wwPDB X-ray Structure Validation Summary Report (i)

Apr 30, 2024 – 06:53 pm BST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

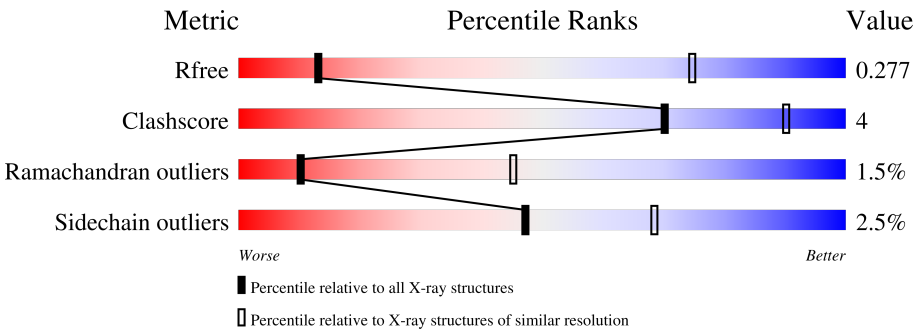
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1133 (4.46-3.70)
Clashscore	141614	1013 (4.42-3.74)
Ramachandran outliers	138981	1151 (4.46-3.70)
Sidechain outliers	138945	1139 (4.46-3.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	480	80% 7% 13%
1	I	480	80% 7% 13%
2	B	447	79% 10% • 10%
2	J	447	79% 11% • 10%
3	C	427	81% 12% • 6%
3	K	427	81% 12% • 6%
4	D	410	88% 11% •

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Mol	Chain	Length	Quality of chain
4	L	410	88% 10% ••
5	E	327	80% 11% 9%
5	M	327	81% 9% • 9%
6	F	331	74% 11% 15%
6	N	331	73% 12% 15%
7	G	222	82% 12% 6%
7	O	222	81% 12% 6%
8	H	213	75% 6% 19%
8	P	213	76% 6% 19%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	419	3348	2113	588	625	22	0	0	0
1	I	419	3348	2113	588	625	22	0	0	0

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
			Total	C	N	O	S			
2	B	403	3304	2102	566	621	15	0	0	0
2	J	403	3304	2102	566	621	15	0	0	0

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
			Total	C	N	O	S			
3	C	401	3191	2032	535	598	26	0	0	0
3	K	401	3191	2032	535	598	26	0	0	0

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
			Total	C	N	O	S			
4	D	406	3251	2047	566	622	16	0	0	0
4	L	406	3251	2047	566	622	16	0	0	0

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
			Total	C	N	O	S			
5	E	298	2366	1510	393	450	13	0	0	0
5	M	298	2366	1510	393	450	13	0	0	0

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
			Total	C	N	O	S			
6	F	281	2236	1429	371	421	15	0	0	0
6	N	281	2236	1429	371	421	15	0	0	0

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
			Total	C	N	O	S			
7	G	208	1631	1028	287	312	4	0	0	0
7	O	208	1631	1028	287	312	4	0	0	0

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
			Total	C	N	O	S			
8	H	173	1383	885	240	254	4	0	0	0
8	P	173	1383	885	240	254	4	0	0	0

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).

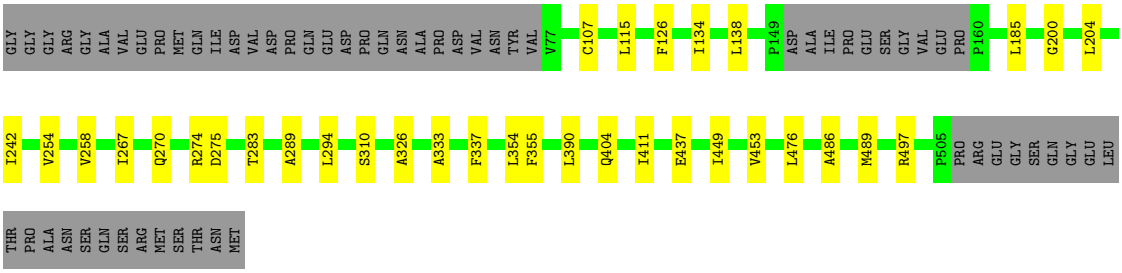
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
9	E	1	1	1	0	0
			Total	Zn		
9	M	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

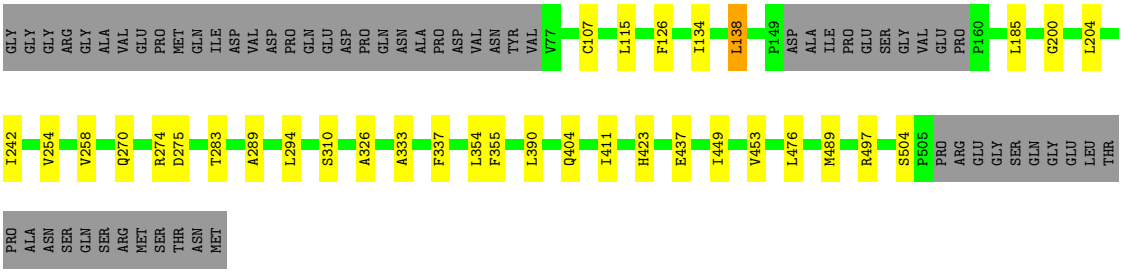
• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain A:



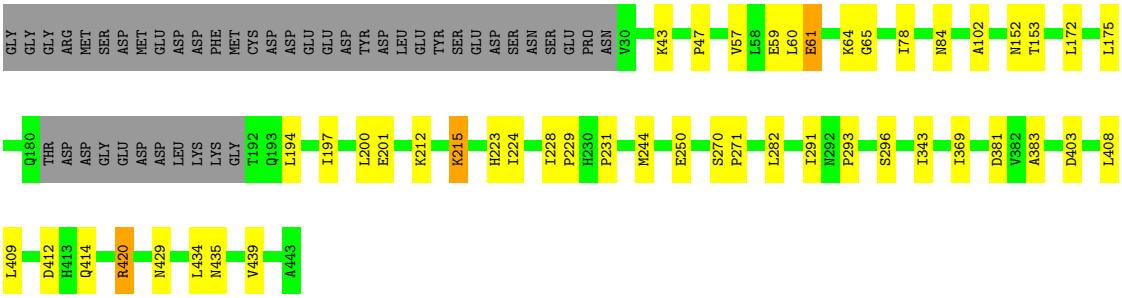
• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain I:



• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

Chain B:



• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

Chain J: 79% 11% • 10%

GLY GLY GLY ARG MET SER ASP MET GLU ASP ASP PHE MET CYS ASP ASP GLU GLU ASP TYR ASP LEU GLU TYR SER GLU ASP SER ASN SER GLU PRO ASN V30 K43 P47 V57 L58 E59 L60 E61 K64 G65 I78 N84 F85 P86 N90 A102 F149

N152 T153 L172 L175 Q180 THR ASP ASP GLY GLU ASP ASP LEU LYS LYS GLY T192 Q193 L194 I197 L200 E201 K212 K215 H223 I224 I228 P229 H230 P231 M244 E250 S270 P271 L282 I291 N292 P293 S296 H334 I343 I369

D403 L408 L409 D412 H413 Q414 R420 A423 N429 L434 N435 A443

• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain C: 81% 12% • 6%

GLY GLY GLY ARG MET ALA S3 T22 G32 E33 L39 S40 H41 T44 V45 V51 L56 G57 V58 M68 V71 P72 S86 R94 F100 R114 P117 I123 L124 M131 Q132 M133 Q137 L138 L148 A152 K153 C154 F155 M167 D168

E172 I191 L221 S246 L275 V295 K296 Q297 C298 L299 S300 S301 L302 Y303 K304 Q308 R309 L310 D321 S329 E343 Q353 K354 E365 P370 L373 L386 E396 I397 F403 VAL GLN LYS SER MET GLY SER GLN GLU ASP ASP SER GLY

ASN LYS PRO SER SER TYR SER

• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain K: 81% 12% • 6%

GLY GLY GLY ARG MET ALA S3 T22 G32 E33 L39 S40 H41 T44 V45 V51 L56 G57 V58 M68 V71 P72 S86 R94 F100 R114 P117 I123 L124 M131 Q132 M133 N136 Q137 L138 L148 A152 K153 C154 F155 M167

D168 E172 I191 A215 L221 L275 V295 K296 Q297 C298 L299 S300 S301 L302 Y303 K304 Q308 R309 L310 D321 S329 E343 E365 N368 N369 P370 L373 L386 E396 I397 F403 VAL GLN LYS SER MET GLY SER GLN GLU ASP ASP SER GLY

ASN LYS PRO SER SER TYR SER

• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

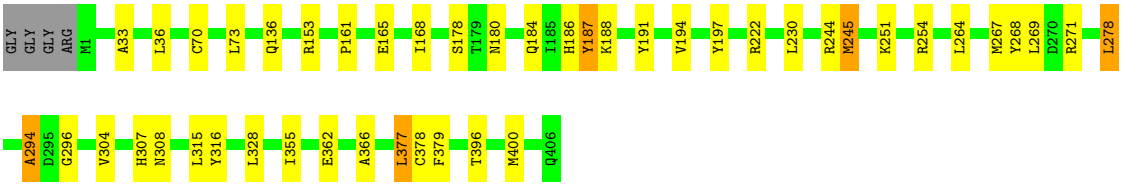
Chain D: 88% 11% •

GLY GLY GLY ARG M1 R6 E40 A47 V60 E83 H86 I97 Q136 L149 P161 E165 I168 Y187 R198 L223 L230 R244 M245 K251 R254 L264 M267 Y268 L269 D270 R271 L278 A294 D295 N308

L315 Y316 F321 E322 E323 L328 I352 I355 D356 G357 I358 E362 A366 L377 C378 F379 T396 M400 Q406

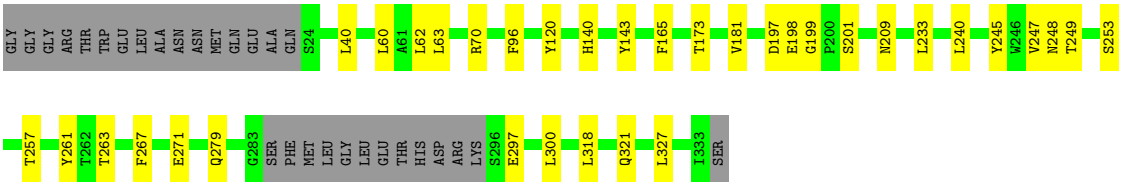
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

Chain L: 88% 10% ••



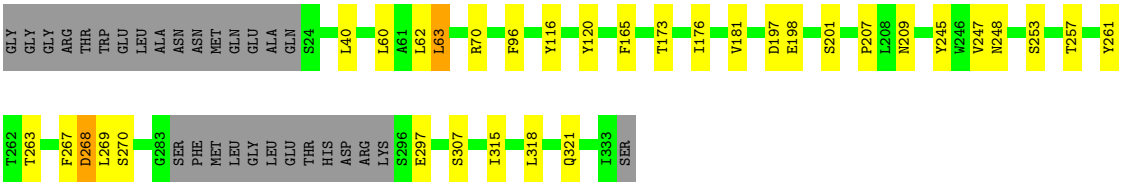
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain E:



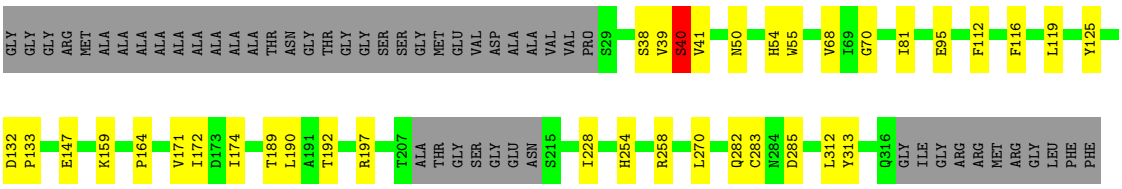
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain M:



• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

Chain F:

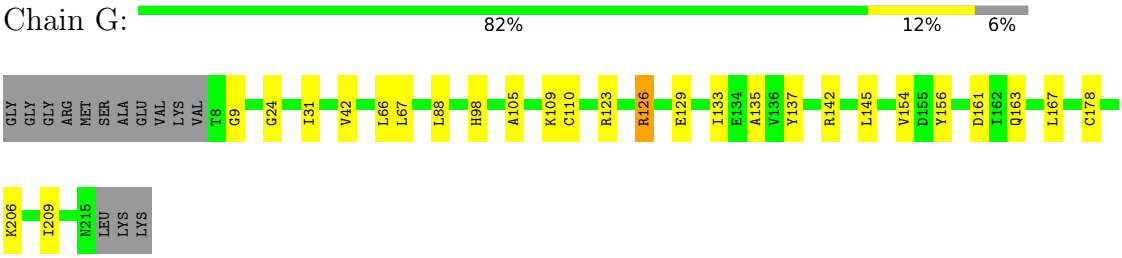


• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

Chain N:

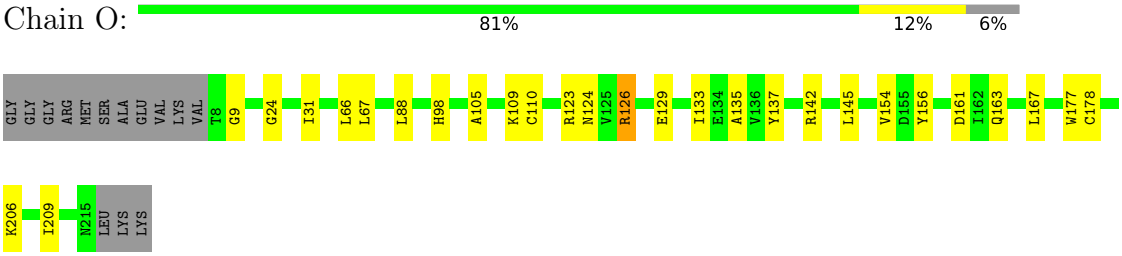
• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A

Chain G:



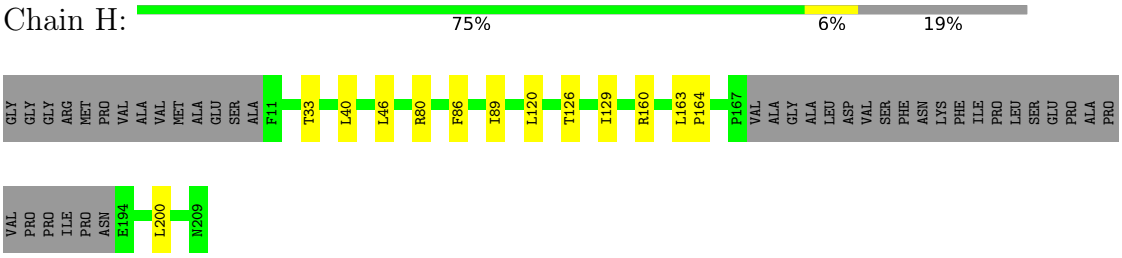
• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A

Chain O:



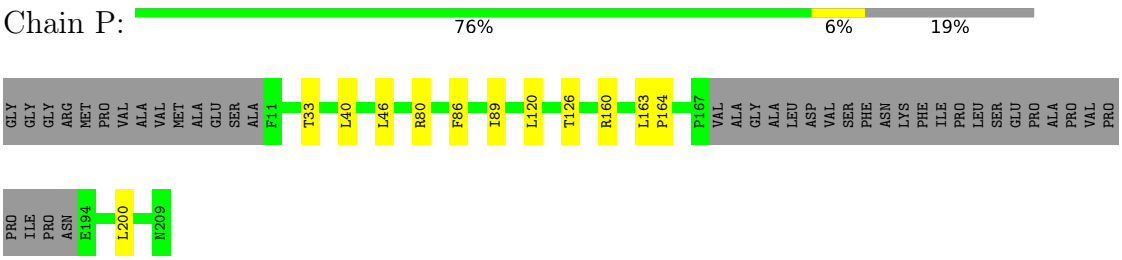
• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8

Chain H:



• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8

Chain P:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.30 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.236 , 0.253 0.263 , 0.277	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 , 196.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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(^{o})	Ideal(^{o})
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%)	15 52
1	I	415/480 (86%)	395 (95%)	17 (4%)	3 (1%)	22 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	5	35
2	J	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	5	35
3	C	399/427 (93%)	360 (90%)	26 (6%)	13 (3%)	4	30
3	K	399/427 (93%)	360 (90%)	25 (6%)	14 (4%)	3	29
4	D	404/410 (98%)	399 (99%)	2 (0%)	3 (1%)	22	61
4	L	404/410 (98%)	400 (99%)	1 (0%)	3 (1%)	22	61
5	E	294/327 (90%)	283 (96%)	8 (3%)	3 (1%)	15	52
5	M	294/327 (90%)	283 (96%)	9 (3%)	2 (1%)	22	61
6	F	277/331 (84%)	267 (96%)	8 (3%)	2 (1%)	22	61
6	N	275/331 (83%)	264 (96%)	8 (3%)	3 (1%)	14	51
7	G	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	10	45
7	O	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	10	45
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%)	10	45

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 (i)

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%)	81	89
1	I	365/415 (88%)	360 (99%)	5 (1%)	67	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/406 (90%)	359 (98%)	8 (2%)	52	71
2	J	367/406 (90%)	358 (98%)	9 (2%)	47	68
3	C	358/378 (95%)	347 (97%)	11 (3%)	40	63
3	K	358/378 (95%)	348 (97%)	10 (3%)	43	65
4	D	347/348 (100%)	334 (96%)	13 (4%)	34	60
4	L	347/348 (100%)	342 (99%)	5 (1%)	67	80
5	E	255/278 (92%)	246 (96%)	9 (4%)	36	61
5	M	255/278 (92%)	247 (97%)	8 (3%)	40	63
6	F	251/277 (91%)	245 (98%)	6 (2%)	49	69
6	N	251/277 (91%)	247 (98%)	4 (2%)	62	79
7	G	174/184 (95%)	168 (97%)	6 (3%)	37	61
7	O	174/184 (95%)	168 (97%)	6 (3%)	37	61
8	H	144/174 (83%)	138 (96%)	6 (4%)	30	56
8	P	144/174 (83%)	138 (96%)	6 (4%)	30	56
All	All	4522/4920 (92%)	4407 (98%)	115 (2%)	47	68

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

Mol	Chain	Res	Type
8	H	40	LEU
8	P	40	LEU
2	J	250	GLU
8	P	33	THR
6	N	38	SER

Sometimes 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	111	GLN
6	N	76	GLN
1	I	324	ASN
7	O	202	GLN
4	L	184	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.