



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:45 PM GMT

PDB ID : 4D18
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

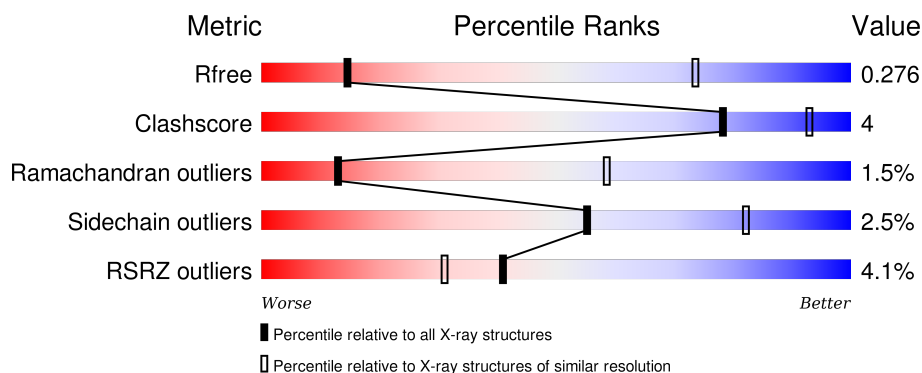
1 Overall quality at a glance ⓘ

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}	91344	1009 (4.52-3.60)
Clashscore	102246	1107 (4.52-3.60)
Ramachandran outliers	100387	1053 (4.52-3.60)
Sidechain outliers	100360	1039 (4.52-3.60)
RSRZ outliers	91569	1012 (4.52-3.60)

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 ≥ 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>80% 7% 13%</div> </div>
1	I	480	<div> <div>3%</div> <div>80% 7% 13%</div> </div>
2	B	447	<div> <div>7%</div> <div>79% 10% 10%</div> </div>
2	J	447	<div> <div>4%</div> <div>79% 11% 10%</div> </div>
3	C	427	<div> <div>4%</div> <div>81% 12% 6%</div> </div>

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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

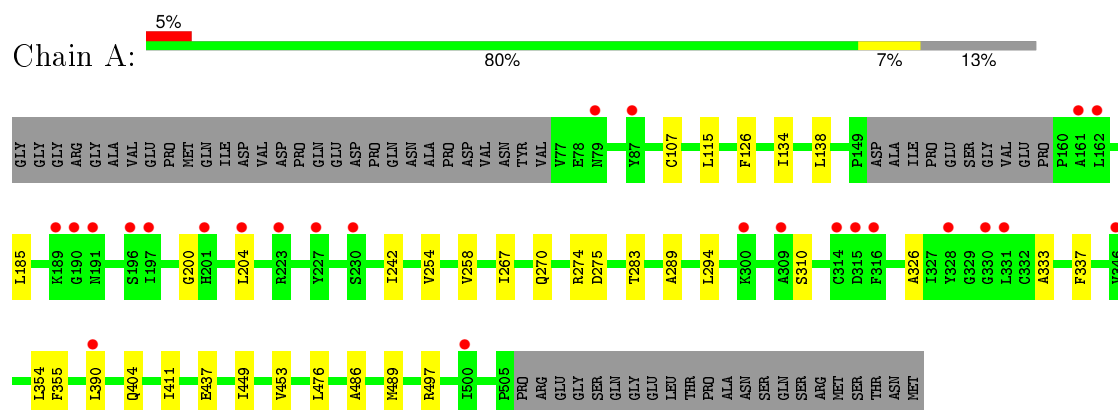
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

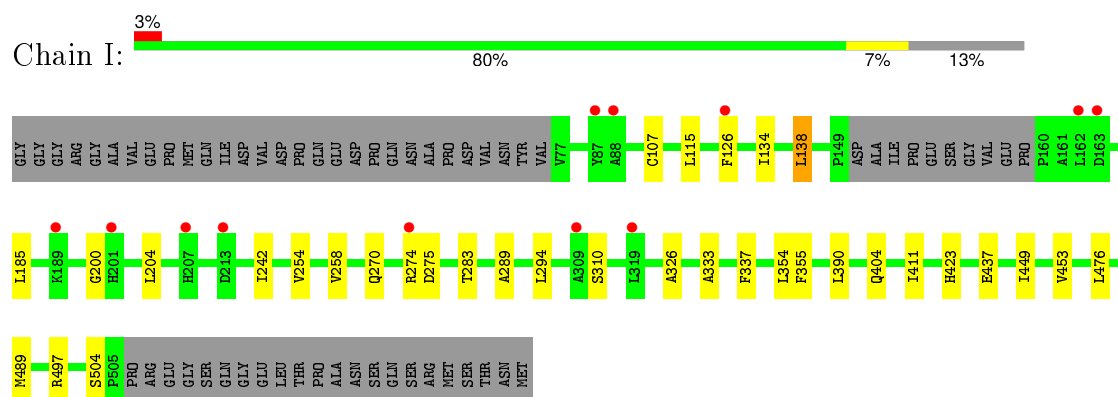
3 Residue-property plots

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 ($RSRZ > 2$). 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.

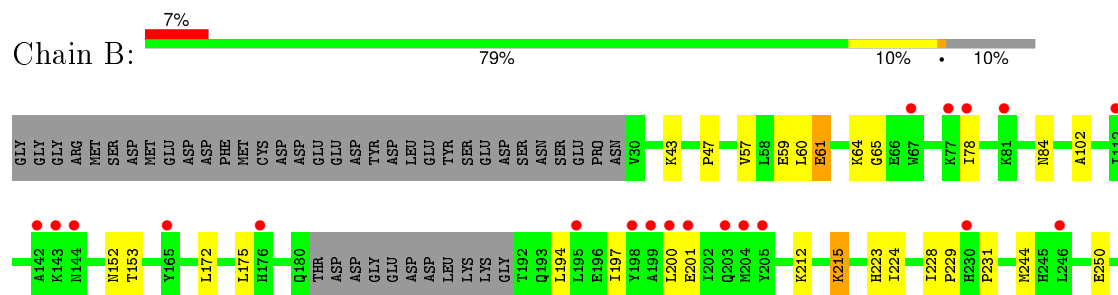
• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

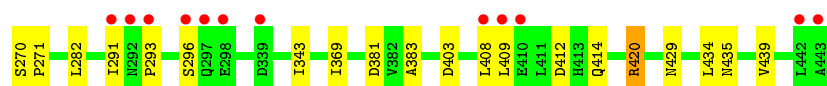


• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

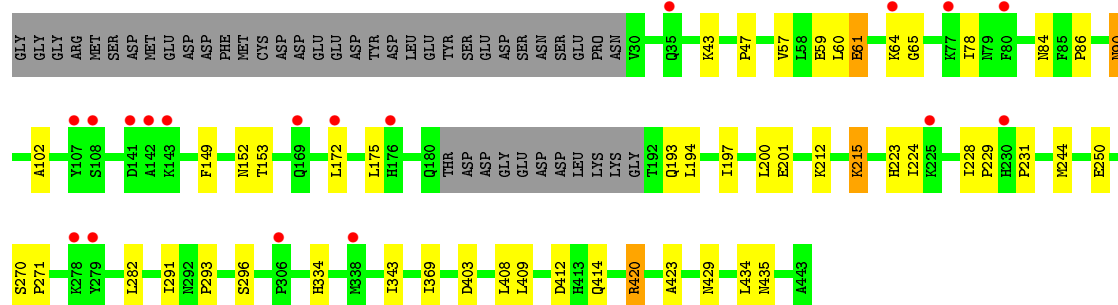
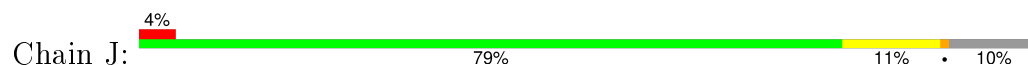


• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

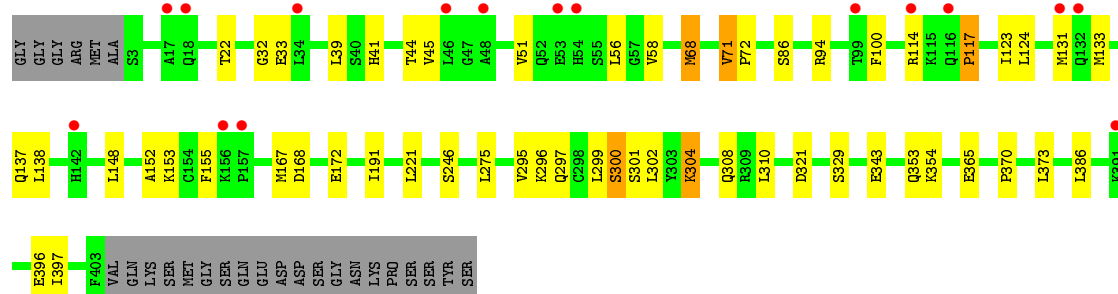
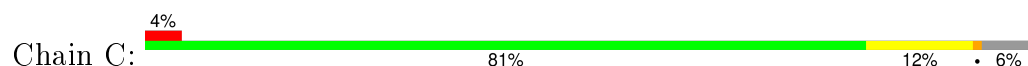




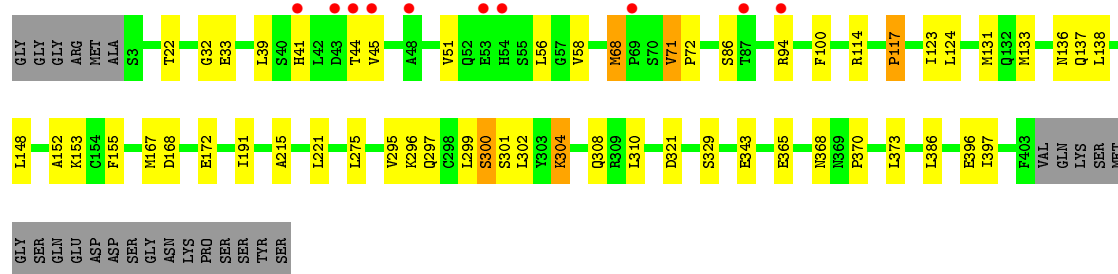
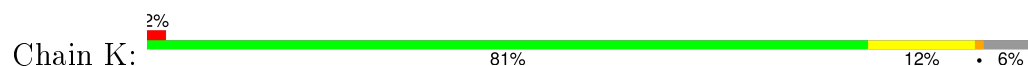
• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2



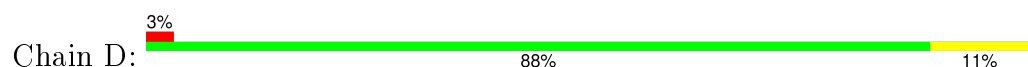
• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3



• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

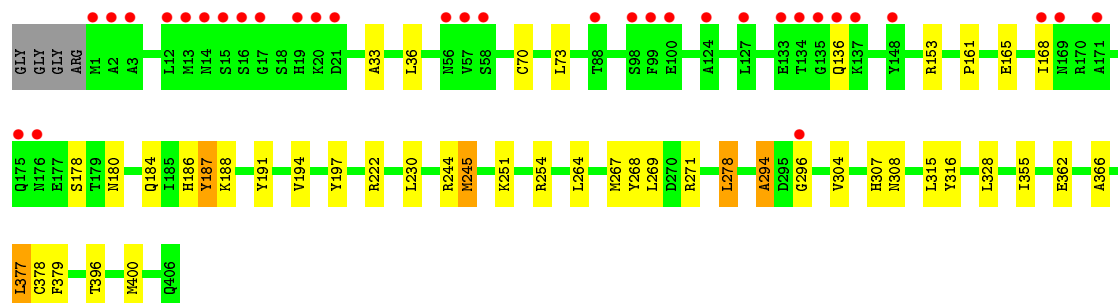
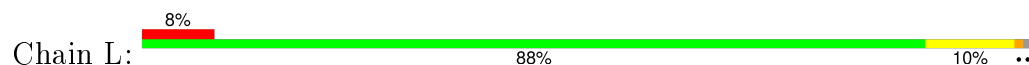


• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

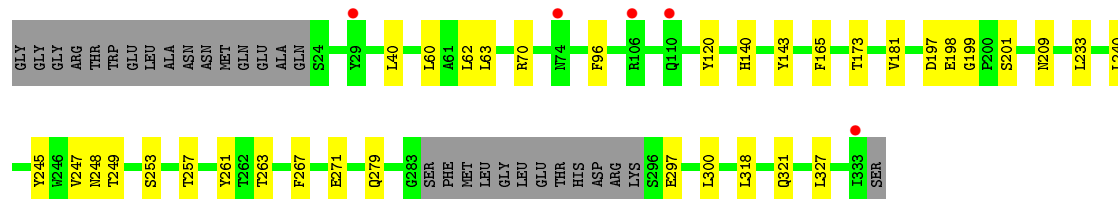




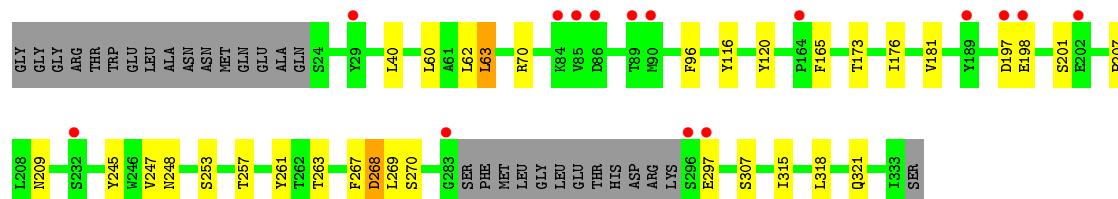
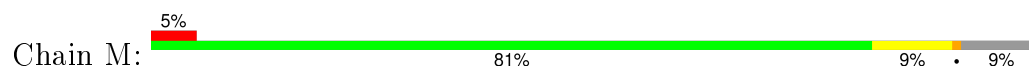
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4



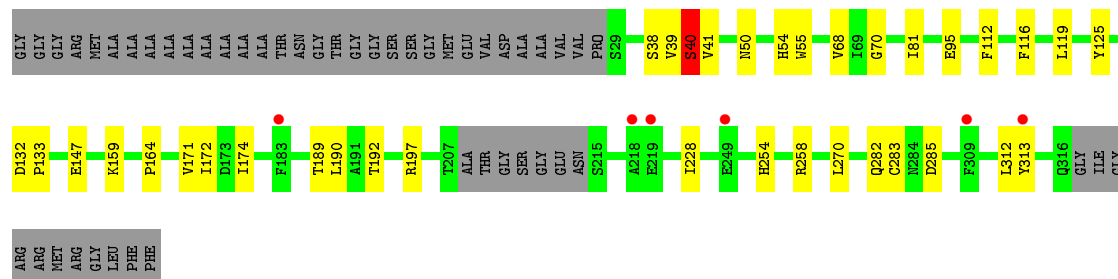
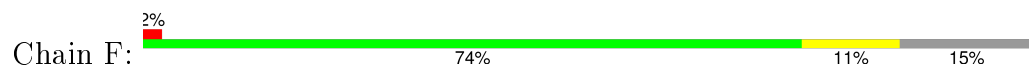
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

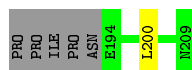


• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5



• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6





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) 100.0 (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 0.260 , 0.276	Depositor DCC
R_{free} test set	3087 reflections (5.01%)	DCC
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 , 196.2	EDS
Estimated twinning fraction	0.059 for -h,-k,l 0.115 for h,-h-k,-l 0.067 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 61643 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/3404	0.48	0/4588
1	I	0.37	0/3404	0.48	0/4588
2	B	0.42	0/3361	0.51	0/4522
2	J	0.42	0/3361	0.51	0/4522
3	C	0.55	2/3250 (0.1%)	0.64	3/4390 (0.1%)
3	K	0.56	2/3250 (0.1%)	0.64	3/4390 (0.1%)
4	D	0.41	0/3303	0.52	0/4460
4	L	0.39	0/3303	0.53	0/4460
5	E	0.40	0/2417	0.54	0/3266
5	M	0.42	0/2417	0.54	0/3266
6	F	0.66	1/2282 (0.0%)	0.57	1/3092 (0.0%)
6	N	0.38	0/2281	0.57	2/3089 (0.1%)
7	G	0.37	0/1652	0.48	0/2239
7	O	0.38	0/1652	0.48	0/2239
8	H	0.39	0/1416	0.49	0/1924
8	P	0.39	0/1416	0.48	0/1924
All	All	0.44	5/42169 (0.0%)	0.54	9/56959 (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
3	C	0	6
3	K	0	6
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	40	SER	C-N	26.22	1.94	1.34
3	K	301	SER	C-O	-5.74	1.12	1.23
3	C	301	SER	C-O	-5.72	1.12	1.23
3	C	297	GLN	C-O	-5.40	1.13	1.23
3	K	297	GLN	C-O	-5.38	1.13	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	40	SER	O-C-N	-7.22	111.15	122.70
3	K	304	LYS	CA-C-O	-5.30	108.97	120.10
3	C	304	LYS	CA-C-O	-5.30	108.98	120.10
3	K	301	SER	CA-C-O	-5.29	109.00	120.10
3	C	301	SER	CA-C-O	-5.26	109.05	120.10

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	22	0
1	I	3348	0	3385	26	0
2	B	3304	0	3351	25	0
2	J	3304	0	3351	35	0
3	C	3191	0	3208	26	0
3	K	3191	0	3208	21	0
4	D	3251	0	3253	31	0
4	L	3251	0	3253	39	0
5	E	2366	0	2340	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	2366	0	2340	31	0
6	F	2236	0	2226	29	0
6	N	2236	0	2226	33	0
7	G	1631	0	1654	18	0
7	O	1631	0	1654	24	0
8	H	1383	0	1366	7	0
8	P	1383	0	1366	5	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
All	All	41422	0	41566	297	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 297 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	1.21
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%)	19 65
1	I	415/480 (86%)	395 (95%)	17 (4%)	3 (1%)	26 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	7	48
2	J	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	7	48
3	C	399/427 (93%)	360 (90%)	26 (6%)	13 (3%)	5	43
3	K	399/427 (93%)	360 (90%)	25 (6%)	14 (4%)	4	42
4	D	404/410 (98%)	399 (99%)	2 (0%)	3 (1%)	26	71
4	L	404/410 (98%)	400 (99%)	1 (0%)	3 (1%)	26	71
5	E	294/327 (90%)	283 (96%)	8 (3%)	3 (1%)	19	65
5	M	294/327 (90%)	283 (96%)	9 (3%)	2 (1%)	26	71
6	F	277/331 (84%)	267 (96%)	8 (3%)	2 (1%)	26	71
6	N	275/331 (83%)	264 (96%)	8 (3%)	3 (1%)	17	64
7	G	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	13	58
7	O	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	13	58
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%)	13	58

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%)	362 (99%)	3 (1%)	86	93
1	I	365/415 (88%)	360 (99%)	5 (1%)	74	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/406 (90%)	359 (98%)	8 (2%)	60	84
2	J	367/406 (90%)	358 (98%)	9 (2%)	55	82
3	C	358/378 (95%)	347 (97%)	11 (3%)	47	78
3	K	358/378 (95%)	348 (97%)	10 (3%)	51	80
4	D	347/348 (100%)	334 (96%)	13 (4%)	41	75
4	L	347/348 (100%)	342 (99%)	5 (1%)	74	89
5	E	255/278 (92%)	246 (96%)	9 (4%)	43	77
5	M	255/278 (92%)	247 (97%)	8 (3%)	47	78
6	F	251/277 (91%)	245 (98%)	6 (2%)	57	83
6	N	251/277 (91%)	247 (98%)	4 (2%)	70	88
7	G	174/184 (95%)	168 (97%)	6 (3%)	44	77
7	O	174/184 (95%)	168 (97%)	6 (3%)	44	77
8	H	144/174 (83%)	138 (96%)	6 (4%)	36	72
8	P	144/174 (83%)	138 (96%)	6 (4%)	36	72
All	All	4522/4920 (92%)	4407 (98%)	115 (2%)	55	82

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	126	ARG
1	I	404	GLN
7	O	161	ASP
7	G	161	ASP
8	H	46	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	76	GLN
1	I	313	HIS
6	N	76	GLN
7	G	202	GLN
1	I	324	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 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](#)

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	A	419/480 (87%)	0.24	25 (5%)	25	17	152, 242, 277, 283	0
1	I	419/480 (87%)	0.10	12 (2%)	55	43	140, 208, 264, 271	0
2	B	403/447 (90%)	0.26	32 (7%)	15	11	147, 264, 281, 288	0
2	J	403/447 (90%)	0.22	18 (4%)	37	28	134, 243, 264, 276	0
3	C	401/427 (93%)	0.13	16 (3%)	42	32	149, 205, 267, 276	0
3	K	401/427 (93%)	0.12	10 (2%)	61	49	121, 179, 260, 268	0
4	D	406/410 (99%)	0.25	14 (3%)	49	38	139, 227, 276, 281	0
4	L	406/410 (99%)	0.36	33 (8%)	15	11	162, 249, 287, 292	0
5	E	298/327 (91%)	0.04	5 (1%)	73	63	132, 172, 222, 242	0
5	M	298/327 (91%)	0.16	15 (5%)	32	24	148, 206, 242, 258	0
6	F	281/331 (84%)	0.07	6 (2%)	67	56	132, 181, 230, 244	0
6	N	281/331 (84%)	0.08	10 (3%)	46	36	132, 213, 247, 259	0
7	G	208/222 (93%)	0.01	4 (1%)	70	60	152, 211, 255, 264	0
7	O	208/222 (93%)	0.04	6 (2%)	55	43	175, 226, 268, 272	0
8	H	173/213 (81%)	0.02	4 (2%)	64	53	165, 200, 231, 241	0
8	P	173/213 (81%)	-0.04	2 (1%)	81	73	160, 193, 228, 239	0
All	All	5178/5714 (90%)	0.15	212 (4%)	41	31	121, 212, 275, 292	0

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	8	THR	12.6
2	B	142	ALA	9.1
5	M	85	VAL	7.7
2	B	204	MET	6.8
4	L	2	ALA	6.8

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
9	ZN	M	999	1/1	0.98	0.13	-1.76	173,173,173,173	0
9	ZN	E	999	1/1	0.99	0.14	-1.84	138,138,138,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.