



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 07:30 PM EDT

PDB ID : 4N9F
Title : Crystal structure of the Vif-CBFbeta-CUL5-EIOB-EIOC 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 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 ⓘ 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

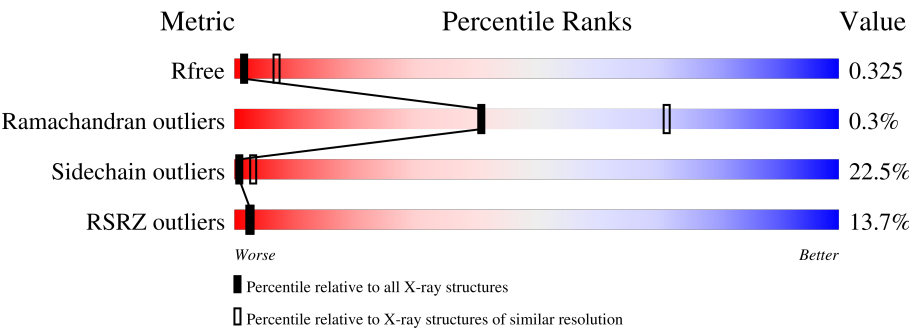
1 Overall quality at a glance i

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	<div><div>12%</div><div>78%</div><div>17%</div><div>5%</div></div>
1	9	311	<div><div>18%</div><div>80%</div><div>15%</div><div>5%</div></div>
1	C	311	<div><div>13%</div><div>75%</div><div>20%</div><div>5%</div></div>
1	I	311	<div><div>11%</div><div>76%</div><div>19%</div><div>5%</div></div>
1	O	311	<div><div>9%</div><div>72%</div><div>23%</div><div>.</div></div>
1	U	311	<div><div>15%</div><div>77%</div><div>20%</div><div>.</div></div>
1	V	311	<div><div>12%</div><div>71%</div><div>24%</div><div>. 5%</div></div>

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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	<div><div>6%</div><div><div></div><div>73%</div><div>23%</div><div></div></div><div></div></div>
5	q	176	<div><div>12%</div><div><div></div><div>69%</div><div>26%</div><div></div></div><div></div></div>
5	v	176	<div><div>10%</div><div><div></div><div>78%</div><div>18%</div><div></div></div><div></div></div>

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 691	C 447	N 111	O 128	S 5	0	0	0
2	E	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	K	86	Total 683	C 442	N 110	O 127	S 4	0	0	0
2	Q	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	Z	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	h	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	n	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	t	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	z	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	5	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	T	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	B	87	Total 691	C 447	N 111	O 128	S 5	0	0	0

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

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

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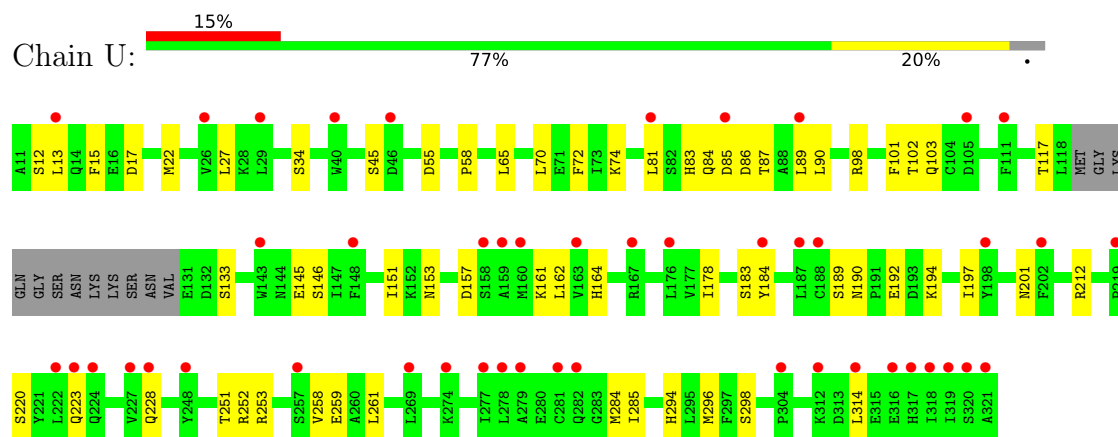
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total 1	Zn 1	0	0
6	S	1	Total 1	Zn 1	0	0
6	d	1	Total 1	Zn 1	0	0
6	j	1	Total 1	Zn 1	0	0
6	p	1	Total 1	Zn 1	0	0
6	v	1	Total 1	Zn 1	0	0
6	1	1	Total 1	Zn 1	0	0
6	7	1	Total 1	Zn 1	0	0
6	q	1	Total 1	Zn 1	0	0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

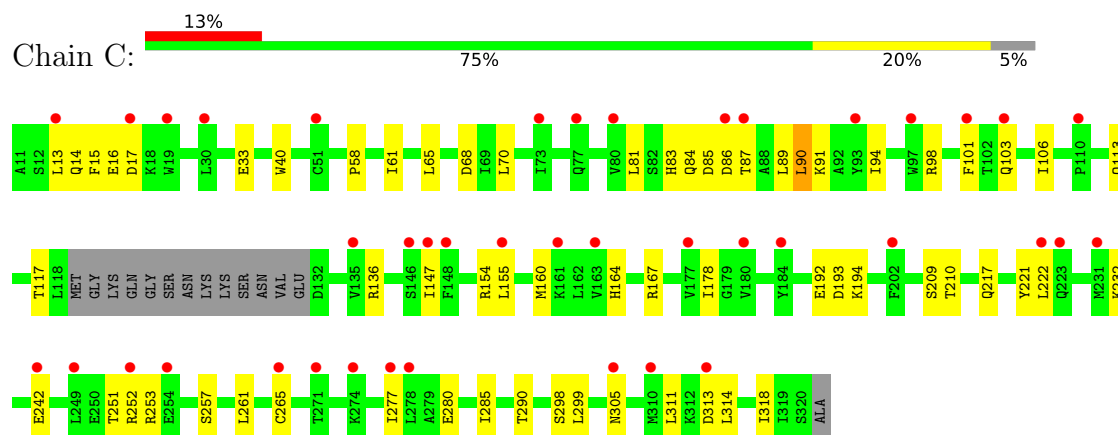
3 Residue-property plots [i](#)

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.

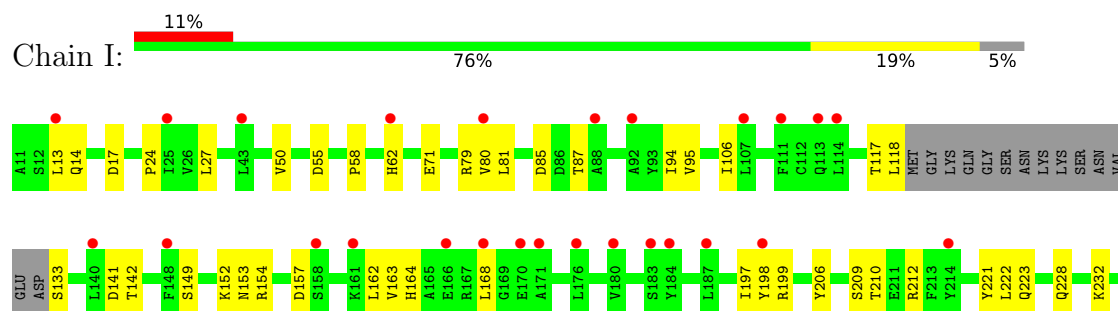
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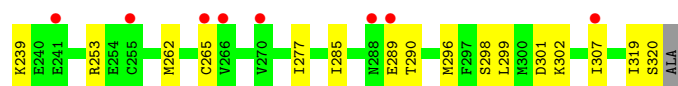


• Molecule 1: Cullin-5

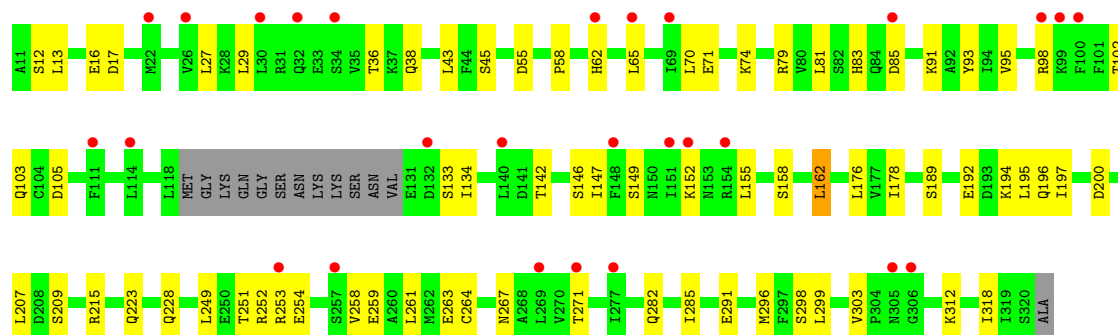
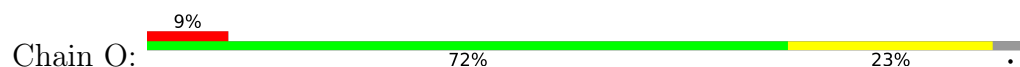


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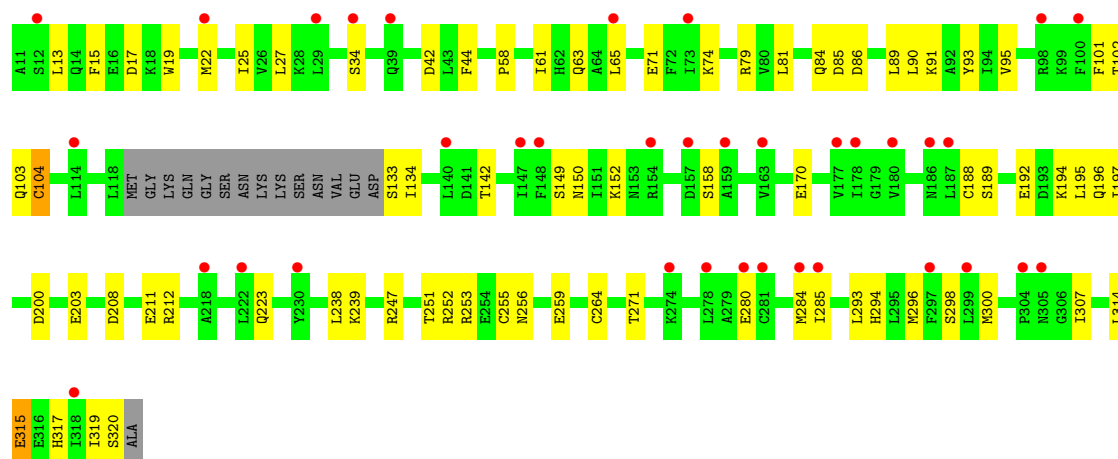




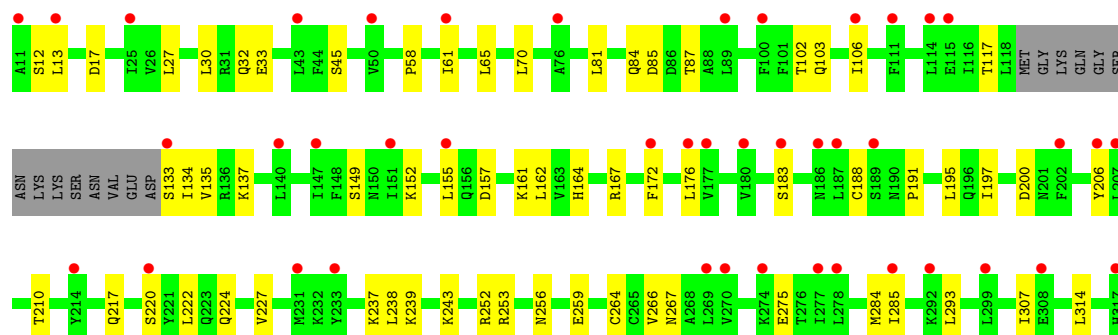
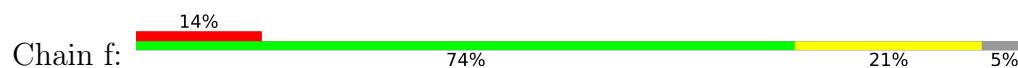
• Molecule 1: Cullin-5



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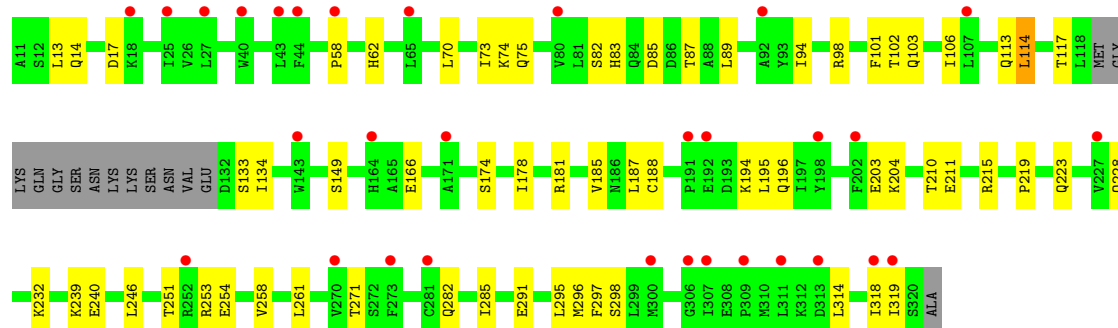
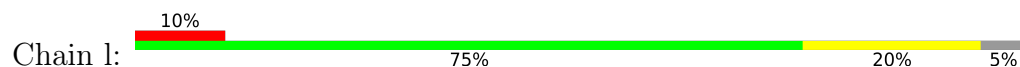


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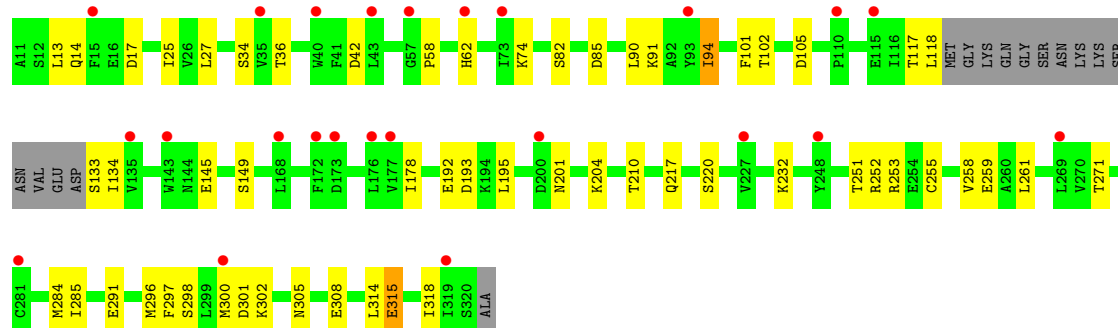
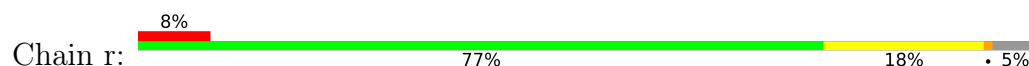




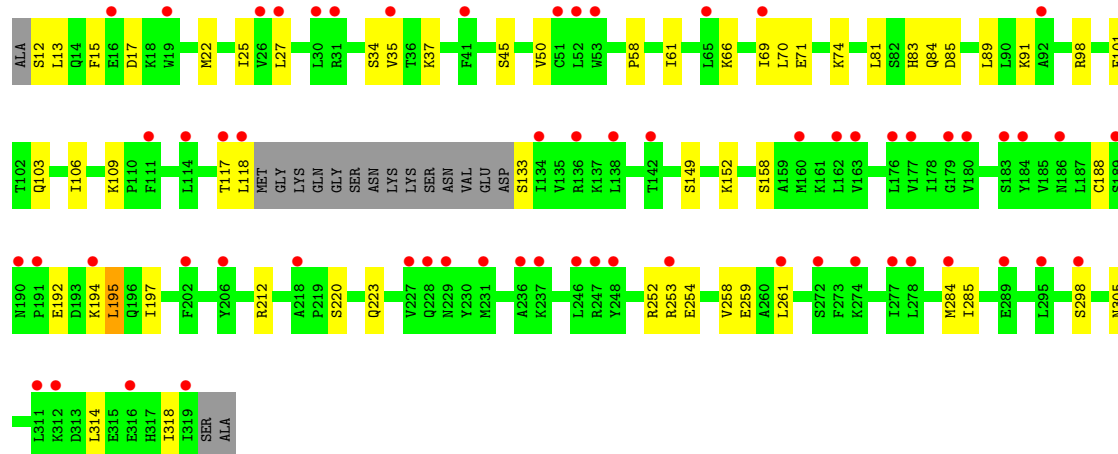
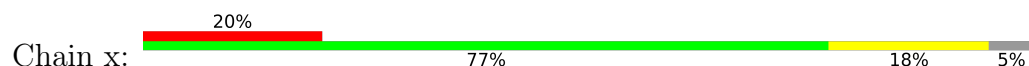
• Molecule 1: Cullin-5



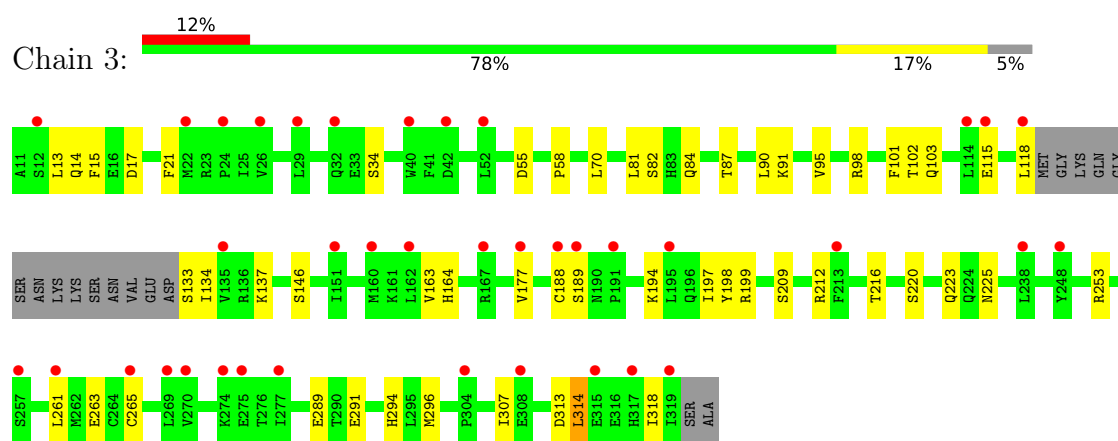
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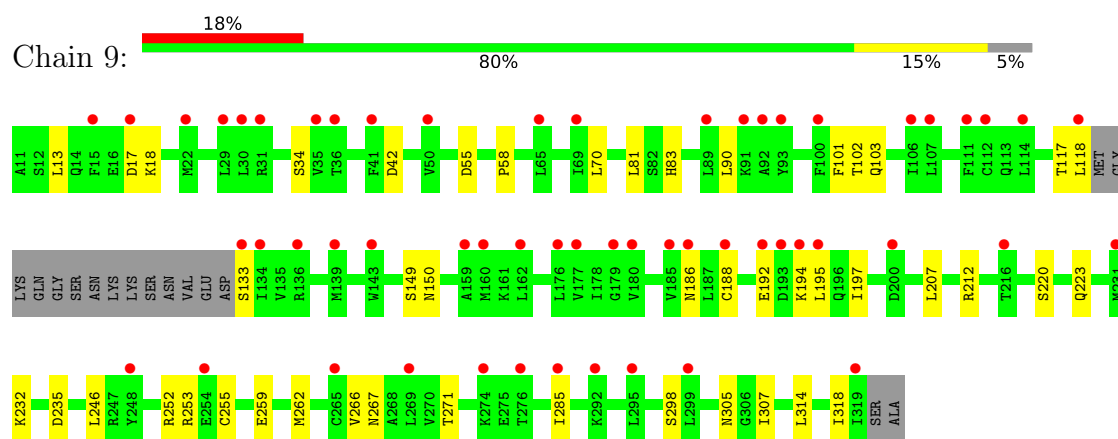
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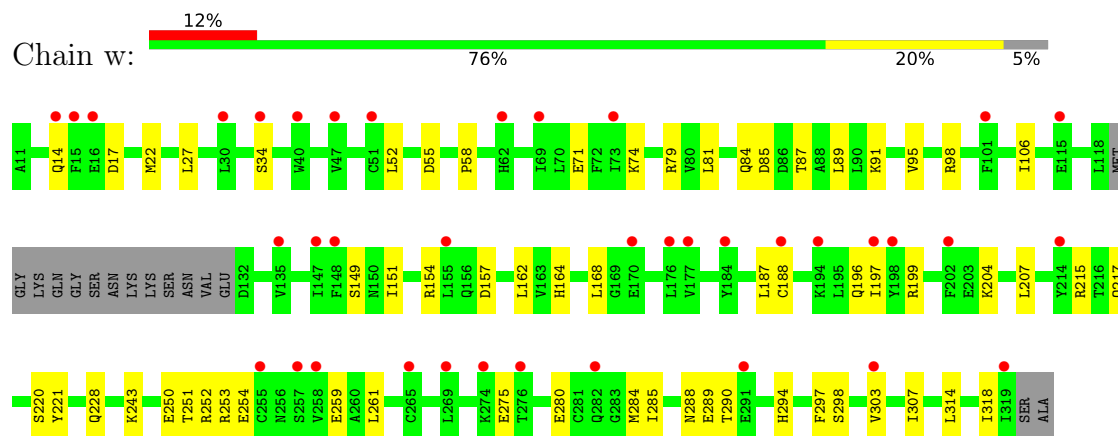
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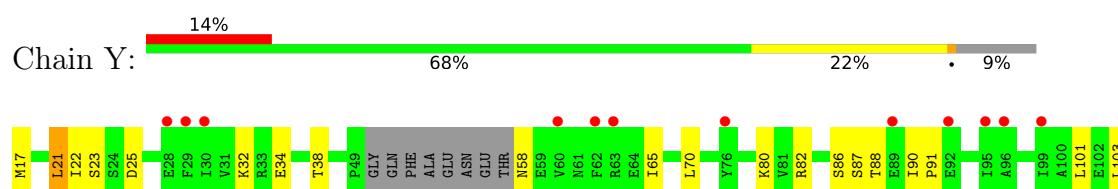
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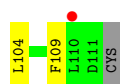


• Molecule 1: Cullin-5

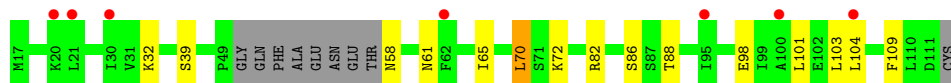
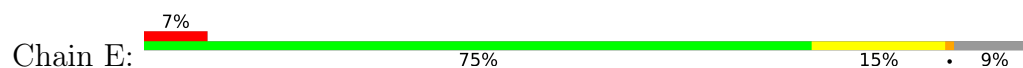


• Molecule 2: Transcription elongation factor B polypeptide 1

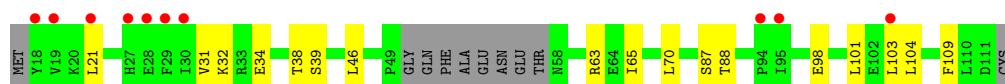
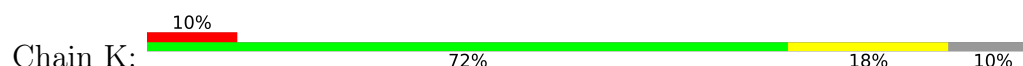




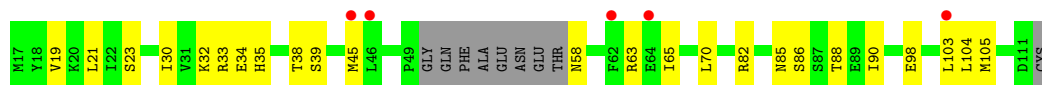
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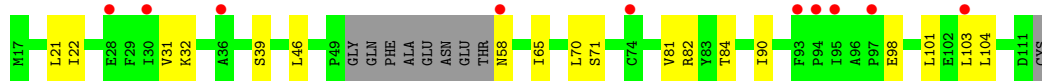
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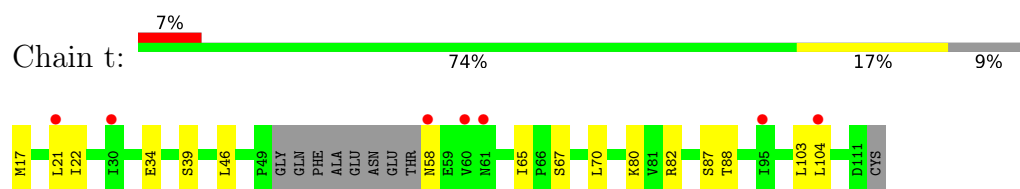
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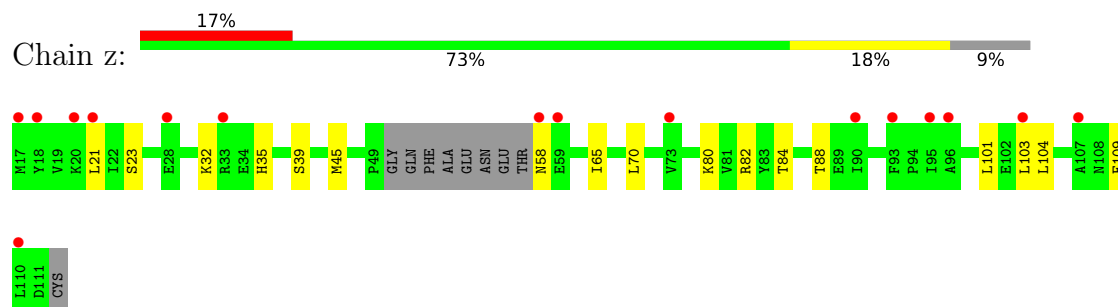
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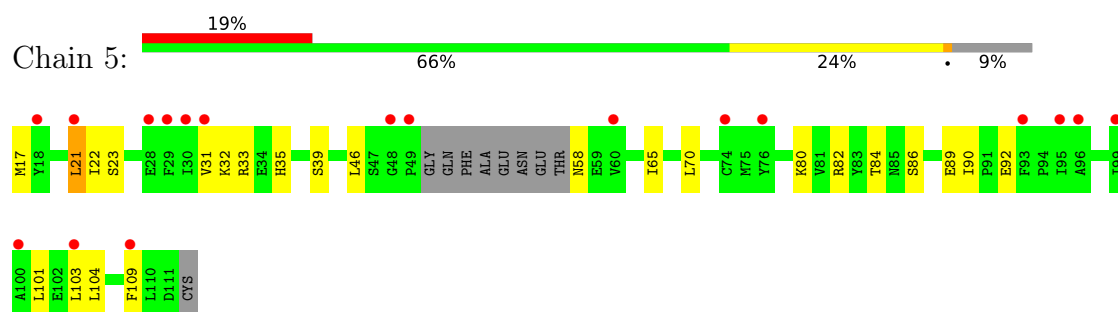
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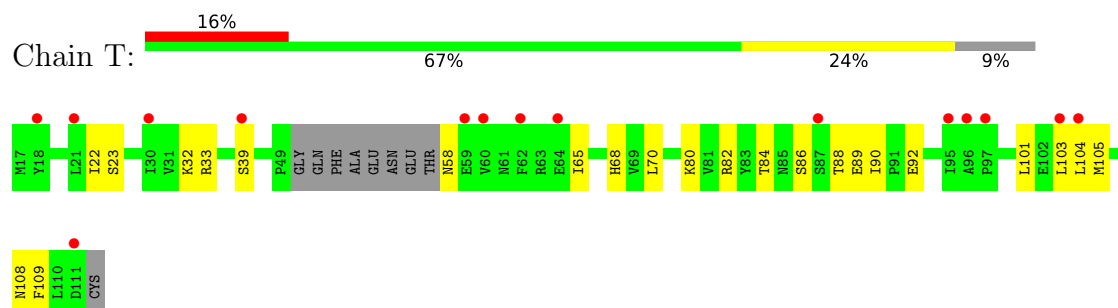
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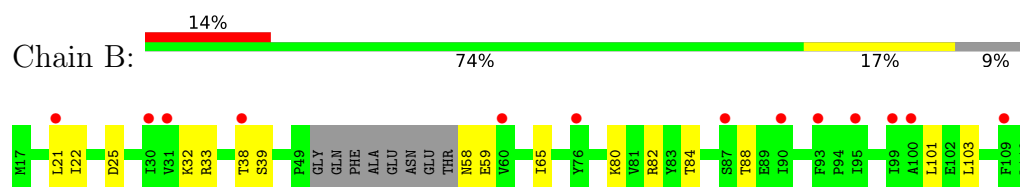
- Molecule 2: Transcription elongation factor B polypeptide 1



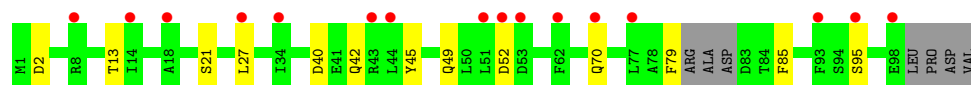
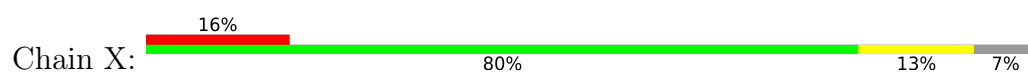
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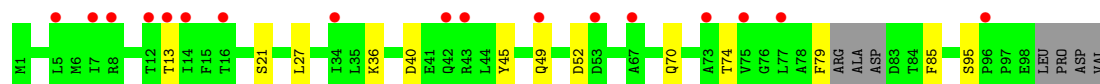
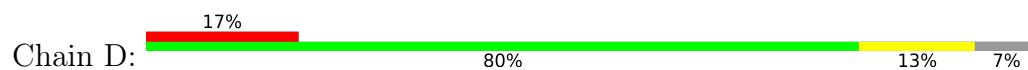
- Molecule 2: Transcription elongation factor B polypeptide 1



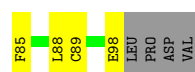
- Molecule 3: Transcription elongation factor B polypeptide 2



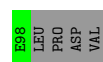
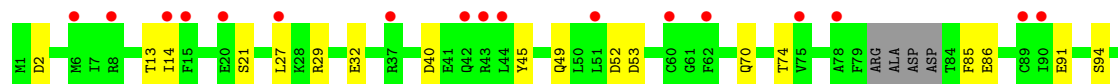
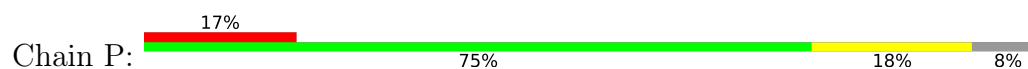
- Molecule 3: Transcription elongation factor B polypeptide 2



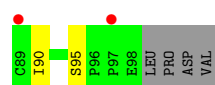
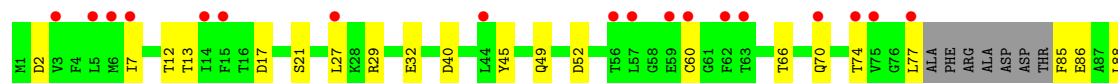
- Molecule 3: Transcription elongation factor B polypeptide 2



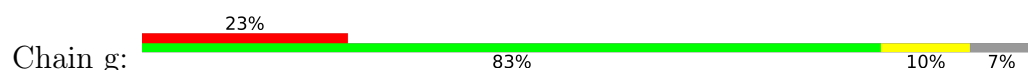
- Molecule 3: Transcription elongation factor B polypeptide 2

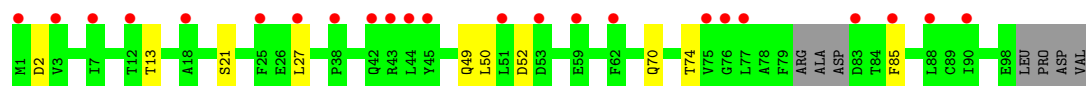


- Molecule 3: Transcription elongation factor B polypeptide 2

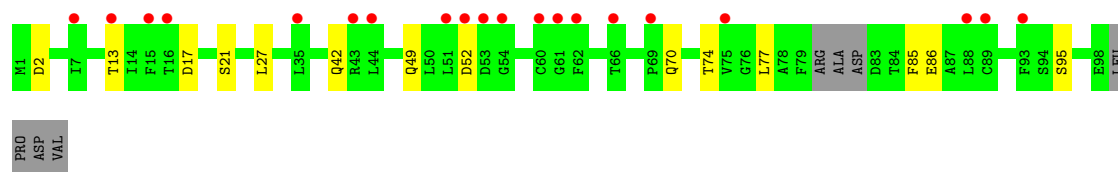
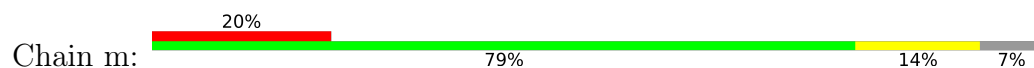


- Molecule 3: Transcription elongation factor B polypeptide 2

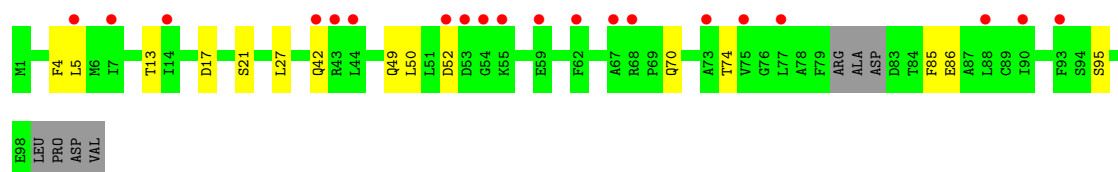
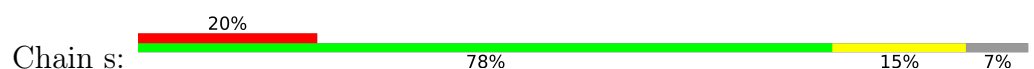




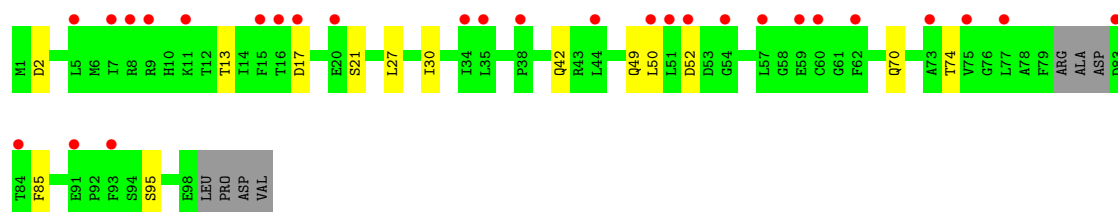
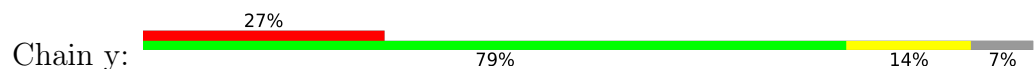
- Molecule 3: Transcription elongation factor B polypeptide 2



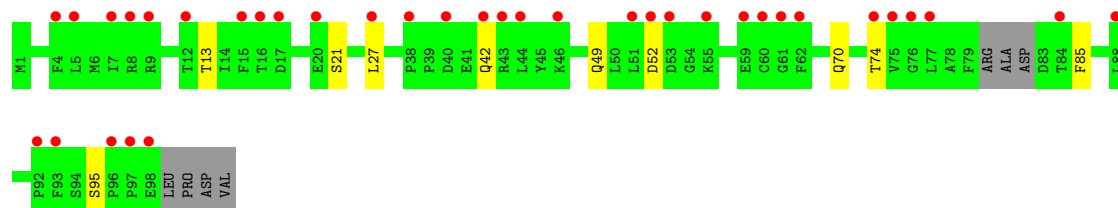
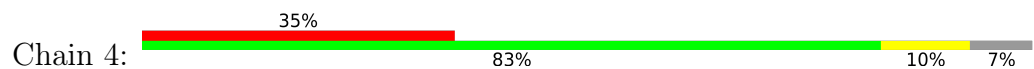
- Molecule 3: Transcription elongation factor B polypeptide 2



- Molecule 3: Transcription elongation factor B polypeptide 2



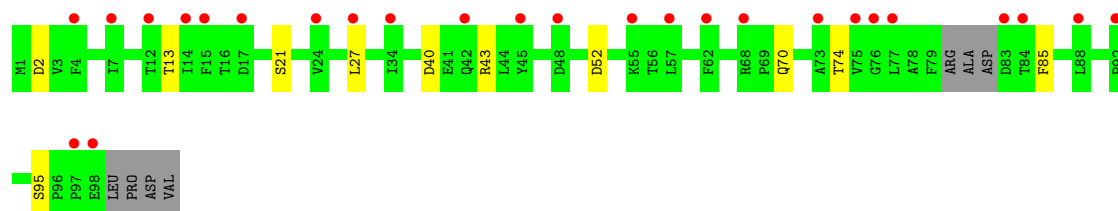
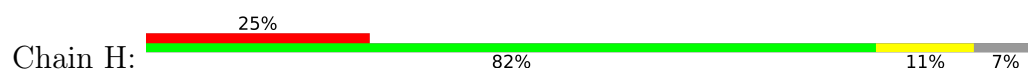
- Molecule 3: Transcription elongation factor B polypeptide 2



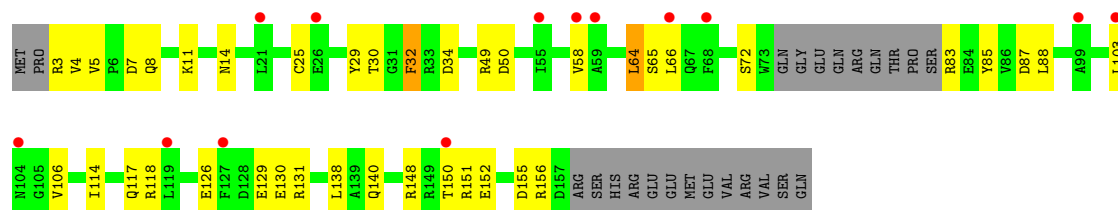
- Molecule 3: Transcription elongation factor B polypeptide 2



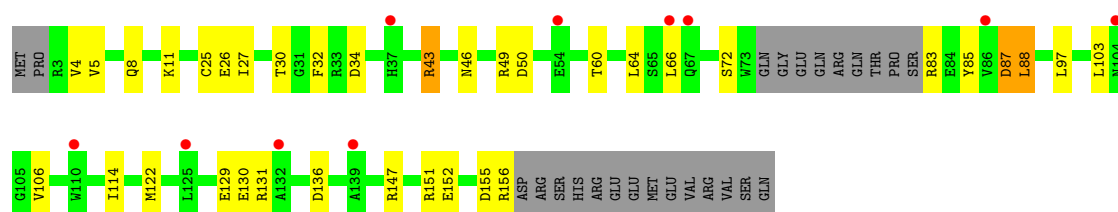
- Molecule 3: Transcription elongation factor B polypeptide 2



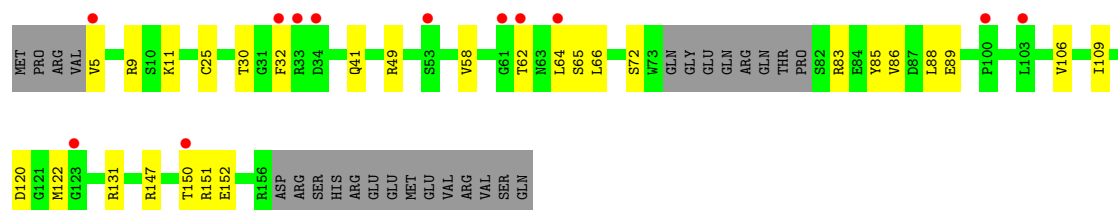
- Molecule 4: Core-binding factor subunit beta



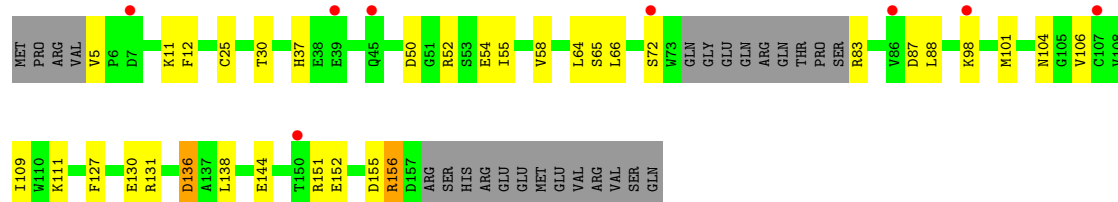
- Molecule 4: Core-binding factor subunit beta



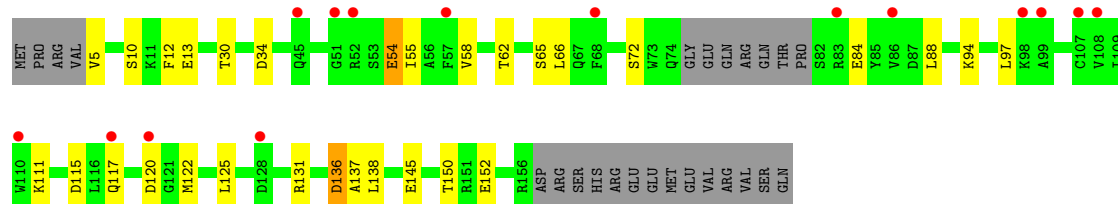
- Molecule 4: Core-binding factor subunit beta



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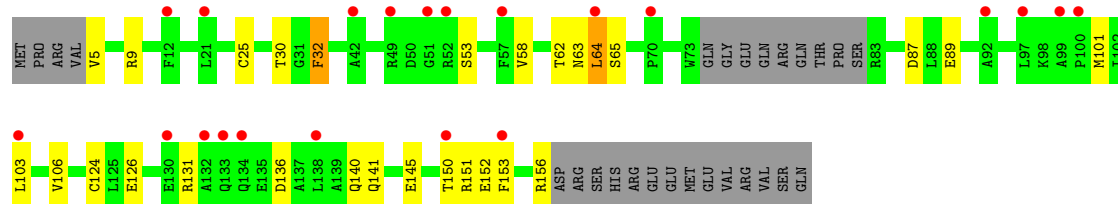
- Molecule 4: Core-binding factor subunit beta



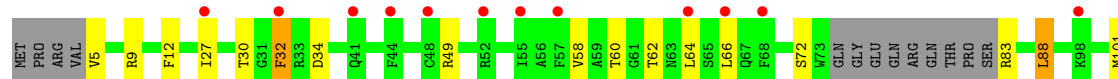
- Molecule 4: Core-binding factor subunit beta

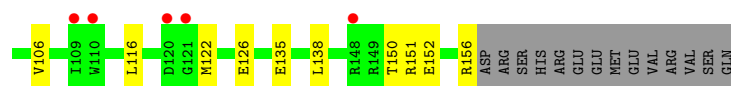


- Molecule 4: Core-binding factor subunit beta

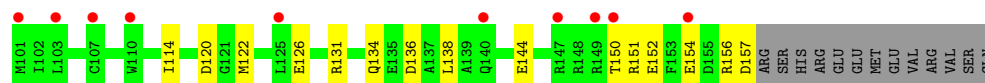
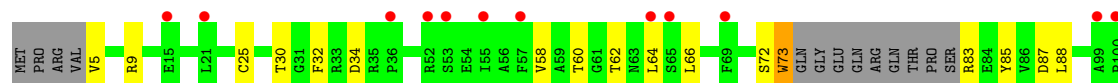


- Molecule 4: Core-binding factor subunit beta

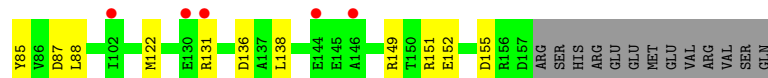
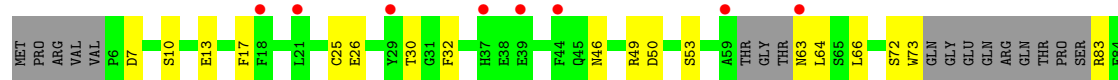




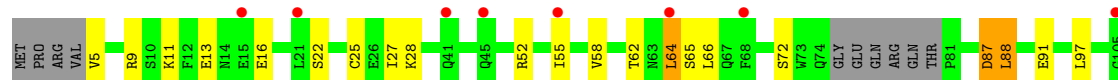
• Molecule 4: Core-binding factor subunit beta



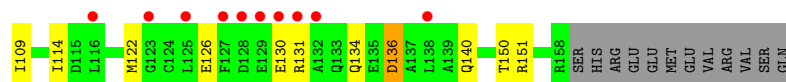
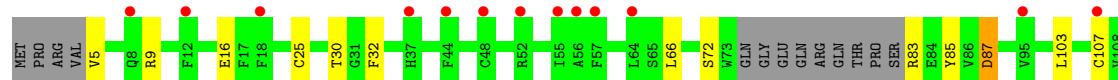
• Molecule 4: Core-binding factor subunit beta



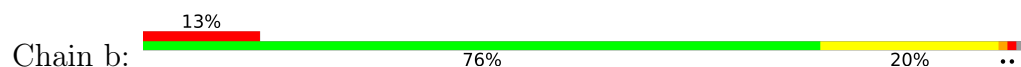
• Molecule 4: Core-binding factor subunit beta

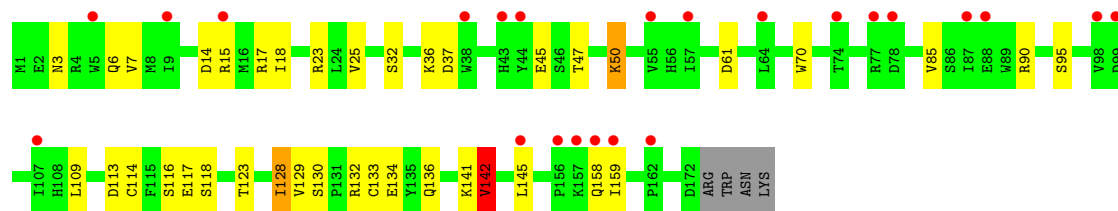


• Molecule 4: Core-binding factor subunit beta

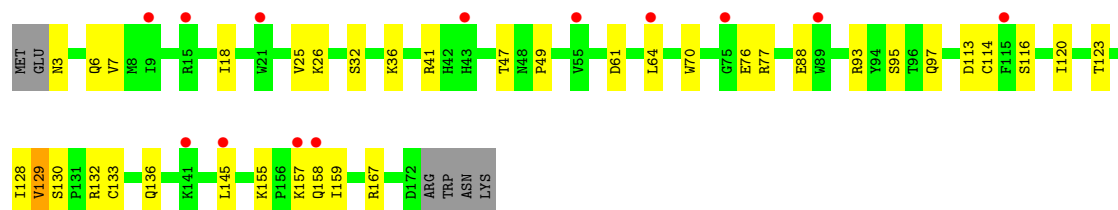
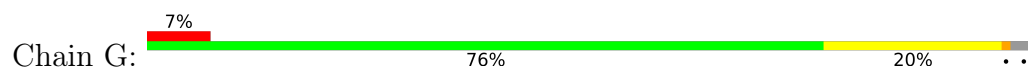


• Molecule 5: Virion infectivity factor

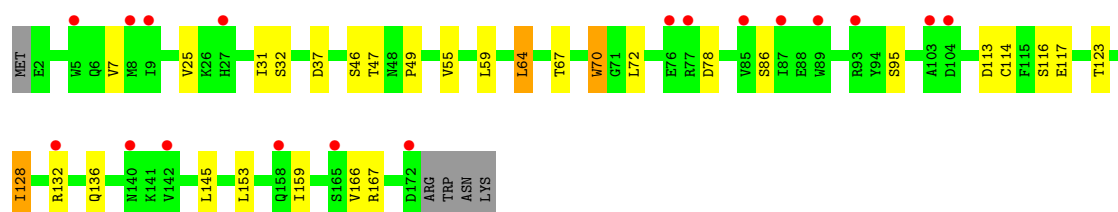
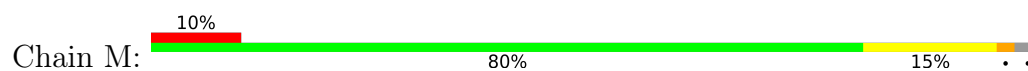




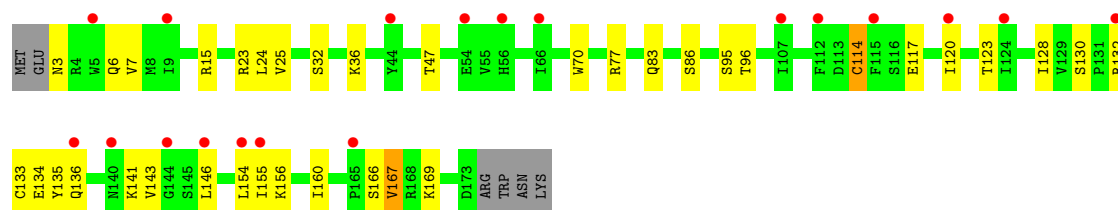
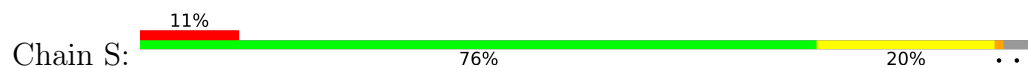
• Molecule 5: Virion infectivity factor



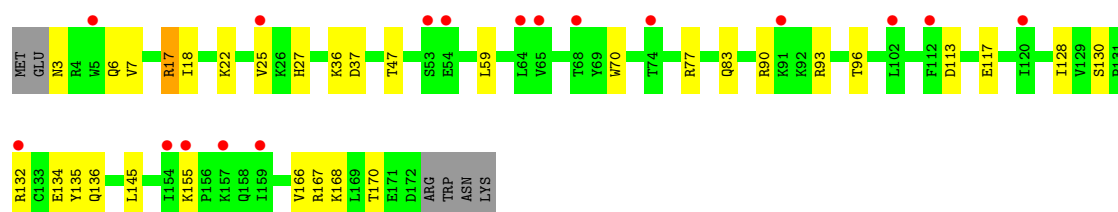
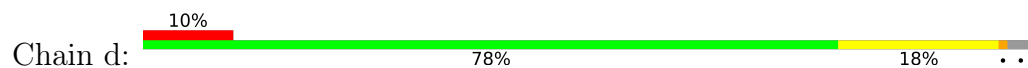
• Molecule 5: Virion infectivity factor



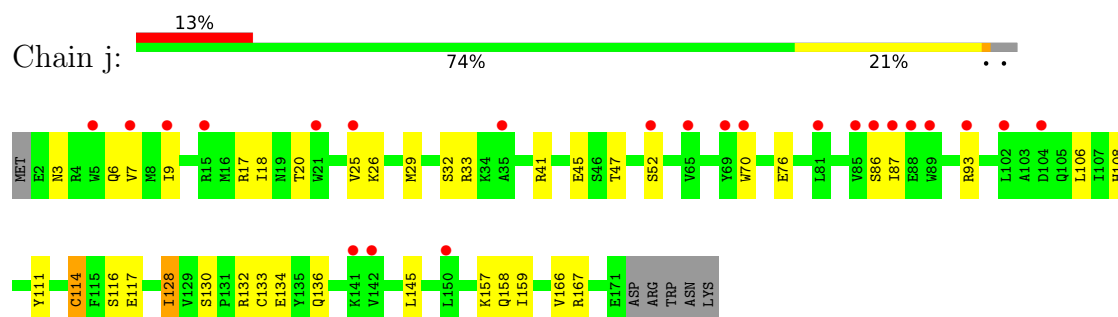
• Molecule 5: Virion infectivity factor



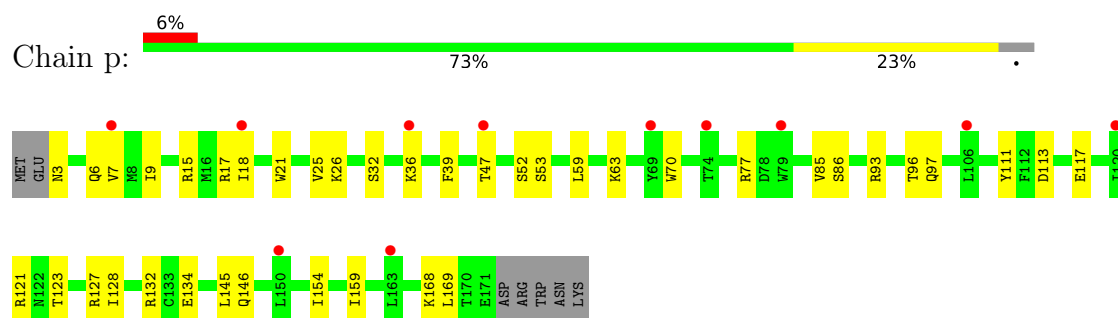
• Molecule 5: Virion infectivity factor



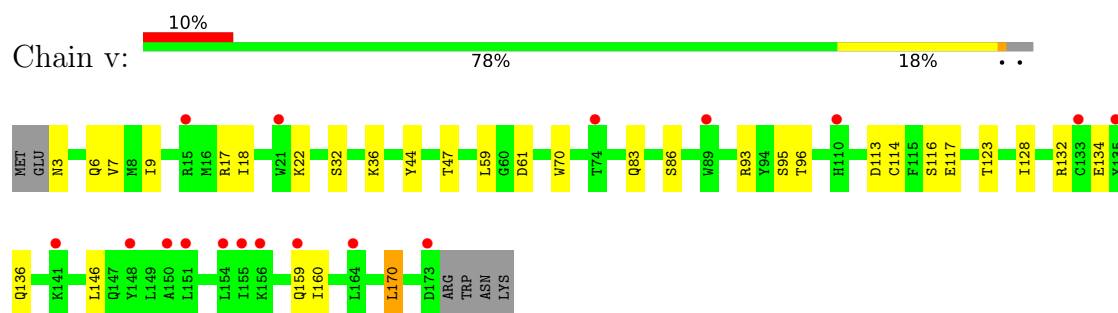
- Molecule 5: Virion infectivity factor



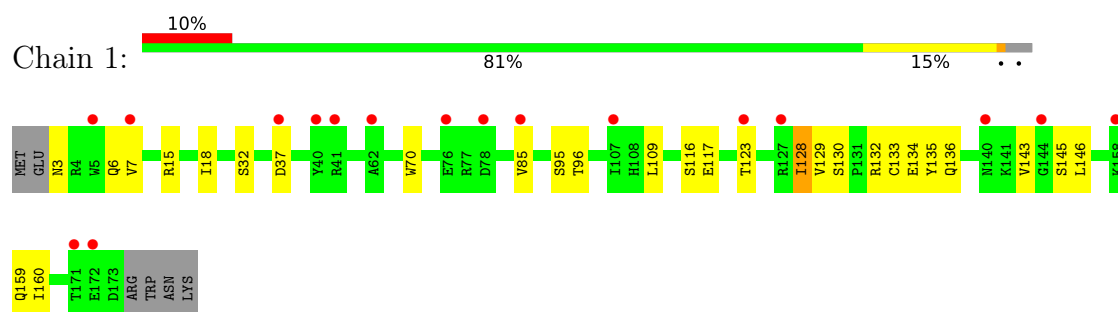
- Molecule 5: Virion infectivity factor



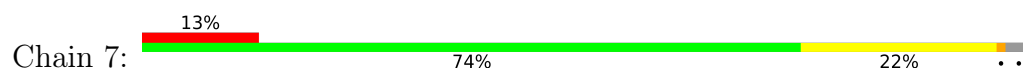
- Molecule 5: Virion infectivity factor

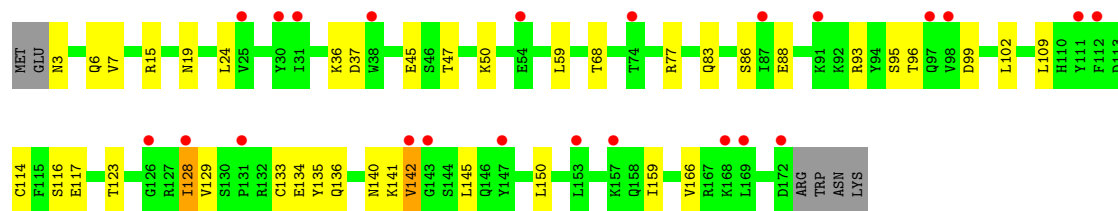


- Molecule 5: Virion infectivity factor

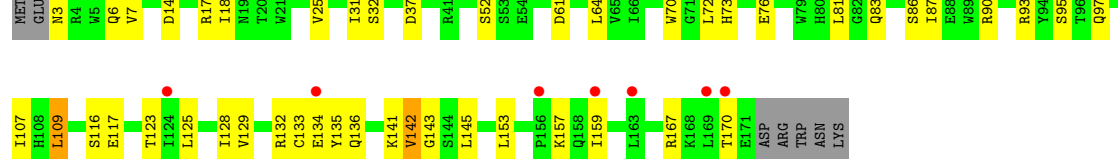


- Molecule 5: Virion infectivity factor

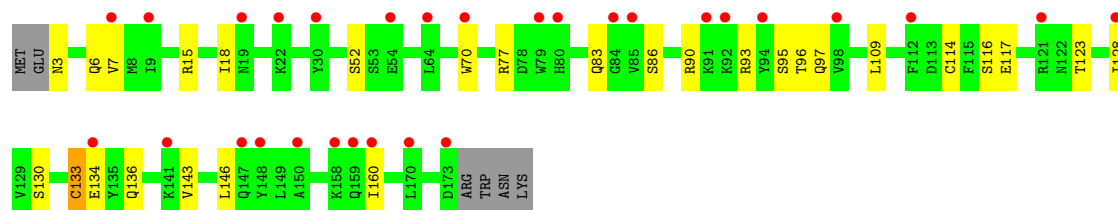
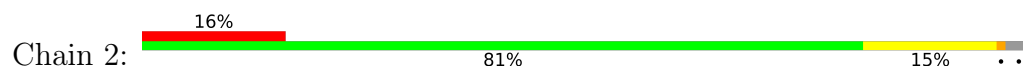




● Molecule 5: Virion infectivity factor



● 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

All (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
1	U	58	PRO	N-CD	5.40	1.55	1.47
4	N	107	CYS	CB-SG	-5.39	1.73	1.81
5	j	114	CYS	CB-SG	5.31	1.91	1.82
4	o	124	CYS	CB-SG	-5.20	1.73	1.81
4	i	73	TRP	CB-CG	-5.16	1.41	1.50
4	L	89	GLU	CB-CG	5.12	1.61	1.52

All (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
1	r	58	PRO	CA-N-CD	-8.88	99.07	111.50
1	9	58	PRO	CA-N-CD	-8.57	99.50	111.50
1	l	58	PRO	CA-N-CD	-8.46	99.66	111.50
5	b	142	VAL	N-CA-C	-8.37	88.40	111.00
1	O	58	PRO	CA-N-CD	-8.29	99.89	111.50
1	x	58	PRO	CA-N-CD	-8.24	99.97	111.50
1	3	58	PRO	CA-N-CD	-8.18	100.04	111.50
1	I	58	PRO	CA-N-CD	-8.18	100.05	111.50
1	C	58	PRO	CA-N-CD	-8.16	100.08	111.50
1	w	58	PRO	CA-N-CD	-7.75	100.65	111.50
4	k	64	LEU	CA-CB-CG	7.28	132.05	115.30
4	F	43	ARG	NE-CZ-NH1	7.23	123.92	120.30
5	q	143	GLY	N-CA-C	7.14	130.96	113.10
4	N	87	ASP	CB-CG-OD1	7.01	124.61	118.30
5	p	111	TYR	N-CA-C	6.91	129.65	111.00
1	l	114	LEU	CA-CB-CG	6.82	130.98	115.30
4	R	156	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	f	167	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	w	52	LEU	CA-CB-CG	6.73	130.77	115.30
4	o	32	PHE	N-CA-C	-6.65	93.03	111.00
4	k	88	LEU	CA-CB-CG	6.64	130.57	115.30
4	R	136	ASP	N-CA-C	6.52	128.60	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	LEU	CB-CG-CD2	-6.51	99.94	111.00
1	I	262	MET	CG-SD-CE	-6.50	89.80	100.20
5	S	167	VAL	CB-CA-C	-6.42	99.20	111.40
1	3	314	LEU	CA-CB-CG	6.41	130.04	115.30
5	7	109	LEU	CA-CB-CG	6.40	130.02	115.30
5	j	111	TYR	N-CA-C	6.36	128.16	111.00
5	v	59	LEU	CB-CG-CD2	-6.35	100.20	111.00
4	F	87	ASP	CB-CG-OD1	6.23	123.91	118.30
3	y	50	LEU	CA-CB-CG	6.06	129.23	115.30
4	u	32	PHE	N-CA-C	-5.94	94.96	111.00
5	S	77	ARG	NE-CZ-NH1	-5.92	117.34	120.30
2	5	21	LEU	CA-CB-CG	5.90	128.87	115.30
4	k	87	ASP	CB-CG-OD1	5.83	123.55	118.30
4	N	136	ASP	CB-CG-OD1	5.81	123.53	118.30
5	b	109	LEU	CA-CB-CG	5.78	128.59	115.30
5	j	114	CYS	CA-CB-SG	5.73	124.31	114.00
1	w	207	LEU	CA-CB-CG	5.70	128.42	115.30
5	q	109	LEU	CA-CB-CG	5.69	128.38	115.30
4	k	138	LEU	CA-CB-CG	-5.68	102.23	115.30
4	u	88	LEU	CA-CB-CG	5.68	128.37	115.30
4	a	64	LEU	CA-CB-CG	5.64	128.27	115.30
2	Y	21	LEU	CA-CB-CG	5.57	128.12	115.30
3	m	77	LEU	CA-CB-CG	5.57	128.12	115.30
4	a	32	PHE	N-CA-C	-5.55	96.02	111.00
4	R	138	LEU	CA-CB-CG	-5.54	102.55	115.30
5	d	59	LEU	CA-CB-CG	5.53	128.03	115.30
2	Z	110	LEU	CA-CB-CG	-5.53	102.59	115.30
4	o	64	LEU	CA-CB-CG	5.49	127.93	115.30
1	f	157	ASP	CB-CG-OD1	-5.46	113.39	118.30
4	L	86	VAL	N-CA-C	-5.45	96.28	111.00
3	e	50	LEU	CA-CB-CG	5.45	127.83	115.30
1	C	90	LEU	CA-CB-CG	5.41	127.75	115.30
1	r	94	ILE	CG1-CB-CG2	-5.41	99.50	111.40
5	S	133	CYS	CA-CB-SG	5.41	123.73	114.00
4	c	97	LEU	CA-CB-CG	5.40	127.73	115.30
2	z	21	LEU	CA-CB-CG	5.38	127.67	115.30
5	b	50	LYS	CD-CE-NZ	-5.37	99.36	111.70
1	f	293	LEU	CA-CB-CG	-5.36	102.98	115.30
2	E	70	LEU	CA-CB-CG	5.35	127.61	115.30
5	l	109	LEU	CA-CB-CG	5.30	127.50	115.30
5	d	17	ARG	NE-CZ-NH1	5.29	122.95	120.30
3	g	50	LEU	CA-CB-CG	5.29	127.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	TRP	CA-CB-CG	5.29	123.74	113.70
4	F	88	LEU	CA-CB-CG	5.26	127.40	115.30
1	w	151	ILE	N-CA-C	5.23	125.11	111.00
5	v	170	LEU	CA-CB-CG	5.22	127.31	115.30
4	c	115	ASP	CB-CG-OD1	5.22	123.00	118.30
5	2	109	LEU	CA-CB-CG	5.22	127.30	115.30
4	c	54	GLU	N-CA-C	-5.21	96.94	111.00
1	f	157	ASP	CB-CG-OD2	5.17	122.95	118.30
3	J	50	LEU	CA-CB-CG	5.16	127.16	115.30
3	J	27	LEU	CA-CB-CG	5.15	127.14	115.30
5	p	59	LEU	CB-CG-CD2	-5.13	102.27	111.00
1	f	134	ILE	N-CA-CB	-5.08	99.13	110.80
1	x	195	LEU	CA-CB-CG	5.07	126.97	115.30
5	M	153	LEU	CA-CB-CG	5.05	126.92	115.30
1	V	90	LEU	CA-CB-CG	5.03	126.86	115.30
1	9	207	LEU	CA-CB-CG	5.01	126.82	115.30
5	M	64	LEU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (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	q	142	VAL	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	X	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	e	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
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

All (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	1	128	ILE
5	1	143	VAL
5	7	128	ILE
5	b	142	VAL
5	G	128	ILE
5	S	128	ILE
4	c	137	ALA
5	q	128	ILE
5	q	129	VAL
5	2	128	ILE
1	U	15	PHE
1	C	15	PHE
4	i	136	ASP
5	v	128	ILE
1	x	15	PHE
4	0	60	THR
5	b	141	LYS
4	c	136	ASP
5	d	128	ILE
5	7	129	VAL
5	7	141	LYS
1	3	15	PHE
5	7	142	VAL
5	1	129	VAL

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (1873) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	12	SER
1	U	13	LEU
1	U	17	ASP
1	U	22	MET
1	U	27	LEU
1	U	34	SER
1	U	45	SER
1	U	55	ASP
1	U	65	LEU
1	U	70	LEU
1	U	72	PHE
1	U	74	LYS
1	U	81	LEU
1	U	83	HIS
1	U	84	GLN
1	U	85	ASP
1	U	86	ASP
1	U	87	THR
1	U	89	LEU
1	U	90	LEU
1	U	98	ARG
1	U	101	PHE
1	U	102	THR
1	U	103	GLN
1	U	117	THR
1	U	133	SER
1	U	145	GLU
1	U	146	SER
1	U	151	ILE
1	U	153	ASN
1	U	157	ASP
1	U	161	LYS
1	U	162	LEU
1	U	164	HIS
1	U	178	ILE
1	U	183	SER
1	U	184	TYR
1	U	189	SER
1	U	190	ASN
1	U	192	GLU
1	U	194	LYS
1	U	197	ILE
1	U	201	ASN

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Mol	Chain	Res	Type
1	U	212	ARG
1	U	220	SER
1	U	223	GLN
1	U	228	GLN
1	U	251	THR
1	U	252	ARG
1	U	253	ARG
1	U	258	VAL
1	U	259	GLU
1	U	261	LEU
1	U	284	MET
1	U	285	ILE
1	U	294	HIS
1	U	296	MET
1	U	298	SER
1	U	314	LEU
2	Y	17	MET
2	Y	21	LEU
2	Y	22	ILE
2	Y	23	SER
2	Y	25	ASP
2	Y	32	LYS
2	Y	34	GLU
2	Y	38	THR
2	Y	58	ASN
2	Y	65	ILE
2	Y	70	LEU
2	Y	80	LYS
2	Y	82	ARG
2	Y	86	SER
2	Y	87	SER
2	Y	88	THR
2	Y	90	ILE
2	Y	101	LEU
2	Y	103	LEU
2	Y	104	LEU
2	Y	109	PHE
3	X	2	ASP
3	X	13	THR
3	X	21	SER
3	X	27	LEU
3	X	40	ASP

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Mol	Chain	Res	Type
3	X	42	GLN
3	X	45	TYR
3	X	49	GLN
3	X	52	ASP
3	X	70	GLN
3	X	79	PHE
3	X	85	PHE
3	X	95	SER
4	a	3	ARG
4	a	4	VAL
4	a	5	VAL
4	a	7	ASP
4	a	8	GLN
4	a	11	LYS
4	a	14	ASN
4	a	25	CYS
4	a	29	TYR
4	a	30	THR
4	a	32	PHE
4	a	34	ASP
4	a	49	ARG
4	a	50	ASP
4	a	58	VAL
4	a	64	LEU
4	a	65	SER
4	a	66	LEU
4	a	72	SER
4	a	83	ARG
4	a	85	TYR
4	a	87	ASP
4	a	88	LEU
4	a	103	LEU
4	a	106	VAL
4	a	114	ILE
4	a	117	GLN
4	a	118	ARG
4	a	126	GLU
4	a	129	GLU
4	a	130	GLU
4	a	131	ARG
4	a	138	LEU
4	a	140	GLN

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Mol	Chain	Res	Type
4	a	148	ARG
4	a	150	THR
4	a	151	ARG
4	a	152	GLU
4	a	155	ASP
4	a	156	ARG
5	b	3	ASN
5	b	6	GLN
5	b	7	VAL
5	b	14	ASP
5	b	15	ARG
5	b	17	ARG
5	b	18	ILE
5	b	23	ARG
5	b	25	VAL
5	b	32	SER
5	b	36	LYS
5	b	37	ASP
5	b	45	GLU
5	b	47	THR
5	b	50	LYS
5	b	61	ASP
5	b	70	TRP
5	b	85	VAL
5	b	90	ARG
5	b	95	SER
5	b	113	ASP
5	b	114	CYS
5	b	116	SER
5	b	117	GLU
5	b	118	SER
5	b	123	THR
5	b	128	ILE
5	b	129	VAL
5	b	130	SER
5	b	132	ARG
5	b	133	CYS
5	b	134	GLU
5	b	136	GLN
5	b	142	VAL
5	b	145	LEU
5	b	158	GLN

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Mol	Chain	Res	Type
5	b	159	ILE
1	C	13	LEU
1	C	14	GLN
1	C	16	GLU
1	C	17	ASP
1	C	33	GLU
1	C	61	ILE
1	C	65	LEU
1	C	68	ASP
1	C	70	LEU
1	C	81	LEU
1	C	83	HIS
1	C	84	GLN
1	C	85	ASP
1	C	86	ASP
1	C	87	THR
1	C	89	LEU
1	C	90	LEU
1	C	91	LYS
1	C	94	ILE
1	C	98	ARG
1	C	101	PHE
1	C	103	GLN
1	C	106	ILE
1	C	113	GLN
1	C	117	THR
1	C	136	ARG
1	C	147	ILE
1	C	154	ARG
1	C	155	LEU
1	C	160	MET
1	C	164	HIS
1	C	167	ARG
1	C	178	ILE
1	C	192	GLU
1	C	193	ASP
1	C	194	LYS
1	C	209	SER
1	C	210	THR
1	C	217	GLN
1	C	221	TYR
1	C	222	LEU

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Mol	Chain	Res	Type
1	C	232	LYS
1	C	242	GLU
1	C	251	THR
1	C	252	ARG
1	C	253	ARG
1	C	257	SER
1	C	261	LEU
1	C	265	CYS
1	C	277	ILE
1	C	280	GLU
1	C	285	ILE
1	C	290	THR
1	C	298	SER
1	C	299	LEU
1	C	305	ASN
1	C	313	ASP
1	C	314	LEU
1	C	318	ILE
2	E	32	LYS
2	E	39	SER
2	E	58	ASN
2	E	61	ASN
2	E	65	ILE
2	E	70	LEU
2	E	72	LYS
2	E	82	ARG
2	E	86	SER
2	E	88	THR
2	E	98	GLU
2	E	101	LEU
2	E	103	LEU
2	E	104	LEU
2	E	109	PHE
3	D	13	THR
3	D	21	SER
3	D	27	LEU
3	D	36	LYS
3	D	40	ASP
3	D	45	TYR
3	D	49	GLN
3	D	52	ASP
3	D	70	GLN

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Mol	Chain	Res	Type
3	D	74	THR
3	D	79	PHE
3	D	85	PHE
3	D	95	SER
4	F	4	VAL
4	F	5	VAL
4	F	8	GLN
4	F	11	LYS
4	F	25	CYS
4	F	26	GLU
4	F	27	ILE
4	F	30	THR
4	F	32	PHE
4	F	34	ASP
4	F	43	ARG
4	F	46	ASN
4	F	49	ARG
4	F	50	ASP
4	F	60	THR
4	F	64	LEU
4	F	66	LEU
4	F	72	SER
4	F	83	ARG
4	F	85	TYR
4	F	87	ASP
4	F	88	LEU
4	F	97	LEU
4	F	103	LEU
4	F	106	VAL
4	F	114	ILE
4	F	122	MET
4	F	129	GLU
4	F	130	GLU
4	F	131	ARG
4	F	136	ASP
4	F	147	ARG
4	F	151	ARG
4	F	152	GLU
4	F	155	ASP
4	F	156	ARG
5	G	3	ASN
5	G	6	GLN

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Mol	Chain	Res	Type
5	G	7	VAL
5	G	18	ILE
5	G	25	VAL
5	G	26	LYS
5	G	32	SER
5	G	36	LYS
5	G	41	ARG
5	G	47	THR
5	G	49	PRO
5	G	61	ASP
5	G	64	LEU
5	G	70	TRP
5	G	76	GLU
5	G	77	ARG
5	G	88	GLU
5	G	93	ARG
5	G	95	SER
5	G	97	GLN
5	G	113	ASP
5	G	114	CYS
5	G	116	SER
5	G	120	ILE
5	G	123	THR
5	G	129	VAL
5	G	130	SER
5	G	132	ARG
5	G	133	CYS
5	G	136	GLN
5	G	145	LEU
5	G	155	LYS
5	G	157	LYS
5	G	158	GLN
5	G	159	ILE
5	G	167	ARG
1	I	13	LEU
1	I	14	GLN
1	I	17	ASP
1	I	24	PRO
1	I	27	LEU
1	I	50	VAL
1	I	55	ASP
1	I	62	HIS

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Mol	Chain	Res	Type
1	I	71	GLU
1	I	79	ARG
1	I	80	VAL
1	I	81	LEU
1	I	85	ASP
1	I	87	THR
1	I	94	ILE
1	I	95	VAL
1	I	106	ILE
1	I	117	THR
1	I	118	LEU
1	I	133	SER
1	I	141	ASP
1	I	142	THR
1	I	149	SER
1	I	152	LYS
1	I	153	ASN
1	I	154	ARG
1	I	157	ASP
1	I	162	LEU
1	I	163	VAL
1	I	164	HIS
1	I	168	LEU
1	I	197	ILE
1	I	198	TYR
1	I	199	ARG
1	I	206	TYR
1	I	209	SER
1	I	210	THR
1	I	212	ARG
1	I	221	TYR
1	I	222	LEU
1	I	223	GLN
1	I	228	GLN
1	I	232	LYS
1	I	239	LYS
1	I	253	ARG
1	I	265	CYS
1	I	277	ILE
1	I	285	ILE
1	I	289	GLU
1	I	290	THR

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Mol	Chain	Res	Type
1	I	296	MET
1	I	298	SER
1	I	299	LEU
1	I	301	ASP
1	I	302	LYS
1	I	307	ILE
1	I	319	ILE
1	I	320	SER
2	K	21	LEU
2	K	31	VAL
2	K	32	LYS
2	K	34	GLU
2	K	38	THR
2	K	39	SER
2	K	46	LEU
2	K	63	ARG
2	K	65	ILE
2	K	70	LEU
2	K	87	SER
2	K	88	THR
2	K	98	GLU
2	K	101	LEU
2	K	103	LEU
2	K	104	LEU
2	K	109	PHE
3	J	9	ARG
3	J	13	THR
3	J	17	ASP
3	J	21	SER
3	J	27	LEU
3	J	29	ARG
3	J	30	ILE
3	J	41	GLU
3	J	44	LEU
3	J	47	ASP
3	J	50	LEU
3	J	52	ASP
3	J	68	ARG
3	J	70	GLN
3	J	74	THR
3	J	84	THR
3	J	85	PHE

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Mol	Chain	Res	Type
3	J	88	LEU
3	J	89	CYS
3	J	98	GLU
4	L	5	VAL
4	L	9	ARG
4	L	11	LYS
4	L	25	CYS
4	L	30	THR
4	L	32	PHE
4	L	41	GLN
4	L	49	ARG
4	L	58	VAL
4	L	62	THR
4	L	64	LEU
4	L	65	SER
4	L	66	LEU
4	L	72	SER
4	L	83	ARG
4	L	85	TYR
4	L	88	LEU
4	L	106	VAL
4	L	109	ILE
4	L	120	ASP
4	L	122	MET
4	L	131	ARG
4	L	147	ARG
4	L	150	THR
4	L	151	ARG
4	L	152	GLU
5	M	7	VAL
5	M	25	VAL
5	M	31	ILE
5	M	32	SER
5	M	37	ASP
5	M	46	SER
5	M	47	THR
5	M	49	PRO
5	M	55	VAL
5	M	59	LEU
5	M	64	LEU
5	M	67	THR
5	M	70	TRP

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Mol	Chain	Res	Type
5	M	72	LEU
5	M	78	ASP
5	M	86	SER
5	M	95	SER
5	M	113	ASP
5	M	114	CYS
5	M	116	SER
5	M	117	GLU
5	M	123	THR
5	M	128	ILE
5	M	132	ARG
5	M	136	GLN
5	M	145	LEU
5	M	159	ILE
5	M	166	VAL
5	M	167	ARG
1	O	12	SER
1	O	13	LEU
1	O	16	GLU
1	O	17	ASP
1	O	27	LEU
1	O	29	LEU
1	O	36	THR
1	O	38	GLN
1	O	43	LEU
1	O	45	SER
1	O	55	ASP
1	O	62	HIS
1	O	65	LEU
1	O	70	LEU
1	O	71	GLU
1	O	74	LYS
1	O	79	ARG
1	O	81	LEU
1	O	83	HIS
1	O	85	ASP
1	O	91	LYS
1	O	93	TYR
1	O	95	VAL
1	O	98	ARG
1	O	102	THR
1	O	103	GLN

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Mol	Chain	Res	Type
1	O	105	ASP
1	O	133	SER
1	O	134	ILE
1	O	142	THR
1	O	146	SER
1	O	147	ILE
1	O	149	SER
1	O	152	LYS
1	O	155	LEU
1	O	158	SER
1	O	162	LEU
1	O	176	LEU
1	O	178	ILE
1	O	189	SER
1	O	192	GLU
1	O	194	LYS
1	O	195	LEU
1	O	196	GLN
1	O	197	ILE
1	O	200	ASP
1	O	207	LEU
1	O	209	SER
1	O	215	ARG
1	O	223	GLN
1	O	228	GLN
1	O	249	LEU
1	O	251	THR
1	O	252	ARG
1	O	253	ARG
1	O	254	GLU
1	O	258	VAL
1	O	259	GLU
1	O	261	LEU
1	O	263	GLU
1	O	264	CYS
1	O	267	ASN
1	O	271	THR
1	O	282	GLN
1	O	285	ILE
1	O	291	GLU
1	O	296	MET
1	O	298	SER

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Mol	Chain	Res	Type
1	O	299	LEU
1	O	303	VAL
1	O	312	LYS
1	O	318	ILE
2	Q	19	VAL
2	Q	21	LEU
2	Q	23	SER
2	Q	30	ILE
2	Q	32	LYS
2	Q	33	ARG
2	Q	34	GLU
2	Q	35	HIS
2	Q	38	THR
2	Q	39	SER
2	Q	45	MET
2	Q	58	ASN
2	Q	63	ARG
2	Q	65	ILE
2	Q	70	LEU
2	Q	82	ARG
2	Q	85	ASN
2	Q	86	SER
2	Q	88	THR
2	Q	90	ILE
2	Q	98	GLU
2	Q	103	LEU
2	Q	104	LEU
2	Q	105	MET
3	P	2	ASP
3	P	13	THR
3	P	14	ILE
3	P	21	SER
3	P	27	LEU
3	P	29	ARG
3	P	32	GLU
3	P	40	ASP
3	P	45	TYR
3	P	49	GLN
3	P	52	ASP
3	P	53	ASP
3	P	70	GLN
3	P	74	THR

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Mol	Chain	Res	Type
3	P	85	PHE
3	P	86	GLU
3	P	91	GLU
3	P	94	SER
4	R	5	VAL
4	R	11	LYS
4	R	12	PHE
4	R	25	CYS
4	R	30	THR
4	R	37	HIS
4	R	50	ASP
4	R	52	ARG
4	R	54	GLU
4	R	55	ILE
4	R	58	VAL
4	R	64	LEU
4	R	65	SER
4	R	66	LEU
4	R	72	SER
4	R	83	ARG
4	R	87	ASP
4	R	88	LEU
4	R	98	LYS
4	R	101	MET
4	R	104	ASN
4	R	106	VAL
4	R	109	ILE
4	R	111	LYS
4	R	127	PHE
4	R	130	GLU
4	R	131	ARG
4	R	136	ASP
4	R	144	GLU
4	R	151	ARG
4	R	152	GLU
4	R	156	ARG
5	S	3	ASN
5	S	6	GLN
5	S	7	VAL
5	S	15	ARG
5	S	23	ARG
5	S	24	LEU

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Mol	Chain	Res	Type
5	S	25	VAL
5	S	32	SER
5	S	36	LYS
5	S	47	THR
5	S	70	TRP
5	S	83	GLN
5	S	86	SER
5	S	95	SER
5	S	96	THR
5	S	114	CYS
5	S	117	GLU
5	S	120	ILE
5	S	123	THR
5	S	130	SER
5	S	132	ARG
5	S	134	GLU
5	S	135	TYR
5	S	136	GLN
5	S	141	LYS
5	S	143	VAL
5	S	146	LEU
5	S	154	LEU
5	S	155	ILE
5	S	156	LYS
5	S	160	ILE
5	S	166	SER
5	S	167	VAL
5	S	169	LYS
1	V	13	LEU
1	V	15	PHE
1	V	17	ASP
1	V	19	TRP
1	V	22	MET
1	V	25	ILE
1	V	27	LEU
1	V	34	SER
1	V	42	ASP
1	V	44	PHE
1	V	61	ILE
1	V	63	GLN
1	V	65	LEU
1	V	71	GLU

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Mol	Chain	Res	Type
1	V	74	LYS
1	V	79	ARG
1	V	81	LEU
1	V	84	GLN
1	V	85	ASP
1	V	86	ASP
1	V	89	LEU
1	V	91	LYS
1	V	93	TYR
1	V	95	VAL
1	V	101	PHE
1	V	102	THR
1	V	103	GLN
1	V	104	CYS
1	V	133	SER
1	V	134	ILE
1	V	142	THR
1	V	149	SER
1	V	150	ASN
1	V	152	LYS
1	V	158	SER
1	V	170	GLU
1	V	188	CYS
1	V	189	SER
1	V	192	GLU
1	V	194	LYS
1	V	195	LEU
1	V	196	GLN
1	V	197	ILE
1	V	200	ASP
1	V	203	GLU
1	V	208	ASP
1	V	211	GLU
1	V	212	ARG
1	V	223	GLN
1	V	238	LEU
1	V	239	LYS
1	V	247	ARG
1	V	251	THR
1	V	252	ARG
1	V	253	ARG
1	V	255	CYS

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Mol	Chain	Res	Type
1	V	256	ASN
1	V	259	GLU
1	V	264	CYS
1	V	271	THR
1	V	280	GLU
1	V	284	MET
1	V	285	ILE
1	V	293	LEU
1	V	294	HIS
1	V	296	MET
1	V	298	SER
1	V	300	MET
1	V	307	ILE
1	V	314	LEU
1	V	315	GLU
1	V	317	HIS
1	V	319	ILE
1	V	320	SER
2	Z	19	VAL
2	Z	21	LEU
2	Z	22	ILE
2	Z	25	ASP
2	Z	30	ILE
2	Z	31	VAL
2	Z	32	LYS
2	Z	39	SER
2	Z	46	LEU
2	Z	58	ASN
2	Z	69	VAL
2	Z	70	LEU
2	Z	80	LYS
2	Z	82	ARG
2	Z	85	ASN
2	Z	95	ILE
2	Z	98	GLU
2	Z	99	ILE
2	Z	101	LEU
2	Z	103	LEU
2	Z	104	LEU
2	Z	105	MET
2	Z	109	PHE
3	W	2	ASP

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Mol	Chain	Res	Type
3	W	7	ILE
3	W	12	THR
3	W	13	THR
3	W	17	ASP
3	W	21	SER
3	W	27	LEU
3	W	29	ARG
3	W	32	GLU
3	W	40	ASP
3	W	45	TYR
3	W	49	GLN
3	W	52	ASP
3	W	60	CYS
3	W	66	THR
3	W	70	GLN
3	W	74	THR
3	W	77	LEU
3	W	85	PHE
3	W	86	GLU
3	W	88	LEU
3	W	90	ILE
3	W	95	SER
4	c	5	VAL
4	c	10	SER
4	c	12	PHE
4	c	13	GLU
4	c	30	THR
4	c	34	ASP
4	c	54	GLU
4	c	55	ILE
4	c	58	VAL
4	c	62	THR
4	c	65	SER
4	c	66	LEU
4	c	72	SER
4	c	84	GLU
4	c	88	LEU
4	c	94	LYS
4	c	111	LYS
4	c	117	GLN
4	c	120	ASP
4	c	122	MET

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Mol	Chain	Res	Type
4	c	125	LEU
4	c	131	ARG
4	c	136	ASP
4	c	138	LEU
4	c	145	GLU
4	c	150	THR
4	c	152	GLU
5	d	3	ASN
5	d	6	GLN
5	d	7	VAL
5	d	17	ARG
5	d	18	ILE
5	d	25	VAL
5	d	27	HIS
5	d	36	LYS
5	d	37	ASP
5	d	47	THR
5	d	70	TRP
5	d	77	ARG
5	d	83	GLN
5	d	90	ARG
5	d	96	THR
5	d	113	ASP
5	d	117	GLU
5	d	130	SER
5	d	132	ARG
5	d	134	GLU
5	d	135	TYR
5	d	136	GLN
5	d	145	LEU
5	d	155	LYS
5	d	166	VAL
5	d	167	ARG
5	d	168	LYS
5	d	170	THR
1	f	12	SER
1	f	13	LEU
1	f	17	ASP
1	f	27	LEU
1	f	30	LEU
1	f	32	GLN
1	f	33	GLU

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Mol	Chain	Res	Type
1	f	45	SER
1	f	61	ILE
1	f	65	LEU
1	f	70	LEU
1	f	81	LEU
1	f	84	GLN
1	f	85	ASP
1	f	87	THR
1	f	102	THR
1	f	103	GLN
1	f	106	ILE
1	f	117	THR
1	f	133	SER
1	f	135	VAL
1	f	137	LYS
1	f	149	SER
1	f	152	LYS
1	f	155	LEU
1	f	161	LYS
1	f	162	LEU
1	f	164	HIS
1	f	172	PHE
1	f	176	LEU
1	f	183	SER
1	f	188	CYS
1	f	191	PRO
1	f	195	LEU
1	f	197	ILE
1	f	200	ASP
1	f	206	TYR
1	f	210	THR
1	f	217	GLN
1	f	220	SER
1	f	222	LEU
1	f	224	GLN
1	f	227	VAL
1	f	237	LYS
1	f	238	LEU
1	f	239	LYS
1	f	243	LYS
1	f	252	ARG
1	f	253	ARG

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Mol	Chain	Res	Type
1	f	256	ASN
1	f	259	GLU
1	f	264	CYS
1	f	266	VAL
1	f	267	ASN
1	f	275	GLU
1	f	284	MET
1	f	285	ILE
1	f	307	ILE
1	f	314	LEU
1	f	319	ILE
2	h	21	LEU
2	h	22	ILE
2	h	31	VAL
2	h	32	LYS
2	h	39	SER
2	h	46	LEU
2	h	58	ASN
2	h	65	ILE
2	h	70	LEU
2	h	71	SER
2	h	81	VAL
2	h	82	ARG
2	h	84	THR
2	h	90	ILE
2	h	98	GLU
2	h	101	LEU
2	h	103	LEU
2	h	104	LEU
3	g	2	ASP
3	g	13	THR
3	g	21	SER
3	g	27	LEU
3	g	49	GLN
3	g	52	ASP
3	g	70	GLN
3	g	74	THR
3	g	85	PHE
4	i	3	ARG
4	i	4	VAL
4	i	5	VAL
4	i	21	LEU

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Mol	Chain	Res	Type
4	i	25	CYS
4	i	29	TYR
4	i	30	THR
4	i	41	GLN
4	i	49	ARG
4	i	50	ASP
4	i	58	VAL
4	i	60	THR
4	i	62	THR
4	i	64	LEU
4	i	65	SER
4	i	66	LEU
4	i	72	SER
4	i	74	GLN
4	i	80	THR
4	i	84	GLU
4	i	85	TYR
4	i	87	ASP
4	i	88	LEU
4	i	111	LYS
4	i	118	ARG
4	i	122	MET
4	i	125	LEU
4	i	126	GLU
4	i	135	GLU
4	i	136	ASP
4	i	147	ARG
4	i	150	THR
4	i	151	ARG
4	i	152	GLU
5	j	3	ASN
5	j	6	GLN
5	j	7	VAL
5	j	9	ILE
5	j	17	ARG
5	j	18	ILE
5	j	20	THR
5	j	25	VAL
5	j	26	LYS
5	j	29	MET
5	j	32	SER
5	j	41	ARG

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Mol	Chain	Res	Type
5	j	45	GLU
5	j	47	THR
5	j	52	SER
5	j	70	TRP
5	j	76	GLU
5	j	86	SER
5	j	87	ILE
5	j	93	ARG
5	j	106	LEU
5	j	108	HIS
5	j	114	CYS
5	j	116	SER
5	j	117	GLU
5	j	128	ILE
5	j	130	SER
5	j	132	ARG
5	j	133	CYS
5	j	134	GLU
5	j	136	GLN
5	j	145	LEU
5	j	157	LYS
5	j	158	GLN
5	j	159	ILE
5	j	166	VAL
5	j	167	ARG
1	l	13	LEU
1	l	14	GLN
1	l	17	ASP
1	l	62	HIS
1	l	70	LEU
1	l	73	ILE
1	l	74	LYS
1	l	75	GLN
1	l	82	SER
1	l	83	HIS
1	l	85	ASP
1	l	87	THR
1	l	89	LEU
1	l	94	ILE
1	l	98	ARG
1	l	101	PHE
1	l	102	THR

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Mol	Chain	Res	Type
1	l	103	GLN
1	l	106	ILE
1	l	113	GLN
1	l	114	LEU
1	l	117	THR
1	l	133	SER
1	l	134	ILE
1	l	149	SER
1	l	166	GLU
1	l	174	SER
1	l	178	ILE
1	l	181	ARG
1	l	185	VAL
1	l	187	LEU
1	l	188	CYS
1	l	194	LYS
1	l	195	LEU
1	l	196	GLN
1	l	203	GLU
1	l	204	LYS
1	l	210	THR
1	l	211	GLU
1	l	215	ARG
1	l	219	PRO
1	l	223	GLN
1	l	228	GLN
1	l	232	LYS
1	l	239	LYS
1	l	240	GLU
1	l	246	LEU
1	l	251	THR
1	l	253	ARG
1	l	254	GLU
1	l	258	VAL
1	l	261	LEU
1	l	271	THR
1	l	282	GLN
1	l	285	ILE
1	l	291	GLU
1	l	295	LEU
1	l	296	MET
1	l	297	PHE

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Mol	Chain	Res	Type
1	l	298	SER
1	l	314	LEU
1	l	318	ILE
1	l	319	ILE
2	n	17	MET
2	n	19	VAL
2	n	35	HIS
2	n	39	SER
2	n	46	LEU
2	n	62	PHE
2	n	64	GLU
2	n	67	SER
2	n	72	LYS
2	n	80	LYS
2	n	82	ARG
2	n	88	THR
2	n	90	ILE
2	n	92	GLU
2	n	99	ILE
2	n	103	LEU
2	n	104	LEU
2	n	109	PHE
3	m	2	ASP
3	m	13	THR
3	m	17	ASP
3	m	21	SER
3	m	27	LEU
3	m	42	GLN
3	m	49	GLN
3	m	52	ASP
3	m	70	GLN
3	m	74	THR
3	m	85	PHE
3	m	86	GLU
3	m	95	SER
4	o	5	VAL
4	o	9	ARG
4	o	25	CYS
4	o	30	THR
4	o	32	PHE
4	o	53	SER
4	o	58	VAL

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Mol	Chain	Res	Type
4	o	62	THR
4	o	63	ASN
4	o	64	LEU
4	o	65	SER
4	o	87	ASP
4	o	89	GLU
4	o	101	MET
4	o	103	LEU
4	o	106	VAL
4	o	126	GLU
4	o	131	ARG
4	o	136	ASP
4	o	140	GLN
4	o	141	GLN
4	o	145	GLU
4	o	150	THR
4	o	151	ARG
4	o	152	GLU
4	o	153	PHE
4	o	156	ARG
5	p	3	ASN
5	p	6	GLN
5	p	7	VAL
5	p	9	ILE
5	p	15	ARG
5	p	17	ARG
5	p	18	ILE
5	p	21	TRP
5	p	25	VAL
5	p	26	LYS
5	p	32	SER
5	p	36	LYS
5	p	39	PHE
5	p	47	THR
5	p	52	SER
5	p	53	SER
5	p	63	LYS
5	p	70	TRP
5	p	77	ARG
5	p	85	VAL
5	p	86	SER
5	p	96	THR

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Mol	Chain	Res	Type
5	p	97	GLN
5	p	113	ASP
5	p	117	GLU
5	p	121	ARG
5	p	123	THR
5	p	127	ARG
5	p	132	ARG
5	p	134	GLU
5	p	145	LEU
5	p	146	GLN
5	p	154	ILE
5	p	159	ILE
5	p	168	LYS
1	r	13	LEU
1	r	14	GLN
1	r	17	ASP
1	r	25	ILE
1	r	27	LEU
1	r	34	SER
1	r	36	THR
1	r	42	ASP
1	r	62	HIS
1	r	74	LYS
1	r	82	SER
1	r	85	ASP
1	r	90	LEU
1	r	91	LYS
1	r	94	ILE
1	r	101	PHE
1	r	102	THR
1	r	105	ASP
1	r	117	THR
1	r	118	LEU
1	r	133	SER
1	r	134	ILE
1	r	145	GLU
1	r	149	SER
1	r	178	ILE
1	r	192	GLU
1	r	193	ASP
1	r	195	LEU
1	r	201	ASN

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Mol	Chain	Res	Type
1	r	204	LYS
1	r	210	THR
1	r	217	GLN
1	r	220	SER
1	r	232	LYS
1	r	251	THR
1	r	252	ARG
1	r	253	ARG
1	r	255	CYS
1	r	258	VAL
1	r	259	GLU
1	r	261	LEU
1	r	271	THR
1	r	284	MET
1	r	285	ILE
1	r	291	GLU
1	r	296	MET
1	r	297	PHE
1	r	298	SER
1	r	300	MET
1	r	301	ASP
1	r	302	LYS
1	r	305	ASN
1	r	308	GLU
1	r	314	LEU
1	r	315	GLU
1	r	318	ILE
2	t	17	MET
2	t	21	LEU
2	t	22	ILE
2	t	34	GLU
2	t	39	SER
2	t	46	LEU
2	t	58	ASN
2	t	65	ILE
2	t	67	SER
2	t	70	LEU
2	t	80	LYS
2	t	82	ARG
2	t	87	SER
2	t	88	THR
2	t	103	LEU

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Mol	Chain	Res	Type
2	t	104	LEU
3	s	4	PHE
3	s	5	LEU
3	s	13	THR
3	s	17	ASP
3	s	21	SER
3	s	27	LEU
3	s	42	GLN
3	s	49	GLN
3	s	50	LEU
3	s	52	ASP
3	s	70	GLN
3	s	74	THR
3	s	85	PHE
3	s	86	GLU
3	s	95	SER
4	u	5	VAL
4	u	9	ARG
4	u	12	PHE
4	u	27	ILE
4	u	30	THR
4	u	32	PHE
4	u	34	ASP
4	u	49	ARG
4	u	58	VAL
4	u	60	THR
4	u	62	THR
4	u	64	LEU
4	u	66	LEU
4	u	72	SER
4	u	83	ARG
4	u	88	LEU
4	u	101	MET
4	u	106	VAL
4	u	116	LEU
4	u	122	MET
4	u	126	GLU
4	u	135	GLU
4	u	138	LEU
4	u	150	THR
4	u	151	ARG
4	u	152	GLU

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Mol	Chain	Res	Type
4	u	156	ARG
5	v	3	ASN
5	v	6	GLN
5	v	7	VAL
5	v	9	ILE
5	v	17	ARG
5	v	18	ILE
5	v	32	SER
5	v	36	LYS
5	v	44	TYR
5	v	47	THR
5	v	61	ASP
5	v	70	TRP
5	v	83	GLN
5	v	86	SER
5	v	93	ARG
5	v	95	SER
5	v	96	THR
5	v	113	ASP
5	v	114	CYS
5	v	116	SER
5	v	117	GLU
5	v	123	THR
5	v	132	ARG
5	v	134	GLU
5	v	136	GLN
5	v	146	LEU
5	v	159	GLN
5	v	160	ILE
5	v	170	LEU
1	x	12	SER
1	x	13	LEU
1	x	17	ASP
1	x	22	MET
1	x	25	ILE
1	x	27	LEU
1	x	34	SER
1	x	35	VAL
1	x	37	LYS
1	x	45	SER
1	x	50	VAL
1	x	61	ILE

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Mol	Chain	Res	Type
1	x	66	LYS
1	x	69	ILE
1	x	70	LEU
1	x	71	GLU
1	x	74	LYS
1	x	81	LEU
1	x	83	HIS
1	x	84	GLN
1	x	85	ASP
1	x	89	LEU
1	x	91	LYS
1	x	98	ARG
1	x	101	PHE
1	x	103	GLN
1	x	106	ILE
1	x	109	LYS
1	x	117	THR
1	x	118	LEU
1	x	133	SER
1	x	149	SER
1	x	152	LYS
1	x	158	SER
1	x	188	CYS
1	x	192	GLU
1	x	194	LYS
1	x	195	LEU
1	x	197	ILE
1	x	212	ARG
1	x	220	SER
1	x	223	GLN
1	x	252	ARG
1	x	253	ARG
1	x	254	GLU
1	x	258	VAL
1	x	259	GLU
1	x	261	LEU
1	x	284	MET
1	x	285	ILE
1	x	298	SER
1	x	305	ASN
1	x	314	LEU
1	x	318	ILE

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Mol	Chain	Res	Type
2	z	23	SER
2	z	32	LYS
2	z	35	HIS
2	z	39	SER
2	z	45	MET
2	z	58	ASN
2	z	65	ILE
2	z	70	LEU
2	z	80	LYS
2	z	82	ARG
2	z	84	THR
2	z	88	THR
2	z	101	LEU
2	z	103	LEU
2	z	104	LEU
2	z	109	PHE
3	y	2	ASP
3	y	13	THR
3	y	17	ASP
3	y	21	SER
3	y	27	LEU
3	y	30	ILE
3	y	42	GLN
3	y	49	GLN
3	y	52	ASP
3	y	70	GLN
3	y	74	THR
3	y	85	PHE
3	y	95	SER
4	0	5	VAL
4	0	9	ARG
4	0	25	CYS
4	0	30	THR
4	0	32	PHE
4	0	34	ASP
4	0	58	VAL
4	0	62	THR
4	0	64	LEU
4	0	66	LEU
4	0	72	SER
4	0	73	TRP
4	0	83	ARG

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Mol	Chain	Res	Type
4	0	85	TYR
4	0	87	ASP
4	0	88	LEU
4	0	114	ILE
4	0	120	ASP
4	0	122	MET
4	0	126	GLU
4	0	131	ARG
4	0	134	GLN
4	0	136	ASP
4	0	138	LEU
4	0	144	GLU
4	0	150	THR
4	0	151	ARG
4	0	152	GLU
4	0	154	GLU
4	0	156	ARG
4	0	157	ASP
5	1	3	ASN
5	1	6	GLN
5	1	7	VAL
5	1	15	ARG
5	1	18	ILE
5	1	32	SER
5	1	37	ASP
5	1	70	TRP
5	1	85	VAL
5	1	95	SER
5	1	96	THR
5	1	116	SER
5	1	117	GLU
5	1	123	THR
5	1	128	ILE
5	1	130	SER
5	1	132	ARG
5	1	133	CYS
5	1	134	GLU
5	1	135	TYR
5	1	136	GLN
5	1	145	SER
5	1	146	LEU
5	1	159	GLN

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Mol	Chain	Res	Type
5	1	160	ILE
1	3	13	LEU
1	3	14	GLN
1	3	17	ASP
1	3	21	PHE
1	3	34	SER
1	3	55	ASP
1	3	70	LEU
1	3	81	LEU
1	3	82	SER
1	3	84	GLN
1	3	87	THR
1	3	90	LEU
1	3	91	LYS
1	3	95	VAL
1	3	98	ARG
1	3	101	PHE
1	3	102	THR
1	3	103	GLN
1	3	115	GLU
1	3	118	LEU
1	3	133	SER
1	3	134	ILE
1	3	137	LYS
1	3	146	SER
1	3	163	VAL
1	3	164	HIS
1	3	177	VAL
1	3	188	CYS
1	3	189	SER
1	3	194	LYS
1	3	197	ILE
1	3	198	TYR
1	3	199	ARG
1	3	209	SER
1	3	212	ARG
1	3	216	THR
1	3	220	SER
1	3	223	GLN
1	3	225	ASN
1	3	261	LEU
1	3	263	GLU

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Mol	Chain	Res	Type
1	3	265	CYS
1	3	289	GLU
1	3	291	GLU
1	3	294	HIS
1	3	296	MET
1	3	307	ILE
1	3	313	ASP
1	3	314	LEU
1	3	318	ILE
2	5	17	MET
2	5	21	LEU
2	5	22	ILE
2	5	23	SER
2	5	31	VAL
2	5	32	LYS
2	5	33	ARG
2	5	35	HIS
2	5	39	SER
2	5	46	LEU
2	5	58	ASN
2	5	65	ILE
2	5	70	LEU
2	5	80	LYS
2	5	82	ARG
2	5	84	THR
2	5	86	SER
2	5	89	GLU
2	5	90	ILE
2	5	92	GLU
2	5	101	LEU
2	5	103	LEU
2	5	104	LEU
2	5	109	PHE
3	4	13	THR
3	4	21	SER
3	4	27	LEU
3	4	42	GLN
3	4	49	GLN
3	4	52	ASP
3	4	70	GLN
3	4	74	THR
3	4	85	PHE

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Mol	Chain	Res	Type
3	4	95	SER
4	6	7	ASP
4	6	10	SER
4	6	13	GLU
4	6	17	PHE
4	6	25	CYS
4	6	26	GLU
4	6	30	THR
4	6	32	PHE
4	6	46	ASN
4	6	49	ARG
4	6	50	ASP
4	6	53	SER
4	6	63	ASN
4	6	64	LEU
4	6	66	LEU
4	6	72	SER
4	6	73	TRP
4	6	83	ARG
4	6	85	TYR
4	6	87	ASP
4	6	88	LEU
4	6	122	MET
4	6	131	ARG
4	6	136	ASP
4	6	138	LEU
4	6	149	ARG
4	6	151	ARG
4	6	152	GLU
4	6	155	ASP
5	7	3	ASN
5	7	6	GLN
5	7	7	VAL
5	7	15	ARG
5	7	19	ASN
5	7	24	LEU
5	7	36	LYS
5	7	37	ASP
5	7	45	GLU
5	7	47	THR
5	7	50	LYS
5	7	59	LEU

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Mol	Chain	Res	Type
5	7	68	THR
5	7	77	ARG
5	7	83	GLN
5	7	86	SER
5	7	88	GLU
5	7	93	ARG
5	7	95	SER
5	7	96	THR
5	7	99	ASP
5	7	102	LEU
5	7	114	CYS
5	7	116	SER
5	7	117	GLU
5	7	123	THR
5	7	128	ILE
5	7	133	CYS
5	7	134	GLU
5	7	135	TYR
5	7	136	GLN
5	7	140	ASN
5	7	142	VAL
5	7	145	LEU
5	7	150	LEU
5	7	159	ILE
5	7	166	VAL
1	9	13	LEU
1	9	17	ASP
1	9	18	LYS
1	9	34	SER
1	9	42	ASP
1	9	55	ASP
1	9	70	LEU
1	9	81	LEU
1	9	83	HIS
1	9	90	LEU
1	9	101	PHE
1	9	102	THR
1	9	103	GLN
1	9	117	THR
1	9	118	LEU
1	9	133	SER
1	9	149	SER

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Mol	Chain	Res	Type
1	9	150	ASN
1	9	186	ASN
1	9	188	CYS
1	9	192	GLU
1	9	194	LYS
1	9	195	LEU
1	9	197	ILE
1	9	212	ARG
1	9	220	SER
1	9	223	GLN
1	9	232	LYS
1	9	235	ASP
1	9	246	LEU
1	9	252	ARG
1	9	253	ARG
1	9	255	CYS
1	9	259	GLU
1	9	262	MET
1	9	266	VAL
1	9	267	ASN
1	9	271	THR
1	9	285	ILE
1	9	298	SER
1	9	305	ASN
1	9	307	ILE
1	9	314	LEU
1	9	318	ILE
2	T	22	ILE
2	T	23	SER
2	T	32	LYS
2	T	33	ARG
2	T	39	SER
2	T	58	ASN
2	T	65	ILE
2	T	68	HIS
2	T	70	LEU
2	T	80	LYS
2	T	82	ARG
2	T	84	THR
2	T	86	SER
2	T	88	THR
2	T	90	ILE

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Mol	Chain	Res	Type
2	T	92	GLU
2	T	101	LEU
2	T	103	LEU
2	T	104	LEU
2	T	105	MET
2	T	108	ASN
2	T	109	PHE
3	e	2	ASP
3	e	4	PHE
3	e	5	LEU
3	e	6	MET
3	e	9	ARG
3	e	13	THR
3	e	17	ASP
3	e	22	SER
3	e	27	LEU
3	e	40	ASP
3	e	43	ARG
3	e	49	GLN
3	e	52	ASP
3	e	70	GLN
3	e	74	THR
4	k	5	VAL
4	k	9	ARG
4	k	11	LYS
4	k	13	GLU
4	k	16	GLU
4	k	22	SER
4	k	25	CYS
4	k	27	ILE
4	k	28	LYS
4	k	52	ARG
4	k	55	ILE
4	k	58	VAL
4	k	62	THR
4	k	64	LEU
4	k	65	SER
4	k	66	LEU
4	k	72	SER
4	k	87	ASP
4	k	88	LEU
4	k	91	GLU

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Mol	Chain	Res	Type
4	k	97	LEU
4	k	106	VAL
4	k	114	ILE
4	k	122	MET
4	k	125	LEU
4	k	126	GLU
4	k	136	ASP
4	k	138	LEU
4	k	145	GLU
4	k	149	ARG
4	k	150	THR
4	k	151	ARG
4	k	152	GLU
4	k	156	ARG
4	k	157	ASP
5	q	3	ASN
5	q	6	GLN
5	q	7	VAL
5	q	14	ASP
5	q	17	ARG
5	q	18	ILE
5	q	25	VAL
5	q	31	ILE
5	q	32	SER
5	q	37	ASP
5	q	52	SER
5	q	61	ASP
5	q	64	LEU
5	q	70	TRP
5	q	72	LEU
5	q	73	HIS
5	q	76	GLU
5	q	81	LEU
5	q	83	GLN
5	q	86	SER
5	q	87	ILE
5	q	90	ARG
5	q	93	ARG
5	q	95	SER
5	q	97	GLN
5	q	107	ILE
5	q	109	LEU

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Mol	Chain	Res	Type
5	q	116	SER
5	q	117	GLU
5	q	123	THR
5	q	125	LEU
5	q	132	ARG
5	q	133	CYS
5	q	134	GLU
5	q	135	TYR
5	q	136	GLN
5	q	141	LYS
5	q	142	VAL
5	q	145	LEU
5	q	153	LEU
5	q	157	LYS
5	q	159	ILE
5	q	167	ARG
5	q	170	THR
1	w	14	GLN
1	w	17	ASP
1	w	22	MET
1	w	27	LEU
1	w	34	SER
1	w	55	ASP
1	w	71	GLU
1	w	74	LYS
1	w	79	ARG
1	w	81	LEU
1	w	84	GLN
1	w	85	ASP
1	w	87	THR
1	w	89	LEU
1	w	91	LYS
1	w	95	VAL
1	w	98	ARG
1	w	106	ILE
1	w	149	SER
1	w	154	ARG
1	w	157	ASP
1	w	162	LEU
1	w	164	HIS
1	w	168	LEU
1	w	187	LEU

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Mol	Chain	Res	Type
1	w	188	CYS
1	w	196	GLN
1	w	197	ILE
1	w	199	ARG
1	w	204	LYS
1	w	215	ARG
1	w	217	GLN
1	w	220	SER
1	w	221	TYR
1	w	228	GLN
1	w	243	LYS
1	w	250	GLU
1	w	251	THR
1	w	252	ARG
1	w	253	ARG
1	w	254	GLU
1	w	259	GLU
1	w	261	LEU
1	w	275	GLU
1	w	280	GLU
1	w	284	MET
1	w	285	ILE
1	w	288	ASN
1	w	289	GLU
1	w	290	THR
1	w	294	HIS
1	w	297	PHE
1	w	298	SER
1	w	303	VAL
1	w	307	ILE
1	w	314	LEU
1	w	318	ILE
2	B	21	LEU
2	B	22	ILE
2	B	25	ASP
2	B	32	LYS
2	B	33	ARG
2	B	38	THR
2	B	39	SER
2	B	58	ASN
2	B	59	GLU
2	B	65	ILE

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Mol	Chain	Res	Type
2	B	80	LYS
2	B	82	ARG
2	B	84	THR
2	B	88	THR
2	B	101	LEU
2	B	103	LEU
3	H	2	ASP
3	H	13	THR
3	H	21	SER
3	H	27	LEU
3	H	40	ASP
3	H	43	ARG
3	H	52	ASP
3	H	70	GLN
3	H	74	THR
3	H	85	PHE
3	H	95	SER
4	N	5	VAL
4	N	9	ARG
4	N	16	GLU
4	N	25	CYS
4	N	30	THR
4	N	32	PHE
4	N	66	LEU
4	N	72	SER
4	N	83	ARG
4	N	85	TYR
4	N	87	ASP
4	N	103	LEU
4	N	109	ILE
4	N	114	ILE
4	N	122	MET
4	N	126	GLU
4	N	130	GLU
4	N	131	ARG
4	N	134	GLN
4	N	136	ASP
4	N	140	GLN
4	N	150	THR
4	N	151	ARG
5	2	3	ASN
5	2	6	GLN

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Mol	Chain	Res	Type
5	2	7	VAL
5	2	15	ARG
5	2	18	ILE
5	2	52	SER
5	2	70	TRP
5	2	77	ARG
5	2	83	GLN
5	2	86	SER
5	2	90	ARG
5	2	93	ARG
5	2	95	SER
5	2	96	THR
5	2	97	GLN
5	2	114	CYS
5	2	116	SER
5	2	117	GLU
5	2	123	THR
5	2	130	SER
5	2	133	CYS
5	2	134	GLU
5	2	136	GLN
5	2	143	VAL
5	2	146	LEU
5	2	160	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	77	GLN
1	U	228	GLN
4	a	41	GLN
4	a	67	GLN
5	b	3	ASN
5	b	19	ASN
1	C	14	GLN
1	C	48	HIS
1	C	228	GLN
3	D	10	HIS
4	F	14	ASN
4	F	134	GLN
1	I	228	GLN
4	L	41	GLN

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Mol	Chain	Res	Type
4	L	63	ASN
4	L	67	GLN
2	Q	27	HIS
4	R	104	ASN
5	S	73	HIS
5	S	139	HIS
1	V	223	GLN
1	V	228	GLN
1	V	305	ASN
5	d	108	HIS
2	h	35	HIS
5	j	73	HIS
1	l	32	GLN
1	l	75	GLN
1	l	317	HIS
2	n	35	HIS
2	n	108	ASN
4	o	140	GLN
5	p	140	ASN
5	p	146	GLN
1	r	14	GLN
1	r	32	GLN
1	r	77	GLN
5	v	27	HIS
5	v	140	ASN
5	v	147	GLN
5	1	140	ASN
1	3	48	HIS
1	3	196	GLN
1	3	223	GLN
1	3	228	GLN
2	5	35	HIS
4	6	37	HIS
4	6	41	GLN
5	7	110	HIS
5	7	139	HIS
1	9	113	GLN
1	9	144	ASN
1	9	164	HIS
1	9	186	ASN
4	k	37	HIS
4	k	41	GLN

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Mol	Chain	Res	Type
5	q	28	HIS
5	q	73	HIS
1	w	32	GLN
1	w	103	GLN
1	w	201	ASN
5	2	73	HIS
5	2	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

All (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
2	z	21	LEU	11.6
1	x	311	LEU	11.5
3	m	52	ASP	11.3
4	o	133	GLN	10.8
5	7	172	ASP	10.6
5	2	173	ASP	10.2
5	2	160	ILE	9.9
3	y	51	LEU	9.3
4	L	34	ASP	9.1
3	s	52	ASP	9.0
3	y	77	LEU	8.9
3	X	52	ASP	8.7
3	4	76	GLY	8.5
1	9	93	TYR	8.5
5	7	112	PHE	8.3
1	x	162	LEU	8.2
3	e	54	GLY	8.0
1	9	176	LEU	7.7
2	Z	86	SER	7.7
3	g	18	ALA	7.7
3	g	76	GLY	7.4
1	l	313	ASP	7.3
1	x	180	VAL	7.3
3	m	54	GLY	7.3
3	D	14	ILE	7.2

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Mol	Chain	Res	Type	RSRZ
1	x	117	THR	7.2
2	T	21	LEU	7.1
3	4	52	ASP	7.1
1	U	320[A]	SER	7.1
3	4	97	PRO	7.0
3	y	44	LEU	7.0
1	9	118	LEU	7.0
3	y	17	ASP	7.0
1	r	172	PHE	6.9
3	H	92	PRO	6.9
3	y	5	LEU	6.8
3	H	77	LEU	6.8
1	9	111	PHE	6.7
4	a	150	THR	6.7
3	J	18	ALA	6.7
1	3	257	SER	6.6
5	q	87	ILE	6.5
1	U	278	LEU	6.5
5	7	126	GLY	6.5
3	y	7	ILE	6.4
4	0	53	SER	6.4
5	2	128	ILE	6.4
3	4	59	GLU	6.3
2	z	95	ILE	6.3
4	N	123	GLY	6.3
4	N	129	GLU	6.3
3	e	75	VAL	6.3
3	P	62	PHE	6.3
3	e	61	GLY	6.2
5	b	78	ASP	6.2
3	e	74	THR	6.2
5	S	120	ILE	6.2
1	9	180	VAL	6.2
4	o	130	GLU	6.1
1	9	160	MET	6.1
1	9	65	LEU	6.0
2	B	30	ILE	6.0
3	4	7	ILE	6.0
2	T	59	GLU	6.0
4	c	86	VAL	6.0
5	7	142	VAL	5.9
3	y	34	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
3	4	96	PRO	5.9
3	4	51	LEU	5.8
3	e	70	GLN	5.8
1	w	257	SER	5.8
1	x	237	LYS	5.7
1	I	214	TYR	5.7
3	H	76	GLY	5.7
3	y	62	PHE	5.7
5	2	141	LYS	5.6
1	x	189	SER	5.6
3	e	53	ASP	5.6
1	x	142	THR	5.6
1	V	65	LEU	5.6
1	x	272	SER	5.5
1	U	274	LYS	5.5
1	9	295	LEU	5.4
3	4	60	CYS	5.4
5	G	75	GLY	5.4
2	T	97	PRO	5.4
1	3	191	PRO	5.4
3	J	44	LEU	5.4
3	4	84	THR	5.4
3	4	62	PHE	5.3
1	l	192	GLU	5.3
4	6	131	ARG	5.3
1	C	146	SER	5.3
3	e	43	ARG	5.3
3	s	53	ASP	5.3
1	w	51	CYS	5.3
3	s	55	LYS	5.3
3	H	75	VAL	5.3
2	h	28	GLU	5.2
3	H	98	GLU	5.2
5	7	87	ILE	5.2
4	c	52	ARG	5.2
3	4	98	GLU	5.2
4	i	80	THR	5.2
3	X	95	SER	5.2
1	U	163	VAL	5.2
1	x	114	LEU	5.2
3	W	15	PHE	5.1
3	H	84	THR	5.1

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Mol	Chain	Res	Type	RSRZ
5	p	7	VAL	5.1
3	4	61	GLY	5.1
2	5	31	VAL	5.1
1	9	143	TRP	5.1
2	z	18	TYR	5.1
4	L	64	LEU	5.1
2	h	93	PHE	5.1
3	e	63	THR	5.1
4	u	41	GLN	5.1
4	0	107	CYS	5.1
2	T	39	SER	5.1
3	W	62	PHE	5.1
1	f	115	GLU	5.0
5	7	30	TYR	5.0
2	Y	96	ALA	5.0
4	R	107	CYS	5.0
1	w	202	PHE	5.0
3	e	51	LEU	5.0
1	9	15	PHE	5.0
2	5	93	PHE	5.0
3	4	55	LYS	4.9
1	x	191	PRO	4.9
2	T	96	ALA	4.9
3	m	51	LEU	4.9
4	6	102	ILE	4.9
2	T	18	TYR	4.9
3	J	52	ASP	4.9
3	g	44	LEU	4.9
4	6	21	LEU	4.9
5	2	84	GLY	4.9
1	9	114	LEU	4.8
1	r	73[A]	ILE	4.8
3	4	93	PHE	4.8
1	9	50	VAL	4.8
2	B	31	VAL	4.8
1	C	305	ASN	4.8
2	T	87	SER	4.8
1	U	314	LEU	4.8
3	e	57	LEU	4.8
1	9	285	ILE	4.8
5	2	79	TRP	4.8
1	9	194	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
2	T	95	ILE	4.7
1	U	321	ALA	4.7
1	I	266	VAL	4.7
3	H	24	VAL	4.7
5	v	141	LYS	4.7
3	H	97	PRO	4.7
2	t	60	VAL	4.7
5	S	124	ILE	4.7
2	K	28	GLU	4.7
3	H	55	LYS	4.7
3	e	20	GLU	4.7
3	e	35	LEU	4.7
5	7	31	ILE	4.7
2	z	20	LYS	4.7
3	g	62	PHE	4.7
5	7	91	LYS	4.6
1	r	177	VAL	4.6
2	K	95	ILE	4.6
1	9	248	TYR	4.6
2	Z	88	THR	4.6
2	T	30	ILE	4.6
3	J	59	GLU	4.6
3	y	83	ASP	4.6
3	y	15	PHE	4.6
3	s	43	ARG	4.6
1	9	195	LEU	4.6
4	o	132	ALA	4.6
2	Z	97	PRO	4.5
1	U	222	LEU	4.5
2	t	21	LEU	4.5
2	z	96	ALA	4.5
3	J	16	THR	4.5
1	x	69	ILE	4.5
3	X	14	ILE	4.5
3	m	7	ILE	4.5
3	m	60	CYS	4.5
1	x	30	LEU	4.5
1	f	43	LEU	4.5
1	U	319	ILE	4.5
3	4	53	ASP	4.4
5	G	43	HIS	4.4
1	U	279	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	f	274	LYS	4.4
3	J	7	ILE	4.4
1	f	114	LEU	4.4
1	r	200	ASP	4.4
1	9	319	ILE	4.4
1	f	177	VAL	4.4
2	5	103	LEU	4.4
1	x	274	LYS	4.4
1	O	277	ILE	4.4
2	Y	62	PHE	4.4
5	j	104	ASP	4.3
3	g	77	LEU	4.3
1	3	188	CYS	4.3
4	N	64	LEU	4.3
3	4	20	GLU	4.3
3	4	46	LYS	4.3
1	3	32	GLN	4.3
5	p	150	LEU	4.3
4	R	150	THR	4.3
5	7	74	THR	4.3
1	f	155	LEU	4.3
2	z	90	ILE	4.3
2	B	95	ILE	4.3
3	g	27	LEU	4.3
2	E	95	ILE	4.3
3	J	51	LEU	4.3
5	M	5	TRP	4.3
3	e	5	LEU	4.3
5	S	140	ASN	4.3
5	2	147	GLN	4.3
3	g	53	ASP	4.3
1	x	186	ASN	4.3
4	R	86	VAL	4.2
1	U	316	GLU	4.2
4	L	150	THR	4.2
1	9	299	LEU	4.2
1	r	135	VAL	4.2
3	D	34	ILE	4.2
3	D	13	THR	4.2
3	P	44	LEU	4.2
1	f	278	LEU	4.2
3	J	33	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	w	319	ILE	4.2
1	C	252	ARG	4.2
3	e	7	ILE	4.2
4	0	101	MET	4.1
1	x	134	ILE	4.1
1	3	151	ILE	4.1
2	5	21	LEU	4.1
3	g	51	LEU	4.1
5	M	8	MET	4.1
4	L	5	VAL	4.1
1	V	98	ARG	4.1
5	v	135	TYR	4.1
1	w	14	GLN	4.1
1	U	85	ASP	4.1
4	u	121	GLY	4.1
1	I	13	LEU	4.1
3	y	35	LEU	4.1
1	x	202	PHE	4.0
5	b	158	GLN	4.0
1	x	190	ASN	4.0
1	C	202	PHE	4.0
1	V	177	VAL	4.0
5	M	9	ILE	4.0
1	x	295	LEU	4.0
1	w	269	LEU	4.0
3	g	38	PRO	4.0
2	5	74	CYS	4.0
3	y	54	GLY	4.0
1	w	47	VAL	4.0
1	3	42	ASP	4.0
3	H	15	PHE	4.0
1	I	187	LEU	4.0
5	v	150	ALA	4.0
5	S	154	LEU	4.0
3	g	42	GLN	4.0
3	g	43	ARG	4.0
1	9	107	LEU	4.0
2	Y	30	ILE	4.0
4	c	99	ALA	4.0
5	2	30	TYR	3.9
1	I	171	ALA	3.9
5	2	112	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
3	X	62	PHE	3.9
5	7	143	GLY	3.9
4	c	120	ASP	3.9
1	w	15	PHE	3.9
3	H	7	ILE	3.9
5	M	103	ALA	3.9
5	p	18	ILE	3.9
1	O	65	LEU	3.9
1	O	26	VAL	3.9
3	y	93	PHE	3.9
1	U	176	LEU	3.9
1	C	254	GLU	3.9
2	E	20	LYS	3.9
4	0	99	ALA	3.9
5	1	78	ASP	3.9
1	w	265	CYS	3.8
2	z	103	LEU	3.8
5	S	112	PHE	3.8
3	e	56	THR	3.8
1	C	310	MET	3.8
5	j	25	VAL	3.8
1	V	305	ASN	3.8
5	G	157	LYS	3.8
5	G	115	PHE	3.8
1	U	282	GLN	3.8
1	U	184	TYR	3.8
3	J	29	ARG	3.8
1	V	163	VAL	3.8
3	D	73	ALA	3.8
4	o	42	ALA	3.8
1	U	227	VAL	3.8
1	f	111	PHE	3.8
4	L	33	ARG	3.8
1	x	176	LEU	3.8
1	9	193	ASP	3.8
1	3	265	CYS	3.8
1	9	200	ASP	3.8
3	X	93	PHE	3.8
2	n	60	VAL	3.8
3	P	90	ILE	3.8
4	0	103	LEU	3.8
1	x	118	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	T	60	VAL	3.7
1	U	89	LEU	3.7
1	O	114	LEU	3.7
3	e	58	GLY	3.7
3	X	18	ALA	3.7
5	1	62	ALA	3.7
1	3	315	GLU	3.7
3	y	50	LEU	3.7
3	4	43	ARG	3.7
1	x	52	LEU	3.7
1	l	40	TRP	3.7
1	l	27	LEU	3.7
1	3	40	TRP	3.7
2	z	59	GLU	3.7
5	b	77	ARG	3.7
1	x	179	GLY	3.7
4	L	61	GLY	3.7
5	v	151	LEU	3.7
1	9	22	MET	3.7
1	9	269	LEU	3.7
1	I	148	PHE	3.7
4	k	127	PHE	3.7
1	I	307	ILE	3.6
3	W	7	ILE	3.6
3	4	15	PHE	3.6
3	g	3	VAL	3.6
2	K	21	LEU	3.6
3	W	74	THR	3.6
1	f	214	TYR	3.6
1	x	248	TYR	3.6
2	5	76	TYR	3.6
3	D	8	ARG	3.6
3	4	42	GLN	3.6
3	e	27	LEU	3.6
1	x	177	VAL	3.6
1	U	317	HIS	3.6
3	D	5	LEU	3.6
3	J	27	LEU	3.6
4	6	37	HIS	3.6
5	S	56	HIS	3.6
2	E	30	ILE	3.6
4	0	150	THR	3.6

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Mol	Chain	Res	Type	RSRZ
5	v	173	ASP	3.6
5	S	5	TRP	3.6
5	b	5	TRP	3.5
1	x	319	ILE	3.5
1	C	13	LEU	3.5
4	a	99	ALA	3.5
5	q	53	SER	3.5
1	3	304	PRO	3.5
3	J	30	ILE	3.5
1	3	308	GLU	3.5
5	b	9	ILE	3.5
3	g	83	ASP	3.5
1	O	22	MET	3.5
3	g	7	ILE	3.5
5	v	148	TYR	3.5
3	e	55	LYS	3.5
5	d	154	ILE	3.5
1	O	148	PHE	3.5
5	G	141	LYS	3.5
3	H	62	PHE	3.5
5	M	132	ARG	3.5
1	x	65	LEU	3.5
1	3	195	LEU	3.5
1	3	115	GLU	3.5
3	W	59	GLU	3.5
5	G	9	ILE	3.5
1	V	186	ASN	3.5
3	s	54	GLY	3.5
5	1	171	THR	3.5
4	a	55	ILE	3.5
3	W	89	CYS	3.5
4	N	55	ILE	3.5
4	F	67	GLN	3.4
1	x	253	ARG	3.4
4	o	64	LEU	3.4
1	l	171	ALA	3.4
1	C	222	LEU	3.4
4	o	150	THR	3.4
1	w	255	CYS	3.4
5	q	159	ILE	3.4
4	N	52	ARG	3.4
3	y	52	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
3	e	69	PRO	3.4
1	I	114	LEU	3.4
1	x	228	GLN	3.4
1	U	318	ILE	3.4
2	B	93	PHE	3.4
1	3	114	LEU	3.4
5	b	98	VAL	3.4
4	c	117	GLN	3.4
2	Z	62	PHE	3.4
5	v	155	ILE	3.4
1	3	160	MET	3.4
1	9	69	ILE	3.4
2	K	94	PRO	3.4
3	m	69	PRO	3.4
1	f	187	LEU	3.4
1	r	227	VAL	3.4
2	n	58	ASN	3.4
1	U	160	MET	3.4
1	V	154	ARG	3.4
5	l	5	TRP	3.4
5	S	107	ILE	3.4
1	w	188	CYS	3.4
2	Z	87	SER	3.4
3	X	27	LEU	3.4
4	c	57	PHE	3.4
5	l	76	GLU	3.4
1	l	65	LEU	3.3
5	q	89	TRP	3.3
4	u	52	ARG	3.3
5	q	169	LEU	3.3
1	l	58	PRO	3.3
3	g	25	PHE	3.3
4	6	146	ALA	3.3
3	X	51	LEU	3.3
1	9	274	LYS	3.3
5	2	170	LEU	3.3
1	U	159	ALA	3.3
3	4	4	PHE	3.3
4	c	68	PHE	3.3
1	C	110	PRO	3.3
1	l	318	ILE	3.3
2	Z	45	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	l	25	ILE	3.3
2	5	95	ILE	3.3
3	e	13	THR	3.3
4	u	110	TRP	3.3
4	o	134	GLN	3.3
3	e	79	PHE	3.3
5	S	155	ILE	3.3
1	x	31	ARG	3.3
3	m	44	LEU	3.3
2	t	58	ASN	3.3
3	W	56	THR	3.3
3	H	27	LEU	3.3
1	I	113	GLN	3.3
1	x	163	VAL	3.3
1	O	306	GLY	3.3
1	C	86	ASP	3.3
5	2	158	LYS	3.3
2	Y	110	LEU	3.3
1	C	17	ASP	3.3
3	J	76	GLY	3.3
4	R	98	LYS	3.3
2	Z	36	ALA	3.3
3	s	75	VAL	3.3
1	9	36	THR	3.2
4	N	127	PHE	3.2
1	V	304	PRO	3.2
1	U	277	ILE	3.2
3	D	42	GLN	3.2
1	9	133	SER	3.2
1	3	269	LEU	3.2
4	N	56	ALA	3.2
1	l	44	PHE	3.2
2	Y	95	ILE	3.2
1	I	176	LEU	3.2
4	o	92	ALA	3.2
4	k	68	PHE	3.2
5	7	25	VAL	3.2
5	7	98	VAL	3.2
4	0	125	LEU	3.2
5	1	140	ASN	3.2
1	r	35	VAL	3.2
2	Y	89	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
5	S	144	GLY	3.2
1	3	275	GLU	3.2
3	J	26	GLU	3.2
2	n	73	VAL	3.2
3	X	98	GLU	3.2
1	x	298	SER	3.2
4	N	128	ASP	3.2
1	r	15	PHE	3.2
1	f	308	GLU	3.2
2	E	104	LEU	3.2
3	m	13	THR	3.2
4	F	37	HIS	3.2
3	4	27	LEU	3.2
4	o	21	LEU	3.2
1	U	281	CYS	3.2
4	R	72	SER	3.2
5	M	93	ARG	3.2
4	k	15	GLU	3.2
1	U	143	TRP	3.1
1	O	111	PHE	3.1
1	9	159	ALA	3.1
1	9	254	GLU	3.1
5	2	19	ASN	3.1
1	l	252	ARG	3.1
3	D	53	ASP	3.1
1	l	227	VAL	3.1
3	H	42	GLN	3.1
5	d	53	SER	3.1
3	X	34	ILE	3.1
1	U	198	TYR	3.1
4	0	100	PRO	3.1
1	f	180	VAL	3.1
3	P	75	VAL	3.1
2	h	30	ILE	3.1
5	q	66	ILE	3.1
1	3	177	VAL	3.1
4	k	143	PHE	3.1
2	t	61	ASN	3.1
3	P	37	ARG	3.1
5	G	89	TRP	3.1
4	N	18	PHE	3.1
1	I	170	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	9	186	ASN	3.1
3	H	83	ASP	3.1
3	g	12	THR	3.1
5	v	164	LEU	3.1
1	C	277	ILE	3.1
4	a	58	VAL	3.1
5	l	7	VAL	3.1
5	d	157	LYS	3.1
5	q	86	SER	3.1
1	r	248	TYR	3.1
3	4	9	ARG	3.1
1	I	107	LEU	3.1
5	d	64	LEU	3.1
3	P	8	ARG	3.1
5	d	120	ILE	3.1
1	C	147	ILE	3.0
1	O	85	ASP	3.0
1	V	318	ILE	3.0
3	J	17	ASP	3.0
2	K	30	ILE	3.0
1	f	50	VAL	3.0
1	9	276	THR	3.0
5	j	7	VAL	3.0
1	9	41	PHE	3.0
1	f	277	ILE	3.0
1	x	16	GLU	3.0
4	N	130	GLU	3.0
5	d	159	ILE	3.0
1	x	231	MET	3.0
1	3	52	LEU	3.0
2	E	21	LEU	3.0
4	L	32	PHE	3.0
2	Y	29	PHE	3.0
2	T	103	LEU	3.0
3	4	44	LEU	3.0
1	x	41	PHE	3.0
1	O	98	ARG	3.0
3	e	8	ARG	3.0
1	O	69	ILE	3.0
1	U	219	PRO	3.0
3	y	11	LYS	3.0
1	U	202	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	Q	62	PHE	3.0
2	K	19	VAL	3.0
1	9	89	LEU	3.0
3	W	27	LEU	3.0
1	V	148	PHE	3.0
3	m	93	PHE	3.0
3	e	60	CYS	3.0
1	U	248	TYR	3.0
5	1	158	LYS	3.0
5	2	80	HIS	3.0
1	9	179	GLY	3.0
3	g	59	GLU	3.0
5	S	54	GLU	3.0
4	L	62	THR	3.0
1	9	100	PHE	3.0
2	z	28	GLU	3.0
2	5	48	GLY	3.0
5	q	124	ILE	3.0
3	4	88	LEU	3.0
1	C	30	LEU	3.0
2	5	109	PHE	3.0
5	d	112	PHE	3.0
2	Q	45	MET	3.0
1	I	166	GLU	2.9
3	4	12	THR	2.9
3	H	12	THR	2.9
5	M	158	GLN	2.9
1	w	69	ILE	2.9
4	u	64	LEU	2.9
5	q	64	LEU	2.9
1	C	223	GLN	2.9
3	s	88	LEU	2.9
5	v	154	LEU	2.9
5	7	169	LEU	2.9
1	f	172	PHE	2.9
2	h	74	CYS	2.9
3	H	4	PHE	2.9
2	t	104	LEU	2.9
5	7	153	LEU	2.9
3	D	16	THR	2.9
5	b	15	ARG	2.9
1	C	231	MET	2.9

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Mol	Chain	Res	Type	RSRZ
4	c	107	CYS	2.9
4	k	105	GLY	2.9
3	P	14	ILE	2.9
5	j	150	LEU	2.9
2	n	47	SER	2.9
4	a	127	PHE	2.9
1	f	133	SER	2.9
5	q	41	ARG	2.9
3	P	78	ALA	2.9
3	g	45	TYR	2.9
5	d	102	LEU	2.9
5	j	85	VAL	2.9
1	C	101	PHE	2.9
1	I	288	ASN	2.9
5	q	79	TRP	2.9
1	9	134	ILE	2.9
2	z	17	MET	2.9
5	b	159	ILE	2.9
5	j	70	TRP	2.9
4	F	139	ALA	2.9
5	b	157	LYS	2.9
2	5	99	ILE	2.8
4	k	110	TRP	2.8
1	U	188	CYS	2.8
1	O	99	LYS	2.8
1	x	92	ALA	2.8
5	j	141	LYS	2.8
1	I	43	LEU	2.8
1	C	148	PHE	2.8
1	9	231	MET	2.8
2	B	99	ILE	2.8
3	H	68	ARG	2.8
4	0	57	PHE	2.8
2	Y	92	GLU	2.8
5	v	21	TRP	2.8
5	G	158	GLN	2.8
5	2	159	GLN	2.8
1	I	168	LEU	2.8
1	x	51	CYS	2.8
4	c	83	ARG	2.8
1	I	111	PHE	2.8
1	U	223	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	184	TYR	2.8
2	K	18	TYR	2.8
5	7	147	TYR	2.8
4	F	104	ASN	2.8
1	3	26	VAL	2.8
1	r	143	TRP	2.8
2	Y	63	ARG	2.8
5	p	69	TYR	2.8
5	M	172	ASP	2.8
5	1	37	ASP	2.8
1	V	278	LEU	2.8
1	w	176	LEU	2.8
2	n	21	LEU	2.8
5	b	145	LEU	2.8
1	f	61	ILE	2.8
5	S	115	PHE	2.8
5	1	172	GLU	2.8
1	V	187	LEU	2.8
2	T	111	ASP	2.8
5	p	163	LEU	2.8
1	w	147	ILE	2.8
2	B	90	ILE	2.8
4	6	39	GLU	2.8
5	j	86	SER	2.8
5	p	106	LEU	2.8
3	y	20	GLU	2.8
1	O	305	ASN	2.8
1	9	112	CYS	2.8
1	I	92	ALA	2.8
1	U	167	ARG	2.8
1	x	35	VAL	2.8
3	J	11	LYS	2.8
4	o	12	PHE	2.8
1	I	88	ALA	2.8
1	I	62	HIS	2.8
1	O	152	LYS	2.8
1	9	216	THR	2.8
5	7	131	PRO	2.8
1	x	289	GLU	2.7
1	l	92	ALA	2.7
3	s	73	ALA	2.7
4	N	44	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	151	ILE	2.7
3	s	42	GLN	2.7
4	i	64	LEU	2.7
1	3	270	VAL	2.7
1	w	258	VAL	2.7
3	W	97	PRO	2.7
3	s	14	ILE	2.7
1	O	132	ASP	2.7
3	D	12	THR	2.7
5	j	88	GLU	2.7
1	U	187	LEU	2.7
1	f	89	LEU	2.7
2	n	109	PHE	2.7
1	9	17	ASP	2.7
2	K	103	LEU	2.7
3	X	8	ARG	2.7
4	L	103	LEU	2.7
4	u	57	PHE	2.7
1	I	158	SER	2.7
4	i	84	GLU	2.7
4	u	109	ILE	2.7
5	M	165	SER	2.7
1	w	155	LEU	2.7
5	S	146	LEU	2.7
3	J	62	PHE	2.7
3	s	62	PHE	2.7
1	w	34	SER	2.7
3	X	77	LEU	2.7
5	b	64	LEU	2.7
2	z	93	PHE	2.7
1	I	180	VAL	2.7
1	9	92	ALA	2.7
1	w	177	VAL	2.7
5	b	55	VAL	2.7
1	V	140	LEU	2.7
3	P	6	MET	2.7
5	j	142	VAL	2.7
1	C	184	TYR	2.7
1	9	192	GLU	2.7
5	1	40	TYR	2.7
3	W	44	LEU	2.7
5	G	145	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	V	274	LYS	2.7
3	y	60	CYS	2.7
1	I	80	VAL	2.7
3	m	75	VAL	2.7
5	2	121	ARG	2.7
2	Y	28	GLU	2.7
1	U	29	LEU	2.7
1	C	77	GLN	2.7
1	l	273	PHE	2.7
3	D	43	ARG	2.7
4	o	70	PRO	2.7
4	u	32	PHE	2.7
1	w	115	GLU	2.7
1	I	198	TYR	2.7
3	H	73	ALA	2.7
1	l	43	LEU	2.7
1	U	224	GLN	2.7
1	9	35	VAL	2.7
3	e	34	ILE	2.7
5	b	87	ILE	2.7
5	2	148	TYR	2.7
1	V	114	LEU	2.7
4	c	98	LYS	2.7
3	W	63	THR	2.7
4	0	64	LEU	2.7
1	I	265	CYS	2.6
3	m	66	THR	2.6
3	y	84	THR	2.6
1	C	177	VAL	2.6
1	I	270	VAL	2.6
1	I	289	GLU	2.6
1	9	177	VAL	2.6
4	0	140	GLN	2.6
5	2	54	GLU	2.6
1	9	91	LYS	2.6
1	V	299	LEU	2.6
5	7	97	GLN	2.6
1	f	285	ILE	2.6
3	e	76	GLY	2.6
1	U	304	PRO	2.6
1	f	140	LEU	2.6
1	x	206	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	3	162	LEU	2.6
5	q	156	PRO	2.6
1	3	12	SER	2.6
1	C	163	VAL	2.6
1	3	167	ARG	2.6
1	O	32	GLN	2.6
3	X	53	ASP	2.6
3	D	75	VAL	2.6
5	j	15	ARG	2.6
4	a	104	ASN	2.6
2	Z	46	LEU	2.6
1	3	274	LYS	2.6
5	d	5	TRP	2.6
1	I	25	ILE	2.6
5	1	107	ILE	2.6
5	1	123	THR	2.6
1	3	317	HIS	2.6
5	q	65	VAL	2.6
1	x	284	MET	2.6
1	x	27	LEU	2.6
3	X	70	GLN	2.6
4	N	138	LEU	2.6
2	h	58	ASN	2.6
4	F	132	ALA	2.6
3	e	15	PHE	2.6
3	y	38	PRO	2.6
4	R	39	GLU	2.6
3	P	60	CYS	2.6
5	j	21	TRP	2.6
1	3	238	LEU	2.6
4	o	103	LEU	2.6
5	M	142	VAL	2.6
1	I	161	LYS	2.6
2	z	107	ALA	2.6
4	u	48	CYS	2.6
1	w	16	GLU	2.6
1	9	30	LEU	2.6
4	u	66	LEU	2.6
1	U	228	GLN	2.6
1	f	76	ALA	2.6
4	N	107	CYS	2.6
1	3	24	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	f	317	HIS	2.6
1	x	261	LEU	2.6
5	v	74	THR	2.6
3	W	3	VAL	2.6
4	o	49	ARG	2.6
3	m	62	PHE	2.5
1	f	206	TYR	2.5
5	2	134	GLU	2.5
1	U	269	LEU	2.5
1	r	173	ASP	2.5
2	n	103	LEU	2.5
1	r	300	MET	2.5
4	N	48	CYS	2.5
1	x	19	TRP	2.5
2	5	28	GLU	2.5
1	w	135	VAL	2.5
4	N	125	LEU	2.5
5	d	91	LYS	2.5
1	C	242	GLU	2.5
3	s	67	ALA	2.5
4	6	144	GLU	2.5
1	9	185	VAL	2.5
1	U	312	LYS	2.5
1	V	100	PHE	2.5
3	W	14	ILE	2.5
5	b	162	PRO	2.5
5	q	19	ASN	2.5
5	q	21	TRP	2.5
1	V	147	ILE	2.5
1	9	136	ARG	2.5
4	o	153	PHE	2.5
3	D	96	PRO	2.5
1	C	135	VAL	2.5
1	f	270	VAL	2.5
1	3	248	TYR	2.5
5	M	27	HIS	2.5
2	z	110	LEU	2.5
3	J	13	THR	2.5
3	e	14	ILE	2.5
3	4	92	PRO	2.5
1	r	62	HIS	2.5
2	5	60	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	J	45	TYR	2.5
5	2	85	VAL	2.5
4	N	12	PHE	2.5
1	w	194	LYS	2.5
4	0	15	GLU	2.5
1	l	164	HIS	2.5
2	h	103	LEU	2.5
3	W	57	LEU	2.5
3	s	44	LEU	2.5
5	2	64	LEU	2.5
1	r	319	ILE	2.5
1	x	277	ILE	2.5
5	p	47	THR	2.5
1	f	11	ALA	2.5
1	l	191	PRO	2.5
1	x	246	LEU	2.5
2	K	29	PHE	2.5
3	e	12	THR	2.5
5	j	9	ILE	2.5
1	w	214	TYR	2.5
4	N	116	LEU	2.5
1	f	220	SER	2.5
1	3	277	ILE	2.5
1	x	227	VAL	2.5
4	a	119	LEU	2.5
4	o	51	GLY	2.5
4	N	95	VAL	2.5
5	M	85	VAL	2.5
5	S	44	TYR	2.5
5	b	57	ILE	2.5
1	C	80	VAL	2.5
2	z	58	ASN	2.5
2	Q	46	LEU	2.5
5	j	69	TYR	2.5
4	N	57	PHE	2.5
2	T	64	GLU	2.5
1	V	29	LEU	2.4
4	u	68	PHE	2.4
1	C	274	LYS	2.4
1	f	269	LEU	2.4
2	T	104	LEU	2.4
4	k	21	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	y	73	ALA	2.4
3	m	16	THR	2.4
4	k	152	GLU	2.4
3	g	1	MET	2.4
3	e	50	LEU	2.4
4	k	107	CYS	2.4
5	p	120	ILE	2.4
5	S	165	PRO	2.4
2	B	60	VAL	2.4
3	m	61	GLY	2.4
4	0	149	ARG	2.4
1	U	111	PHE	2.4
4	6	29	TYR	2.4
1	x	312	LYS	2.4
4	6	63	ASN	2.4
5	b	88	GLU	2.4
4	k	41	GLN	2.4
1	l	80	VAL	2.4
3	D	77	LEU	2.4
3	4	8	ARG	2.4
4	o	97	LEU	2.4
5	j	93	ARG	2.4
2	K	27	HIS	2.4
1	C	97	TRP	2.4
5	7	111	TYR	2.4
5	7	157	LYS	2.4
4	u	27	ILE	2.4
4	c	108	VAL	2.4
1	O	62	HIS	2.4
1	x	111	PHE	2.4
1	V	230	TYR	2.4
1	r	93	TYR	2.4
5	7	38	TRP	2.4
3	P	42	GLN	2.4
5	M	77	ARG	2.4
1	f	299	LEU	2.4
1	w	148	PHE	2.4
3	P	15	PHE	2.4
1	w	184	TYR	2.4
2	n	35	HIS	2.4
5	b	43	HIS	2.4
3	H	34	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	l	306	GLY	2.4
1	C	87	THR	2.4
4	N	132	ALA	2.4
1	x	138	LEU	2.4
3	W	75	VAL	2.4
4	R	45	GLN	2.4
1	f	186	ASN	2.4
1	w	198	TYR	2.4
4	i	15	GLU	2.4
5	q	170	THR	2.4
3	H	48	ASP	2.4
3	P	51	LEU	2.4
1	f	202	PHE	2.4
2	B	87	SER	2.4
1	V	159	ALA	2.4
3	s	7	ILE	2.4
5	S	66	ILE	2.4
1	C	155	LEU	2.4
1	9	188	CYS	2.4
2	h	94	PRO	2.4
1	w	73[A]	ILE	2.4
4	6	59	ALA	2.4
2	B	21	LEU	2.4
2	B	38	THR	2.4
4	a	21	LEU	2.4
5	2	70	TRP	2.3
1	V	39	GLN	2.3
1	V	178	ILE	2.3
1	V	285	ILE	2.3
5	j	35	ALA	2.3
3	m	89	CYS	2.3
3	y	57	LEU	2.3
5	j	102	LEU	2.3
5	S	132	ARG	2.3
3	J	54	GLY	2.3
5	b	38	TRP	2.3
5	j	65	VAL	2.3
1	3	22	MET	2.3
4	c	45	GLN	2.3
1	C	93	TYR	2.3
1	U	148	PHE	2.3
2	E	62	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
5	v	110	HIS	2.3
3	J	53	ASP	2.3
5	v	159	GLN	2.3
1	V	218	ALA	2.3
1	f	151	ILE	2.3
4	0	55	ILE	2.3
5	q	163	LEU	2.3
5	p	79	TRP	2.3
4	N	131	ARG	2.3
1	V	222	LEU	2.3
1	f	25	ILE	2.3
1	x	236	ALA	2.3
1	3	319	ILE	2.3
2	5	18	TYR	2.3
2	h	97	PRO	2.3
4	a	26	GLU	2.3
2	Z	33	ARG	2.3
4	0	147	ARG	2.3
1	x	184	TYR	2.3
3	g	90	ILE	2.3
4	0	21	LEU	2.3
5	S	136	GLN	2.3
1	C	278	LEU	2.3
1	l	198	TYR	2.3
2	E	100	ALA	2.3
2	h	95	ILE	2.3
4	c	128	ASP	2.3
1	l	281	CYS	2.3
1	r	57	GLY	2.3
3	g	85	PHE	2.3
4	6	18	PHE	2.3
1	r	110	PRO	2.3
1	C	161	LYS	2.3
3	J	19	LYS	2.3
2	T	62	PHE	2.3
5	v	15	ARG	2.3
4	F	54	GLU	2.3
5	q	54	GLU	2.3
1	V	281	CYS	2.3
4	i	107	CYS	2.3
1	f	207	LEU	2.3
3	4	5	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	73[A]	ILE	2.3
4	u	44	PHE	2.3
5	2	150	ALA	2.3
1	I	241	GLU	2.3
2	5	49	PRO	2.3
1	l	311	LEU	2.3
4	a	66	LEU	2.3
4	a	103	LEU	2.3
3	D	7	ILE	2.3
2	Y	60	VAL	2.3
5	d	74	THR	2.3
5	2	91	LYS	2.3
1	U	105	ASP	2.3
3	m	88	LEU	2.3
5	b	156	PRO	2.3
1	V	12	SER	2.3
1	f	183	SER	2.3
4	N	8	GLN	2.3
5	S	9	ILE	2.3
2	5	96	ALA	2.3
3	J	67	ALA	2.3
4	o	57	PHE	2.3
5	q	5	TRP	2.3
2	n	85	ASN	2.3
3	4	38	PRO	2.3
1	V	73[A]	ILE	2.3
2	B	109	PHE	2.3
5	v	156	LYS	2.3
3	W	60	CYS	2.2
1	O	30	LEU	2.2
3	J	43	ARG	2.2
1	O	100	PHE	2.2
5	j	87	ILE	2.2
1	3	135	VAL	2.2
5	d	25	VAL	2.2
5	M	89	TRP	2.2
3	P	43	ARG	2.2
1	l	18	LYS	2.2
1	r	281	CYS	2.2
1	w	276	THR	2.2
2	5	30	ILE	2.2
1	3	189	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	n	105	MET	2.2
2	t	95	ILE	2.2
3	H	57	LEU	2.2
5	j	52	SER	2.2
1	U	26	VAL	2.2
4	i	95	VAL	2.2
1	x	218	ALA	2.2
1	x	316	GLU	2.2
3	e	46	LYS	2.2
1	I	140	LEU	2.2
3	W	77	LEU	2.2
1	f	233	TYR	2.2
3	H	17	ASP	2.2
5	2	22	LYS	2.2
3	4	74	THR	2.2
1	U	81	LEU	2.2
1	r	168	LEU	2.2
1	r	176	LEU	2.2
2	Z	74	CYS	2.2
4	N	37	HIS	2.2
1	f	189	SER	2.2
1	x	26	VAL	2.2
3	s	68	ARG	2.2
4	F	86	VAL	2.2
4	k	55	ILE	2.2
1	V	280	GLU	2.2
1	w	170	GLU	2.2
1	V	157	ASP	2.2
3	g	88	LEU	2.2
1	9	31	ARG	2.2
5	1	127	ARG	2.2
3	P	89	CYS	2.2
3	s	90	ILE	2.2
1	V	34	SER	2.2
1	w	291	GLU	2.2
5	2	7	VAL	2.2
2	Y	76	TYR	2.2
3	H	45	TYR	2.2
1	O	140	LEU	2.2
1	w	101	PHE	2.2
3	W	6	MET	2.2
4	c	110	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
4	u	55	ILE	2.2
1	U	158	SER	2.2
2	h	36	ALA	2.2
5	b	44	TYR	2.2
3	m	35	LEU	2.2
1	C	313	ASP	2.2
1	x	194	LYS	2.2
3	m	43	ARG	2.2
1	f	106	ILE	2.2
1	U	40	TRP	2.2
1	O	253	ARG	2.2
1	x	136	ARG	2.2
1	9	162	LEU	2.2
3	J	50	LEU	2.2
5	G	15	ARG	2.2
1	l	309	PRO	2.2
4	L	100	PRO	2.2
1	f	147	ILE	2.2
2	n	19	VAL	2.2
5	2	9	ILE	2.2
1	l	202	PHE	2.2
1	V	22	MET	2.2
4	0	154	GLU	2.2
5	7	54	GLU	2.2
1	x	53	TRP	2.1
1	w	274	LYS	2.2
3	e	4	PHE	2.1
4	0	69	PHE	2.1
1	l	307	ILE	2.1
4	L	123	GLY	2.1
1	w	40	TRP	2.1
4	F	66	LEU	2.1
5	p	74	THR	2.1
3	m	15	PHE	2.1
1	O	154	ARG	2.1
2	Y	99	ILE	2.1
3	X	43	ARG	2.1
4	L	53	SER	2.1
4	0	65	SER	2.1
5	d	54	GLU	2.1
1	U	13	LEU	2.1
1	r	269	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	255	CYS	2.1
1	V	297	PHE	2.1
1	r	40	TRP	2.1
3	W	70	GLN	2.1
5	p	36	LYS	2.1
5	d	65	VAL	2.1
5	2	98	VAL	2.1
1	x	160	MET	2.1
1	9	139	MET	2.1
1	3	29	LEU	2.1
1	3	261	LEU	2.1
4	u	120	ASP	2.1
5	d	132	ARG	2.1
5	7	168	LYS	2.1
4	6	130	GLU	2.1
4	k	45	GLN	2.1
5	M	76	GLU	2.1
5	7	128	ILE	2.1
1	f	231	MET	2.1
3	P	27	LEU	2.1
1	x	247	ARG	2.1
3	4	17	ASP	2.1
1	w	62	HIS	2.1
5	v	89	TRP	2.1
1	O	271	THR	2.1
1	w	197	ILE	2.1
3	D	49	GLN	2.1
1	f	176	LEU	2.1
3	s	5	LEU	2.1
4	c	51	GLY	2.1
1	O	257	SER	2.1
4	i	90	ARG	2.1
5	2	92	LYS	2.1
2	5	29	PHE	2.1
3	4	40	ASP	2.1
3	g	75	VAL	2.1
4	0	110	TRP	2.1
3	H	14	ILE	2.1
1	x	278	LEU	2.1
1	9	29	LEU	2.1
3	y	8	ARG	2.1
5	j	81	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	9	265	CYS	2.1
1	I	183	SER	2.1
3	e	21	SER	2.1
3	D	67	ALA	2.1
4	o	99	ALA	2.1
4	F	110	TRP	2.1
1	f	292	LYS	2.1
1	w	282	GLN	2.1
4	u	148	ARG	2.1
5	G	64	LEU	2.1
1	f	100	PHE	2.1
5	v	133	CYS	2.1
2	z	73	VAL	2.1
1	l	143	TRP	2.1
1	r	115	GLU	2.1
2	B	100	ALA	2.1
3	y	91	GLU	2.1
3	y	75	VAL	2.1
5	d	155	LYS	2.1
3	s	77	LEU	2.1
1	C	103	GLN	2.1
5	G	21	TRP	2.1
5	j	5	TRP	2.1
1	w	303	VAL	2.1
2	5	100	ALA	2.1
5	2	94	TYR	2.1
1	9	106	ILE	2.1
4	i	55	ILE	2.1
1	O	269	LEU	2.1
1	f	13	LEU	2.1
3	X	44	LEU	2.1
3	H	88	LEU	2.1
4	k	64	LEU	2.1
1	V	284	MET	2.1
5	q	70	TRP	2.1
4	0	52	ARG	2.1
4	a	59	ALA	2.1
1	C	249	LEU	2.1
1	U	257	SER	2.1
5	1	144	GLY	2.1
1	9	292	LYS	2.0
3	s	93	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	51	CYS	2.0
2	z	33	ARG	2.0
3	s	59	GLU	2.0
4	o	52	ARG	2.0
1	C	180	VAL	2.0
5	d	68	THR	2.0
5	l	85	VAL	2.0
1	w	30	LEU	2.0
1	3	213	PHE	2.0
1	U	46	ASP	2.0
3	y	9	ARG	2.0
4	R	7	ASP	2.0
1	l	270	VAL	2.0
1	l	107	LEU	2.0
1	3	118	LEU	2.0
4	o	138	LEU	2.0
3	P	20	GLU	2.0
5	G	55	VAL	2.0
2	t	30	ILE	2.0
1	C	271	THR	2.0
5	l	41	ARG	2.0
1	l	300	MET	2.0
3	y	59	GLU	2.0
5	q	134	GLU	2.0
1	x	183	SER	2.0
5	b	99	ASP	2.0
5	j	89	TRP	2.0
1	V	180	VAL	2.0
2	B	76	TYR	2.0
1	l	319	ILE	2.0
5	M	87	ILE	2.0
4	a	68	PHE	2.0
4	o	100	PRO	2.0
4	0	36	PRO	2.0
1	C	265	CYS	2.0
3	4	16	THR	2.0
3	e	6	MET	2.0
5	M	140	ASN	2.0
2	Q	64	GLU	2.0
1	C	19	TRP	2.0
1	O	34	SER	2.0
4	u	98	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	Q	103	LEU	2.0
3	W	5	LEU	2.0
4	F	125	LEU	2.0
5	M	104	ASP	2.0
5	b	107	ILE	2.0
4	6	44	PHE	2.0
1	x	229	ASN	2.0
5	b	74	THR	2.0
1	r	43	LEU	2.0
3	e	68	ARG	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.

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
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.