



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 07:30 PM EDT

PDB ID : 4N9F
Title : Crystal structure of the Vif-CBFbeta-CUL5-ElOB-ElOC pentameric complex
Authors : Guo, Y.Y.; Dong, L.Y.; Huang, Z.W.
Deposited on : 2013-10-21
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

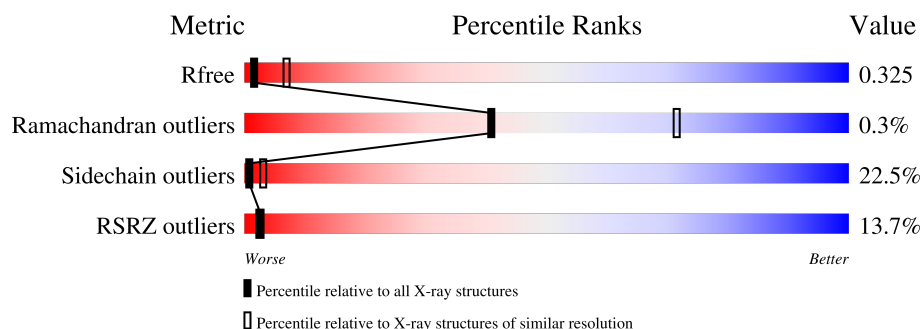
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




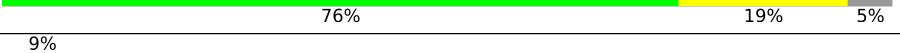
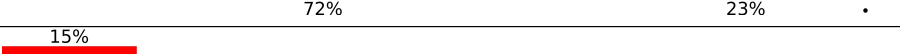
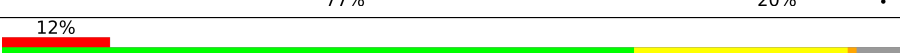
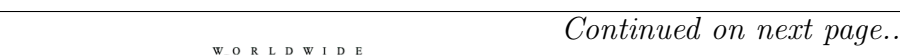
The reported resolution of this entry is 3.30 Å.

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	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	311	
1	9	311	
1	C	311	
1	I	311	
1	O	311	
1	U	311	
1	V	311	

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Mol	Chain	Length	Quality of chain
1	f	311	
1	l	311	
1	r	311	
1	w	311	
1	x	311	
2	5	96	
2	B	96	
2	E	96	
2	K	96	
2	Q	96	
2	T	96	
2	Y	96	
2	Z	96	
2	h	96	
2	n	96	
2	t	96	
2	z	96	
3	4	102	
3	D	102	
3	H	102	
3	J	102	
3	P	102	
3	W	102	
3	X	102	
3	e	102	




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Mol	Chain	Length	Quality of chain
3	g	102	
3	m	102	
3	s	102	
3	y	102	
4	0	170	
4	6	170	
4	F	170	
4	L	170	
4	N	170	
4	R	170	
4	a	170	
4	c	170	
4	i	170	
4	k	170	
4	o	170	
4	u	170	
5	1	176	
5	2	176	
5	7	176	
5	G	176	
5	M	176	
5	S	176	
5	b	176	
5	d	176	
5	j	176	

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Mol	Chain	Length	Quality of chain
5	p	176	
5	q	176	
5	v	176	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 77274 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 Cullin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	299	Total	C	N	O	S	0	2	0
			2469	1567	420	465	17			
1	C	297	Total	C	N	O	S	0	1	0
			2446	1555	417	457	17			
1	I	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	O	298	Total	C	N	O	S	0	1	0
			2451	1558	418	458	17			
1	V	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	f	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	l	297	Total	C	N	O	S	0	0	0
			2444	1555	416	456	17			
1	r	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	x	294	Total	C	N	O	S	0	0	0
			2419	1540	410	452	17			
1	3	295	Total	C	N	O	S	0	1	0
			2435	1549	415	454	17			
1	9	295	Total	C	N	O	S	0	1	0
			2435	1549	415	454	17			
1	w	296	Total	C	N	O	S	0	1	0
			2440	1552	416	455	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	11	ALA	-	expression tag	UNP Q93034
C	11	ALA	-	expression tag	UNP Q93034
I	11	ALA	-	expression tag	UNP Q93034
O	11	ALA	-	expression tag	UNP Q93034
V	11	ALA	-	expression tag	UNP Q93034

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Chain	Residue	Modelled	Actual	Comment	Reference
f	11	ALA	-	expression tag	UNP Q93034
l	11	ALA	-	expression tag	UNP Q93034
r	11	ALA	-	expression tag	UNP Q93034
x	11	ALA	-	expression tag	UNP Q93034
3	11	ALA	-	expression tag	UNP Q93034
9	11	ALA	-	expression tag	UNP Q93034
w	11	ALA	-	expression tag	UNP Q93034

- Molecule 2 is a protein called Transcription elongation factor B polypeptide 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	E	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	K	86	Total	C	N	O	S	0	0	0
			683	442	110	127	4			
2	Q	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	Z	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	h	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	n	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	t	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	z	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	5	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	T	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			
2	B	87	Total	C	N	O	S	0	0	0
			691	447	111	128	5			

- Molecule 3 is a protein called Transcription elongation factor B polypeptide 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	D	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	90	Total	C	N	O	S	0	0	0
			711	449	120	139	3			
3	P	94	Total	C	N	O	S	0	0	0
			740	470	124	143	3			
3	W	91	Total	C	N	O	S	0	0	0
			717	454	121	139	3			
3	g	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	m	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	s	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	y	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	4	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	e	79	Total	C	N	O	S	0	0	0
			624	394	109	119	2			
3	H	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			

- Molecule 4 is a protein called Core-binding factor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	a	146	Total	C	N	O	S	0	0	0
			1193	745	217	225	6			
4	F	145	Total	C	N	O	S	0	0	0
			1185	741	216	222	6			
4	L	144	Total	C	N	O	S	0	0	0
			1154	723	211	214	6			
4	R	144	Total	C	N	O	S	0	0	0
			1175	734	212	223	6			
4	c	145	Total	C	N	O	S	0	0	0
			1180	737	213	224	6			
4	i	155	Total	C	N	O	S	0	0	0
			1271	790	232	243	6			
4	o	143	Total	C	N	O	S	0	0	0
			1167	730	211	220	6			
4	u	143	Total	C	N	O	S	0	0	0
			1167	730	211	220	6			
4	0	144	Total	C	N	O	S	0	0	0
			1175	734	212	223	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	6	140	Total	C	N	O	S	0	0	0
			1147	718	208	215	6			
4	k	147	Total	C	N	O	S	0	0	0
			1196	746	215	229	6			
4	N	145	Total	C	N	O	S	0	0	0
			1173	734	213	220	6			

- Molecule 5 is a protein called Virion infectivity factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	b	172	Total	C	N	O	S	0	0	0
			1414	908	258	243	5			
5	G	170	Total	C	N	O	S	0	0	0
			1397	898	256	239	4			
5	M	171	Total	C	N	O	S	0	0	0
			1402	901	257	240	4			
5	S	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	d	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	j	170	Total	C	N	O	S	0	0	0
			1397	898	256	239	4			
5	p	169	Total	C	N	O	S	0	0	0
			1380	887	251	238	4			
5	v	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	1	170	Total	C	N	O	S	0	0	0
			1385	890	252	239	4			
5	7	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	q	169	Total	C	N	O	S	0	0	0
			1386	892	252	238	4			
5	2	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	b	1	Total	Zn	0	0
			1	1		
6	G	1	Total	Zn	0	0
			1	1		

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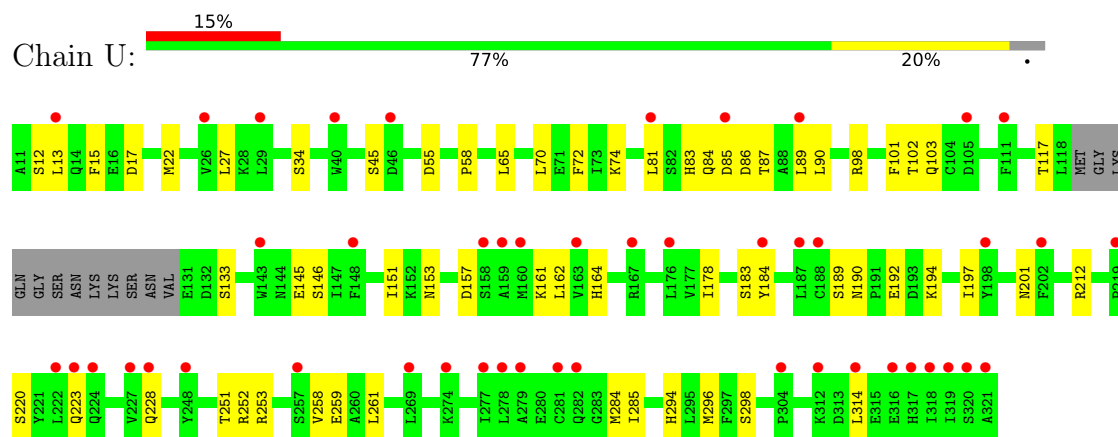
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total 1	Zn 1	0	0
6	S	1	Total 1	Zn 1	0	0
6	d	1	Total 1	Zn 1	0	0
6	j	1	Total 1	Zn 1	0	0
6	p	1	Total 1	Zn 1	0	0
6	v	1	Total 1	Zn 1	0	0
6	1	1	Total 1	Zn 1	0	0
6	7	1	Total 1	Zn 1	0	0
6	q	1	Total 1	Zn 1	0	0
6	2	1	Total 1	Zn 1	0	0

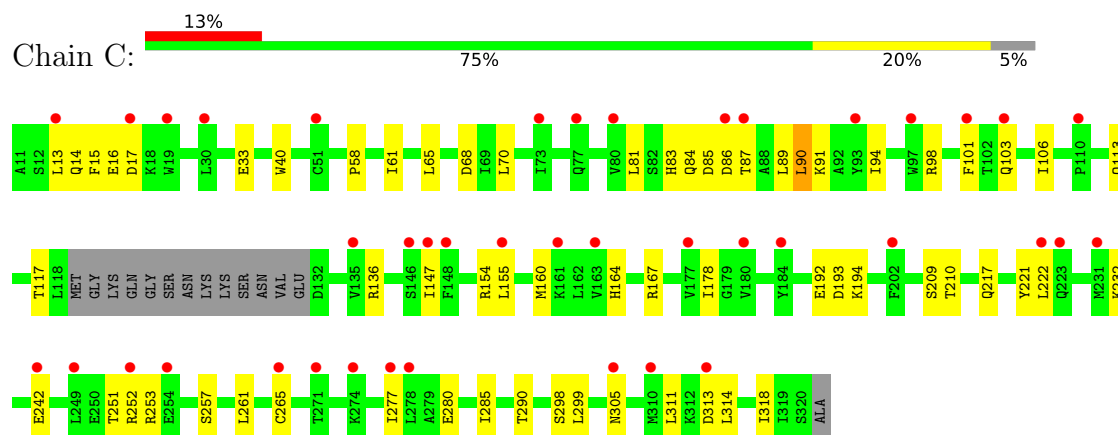
3 Residue-property plots [i](#)

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.

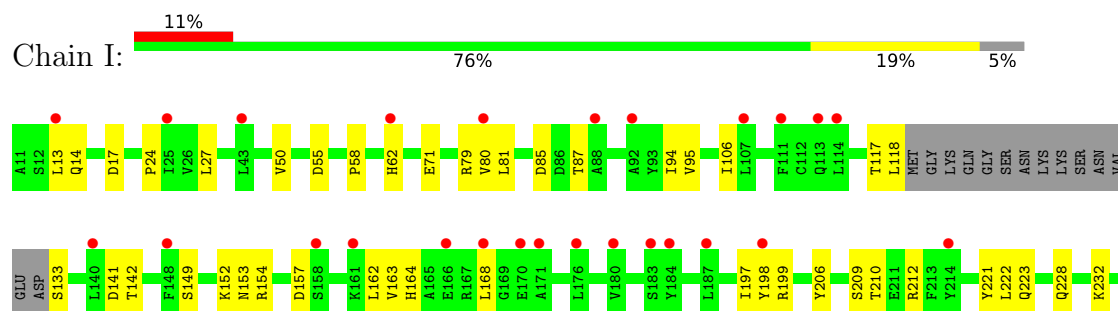
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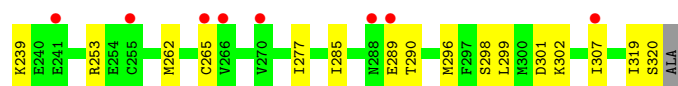


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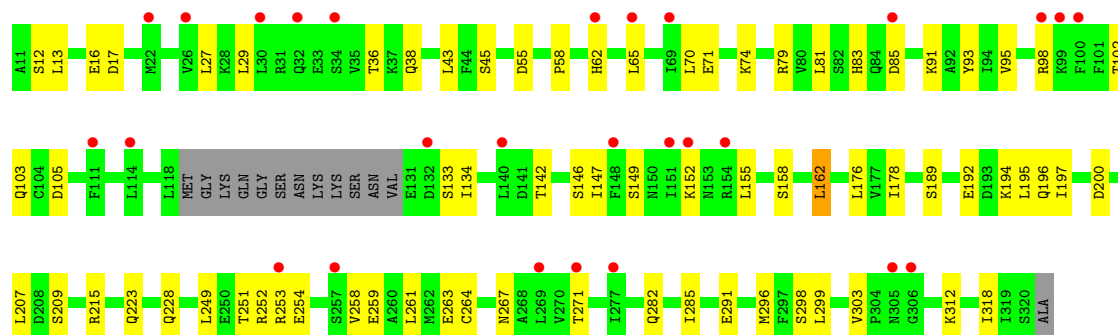
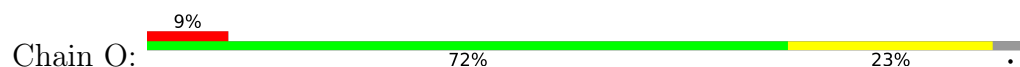


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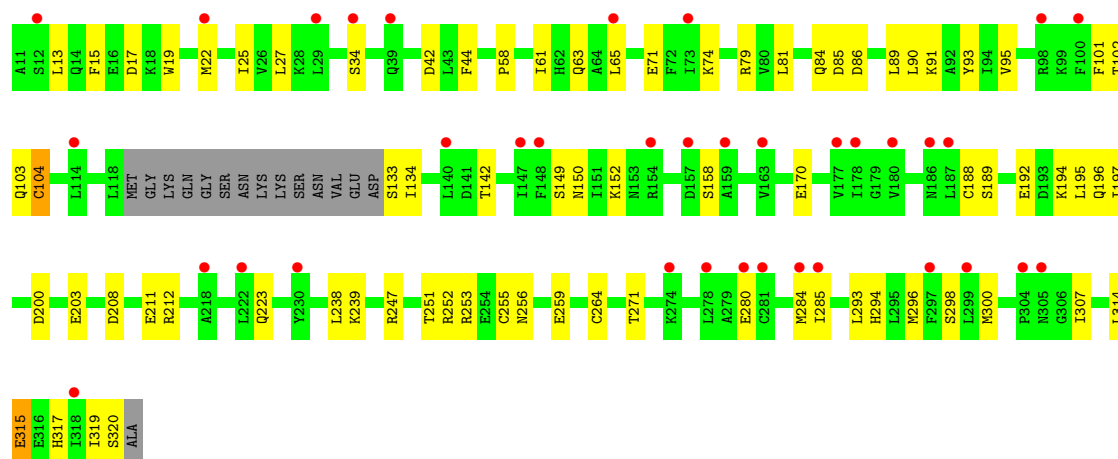




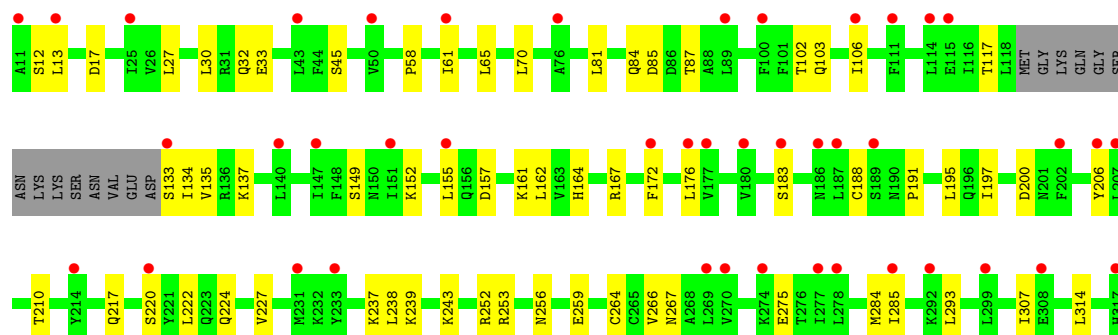
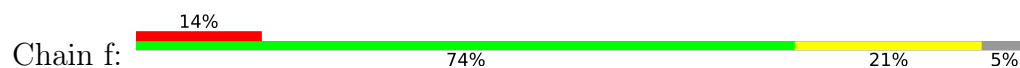
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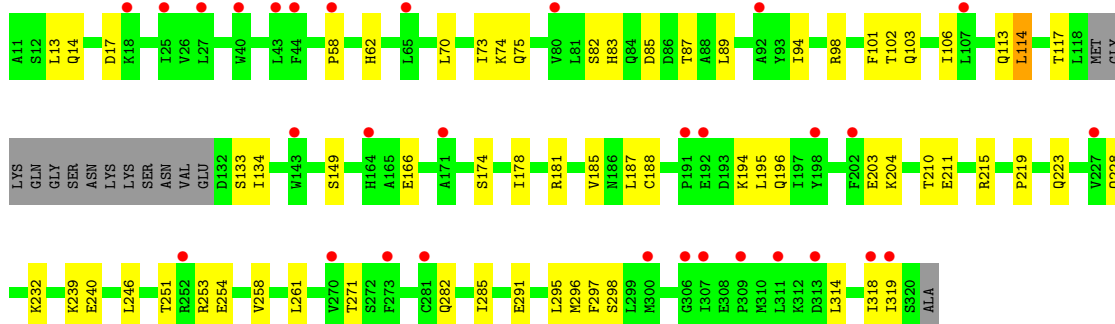
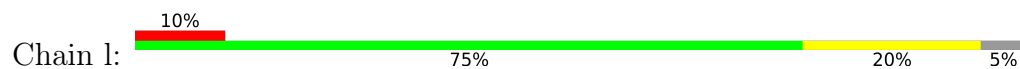


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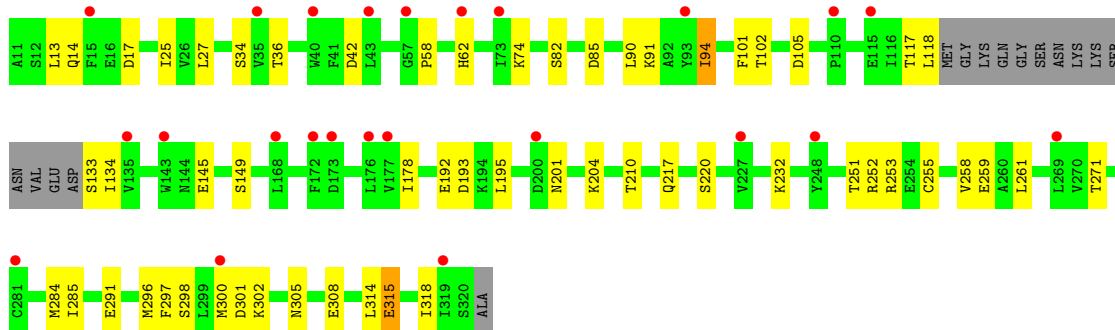
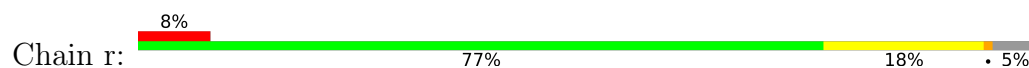




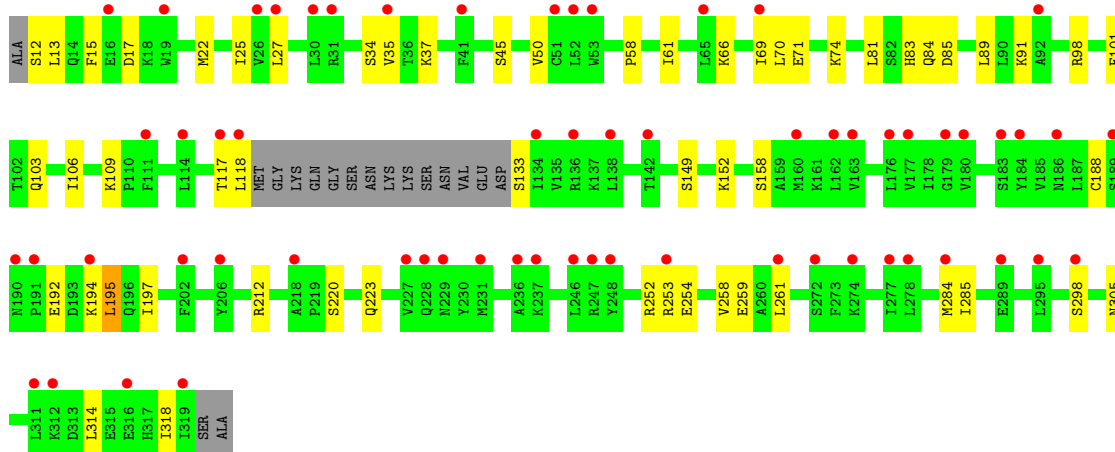
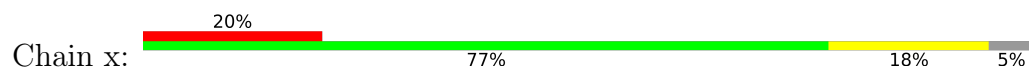
• Molecule 1: Cullin-5



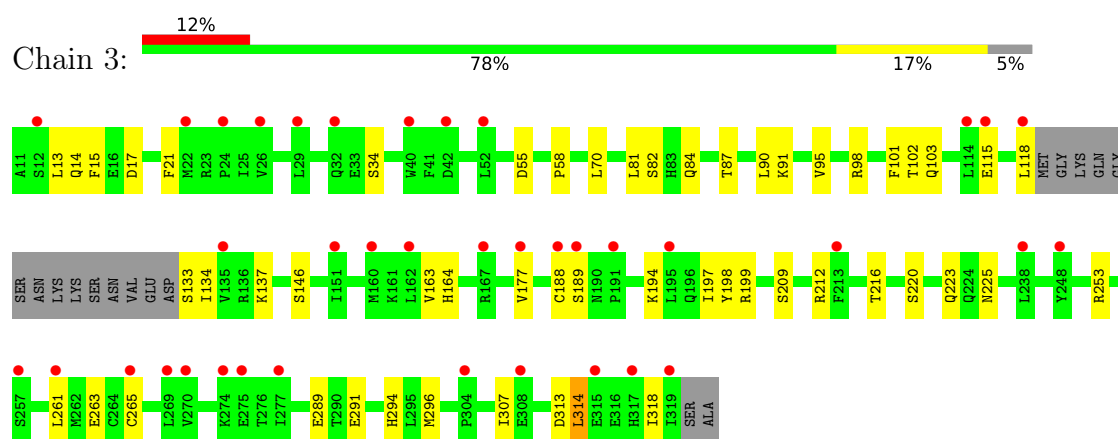
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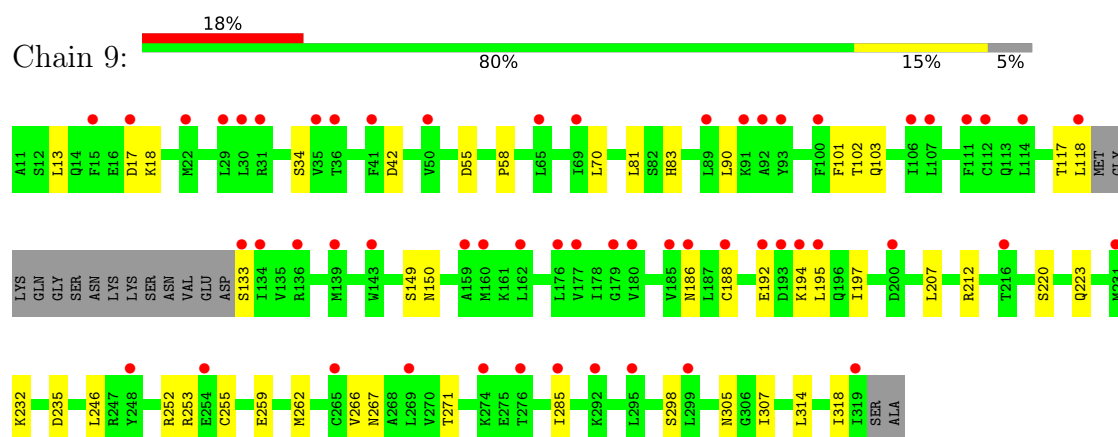
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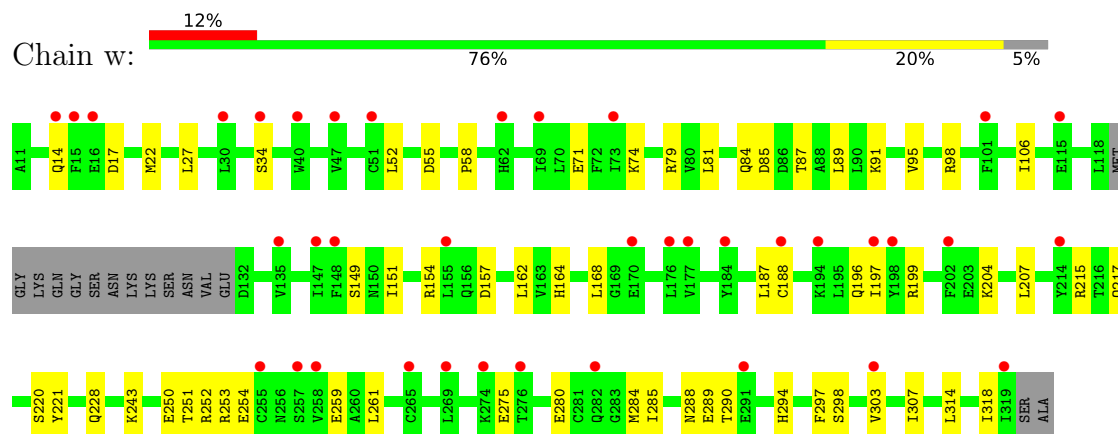
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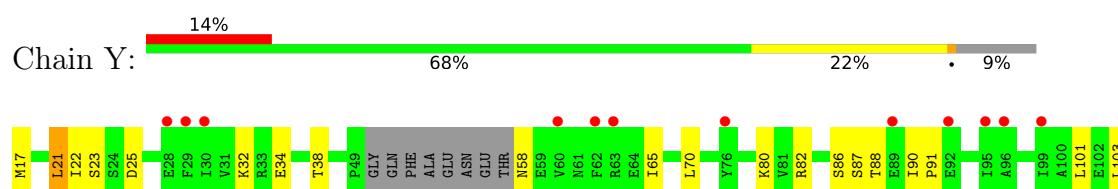
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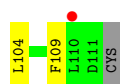


• Molecule 1: Cullin-5

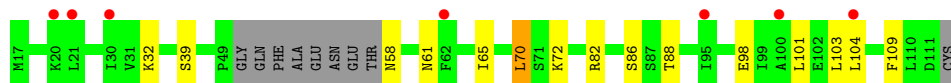
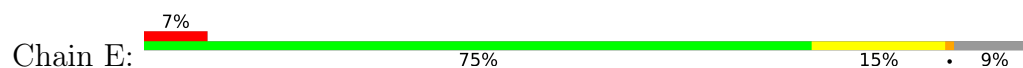


• Molecule 2: Transcription elongation factor B polypeptide 1

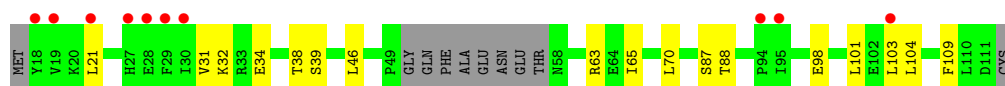




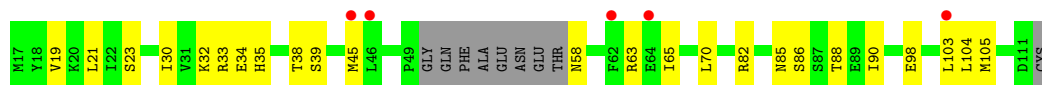
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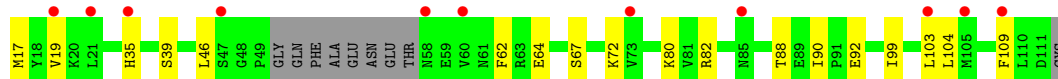
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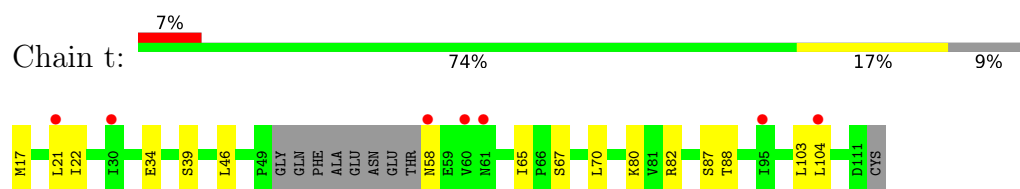
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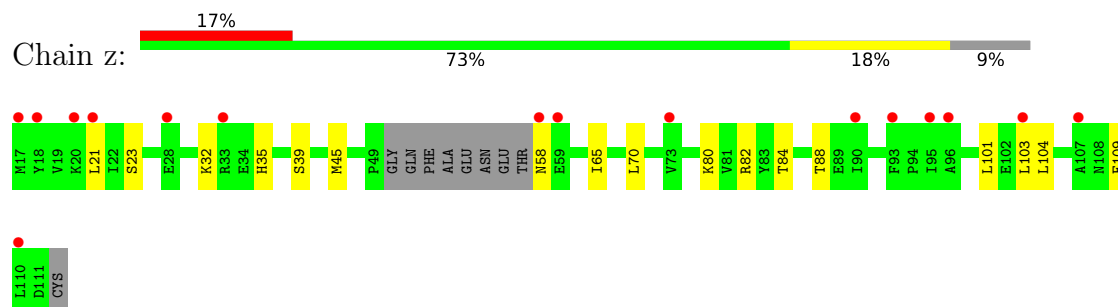
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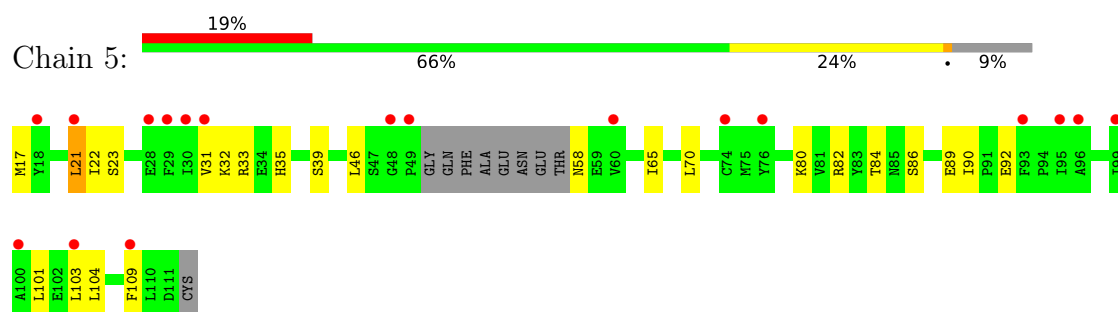
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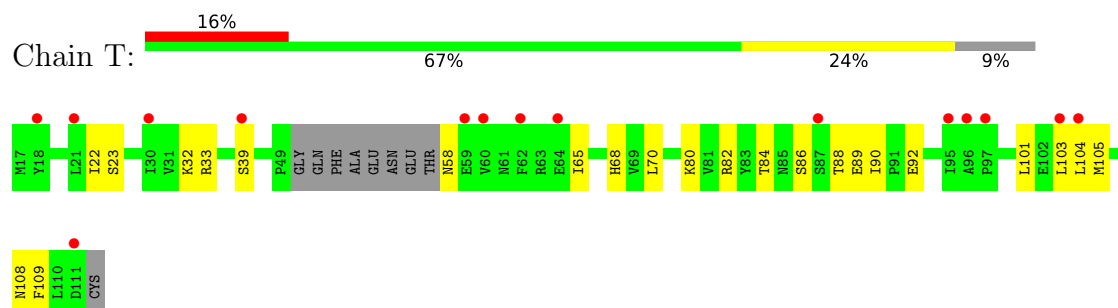
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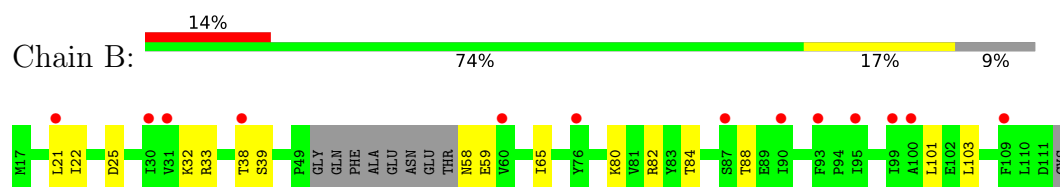
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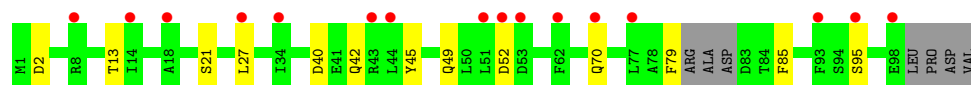
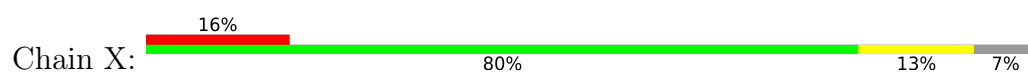
- Molecule 2: Transcription elongation factor B polypeptide 1



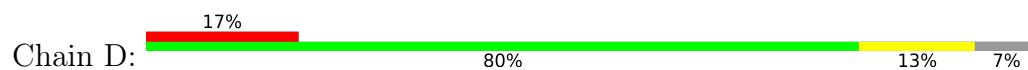
- Molecule 2: Transcription elongation factor B polypeptide 1



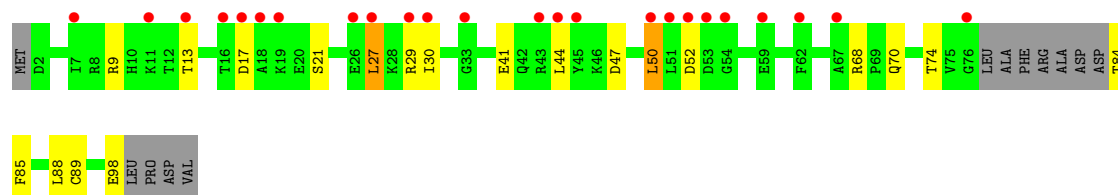
- Molecule 3: Transcription elongation factor B polypeptide 2



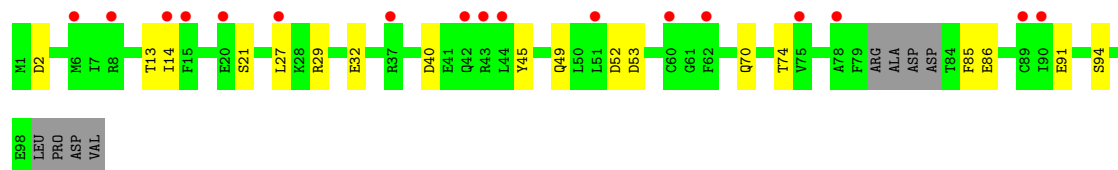
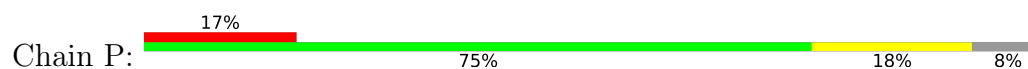
- Molecule 3: Transcription elongation factor B polypeptide 2



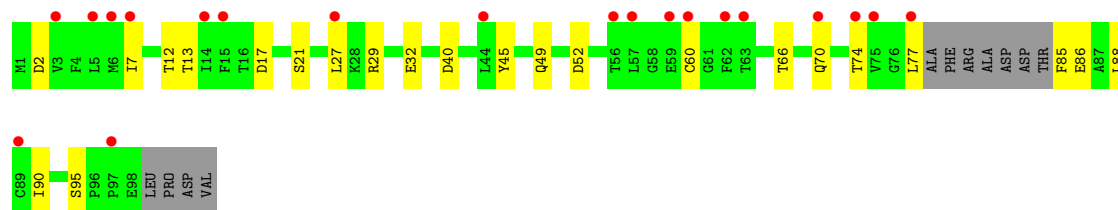
- Molecule 3: Transcription elongation factor B polypeptide 2



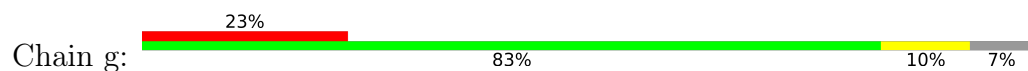
- Molecule 3: Transcription elongation factor B polypeptide 2

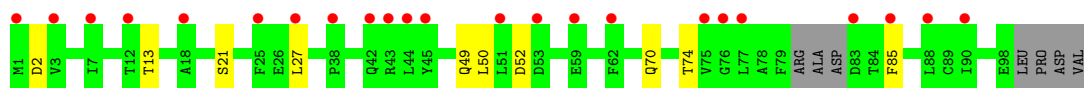


- Molecule 3: Transcription elongation factor B polypeptide 2

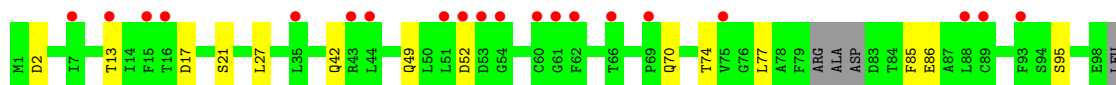
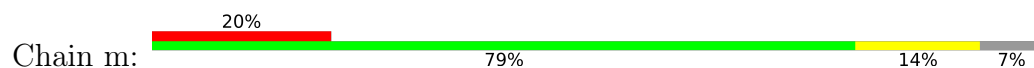


- Molecule 3: Transcription elongation factor B polypeptide 2

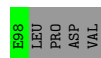
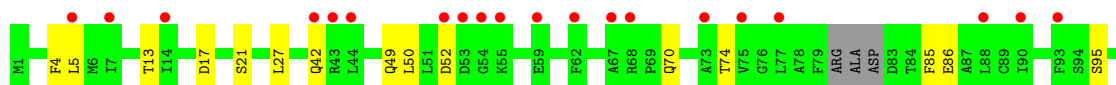
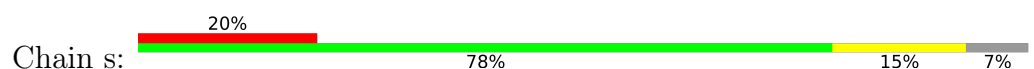




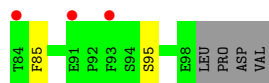
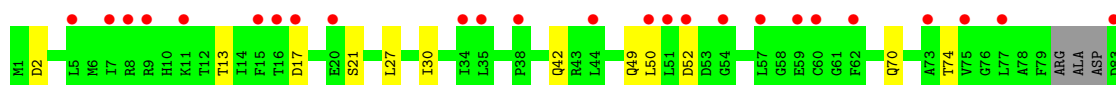
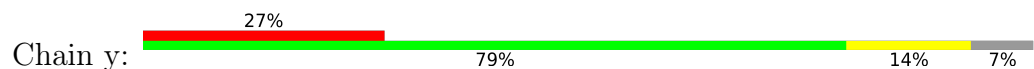
- Molecule 3: Transcription elongation factor B polypeptide 2



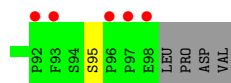
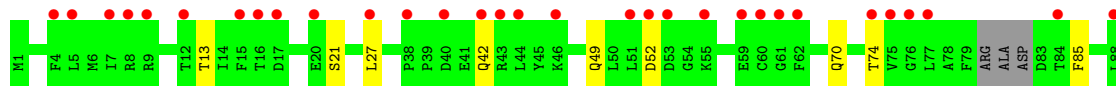
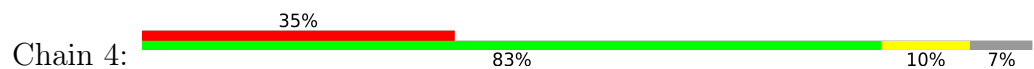
- Molecule 3: Transcription elongation factor B polypeptide 2



- Molecule 3: Transcription elongation factor B polypeptide 2

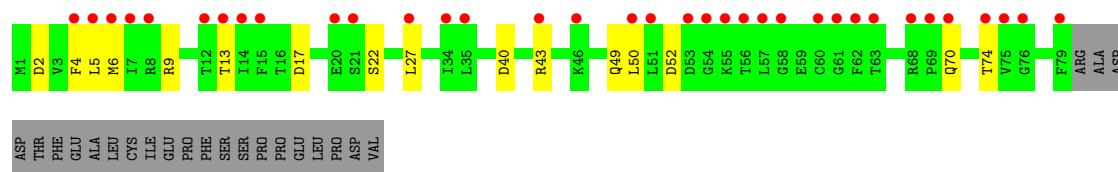


- Molecule 3: Transcription elongation factor B polypeptide 2

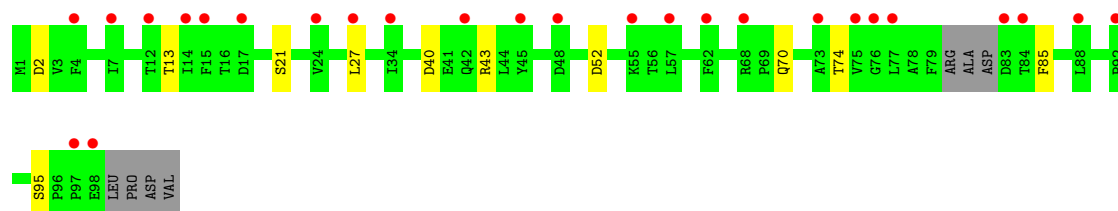
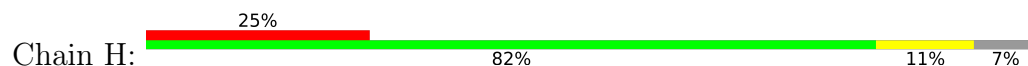


- Molecule 3: Transcription elongation factor B polypeptide 2

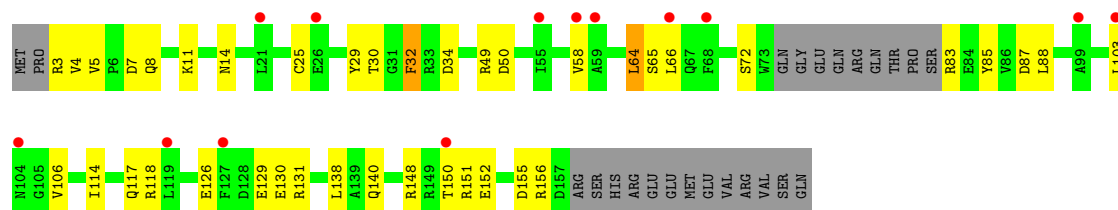




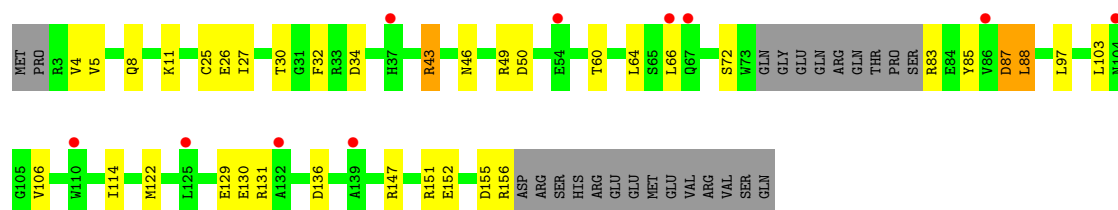
• Molecule 3: Transcription elongation factor B polypeptide 2



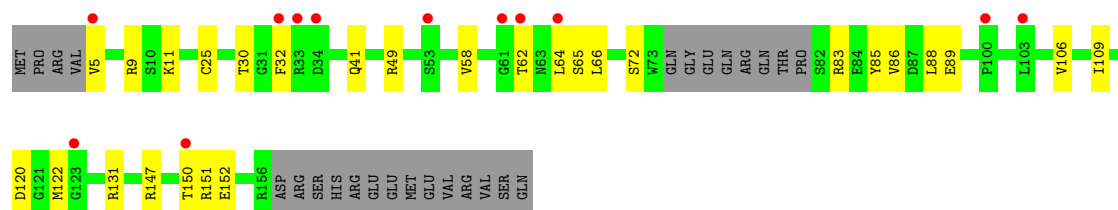
• Molecule 4: Core-binding factor subunit beta



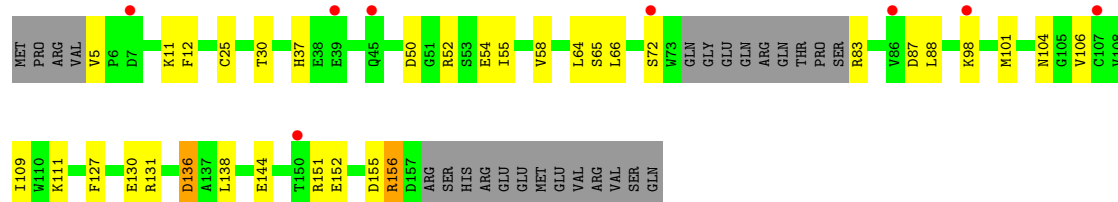
• Molecule 4: Core-binding factor subunit beta



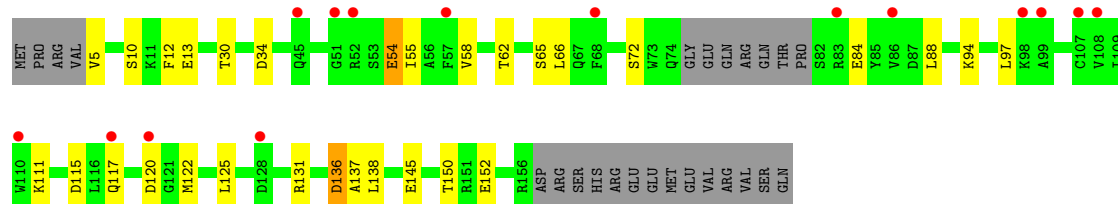
• Molecule 4: Core-binding factor subunit beta



- Molecule 4: Core-binding factor subunit beta



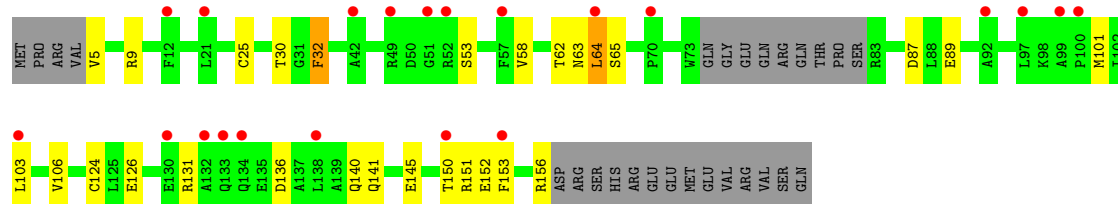
- Molecule 4: Core-binding factor subunit beta



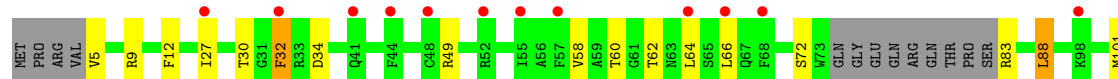
- Molecule 4: Core-binding factor subunit beta

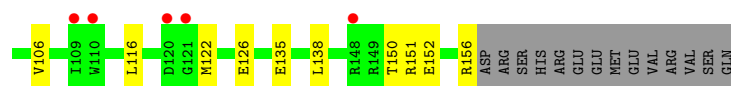


- Molecule 4: Core-binding factor subunit beta

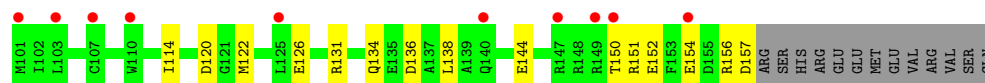
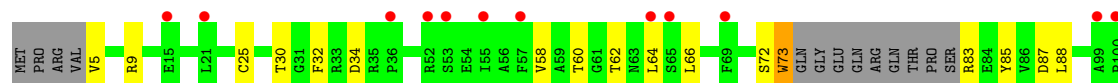


- Molecule 4: Core-binding factor subunit beta

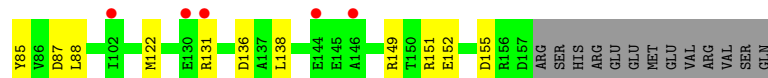
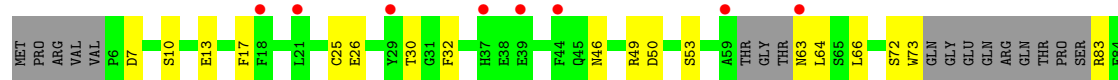




• Molecule 4: Core-binding factor subunit beta



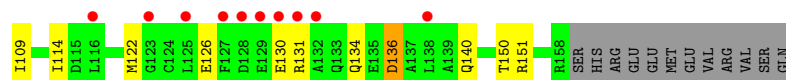
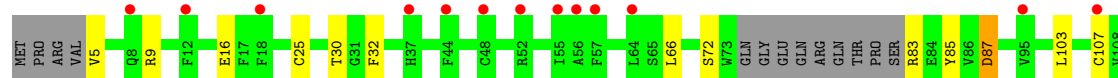
• Molecule 4: Core-binding factor subunit beta



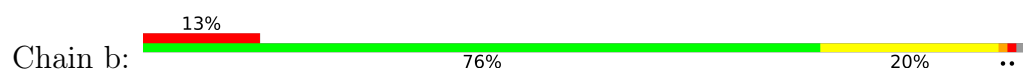
• Molecule 4: Core-binding factor subunit beta

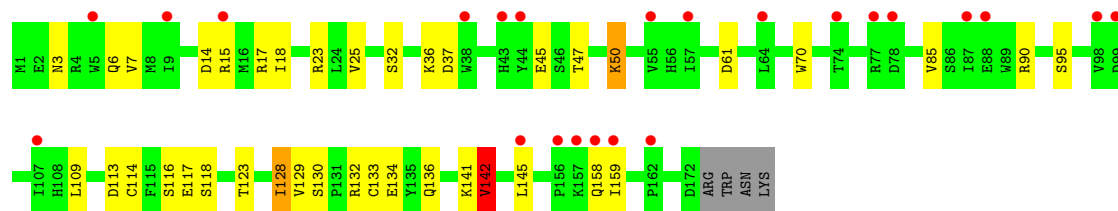


• Molecule 4: Core-binding factor subunit beta

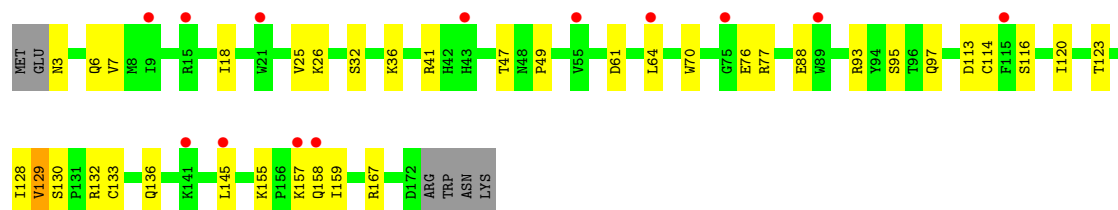
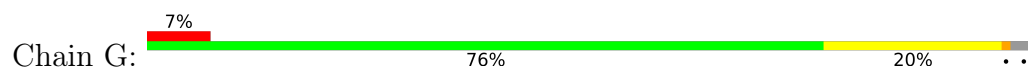


• Molecule 5: Virion infectivity factor

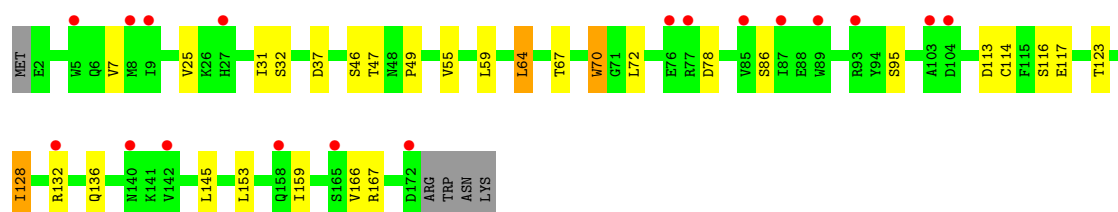
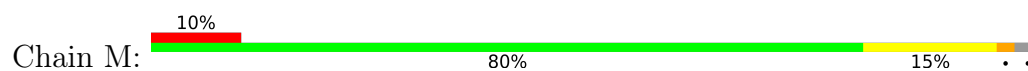




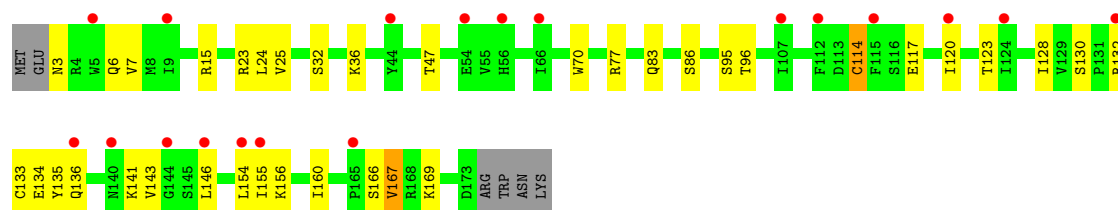
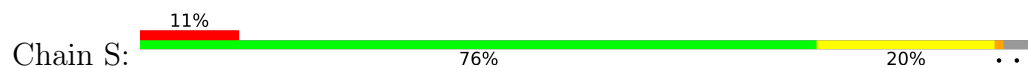
• Molecule 5: Virion infectivity factor



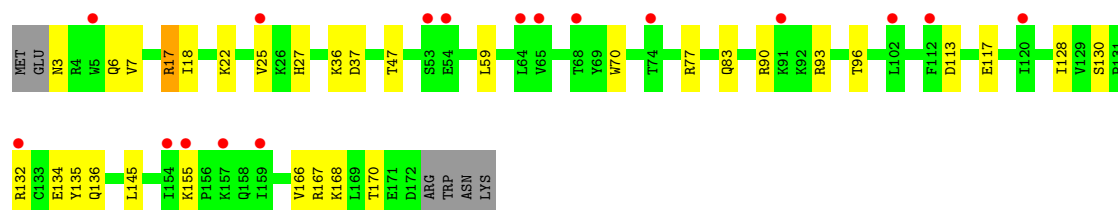
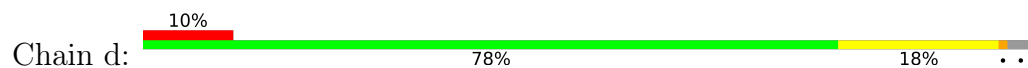
• Molecule 5: Virion infectivity factor



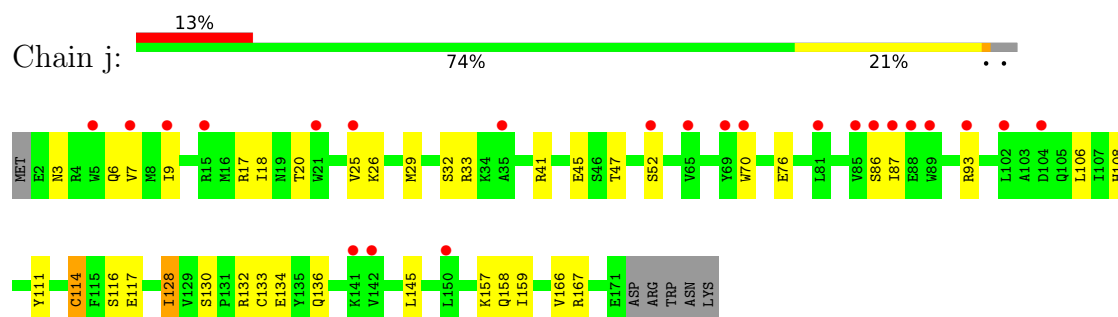
• Molecule 5: Virion infectivity factor



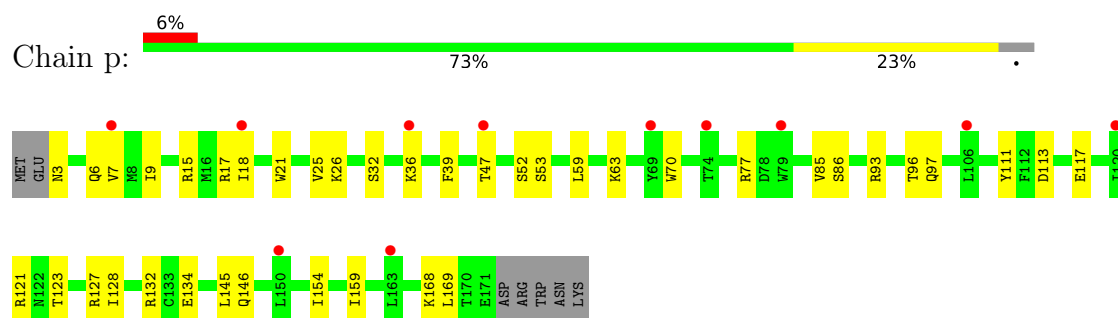
• Molecule 5: Virion infectivity factor



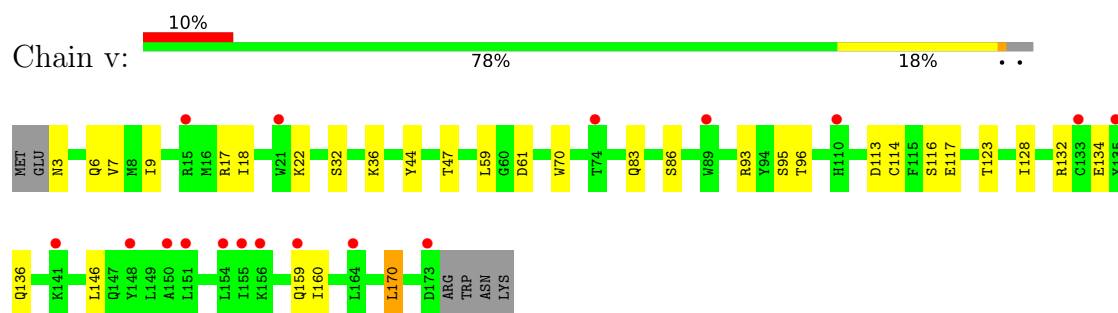
- Molecule 5: Virion infectivity factor



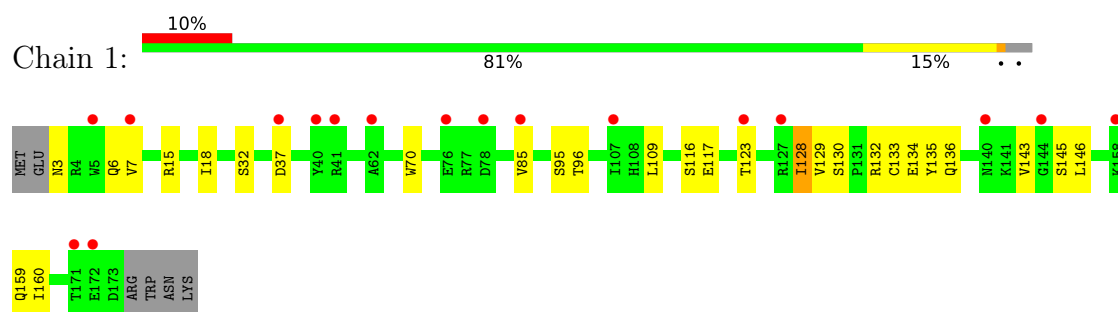
- Molecule 5: Virion infectivity factor



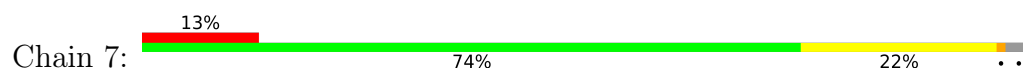
- Molecule 5: Virion infectivity factor

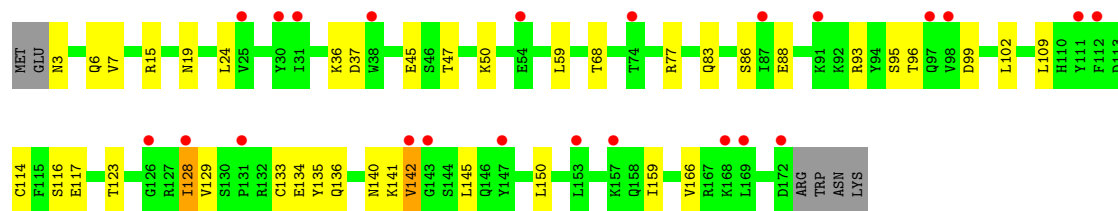


- Molecule 5: Virion infectivity factor

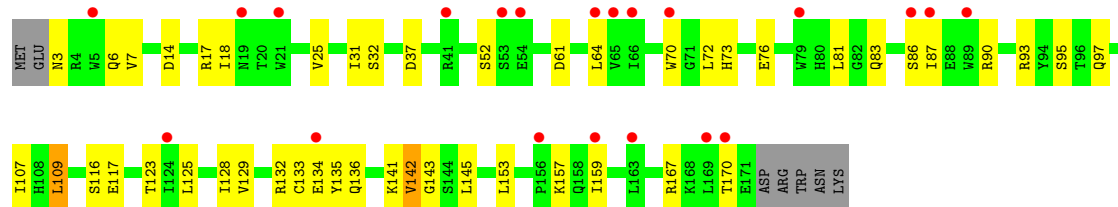


- Molecule 5: Virion infectivity factor

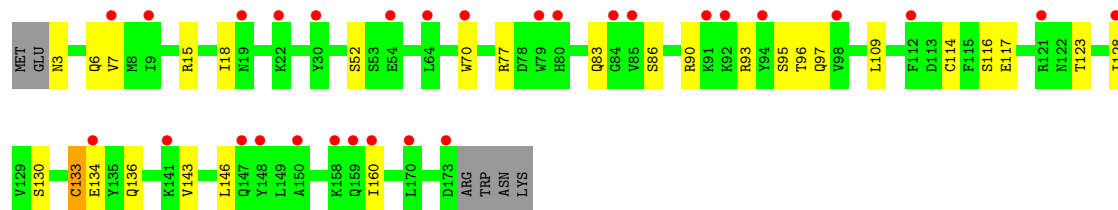
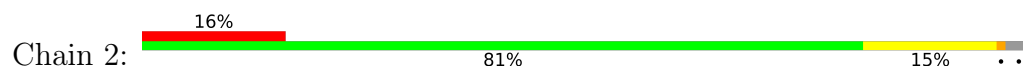




● Molecule 5: Virion infectivity factor



● Molecule 5: Virion infectivity factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.92Å 204.00Å 247.87Å 65.51° 90.28° 90.50°	Depositor
Resolution (Å)	49.53 – 3.30 49.54 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.53-3.30) 93.8 (49.54-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.262 , 0.324 0.265 , 0.325	Depositor DCC
R_{free} test set	14295 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	100.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l 0.327 for -h,k,k-l 0.196 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	77274	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	3	0.60	0/2480	0.83	2/3340 (0.1%)
1	9	0.48	0/2480	0.75	2/3340 (0.1%)
1	C	0.60	0/2491	0.85	4/3355 (0.1%)
1	I	0.57	0/2486	0.87	2/3348 (0.1%)
1	O	0.61	0/2496	0.87	2/3362 (0.1%)
1	U	0.57	1/2514 (0.0%)	0.83	1/3386 (0.0%)
1	V	0.63	1/2486 (0.0%)	0.89	2/3348 (0.1%)
1	f	0.57	0/2486	0.86	6/3348 (0.2%)
1	l	0.60	0/2489	0.88	2/3352 (0.1%)
1	r	0.61	0/2486	0.85	2/3348 (0.1%)
1	w	0.57	0/2485	0.84	4/3347 (0.1%)
1	x	0.49	0/2464	0.73	2/3319 (0.1%)
2	5	0.52	0/706	0.86	1/954 (0.1%)
2	B	0.54	0/706	0.79	0/954
2	E	0.58	0/706	0.81	1/954 (0.1%)
2	K	0.55	0/698	0.85	0/944
2	Q	0.60	0/706	0.80	0/954
2	T	0.51	0/706	0.78	0/954
2	Y	0.62	0/706	0.84	1/954 (0.1%)
2	Z	0.54	0/706	0.73	1/954 (0.1%)
2	h	0.60	0/706	0.88	0/954
2	n	0.61	0/706	0.85	0/954
2	t	0.58	0/706	0.83	0/954
2	z	0.52	0/706	0.77	1/954 (0.1%)
3	4	0.40	0/762	0.72	0/1029
3	D	0.44	0/762	0.71	0/1029
3	H	0.40	0/762	0.72	0/1029
3	J	0.54	0/724	0.92	2/977 (0.2%)
3	P	0.49	0/754	0.81	0/1018
3	W	0.46	0/730	0.79	0/985
3	X	0.48	0/762	0.75	0/1029
3	e	0.42	0/634	0.75	1/854 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	g	0.45	0/762	0.75	1/1029 (0.1%)
3	m	0.46	0/762	0.77	1/1029 (0.1%)
3	s	0.52	0/762	0.78	0/1029
3	y	0.42	0/762	0.70	1/1029 (0.1%)
4	0	0.62	1/1198 (0.1%)	0.85	0/1610
4	6	0.65	0/1169	0.85	0/1567
4	F	0.68	0/1208	1.00	3/1623 (0.2%)
4	L	0.67	1/1177 (0.1%)	0.88	1/1583 (0.1%)
4	N	0.61	1/1196 (0.1%)	0.87	2/1608 (0.1%)
4	R	0.69	0/1198	0.98	3/1610 (0.2%)
4	a	0.69	0/1216	0.92	2/1634 (0.1%)
4	c	0.73	0/1203	0.93	3/1616 (0.2%)
4	i	0.64	1/1297 (0.1%)	0.87	0/1744
4	k	0.60	0/1220	0.90	4/1639 (0.2%)
4	o	0.69	1/1190 (0.1%)	0.90	2/1599 (0.1%)
4	u	0.73	0/1190	0.92	2/1599 (0.1%)
5	1	0.60	0/1427	0.84	1/1942 (0.1%)
5	2	0.57	1/1433 (0.1%)	0.82	1/1949 (0.1%)
5	7	0.53	0/1433	0.82	1/1949 (0.1%)
5	G	0.62	0/1439	0.86	0/1956
5	M	0.64	1/1444 (0.1%)	0.87	2/1963 (0.1%)
5	S	0.70	1/1433 (0.1%)	0.94	3/1949 (0.2%)
5	b	0.68	0/1456	0.95	3/1978 (0.2%)
5	d	0.71	0/1433	0.95	2/1949 (0.1%)
5	j	0.67	1/1439 (0.1%)	0.91	2/1956 (0.1%)
5	p	0.68	0/1422	0.96	3/1935 (0.2%)
5	q	0.64	0/1428	0.86	2/1942 (0.1%)
5	v	0.68	0/1433	0.90	2/1949 (0.1%)
All	All	0.60	11/78927 (0.0%)	0.85	86/106546 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	1
2	T	0	1
2	Y	0	1
4	R	0	1
5	j	0	1
5	q	0	1
All	All	0	6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	114	CYS	CB-SG	-6.59	1.71	1.82
1	V	104	CYS	CB-SG	-6.54	1.71	1.82
5	M	70	TRP	CB-CG	-6.26	1.39	1.50
5	2	133	CYS	CB-SG	-5.83	1.72	1.81
4	0	73	TRP	CB-CG	5.63	1.60	1.50

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	162	LEU	CB-CG-CD2	-11.08	92.16	111.00
1	U	58	PRO	CA-N-CD	-9.22	98.58	111.50
5	p	169	LEU	CA-CB-CG	9.16	136.38	115.30
1	f	58	PRO	CA-N-CD	-9.00	98.90	111.50
1	V	58	PRO	CA-N-CD	-8.90	99.04	111.50

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	253	ARG	Peptide
4	R	155	ASP	Peptide
2	T	89	GLU	Peptide
2	Y	91	PRO	Peptide
5	j	33	ARG	Peptide

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	3	292/311 (94%)	289 (99%)	2 (1%)	1 (0%)	41	71
1	9	292/311 (94%)	279 (96%)	13 (4%)	0	100	100
1	C	294/311 (94%)	290 (99%)	3 (1%)	1 (0%)	41	71
1	I	293/311 (94%)	288 (98%)	5 (2%)	0	100	100
1	O	295/311 (95%)	291 (99%)	4 (1%)	0	100	100
1	U	297/311 (96%)	290 (98%)	6 (2%)	1 (0%)	41	71
1	V	293/311 (94%)	288 (98%)	5 (2%)	0	100	100
1	f	293/311 (94%)	287 (98%)	6 (2%)	0	100	100
1	l	293/311 (94%)	287 (98%)	6 (2%)	0	100	100
1	r	293/311 (94%)	287 (98%)	6 (2%)	0	100	100
1	w	293/311 (94%)	289 (99%)	4 (1%)	0	100	100
1	x	290/311 (93%)	287 (99%)	2 (1%)	1 (0%)	41	71
2	5	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	B	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	E	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	K	82/96 (85%)	81 (99%)	1 (1%)	0	100	100
2	Q	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	T	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	Y	83/96 (86%)	77 (93%)	6 (7%)	0	100	100
2	Z	83/96 (86%)	79 (95%)	4 (5%)	0	100	100
2	h	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	n	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	t	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	z	83/96 (86%)	79 (95%)	4 (5%)	0	100	100
3	4	91/102 (89%)	86 (94%)	5 (6%)	0	100	100
3	D	91/102 (89%)	87 (96%)	4 (4%)	0	100	100
3	H	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	J	86/102 (84%)	83 (96%)	3 (4%)	0	100	100
3	P	90/102 (88%)	87 (97%)	3 (3%)	0	100	100
3	W	87/102 (85%)	84 (97%)	3 (3%)	0	100	100
3	X	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	e	77/102 (76%)	72 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	m	91/102 (89%)	86 (94%)	5 (6%)	0	100	100
3	s	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	y	91/102 (89%)	86 (94%)	5 (6%)	0	100	100
4	0	140/170 (82%)	137 (98%)	2 (1%)	1 (1%)	22	54
4	6	134/170 (79%)	130 (97%)	4 (3%)	0	100	100
4	F	141/170 (83%)	137 (97%)	4 (3%)	0	100	100
4	L	140/170 (82%)	136 (97%)	4 (3%)	0	100	100
4	N	141/170 (83%)	136 (96%)	5 (4%)	0	100	100
4	R	140/170 (82%)	135 (96%)	5 (4%)	0	100	100
4	a	142/170 (84%)	138 (97%)	4 (3%)	0	100	100
4	c	141/170 (83%)	135 (96%)	4 (3%)	2 (1%)	11	38
4	i	153/170 (90%)	148 (97%)	4 (3%)	1 (1%)	22	54
4	k	143/170 (84%)	140 (98%)	3 (2%)	0	100	100
4	o	139/170 (82%)	136 (98%)	3 (2%)	0	100	100
4	u	139/170 (82%)	136 (98%)	3 (2%)	0	100	100
5	1	168/176 (96%)	161 (96%)	4 (2%)	3 (2%)	8	35
5	2	168/176 (96%)	162 (96%)	5 (3%)	1 (1%)	25	57
5	7	168/176 (96%)	160 (95%)	4 (2%)	4 (2%)	6	28
5	G	168/176 (96%)	159 (95%)	7 (4%)	2 (1%)	13	42
5	M	169/176 (96%)	161 (95%)	7 (4%)	1 (1%)	25	57
5	S	168/176 (96%)	162 (96%)	5 (3%)	1 (1%)	25	57
5	b	170/176 (97%)	161 (95%)	6 (4%)	3 (2%)	8	35
5	d	168/176 (96%)	162 (96%)	5 (3%)	1 (1%)	25	57
5	j	168/176 (96%)	163 (97%)	4 (2%)	1 (1%)	25	57
5	p	167/176 (95%)	164 (98%)	2 (1%)	1 (1%)	25	57
5	q	167/176 (95%)	161 (96%)	4 (2%)	2 (1%)	13	42
5	v	168/176 (96%)	161 (96%)	6 (4%)	1 (1%)	25	57
All	All	9291/10260 (91%)	9012 (97%)	250 (3%)	29 (0%)	41	71

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	b	128	ILE
5	G	129	VAL
5	M	128	ILE
5	j	128	ILE
5	p	128	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	269/283 (95%)	219 (81%)	50 (19%)	1	7
1	9	269/283 (95%)	225 (84%)	44 (16%)	2	10
1	C	270/283 (95%)	211 (78%)	59 (22%)	1	3
1	I	270/283 (95%)	212 (78%)	58 (22%)	1	4
1	O	270/283 (95%)	198 (73%)	72 (27%)	0	1
1	U	273/283 (96%)	214 (78%)	59 (22%)	1	4
1	V	270/283 (95%)	196 (73%)	74 (27%)	0	1
1	f	270/283 (95%)	210 (78%)	60 (22%)	1	3
1	l	271/283 (96%)	208 (77%)	63 (23%)	1	3
1	r	270/283 (95%)	214 (79%)	56 (21%)	1	4
1	w	269/283 (95%)	212 (79%)	57 (21%)	1	4
1	x	268/283 (95%)	214 (80%)	54 (20%)	1	5
2	5	78/85 (92%)	54 (69%)	24 (31%)	0	1
2	B	78/85 (92%)	62 (80%)	16 (20%)	1	4
2	E	78/85 (92%)	63 (81%)	15 (19%)	1	6
2	K	77/85 (91%)	60 (78%)	17 (22%)	1	3
2	Q	78/85 (92%)	54 (69%)	24 (31%)	0	1
2	T	78/85 (92%)	56 (72%)	22 (28%)	0	1
2	Y	78/85 (92%)	57 (73%)	21 (27%)	0	1
2	Z	78/85 (92%)	55 (70%)	23 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	h	78/85 (92%)	60 (77%)	18 (23%)	1	3
2	n	78/85 (92%)	60 (77%)	18 (23%)	1	3
2	t	78/85 (92%)	62 (80%)	16 (20%)	1	4
2	z	78/85 (92%)	62 (80%)	16 (20%)	1	4
3	4	83/90 (92%)	73 (88%)	10 (12%)	5	20
3	D	83/90 (92%)	70 (84%)	13 (16%)	2	12
3	H	83/90 (92%)	72 (87%)	11 (13%)	4	17
3	J	80/90 (89%)	60 (75%)	20 (25%)	0	2
3	P	82/90 (91%)	64 (78%)	18 (22%)	1	3
3	W	80/90 (89%)	57 (71%)	23 (29%)	0	1
3	X	83/90 (92%)	70 (84%)	13 (16%)	2	12
3	e	68/90 (76%)	53 (78%)	15 (22%)	1	3
3	g	83/90 (92%)	74 (89%)	9 (11%)	6	24
3	m	83/90 (92%)	70 (84%)	13 (16%)	2	12
3	s	83/90 (92%)	68 (82%)	15 (18%)	1	7
3	y	83/90 (92%)	70 (84%)	13 (16%)	2	12
4	0	118/149 (79%)	87 (74%)	31 (26%)	0	2
4	6	114/149 (76%)	85 (75%)	29 (25%)	0	2
4	F	119/149 (80%)	83 (70%)	36 (30%)	0	1
4	L	112/149 (75%)	86 (77%)	26 (23%)	1	3
4	N	116/149 (78%)	93 (80%)	23 (20%)	1	5
4	R	118/149 (79%)	86 (73%)	32 (27%)	0	1
4	a	120/149 (80%)	80 (67%)	40 (33%)	0	1
4	c	118/149 (79%)	91 (77%)	27 (23%)	1	3
4	i	130/149 (87%)	96 (74%)	34 (26%)	0	2
4	k	121/149 (81%)	86 (71%)	35 (29%)	0	1
4	o	117/149 (78%)	90 (77%)	27 (23%)	1	3
4	u	117/149 (78%)	90 (77%)	27 (23%)	1	3
5	1	145/160 (91%)	120 (83%)	25 (17%)	2	9
5	2	147/160 (92%)	121 (82%)	26 (18%)	2	8
5	7	147/160 (92%)	110 (75%)	37 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	148/160 (92%)	112 (76%)	36 (24%)	0	2
5	M	148/160 (92%)	119 (80%)	29 (20%)	1	5
5	S	147/160 (92%)	113 (77%)	34 (23%)	1	3
5	b	150/160 (94%)	113 (75%)	37 (25%)	0	2
5	d	147/160 (92%)	119 (81%)	28 (19%)	1	6
5	j	148/160 (92%)	111 (75%)	37 (25%)	0	2
5	p	145/160 (91%)	110 (76%)	35 (24%)	0	2
5	q	147/160 (92%)	103 (70%)	44 (30%)	0	1
5	v	147/160 (92%)	118 (80%)	29 (20%)	1	5
All	All	8334/9204 (90%)	6461 (78%)	1873 (22%)	1	3

5 of 1873 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	i	29	TYR
1	w	221	TYR
5	p	159	ILE
1	w	91	LYS
1	9	188	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	l	317	HIS
4	k	41	GLN
1	r	32	GLN
4	k	37	HIS
1	w	103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	3	295/311 (94%)	0.74	38 (12%)	3 3	20, 60, 139, 214	0
1	9	295/311 (94%)	1.02	56 (18%)	1 1	42, 104, 191, 306	0
1	C	297/311 (95%)	0.72	41 (13%)	2 2	23, 57, 124, 228	0
1	I	296/311 (95%)	0.71	34 (11%)	4 4	24, 69, 144, 252	0
1	O	298/311 (95%)	0.53	27 (9%)	9 9	20, 60, 126, 207	0
1	U	299/311 (96%)	0.88	47 (15%)	2 2	20, 59, 135, 250	0
1	V	296/311 (95%)	0.56	36 (12%)	4 3	17, 60, 125, 228	0
1	f	296/311 (95%)	0.77	43 (14%)	2 2	26, 67, 147, 223	0
1	l	297/311 (95%)	0.62	31 (10%)	6 6	19, 47, 105, 176	0
1	r	296/311 (95%)	0.50	24 (8%)	12 11	13, 48, 118, 195	0
1	w	296/311 (95%)	0.77	38 (12%)	3 3	4, 60, 145, 197	0
1	x	294/311 (94%)	1.07	62 (21%)	1 1	41, 107, 198, 297	0
2	5	87/96 (90%)	0.92	18 (20%)	1 1	44, 76, 172, 193	0
2	B	87/96 (90%)	0.87	13 (14%)	2 2	45, 76, 169, 246	0
2	E	87/96 (90%)	0.60	7 (8%)	12 11	23, 46, 121, 189	0
2	K	86/96 (89%)	0.65	10 (11%)	4 4	32, 54, 134, 201	0
2	Q	87/96 (90%)	0.62	5 (5%)	23 23	36, 61, 138, 195	0
2	T	87/96 (90%)	1.10	15 (17%)	1 1	60, 92, 168, 226	0
2	Y	87/96 (90%)	0.82	13 (14%)	2 2	23, 49, 129, 184	0
2	Z	87/96 (90%)	0.88	10 (11%)	4 4	34, 61, 143, 184	0
2	h	87/96 (90%)	0.91	10 (11%)	4 4	35, 63, 141, 175	0
2	n	87/96 (90%)	0.73	11 (12%)	3 3	24, 51, 110, 176	0
2	t	87/96 (90%)	0.65	7 (8%)	12 11	28, 51, 127, 198	0
2	z	87/96 (90%)	1.08	16 (18%)	1 1	55, 91, 168, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	4	95/102 (93%)	2.03	36 (37%) 0 0	61, 115, 212, 286	0
3	D	95/102 (93%)	1.04	17 (17%) 1 1	51, 86, 177, 225	0
3	H	95/102 (93%)	1.36	26 (27%) 0 0	71, 107, 209, 248	0
3	J	90/102 (88%)	1.29	24 (26%) 0 0	62, 87, 171, 260	0
3	P	94/102 (92%)	0.89	17 (18%) 1 1	38, 79, 151, 174	0
3	W	91/102 (89%)	0.97	20 (21%) 0 1	41, 72, 141, 208	0
3	X	95/102 (93%)	0.92	16 (16%) 1 1	44, 80, 177, 216	0
3	e	79/102 (77%)	2.09	35 (44%) 0 0	79, 106, 177, 210	0
3	g	95/102 (93%)	1.22	23 (24%) 0 0	73, 99, 210, 260	0
3	m	95/102 (93%)	1.23	20 (21%) 1 1	45, 78, 164, 226	0
3	s	95/102 (93%)	1.08	20 (21%) 1 1	42, 68, 142, 188	0
3	y	95/102 (93%)	1.70	28 (29%) 0 0	76, 106, 219, 290	0
4	0	144/170 (84%)	0.71	22 (15%) 2 2	26, 56, 122, 194	0
4	6	140/170 (82%)	0.65	13 (9%) 8 9	33, 66, 121, 195	0
4	F	145/170 (85%)	0.48	10 (6%) 16 16	22, 49, 101, 164	0
4	L	144/170 (84%)	0.65	12 (8%) 11 11	20, 52, 114, 170	0
4	N	145/170 (85%)	0.79	23 (15%) 1 2	34, 70, 135, 198	0
4	R	144/170 (84%)	0.57	8 (5%) 24 23	16, 45, 99, 223	0
4	a	146/170 (85%)	0.70	13 (8%) 9 10	20, 48, 96, 214	0
4	c	145/170 (85%)	0.65	15 (10%) 6 6	22, 43, 97, 160	0
4	i	155/170 (91%)	0.55	8 (5%) 27 25	24, 55, 120, 177	0
4	k	147/170 (86%)	0.52	13 (8%) 10 10	32, 58, 128, 183	0
4	o	143/170 (84%)	0.86	21 (14%) 2 2	18, 46, 103, 149	0
4	u	143/170 (84%)	0.74	17 (11%) 4 4	20, 48, 105, 152	0
5	1	170/176 (96%)	0.68	17 (10%) 7 7	36, 62, 141, 239	0
5	2	170/176 (96%)	1.01	29 (17%) 1 1	34, 67, 151, 221	0
5	7	170/176 (96%)	0.91	23 (13%) 3 3	30, 65, 158, 254	0
5	G	170/176 (96%)	0.66	13 (7%) 13 13	16, 41, 95, 173	0
5	M	171/176 (97%)	0.77	18 (10%) 6 6	24, 46, 103, 189	0
5	S	170/176 (96%)	0.76	19 (11%) 5 5	21, 36, 106, 233	0
5	b	172/176 (97%)	0.85	23 (13%) 3 3	22, 41, 93, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	d	170/176 (96%)	0.68	17 (10%) 7 7	18, 39, 106, 172	0
5	j	170/176 (96%)	0.81	23 (13%) 3 3	19, 42, 108, 180	0
5	p	169/176 (96%)	0.68	11 (6%) 18 18	21, 38, 83, 138	0
5	q	169/176 (96%)	0.71	21 (12%) 4 3	33, 59, 125, 190	0
5	v	170/176 (96%)	0.74	17 (10%) 7 7	21, 37, 105, 186	0
All	All	9494/10260 (92%)	0.81	1300 (13%) 3 2	4, 62, 151, 306	0

The worst 5 of 1300 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	m	53	ASP	13.4
3	4	77	LEU	12.6
3	y	16	THR	12.3
3	4	75	VAL	11.7
3	e	62	PHE	11.7

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ZN	v	201	1/1	0.89	0.20	24,24,24,24	0
6	ZN	p	201	1/1	0.91	0.23	19,19,19,19	0
6	ZN	7	201	1/1	0.93	0.20	51,51,51,51	0
6	ZN	d	201	1/1	0.94	0.22	25,25,25,25	0
6	ZN	b	201	1/1	0.94	0.19	33,33,33,33	0
6	ZN	j	201	1/1	0.95	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ZN	q	201	1/1	0.95	0.13	50,50,50,50	0
6	ZN	S	201	1/1	0.96	0.23	32,32,32,32	0
6	ZN	2	201	1/1	0.96	0.24	36,36,36,36	0
6	ZN	G	201	1/1	0.97	0.21	47,47,47,47	0
6	ZN	1	201	1/1	0.98	0.14	65,65,65,65	0
6	ZN	M	201	1/1	0.99	0.23	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.