Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:42 PM GMT

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 Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

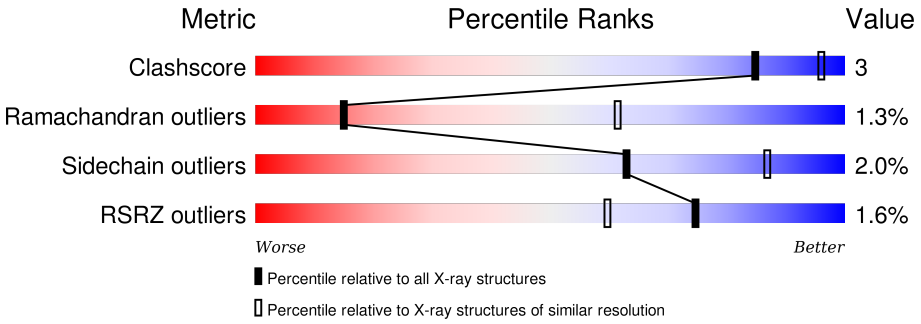
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

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))
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 <=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	3% 82% 5% 13%
1	I	480	2% 82% 5% 13%
2	B	447	2% 80% 9% • 10%
2	J	447	2% 81% 8% • 10%
3	C	423	86% 9% • 5%
3	K	423	% 86% 8% • 5%
4	D	410	2% 90% 9% •

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Mol	Chain	Length	Quality of chain
4	L	410	49% 5% 45%
5	E	334	% 82% 7% 11%
5	M	334	80% 8% 11%
6	F	331	76% 9% 15%
6	N	331	% 75% 10% 15%
7	G	222	% 84% 9% 6%
7	O	222	% 82% 10% 6%
8	H	212	74% 8% 18%
8	P	212	74% 7% 18%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 39976 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			

- 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).

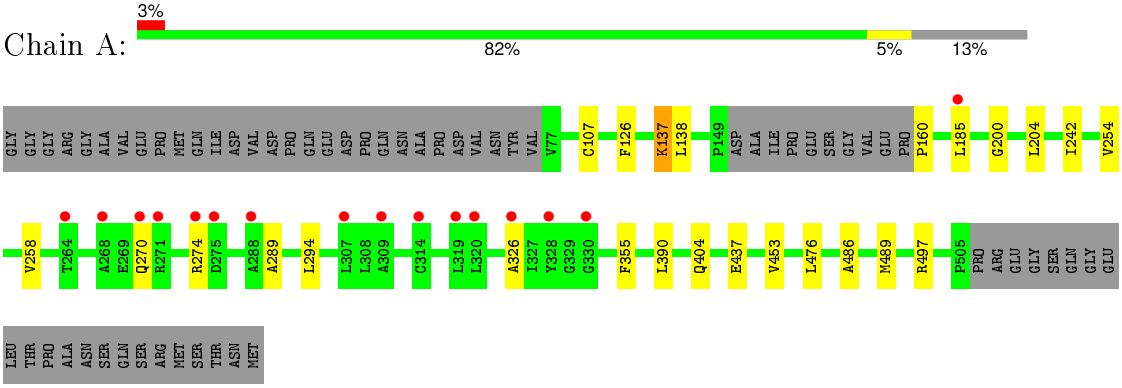
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Zn	0	0
			1	1		
9	E	1	Total	Zn	0	0
			1	1		

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.

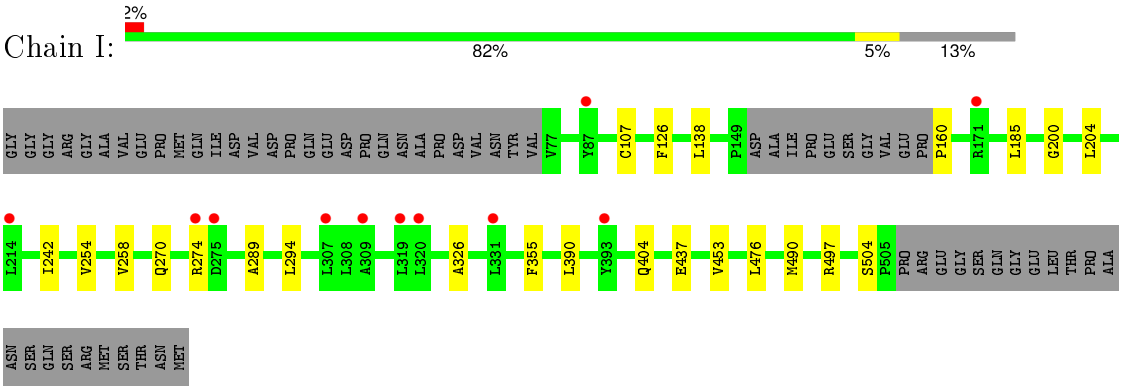
- Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain A:



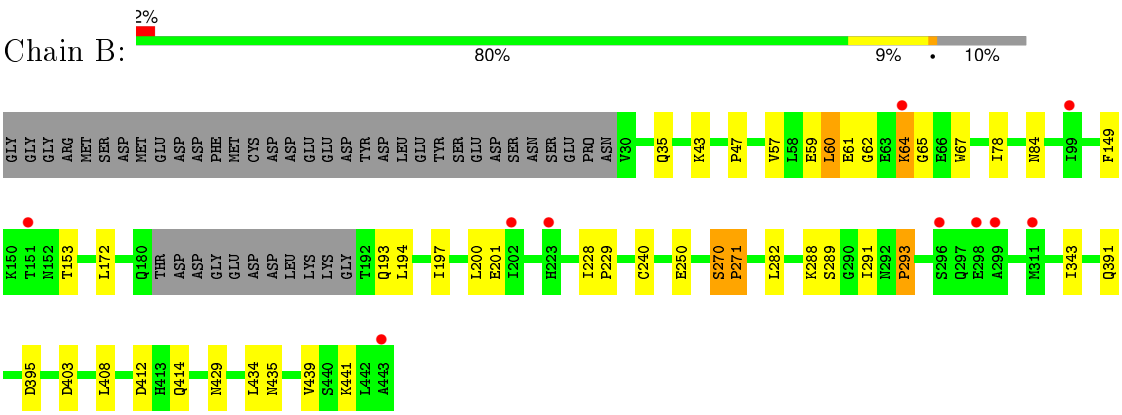
- Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain I:



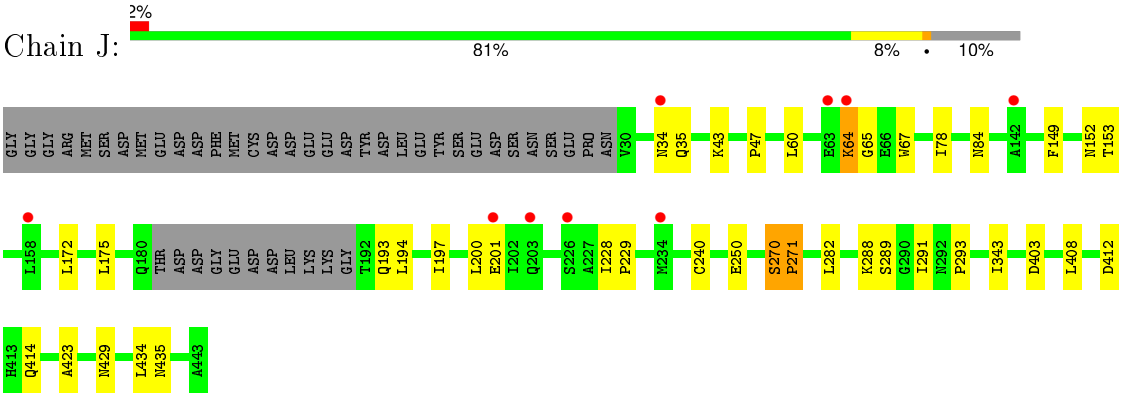
- Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

Chain B:



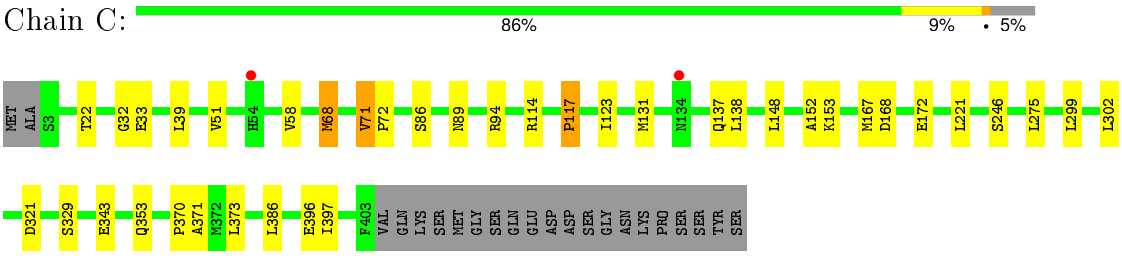
• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

Chain J:



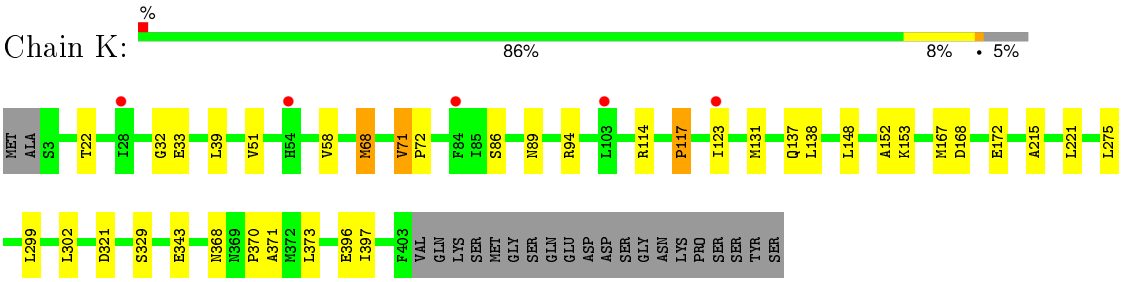
• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain C:



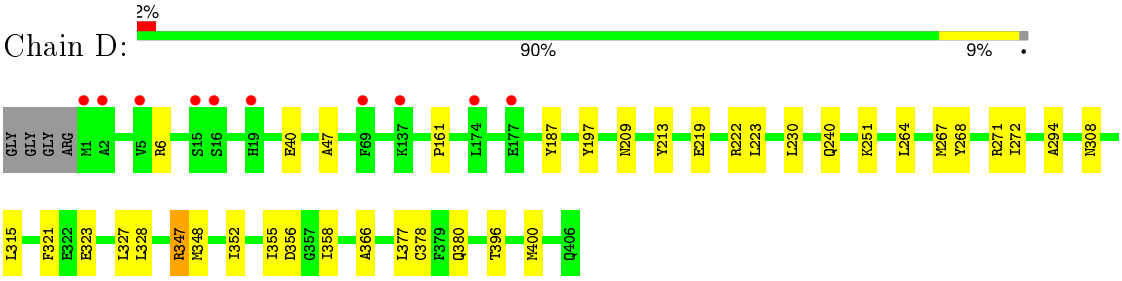
• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain K:



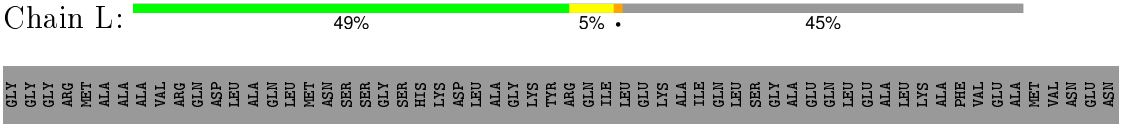
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

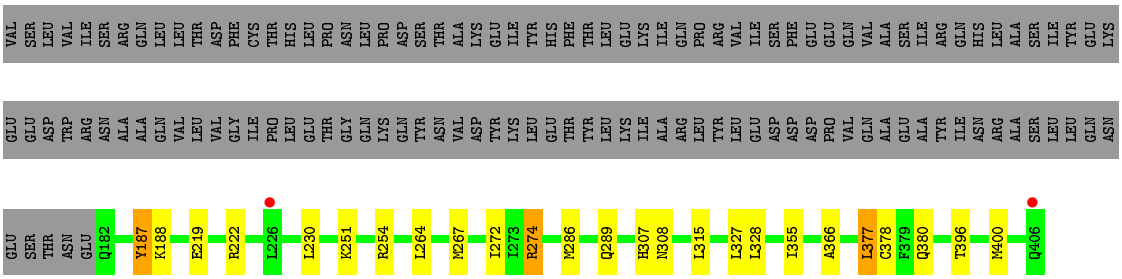
Chain D:



• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

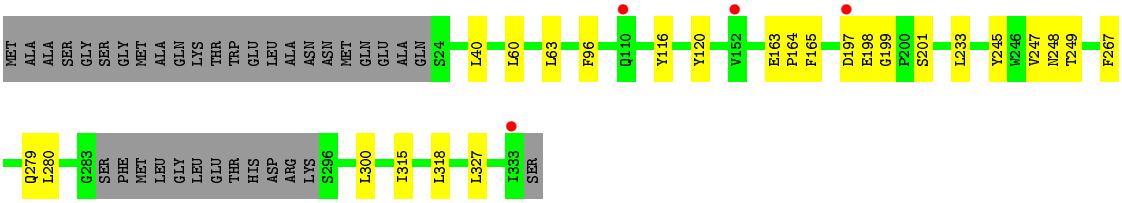
Chain L:





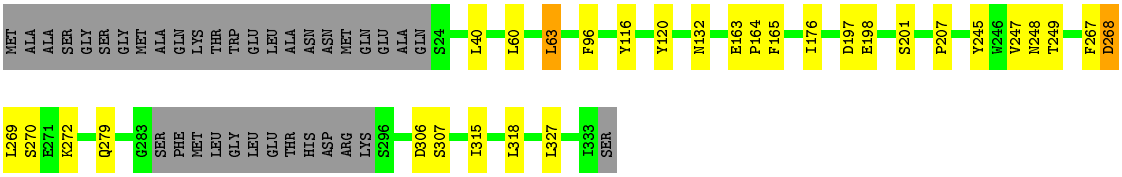
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain E:



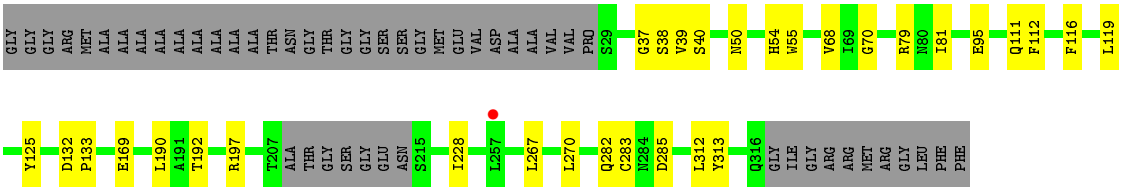
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain M:



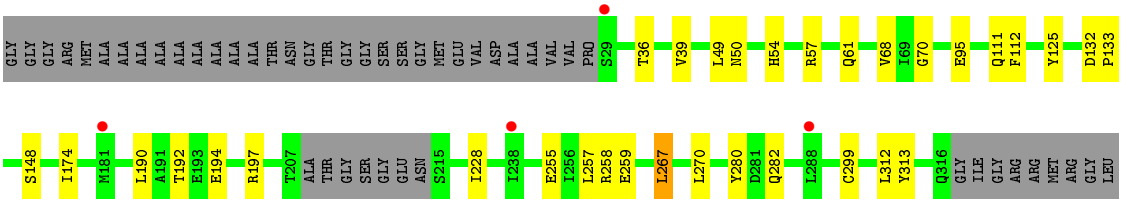
• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

Chain F:



• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

Chain N:

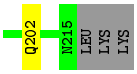


• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A

Chain G:

• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A

Chain O:

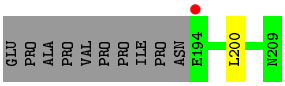


• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8

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	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
$< I/\sigma(I) >$ [1]	1.28 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.199 , 0.228 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	156.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.54	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(^{o})	Ideal(^{o})
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.

All (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,Peptide
6	F	267	LEU	Peptide
8	H	28	PRO	Mainchain,Peptide
2	J	270	SER	Mainchain,Peptide
2	J	288	LYS	Mainchain,Peptide
2	J	64	LYS	Mainchain,Peptide
3	K	68	MET	Mainchain,Peptide
5	M	163	GLU	Mainchain,Peptide
6	N	267	LEU	Mainchain,Peptide
8	P	28	PRO	Mainchain,Peptide

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	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

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 3.

All (233) 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)
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
5:M:96:PHE:CD2	5:M:120:TYR:CE2	2.40	1.09
4:L:274:ARG:NH2	4:L:327:LEU:HD12	1.81	0.95
5:E:96:PHE:CD2	5:E:120:TYR:CE2	2.57	0.92
1:I:200:GLY:O	1:I:204:LEU:CD1	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLY:O	1:A:204:LEU:CD1	2.21	0.88
6:F:39:VAL:HG11	6:F:81:ILE:HD11	1.60	0.83
5:M:96:PHE:CE2	5:M:120:TYR:CE2	2.67	0.82
1:I:185:LEU:HD22	1:I:204:LEU:HD21	1.62	0.80
1:A:185:LEU:HD22	1:A:204:LEU:HD21	1.62	0.80
2:B:61:GLU:C	2:B:62:GLY:N	2.35	0.79
7:G:126:ARG:NH2	7:G:129:GLU:HB3	1.97	0.79
4:D:251:LYS:NZ	6:F:38:SER:HB2	1.97	0.77
7:O:126:ARG:NH2	7:O:129:GLU:HB3	1.99	0.77
6:F:39:VAL:HG11	6:F:81:ILE:CD1	2.15	0.76
4:D:251:LYS:HZ2	6:F:38:SER:HB2	1.53	0.73
5:M:96:PHE:CD2	5:M:120:TYR:HE2	2.00	0.73
6:F:39:VAL:HG21	6:F:81:ILE:HD12	1.72	0.72
7:G:126:ARG:NH2	7:G:129:GLU:CB	2.53	0.71
7:O:126:ARG:NH2	7:O:129:GLU:CB	2.54	0.70
4:L:274:ARG:HH22	4:L:327:LEU:HD12	1.56	0.69
2:B:60:LEU:C	2:B:61:GLU:O	2.31	0.69
6:F:116:PHE:HB3	6:F:119:LEU:HD13	1.74	0.69
1:A:138:LEU:HD21	1:A:160:PRO:HG3	1.75	0.68
1:I:490:MET:SD	3:K:167:MET:SD	2.92	0.68
2:J:64:LYS:HB3	2:J:65:GLY:HA2	1.76	0.67
5:M:198:GLU:OE1	5:M:198:GLU:HA	1.95	0.66
5:M:96:PHE:CE2	5:M:120:TYR:CD2	2.83	0.66
2:B:64:LYS:HB3	2:B:65:GLY:HA2	1.77	0.64
4:D:315:LEU:HD13	7:G:133:ILE:HG12	1.79	0.64
1:I:200:GLY:C	1:I:204:LEU:HD13	2.17	0.64
1:I:138:LEU:HD21	1:I:160:PRO:HG3	1.79	0.63
5:E:96:PHE:CE2	5:E:120:TYR:CE2	2.87	0.63
3:K:370:PRO:O	3:K:373:LEU:N	2.32	0.63
1:A:200:GLY:C	1:A:204:LEU:HD13	2.18	0.63
5:E:249:THR:HG23	6:F:197:ARG:NH1	2.14	0.62
3:C:353:GLN:O	7:O:123:ARG:NH1	2.33	0.62
3:C:370:PRO:O	3:C:373:LEU:N	2.32	0.62
4:D:268:TYR:OH	6:F:38:SER:HA	2.00	0.61
6:F:38:SER:OG	6:F:39:VAL:HG13	2.01	0.61
3:C:343:GLU:HG3	8:H:120:LEU:HD13	1.82	0.61
2:B:391:GLN:NE2	2:B:395:ASP:OD2	2.30	0.60
4:L:286:MET:HB2	4:L:289:GLN:OE1	2.02	0.60
2:J:34:ASN:OD1	2:J:60:LEU:HD12	2.01	0.60
4:L:378:CYS:HB3	5:M:247:VAL:HG22	1.84	0.59
8:P:126:THR:O	8:P:164:PRO:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:153:THR:HG23	2:J:200:LEU:HD11	1.85	0.58
5:E:96:PHE:CD2	5:E:120:TYR:HE2	2.17	0.58
1:A:138:LEU:CD2	1:A:160:PRO:HG3	2.34	0.58
2:B:153:THR:HG23	2:B:200:LEU:HD11	1.86	0.57
4:L:187:TYR:CD1	4:L:188:LYS:N	2.72	0.57
5:M:96:PHE:CE2	5:M:120:TYR:HE2	2.17	0.57
6:F:38:SER:OG	6:F:39:VAL:N	2.37	0.57
8:H:126:THR:O	8:H:164:PRO:HD2	2.03	0.57
5:M:96:PHE:CZ	5:M:120:TYR:CD2	2.92	0.57
4:D:219:GLU:O	4:D:223:LEU:HD13	2.04	0.57
3:K:71:VAL:HB	3:K:72:PRO:CD	2.35	0.57
4:D:321:PHE:HZ	4:D:352:ILE:HG23	1.69	0.57
1:I:497:ARG:HG3	6:N:313:TYR:CE1	2.39	0.57
4:D:323:GLU:OE2	7:G:126:ARG:HB2	2.04	0.57
5:M:60:LEU:HD11	6:N:50:ASN:OD1	2.05	0.57
1:I:185:LEU:HD22	1:I:204:LEU:CD2	2.33	0.56
3:C:71:VAL:HB	3:C:72:PRO:CD	2.35	0.56
2:B:434:LEU:HD21	5:E:300:LEU:HD11	1.87	0.56
1:A:185:LEU:HD22	1:A:204:LEU:CD2	2.33	0.56
5:M:315:ILE:HG23	8:P:200:LEU:HD22	1.87	0.55
4:L:308:ASN:HB3	4:L:328:LEU:HD22	1.88	0.55
4:D:251:LYS:NZ	6:F:38:SER:CB	2.68	0.55
4:L:315:LEU:HD13	7:O:133:ILE:HG12	1.89	0.55
6:N:255:GLU:OE1	6:N:258:ARG:NE	2.40	0.55
2:J:194:LEU:HA	2:J:197:ILE:HD12	1.88	0.55
3:K:343:GLU:HG3	8:P:120:LEU:HD13	1.88	0.54
1:I:138:LEU:CD2	1:I:160:PRO:HG3	2.38	0.54
5:M:248:ASN:OD1	6:N:192:THR:HG22	2.08	0.54
5:M:249:THR:HG23	6:N:197:ARG:NH1	2.23	0.54
4:L:251:LYS:NZ	6:N:148:SER:OG	2.41	0.54
4:D:308:ASN:HB3	4:D:328:LEU:HD22	1.89	0.54
2:B:194:LEU:HA	2:B:197:ILE:HD12	1.88	0.54
5:M:120:TYR:N	6:N:111:GLN:HE22	2.05	0.54
4:D:378:CYS:HB3	5:E:247:VAL:HG22	1.89	0.53
5:E:60:LEU:HD11	6:F:50:ASN:OD1	2.08	0.53
6:N:255:GLU:OE2	6:N:259:GLU:OE2	2.26	0.53
3:K:275:LEU:HD23	3:K:299:LEU:HD12	1.90	0.53
4:D:161:PRO:HB3	4:D:197:TYR:HB3	1.91	0.52
5:M:272:LYS:NZ	5:M:306:ASP:OD2	2.26	0.52
4:D:271:ARG:HB3	7:G:137:TYR:CE2	2.44	0.52
4:D:219:GLU:HA	4:D:222:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:ARG:NH2	7:G:129:GLU:HB2	2.24	0.52
5:E:327:LEU:HD11	6:F:228:ILE:HG12	1.91	0.52
2:J:434:LEU:HD23	6:N:299:CYS:SG	2.50	0.52
6:N:255:GLU:OE1	6:N:255:GLU:HA	2.10	0.51
4:L:219:GLU:HA	4:L:222:ARG:HE	1.76	0.51
4:L:254:ARG:HD3	6:N:174:ILE:HD12	1.92	0.51
6:N:267:LEU:HD11	7:O:177:TRP:CE3	2.45	0.51
2:J:282:LEU:HD13	2:J:343:ILE:HG23	1.92	0.51
6:F:37:GLY:HA3	6:F:169:GLU:OE2	2.10	0.51
4:L:267:MET:HA	4:L:307:HIS:CE1	2.46	0.51
2:B:282:LEU:HD13	2:B:343:ILE:HG23	1.92	0.51
3:C:275:LEU:HD23	3:C:299:LEU:HD12	1.91	0.51
2:B:270:SER:HB2	2:B:271:PRO:HA	1.93	0.51
5:M:96:PHE:CG	5:M:120:TYR:CE2	2.96	0.50
7:O:126:ARG:NH2	7:O:129:GLU:HB2	2.25	0.50
2:J:270:SER:HB2	2:J:271:PRO:HA	1.93	0.50
5:M:63:LEU:HD12	6:N:49:LEU:HD12	1.92	0.50
5:M:116:TYR:CD1	5:M:116:TYR:C	2.85	0.50
1:A:326:ALA:HB2	1:A:355:PHE:HB3	1.93	0.50
3:K:117:PRO:HD2	3:K:152:ALA:HB2	1.93	0.50
1:I:326:ALA:HB2	1:I:355:PHE:HB3	1.94	0.49
7:O:126:ARG:HH22	7:O:129:GLU:HB3	1.75	0.49
3:C:117:PRO:HD2	3:C:152:ALA:HB2	1.93	0.49
7:G:126:ARG:HH22	7:G:129:GLU:HB3	1.73	0.49
1:A:497:ARG:HG3	6:F:313:TYR:CE1	2.48	0.48
5:M:176:ILE:HG23	6:N:194:GLU:HG2	1.94	0.48
2:B:441:LYS:HE3	5:E:280:LEU:HD22	1.94	0.48
4:L:187:TYR:HE1	4:L:188:LYS:HD3	1.78	0.48
5:E:96:PHE:CE2	5:E:120:TYR:CD2	3.02	0.48
8:H:159:THR:HA	7:O:117:LEU:HD13	1.95	0.48
2:J:423:ALA:HB2	5:M:267:PHE:CE2	2.49	0.47
5:M:96:PHE:CZ	5:M:120:TYR:HD2	2.32	0.47
1:A:486:ALA:CB	3:C:386:LEU:HD21	2.45	0.47
4:D:347:ARG:C	4:D:348:MET:CA	2.76	0.47
7:O:105:ALA:HB1	7:O:154:VAL:HG11	1.97	0.47
5:E:233:LEU:HD22	6:F:55:TRP:CE3	2.49	0.47
1:I:437:GLU:HG3	1:I:453:VAL:HG11	1.96	0.47
7:G:105:ALA:HB1	7:G:154:VAL:HG11	1.97	0.46
4:D:6:ARG:HG2	4:D:47:ALA:HB1	1.97	0.46
2:B:172:LEU:HD22	2:B:201:GLU:HG3	1.95	0.46
5:E:245:TYR:HD1	6:F:190:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:318:LEU:HD11	6:F:283:CYS:HA	1.97	0.46
4:D:347:ARG:CA	4:D:348:MET:N	2.72	0.46
1:A:437:GLU:HG3	1:A:453:VAL:HG11	1.96	0.46
2:J:172:LEU:HD22	2:J:201:GLU:HG3	1.96	0.46
3:K:368:ASN:O	6:N:280:TYR:HB3	2.16	0.46
3:C:117:PRO:HB2	3:C:148:LEU:HD22	1.98	0.46
7:O:188:ILE:O	7:O:189:GLU:C	2.54	0.46
5:E:116:TYR:C	5:E:116:TYR:CD1	2.89	0.46
5:E:248:ASN:OD1	6:F:192:THR:HG22	2.16	0.46
7:G:188:ILE:O	7:G:189:GLU:C	2.53	0.46
3:K:117:PRO:HB2	3:K:148:LEU:HD22	1.98	0.46
1:I:107:CYS:HB2	1:I:390:LEU:HD22	1.97	0.46
2:B:408:LEU:HD22	4:D:355:ILE:HG12	1.97	0.46
1:A:107:CYS:HB2	1:A:390:LEU:HD22	1.97	0.45
2:B:149:PHE:CZ	2:B:193:GLN:HB2	2.51	0.45
5:M:318:LEU:HD23	8:P:200:LEU:HD21	1.98	0.45
2:J:149:PHE:CZ	2:J:193:GLN:HB2	2.52	0.45
8:P:86:PHE:HA	8:P:89:ILE:HD12	1.98	0.45
3:K:370:PRO:O	3:K:371:ALA:C	2.54	0.45
3:C:370:PRO:O	3:C:373:LEU:HB3	2.15	0.45
3:K:397:ILE:HG23	6:N:312:LEU:HD12	1.98	0.45
8:P:141:VAL:HG11	8:P:160:ARG:NH2	2.31	0.45
4:D:378:CYS:HB2	5:E:247:VAL:HG13	1.98	0.45
4:D:268:TYR:CE2	6:F:79:ARG:HD3	2.52	0.45
3:K:370:PRO:O	3:K:373:LEU:HB3	2.16	0.45
5:M:269:LEU:HD21	5:M:307:SER:HB3	1.99	0.45
5:M:207:PRO:HB3	5:M:268:ASP:OD2	2.17	0.45
3:C:397:ILE:HG23	6:F:312:LEU:HD12	1.98	0.45
4:L:187:TYR:CD1	4:L:187:TYR:C	2.90	0.45
3:C:39:LEU:HD22	3:C:58:VAL:HG22	1.98	0.45
1:A:138:LEU:CD2	1:A:160:PRO:CG	2.95	0.44
2:B:59:GLU:O	2:B:61:GLU:N	2.48	0.44
4:L:187:TYR:CE1	4:L:188:LYS:HD3	2.52	0.44
5:E:318:LEU:HD11	6:F:283:CYS:SG	2.56	0.44
8:H:86:PHE:HA	8:H:89:ILE:HD12	1.98	0.44
2:B:57:VAL:HA	2:B:60:LEU:HD12	1.99	0.44
1:I:242:ILE:HG23	1:I:254:VAL:HG13	1.99	0.44
2:B:47:PRO:HB3	2:B:78:ILE:HG21	2.00	0.44
3:K:39:LEU:HD22	3:K:58:VAL:HG22	1.98	0.44
2:J:47:PRO:HB3	2:J:78:ILE:HG21	1.99	0.44
3:C:370:PRO:O	3:C:371:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:66:LEU:HD21	7:G:88:LEU:HD21	2.00	0.44
4:D:272:ILE:CD1	4:D:327:LEU:HD21	2.48	0.44
1:A:242:ILE:HG23	1:A:254:VAL:HG13	2.00	0.44
1:I:504:SER:HA	3:K:215:ALA:HB2	1.99	0.44
3:K:71:VAL:HB	3:K:72:PRO:HD2	1.98	0.44
3:C:71:VAL:HB	3:C:72:PRO:HD2	1.98	0.44
3:K:94:ARG:HH22	3:K:137:GLN:HE22	1.66	0.43
4:D:356:ASP:HB3	4:D:358:ILE:HD12	1.99	0.43
7:O:66:LEU:HD21	7:O:88:LEU:HD21	2.01	0.43
6:F:39:VAL:CG2	6:F:81:ILE:HD12	2.44	0.43
4:L:378:CYS:HB2	5:M:247:VAL:HG13	1.99	0.43
7:O:31:ILE:HG23	7:O:67:LEU:HD13	1.99	0.43
4:L:230:LEU:HD11	4:L:264:LEU:HB2	2.01	0.43
6:N:54:HIS:CE1	6:N:68:VAL:HB	2.54	0.43
1:A:486:ALA:HB1	3:C:386:LEU:HD21	1.99	0.43
5:E:318:LEU:HD23	8:H:200:LEU:HD21	2.01	0.43
6:F:132:ASP:HB2	6:F:133:PRO:CD	2.49	0.43
4:D:396:THR:O	4:D:400:MET:HB2	2.18	0.43
2:J:403:ASP:HB3	2:J:408:LEU:HG	2.00	0.43
2:B:403:ASP:HB3	2:B:408:LEU:HG	2.00	0.43
7:G:31:ILE:HG23	7:G:67:LEU:HD13	2.00	0.43
4:L:377:LEU:HD21	7:O:177:TRP:CH2	2.53	0.43
4:L:396:THR:O	4:L:400:MET:HB2	2.18	0.43
6:N:132:ASP:HB2	6:N:133:PRO:CD	2.48	0.43
6:F:54:HIS:CE1	6:F:68:VAL:HB	2.54	0.43
4:L:272:ILE:CD1	4:L:327:LEU:HD21	2.49	0.43
4:L:274:ARG:NH2	4:L:327:LEU:CD1	2.68	0.43
3:C:94:ARG:HH22	3:C:137:GLN:HE22	1.67	0.42
4:D:230:LEU:HD11	4:D:264:LEU:HB2	2.01	0.42
1:I:258:VAL:HG11	1:I:289:ALA:HB2	2.01	0.42
6:F:39:VAL:HA	6:F:79:ARG:O	2.20	0.42
3:K:275:LEU:HD22	3:K:302:LEU:HD22	2.01	0.42
5:E:96:PHE:CE2	5:E:120:TYR:HE2	2.37	0.42
1:A:258:VAL:HG11	1:A:289:ALA:HB2	2.01	0.42
6:N:257:LEU:HD22	7:O:167:LEU:HD21	2.02	0.42
4:L:187:TYR:HD1	4:L:188:LYS:N	2.15	0.41
2:J:408:LEU:HD22	4:L:355:ILE:HG12	2.02	0.41
1:A:489:MET:HB3	2:B:439:VAL:HG13	2.01	0.41
7:G:98:HIS:HD2	7:G:135:ALA:HB2	1.85	0.41
3:C:275:LEU:HD22	3:C:302:LEU:HD22	2.01	0.41
6:N:36:THR:HB	6:N:39:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:98:HIS:HD2	7:O:135:ALA:HB2	1.85	0.41
1:I:138:LEU:CD2	1:I:160:PRO:CG	2.98	0.41
2:J:35:GLN:HG2	2:J:67:TRP:CZ2	2.56	0.41
5:E:96:PHE:CG	5:E:120:TYR:CE2	3.07	0.41
4:D:209:ASN:O	4:D:213:TYR:CD2	2.74	0.41
6:F:70:GLY:HA3	6:F:125:TYR:CE2	2.55	0.41
5:M:245:TYR:HD1	6:N:190:LEU:HD13	1.84	0.41
5:E:120:TYR:N	6:F:111:GLN:HE22	2.19	0.41
6:N:70:GLY:HA3	6:N:125:TYR:CE2	2.55	0.41
8:H:78:GLY:HA2	8:H:81:ILE:HD12	2.03	0.41
5:M:327:LEU:HD11	6:N:228:ILE:HG12	2.02	0.41
7:O:164:ARG:HA	7:O:167:LEU:HD12	2.03	0.40
2:B:35:GLN:HG2	2:B:67:TRP:CZ2	2.56	0.40
5:E:315:ILE:HG23	8:H:200:LEU:HD22	2.03	0.40
8:P:78:GLY:HA2	8:P:81:ILE:HD12	2.04	0.40
6:F:132:ASP:HB2	6:F:133:PRO:HD2	2.02	0.40
5:M:96:PHE:CD2	5:M:120:TYR:CD2	3.01	0.40
2:J:152:ASN:HB3	2:J:175:LEU:HD21	2.03	0.40
6:N:57:ARG:HG2	6:N:61:GLN:HE21	1.86	0.40

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%)	394 (95%)	18 (4%)	3 (1%)	26 72
1	I	415/480 (86%)	394 (95%)	18 (4%)	3 (1%)	26 72
2	B	397/447 (89%)	366 (92%)	23 (6%)	8 (2%)	9 54
2	J	399/447 (89%)	369 (92%)	23 (6%)	7 (2%)	11 55
3	C	399/423 (94%)	362 (91%)	24 (6%)	13 (3%)	5 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	K	399/423 (94%)	362 (91%)	24 (6%)	13 (3%)	5 43
4	D	404/410 (98%)	399 (99%)	3 (1%)	2 (0%)	34 77
4	L	223/410 (54%)	219 (98%)	3 (1%)	1 (0%)	39 80
5	E	294/334 (88%)	281 (96%)	10 (3%)	3 (1%)	19 66
5	M	294/334 (88%)	281 (96%)	11 (4%)	2 (1%)	26 72
6	F	277/331 (84%)	266 (96%)	9 (3%)	2 (1%)	26 72
6	N	277/331 (84%)	265 (96%)	10 (4%)	2 (1%)	26 72
7	G	206/222 (93%)	194 (94%)	10 (5%)	2 (1%)	19 66
7	O	206/222 (93%)	194 (94%)	10 (5%)	2 (1%)	19 66
8	H	169/212 (80%)	161 (95%)	7 (4%)	1 (1%)	30 74
8	P	169/212 (80%)	161 (95%)	7 (4%)	1 (1%)	30 74
All	All	4943/5718 (86%)	4668 (94%)	210 (4%)	65 (1%)	15 61

All (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
8	P	29	GLY
1	A	274	ARG
3	C	71	VAL
3	C	153	LYS
3	C	172	GLU
7	G	24	GLY
1	I	274	ARG
2	J	414	GLN
3	K	71	VAL
3	K	153	LYS
3	K	172	GLU
7	O	24	GLY
2	B	43	LYS
2	B	271	PRO
2	B	414	GLN
3	C	33	GLU
3	C	89	ASN

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Mol	Chain	Res	Type
3	C	114	ARG
3	C	168	ASP
4	D	294	ALA
1	I	270	GLN
2	J	43	LYS
2	J	271	PRO
3	K	33	GLU
3	K	89	ASN
3	K	114	ARG
3	K	168	ASP
1	A	126	PHE
1	A	270	GLN
2	B	84	ASN
3	C	86	SER
3	C	117	PRO
4	D	366	ALA
6	F	95	GLU
6	F	270	LEU
7	G	9	GLY
1	I	126	PHE
2	J	84	ASN
3	K	86	SER
3	K	117	PRO
4	L	366	ALA
6	N	95	GLU
6	N	270	LEU
7	O	9	GLY
2	B	60	LEU
2	B	229	PRO
2	B	291	ILE
3	C	329	SER
5	E	164	PRO
5	E	201	SER
2	J	229	PRO
2	J	291	ILE
3	K	329	SER
5	M	164	PRO
5	M	201	SER
5	E	199	GLY
3	K	32	GLY
3	C	32	GLY
2	J	293	PRO

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Mol	Chain	Res	Type
2	B	293	PRO

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%)	86	94
1	I	365/415 (88%)	362 (99%)	3 (1%)	86	94
2	B	367/406 (90%)	360 (98%)	7 (2%)	65	87
2	J	367/406 (90%)	361 (98%)	6 (2%)	70	89
3	C	358/377 (95%)	349 (98%)	9 (2%)	55	83
3	K	358/377 (95%)	351 (98%)	7 (2%)	63	87
4	D	347/348 (100%)	342 (99%)	5 (1%)	74	90
4	L	190/348 (55%)	186 (98%)	4 (2%)	61	86
5	E	255/283 (90%)	248 (97%)	7 (3%)	52	82
5	M	255/283 (90%)	247 (97%)	8 (3%)	47	80
6	F	251/277 (91%)	247 (98%)	4 (2%)	70	89
6	N	251/277 (91%)	249 (99%)	2 (1%)	86	94
7	G	174/184 (95%)	167 (96%)	7 (4%)	38	75
7	O	174/184 (95%)	167 (96%)	7 (4%)	38	75
8	H	144/173 (83%)	138 (96%)	6 (4%)	36	74
8	P	144/173 (83%)	140 (97%)	4 (3%)	51	81
All	All	4365/4926 (89%)	4276 (98%)	89 (2%)	63	87

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	LEU
1	A	404	GLN
1	A	476	LEU

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Mol	Chain	Res	Type
2	B	228	ILE
2	B	240	CYS
2	B	250	GLU
2	B	293	PRO
2	B	412	ASP
2	B	429	ASN
2	B	435	ASN
3	C	22	THR
3	C	123	ILE
3	C	131	MET
3	C	138	LEU
3	C	167	MET
3	C	221	LEU
3	C	246	SER
3	C	321	ASP
3	C	396	GLU
4	D	40	GLU
4	D	240	GLN
4	D	267	MET
4	D	377	LEU
4	D	380	GLN
5	E	40	LEU
5	E	63	LEU
5	E	165	PHE
5	E	197	ASP
5	E	198	GLU
5	E	267	PHE
5	E	279	GLN
6	F	40	SER
6	F	112	PHE
6	F	282	GLN
6	F	285	ASP
7	G	52	VAL
7	G	109	LYS
7	G	110	CYS
7	G	126	ARG
7	G	161	ASP
7	G	167	LEU
7	G	178	CYS
8	H	33	THR
8	H	40	LEU
8	H	46	LEU

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Mol	Chain	Res	Type
8	H	160	ARG
8	H	163	LEU
8	H	165	ARG
1	I	294	LEU
1	I	404	GLN
1	I	476	LEU
2	J	228	ILE
2	J	240	CYS
2	J	250	GLU
2	J	412	ASP
2	J	429	ASN
2	J	435	ASN
3	K	22	THR
3	K	123	ILE
3	K	131	MET
3	K	138	LEU
3	K	221	LEU
3	K	321	ASP
3	K	396	GLU
4	L	187	TYR
4	L	274	ARG
4	L	377	LEU
4	L	380	GLN
5	M	40	LEU
5	M	63	LEU
5	M	132	ASN
5	M	165	PHE
5	M	197	ASP
5	M	268	ASP
5	M	270	SER
5	M	279	GLN
6	N	112	PHE
6	N	282	GLN
7	O	52	VAL
7	O	110	CYS
7	O	126	ARG
7	O	161	ASP
7	O	167	LEU
7	O	178	CYS
7	O	202	GLN
8	P	33	THR
8	P	40	LEU

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Mol	Chain	Res	Type
8	P	46	LEU
8	P	163	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	324	ASN
1	A	412	GLN
2	B	90	ASN
2	B	319	GLN
3	C	41	HIS
3	C	89	ASN
5	E	321	GLN
6	F	61	GLN
6	F	111	GLN
7	G	202	GLN
1	I	187	ASN
1	I	324	ASN
1	I	412	GLN
2	J	90	ASN
2	J	319	GLN
3	K	41	HIS
3	K	89	ASN
4	L	403	GLN
5	M	321	GLN
6	N	61	GLN
6	N	111	GLN
6	N	284	ASN
7	O	202	GLN

5.3.3 RNA

There are no RNA molecules 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.

No monomer is involved in short contacts.

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, 95^{th} 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%)	0.09	16 (3%) 44 30	130, 224, 265, 285	0
1	I	419/480 (87%)	-0.01	11 (2%) 59 43	127, 198, 253, 268	0
2	B	403/447 (90%)	-0.06	10 (2%) 61 44	132, 224, 253, 270	0
2	J	403/447 (90%)	-0.04	9 (2%) 65 50	121, 208, 243, 263	0
3	C	401/423 (94%)	0.03	2 (0%) 91 85	129, 172, 261, 280	0
3	K	401/423 (94%)	0.08	5 (1%) 81 67	133, 186, 261, 276	0
4	D	406/410 (99%)	0.02	10 (2%) 61 44	133, 191, 268, 297	0
4	L	225/410 (54%)	0.02	2 (0%) 85 74	136, 189, 232, 249	0
5	E	298/334 (89%)	0.06	4 (1%) 79 65	142, 176, 217, 258	0
5	M	298/334 (89%)	-0.05	0 100 100	128, 156, 187, 222	0
6	F	281/331 (84%)	0.01	1 (0%) 93 87	133, 180, 208, 224	0
6	N	281/331 (84%)	0.06	4 (1%) 78 63	130, 177, 212, 221	0
7	G	208/222 (93%)	-0.14	2 (0%) 84 72	140, 194, 247, 256	0
7	O	208/222 (93%)	-0.19	2 (0%) 84 72	133, 186, 238, 250	0
8	H	173/212 (81%)	-0.07	0 100 100	135, 175, 215, 232	0
8	P	173/212 (81%)	0.02	1 (0%) 90 82	162, 198, 230, 240	0
All	All	4997/5718 (87%)	-0.00	79 (1%) 74 60	121, 187, 253, 297	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	54	HIS	7.4
3	K	54	HIS	7.1
1	A	275	ASP	5.4
1	A	320	LEU	5.0
1	A	319	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
8	P	194	GLU	4.3
1	I	319	LEU	4.0
2	J	64	LYS	3.9
2	B	298	GLU	3.6
4	D	1	MET	3.5
1	A	264	THR	3.2
3	C	134	ASN	3.2
4	D	5	VAL	3.2
1	I	309	ALA	3.2
1	I	214	LEU	3.2
2	B	64	LYS	3.1
1	A	268	ALA	3.1
1	A	274	ARG	3.1
4	D	177	GLU	3.1
2	J	142	ALA	3.0
1	I	320	LEU	3.0
5	E	197	ASP	3.0
4	D	19	HIS	2.9
1	A	330	GLY	2.9
2	B	296	SER	2.9
3	K	28	ILE	2.9
6	N	238	ILE	2.8
4	L	406	GLN	2.8
6	F	257	LEU	2.8
2	J	63	GLU	2.7
4	D	16	SER	2.7
2	B	202	ILE	2.7
1	A	271	ARG	2.7
7	O	35	LEU	2.7
4	D	174	LEU	2.6
1	A	270	GLN	2.6
2	J	201	GLU	2.6
4	L	226	LEU	2.6
1	A	309	ALA	2.6
1	I	87	TYR	2.6
2	B	311	MET	2.5
4	D	137	LYS	2.5
3	K	123	ILE	2.5
2	J	34	ASN	2.5
7	G	70	PHE	2.5
1	I	331	LEU	2.4
1	I	307	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	299	ALA	2.4
4	D	69	PHE	2.3
5	E	110	GLN	2.3
5	E	152	VAL	2.3
5	E	333	ILE	2.3
2	J	203	GLN	2.3
1	I	171	ARG	2.2
2	J	158	LEU	2.2
6	N	181	MET	2.2
1	I	275	ASP	2.2
1	A	185	LEU	2.2
6	N	288	LEU	2.2
3	K	84	PHE	2.2
4	D	15	SER	2.1
2	B	99	ILE	2.1
1	A	326	ALA	2.1
7	O	43	PHE	2.1
7	G	35	LEU	2.1
2	B	223	HIS	2.1
1	I	274	ARG	2.1
1	A	307	LEU	2.1
2	B	443	ALA	2.1
2	J	234	MET	2.1
1	A	288	ALA	2.1
3	K	103	LEU	2.0
1	A	314	CYS	2.0
1	A	328	TYR	2.0
4	D	2	ALA	2.0
1	I	393	TYR	2.0
6	N	29	SER	2.0
2	B	151	THR	2.0
2	J	226	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
9	ZN	M	999	1/1	0.99	0.25	0.09	127,127,127,127	0
9	ZN	E	999	1/1	0.98	0.18	-1.51	149,149,149,149	0

6.5 Other polymers

There are no such residues in this entry.