



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 11:09 AM EDT

PDB ID : 4D18 / pdb_00004d18
Title : Crystal structure of the COP9 signalosome
Authors : Bunker, R.D.; Lingaraju, G.M.; Thoma, N.H.
Deposited on : 2014-05-01
Resolution : 4.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

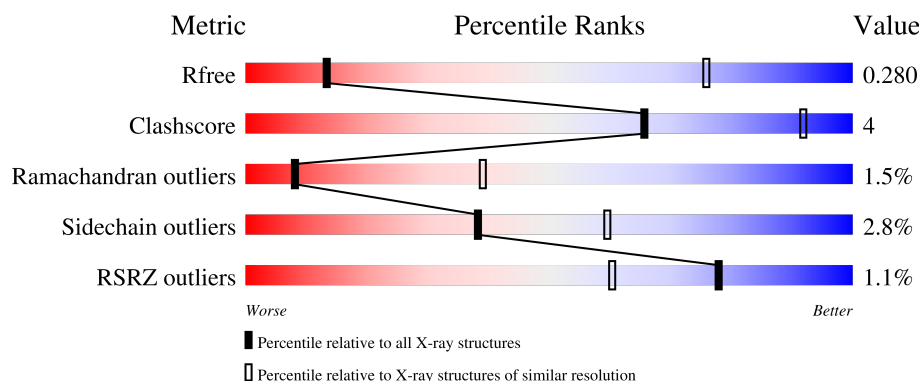
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.08 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}	180053	1200 (4.36-3.80)
Clashscore	190562	1249 (4.36-3.80)
Ramachandran outliers	187476	1169 (4.36-3.80)
Sidechain outliers	187428	1158 (4.36-3.80)
RSRZ outliers	180081	1199 (4.36-3.80)

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	A	480	79% 8% 13%
1	I	480	80% 7% 13%
2	B	447	78% 11% 10%
2	J	447	78% 11% 10%
3	C	427	78% 13% 6%

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Mol	Chain	Length	Quality of chain
3	K	427	
4	D	410	
4	L	410	
5	E	327	
5	M	327	
6	F	331	
6	N	331	
7	G	222	
7	O	222	
8	H	213	
8	P	213	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 41422 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			

There are 8 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

- 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			

There are 8 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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			

There are 8 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

- 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			

There are 8 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

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	GLY	-	expression tag	UNP Q9BT78
L	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			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	GLY	-	expression tag	UNP Q92905
E	9	GLY	-	expression tag	UNP Q92905
E	10	GLY	-	expression tag	UNP Q92905
E	11	ARG	-	expression tag	UNP Q92905
M	8	GLY	-	expression tag	UNP Q92905
M	9	GLY	-	expression tag	UNP Q92905
M	10	GLY	-	expression tag	UNP Q92905
M	11	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	281	Total	C	N	O	S	0	0	0
			2236	1429	371	421	15			
6	N	281	Total	C	N	O	S	0	0	0
			2236	1429	371	421	15			

There are 8 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
N	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			

There are 8 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
O	-2	GLY	-	expression tag	UNP Q9UBW8
O	-1	GLY	-	expression tag	UNP Q9UBW8
O	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			

There are 8 discrepancies between the modelled and reference sequences:

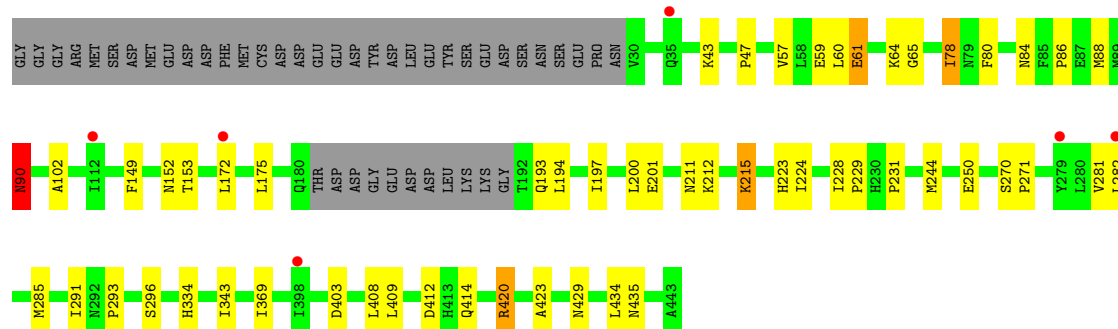
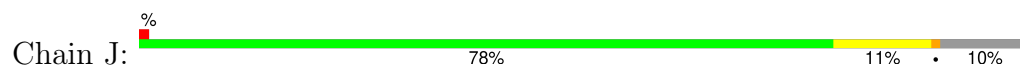
Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP Q99627
H	-2	GLY	-	expression tag	UNP Q99627
H	-1	GLY	-	expression tag	UNP Q99627
H	0	ARG	-	expression tag	UNP Q99627
P	-3	GLY	-	expression tag	UNP Q99627
P	-2	GLY	-	expression tag	UNP Q99627
P	-1	GLY	-	expression tag	UNP Q99627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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

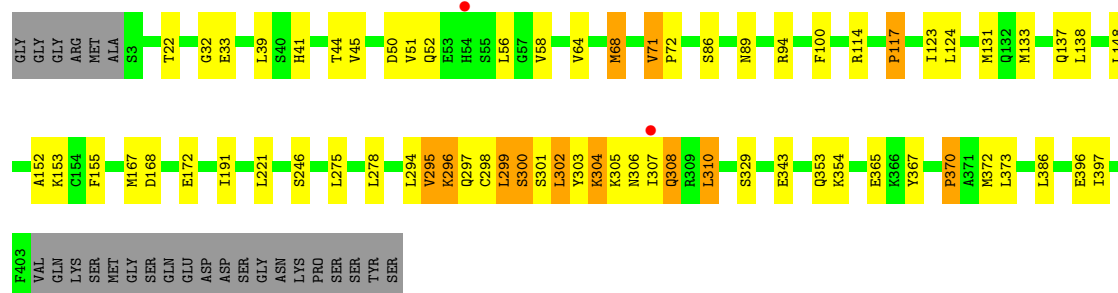
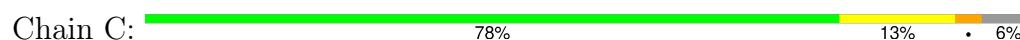
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total 1	Zn 1	0	0
9	M	1	Total 1	Zn 1	0	0



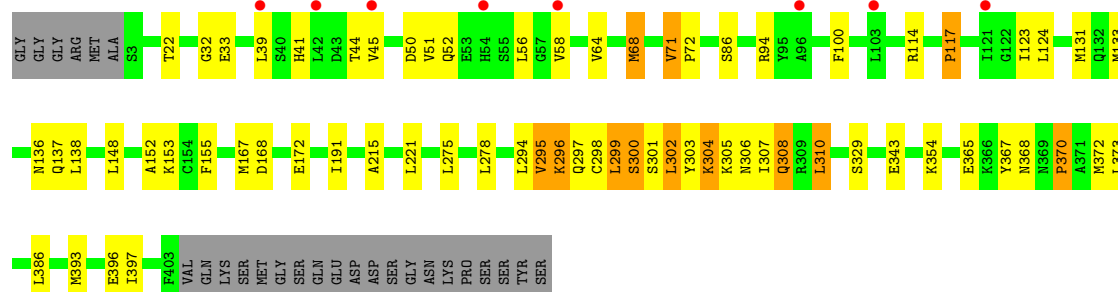
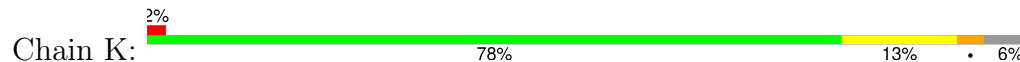
• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2



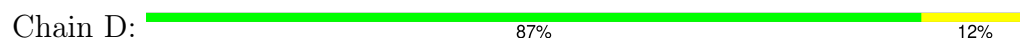
• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

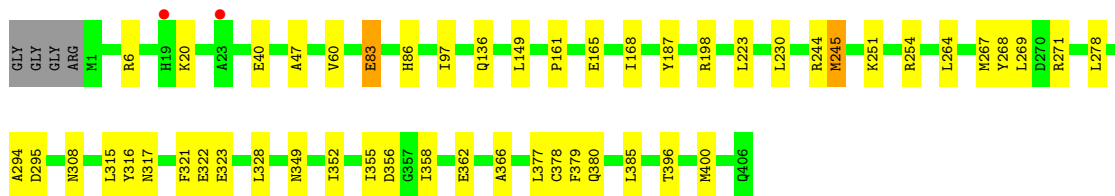


• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3



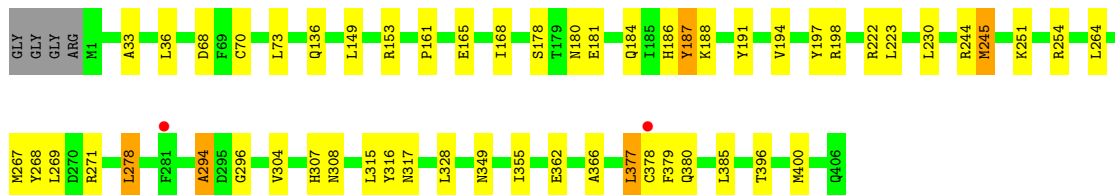
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4





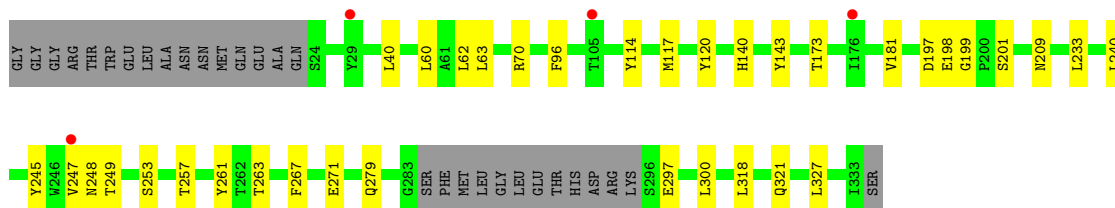
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

Chain L: 86% 12% ..



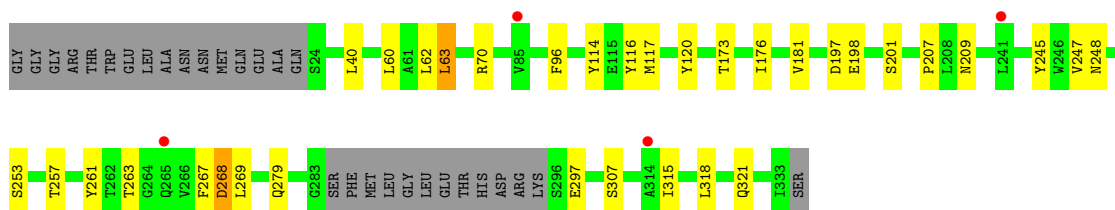
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain E: 80% 11% 9%



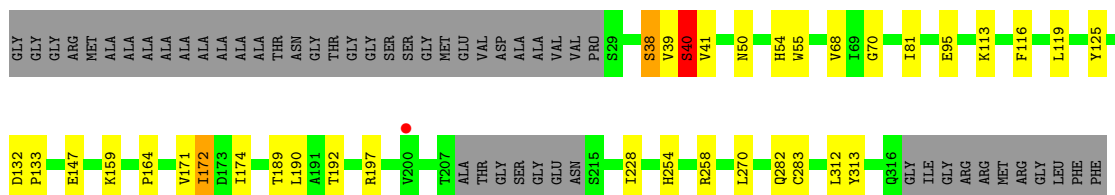
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain M: 81% 10% 9%

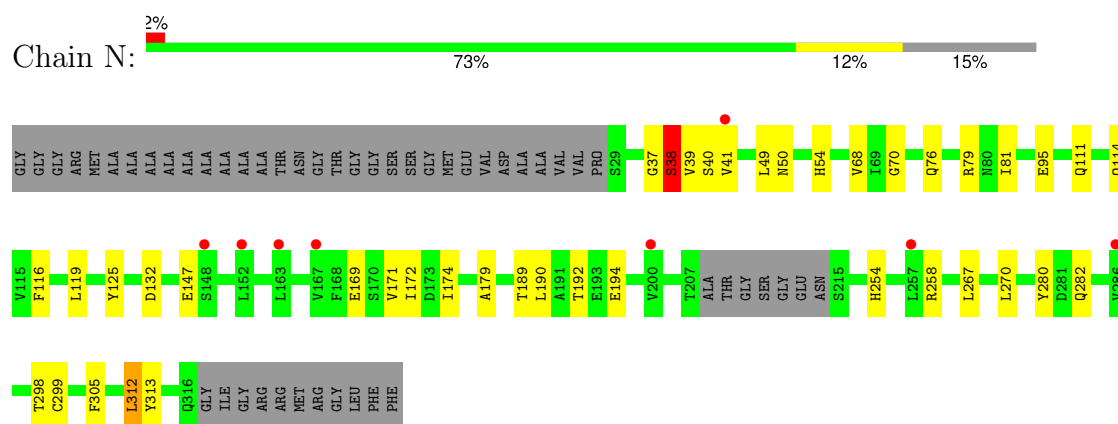


• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

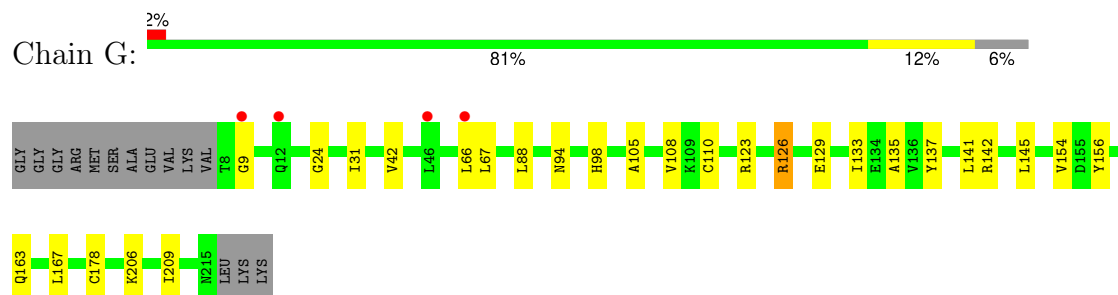
Chain F: 74% 10% 15%



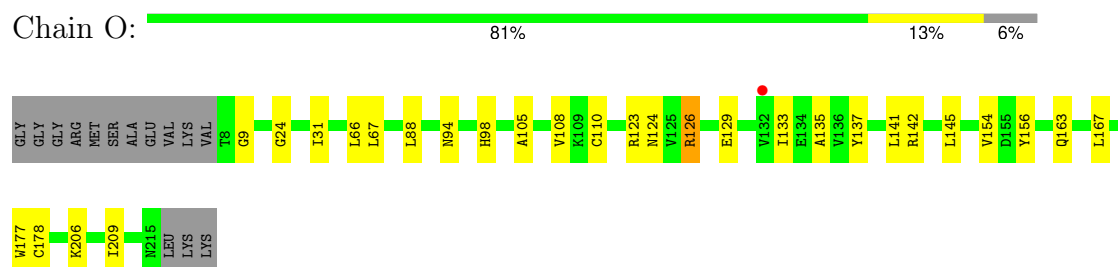
• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6



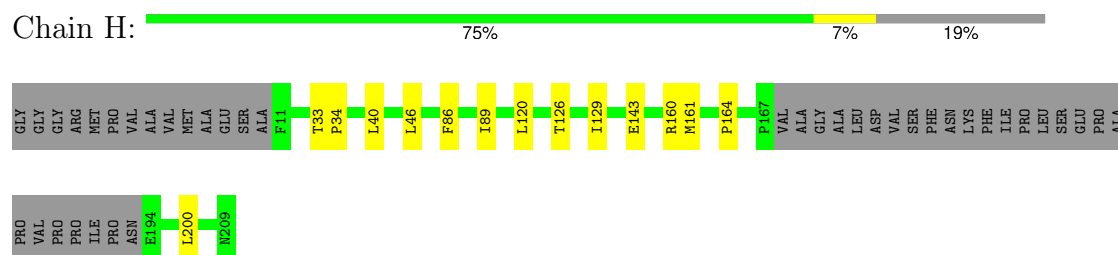
- Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



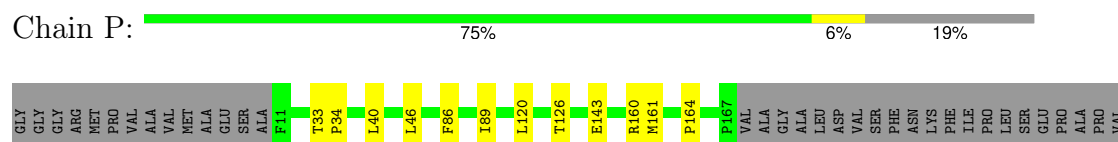
- Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



- Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



- Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



PRO	
PRO	
ILE	
PRO	
ASN	
E194	
L200	
N209	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	147.68Å 147.68Å 317.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.98 – 4.08 52.98 – 4.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.98-4.08) 99.9 (52.98-4.08)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.236 , 0.253 0.264 , 0.280	Depositor DCC
R_{free} test set	3085 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	175.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 194.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l 0.115 for h,-h-k,-l 0.067 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	41422	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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	A	0.67	1/3404 (0.0%)	1.12	2/4588 (0.0%)
1	I	0.64	0/3404	1.13	0/4588
2	B	0.71	0/3361	1.13	2/4522 (0.0%)
2	J	0.71	0/3361	1.14	3/4522 (0.1%)
3	C	0.94	19/3250 (0.6%)	1.35	46/4390 (1.0%)
3	K	0.94	19/3250 (0.6%)	1.35	45/4390 (1.0%)
4	D	0.70	0/3303	1.12	1/4460 (0.0%)
4	L	0.69	1/3303 (0.0%)	1.19	5/4460 (0.1%)
5	E	0.67	0/2417	1.07	0/3266
5	M	0.69	0/2417	1.06	0/3266
6	F	1.07	1/2282 (0.0%)	1.15	7/3092 (0.2%)
6	N	0.65	0/2281	1.12	5/3089 (0.2%)
7	G	0.65	0/1652	1.13	0/2239
7	O	0.65	0/1652	1.13	0/2239
8	H	0.67	0/1416	1.11	1/1924 (0.1%)
8	P	0.67	0/1416	1.10	1/1924 (0.1%)
All	All	0.75	41/42169 (0.1%)	1.16	118/56959 (0.2%)

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
3	C	0	6
3	K	0	6
All	All	0	12

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	40	SER	C-N	41.13	1.94	1.33
3	K	301	SER	C-O	-9.23	1.12	1.24
3	C	301	SER	C-O	-9.21	1.12	1.24
3	C	297	GLN	C-O	-8.73	1.13	1.24
3	K	297	GLN	C-O	-8.70	1.13	1.24

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	304	LYS	CA-C-O	-10.93	108.97	120.55
3	C	304	LYS	CA-C-O	-10.92	108.98	120.55
3	C	300	SER	CA-C-O	-10.46	109.47	120.55
3	K	300	SER	CA-C-O	-10.32	109.48	120.42
6	F	40	SER	O-C-N	-10.00	111.15	123.05

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	295	VAL	Mainchain
3	C	296	LYS	Mainchain
3	C	300	SER	Mainchain
3	C	304	LYS	Mainchain
3	C	308	GLN	Mainchain

5.2 Too-close contacts [i](#)

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	23	0
1	I	3348	0	3385	27	0
2	B	3304	0	3351	27	0
2	J	3304	0	3351	37	0
3	C	3191	0	3208	29	0
3	K	3191	0	3208	25	0
4	D	3251	0	3253	31	0
4	L	3251	0	3253	41	0
5	E	2366	0	2340	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	2366	0	2340	32	0
6	F	2236	0	2226	30	0
6	N	2236	0	2226	34	0
7	G	1631	0	1654	19	0
7	O	1631	0	1654	25	0
8	H	1383	0	1366	8	0
8	P	1383	0	1366	6	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
All	All	41422	0	41566	317	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 4.

The worst 5 of 317 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:F:40:SER:C	6:F:41:VAL:N	1.94	1.25
1:A:200:GLY:O	1:A:204:LEU:HD13	1.63	0.98
1:I:200:GLY:O	1:I:204:LEU:HD13	1.64	0.98
5:M:70:ARG:NH2	5:M:257:THR:HG22	1.78	0.97
3:K:41:HIS:O	3:K:44:THR:HG22	1.63	0.96

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%)	395 (95%)	16 (4%)	4 (1%)	12	46
1	I	415/480 (86%)	395 (95%)	17 (4%)	3 (1%)	18	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	4	29
2	J	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	4	29
3	C	399/427 (93%)	360 (90%)	26 (6%)	13 (3%)	3	24
3	K	399/427 (93%)	360 (90%)	25 (6%)	14 (4%)	3	23
4	D	404/410 (98%)	399 (99%)	2 (0%)	3 (1%)	18	55
4	L	404/410 (98%)	400 (99%)	1 (0%)	3 (1%)	18	55
5	E	294/327 (90%)	283 (96%)	8 (3%)	3 (1%)	12	46
5	M	294/327 (90%)	283 (96%)	9 (3%)	2 (1%)	18	55
6	F	277/331 (84%)	267 (96%)	8 (3%)	2 (1%)	18	55
6	N	275/331 (83%)	264 (96%)	8 (3%)	3 (1%)	11	44
7	G	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	8	39
7	O	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	8	39
8	H	169/213 (79%)	162 (96%)	7 (4%)	0	100	100
8	P	169/213 (79%)	162 (96%)	7 (4%)	0	100	100
All	All	5124/5714 (90%)	4850 (95%)	198 (4%)	76 (2%)	8	39

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	51	VAL
3	C	68	MET
3	C	153	LYS
4	D	294	ALA
5	E	297	GLU

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%)	360 (99%)	5 (1%)	59	71
1	I	365/415 (88%)	360 (99%)	5 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/406 (90%)	358 (98%)	9 (2%)	42	62
2	J	367/406 (90%)	357 (97%)	10 (3%)	39	60
3	C	358/378 (95%)	346 (97%)	12 (3%)	32	55
3	K	358/378 (95%)	347 (97%)	11 (3%)	35	57
4	D	347/348 (100%)	329 (95%)	18 (5%)	21	45
4	L	347/348 (100%)	337 (97%)	10 (3%)	37	58
5	E	255/278 (92%)	247 (97%)	8 (3%)	35	57
5	M	255/278 (92%)	248 (97%)	7 (3%)	39	60
6	F	251/277 (91%)	246 (98%)	5 (2%)	48	66
6	N	251/277 (91%)	248 (99%)	3 (1%)	63	73
7	G	174/184 (95%)	168 (97%)	6 (3%)	32	55
7	O	174/184 (95%)	168 (97%)	6 (3%)	32	55
8	H	144/174 (83%)	139 (96%)	5 (4%)	32	54
8	P	144/174 (83%)	139 (96%)	5 (4%)	32	54
All	All	4522/4920 (92%)	4397 (97%)	125 (3%)	38	59

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	108	VAL
5	M	279	GLN
1	I	404	GLN
5	M	268	ASP
7	O	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
3	K	116	GLN
5	M	132	ASN
3	K	147	GLN
3	K	375	ASN
6	N	76	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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
6	N	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	40:SER	C	41:VAL	N	2.59

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	40:SER	C	41:VAL	N	1.94

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	A	419/480 (87%)	-0.00	4 (0%) 79 62	152, 242, 277, 283	0
1	I	419/480 (87%)	0.03	5 (1%) 76 59	140, 208, 264, 271	0
2	B	403/447 (90%)	0.05	5 (1%) 76 59	147, 264, 281, 288	0
2	J	403/447 (90%)	0.03	6 (1%) 72 54	134, 243, 264, 276	0
3	C	401/427 (93%)	0.09	2 (0%) 87 74	149, 205, 267, 276	0
3	K	401/427 (93%)	0.18	8 (1%) 65 48	121, 179, 260, 268	0
4	D	406/410 (99%)	0.04	2 (0%) 87 74	139, 227, 276, 281	0
4	L	406/410 (99%)	0.04	2 (0%) 87 74	162, 249, 287, 292	0
5	E	298/327 (91%)	0.02	4 (1%) 75 57	132, 172, 222, 242	0
5	M	298/327 (91%)	0.08	4 (1%) 75 57	148, 206, 242, 258	0
6	F	281/331 (84%)	0.15	1 (0%) 88 76	132, 181, 230, 244	0
6	N	281/331 (84%)	0.13	8 (2%) 55 41	132, 213, 247, 259	0
7	G	208/222 (93%)	0.08	4 (1%) 66 49	152, 211, 255, 264	0
7	O	208/222 (93%)	-0.05	1 (0%) 87 74	175, 226, 268, 272	0
8	H	173/213 (81%)	-0.07	0 100 100	165, 200, 231, 241	0
8	P	173/213 (81%)	-0.10	0 100 100	160, 193, 228, 239	0
All	All	5178/5714 (90%)	0.05	56 (1%) 78 60	121, 212, 275, 292	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	54	HIS	9.5
1	I	309	ALA	4.9
2	B	204	MET	4.1
2	J	172	LEU	3.6
1	A	331	LEU	3.6

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
9	ZN	M	999	1/1	0.98	0.06	173,173,173,173	0
9	ZN	E	999	1/1	0.99	0.04	138,138,138,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.