



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 3, 2016 – 11:59 AM EDT

PDB ID : 4WSN  
Title : Crystal structure of the COP9 signalosome, a P1 crystal form  
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Deposited on : 2014-10-28  
Resolution : 5.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

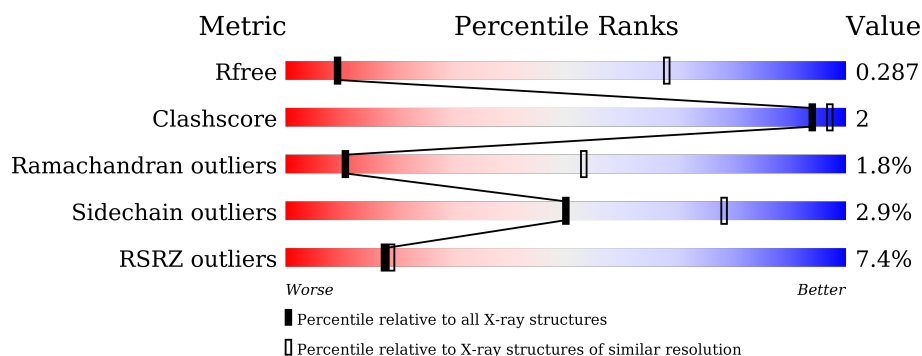
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	480	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	I	480	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	Q	480	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	Y	480	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	g	480	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>•</div> <div>13%</div> </div> </div>
1	o	480	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	447	
2	J	447	
2	R	447	
2	Z	447	
2	h	447	
2	p	447	
3	C	427	
3	K	427	
3	S	427	
3	a	427	
3	i	427	
3	q	427	
4	D	410	
4	L	410	
4	T	410	
4	b	410	
4	j	410	
4	r	410	
5	E	325	
5	M	325	
5	U	325	
5	c	325	
5	k	325	
5	s	325	
6	F	331	

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Mol	Chain	Length	Quality of chain
6	N	331	
6	V	331	
6	d	331	
6	l	331	
6	t	331	
7	G	222	
7	O	222	
7	W	222	
7	e	222	
7	m	222	
7	u	222	
8	H	213	
8	P	213	
8	X	213	
8	f	213	
8	n	213	
8	v	213	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 124428 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	I	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	Q	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	Y	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	g	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	o	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP Q13098
A	49	GLY	-	expression tag	UNP Q13098
A	50	GLY	-	expression tag	UNP Q13098
A	51	ARG	-	expression tag	UNP Q13098
I	48	GLY	-	expression tag	UNP Q13098
I	49	GLY	-	expression tag	UNP Q13098
I	50	GLY	-	expression tag	UNP Q13098
I	51	ARG	-	expression tag	UNP Q13098
Q	48	GLY	-	expression tag	UNP Q13098
Q	49	GLY	-	expression tag	UNP Q13098
Q	50	GLY	-	expression tag	UNP Q13098
Q	51	ARG	-	expression tag	UNP Q13098
Y	48	GLY	-	expression tag	UNP Q13098
Y	49	GLY	-	expression tag	UNP Q13098
Y	50	GLY	-	expression tag	UNP Q13098
Y	51	ARG	-	expression tag	UNP Q13098
g	48	GLY	-	expression tag	UNP Q13098

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Chain	Residue	Modelled	Actual	Comment	Reference
g	49	GLY	-	expression tag	UNP Q13098
g	50	GLY	-	expression tag	UNP Q13098
g	51	ARG	-	expression tag	UNP Q13098
o	48	GLY	-	expression tag	UNP Q13098
o	49	GLY	-	expression tag	UNP Q13098
o	50	GLY	-	expression tag	UNP Q13098
o	51	ARG	-	expression tag	UNP Q13098

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	J	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	R	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	Z	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	h	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	p	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P61201
B	-2	GLY	-	expression tag	UNP P61201
B	-1	GLY	-	expression tag	UNP P61201
B	0	ARG	-	expression tag	UNP P61201
J	-3	GLY	-	expression tag	UNP P61201
J	-2	GLY	-	expression tag	UNP P61201
J	-1	GLY	-	expression tag	UNP P61201
J	0	ARG	-	expression tag	UNP P61201
R	-3	GLY	-	expression tag	UNP P61201
R	-2	GLY	-	expression tag	UNP P61201
R	-1	GLY	-	expression tag	UNP P61201
R	0	ARG	-	expression tag	UNP P61201
Z	-3	GLY	-	expression tag	UNP P61201
Z	-2	GLY	-	expression tag	UNP P61201
Z	-1	GLY	-	expression tag	UNP P61201

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	ARG	-	expression tag	UNP P61201
h	-3	GLY	-	expression tag	UNP P61201
h	-2	GLY	-	expression tag	UNP P61201
h	-1	GLY	-	expression tag	UNP P61201
h	0	ARG	-	expression tag	UNP P61201
p	-3	GLY	-	expression tag	UNP P61201
p	-2	GLY	-	expression tag	UNP P61201
p	-1	GLY	-	expression tag	UNP P61201
p	0	ARG	-	expression tag	UNP P61201

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	K	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	S	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	a	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	i	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	q	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9UNS2
C	-2	GLY	-	expression tag	UNP Q9UNS2
C	-1	GLY	-	expression tag	UNP Q9UNS2
C	0	ARG	-	expression tag	UNP Q9UNS2
K	-3	GLY	-	expression tag	UNP Q9UNS2
K	-2	GLY	-	expression tag	UNP Q9UNS2
K	-1	GLY	-	expression tag	UNP Q9UNS2
K	0	ARG	-	expression tag	UNP Q9UNS2
S	-3	GLY	-	expression tag	UNP Q9UNS2
S	-2	GLY	-	expression tag	UNP Q9UNS2
S	-1	GLY	-	expression tag	UNP Q9UNS2
S	0	ARG	-	expression tag	UNP Q9UNS2
a	-3	GLY	-	expression tag	UNP Q9UNS2

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-2	GLY	-	expression tag	UNP Q9UNS2
a	-1	GLY	-	expression tag	UNP Q9UNS2
a	0	ARG	-	expression tag	UNP Q9UNS2
i	-3	GLY	-	expression tag	UNP Q9UNS2
i	-2	GLY	-	expression tag	UNP Q9UNS2
i	-1	GLY	-	expression tag	UNP Q9UNS2
i	0	ARG	-	expression tag	UNP Q9UNS2
q	-3	GLY	-	expression tag	UNP Q9UNS2
q	-2	GLY	-	expression tag	UNP Q9UNS2
q	-1	GLY	-	expression tag	UNP Q9UNS2
q	0	ARG	-	expression tag	UNP Q9UNS2

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	L	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	T	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	b	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	j	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	r	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q9BT78
D	-2	GLY	-	expression tag	UNP Q9BT78
D	-1	GLY	-	expression tag	UNP Q9BT78
D	0	ARG	-	expression tag	UNP Q9BT78
L	-3	GLY	-	expression tag	UNP Q9BT78
L	-2	GLY	-	expression tag	UNP Q9BT78
L	-1	GLY	-	expression tag	UNP Q9BT78
L	0	ARG	-	expression tag	UNP Q9BT78
T	-3	GLY	-	expression tag	UNP Q9BT78
T	-2	GLY	-	expression tag	UNP Q9BT78
T	-1	GLY	-	expression tag	UNP Q9BT78

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Chain	Residue	Modelled	Actual	Comment	Reference
T	0	ARG	-	expression tag	UNP Q9BT78
b	-3	GLY	-	expression tag	UNP Q9BT78
b	-2	GLY	-	expression tag	UNP Q9BT78
b	-1	GLY	-	expression tag	UNP Q9BT78
b	0	ARG	-	expression tag	UNP Q9BT78
j	-3	GLY	-	expression tag	UNP Q9BT78
j	-2	GLY	-	expression tag	UNP Q9BT78
j	-1	GLY	-	expression tag	UNP Q9BT78
j	0	ARG	-	expression tag	UNP Q9BT78
r	-3	GLY	-	expression tag	UNP Q9BT78
r	-2	GLY	-	expression tag	UNP Q9BT78
r	-1	GLY	-	expression tag	UNP Q9BT78
r	0	ARG	-	expression tag	UNP Q9BT78

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	M	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	U	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	c	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	k	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	s	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	expression tag	UNP Q92905
E	11	GLY	-	expression tag	UNP Q92905
E	12	GLY	-	expression tag	UNP Q92905
E	13	ARG	-	expression tag	UNP Q92905
M	10	GLY	-	expression tag	UNP Q92905
M	11	GLY	-	expression tag	UNP Q92905
M	12	GLY	-	expression tag	UNP Q92905
M	13	ARG	-	expression tag	UNP Q92905
U	10	GLY	-	expression tag	UNP Q92905

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Chain	Residue	Modelled	Actual	Comment	Reference
U	11	GLY	-	expression tag	UNP Q92905
U	12	GLY	-	expression tag	UNP Q92905
U	13	ARG	-	expression tag	UNP Q92905
c	10	GLY	-	expression tag	UNP Q92905
c	11	GLY	-	expression tag	UNP Q92905
c	12	GLY	-	expression tag	UNP Q92905
c	13	ARG	-	expression tag	UNP Q92905
k	10	GLY	-	expression tag	UNP Q92905
k	11	GLY	-	expression tag	UNP Q92905
k	12	GLY	-	expression tag	UNP Q92905
k	13	ARG	-	expression tag	UNP Q92905
s	10	GLY	-	expression tag	UNP Q92905
s	11	GLY	-	expression tag	UNP Q92905
s	12	GLY	-	expression tag	UNP Q92905
s	13	ARG	-	expression tag	UNP Q92905

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	N	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	V	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	d	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	l	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	t	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP Q7L5N1
F	-2	GLY	-	expression tag	UNP Q7L5N1
F	-1	GLY	-	expression tag	UNP Q7L5N1
F	0	ARG	-	expression tag	UNP Q7L5N1
N	-3	GLY	-	expression tag	UNP Q7L5N1
N	-2	GLY	-	expression tag	UNP Q7L5N1
N	-1	GLY	-	expression tag	UNP Q7L5N1

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Chain	Residue	Modelled	Actual	Comment	Reference
N	0	ARG	-	expression tag	UNP Q7L5N1
V	-3	GLY	-	expression tag	UNP Q7L5N1
V	-2	GLY	-	expression tag	UNP Q7L5N1
V	-1	GLY	-	expression tag	UNP Q7L5N1
V	0	ARG	-	expression tag	UNP Q7L5N1
d	-3	GLY	-	expression tag	UNP Q7L5N1
d	-2	GLY	-	expression tag	UNP Q7L5N1
d	-1	GLY	-	expression tag	UNP Q7L5N1
d	0	ARG	-	expression tag	UNP Q7L5N1
l	-3	GLY	-	expression tag	UNP Q7L5N1
l	-2	GLY	-	expression tag	UNP Q7L5N1
l	-1	GLY	-	expression tag	UNP Q7L5N1
l	0	ARG	-	expression tag	UNP Q7L5N1
t	-3	GLY	-	expression tag	UNP Q7L5N1
t	-2	GLY	-	expression tag	UNP Q7L5N1
t	-1	GLY	-	expression tag	UNP Q7L5N1
t	0	ARG	-	expression tag	UNP Q7L5N1

- Molecule 7 is a protein called COP9 signalosome complex subunit 7a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	O	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	W	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	e	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	m	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	u	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q9UBW8
G	-2	GLY	-	expression tag	UNP Q9UBW8
G	-1	GLY	-	expression tag	UNP Q9UBW8
G	0	ARG	-	expression tag	UNP Q9UBW8
O	-3	GLY	-	expression tag	UNP Q9UBW8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	expression tag	UNP Q9UBW8
O	-1	GLY	-	expression tag	UNP Q9UBW8
O	0	ARG	-	expression tag	UNP Q9UBW8
W	-3	GLY	-	expression tag	UNP Q9UBW8
W	-2	GLY	-	expression tag	UNP Q9UBW8
W	-1	GLY	-	expression tag	UNP Q9UBW8
W	0	ARG	-	expression tag	UNP Q9UBW8
e	-3	GLY	-	expression tag	UNP Q9UBW8
e	-2	GLY	-	expression tag	UNP Q9UBW8
e	-1	GLY	-	expression tag	UNP Q9UBW8
e	0	ARG	-	expression tag	UNP Q9UBW8
m	-3	GLY	-	expression tag	UNP Q9UBW8
m	-2	GLY	-	expression tag	UNP Q9UBW8
m	-1	GLY	-	expression tag	UNP Q9UBW8
m	0	ARG	-	expression tag	UNP Q9UBW8
u	-3	GLY	-	expression tag	UNP Q9UBW8
u	-2	GLY	-	expression tag	UNP Q9UBW8
u	-1	GLY	-	expression tag	UNP Q9UBW8
u	0	ARG	-	expression tag	UNP Q9UBW8

- Molecule 8 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	P	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	X	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	f	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	n	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	v	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP Q99627
H	-2	GLY	-	expression tag	UNP Q99627
H	-1	GLY	-	expression tag	UNP Q99627

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ARG	-	expression tag	UNP Q99627
P	-3	GLY	-	expression tag	UNP Q99627
P	-2	GLY	-	expression tag	UNP Q99627
P	-1	GLY	-	expression tag	UNP Q99627
P	0	ARG	-	expression tag	UNP Q99627
X	-3	GLY	-	expression tag	UNP Q99627
X	-2	GLY	-	expression tag	UNP Q99627
X	-1	GLY	-	expression tag	UNP Q99627
X	0	ARG	-	expression tag	UNP Q99627
f	-3	GLY	-	expression tag	UNP Q99627
f	-2	GLY	-	expression tag	UNP Q99627
f	-1	GLY	-	expression tag	UNP Q99627
f	0	ARG	-	expression tag	UNP Q99627
n	-3	GLY	-	expression tag	UNP Q99627
n	-2	GLY	-	expression tag	UNP Q99627
n	-1	GLY	-	expression tag	UNP Q99627
n	0	ARG	-	expression tag	UNP Q99627
v	-3	GLY	-	expression tag	UNP Q99627
v	-2	GLY	-	expression tag	UNP Q99627
v	-1	GLY	-	expression tag	UNP Q99627
v	0	ARG	-	expression tag	UNP Q99627

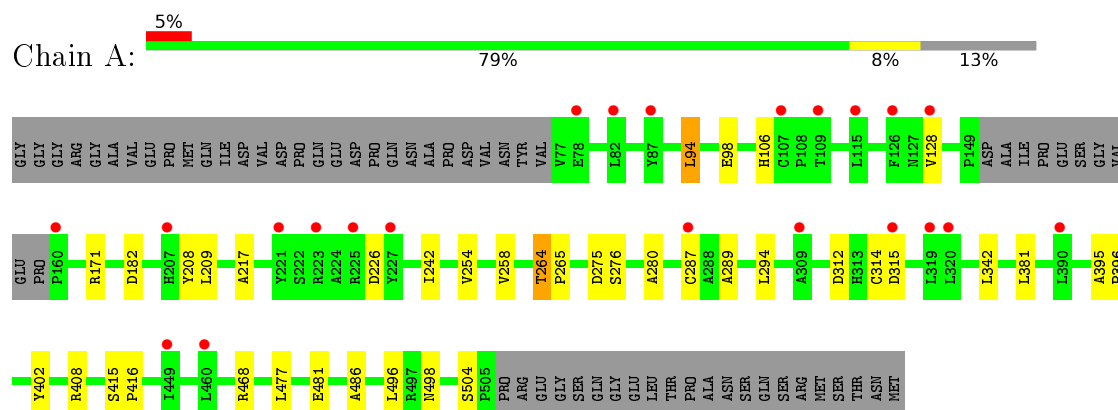
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	k	1	Total Zn 1 1	0	0
9	E	1	Total Zn 1 1	0	0
9	c	1	Total Zn 1 1	0	0
9	U	1	Total Zn 1 1	0	0
9	s	1	Total Zn 1 1	0	0
9	M	1	Total Zn 1 1	0	0

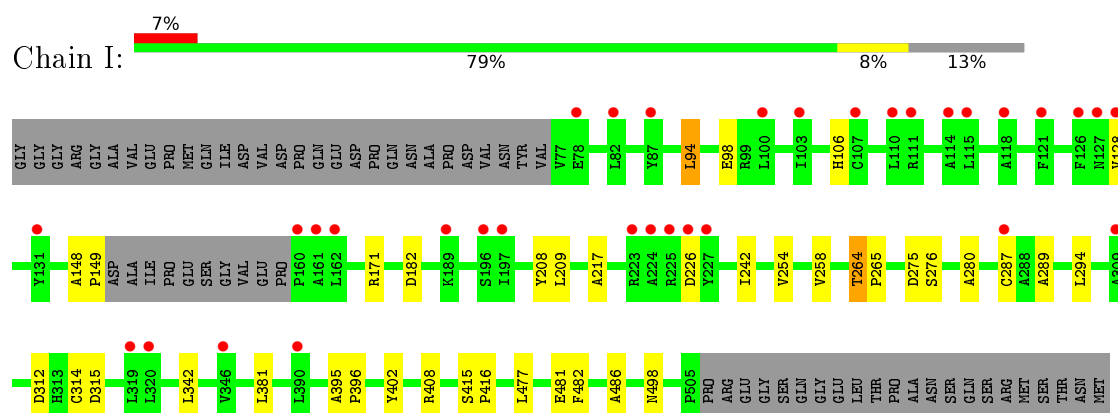
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

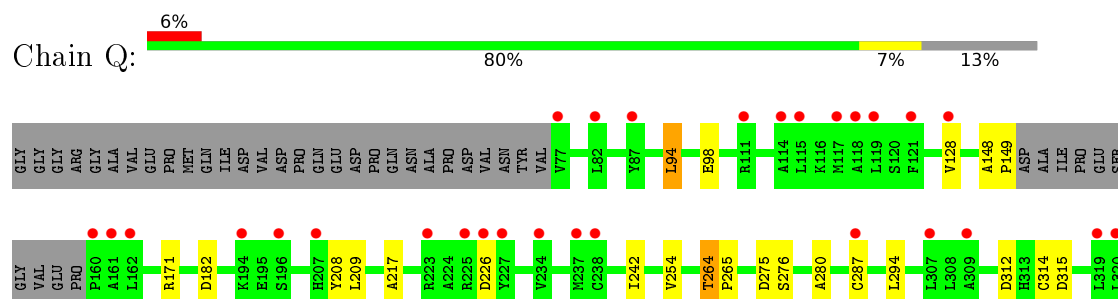
- Molecule 1: COP9 signalosome complex subunit 1



- Molecule 1: COP9 signalosome complex subunit 1

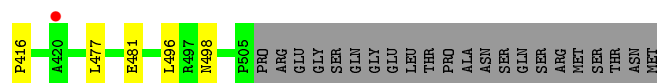
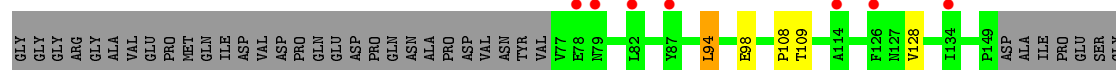
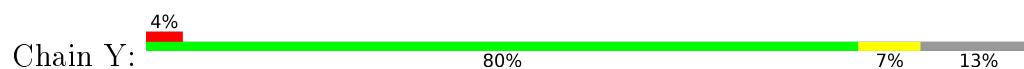


- Molecule 1: COP9 signalosome complex subunit 1

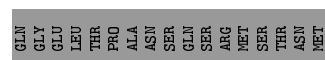
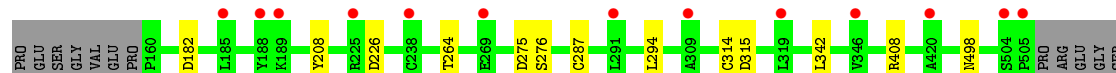
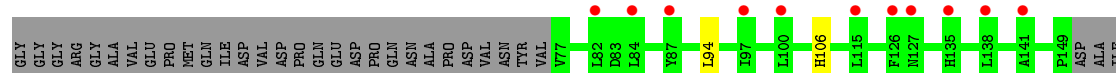
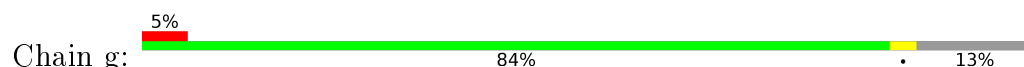




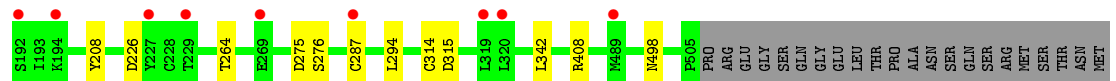
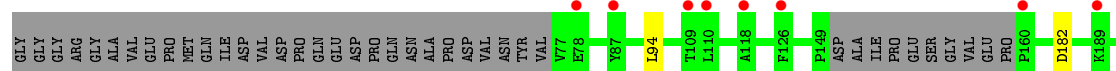
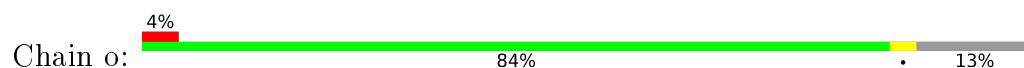
• Molecule 1: COP9 signalosome complex subunit 1



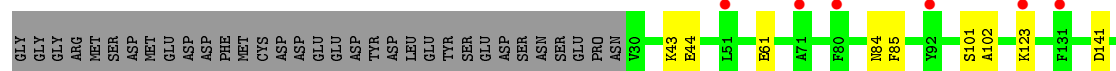
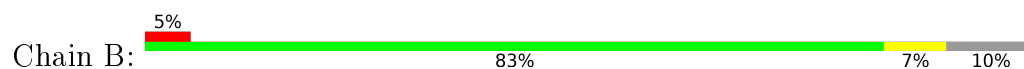
• Molecule 1: COP9 signalosome complex subunit 1

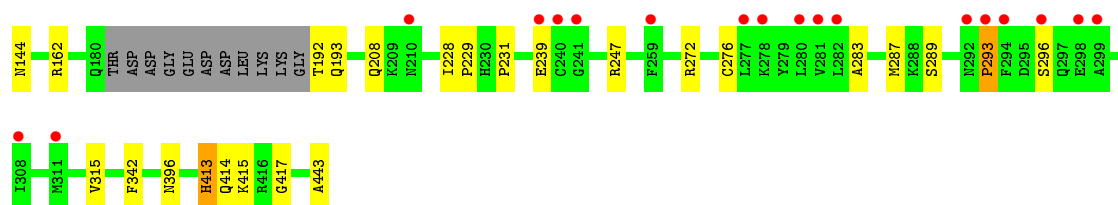


• Molecule 1: COP9 signalosome complex subunit 1

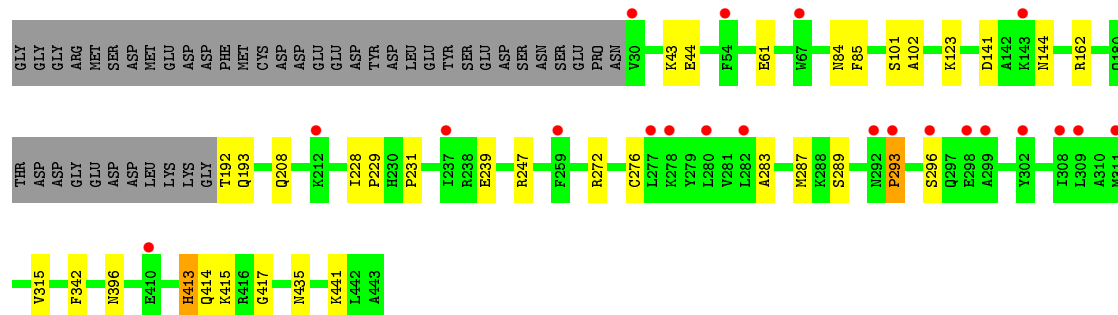
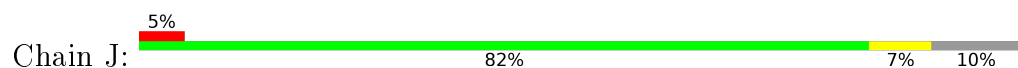


• Molecule 2: COP9 signalosome complex subunit 2

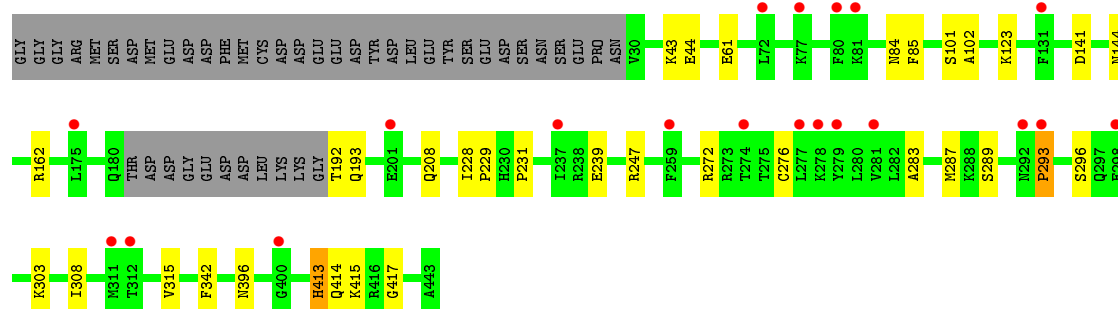
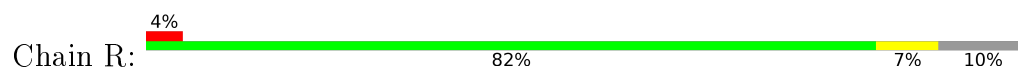




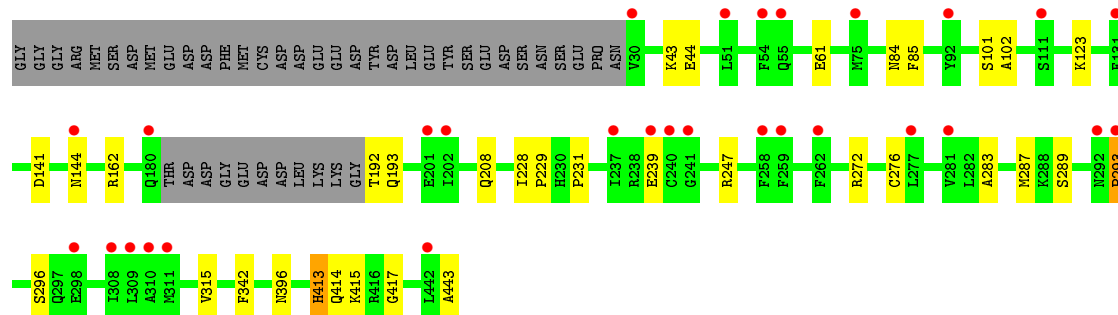
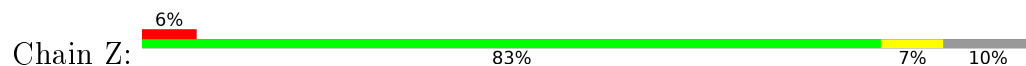
- Molecule 2: COP9 signalosome complex subunit 2



- Molecule 2: COP9 signalosome complex subunit 2

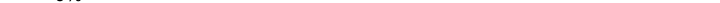


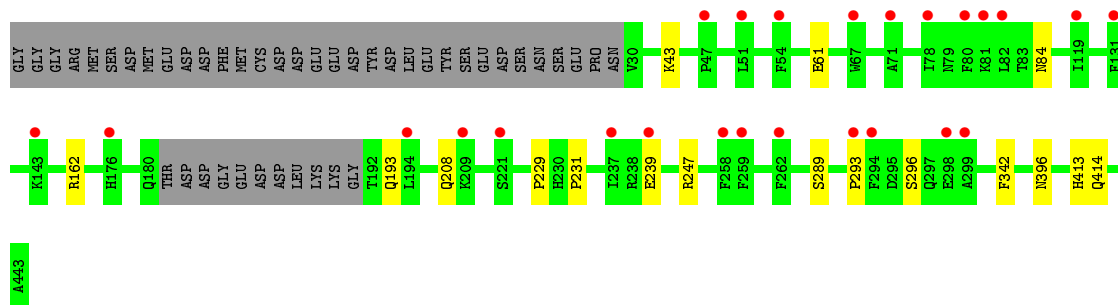
- Molecule 2: COP9 signalosome complex subunit 2



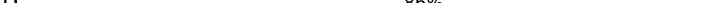
- Molecule 2: COP9 signalosome complex subunit 2

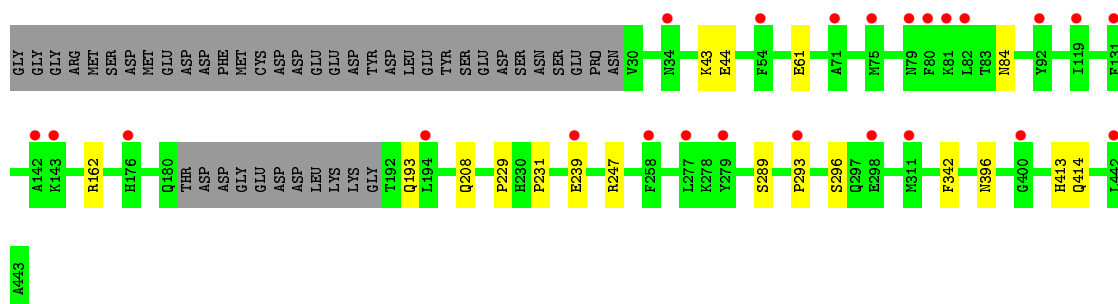


Chain h: 




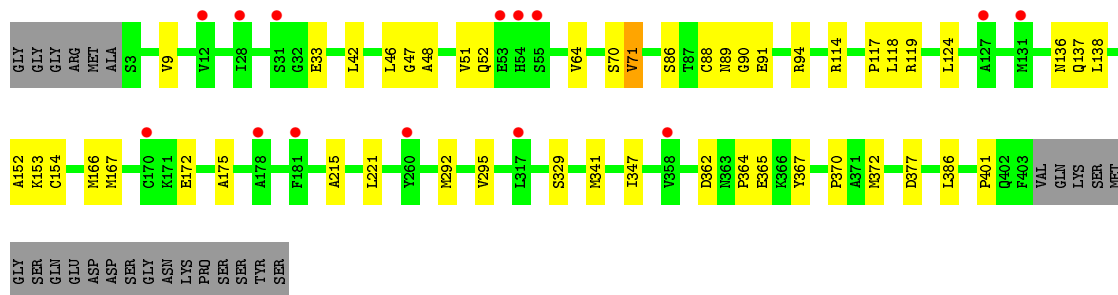
- Molecule 2: COP9 signalosome complex subunit 2

Chain p:  5% 86% 10%




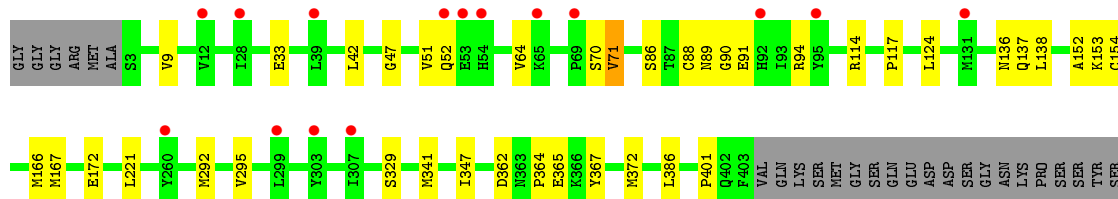
- Molecule 3: COP9 signalosome complex subunit 3

Chain C:  3% 83% 11% 6%

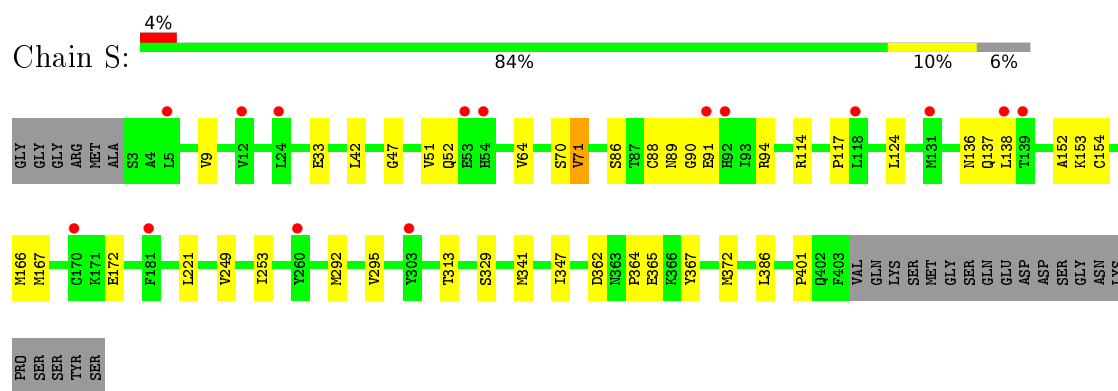


- Molecule 3: COP9 signalosome complex subunit 3

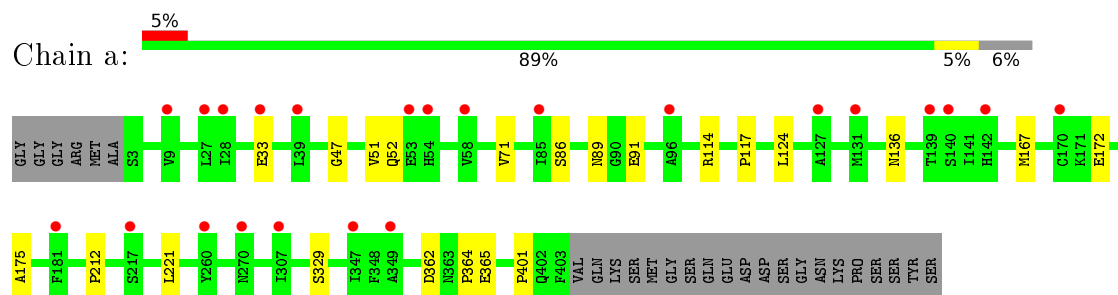
Chain K: 



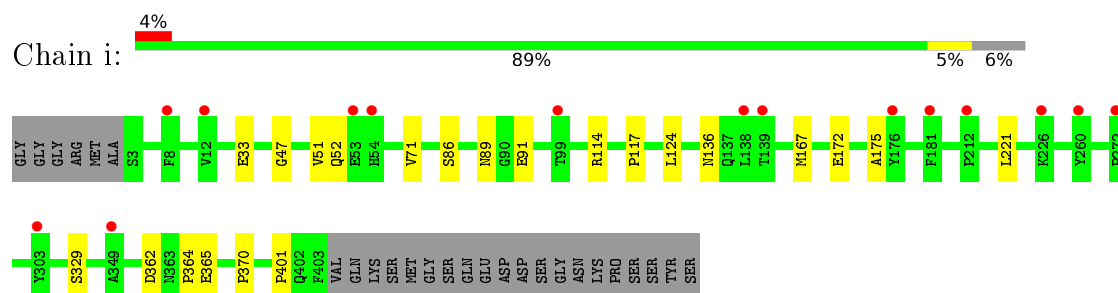
- Molecule 3: COP9 signalosome complex subunit 3



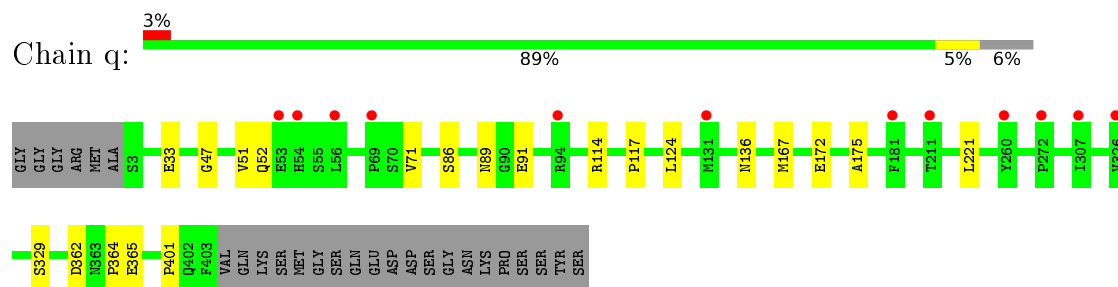
- Molecule 3: COP9 signalosome complex subunit 3



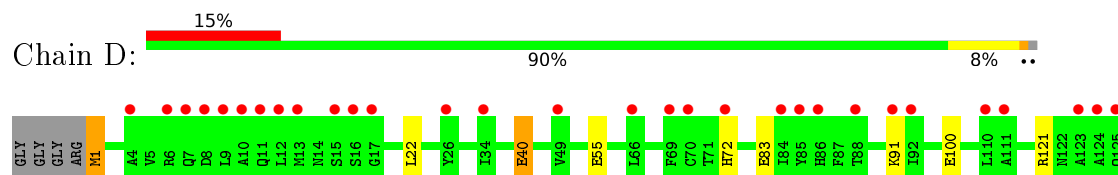
- Molecule 3: COP9 signalosome complex subunit 3

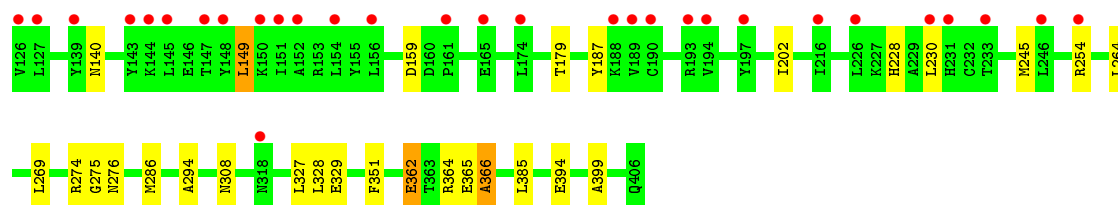


- Molecule 3: COP9 signalosome complex subunit 3

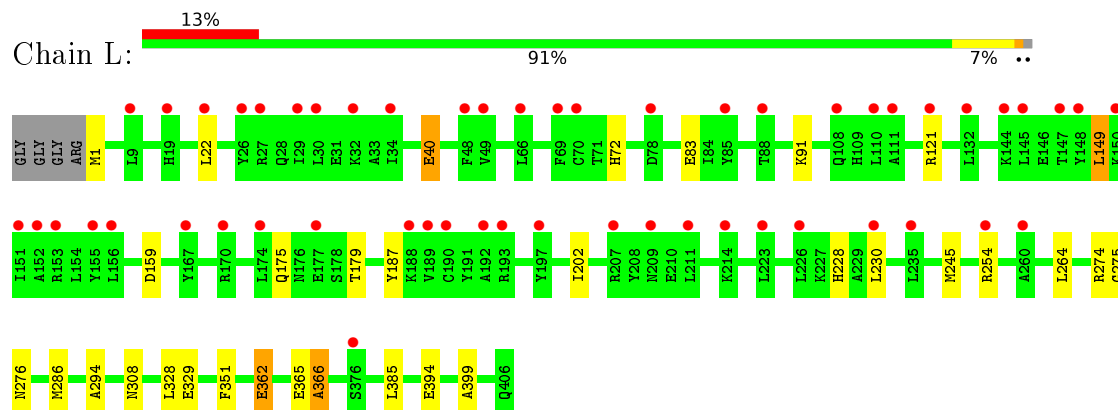


- Molecule 4: COP9 signalosome complex subunit 4

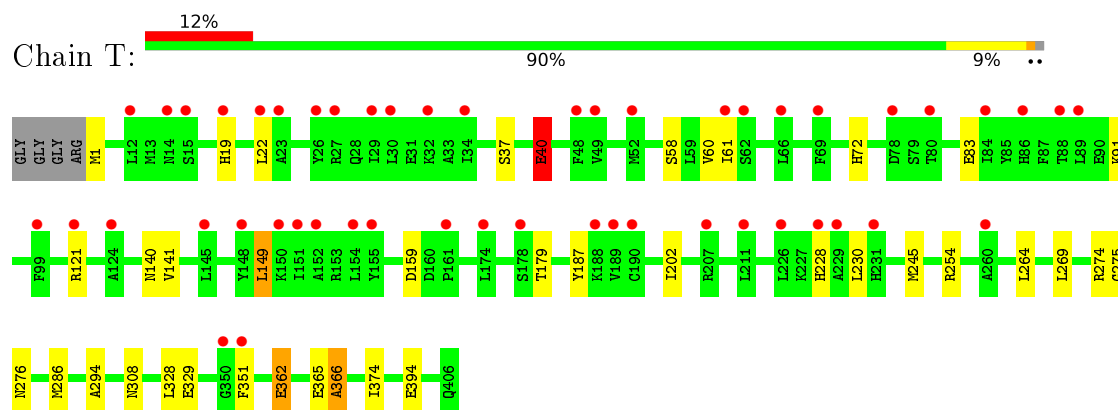




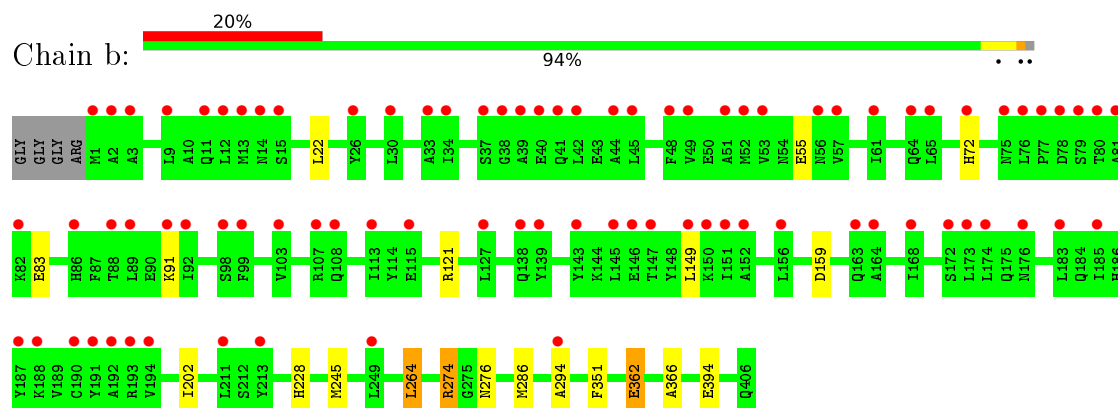
• Molecule 4: COP9 signalosome complex subunit 4



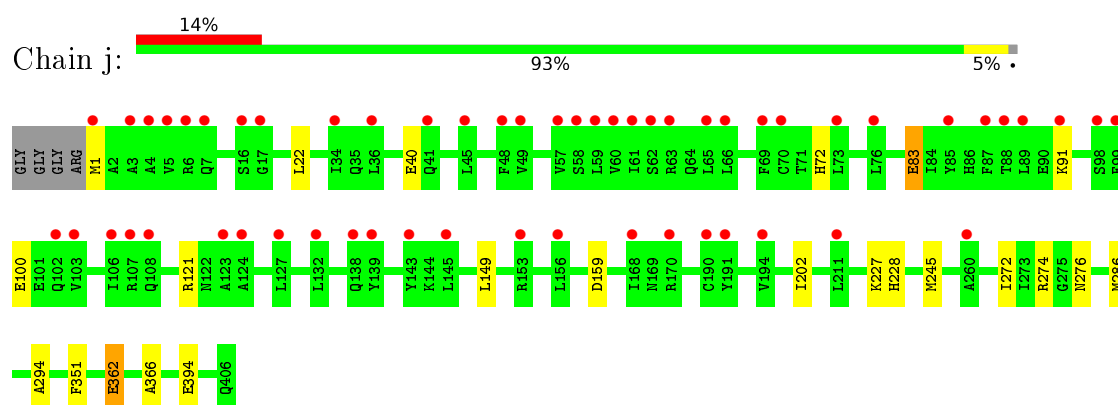
• Molecule 4: COP9 signalosome complex subunit 4



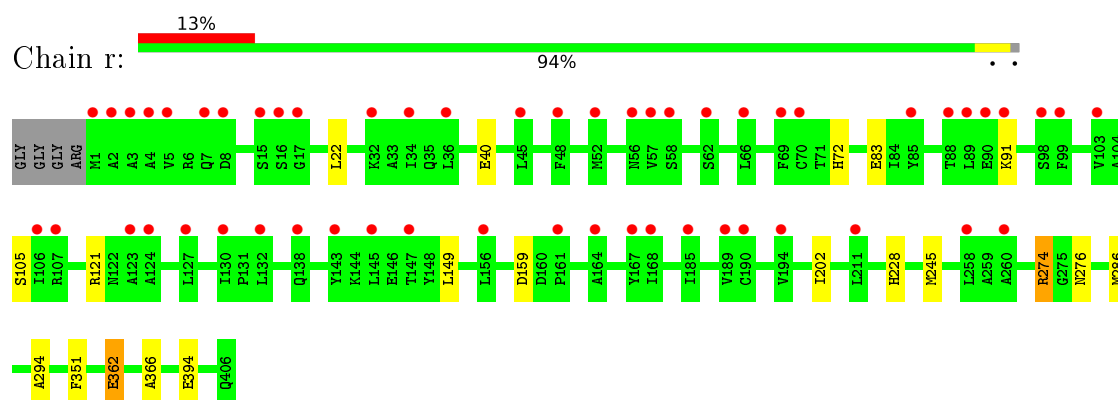
• Molecule 4: COP9 signalosome complex subunit 4



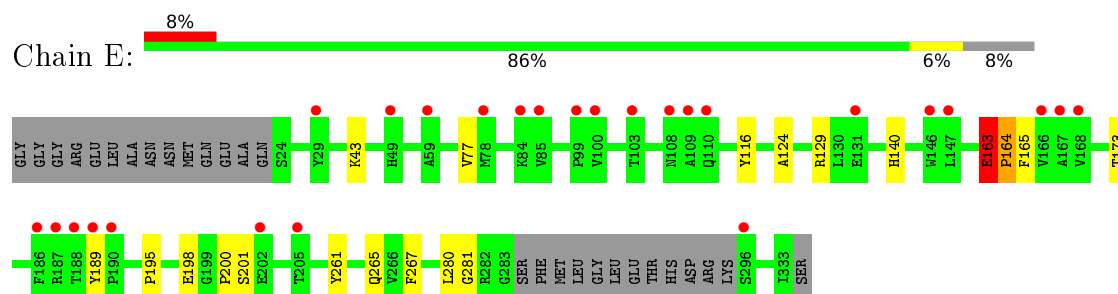
• Molecule 4: COP9 signalosome complex subunit 4



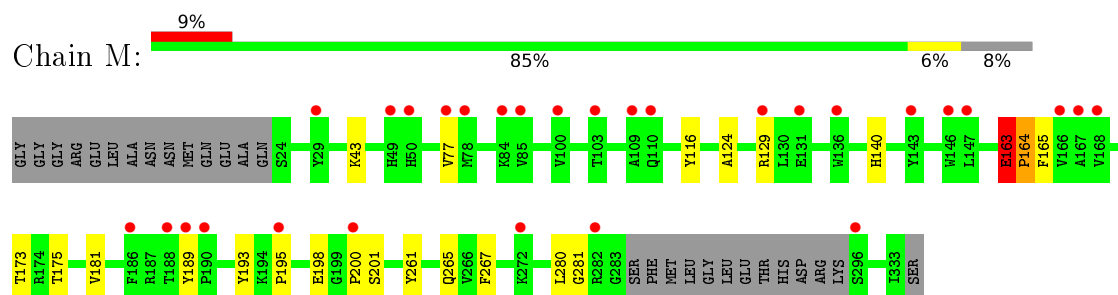
- Molecule 4: COP9 signalosome complex subunit 4



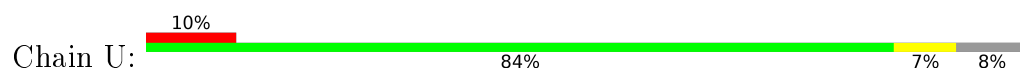
- Molecule 5: COP9 signalosome complex subunit 5

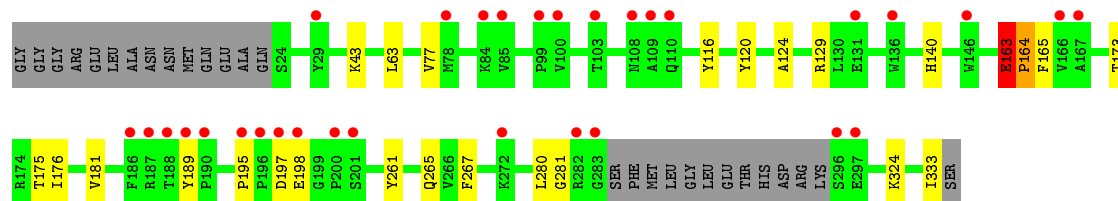


- Molecule 5: COP9 signalosome complex subunit 5

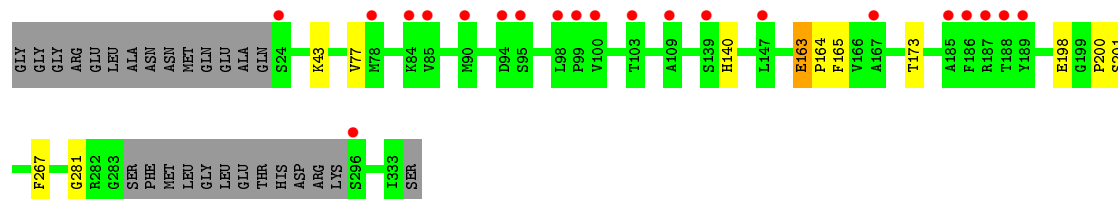
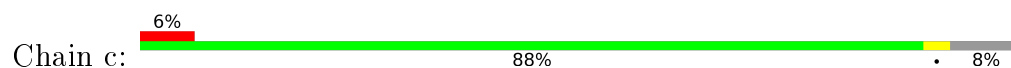


- Molecule 5: COP9 signalosome complex subunit 5

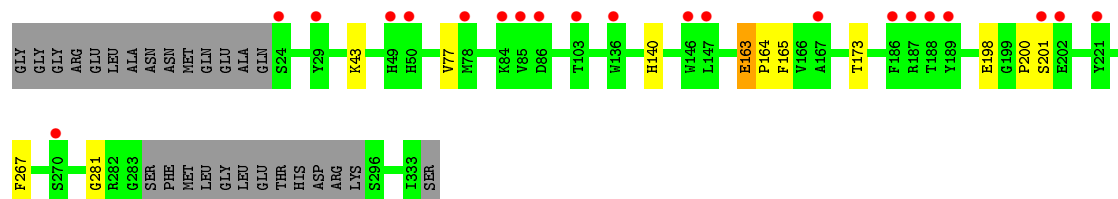
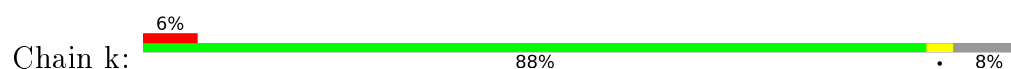




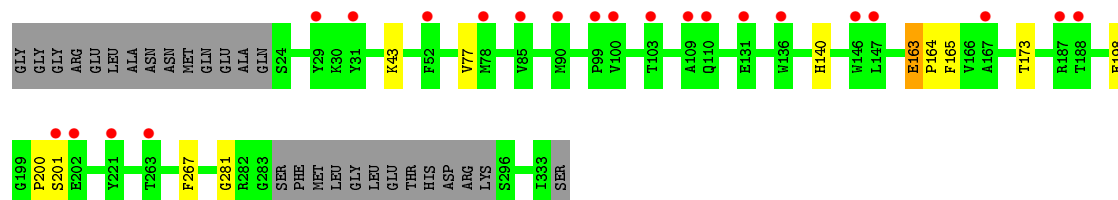
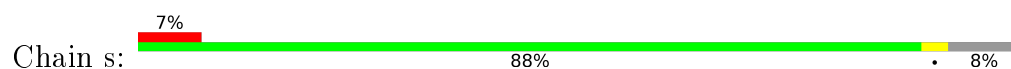
- Molecule 5: COP9 signalosome complex subunit 5



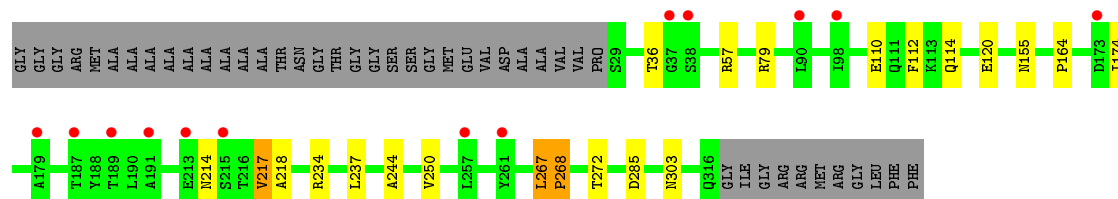
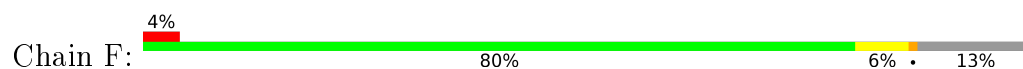
- Molecule 5: COP9 signalosome complex subunit 5



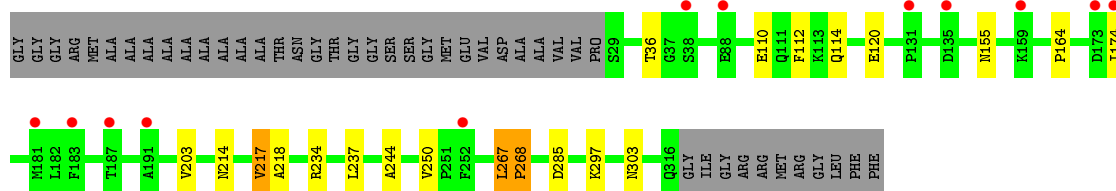
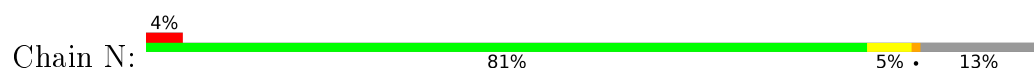
- Molecule 5: COP9 signalosome complex subunit 5



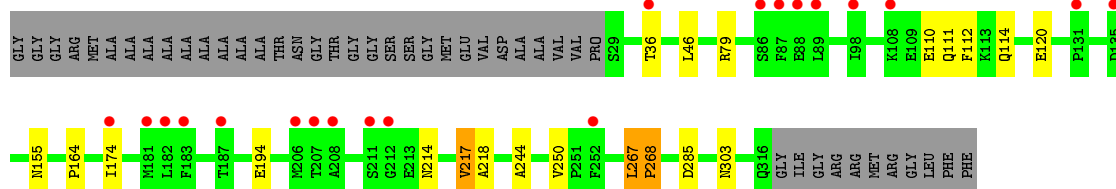
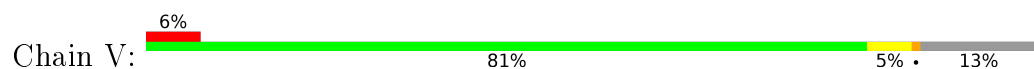
- Molecule 6: COP9 signalosome complex subunit 6



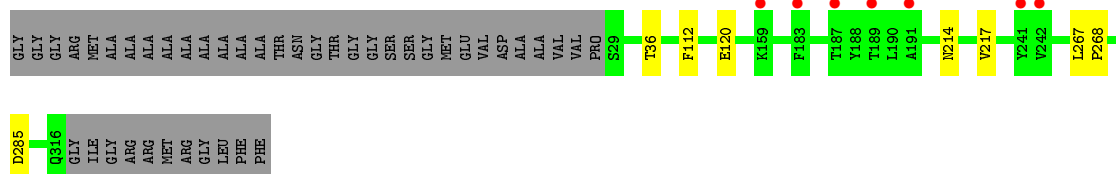
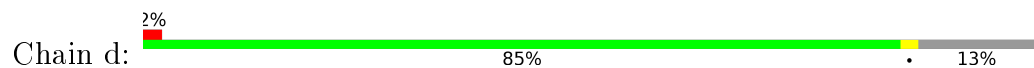
- Molecule 6: COP9 signalosome complex subunit 6



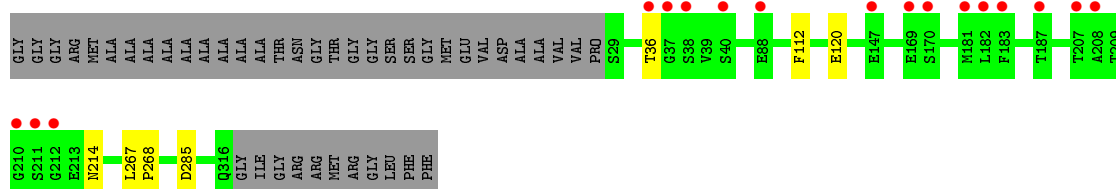
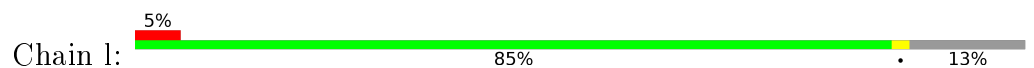
- Molecule 6: COP9 signalosome complex subunit 6



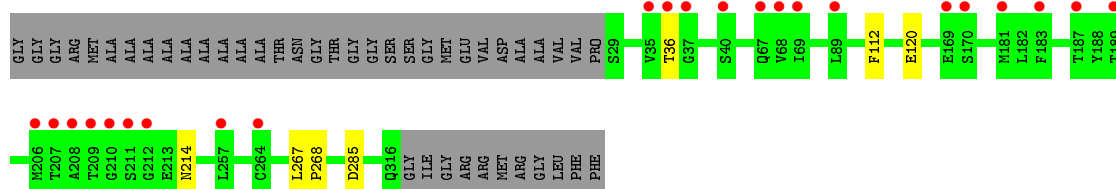
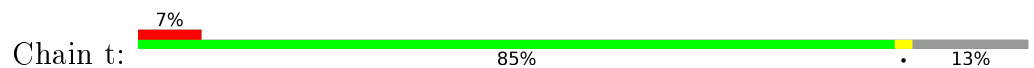
- Molecule 6: COP9 signalosome complex subunit 6



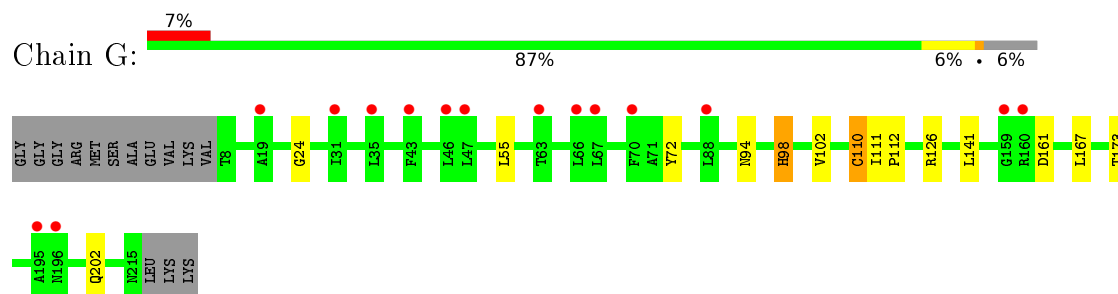
- Molecule 6: COP9 signalosome complex subunit 6



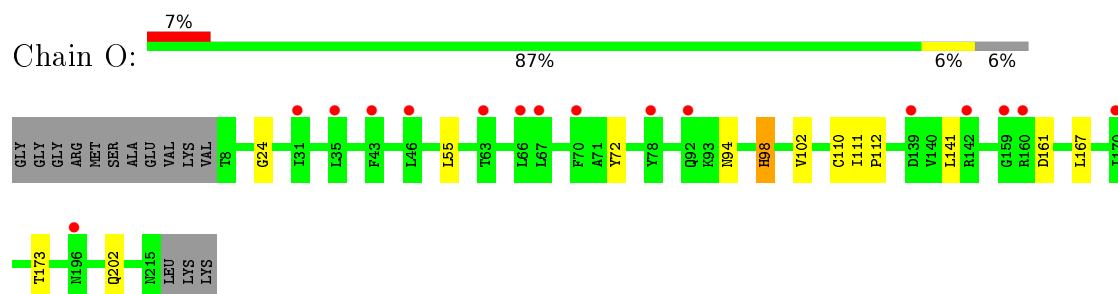
- Molecule 6: COP9 signalosome complex subunit 6



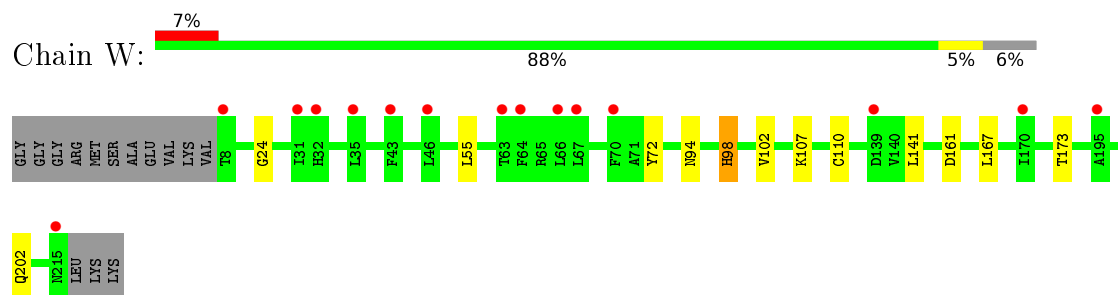
- Molecule 7: COP9 signalosome complex subunit 7a



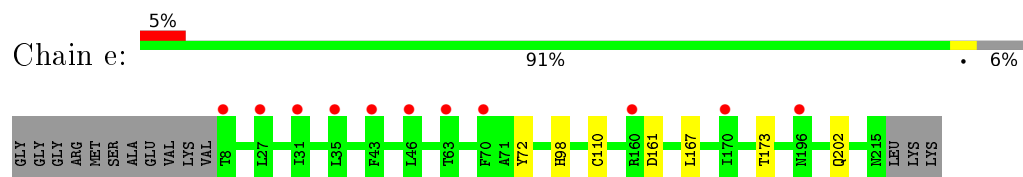
- Molecule 7: COP9 signalosome complex subunit 7a



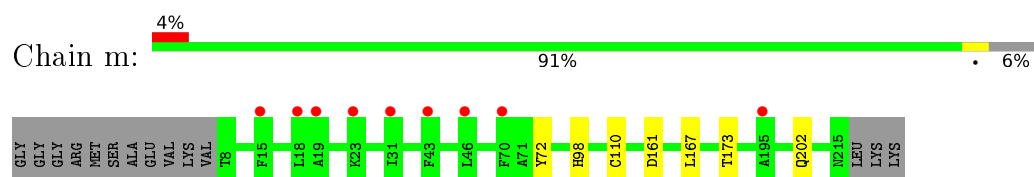
- Molecule 7: COP9 signalosome complex subunit 7a



- Molecule 7: COP9 signalosome complex subunit 7a

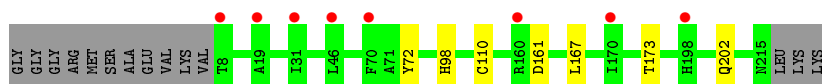


- Molecule 7: COP9 signalosome complex subunit 7a

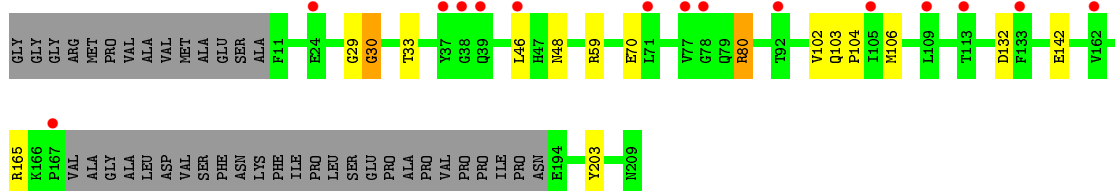
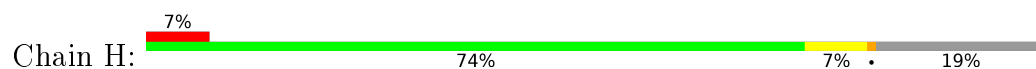


- Molecule 7: COP9 signalosome complex subunit 7a

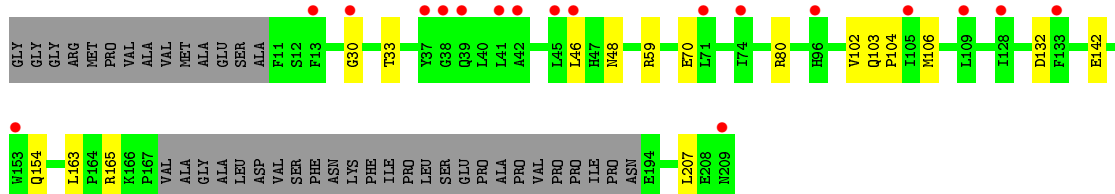




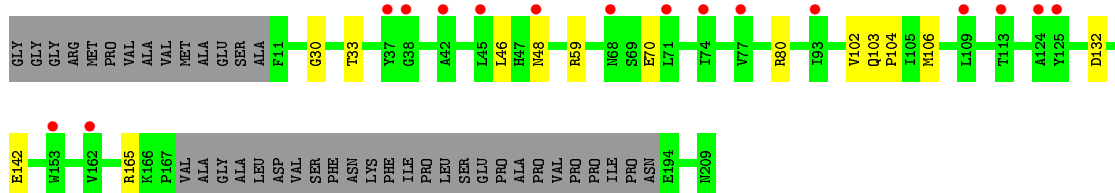
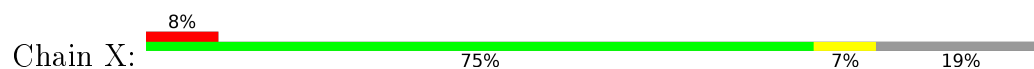
- Molecule 8: COP9 signalosome complex subunit 8



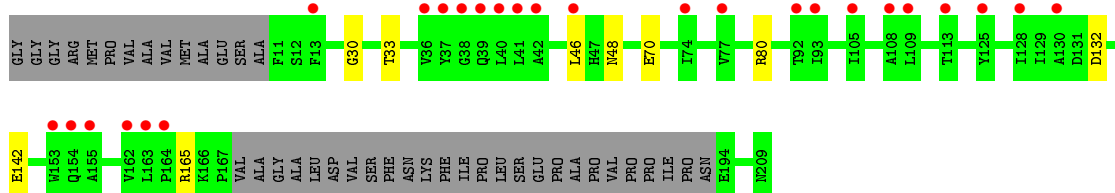
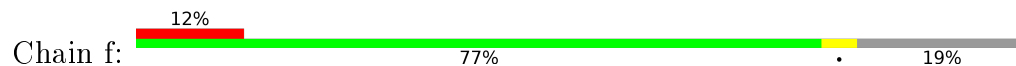
- Molecule 8: COP9 signalosome complex subunit 8



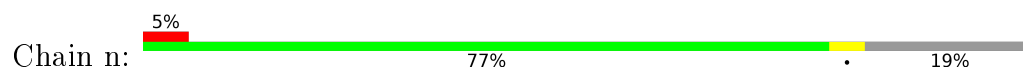
- Molecule 8: COP9 signalosome complex subunit 8



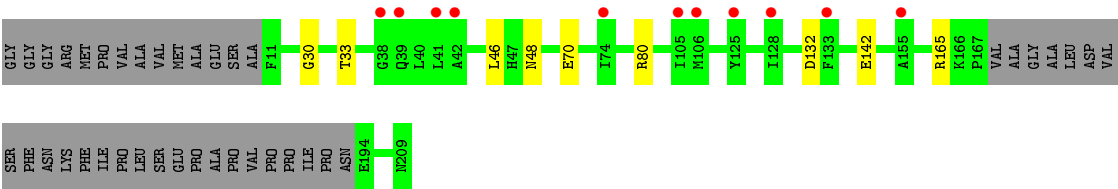
- Molecule 8: COP9 signalosome complex subunit 8



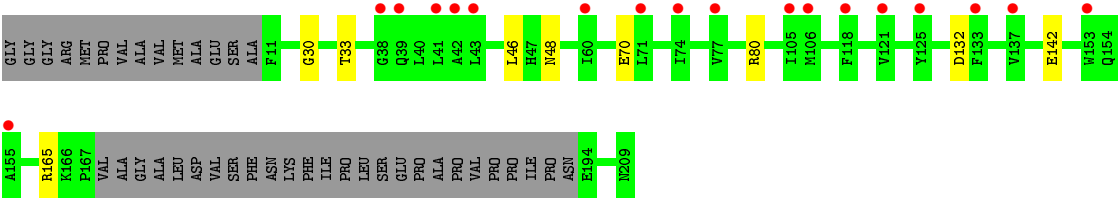
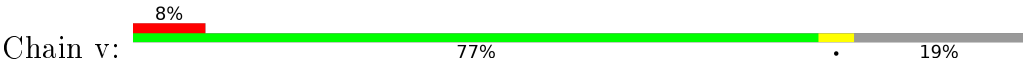
- Molecule 8: COP9 signalosome complex subunit 8







● Molecule 8: COP9 signalosome complex subunit 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.64Å 150.98Å 336.72Å 92.34° 92.62° 119.88°	Depositor
Resolution (Å)	49.64 – 5.50 49.63 – 5.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.64-5.50) 82.0 (49.63-5.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 5.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.254 , 0.282 0.250 , 0.287	Depositor DCC
$R_{free}$ test set	3398 reflections (2.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	258.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 123.7	EDS
Estimated twinning fraction	0.084 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 79094 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	124428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.30	0/3404	0.46	0/4588
1	I	0.30	0/3404	0.47	0/4588
1	Q	0.30	0/3404	0.47	0/4588
1	Y	0.30	0/3404	0.47	0/4588
1	g	0.30	0/3404	0.47	0/4588
1	o	0.30	0/3404	0.47	0/4588
2	B	0.30	0/3360	0.45	0/4519
2	J	0.30	0/3360	0.45	0/4519
2	R	0.31	0/3360	0.45	0/4519
2	Z	0.30	0/3360	0.44	0/4519
2	h	0.30	0/3360	0.45	0/4519
2	p	0.30	0/3360	0.45	0/4519
3	C	0.29	0/3250	0.45	0/4390
3	K	0.29	0/3250	0.45	0/4390
3	S	0.29	0/3250	0.45	0/4390
3	a	0.29	0/3250	0.45	0/4390
3	i	0.29	0/3250	0.45	0/4390
3	q	0.29	0/3250	0.45	0/4390
4	D	0.33	0/3303	0.50	1/4460 (0.0%)
4	L	0.34	0/3303	0.49	0/4460
4	T	0.35	0/3303	0.51	1/4460 (0.0%)
4	b	0.34	0/3303	0.51	2/4460 (0.0%)
4	j	0.34	0/3302	0.52	1/4457 (0.0%)
4	r	0.35	0/3302	0.51	1/4457 (0.0%)
5	E	0.29	0/2417	0.44	0/3266
5	M	0.29	0/2417	0.44	0/3266
5	U	0.29	0/2417	0.45	0/3266
5	c	0.29	0/2417	0.44	0/3266
5	k	0.30	0/2417	0.45	0/3266
5	s	0.29	0/2417	0.45	0/3266
6	F	0.51	1/2310 (0.0%)	0.46	1/3133 (0.0%)
6	N	0.51	1/2310 (0.0%)	0.47	1/3133 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	V	0.48	1/2310 (0.0%)	0.47	1/3133 (0.0%)
6	d	0.50	1/2310 (0.0%)	0.46	1/3133 (0.0%)
6	l	0.31	0/2310	0.45	0/3133
6	t	0.30	0/2310	0.45	0/3133
7	G	0.31	0/1652	0.46	0/2239
7	O	0.30	0/1652	0.46	0/2239
7	W	0.30	0/1652	0.46	0/2239
7	e	0.31	0/1652	0.46	0/2239
7	m	0.31	0/1652	0.46	0/2239
7	u	0.31	0/1652	0.46	0/2239
8	H	0.30	0/1416	0.44	0/1924
8	P	0.30	0/1416	0.45	0/1924
8	X	0.30	0/1416	0.45	0/1924
8	f	0.29	0/1416	0.44	0/1924
8	n	0.30	0/1416	0.45	0/1924
8	v	0.30	0/1416	0.45	0/1924
All	All	0.32	4/126670 (0.0%)	0.46	10/171108 (0.0%)

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
5	E	0	1
5	M	0	1
5	U	0	1
5	c	0	1
5	k	0	1
5	s	0	1
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	217	VAL	C-N	20.09	1.80	1.34
6	N	217	VAL	C-N	19.82	1.79	1.34
6	d	217	VAL	C-N	19.29	1.78	1.34
6	V	217	VAL	C-N	17.96	1.75	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	217	VAL	O-C-N	-7.51	110.69	122.70
4	b	264	LEU	CB-CG-CD1	6.28	121.67	111.00
4	r	274	ARG	NE-CZ-NH1	6.18	123.39	120.30
4	T	40	GLU	CB-CA-C	6.08	122.56	110.40
4	D	364	ARG	NE-CZ-NH1	6.00	123.30	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	163	GLU	Peptide
5	M	163	GLU	Peptide
5	U	163	GLU	Peptide
5	c	163	GLU	Peptide
5	k	163	GLU	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3348	0	3385	16	0
1	I	3348	0	3385	14	0
1	Q	3348	0	3385	14	0
1	Y	3348	0	3385	12	0
1	g	3348	0	3385	0	0
1	o	3348	0	3385	0	0
2	B	3304	0	3350	9	0
2	J	3304	0	3350	10	0
2	R	3304	0	3350	9	0
2	Z	3304	0	3350	9	0
2	h	3304	0	3350	0	0
2	p	3304	0	3350	0	0
3	C	3191	0	3208	19	0
3	K	3191	0	3208	12	0
3	S	3191	0	3208	15	0
3	a	3191	0	3208	0	0
3	i	3191	0	3208	0	0
3	q	3191	0	3208	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3251	0	3253	15	0
4	L	3251	0	3253	9	0
4	T	3251	0	3253	12	0
4	b	3251	0	3253	0	0
4	j	3251	0	3252	0	0
4	r	3251	0	3252	0	0
5	E	2366	0	2340	8	0
5	M	2366	0	2340	11	0
5	U	2366	0	2340	15	0
5	c	2366	0	2340	0	0
5	k	2366	0	2340	0	0
5	s	2366	0	2340	0	0
6	F	2263	0	2235	14	0
6	N	2263	0	2235	11	0
6	V	2263	0	2235	14	0
6	d	2263	0	2235	0	0
6	l	2263	0	2236	0	0
6	t	2263	0	2236	0	0
7	G	1631	0	1654	7	0
7	O	1631	0	1654	4	0
7	W	1631	0	1654	5	0
7	e	1631	0	1654	0	0
7	m	1631	0	1654	0	0
7	u	1631	0	1654	0	0
8	H	1383	0	1366	7	0
8	P	1383	0	1366	5	0
8	X	1383	0	1366	3	0
8	f	1383	0	1366	0	0
8	n	1383	0	1366	0	0
8	v	1383	0	1366	0	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
9	U	1	0	0	0	0
9	c	1	0	0	0	0
9	k	1	0	0	0	0
9	s	1	0	0	0	0
All	All	124428	0	124746	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 232 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:217:VAL:C	6:V:218:ALA:N	1.75	1.39
6:N:217:VAL:C	6:N:218:ALA:N	1.79	1.35
6:F:217:VAL:C	6:F:218:ALA:N	1.80	1.32
5:U:116:TYR:CE2	6:V:114:GLN:HG3	2.32	0.65
4:T:37:SER:O	4:T:40:GLU:OE1	2.17	0.61

There are no symmetry-related clashes.

## 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	A	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	19	64
1	I	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	19	64
1	Q	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	19	64
1	Y	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	19	64
1	g	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	19	64
1	o	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	19	64
2	B	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	5	42
2	J	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	5	42
2	R	397/447 (89%)	353 (89%)	32 (8%)	12 (3%)	5	42
2	Z	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	5	42
2	h	397/447 (89%)	351 (88%)	36 (9%)	10 (2%)	7	46
2	p	397/447 (89%)	351 (88%)	35 (9%)	11 (3%)	6	44
3	C	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	4	37
3	K	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	4	39
3	S	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	4	39
3	a	399/427 (93%)	341 (86%)	43 (11%)	15 (4%)	4	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	i	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	4	37
3	q	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	4	37
4	D	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	19	64
4	L	404/410 (98%)	373 (92%)	27 (7%)	4 (1%)	19	64
4	T	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	19	64
4	b	404/410 (98%)	374 (93%)	26 (6%)	4 (1%)	19	64
4	j	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	19	64
4	r	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	19	64
5	E	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	9	51
5	M	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	9	51
5	U	294/325 (90%)	262 (89%)	28 (10%)	4 (1%)	14	58
5	c	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	9	51
5	k	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	9	51
5	s	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	9	51
6	F	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	N	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	V	286/331 (86%)	258 (90%)	24 (8%)	4 (1%)	14	58
6	d	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	l	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	t	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
7	G	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
7	O	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	34	77
7	W	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	34	77
7	e	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
7	m	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
7	u	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
8	H	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	P	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	X	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	f	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	n	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	v	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
All	All	15416/17130 (90%)	13844 (90%)	1291 (8%)	281 (2%)	11	53

5 of 281 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	229	PRO
2	B	414	GLN
3	C	51	VAL
3	C	89	ASN
3	C	364	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	365/415 (88%)	354 (97%)	11 (3%)	48	77
1	I	365/415 (88%)	354 (97%)	11 (3%)	48	77
1	Q	365/415 (88%)	355 (97%)	10 (3%)	52	79
1	Y	365/415 (88%)	355 (97%)	10 (3%)	52	79
1	g	365/415 (88%)	354 (97%)	11 (3%)	48	77
1	o	365/415 (88%)	355 (97%)	10 (3%)	52	79
2	B	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	J	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	R	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	Z	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	h	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	p	367/406 (90%)	360 (98%)	7 (2%)	65	86
3	C	358/378 (95%)	351 (98%)	7 (2%)	63	85
3	K	358/378 (95%)	352 (98%)	6 (2%)	68	88
3	S	358/378 (95%)	352 (98%)	6 (2%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	a	358/378 (95%)	351 (98%)	7 (2%)	63	85
3	i	358/378 (95%)	351 (98%)	7 (2%)	63	85
3	q	358/378 (95%)	352 (98%)	6 (2%)	68	88
4	D	347/348 (100%)	328 (94%)	19 (6%)	27	64
4	L	347/348 (100%)	329 (95%)	18 (5%)	29	65
4	T	347/348 (100%)	329 (95%)	18 (5%)	29	65
4	b	347/348 (100%)	330 (95%)	17 (5%)	31	67
4	j	347/348 (100%)	327 (94%)	20 (6%)	25	62
4	r	347/348 (100%)	330 (95%)	17 (5%)	31	67
5	E	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	M	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	U	255/276 (92%)	248 (97%)	7 (3%)	52	79
5	c	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	k	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	s	255/276 (92%)	249 (98%)	6 (2%)	57	82
6	F	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	N	250/277 (90%)	246 (98%)	4 (2%)	70	88
6	V	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	d	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	l	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	t	250/277 (90%)	247 (99%)	3 (1%)	78	90
7	G	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	O	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	W	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	e	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	m	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	u	174/184 (95%)	168 (97%)	6 (3%)	44	76
8	H	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	P	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	X	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	f	144/174 (83%)	137 (95%)	7 (5%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	n	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	v	144/174 (83%)	137 (95%)	7 (5%)	31	67
All	All	13560/14748 (92%)	13173 (97%)	387 (3%)	50	78

5 of 387 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	U	165	PHE
3	a	221	LEU
4	r	228	HIS
6	V	120	GLU
1	Y	182	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	324	ASN
5	c	321	GLN
4	r	277	GLN
2	Z	35	GLN
2	Z	84	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	p	1
2	J	1
6	d	1
2	h	1
2	B	1
4	j	1
6	V	1
2	Z	1
6	N	1
4	r	1
2	R	1
6	F	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	290:LYS	C	291:ALA	N	3.62
1	J	193:GLN	C	194:LEU	N	2.88
1	B	193:GLN	C	194:LEU	N	2.87
1	R	193:GLN	C	194:LEU	N	2.86
1	p	193:GLN	C	194:LEU	N	2.85

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/480 (87%)	0.42	22 (5%) 30 29	60, 128, 170, 185	0
1	I	419/480 (87%)	0.49	33 (7%) 15 17	67, 120, 169, 191	0
1	Q	419/480 (87%)	0.48	31 (7%) 17 19	81, 121, 167, 197	0
1	Y	419/480 (87%)	0.31	17 (4%) 41 37	68, 108, 148, 176	0
1	g	419/480 (87%)	0.40	24 (5%) 27 26	80, 111, 161, 190	0
1	o	419/480 (87%)	0.29	17 (4%) 41 37	75, 109, 168, 189	0
2	B	403/447 (90%)	0.42	24 (5%) 25 24	65, 127, 155, 189	0
2	J	403/447 (90%)	0.34	21 (5%) 31 29	70, 125, 159, 172	0
2	R	403/447 (90%)	0.30	20 (4%) 32 30	75, 108, 139, 163	0
2	Z	403/447 (90%)	0.46	29 (7%) 18 19	68, 139, 167, 189	0
2	h	403/447 (90%)	0.43	25 (6%) 24 23	85, 135, 176, 202	0
2	p	403/447 (90%)	0.38	24 (5%) 25 24	81, 126, 165, 179	0
3	C	401/427 (93%)	0.32	14 (3%) 48 43	58, 118, 219, 260	0
3	K	401/427 (93%)	0.34	15 (3%) 45 41	69, 118, 201, 220	0
3	S	401/427 (93%)	0.28	15 (3%) 45 41	68, 99, 195, 216	0
3	a	401/427 (93%)	0.43	23 (5%) 27 26	69, 134, 218, 238	0
3	i	401/427 (93%)	0.30	15 (3%) 45 41	81, 114, 207, 257	0
3	q	401/427 (93%)	0.25	12 (2%) 54 47	77, 116, 208, 249	0
4	D	406/410 (99%)	0.86	60 (14%) 3 7	68, 145, 251, 272	0
4	L	406/410 (99%)	0.70	53 (13%) 5 8	80, 152, 188, 216	0
4	T	406/410 (99%)	0.72	50 (12%) 5 9	88, 131, 183, 209	0
4	b	406/410 (99%)	1.13	84 (20%) 1 5	73, 166, 243, 253	0
4	j	406/410 (99%)	0.76	56 (13%) 4 8	86, 132, 269, 285	0
4	r	406/410 (99%)	0.82	54 (13%) 4 8	81, 162, 253, 272	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
5	E	298/325 (91%)	0.54	26 (8%) 13 15	73, 112, 148, 170	0
5	M	298/325 (91%)	0.59	29 (9%) 10 13	78, 107, 159, 185	0
5	U	298/325 (91%)	0.60	31 (10%) 8 12	89, 121, 174, 198	0
5	c	298/325 (91%)	0.43	21 (7%) 19 20	61, 88, 126, 144	0
5	k	298/325 (91%)	0.46	21 (7%) 19 20	85, 107, 145, 166	0
5	s	298/325 (91%)	0.52	22 (7%) 17 19	84, 108, 148, 170	0
6	F	288/331 (87%)	0.37	13 (4%) 37 34	62, 114, 153, 184	0
6	N	288/331 (87%)	0.41	12 (4%) 40 36	73, 113, 165, 193	0
6	V	288/331 (87%)	0.46	20 (6%) 20 20	84, 120, 160, 194	0
6	d	288/331 (87%)	0.33	7 (2%) 62 57	63, 97, 150, 185	0
6	l	288/331 (87%)	0.45	17 (5%) 26 25	84, 116, 156, 182	0
6	t	288/331 (87%)	0.45	23 (7%) 15 17	77, 116, 160, 190	0
7	G	208/222 (93%)	0.37	15 (7%) 18 19	92, 114, 162, 187	0
7	O	208/222 (93%)	0.32	16 (7%) 16 17	68, 115, 160, 181	0
7	W	208/222 (93%)	0.33	15 (7%) 18 19	111, 135, 161, 174	0
7	e	208/222 (93%)	0.32	11 (5%) 30 29	84, 106, 145, 168	0
7	m	208/222 (93%)	0.19	9 (4%) 39 35	72, 98, 143, 188	0
7	u	208/222 (93%)	0.27	8 (3%) 44 40	73, 111, 149, 164	0
8	H	173/213 (81%)	0.45	15 (8%) 13 15	82, 123, 154, 168	0
8	P	173/213 (81%)	0.46	18 (10%) 8 12	91, 121, 147, 161	0
8	X	173/213 (81%)	0.49	16 (9%) 11 14	91, 114, 142, 150	0
8	f	173/213 (81%)	0.60	26 (15%) 3 7	81, 169, 190, 196	0
8	n	173/213 (81%)	0.42	11 (6%) 23 22	98, 129, 164, 181	0
8	v	173/213 (81%)	0.53	18 (10%) 8 12	94, 139, 175, 187	0
All	All	15576/17130 (90%)	0.47	1158 (7%) 17 19	58, 119, 209, 285	0

The worst 5 of 1158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	b	78	ASP	15.2
1	I	160	PRO	8.6
4	b	2	ALA	8.2
5	U	189	TYR	7.3
3	C	54	HIS	7.3

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	ZN	M	401	1/1	0.92	0.16	-0.82	130,130,130,130	0
9	ZN	E	401	1/1	0.98	0.17	-1.06	130,130,130,130	0
9	ZN	s	401	1/1	0.80	0.09	-1.31	130,130,130,130	0
9	ZN	k	401	1/1	0.98	0.09	-1.51	130,130,130,130	0
9	ZN	c	401	1/1	0.97	0.09	-1.72	130,130,130,130	0
9	ZN	U	401	1/1	0.94	0.08	-1.93	130,130,130,130	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.