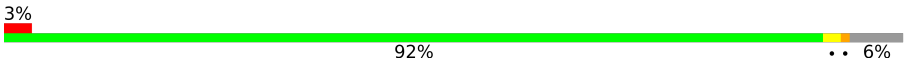
Chain y:

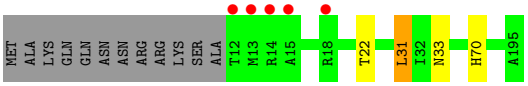




• Molecule 1: Coat protein

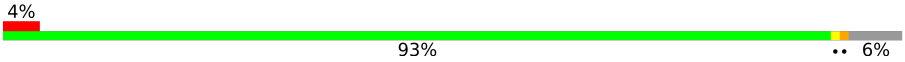
Chain z:

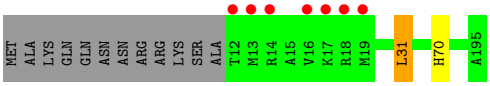




• Molecule 1: Coat protein

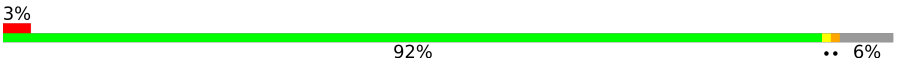
Chain 0:

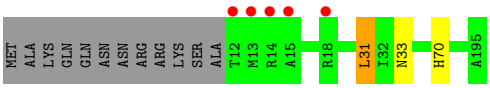




• Molecule 1: Coat protein

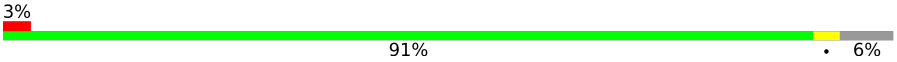
Chain 1:

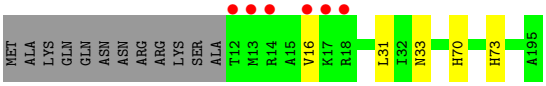




• Molecule 1: Coat protein

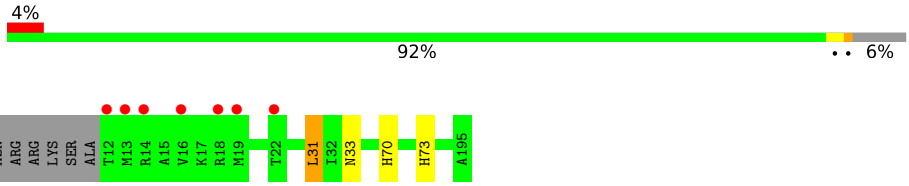
Chain 2:





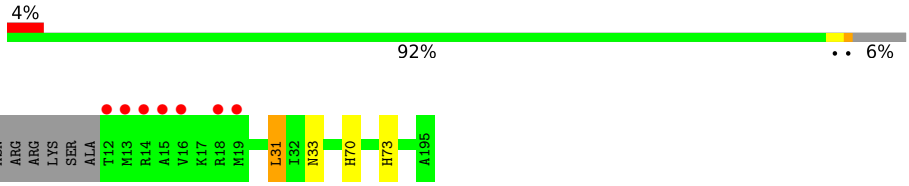
• Molecule 1: Coat protein

Chain 3:



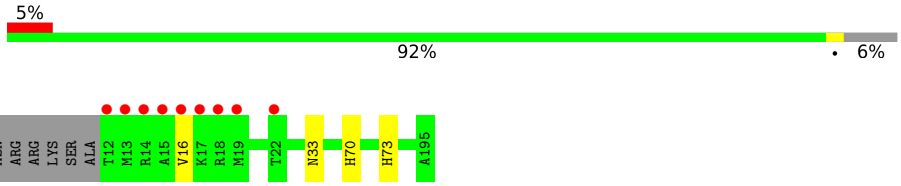
• Molecule 1: Coat protein

Chain 4:



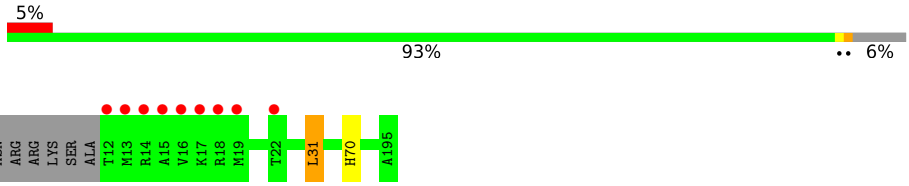
• Molecule 1: Coat protein

Chain 5:



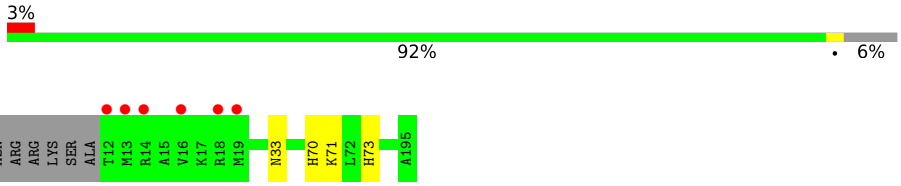
• Molecule 1: Coat protein

Chain 6:



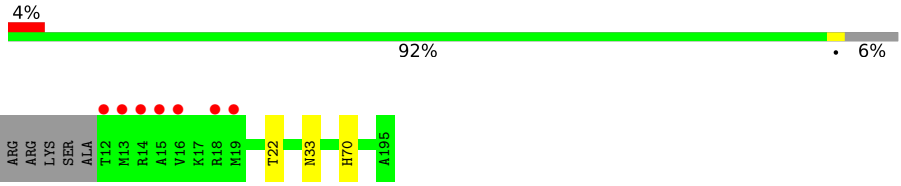
• Molecule 1: Coat protein

Chain 7:



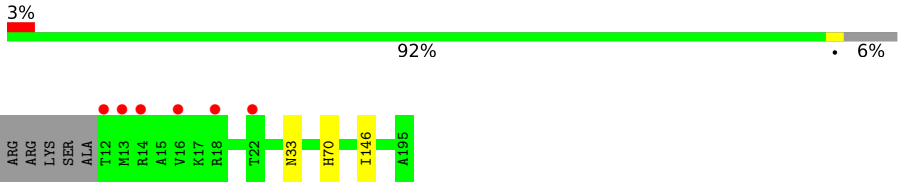
• Molecule 1: Coat protein

Chain A:



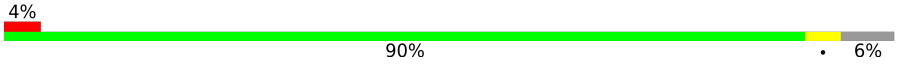
• Molecule 1: Coat protein

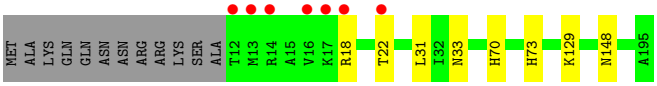
Chain B:



• Molecule 1: Coat protein

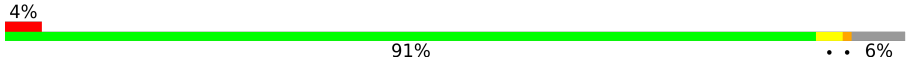
Chain C:

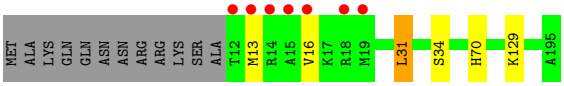




• Molecule 1: Coat protein

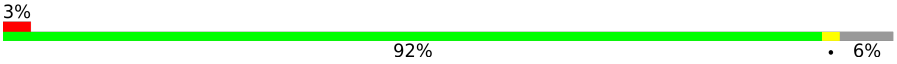
Chain D:

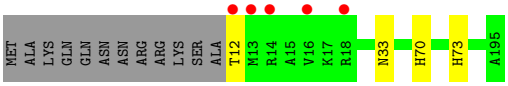




• Molecule 1: Coat protein

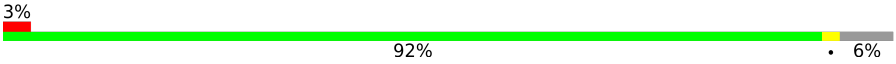
Chain E:

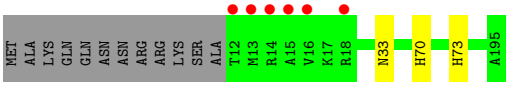




• Molecule 1: Coat protein

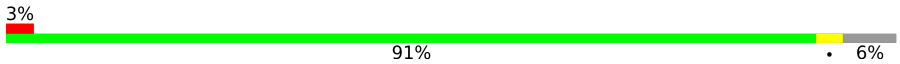
Chain F:

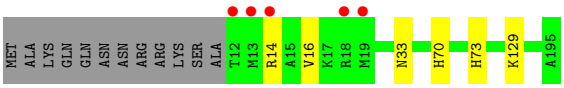




• Molecule 1: Coat protein

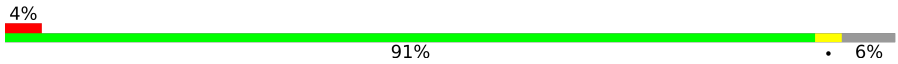
Chain G:

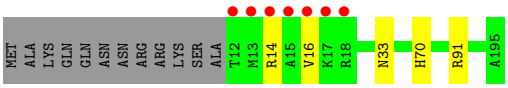




• Molecule 1: Coat protein

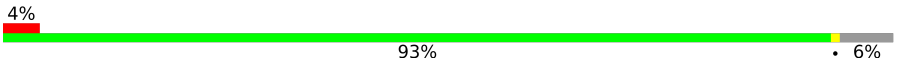
Chain H:

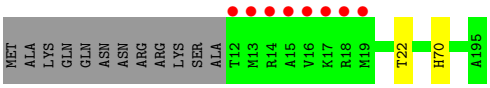




• Molecule 1: Coat protein

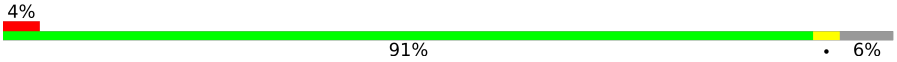
Chain I:

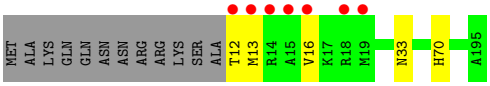




• Molecule 1: Coat protein

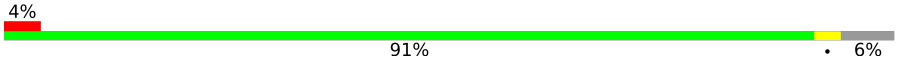
Chain J:

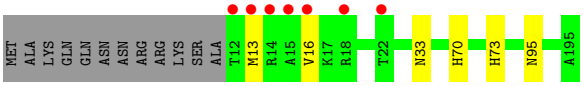




• Molecule 1: Coat protein

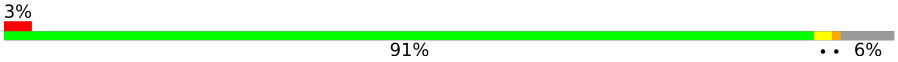
Chain K:

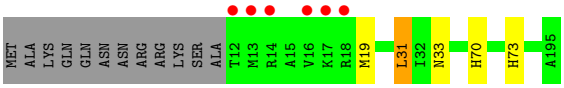




• Molecule 1: Coat protein

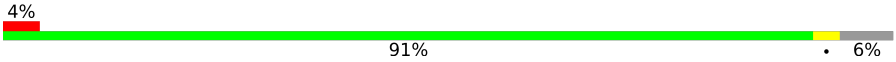
Chain L:

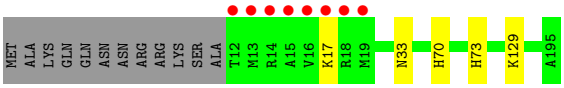




• Molecule 1: Coat protein

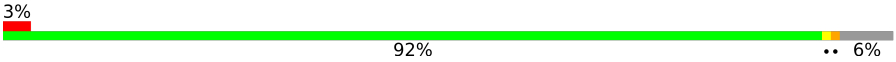
Chain M:

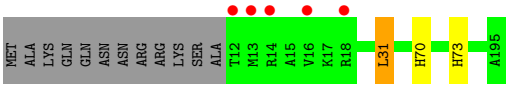




• Molecule 1: Coat protein

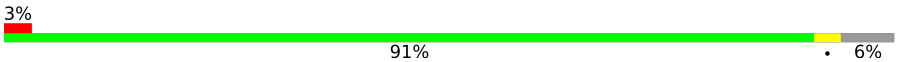
Chain N:

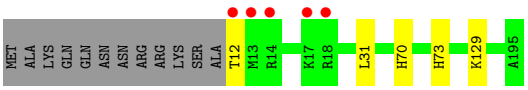




• Molecule 1: Coat protein

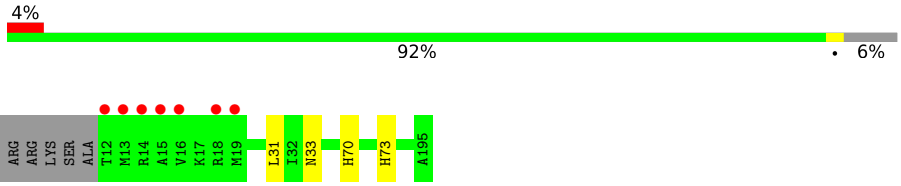
Chain O:





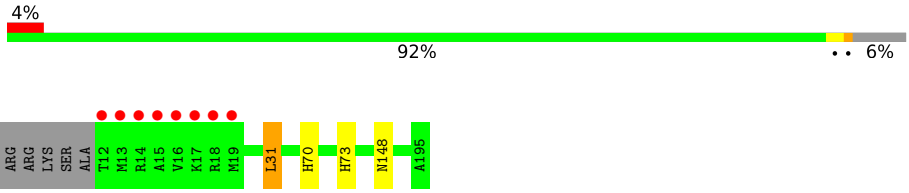
• Molecule 1: Coat protein

Chain P:



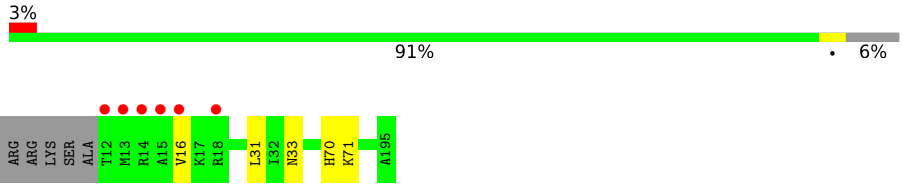
• Molecule 1: Coat protein

Chain Q:



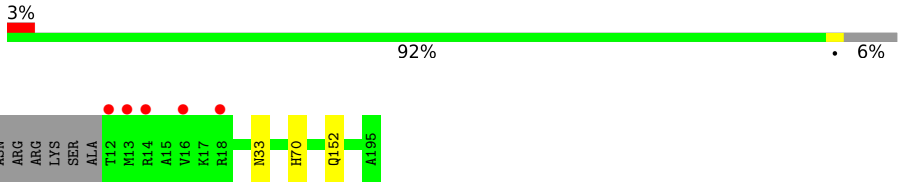
• Molecule 1: Coat protein

Chain R:



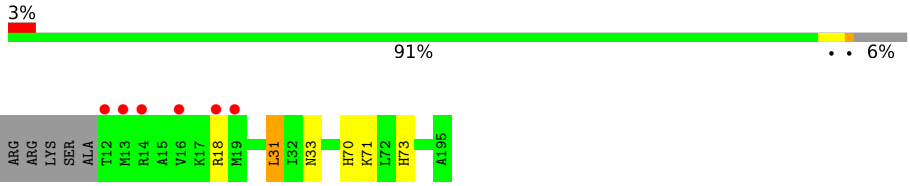
• Molecule 1: Coat protein

Chain S:



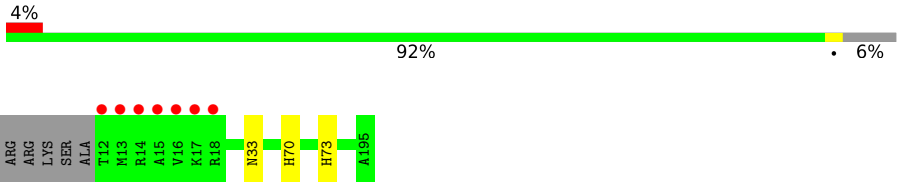
• Molecule 1: Coat protein

Chain T:



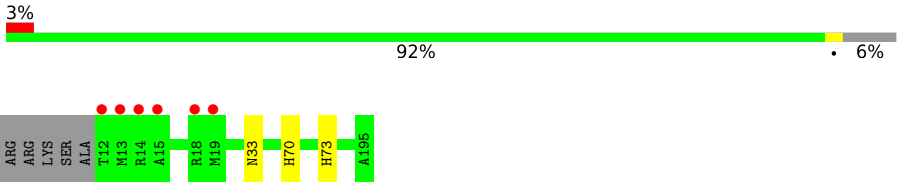
• Molecule 1: Coat protein

Chain U:



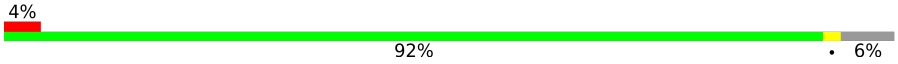
• Molecule 1: Coat protein

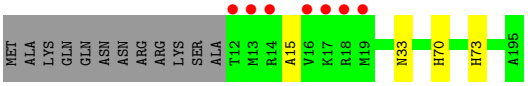
Chain V:



- Molecule 1: Coat protein

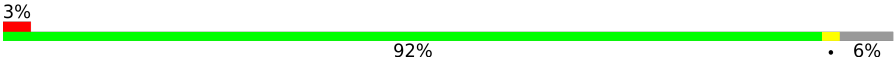
Chain W:

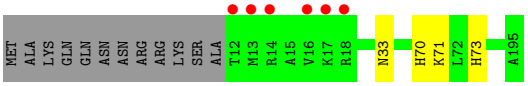




- Molecule 1: Coat protein

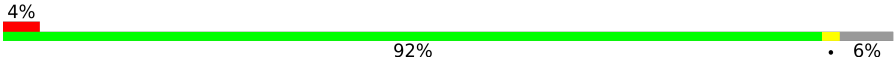
Chain X:

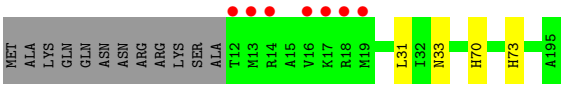




- Molecule 1: Coat protein

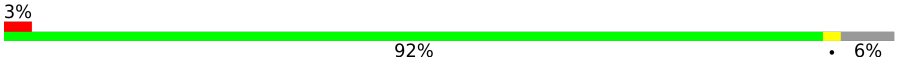
Chain Y:

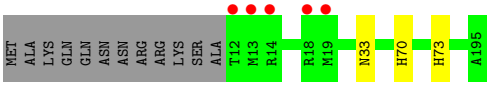




- Molecule 1: Coat protein

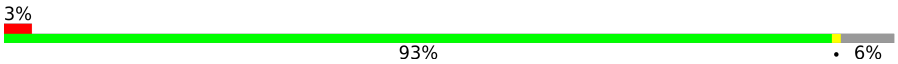
Chain Z:

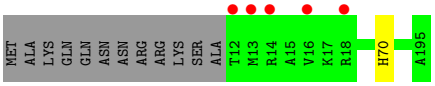




- Molecule 1: Coat protein

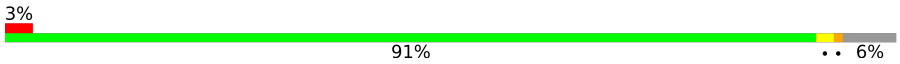
Chain a:

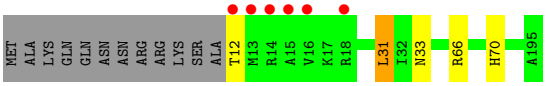




- Molecule 1: Coat protein

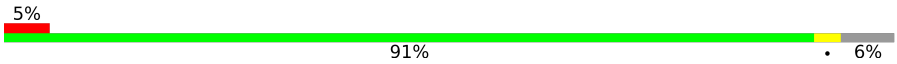
Chain b:

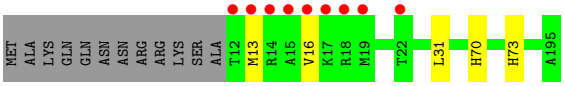




- Molecule 1: Coat protein

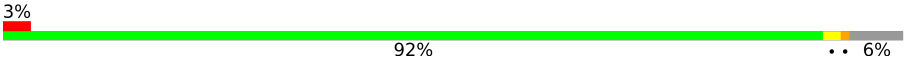
Chain c:

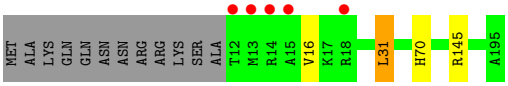




• Molecule 1: Coat protein

Chain d:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	307.58Å 302.26Å 181.92Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	12.00 – 1.45 12.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (12.00-1.45) 76.2 (12.00-1.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.175 , 0.208 0.185 , 0.209	Depositor DCC
R_{free} test set	111080 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	10.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l 0.009 for -k,-h,-l 0.013 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	102135	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0	0.47	0/1468	0.64	1/1988 (0.1%)
1	1	0.45	0/1477	0.64	1/2000 (0.1%)
1	2	0.45	0/1486	0.62	0/2012
1	3	0.45	0/1488	0.63	1/2014 (0.0%)
1	4	0.46	0/1474	0.62	1/1997 (0.1%)
1	5	0.46	0/1457	0.61	0/1975
1	6	0.44	0/1479	0.62	1/2002 (0.0%)
1	7	0.44	0/1466	0.62	0/1986
1	A	0.46	0/1500	0.65	0/2032
1	B	0.46	0/1504	0.63	0/2036
1	C	0.44	0/1485	0.61	0/2011
1	D	0.44	0/1479	0.64	2/2004 (0.1%)
1	E	0.43	0/1465	0.62	0/1985
1	F	0.44	0/1466	0.62	0/1986
1	G	0.43	0/1484	0.62	0/2010
1	H	0.45	0/1468	0.61	0/1988
1	I	0.45	0/1474	0.62	0/1997
1	J	0.46	0/1468	0.64	0/1988
1	K	0.45	0/1513	0.67	0/2048
1	L	0.44	0/1495	0.60	1/2024 (0.0%)
1	M	0.46	0/1473	0.61	0/1996
1	N	0.43	0/1476	0.63	1/1999 (0.1%)
1	O	0.43	0/1468	0.61	0/1988
1	P	0.46	0/1505	0.62	0/2036
1	Q	0.45	0/1465	0.62	1/1985 (0.1%)
1	R	0.46	0/1473	0.63	0/1996
1	S	0.47	0/1505	0.63	0/2037
1	T	0.47	0/1471	0.67	2/1993 (0.1%)
1	U	0.46	0/1485	0.64	0/2011
1	V	0.47	0/1474	0.64	0/1997
1	W	0.44	0/1457	0.62	0/1974
1	X	0.46	0/1465	0.61	0/1985

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Y	0.47	0/1476	0.62	0/1999
1	Z	0.47	0/1479	0.65	0/2002
1	a	0.45	0/1493	0.64	0/2022
1	b	0.47	0/1457	0.65	1/1974 (0.1%)
1	c	0.48	0/1479	0.62	0/2002
1	d	0.47	0/1464	0.64	1/1984 (0.1%)
1	e	0.46	0/1464	0.64	0/1984
1	f	0.44	0/1484	0.61	0/2010
1	g	0.44	0/1465	0.62	0/1985
1	h	0.47	0/1485	0.65	0/2012
1	i	0.45	0/1476	0.61	0/1999
1	j	0.45	0/1469	0.63	0/1990
1	k	0.48	0/1468	0.64	0/1989
1	l	0.46	0/1457	0.64	1/1974 (0.1%)
1	m	0.43	0/1468	0.60	0/1988
1	n	0.43	0/1484	0.62	0/2010
1	o	0.45	0/1458	0.62	0/1976
1	p	0.45	0/1457	0.64	1/1974 (0.1%)
1	q	0.47	0/1457	0.64	1/1974 (0.1%)
1	r	0.47	0/1479	0.65	1/2002 (0.0%)
1	s	0.46	0/1464	0.63	0/1984
1	t	0.44	0/1515	0.62	1/2050 (0.0%)
1	u	0.46	0/1468	0.61	0/1988
1	v	0.46	0/1468	0.64	0/1988
1	w	0.47	0/1475	0.65	0/1998
1	x	0.46	0/1476	0.63	0/1999
1	y	0.46	0/1464	0.64	0/1984
1	z	0.46	0/1485	0.64	2/2011 (0.1%)
All	All	0.45	0/88547	0.63	21/119932 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	l	31	LEU	CA-CB-CG	6.64	130.58	115.30
1	q	31	LEU	CA-CB-CG	6.54	130.35	115.30
1	p	31	LEU	CA-CB-CG	6.10	129.32	115.30
1	4	31	LEU	CA-CB-CG	5.94	128.96	115.30
1	3	31	LEU	CA-CB-CG	5.89	128.85	115.30
1	t	31	LEU	CA-CB-CG	5.82	128.68	115.30
1	1	31	LEU	CA-CB-CG	5.75	128.52	115.30
1	N	31	LEU	CA-CB-CG	5.72	128.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	r	31	LEU	CA-CB-CG	5.54	128.05	115.30
1	D	31[A]	LEU	CA-CB-CG	5.49	127.93	115.30
1	D	31[B]	LEU	CA-CB-CG	5.49	127.93	115.30
1	6	31	LEU	CA-CB-CG	5.37	127.65	115.30
1	d	31	LEU	CA-CB-CG	5.32	127.53	115.30
1	T	31[A]	LEU	CA-CB-CG	5.31	127.52	115.30
1	T	31[B]	LEU	CA-CB-CG	5.31	127.52	115.30
1	0	31	LEU	CA-CB-CG	5.30	127.50	115.30
1	L	31	LEU	CA-CB-CG	5.28	127.45	115.30
1	Q	31	LEU	CA-CB-CG	5.12	127.09	115.30
1	z	31[A]	LEU	CA-CB-CG	5.10	127.03	115.30
1	z	31[B]	LEU	CA-CB-CG	5.10	127.03	115.30
1	b	31	LEU	CA-CB-CG	5.09	127.00	115.30

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	1	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	2	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	3	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	4	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	5	183/196 (93%)	179 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	7	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	A	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
1	B	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
1	C	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	D	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	E	184/196 (94%)	176 (96%)	8 (4%)	0	100	100
1	F	184/196 (94%)	176 (96%)	8 (4%)	0	100	100
1	G	186/196 (95%)	178 (96%)	7 (4%)	1 (0%)	29	9
1	H	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	I	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	J	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	K	189/196 (96%)	184 (97%)	4 (2%)	1 (0%)	29	9
1	L	187/196 (95%)	182 (97%)	5 (3%)	0	100	100
1	M	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	N	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	O	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	P	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
1	Q	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	R	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	S	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
1	T	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	U	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	V	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	W	183/196 (93%)	176 (96%)	6 (3%)	1 (0%)	29	9
1	X	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	Y	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	Z	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	a	187/196 (95%)	182 (97%)	5 (3%)	0	100	100
1	b	183/196 (93%)	179 (98%)	4 (2%)	0	100	100
1	c	185/196 (94%)	179 (97%)	5 (3%)	1 (0%)	29	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	e	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	f	186/196 (95%)	178 (96%)	8 (4%)	0	100	100
1	g	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	h	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	i	185/196 (94%)	179 (97%)	5 (3%)	1 (0%)	29	9
1	j	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	k	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	l	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	m	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	n	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	o	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	p	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	q	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	r	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	s	184/196 (94%)	177 (96%)	7 (4%)	0	100	100
1	t	189/196 (96%)	183 (97%)	6 (3%)	0	100	100
1	u	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	v	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	w	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
1	x	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	y	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	z	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
All	All	11101/11760 (94%)	10766 (97%)	330 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	15	ALA
1	G	14	ARG
1	K	13	MET
1	i	14	ARG
1	c	13	MET

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	159/167 (95%)	157 (99%)	2 (1%)	69	40
1	1	160/167 (96%)	157 (98%)	3 (2%)	57	23
1	2	161/167 (96%)	156 (97%)	5 (3%)	40	9
1	3	161/167 (96%)	157 (98%)	4 (2%)	47	14
1	4	160/167 (96%)	156 (98%)	4 (2%)	47	14
1	5	158/167 (95%)	154 (98%)	4 (2%)	47	14
1	6	160/167 (96%)	158 (99%)	2 (1%)	69	40
1	7	159/167 (95%)	155 (98%)	4 (2%)	47	14
1	A	163/167 (98%)	160 (98%)	3 (2%)	59	26
1	B	163/167 (98%)	159 (98%)	4 (2%)	47	14
1	C	161/167 (96%)	152 (94%)	9 (6%)	21	1
1	D	161/167 (96%)	153 (95%)	8 (5%)	24	2
1	E	159/167 (95%)	155 (98%)	4 (2%)	47	14
1	F	159/167 (95%)	156 (98%)	3 (2%)	57	23
1	G	161/167 (96%)	156 (97%)	5 (3%)	40	9
1	H	159/167 (95%)	153 (96%)	6 (4%)	33	5
1	I	160/167 (96%)	158 (99%)	2 (1%)	69	40
1	J	159/167 (95%)	154 (97%)	5 (3%)	40	9
1	K	164/167 (98%)	159 (97%)	5 (3%)	41	9
1	L	162/167 (97%)	157 (97%)	5 (3%)	40	9
1	M	160/167 (96%)	155 (97%)	5 (3%)	40	9
1	N	160/167 (96%)	157 (98%)	3 (2%)	57	23
1	O	159/167 (95%)	154 (97%)	5 (3%)	40	9
1	P	163/167 (98%)	159 (98%)	4 (2%)	47	14
1	Q	159/167 (95%)	154 (97%)	5 (3%)	40	9
1	R	160/167 (96%)	154 (96%)	6 (4%)	33	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	163/167 (98%)	159 (98%)	4 (2%)	47	14
1	T	160/167 (96%)	153 (96%)	7 (4%)	28	3
1	U	161/167 (96%)	158 (98%)	3 (2%)	57	23
1	V	160/167 (96%)	157 (98%)	3 (2%)	57	23
1	W	158/167 (95%)	155 (98%)	3 (2%)	57	23
1	X	159/167 (95%)	155 (98%)	4 (2%)	47	14
1	Y	160/167 (96%)	156 (98%)	4 (2%)	47	14
1	Z	160/167 (96%)	157 (98%)	3 (2%)	57	23
1	a	162/167 (97%)	161 (99%)	1 (1%)	86	69
1	b	158/167 (95%)	153 (97%)	5 (3%)	39	8
1	c	160/167 (96%)	156 (98%)	4 (2%)	47	14
1	d	159/167 (95%)	155 (98%)	4 (2%)	47	14
1	e	159/167 (95%)	156 (98%)	3 (2%)	57	23
1	f	161/167 (96%)	156 (97%)	5 (3%)	40	9
1	g	159/167 (95%)	156 (98%)	3 (2%)	57	23
1	h	161/167 (96%)	158 (98%)	3 (2%)	57	23
1	i	160/167 (96%)	157 (98%)	3 (2%)	57	23
1	j	159/167 (95%)	157 (99%)	2 (1%)	69	40
1	k	159/167 (95%)	156 (98%)	3 (2%)	57	23
1	l	158/167 (95%)	154 (98%)	4 (2%)	47	14
1	m	159/167 (95%)	155 (98%)	4 (2%)	47	14
1	n	161/167 (96%)	158 (98%)	3 (2%)	57	23
1	o	158/167 (95%)	155 (98%)	3 (2%)	57	23
1	p	158/167 (95%)	154 (98%)	4 (2%)	47	14
1	q	158/167 (95%)	154 (98%)	4 (2%)	47	14
1	r	160/167 (96%)	152 (95%)	8 (5%)	24	2
1	s	159/167 (95%)	154 (97%)	5 (3%)	40	9
1	t	164/167 (98%)	159 (97%)	5 (3%)	41	9
1	u	159/167 (95%)	154 (97%)	5 (3%)	40	9
1	v	159/167 (95%)	155 (98%)	4 (2%)	47	14
1	w	160/167 (96%)	158 (99%)	2 (1%)	69	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	x	160/167 (96%)	157 (98%)	3 (2%)	57 23
1	y	159/167 (95%)	156 (98%)	3 (2%)	57 23
1	z	161/167 (96%)	156 (97%)	5 (3%)	40 9
All	All	9601/10020 (96%)	9357 (98%)	244 (2%)	47 14

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	33	ASN
1	e	70	HIS
1	e	145	ARG
1	f	12	THR
1	f	28	ARG
1	f	33	ASN
1	f	70	HIS
1	f	73	HIS
1	g	33	ASN
1	g	70	HIS
1	g	73	HIS
1	h	33	ASN
1	h	70	HIS
1	h	73	HIS
1	i	33	ASN
1	i	70	HIS
1	i	73	HIS
1	j	70	HIS
1	j	73	HIS
1	k	31	LEU
1	k	33	ASN
1	k	70	HIS
1	l	31	LEU
1	l	33	ASN
1	l	70	HIS
1	l	73	HIS
1	m	22	THR
1	m	31	LEU
1	m	33	ASN
1	m	70	HIS
1	n	21	ASN
1	n	22	THR
1	n	70	HIS

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Mol	Chain	Res	Type
1	o	16	VAL
1	o	70	HIS
1	o	73	HIS
1	p	13	MET
1	p	31	LEU
1	p	33	ASN
1	p	70	HIS
1	q	16	VAL
1	q	28	ARG
1	q	31	LEU
1	q	70	HIS
1	r	12	THR
1	r	16	VAL
1	r	31	LEU
1	r	33	ASN
1	r	70	HIS
1	r	73	HIS
1	r	145[A]	ARG
1	r	145[B]	ARG
1	s	31	LEU
1	s	33	ASN
1	s	70	HIS
1	s	181[A]	VAL
1	s	181[B]	VAL
1	t	22	THR
1	t	31	LEU
1	t	33	ASN
1	t	70	HIS
1	t	73	HIS
1	u	16	VAL
1	u	31	LEU
1	u	33	ASN
1	u	70	HIS
1	u	73	HIS
1	v	13	MET
1	v	31	LEU
1	v	70	HIS
1	v	73	HIS
1	w	70	HIS
1	w	73	HIS
1	x	66	ARG
1	x	70	HIS

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Mol	Chain	Res	Type
1	x	73	HIS
1	y	16	VAL
1	y	70	HIS
1	y	73	HIS
1	z	22	THR
1	z	31[A]	LEU
1	z	31[B]	LEU
1	z	33	ASN
1	z	70	HIS
1	0	31	LEU
1	0	70	HIS
1	1	31	LEU
1	1	33	ASN
1	1	70	HIS
1	2	16	VAL
1	2	31	LEU
1	2	33	ASN
1	2	70	HIS
1	2	73	HIS
1	3	31	LEU
1	3	33	ASN
1	3	70	HIS
1	3	73	HIS
1	4	31	LEU
1	4	33	ASN
1	4	70	HIS
1	4	73	HIS
1	5	16	VAL
1	5	33	ASN
1	5	70	HIS
1	5	73	HIS
1	6	31	LEU
1	6	70	HIS
1	7	33	ASN
1	7	70	HIS
1	7	71	LYS
1	7	73	HIS
1	A	22	THR
1	A	33	ASN
1	A	70	HIS
1	B	33	ASN
1	B	70	HIS

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Mol	Chain	Res	Type
1	B	146[A]	ILE
1	B	146[B]	ILE
1	C	18	ARG
1	C	22	THR
1	C	31	LEU
1	C	33	ASN
1	C	70	HIS
1	C	73	HIS
1	C	129	LYS
1	C	148[A]	ASN
1	C	148[B]	ASN
1	D	13	MET
1	D	16	VAL
1	D	31[A]	LEU
1	D	31[B]	LEU
1	D	34[A]	SER
1	D	34[B]	SER
1	D	70	HIS
1	D	129	LYS
1	E	12	THR
1	E	33	ASN
1	E	70	HIS
1	E	73	HIS
1	F	33	ASN
1	F	70	HIS
1	F	73	HIS
1	G	16	VAL
1	G	33	ASN
1	G	70	HIS
1	G	73	HIS
1	G	129	LYS
1	H	14	ARG
1	H	16	VAL
1	H	33	ASN
1	H	70	HIS
1	H	91[A]	ARG
1	H	91[B]	ARG
1	I	22	THR
1	I	70	HIS
1	J	12	THR
1	J	13	MET
1	J	16	VAL

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Mol	Chain	Res	Type
1	J	33	ASN
1	J	70	HIS
1	K	16	VAL
1	K	33	ASN
1	K	70	HIS
1	K	73	HIS
1	K	95	ASN
1	L	19	MET
1	L	31	LEU
1	L	33	ASN
1	L	70	HIS
1	L	73	HIS
1	M	17	LYS
1	M	33	ASN
1	M	70	HIS
1	M	73	HIS
1	M	129	LYS
1	N	31	LEU
1	N	70	HIS
1	N	73	HIS
1	O	12	THR
1	O	31	LEU
1	O	70	HIS
1	O	73	HIS
1	O	129	LYS
1	P	31	LEU
1	P	33	ASN
1	P	70	HIS
1	P	73	HIS
1	Q	31	LEU
1	Q	70	HIS
1	Q	73	HIS
1	Q	148[A]	ASN
1	Q	148[B]	ASN
1	R	16	VAL
1	R	31[A]	LEU
1	R	31[B]	LEU
1	R	33	ASN
1	R	70	HIS
1	R	71	LYS
1	S	33	ASN
1	S	70	HIS

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Mol	Chain	Res	Type
1	S	152[A]	GLN
1	S	152[B]	GLN
1	T	18	ARG
1	T	31[A]	LEU
1	T	31[B]	LEU
1	T	33	ASN
1	T	70	HIS
1	T	71	LYS
1	T	73	HIS
1	U	33	ASN
1	U	70	HIS
1	U	73	HIS
1	V	33	ASN
1	V	70	HIS
1	V	73	HIS
1	W	33	ASN
1	W	70	HIS
1	W	73	HIS
1	X	33	ASN
1	X	70	HIS
1	X	71	LYS
1	X	73	HIS
1	Y	31	LEU
1	Y	33	ASN
1	Y	70	HIS
1	Y	73	HIS
1	Z	33	ASN
1	Z	70	HIS
1	Z	73	HIS
1	a	70	HIS
1	b	12	THR
1	b	31	LEU
1	b	33	ASN
1	b	66	ARG
1	b	70	HIS
1	c	16	VAL
1	c	31	LEU
1	c	70	HIS
1	c	73	HIS
1	d	16	VAL
1	d	31	LEU
1	d	70	HIS

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Mol	Chain	Res	Type
1	d	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (487) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	21	ASN
1	e	23	HIS
1	e	26	HIS
1	e	33	ASN
1	e	36	ASN
1	e	73	HIS
1	e	93	ASN
1	e	95	ASN
1	e	134	ASN
1	f	23	HIS
1	f	26	HIS
1	f	33	ASN
1	f	36	ASN
1	f	73	HIS
1	f	93	ASN
1	f	95	ASN
1	f	134	ASN
1	g	23	HIS
1	g	26	HIS
1	g	33	ASN
1	g	36	ASN
1	g	73	HIS
1	g	93	ASN
1	g	95	ASN
1	g	134	ASN
1	g	152	GLN
1	h	23	HIS
1	h	26	HIS
1	h	73	HIS
1	h	93	ASN
1	h	95	ASN
1	h	134	ASN
1	i	23	HIS
1	i	26	HIS
1	i	33	ASN
1	i	36	ASN
1	i	73	HIS

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Mol	Chain	Res	Type
1	i	93	ASN
1	i	95	ASN
1	i	134	ASN
1	j	23	HIS
1	j	26	HIS
1	j	33	ASN
1	j	73	HIS
1	j	93	ASN
1	j	95	ASN
1	j	134	ASN
1	k	26	HIS
1	k	33	ASN
1	k	36	ASN
1	k	73	HIS
1	k	93	ASN
1	k	95	ASN
1	k	134	ASN
1	l	26	HIS
1	l	33	ASN
1	l	36	ASN
1	l	45	GLN
1	l	73	HIS
1	l	93	ASN
1	l	95	ASN
1	l	134	ASN
1	m	21	ASN
1	m	26	HIS
1	m	33	ASN
1	m	36	ASN
1	m	73	HIS
1	m	93	ASN
1	m	95	ASN
1	m	134	ASN
1	n	21	ASN
1	n	23	HIS
1	n	26	HIS
1	n	33	ASN
1	n	36	ASN
1	n	73	HIS
1	n	93	ASN
1	n	95	ASN
1	n	134	ASN

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Mol	Chain	Res	Type
1	o	21	ASN
1	o	23	HIS
1	o	26	HIS
1	o	73	HIS
1	o	93	ASN
1	o	95	ASN
1	o	134	ASN
1	p	21	ASN
1	p	23	HIS
1	p	26	HIS
1	p	33	ASN
1	p	36	ASN
1	p	73	HIS
1	p	93	ASN
1	p	95	ASN
1	p	134	ASN
1	q	21	ASN
1	q	23	HIS
1	q	26	HIS
1	q	33	ASN
1	q	36	ASN
1	q	73	HIS
1	q	93	ASN
1	q	95	ASN
1	q	134	ASN
1	q	175	GLN
1	r	21	ASN
1	r	23	HIS
1	r	26	HIS
1	r	33	ASN
1	r	36	ASN
1	r	73	HIS
1	r	93	ASN
1	r	95	ASN
1	r	134	ASN
1	s	23	HIS
1	s	26	HIS
1	s	33	ASN
1	s	36	ASN
1	s	73	HIS
1	s	93	ASN
1	s	95	ASN

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Mol	Chain	Res	Type
1	s	134	ASN
1	t	21	ASN
1	t	23	HIS
1	t	26	HIS
1	t	33	ASN
1	t	36	ASN
1	t	45	GLN
1	t	73	HIS
1	t	93	ASN
1	t	95	ASN
1	t	134	ASN
1	u	21	ASN
1	u	23	HIS
1	u	26	HIS
1	u	33	ASN
1	u	36	ASN
1	u	73	HIS
1	u	93	ASN
1	u	95	ASN
1	u	134	ASN
1	v	26	HIS
1	v	33	ASN
1	v	36	ASN
1	v	73	HIS
1	v	93	ASN
1	v	95	ASN
1	v	134	ASN
1	w	23	HIS
1	w	26	HIS
1	w	33	ASN
1	w	36	ASN
1	w	73	HIS
1	w	93	ASN
1	w	95	ASN
1	w	134	ASN
1	x	23	HIS
1	x	26	HIS
1	x	33	ASN
1	x	36	ASN
1	x	73	HIS
1	x	93	ASN
1	x	95	ASN

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Mol	Chain	Res	Type
1	x	134	ASN
1	x	152	GLN
1	y	21	ASN
1	y	23	HIS
1	y	26	HIS
1	y	33	ASN
1	y	36	ASN
1	y	73	HIS
1	y	93	ASN
1	y	95	ASN
1	y	134	ASN
1	z	21	ASN
1	z	26	HIS
1	z	33	ASN
1	z	36	ASN
1	z	73	HIS
1	z	93	ASN
1	z	95	ASN
1	z	134	ASN
1	0	23	HIS
1	0	26	HIS
1	0	33	ASN
1	0	36	ASN
1	0	73	HIS
1	0	93	ASN
1	0	95	ASN
1	0	134	ASN
1	1	21	ASN
1	1	26	HIS
1	1	33	ASN
1	1	36	ASN
1	1	73	HIS
1	1	93	ASN
1	1	95	ASN
1	1	134	ASN
1	2	21	ASN
1	2	26	HIS
1	2	33	ASN
1	2	36	ASN
1	2	73	HIS
1	2	93	ASN
1	2	95	ASN

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Mol	Chain	Res	Type
1	2	134	ASN
1	3	23	HIS
1	3	26	HIS
1	3	73	HIS
1	3	93	ASN
1	3	95	ASN
1	3	134	ASN
1	4	23	HIS
1	4	26	HIS
1	4	33	ASN
1	4	36	ASN
1	4	73	HIS
1	4	93	ASN
1	4	95	ASN
1	4	134	ASN
1	5	23	HIS
1	5	26	HIS
1	5	33	ASN
1	5	36	ASN
1	5	73	HIS
1	5	93	ASN
1	5	95	ASN
1	5	134	ASN
1	6	21	ASN
1	6	23	HIS
1	6	26	HIS
1	6	33	ASN
1	6	36	ASN
1	6	73	HIS
1	6	93	ASN
1	6	95	ASN
1	6	134	ASN
1	7	26	HIS
1	7	33	ASN
1	7	73	HIS
1	7	93	ASN
1	7	95	ASN
1	7	134	ASN
1	A	21	ASN
1	A	26	HIS
1	A	33	ASN
1	A	36	ASN

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Mol	Chain	Res	Type
1	A	73	HIS
1	A	93	ASN
1	A	95	ASN
1	A	134	ASN
1	B	21	ASN
1	B	23	HIS
1	B	26	HIS
1	B	33	ASN
1	B	36	ASN
1	B	73	HIS
1	B	93	ASN
1	B	95	ASN
1	B	134	ASN
1	C	26	HIS
1	C	33	ASN
1	C	36	ASN
1	C	73	HIS
1	C	93	ASN
1	C	95	ASN
1	C	134	ASN
1	D	23	HIS
1	D	26	HIS
1	D	33	ASN
1	D	36	ASN
1	D	73	HIS
1	D	93	ASN
1	D	95	ASN
1	D	134	ASN
1	E	21	ASN
1	E	23	HIS
1	E	26	HIS
1	E	33	ASN
1	E	36	ASN
1	E	73	HIS
1	E	93	ASN
1	E	95	ASN
1	E	134	ASN
1	F	26	HIS
1	F	73	HIS
1	F	93	ASN
1	F	95	ASN
1	F	134	ASN

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Mol	Chain	Res	Type
1	G	21	ASN
1	G	26	HIS
1	G	33	ASN
1	G	36	ASN
1	G	73	HIS
1	G	93	ASN
1	G	95	ASN
1	G	134	ASN
1	H	21	ASN
1	H	23	HIS
1	H	26	HIS
1	H	33	ASN
1	H	36	ASN
1	H	73	HIS
1	H	93	ASN
1	H	95	ASN
1	H	134	ASN
1	I	23	HIS
1	I	26	HIS
1	I	33	ASN
1	I	36	ASN
1	I	73	HIS
1	I	93	ASN
1	I	95	ASN
1	I	134	ASN
1	J	21	ASN
1	J	23	HIS
1	J	26	HIS
1	J	33	ASN
1	J	36	ASN
1	J	73	HIS
1	J	93	ASN
1	J	95	ASN
1	J	134	ASN
1	K	26	HIS
1	K	33	ASN
1	K	36	ASN
1	K	73	HIS
1	K	93	ASN
1	K	95	ASN
1	K	134	ASN
1	L	21	ASN

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Mol	Chain	Res	Type
1	L	23	HIS
1	L	26	HIS
1	L	33	ASN
1	L	36	ASN
1	L	73	HIS
1	L	93	ASN
1	L	95	ASN
1	L	134	ASN
1	M	21	ASN
1	M	26	HIS
1	M	33	ASN
1	M	36	ASN
1	M	73	HIS
1	M	93	ASN
1	M	95	ASN
1	M	134	ASN
1	N	21	ASN
1	N	23	HIS
1	N	26	HIS
1	N	33	ASN
1	N	36	ASN
1	N	73	HIS
1	N	93	ASN
1	N	95	ASN
1	N	134	ASN
1	N	152	GLN
1	O	23	HIS
1	O	26	HIS
1	O	33	ASN
1	O	73	HIS
1	O	93	ASN
1	O	95	ASN
1	O	134	ASN
1	P	21	ASN
1	P	23	HIS
1	P	26	HIS
1	P	33	ASN
1	P	36	ASN
1	P	73	HIS
1	P	93	ASN
1	P	95	ASN
1	P	134	ASN

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Mol	Chain	Res	Type
1	Q	21	ASN
1	Q	23	HIS
1	Q	26	HIS
1	Q	33	ASN
1	Q	73	HIS
1	Q	93	ASN
1	Q	95	ASN
1	Q	134	ASN
1	R	21	ASN
1	R	26	HIS
1	R	33	ASN
1	R	36	ASN
1	R	73	HIS
1	R	93	ASN
1	R	95	ASN
1	R	134	ASN
1	S	23	HIS
1	S	26	HIS
1	S	33	ASN
1	S	36	ASN
1	S	73	HIS
1	S	93	ASN
1	S	95	ASN
1	S	134	ASN
1	T	23	HIS
1	T	26	HIS
1	T	33	ASN
1	T	73	HIS
1	T	93	ASN
1	T	95	ASN
1	T	134	ASN
1	U	23	HIS
1	U	26	HIS
1	U	33	ASN
1	U	36	ASN
1	U	73	HIS
1	U	93	ASN
1	U	95	ASN
1	U	134	ASN
1	V	23	HIS
1	V	26	HIS
1	V	33	ASN

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Mol	Chain	Res	Type
1	V	36	ASN
1	V	73	HIS
1	V	93	ASN
1	V	95	ASN
1	V	134	ASN
1	W	21	ASN
1	W	26	HIS
1	W	33	ASN
1	W	36	ASN
1	W	73	HIS
1	W	93	ASN
1	W	95	ASN
1	W	134	ASN
1	X	21	ASN
1	X	23	HIS
1	X	26	HIS
1	X	33	ASN
1	X	36	ASN
1	X	73	HIS
1	X	93	ASN
1	X	95	ASN
1	X	134	ASN
1	Y	26	HIS
1	Y	33	ASN
1	Y	36	ASN
1	Y	73	HIS
1	Y	93	ASN
1	Y	95	ASN
1	Y	134	ASN
1	Z	21	ASN
1	Z	26	HIS
1	Z	33	ASN
1	Z	36	ASN
1	Z	73	HIS
1	Z	93	ASN
1	Z	95	ASN
1	Z	134	ASN
1	a	23	HIS
1	a	26	HIS
1	a	33	ASN
1	a	36	ASN
1	a	73	HIS

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Mol	Chain	Res	Type
1	a	93	ASN
1	a	95	ASN
1	a	134	ASN
1	b	21	ASN
1	b	23	HIS
1	b	26	HIS
1	b	33	ASN
1	b	36	ASN
1	b	73	HIS
1	b	93	ASN
1	b	95	ASN
1	b	134	ASN
1	b	152	GLN
1	c	21	ASN
1	c	23	HIS
1	c	26	HIS
1	c	33	ASN
1	c	36	ASN
1	c	73	HIS
1	c	93	ASN
1	c	95	ASN
1	c	134	ASN
1	d	23	HIS
1	d	26	HIS
1	d	33	ASN
1	d	36	ASN
1	d	73	HIS
1	d	93	ASN
1	d	95	ASN
1	d	134	ASN

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)

Of 92 ligands modelled in this entry, 92 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.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	0	184/196 (93%)	-0.50	7 (3%)	40	43	7, 10, 27, 62	0
1	1	184/196 (93%)	-0.44	5 (2%)	54	56	8, 10, 26, 63	0
1	2	184/196 (93%)	-0.51	6 (3%)	46	48	7, 10, 25, 61	0
1	3	184/196 (93%)	-0.45	7 (3%)	40	43	8, 11, 29, 61	0
1	4	184/196 (93%)	-0.52	7 (3%)	40	43	7, 10, 25, 58	0
1	5	184/196 (93%)	-0.43	9 (4%)	29	32	9, 11, 29, 64	0
1	6	184/196 (93%)	-0.44	9 (4%)	29	32	8, 11, 29, 64	0
1	7	184/196 (93%)	-0.46	6 (3%)	46	48	8, 11, 28, 61	0
1	A	184/196 (93%)	-0.44	7 (3%)	40	43	8, 10, 29, 63	0
1	B	184/196 (93%)	-0.47	6 (3%)	46	48	8, 11, 29, 62	0
1	C	184/196 (93%)	-0.47	7 (3%)	40	43	9, 12, 28, 61	0
1	D	184/196 (93%)	-0.50	7 (3%)	40	43	8, 10, 27, 64	0
1	E	184/196 (93%)	-0.42	5 (2%)	54	56	9, 12, 27, 63	0
1	F	184/196 (93%)	-0.43	6 (3%)	46	48	9, 12, 28, 63	0
1	G	184/196 (93%)	-0.43	5 (2%)	54	56	9, 12, 29, 62	0
1	H	184/196 (93%)	-0.47	7 (3%)	40	43	8, 11, 29, 64	0
1	I	184/196 (93%)	-0.45	8 (4%)	35	38	9, 11, 29, 62	0
1	J	184/196 (93%)	-0.47	7 (3%)	40	43	8, 11, 27, 60	0
1	K	184/196 (93%)	-0.51	7 (3%)	40	43	7, 9, 27, 61	0
1	L	184/196 (93%)	-0.45	6 (3%)	46	48	8, 11, 28, 62	0
1	M	184/196 (93%)	-0.44	8 (4%)	35	38	7, 11, 28, 64	0
1	N	184/196 (93%)	-0.40	5 (2%)	54	56	9, 12, 29, 63	0
1	O	184/196 (93%)	-0.48	5 (2%)	54	56	9, 12, 29, 62	0
1	P	184/196 (93%)	-0.46	7 (3%)	40	43	8, 11, 28, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Q	184/196 (93%)	-0.43	8 (4%)	35	38	8, 11, 28, 62	0
1	R	184/196 (93%)	-0.51	6 (3%)	46	48	7, 10, 27, 61	0
1	S	184/196 (93%)	-0.44	5 (2%)	54	56	8, 10, 27, 62	0
1	T	184/196 (93%)	-0.53	6 (3%)	46	48	7, 9, 27, 63	0
1	U	184/196 (93%)	-0.48	7 (3%)	40	43	7, 9, 27, 64	0
1	V	184/196 (93%)	-0.52	6 (3%)	46	48	7, 10, 26, 59	0
1	W	184/196 (93%)	-0.45	7 (3%)	40	43	9, 11, 29, 65	0
1	X	184/196 (93%)	-0.47	6 (3%)	46	48	8, 10, 28, 60	0
1	Y	184/196 (93%)	-0.50	7 (3%)	40	43	7, 10, 28, 61	0
1	Z	184/196 (93%)	-0.53	5 (2%)	54	56	6, 9, 28, 64	0
1	a	184/196 (93%)	-0.48	5 (2%)	54	56	8, 11, 28, 59	0
1	b	184/196 (93%)	-0.50	6 (3%)	46	48	7, 10, 27, 58	0
1	c	184/196 (93%)	-0.49	9 (4%)	29	32	7, 10, 27, 64	0
1	d	184/196 (93%)	-0.51	5 (2%)	54	56	7, 9, 27, 62	0
1	e	184/196 (93%)	-0.46	6 (3%)	46	48	7, 10, 27, 63	0
1	f	184/196 (93%)	-0.47	6 (3%)	46	48	9, 12, 29, 60	0
1	g	184/196 (93%)	-0.46	6 (3%)	46	48	8, 11, 28, 63	0
1	h	184/196 (93%)	-0.46	6 (3%)	46	48	7, 10, 25, 61	0
1	i	184/196 (93%)	-0.46	7 (3%)	40	43	7, 10, 28, 60	0
1	j	184/196 (93%)	-0.47	8 (4%)	35	38	7, 11, 26, 62	0
1	k	184/196 (93%)	-0.47	7 (3%)	40	43	7, 10, 27, 61	0
1	l	184/196 (93%)	-0.46	8 (4%)	35	38	7, 10, 27, 61	0
1	m	184/196 (93%)	-0.43	6 (3%)	46	48	9, 12, 29, 64	0
1	n	184/196 (93%)	-0.37	5 (2%)	54	56	9, 12, 30, 63	0
1	o	184/196 (93%)	-0.51	7 (3%)	40	43	8, 11, 29, 64	0
1	p	184/196 (93%)	-0.47	7 (3%)	40	43	8, 11, 26, 61	0
1	q	184/196 (93%)	-0.50	5 (2%)	54	56	7, 10, 26, 61	0
1	r	184/196 (93%)	-0.47	5 (2%)	54	56	7, 9, 27, 62	0
1	s	184/196 (93%)	-0.47	9 (4%)	29	32	8, 11, 28, 61	0
1	t	184/196 (93%)	-0.50	5 (2%)	54	56	8, 11, 29, 61	0
1	u	184/196 (93%)	-0.48	7 (3%)	40	43	8, 11, 29, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	v	184/196 (93%)	-0.46	7 (3%)	40	43	7, 10, 27, 61	0
1	w	184/196 (93%)	-0.53	6 (3%)	46	48	7, 10, 25, 60	0
1	x	184/196 (93%)	-0.50	7 (3%)	40	43	6, 10, 27, 62	0
1	y	184/196 (93%)	-0.49	7 (3%)	40	43	7, 9, 26, 58	0
1	z	184/196 (93%)	-0.42	5 (2%)	54	56	8, 11, 27, 61	0
All	All	11040/11760 (93%)	-0.47	389 (3%)	44	47	6, 11, 34, 65	0

All (389) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	x	12	THR	9.1
1	k	12	THR	8.7
1	h	13	MET	8.7
1	3	12	THR	8.5
1	1	13	MET	8.2
1	6	12	THR	8.1
1	G	12	THR	8.1
1	7	13	MET	7.9
1	Z	13	MET	7.8
1	5	13	MET	7.8
1	z	14	ARG	7.8
1	2	12	THR	7.8
1	D	13	MET	7.6
1	S	12	THR	7.5
1	L	12	THR	7.5
1	z	12	THR	7.4
1	K	12	THR	7.4
1	e	14	ARG	7.4
1	q	14	ARG	7.4
1	j	12	THR	7.3
1	U	12	THR	7.3
1	l	12	THR	7.3
1	p	12	THR	7.3
1	v	12	THR	7.3
1	6	14	ARG	7.3
1	X	12	THR	7.2
1	W	14	ARG	7.2
1	S	13	MET	7.1
1	O	12	THR	7.1
1	f	12	THR	7.0

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Mol	Chain	Res	Type	RSRZ
1	u	12	THR	7.0
1	I	13	MET	7.0
1	g	13	MET	7.0
1	U	14	ARG	6.9
1	Z	12	THR	6.9
1	B	12	THR	6.8
1	5	12	THR	6.8
1	r	13	MET	6.8
1	r	12	THR	6.8
1	J	14	ARG	6.8
1	h	12	THR	6.8
1	2	14	ARG	6.8
1	4	14	ARG	6.8
1	v	13	MET	6.8
1	v	14	ARG	6.7
1	r	14	ARG	6.7
1	F	14	ARG	6.7
1	N	12	THR	6.7
1	1	12	THR	6.7
1	M	14	ARG	6.7
1	i	12	THR	6.6
1	y	14	ARG	6.6
1	j	14	ARG	6.6
1	p	13	MET	6.5
1	C	12	THR	6.5
1	A	14	ARG	6.5
1	F	13	MET	6.4
1	f	14	ARG	6.4
1	e	12	THR	6.4
1	3	13	MET	6.4
1	m	14	ARG	6.4
1	w	14	ARG	6.3
1	E	14	ARG	6.3
1	T	13	MET	6.3
1	u	13	MET	6.3
1	h	14	ARG	6.2
1	0	14	ARG	6.2
1	Q	13	MET	6.2
1	5	14	ARG	6.2
1	Z	14	ARG	6.2
1	m	13	MET	6.2
1	I	12	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	X	14	ARG	6.1
1	p	14	ARG	6.1
1	a	14	ARG	6.0
1	J	18	ARG	6.0
1	o	14	ARG	6.0
1	J	13	MET	6.0
1	Q	14	ARG	5.9
1	E	13	MET	5.9
1	D	12	THR	5.9
1	L	14	ARG	5.8
1	Y	14	ARG	5.8
1	s	12	THR	5.8
1	R	14	ARG	5.7
1	i	13	MET	5.7
1	l	13	MET	5.7
1	e	13	MET	5.7
1	j	13	MET	5.7
1	C	13	MET	5.7
1	3	14	ARG	5.7
1	T	12	THR	5.6
1	V	12	THR	5.6
1	g	14	ARG	5.6
1	m	12	THR	5.6
1	n	12	THR	5.6
1	0	12	THR	5.6
1	K	15	ALA	5.6
1	x	13	MET	5.6
1	4	13	MET	5.6
1	A	12	THR	5.6
1	P	14	ARG	5.5
1	L	13	MET	5.5
1	X	16	VAL	5.5
1	n	18	ARG	5.5
1	S	14	ARG	5.5
1	w	12	THR	5.5
1	k	13	MET	5.5
1	r	18	ARG	5.5
1	F	12	THR	5.4
1	g	12	THR	5.4
1	7	12	THR	5.4
1	W	13	MET	5.4
1	b	13	MET	5.3

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Mol	Chain	Res	Type	RSRZ
1	N	18	ARG	5.3
1	c	12	THR	5.3
1	I	14	ARG	5.3
1	d	14	ARG	5.3
1	X	13	MET	5.3
1	d	12	THR	5.2
1	O	14	ARG	5.2
1	Y	12	THR	5.2
1	1	14	ARG	5.1
1	G	14	ARG	5.1
1	s	14	ARG	5.1
1	R	12	THR	5.1
1	t	12	THR	5.1
1	6	18	ARG	5.1
1	o	12	THR	5.0
1	g	18	ARG	5.0
1	H	18	ARG	5.0
1	W	18	ARG	5.0
1	b	18	ARG	5.0
1	x	14	ARG	5.0
1	2	13	MET	5.0
1	p	18	ARG	5.0
1	b	14	ARG	5.0
1	W	12	THR	5.0
1	L	16	VAL	5.0
1	w	18	ARG	4.9
1	y	12	THR	4.9
1	0	18	ARG	4.9
1	D	18	ARG	4.9
1	o	18	ARG	4.8
1	F	18	ARG	4.8
1	K	14	ARG	4.8
1	c	14	ARG	4.8
1	k	14	ARG	4.8
1	d	18	ARG	4.8
1	H	13	MET	4.8
1	Y	13	MET	4.8
1	4	18	ARG	4.7
1	T	14	ARG	4.7
1	c	16	VAL	4.7
1	N	14	ARG	4.7
1	E	16	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	14	ARG	4.7
1	z	18	ARG	4.7
1	K	13	MET	4.7
1	M	13	MET	4.6
1	c	13	MET	4.6
1	A	18	ARG	4.6
1	w	13	MET	4.6
1	e	18	ARG	4.6
1	i	14	ARG	4.6
1	t	13	MET	4.6
1	7	14	ARG	4.6
1	a	12	THR	4.6
1	7	18	ARG	4.6
1	B	18	ARG	4.6
1	n	13	MET	4.6
1	G	13	MET	4.6
1	R	18	ARG	4.5
1	4	12	THR	4.5
1	j	18	ARG	4.5
1	l	18	ARG	4.5
1	5	18	ARG	4.5
1	H	14	ARG	4.5
1	R	13	MET	4.5
1	Q	15	ALA	4.5
1	Q	18	ARG	4.5
1	X	18	ARG	4.5
1	t	18	ARG	4.4
1	m	16	VAL	4.4
1	q	12	THR	4.4
1	6	15	ALA	4.4
1	t	14	ARG	4.4
1	Q	12	THR	4.4
1	l	14	ARG	4.4
1	x	18	ARG	4.4
1	5	15	ALA	4.4
1	q	13	MET	4.4
1	a	13	MET	4.4
1	Y	18	ARG	4.3
1	P	12	THR	4.3
1	h	16	VAL	4.3
1	I	16	VAL	4.3
1	y	18	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	14	ARG	4.3
1	y	13	MET	4.3
1	N	13	MET	4.3
1	h	18	ARG	4.3
1	M	18	ARG	4.3
1	V	14	ARG	4.3
1	D	14	ARG	4.2
1	U	18	ARG	4.2
1	f	13	MET	4.2
1	O	13	MET	4.2
1	U	13	MET	4.2
1	z	13	MET	4.2
1	d	13	MET	4.2
1	u	14	ARG	4.2
1	T	18	ARG	4.2
1	q	18	ARG	4.1
1	v	18	ARG	4.1
1	6	13	MET	4.1
1	n	14	ARG	4.1
1	E	18	ARG	4.1
1	P	18	ARG	4.1
1	m	18	ARG	4.1
1	H	12	THR	4.0
1	c	18	ARG	4.0
1	U	15	ALA	4.0
1	I	18	ARG	3.9
1	J	12	THR	3.9
1	P	13	MET	3.9
1	A	15	ALA	3.9
1	5	16	VAL	3.9
1	p	16	VAL	3.8
1	u	18	ARG	3.8
1	L	18	ARG	3.8
1	1	18	ARG	3.8
1	s	18	ARG	3.7
1	7	16	VAL	3.7
1	M	12	THR	3.7
1	2	18	ARG	3.7
1	V	15	ALA	3.7
1	S	18	ARG	3.7
1	u	16	VAL	3.7
1	V	13	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	k	18	ARG	3.6
1	w	16	VAL	3.6
1	E	12	THR	3.6
1	B	13	MET	3.6
1	i	18	ARG	3.6
1	o	13	MET	3.6
1	0	13	MET	3.6
1	A	13	MET	3.6
1	b	12	THR	3.6
1	V	18	ARG	3.5
1	P	15	ALA	3.5
1	3	18	ARG	3.5
1	a	18	ARG	3.5
1	K	18	ARG	3.5
1	6	17	LYS	3.5
1	f	18	ARG	3.5
1	H	15	ALA	3.4
1	s	17	LYS	3.3
1	C	18	ARG	3.3
1	5	19	MET	3.3
1	e	16	VAL	3.3
1	R	15	ALA	3.3
1	A	16	VAL	3.2
1	P	16	VAL	3.2
1	j	16	VAL	3.2
1	i	16	VAL	3.1
1	v	16	VAL	3.1
1	f	16	VAL	3.1
1	O	18	ARG	3.0
1	1	15	ALA	3.0
1	C	16	VAL	3.0
1	7	19	MET	3.0
1	x	16	VAL	2.9
1	D	16	VAL	2.9
1	s	13	MET	2.9
1	P	19	MET	2.9
1	d	15	ALA	2.9
1	l	15	ALA	2.9
1	w	15	ALA	2.9
1	F	16	VAL	2.9
1	J	16	VAL	2.9
1	T	16	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	b	16	VAL	2.9
1	g	16	VAL	2.8
1	v	17	LYS	2.8
1	U	16	VAL	2.8
1	W	16	VAL	2.8
1	M	17	LYS	2.8
1	s	19	MET	2.8
1	c	15	ALA	2.7
1	Z	18	ARG	2.7
1	4	16	VAL	2.7
1	V	19	MET	2.7
1	W	17	LYS	2.7
1	G	18	ARG	2.6
1	b	15	ALA	2.6
1	0	19	MET	2.6
1	M	19	MET	2.6
1	g	15	ALA	2.6
1	o	16	VAL	2.6
1	y	16	VAL	2.6
1	s	22	THR	2.6
1	5	17	LYS	2.6
1	q	17	LYS	2.5
1	v	15	ALA	2.5
1	4	15	ALA	2.5
1	3	19	MET	2.5
1	3	22	THR	2.5
1	A	19	MET	2.5
1	Y	19	MET	2.5
1	Y	17	LYS	2.5
1	p	15	ALA	2.5
1	p	19	MET	2.5
1	L	17	LYS	2.4
1	r	16	VAL	2.4
1	M	16	VAL	2.4
1	Y	16	VAL	2.4
1	0	17	LYS	2.4
1	6	19	MET	2.4
1	Q	19	MET	2.4
1	h	15	ALA	2.4
1	y	15	ALA	2.4
1	j	19	MET	2.4
1	I	19	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	c	22	THR	2.4
1	T	19	MET	2.4
1	z	15	ALA	2.4
1	l	22	THR	2.4
1	k	17	LYS	2.3
1	R	16	VAL	2.3
1	i	15	ALA	2.3
1	k	16	VAL	2.3
1	2	16	VAL	2.3
1	3	16	VAL	2.3
1	H	16	VAL	2.3
1	I	17	LYS	2.3
1	D	15	ALA	2.3
1	C	22	THR	2.3
1	o	17	LYS	2.3
1	N	16	VAL	2.3
1	m	17	LYS	2.3
1	k	15	ALA	2.3
1	s	15	ALA	2.3
1	6	22	THR	2.2
1	W	19	MET	2.2
1	u	17	LYS	2.2
1	H	17	LYS	2.2
1	G	19	MET	2.2
1	x	22	THR	2.2
1	l	16	VAL	2.2
1	s	16	VAL	2.2
1	t	16	VAL	2.2
1	0	16	VAL	2.2
1	S	16	VAL	2.2
1	l	17	LYS	2.2
1	e	15	ALA	2.2
1	u	22	THR	2.2
1	K	16	VAL	2.2
1	O	17	LYS	2.2
1	Q	17	LYS	2.2
1	Z	19	MET	2.2
1	c	19	MET	2.2
1	x	15	ALA	2.1
1	I	15	ALA	2.1
1	C	17	LYS	2.1
1	6	16	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	16	VAL	2.1
1	y	22	THR	2.1
1	j	15	ALA	2.1
1	n	15	ALA	2.1
1	M	15	ALA	2.1
1	F	15	ALA	2.1
1	4	19	MET	2.1
1	c	17	LYS	2.1
1	j	21	ASN	2.1
1	B	22	THR	2.1
1	o	19	MET	2.1
1	J	19	MET	2.1
1	K	22	THR	2.1
1	J	15	ALA	2.1
1	D	19	MET	2.0
1	X	17	LYS	2.0
1	5	22	THR	2.0
1	f	17	LYS	2.0
1	Q	16	VAL	2.0
1	a	16	VAL	2.0
1	i	17	LYS	2.0
1	2	17	LYS	2.0
1	U	17	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	N	202	1/1	0.98	0.06	10,10,10,10	0
2	CA	0	201	1/1	0.99	0.06	8,8,8,8	0
2	CA	1	202	1/1	0.99	0.06	8,8,8,8	0
2	CA	3	202	1/1	0.99	0.05	9,9,9,9	0
2	CA	5	202	1/1	0.99	0.06	9,9,9,9	0
2	CA	6	202	1/1	0.99	0.07	9,9,9,9	0
2	CA	A	202	1/1	0.99	0.07	9,9,9,9	0
2	CA	B	203	1/1	0.99	0.08	9,9,9,9	0
2	CA	E	202	1/1	0.99	0.04	9,9,9,9	0
2	CA	G	202	1/1	0.99	0.03	12,12,12,12	0
2	CA	G	203	1/1	0.99	0.05	9,9,9,9	0
2	CA	I	201	1/1	0.99	0.06	10,10,10,10	0
2	CA	N	201	1/1	0.99	0.04	11,11,11,11	0
2	CA	n	202	1/1	0.99	0.03	11,11,11,11	0
2	CA	P	201	1/1	0.99	0.04	10,10,10,10	0
2	CA	Q	202	1/1	0.99	0.05	8,8,8,8	0
2	CA	S	202	1/1	0.99	0.08	8,8,8,8	0
2	CA	T	202	1/1	0.99	0.07	7,7,7,7	0
2	CA	U	203	1/1	0.99	0.08	8,8,8,8	0
2	CA	V	201	1/1	0.99	0.05	6,6,6,6	0
2	CA	W	201	1/1	0.99	0.03	10,10,10,10	0
2	CA	u	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	v	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	w	201	1/1	1.00	0.04	8,8,8,8	0
2	CA	x	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	y	201	1/1	1.00	0.02	8,8,8,8	0
2	CA	z	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	f	201	1/1	1.00	0.02	10,10,10,10	0
2	CA	0	202	1/1	1.00	0.02	8,8,8,8	0
2	CA	1	201	1/1	1.00	0.04	9,9,9,9	0
2	CA	g	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	1	203	1/1	1.00	0.03	10,10,10,10	0
2	CA	2	201	1/1	1.00	0.02	10,10,10,10	0
2	CA	2	202	1/1	1.00	0.03	9,9,9,9	0
2	CA	3	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	h	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	4	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	4	202	1/1	1.00	0.04	8,8,8,8	0
2	CA	5	201	1/1	1.00	0.03	10,10,10,10	0
2	CA	i	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	6	201	1/1	1.00	0.03	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	i	202	1/1	1.00	0.04	11,11,11,11	0
2	CA	7	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	A	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	j	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	B	201	1/1	1.00	0.02	10,10,10,10	0
2	CA	B	202	1/1	1.00	0.02	10,10,10,10	0
2	CA	j	202	1/1	1.00	0.06	8,8,8,8	0
2	CA	C	201	1/1	1.00	0.04	10,10,10,10	0
2	CA	D	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	E	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	k	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	E	203	1/1	1.00	0.02	11,11,11,11	0
2	CA	F	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	G	201	1/1	1.00	0.02	10,10,10,10	0
2	CA	l	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	m	201	1/1	1.00	0.04	11,11,11,11	0
2	CA	H	201	1/1	1.00	0.03	10,10,10,10	0
2	CA	n	201	1/1	1.00	0.02	11,11,11,11	0
2	CA	I	202	1/1	1.00	0.02	10,10,10,10	0
2	CA	J	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	K	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	K	202	1/1	1.00	0.02	9,9,9,9	0
2	CA	L	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	M	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	e	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	o	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	O	201	1/1	1.00	0.03	10,10,10,10	0
2	CA	o	202	1/1	1.00	0.02	12,12,12,12	0
2	CA	Q	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	p	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	R	201	1/1	1.00	0.04	8,8,8,8	0
2	CA	R	202	1/1	1.00	0.02	8,8,8,8	0
2	CA	S	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	q	201	1/1	1.00	0.02	7,7,7,7	0
2	CA	T	201	1/1	1.00	0.02	8,8,8,8	0
2	CA	q	202	1/1	1.00	0.02	10,10,10,10	0
2	CA	U	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	U	202	1/1	1.00	0.03	8,8,8,8	0
2	CA	r	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	s	201	1/1	1.00	0.02	8,8,8,8	0
2	CA	V	202	1/1	1.00	0.02	8,8,8,8	0
2	CA	t	201	1/1	1.00	0.02	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	X	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	Y	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	Z	201	1/1	1.00	0.03	8,8,8,8	0
2	CA	a	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	b	201	1/1	1.00	0.03	9,9,9,9	0
2	CA	b	202	1/1	1.00	0.06	8,8,8,8	0
2	CA	c	201	1/1	1.00	0.03	7,7,7,7	0
2	CA	c	202	1/1	1.00	0.03	10,10,10,10	0
2	CA	d	201	1/1	1.00	0.03	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.