



wwPDB X-ray Structure Validation Summary Report

Aug 15, 2014 – 10:41 AM EDT

PDB ID : 4D10
Title : Crystal structure of the COP9 signalosome
Authors : Bunker, R.D.; Lingaraju, G.M.; Thoma, N.H.
Deposited on : 2014-04-30
Resolution : 3.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

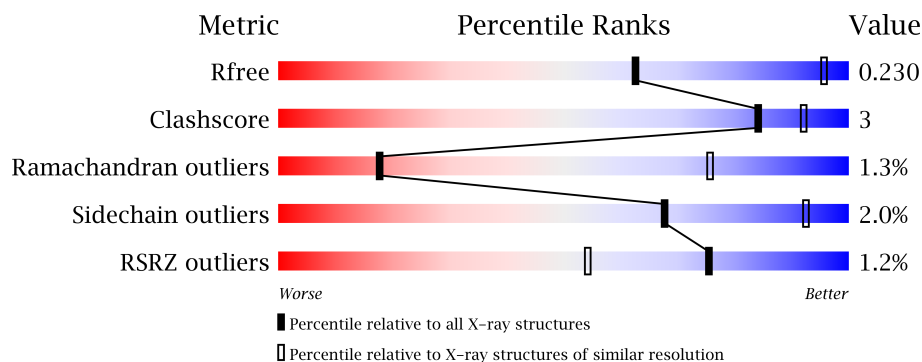
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	480	
1	I	480	
2	B	447	
2	J	447	
3	C	423	
3	K	423	
4	D	410	
4	L	410	
5	E	334	
5	M	334	
6	F	331	
6	N	331	
7	G	222	
7	O	222	

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Mol	Chain	Length	Quality of chain
8	H	212	
8	P	212	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 39976 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

- 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	225	Total	C	N	O	S	0	0	0
			1805	1137	319	337	12			

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
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			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	-2	GLY	-	EXPRESSION TAG	UNP Q99627
H	-1	GLY	-	EXPRESSION TAG	UNP Q99627
H	0	GLY	-	EXPRESSION TAG	UNP Q99627
H	1	ARG	-	EXPRESSION TAG	UNP Q99627
P	-2	GLY	-	EXPRESSION TAG	UNP Q99627
P	-1	GLY	-	EXPRESSION TAG	UNP Q99627
P	0	GLY	-	EXPRESSION TAG	UNP Q99627
P	1	ARG	-	EXPRESSION TAG	UNP Q99627

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

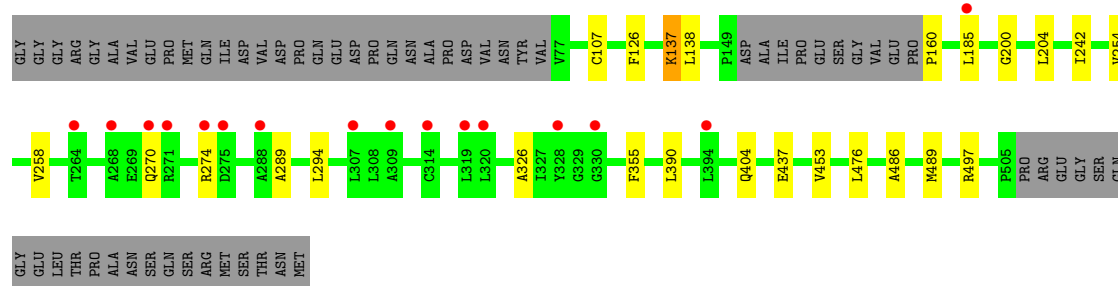
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Zn	0	0
			1	1		
9	E	1	Total	Zn	0	0
			1	1		

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.

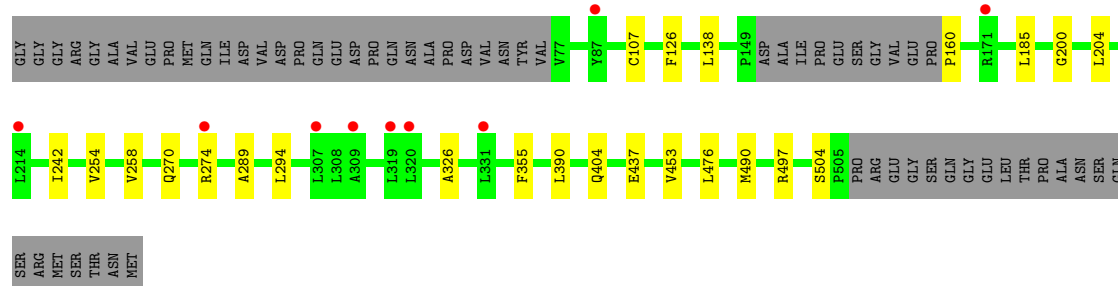
• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain A: 



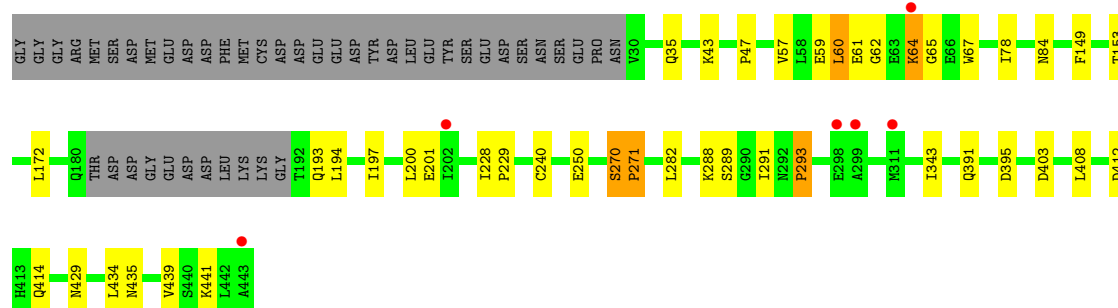
• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain I: 

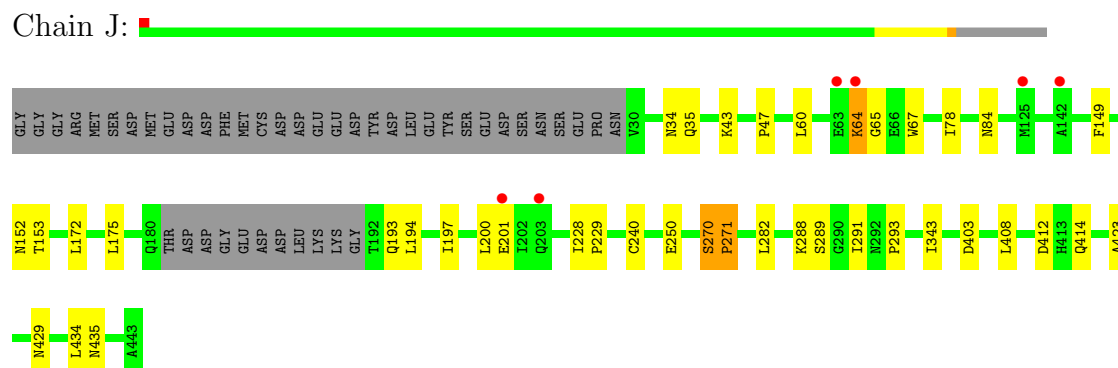


• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

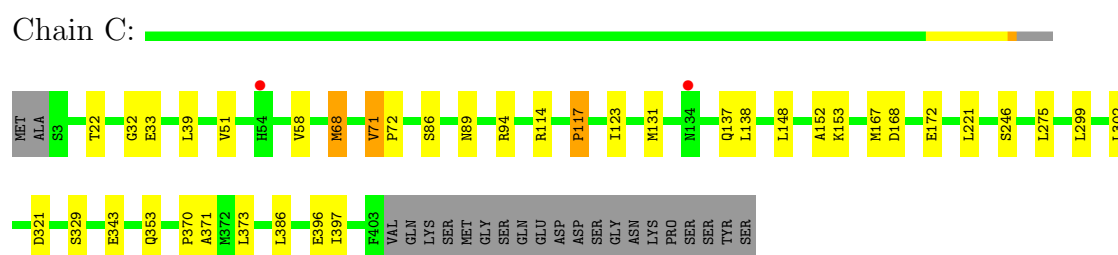
Chain B: 



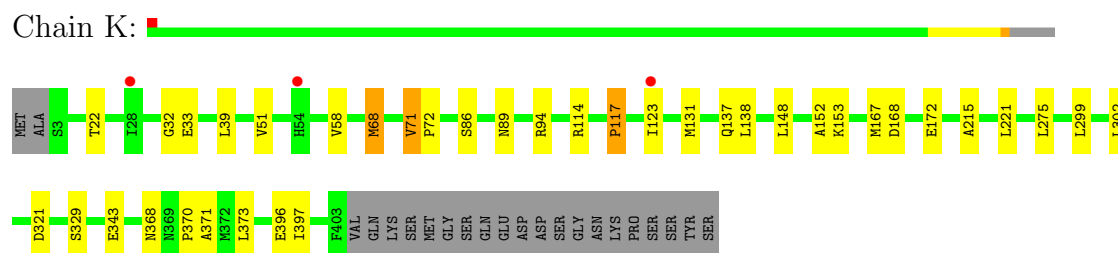
- Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2



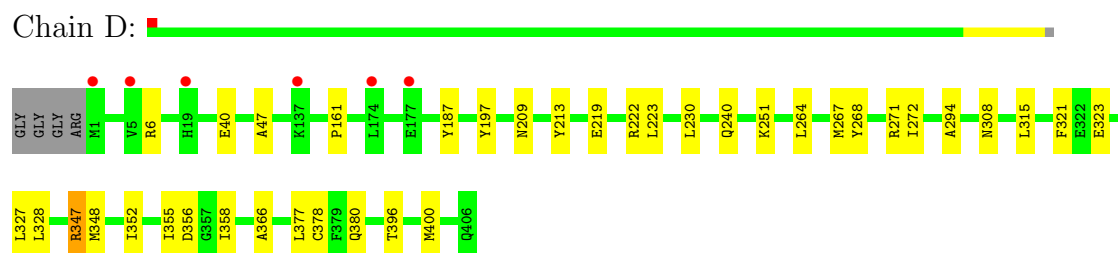
- Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3



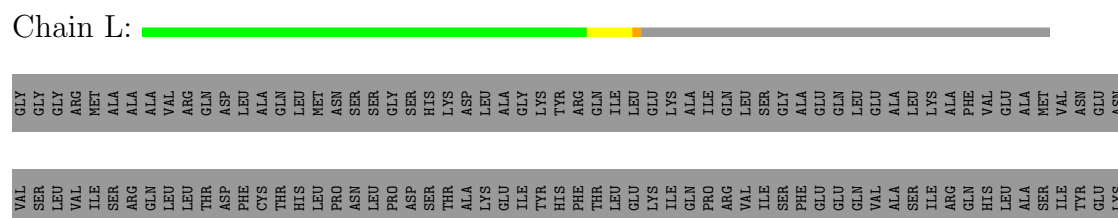
- Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3



- Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4



- Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4



GLU GLU ASP TRP ARG ASN ALA ALA GLN VAL LEU VAL GLY ILE PRO LEU GLU THR GLN GLN LYS GLN TYR ASN VAL ASP TYR LYS LEU GLU THR TYR LEU ILE ALA ARG LEU TYR LEU GLU ASP ASP PRO VAL GLN ALA GLU ALA TYR ILE ALA ARG ALA Q182 Y187 K188 E219 R222 L225 L230 K251 R254 L264 M267 T272 L273 R274 M286 Q289 H307 N308 L315 L327 L328 L355 A366 L377 C378 F379 Q380 T396 M400 Q405

• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain E:

MET ALA SER MET GLY SER MET MET ALA GLN THR TRP GLU LEU ALA ASN MET GLN ALA S24 L40 L60 L63 F96 Y116 Y120 E163 P164 F165 D197 E198 G199 P200 S201 L233 Y245 V246 N248 T249 F267 Q279 L280

Q283 SER PHE MET GLY GLU THR HIS ASP ARG LYS S296 L300 L315 L318 L327 L333 SER

• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain M:

MET ALA SER MET GLY MET ALA GLN THR TRP GLU LEU ALA ASN MET GLN ALA S24 L40 L60 L63 F96 Y116 Y120 M132 E163 P164 F165 I176 D197 E198 S201 P207 Y245 V246 N248 T249

F267 D268 L269 S270 K271 K272 Q279 Q283 SER PHE MET LEU GLY LEU GLU THR HIS ASP ARG LYS S296 D306 S307 L315 L318 L327 L333 SER

• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

Chain F:

GLY GLY ARG MET ALA ALA ALA ALA ALA ALA THR ASN GLY THR GLY GLY GLY SER GLY MET GLU VAL ASP ALA ALA VAL VAL PRO G37 S38 V39 S40 N50 H54 W55 V68 I69 G70 R79 N80 I81 E95 Q111 F112 F116 L119

Y125 D132 P133 E169 L190 A191 T192 R197 T207 ALA THR GLY SER GLY GLU ASN S215 L228 L257 L267 L270 Q282 Q283 N284 D285 R302 L312 Y313 Q316 GLY ILE GLY ARG ARG MET ARG GLY LEU PHE

• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

Chain N:

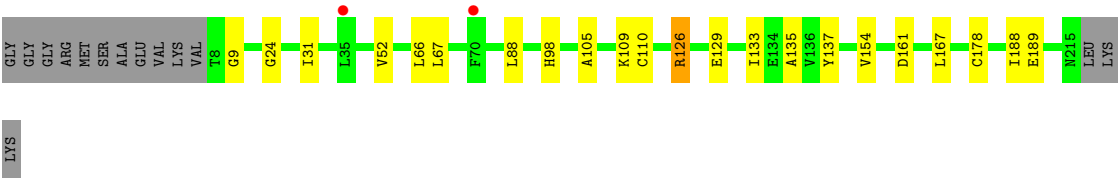
GLY GLY ARG MET ALA ALA ALA ALA ALA ALA THR ASN GLY THR GLY GLY GLY SER GLY GLY MET GLU VAL ASP ALA ALA VAL VAL PRO S29 T36 V39 L49 N50 H54 R57 Q61 V68 I69 G70 E95 Q111 F112 Y125 D132 P133

S148 I174 M181 L190 A191 T192 E193 E194 R197 T207 ALA THR GLY SER GLY GLU ASN S215 L228 L238 E255 T256 L257 R258 E259 L267 L270 Y280 D281 Q282 L288 C299 L312 Y313 Q316 GLY ILE GLY ARG ARG MET ARG GLY LEU

PHE PHE

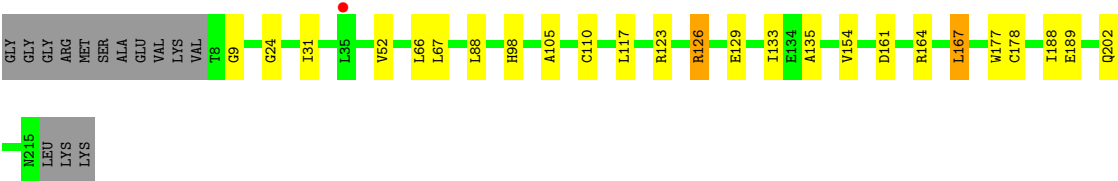
• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A

Chain G:



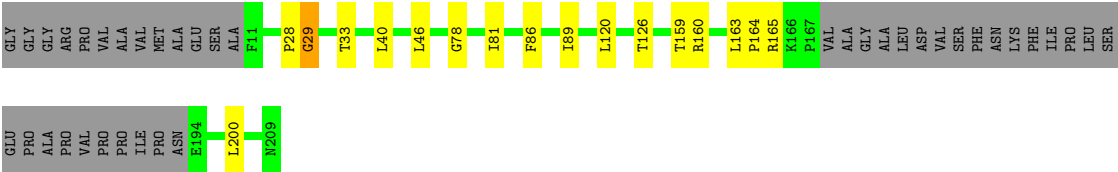
• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A

Chain O:



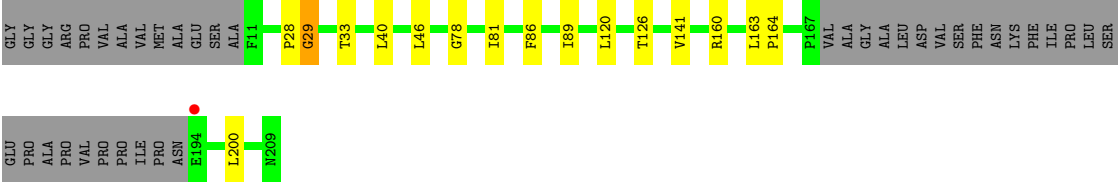
• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8

Chain H:



• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	151.62Å 151.62Å 343.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.87 – 3.80 50.87 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.87-3.80) 100.0 (50.87-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.199 , 0.228 0.208 , 0.230	Depositor DCC
R_{free} test set	1656 reflections (1.94%)	DCC
Wilson B-factor (Å ²)	156.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 110.4	EDS
Estimated twinning fraction	0.636 for H, K, L 0.364 for K, H, -L 0.096 for -h,-k,l 0.277 for h,-h-k,-l 0.097 for -k,-h,-l	Xtriage
Reported twinning fraction	0.636 for H, K, L 0.364 for K, H, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 86819 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39976	wwPDB-VP
Average B, all atoms (Å ²)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.54	1/3404 (0.0%)	0.53	1/4588 (0.0%)
1	I	0.43	0/3404	0.52	0/4588
2	B	0.43	0/3360	0.53	1/4519 (0.0%)
2	J	0.43	0/3361	0.53	1/4522 (0.0%)
3	C	0.43	0/3250	0.54	0/4390
3	K	0.42	0/3250	0.53	0/4390
4	D	0.55	2/3303 (0.1%)	0.56	0/4460
4	L	0.41	0/1834	0.55	0/2470
5	E	0.40	0/2417	0.54	0/3266
5	M	0.42	0/2417	0.55	0/3266
6	F	0.43	0/2282	0.56	0/3092
6	N	0.42	0/2282	0.54	0/3092
7	G	0.40	0/1652	0.51	0/2239
7	O	0.40	0/1652	0.52	0/2239
8	H	0.44	0/1416	0.58	1/1924 (0.1%)
8	P	0.44	0/1416	0.58	1/1924 (0.1%)
All	All	0.45	3/40700 (0.0%)	0.54	5/54969 (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
2	B	0	6
2	J	0	6
3	C	0	2
3	K	0	2
5	E	0	2
5	M	0	2
6	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	N	0	2
8	H	0	2
8	P	0	2
All	All	0	27

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	LYS	C-N	18.80	1.77	1.34
4	D	347	ARG	C-N	18.29	1.76	1.34
4	D	187	TYR	C-N	-7.67	1.16	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	29	GLY	N-CA-C	8.48	134.30	113.10
8	H	29	GLY	N-CA-C	8.42	134.16	113.10
2	J	289	SER	N-CA-CB	5.50	118.75	110.50
2	B	289	SER	N-CA-CB	5.46	118.69	110.50
1	A	137	LYS	O-C-N	-5.34	114.15	122.70

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	270	SER	Mainchain,Peptide
2	B	288	LYS	Mainchain,Peptide
2	B	64	LYS	Mainchain,Peptide
3	C	68	MET	Mainchain,Peptide
5	E	163	GLU	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3348	0	3384	18	0
1	I	3348	0	3385	16	0
2	B	3304	0	3350	20	0
2	J	3304	0	3351	15	0
3	C	3191	0	3208	16	0
3	K	3191	0	3208	16	0
4	D	3251	0	3251	25	0
4	L	1805	0	1812	22	0
5	E	2366	0	2340	22	0
5	M	2366	0	2340	27	0
6	F	2236	0	2227	29	0
6	N	2236	0	2227	24	0
7	G	1631	0	1654	12	0
7	O	1631	0	1654	16	0
8	H	1383	0	1366	7	0
8	P	1383	0	1366	7	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
All	All	39976	0	40123	233	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 233 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:347:ARG:C	4:D:348:MET:N	1.76	1.38
1:A:137:LYS:C	1:A:138:LEU:N	1.77	1.36
1:A:200:GLY:O	1:A:204:LEU:HD13	1.45	1.15
1:I:200:GLY:O	1:I:204:LEU:HD13	1.45	1.14
2:B:60:LEU:O	2:B:61:GLU:O	1.68	1.12

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	394 (95%)	18 (4%)	3 (1%)	30	84
1	I	415/480 (86%)	394 (95%)	18 (4%)	3 (1%)	30	84
2	B	397/447 (89%)	366 (92%)	23 (6%)	8 (2%)	11	68
2	J	399/447 (89%)	369 (92%)	23 (6%)	7 (2%)	13	70
3	C	399/423 (94%)	362 (91%)	24 (6%)	13 (3%)	6	57
3	K	399/423 (94%)	362 (91%)	24 (6%)	13 (3%)	6	57
4	D	404/410 (98%)	399 (99%)	3 (1%)	2 (0%)	38	88
4	L	223/410 (54%)	219 (98%)	3 (1%)	1 (0%)	43	90
5	E	294/334 (88%)	281 (96%)	10 (3%)	3 (1%)	22	80
5	M	294/334 (88%)	281 (96%)	11 (4%)	2 (1%)	30	84
6	F	277/331 (84%)	266 (96%)	9 (3%)	2 (1%)	30	84
6	N	277/331 (84%)	265 (96%)	10 (4%)	2 (1%)	30	84
7	G	206/222 (93%)	194 (94%)	10 (5%)	2 (1%)	22	80
7	O	206/222 (93%)	194 (94%)	10 (5%)	2 (1%)	22	80
8	H	169/212 (80%)	161 (95%)	7 (4%)	1 (1%)	33	86
8	P	169/212 (80%)	161 (95%)	7 (4%)	1 (1%)	33	86
All	All	4943/5718 (86%)	4668 (94%)	210 (4%)	65 (1%)	18	76

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	51	VAL
3	C	68	MET
8	H	29	GLY
3	K	51	VAL
3	K	68	MET

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%)	89	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	365/415 (88%)	362 (99%)	3 (1%)	89	98
2	B	367/406 (90%)	360 (98%)	7 (2%)	69	93
2	J	367/406 (90%)	361 (98%)	6 (2%)	75	94
3	C	358/377 (95%)	349 (98%)	9 (2%)	60	91
3	K	358/377 (95%)	351 (98%)	7 (2%)	68	92
4	D	347/348 (100%)	342 (99%)	5 (1%)	78	95
4	L	190/348 (55%)	186 (98%)	4 (2%)	66	92
5	E	255/283 (90%)	248 (97%)	7 (3%)	57	90
5	M	255/283 (90%)	247 (97%)	8 (3%)	52	89
6	F	251/277 (91%)	247 (98%)	4 (2%)	75	94
6	N	251/277 (91%)	249 (99%)	2 (1%)	89	98
7	G	174/184 (95%)	167 (96%)	7 (4%)	42	85
7	O	174/184 (95%)	167 (96%)	7 (4%)	42	85
8	H	144/173 (83%)	138 (96%)	6 (4%)	40	84
8	P	144/173 (83%)	140 (97%)	4 (3%)	56	89
All	All	4365/4926 (89%)	4276 (98%)	89 (2%)	68	92

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	167	LEU
1	I	404	GLN
7	O	167	LEU
7	G	178	CYS
8	H	160	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	202	GLN
1	I	412	GLN
6	N	284	ASN
1	I	187	ASN
1	I	324	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	419/480 (87%)	0.28	16 (3%) 38 26	130, 224, 265, 285	0
1	I	419/480 (87%)	0.22	9 (2%) 60 40	127, 198, 253, 268	0
2	B	403/447 (90%)	0.17	6 (1%) 70 48	132, 224, 253, 270	0
2	J	403/447 (90%)	0.19	6 (1%) 70 48	121, 208, 243, 263	0
3	C	401/423 (94%)	0.21	2 (0%) 88 74	129, 172, 261, 280	0
3	K	401/423 (94%)	0.26	3 (0%) 84 67	133, 186, 261, 276	0
4	D	406/410 (99%)	0.19	6 (1%) 70 48	133, 191, 268, 297	0
4	L	225/410 (54%)	0.21	2 (0%) 81 62	136, 189, 232, 249	0
5	E	298/334 (89%)	0.20	0 100 100	142, 176, 217, 258	0
5	M	298/334 (89%)	0.13	1 (0%) 91 83	128, 156, 187, 222	0
6	F	281/331 (84%)	0.18	2 (0%) 84 67	133, 180, 208, 224	0
6	N	281/331 (84%)	0.23	3 (1%) 77 56	130, 177, 212, 221	0
7	G	208/222 (93%)	0.08	2 (0%) 79 59	140, 194, 247, 256	0
7	O	208/222 (93%)	0.04	1 (0%) 88 74	133, 186, 238, 250	0
8	H	173/212 (81%)	0.14	0 100 100	135, 175, 215, 232	0
8	P	173/212 (81%)	0.21	1 (0%) 86 70	162, 198, 230, 240	0
All	All	4997/5718 (87%)	0.19	60 (1%) 75 54	121, 187, 253, 297	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	54	HIS	6.2
3	K	54	HIS	6.2
2	J	64	LYS	4.3
1	A	320	LEU	4.1
1	A	319	LEU	4.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	ZN	M	999	1/1	0.27	0.68	127,127,127,127	0
9	ZN	E	999	1/1	0.20	-1.14	149,149,149,149	0

6.5 Other polymers ⓘ

There are no such residues in this entry.