Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:37 am BST

PDB ID	:	4WSN
Title	:	Crystal structure of the COP9 signalosome, a P1 crystal form
Authors	:	Bunker, R.D.; Lingaraju, G.M.; Thoma, N.H.
Deposited on	:	2014-10-28
Resolution	:	5.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

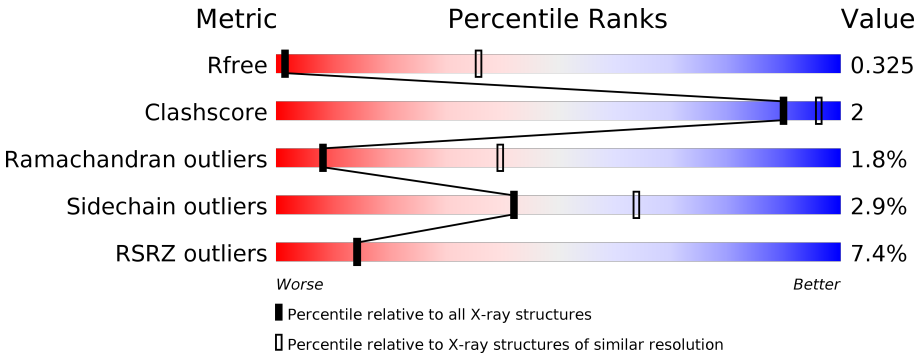
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 5.50 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	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)

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 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% 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	4% 79% 8% 13%
1	I	480	7% 79% 8% 13%
1	Q	480	6% 80% 7% 13%
1	Y	480	4% 80% 7% 13%
1	g	480	5% 84% • 13%
1	o	480	3% 84% • 13%

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Mol	Chain	Length	Quality of chain
2	B	447	6% 83% 7% 10%
2	J	447	5% 82% 7% 10%
2	R	447	4% 82% 7% 10%
2	Z	447	6% 83% 7% 10%
2	h	447	6% 86% 10%
2	p	447	5% 86% 10%
3	C	427	3% 83% 11% 6%
3	K	427	4% 85% 9% 6%
3	S	427	4% 84% 10% 6%
3	a	427	5% 89% 5% 6%
3	i	427	3% 89% 5% 6%
3	q	427	3% 89% 5% 6%
4	D	410	15% 90% 8%
4	L	410	13% 91% 7%
4	T	410	12% 90% 9%
4	b	410	20% 94%
4	j	410	14% 93% 5%
4	r	410	13% 94%
5	E	325	8% 86% 6% 8%
5	M	325	8% 85% 6% 8%
5	U	325	9% 84% 7% 8%
5	c	325	6% 88% 8%
5	k	325	6% 88% 8%
5	s	325	7% 88% 8%
6	F	331	3% 80% 6% 13%

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Mol	Chain	Length	Quality of chain
6	N	331	4% 81% 5% 13%
6	V	331	6% 81% 5% 13%
6	d	331	2% 85% 13%
6	l	331	5% 85% 13%
6	t	331	7% 85% 13%
7	G	222	7% 87% 6% 6%
7	O	222	7% 87% 6% 6%
7	W	222	7% 88% 5% 6%
7	e	222	5% 91% 6%
7	m	222	4% 91% 6%
7	u	222	3% 91% 6%
8	H	213	7% 74% 7% 19%
8	P	213	8% 73% 8% 19%
8	X	213	8% 75% 7% 19%
8	f	213	12% 77% 19%
8	n	213	5% 77% 19%
8	v	213	8% 77% 19%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 124428 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			
1	Q	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	Y	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	g	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	o	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			

There are 24 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
Q	48	GLY	-	expression tag	UNP Q13098
Q	49	GLY	-	expression tag	UNP Q13098
Q	50	GLY	-	expression tag	UNP Q13098
Q	51	ARG	-	expression tag	UNP Q13098
Y	48	GLY	-	expression tag	UNP Q13098
Y	49	GLY	-	expression tag	UNP Q13098
Y	50	GLY	-	expression tag	UNP Q13098
Y	51	ARG	-	expression tag	UNP Q13098
g	48	GLY	-	expression tag	UNP Q13098

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Chain	Residue	Modelled	Actual	Comment	Reference
g	49	GLY	-	expression tag	UNP Q13098
g	50	GLY	-	expression tag	UNP Q13098
g	51	ARG	-	expression tag	UNP Q13098
o	48	GLY	-	expression tag	UNP Q13098
o	49	GLY	-	expression tag	UNP Q13098
o	50	GLY	-	expression tag	UNP Q13098
o	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			
2	R	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	Z	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	h	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	p	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			

There are 24 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
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
R	-3	GLY	-	expression tag	UNP P61201
R	-2	GLY	-	expression tag	UNP P61201
R	-1	GLY	-	expression tag	UNP P61201
R	0	ARG	-	expression tag	UNP P61201
Z	-3	GLY	-	expression tag	UNP P61201
Z	-2	GLY	-	expression tag	UNP P61201
Z	-1	GLY	-	expression tag	UNP P61201

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	ARG	-	expression tag	UNP P61201
h	-3	GLY	-	expression tag	UNP P61201
h	-2	GLY	-	expression tag	UNP P61201
h	-1	GLY	-	expression tag	UNP P61201
h	0	ARG	-	expression tag	UNP P61201
p	-3	GLY	-	expression tag	UNP P61201
p	-2	GLY	-	expression tag	UNP P61201
p	-1	GLY	-	expression tag	UNP P61201
p	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			
3	S	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	a	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	i	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	q	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			

There are 24 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
S	-3	GLY	-	expression tag	UNP Q9UNS2
S	-2	GLY	-	expression tag	UNP Q9UNS2
S	-1	GLY	-	expression tag	UNP Q9UNS2
S	0	ARG	-	expression tag	UNP Q9UNS2
a	-3	GLY	-	expression tag	UNP Q9UNS2

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-2	GLY	-	expression tag	UNP Q9UNS2
a	-1	GLY	-	expression tag	UNP Q9UNS2
a	0	ARG	-	expression tag	UNP Q9UNS2
i	-3	GLY	-	expression tag	UNP Q9UNS2
i	-2	GLY	-	expression tag	UNP Q9UNS2
i	-1	GLY	-	expression tag	UNP Q9UNS2
i	0	ARG	-	expression tag	UNP Q9UNS2
q	-3	GLY	-	expression tag	UNP Q9UNS2
q	-2	GLY	-	expression tag	UNP Q9UNS2
q	-1	GLY	-	expression tag	UNP Q9UNS2
q	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			
4	T	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	b	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	j	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	r	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			

There are 24 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
T	-3	GLY	-	expression tag	UNP Q9BT78
T	-2	GLY	-	expression tag	UNP Q9BT78
T	-1	GLY	-	expression tag	UNP Q9BT78

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Chain	Residue	Modelled	Actual	Comment	Reference
T	0	ARG	-	expression tag	UNP Q9BT78
b	-3	GLY	-	expression tag	UNP Q9BT78
b	-2	GLY	-	expression tag	UNP Q9BT78
b	-1	GLY	-	expression tag	UNP Q9BT78
b	0	ARG	-	expression tag	UNP Q9BT78
j	-3	GLY	-	expression tag	UNP Q9BT78
j	-2	GLY	-	expression tag	UNP Q9BT78
j	-1	GLY	-	expression tag	UNP Q9BT78
j	0	ARG	-	expression tag	UNP Q9BT78
r	-3	GLY	-	expression tag	UNP Q9BT78
r	-2	GLY	-	expression tag	UNP Q9BT78
r	-1	GLY	-	expression tag	UNP Q9BT78
r	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			
5	U	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	c	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	k	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	s	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	expression tag	UNP Q92905
E	11	GLY	-	expression tag	UNP Q92905
E	12	GLY	-	expression tag	UNP Q92905
E	13	ARG	-	expression tag	UNP Q92905
M	10	GLY	-	expression tag	UNP Q92905
M	11	GLY	-	expression tag	UNP Q92905
M	12	GLY	-	expression tag	UNP Q92905
M	13	ARG	-	expression tag	UNP Q92905
U	10	GLY	-	expression tag	UNP Q92905

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Chain	Residue	Modelled	Actual	Comment	Reference
U	11	GLY	-	expression tag	UNP Q92905
U	12	GLY	-	expression tag	UNP Q92905
U	13	ARG	-	expression tag	UNP Q92905
c	10	GLY	-	expression tag	UNP Q92905
c	11	GLY	-	expression tag	UNP Q92905
c	12	GLY	-	expression tag	UNP Q92905
c	13	ARG	-	expression tag	UNP Q92905
k	10	GLY	-	expression tag	UNP Q92905
k	11	GLY	-	expression tag	UNP Q92905
k	12	GLY	-	expression tag	UNP Q92905
k	13	ARG	-	expression tag	UNP Q92905
s	10	GLY	-	expression tag	UNP Q92905
s	11	GLY	-	expression tag	UNP Q92905
s	12	GLY	-	expression tag	UNP Q92905
s	13	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	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	N	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	V	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	d	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	l	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	t	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			

There are 24 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

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Chain	Residue	Modelled	Actual	Comment	Reference
N	0	ARG	-	expression tag	UNP Q7L5N1
V	-3	GLY	-	expression tag	UNP Q7L5N1
V	-2	GLY	-	expression tag	UNP Q7L5N1
V	-1	GLY	-	expression tag	UNP Q7L5N1
V	0	ARG	-	expression tag	UNP Q7L5N1
d	-3	GLY	-	expression tag	UNP Q7L5N1
d	-2	GLY	-	expression tag	UNP Q7L5N1
d	-1	GLY	-	expression tag	UNP Q7L5N1
d	0	ARG	-	expression tag	UNP Q7L5N1
l	-3	GLY	-	expression tag	UNP Q7L5N1
l	-2	GLY	-	expression tag	UNP Q7L5N1
l	-1	GLY	-	expression tag	UNP Q7L5N1
l	0	ARG	-	expression tag	UNP Q7L5N1
t	-3	GLY	-	expression tag	UNP Q7L5N1
t	-2	GLY	-	expression tag	UNP Q7L5N1
t	-1	GLY	-	expression tag	UNP Q7L5N1
t	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			
7	W	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	e	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	m	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	u	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			

There are 24 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

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	expression tag	UNP Q9UBW8
O	-1	GLY	-	expression tag	UNP Q9UBW8
O	0	ARG	-	expression tag	UNP Q9UBW8
W	-3	GLY	-	expression tag	UNP Q9UBW8
W	-2	GLY	-	expression tag	UNP Q9UBW8
W	-1	GLY	-	expression tag	UNP Q9UBW8
W	0	ARG	-	expression tag	UNP Q9UBW8
e	-3	GLY	-	expression tag	UNP Q9UBW8
e	-2	GLY	-	expression tag	UNP Q9UBW8
e	-1	GLY	-	expression tag	UNP Q9UBW8
e	0	ARG	-	expression tag	UNP Q9UBW8
m	-3	GLY	-	expression tag	UNP Q9UBW8
m	-2	GLY	-	expression tag	UNP Q9UBW8
m	-1	GLY	-	expression tag	UNP Q9UBW8
m	0	ARG	-	expression tag	UNP Q9UBW8
u	-3	GLY	-	expression tag	UNP Q9UBW8
u	-2	GLY	-	expression tag	UNP Q9UBW8
u	-1	GLY	-	expression tag	UNP Q9UBW8
u	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			
8	X	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	f	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	n	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	v	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			

There are 24 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
X	-3	GLY	-	expression tag	UNP Q99627
X	-2	GLY	-	expression tag	UNP Q99627
X	-1	GLY	-	expression tag	UNP Q99627
X	0	ARG	-	expression tag	UNP Q99627
f	-3	GLY	-	expression tag	UNP Q99627
f	-2	GLY	-	expression tag	UNP Q99627
f	-1	GLY	-	expression tag	UNP Q99627
f	0	ARG	-	expression tag	UNP Q99627
n	-3	GLY	-	expression tag	UNP Q99627
n	-2	GLY	-	expression tag	UNP Q99627
n	-1	GLY	-	expression tag	UNP Q99627
n	0	ARG	-	expression tag	UNP Q99627
v	-3	GLY	-	expression tag	UNP Q99627
v	-2	GLY	-	expression tag	UNP Q99627
v	-1	GLY	-	expression tag	UNP Q99627
v	0	ARG	-	expression tag	UNP Q99627

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

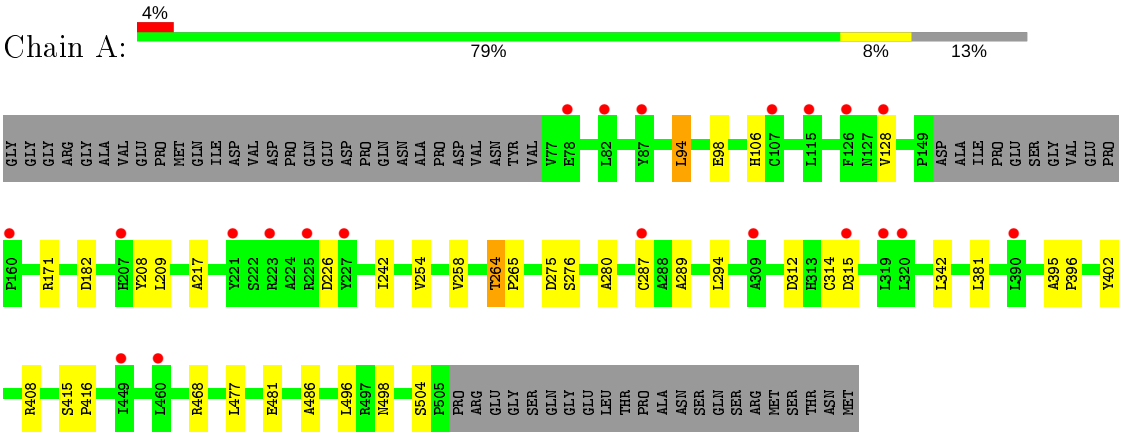
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	k	1	Total Zn 1 1	0	0
9	E	1	Total Zn 1 1	0	0
9	c	1	Total Zn 1 1	0	0
9	U	1	Total Zn 1 1	0	0
9	s	1	Total Zn 1 1	0	0
9	M	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 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.

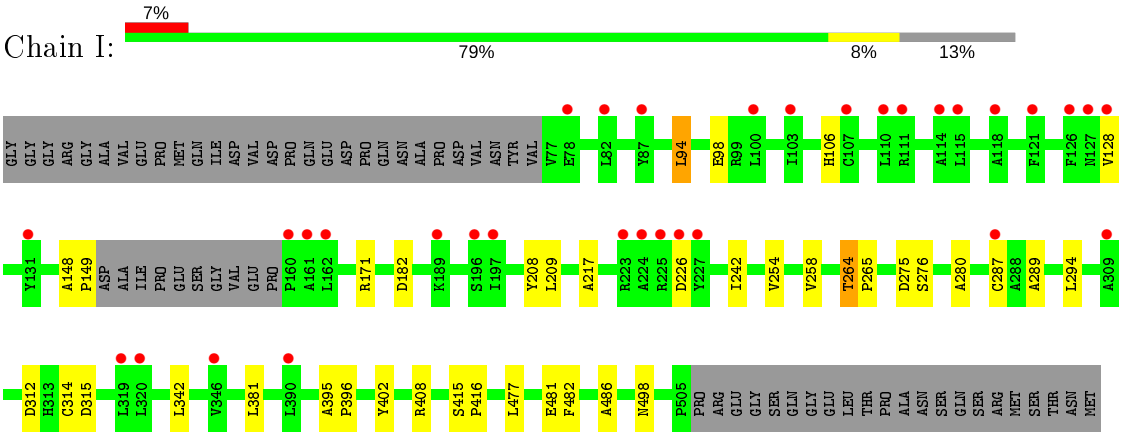
- Molecule 1: COP9 signalosome complex subunit 1

Chain A:



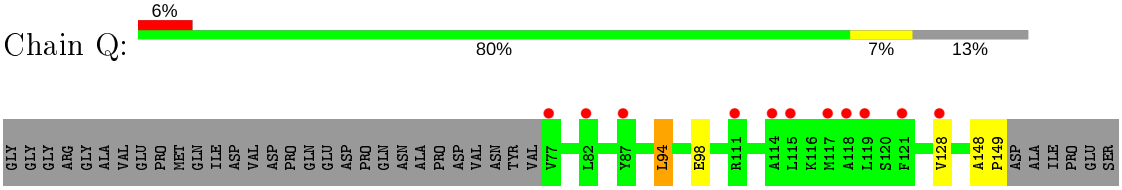
- Molecule 1: COP9 signalosome complex subunit 1

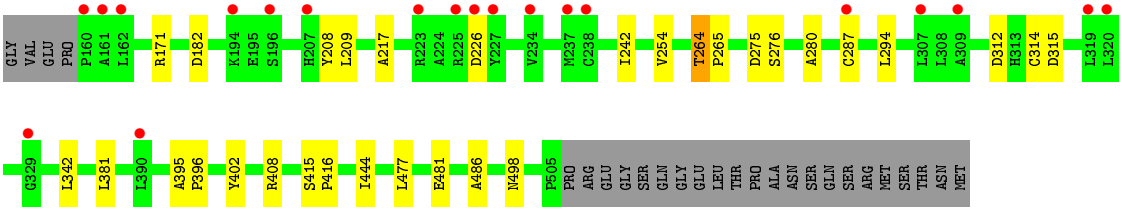
Chain I:



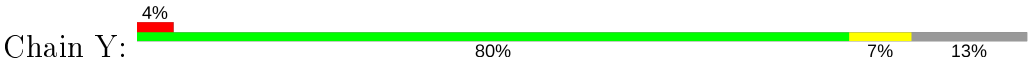
- Molecule 1: COP9 signalosome complex subunit 1

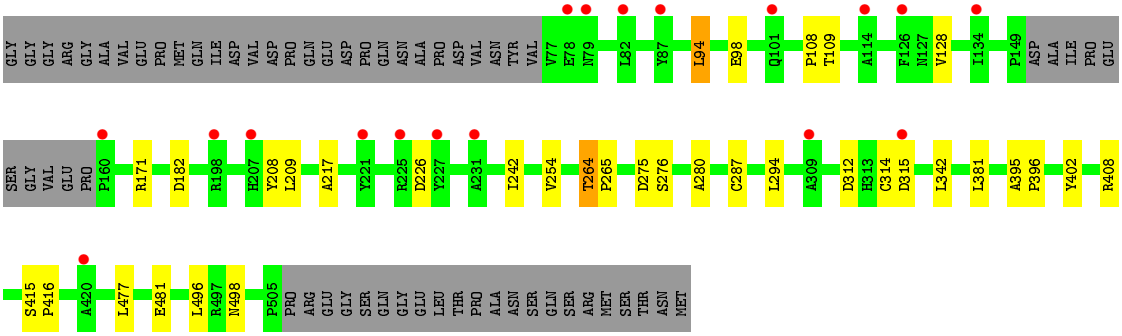
Chain Q:



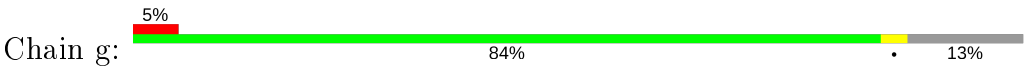


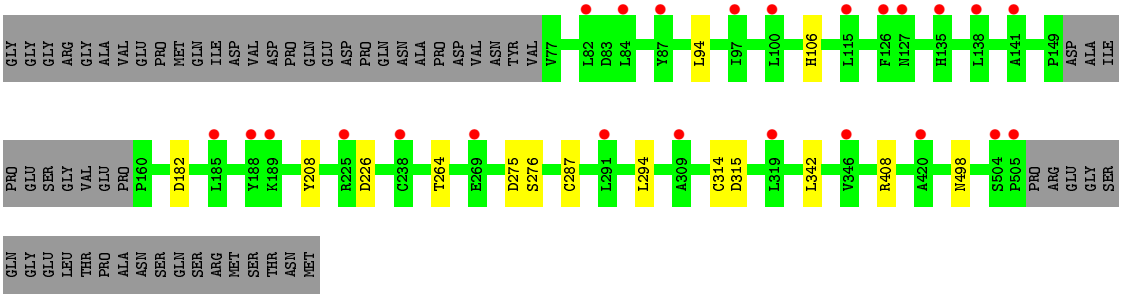
• Molecule 1: COP9 signalosome complex subunit 1



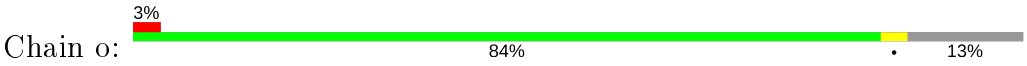


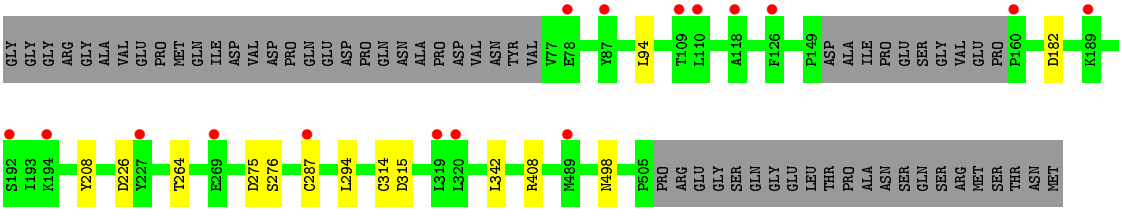
• Molecule 1: COP9 signalosome complex subunit 1



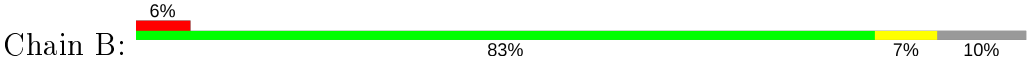


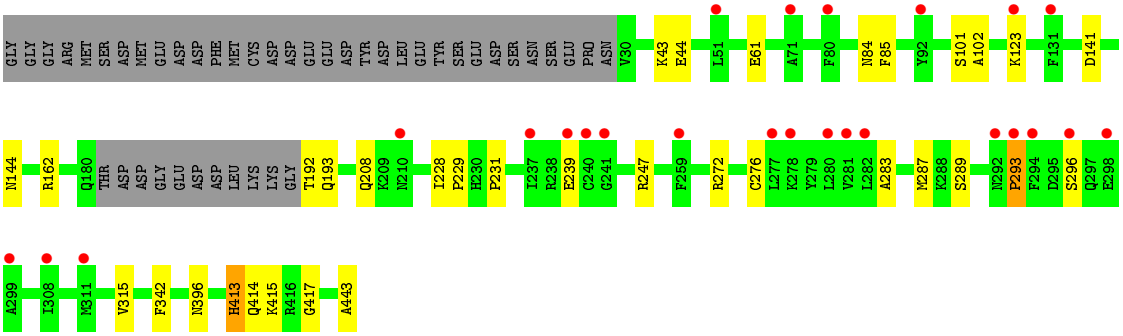
• Molecule 1: COP9 signalosome complex subunit 1





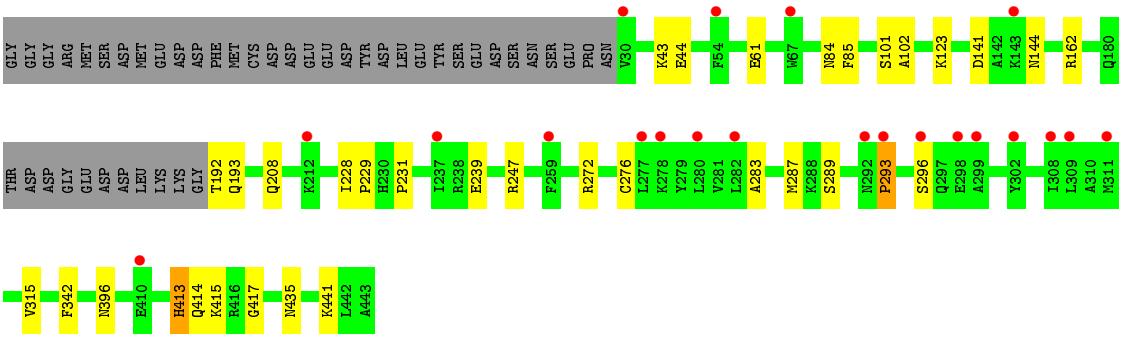
• Molecule 2: COP9 signalosome complex subunit 2





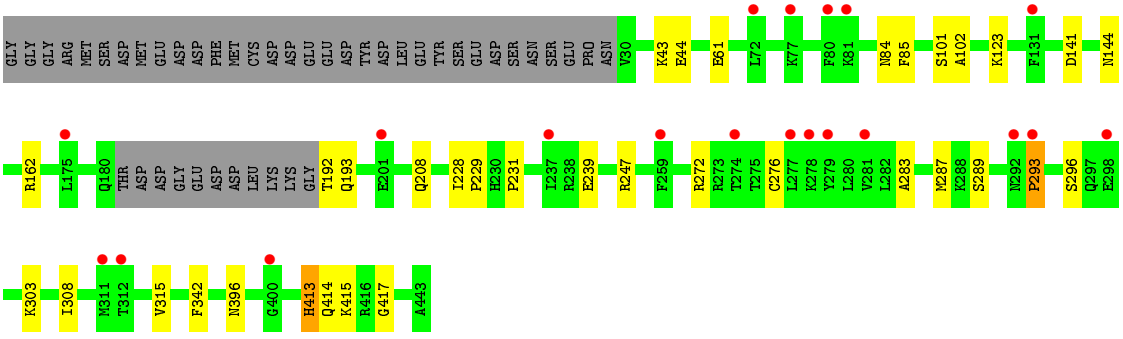
• Molecule 2: COP9 signalosome complex subunit 2

Chain J:



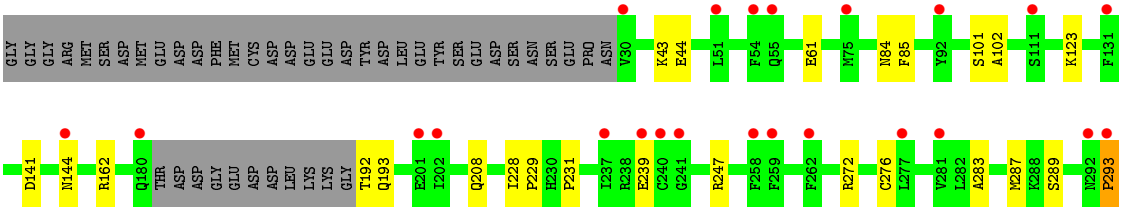
• Molecule 2: COP9 signalosome complex subunit 2

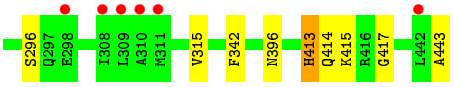
Chain R:



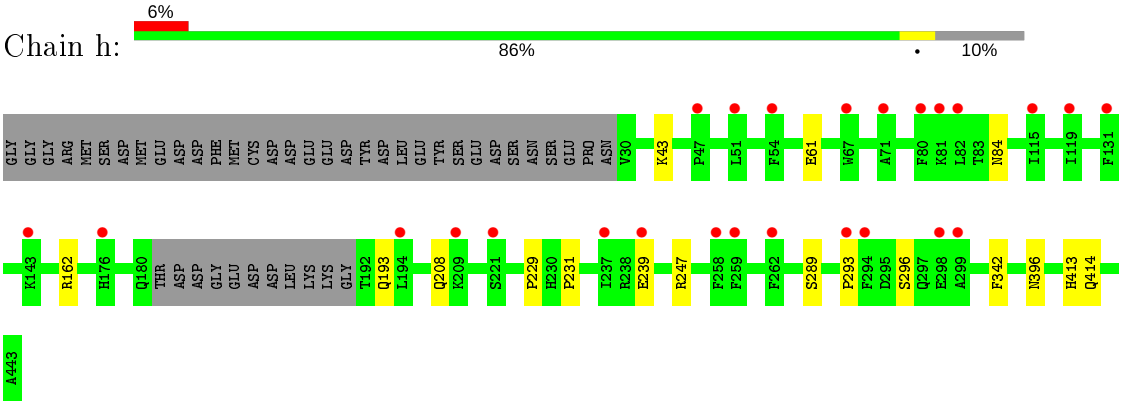
• Molecule 2: COP9 signalosome complex subunit 2

Chain Z:

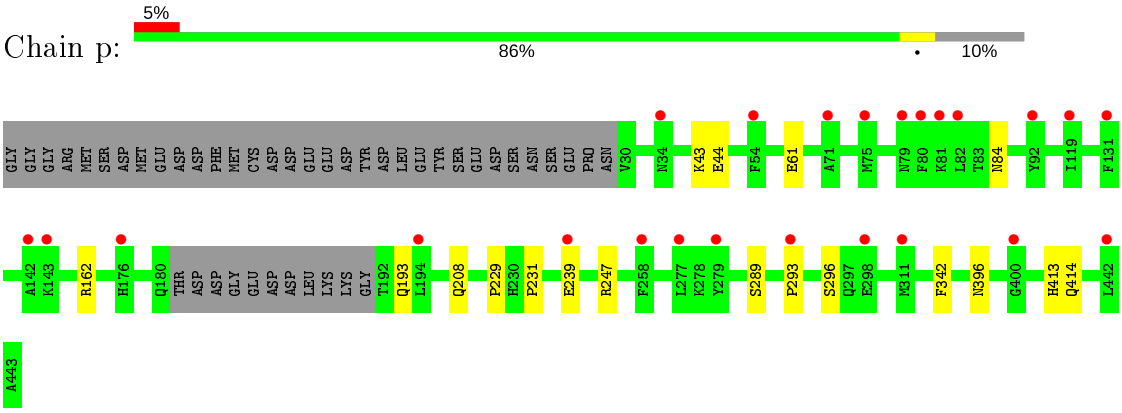




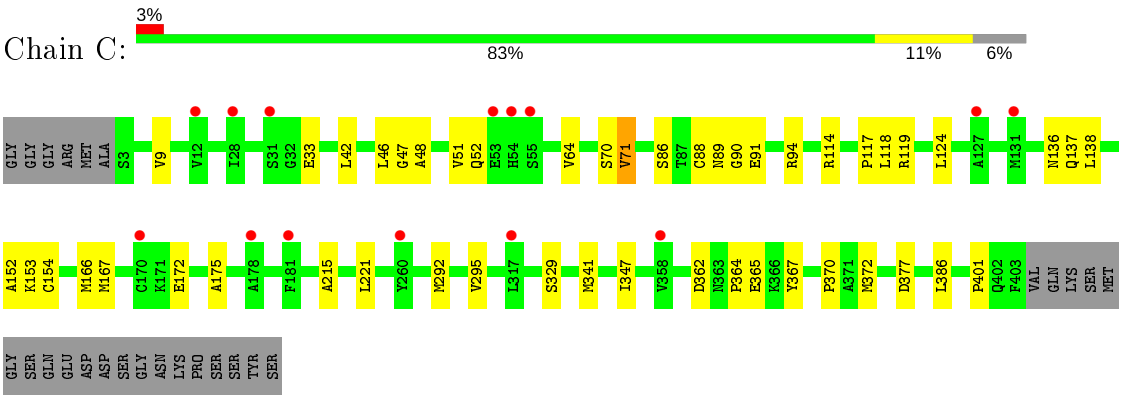
- Molecule 2: COP9 signalosome complex subunit 2



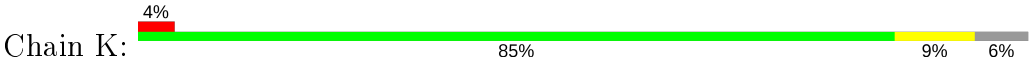
- Molecule 2: COP9 signalosome complex subunit 2

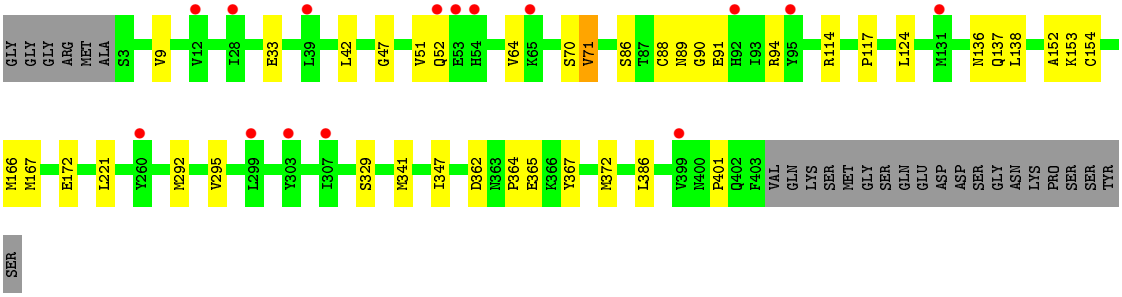


- Molecule 3: COP9 signalosome complex subunit 3



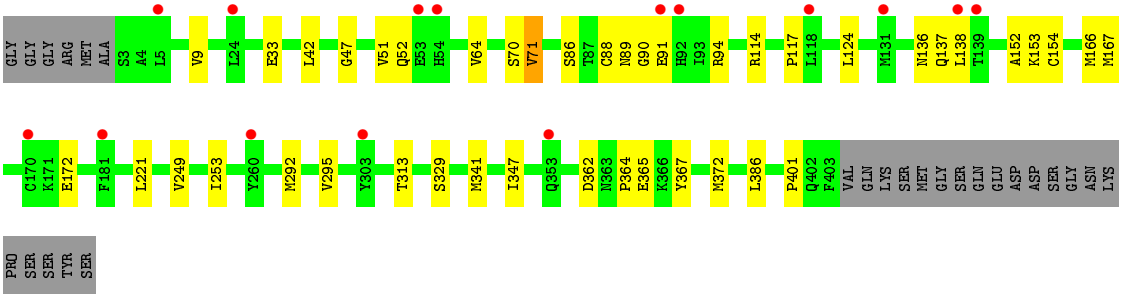
- Molecule 3: COP9 signalosome complex subunit 3





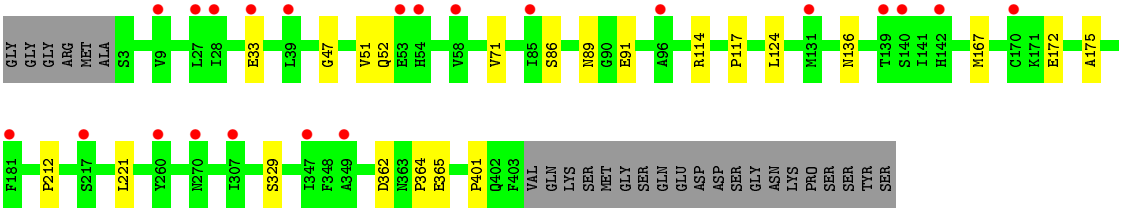
- Molecule 3: COP9 signalosome complex subunit 3

Chain S:



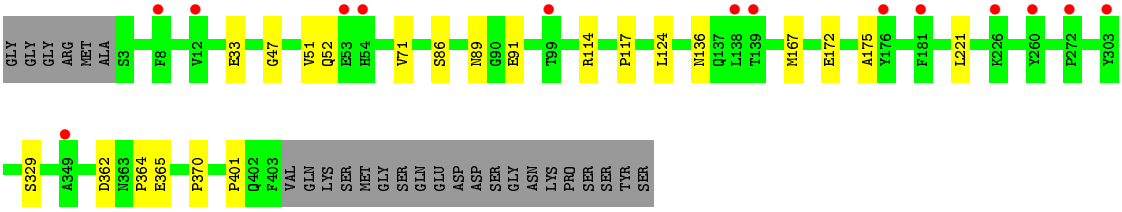
- Molecule 3: COP9 signalosome complex subunit 3

Chain a:



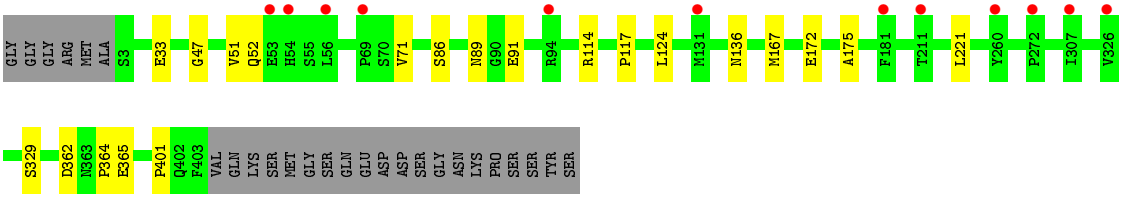
- Molecule 3: COP9 signalosome complex subunit 3

Chain i:



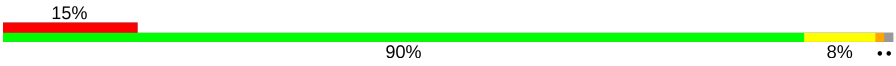
- Molecule 3: COP9 signalosome complex subunit 3

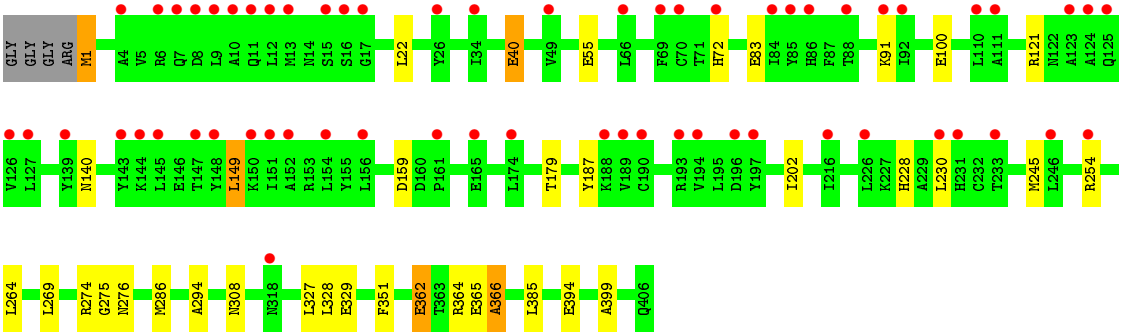
Chain q:



• Molecule 4: COP9 signalosome complex subunit 4

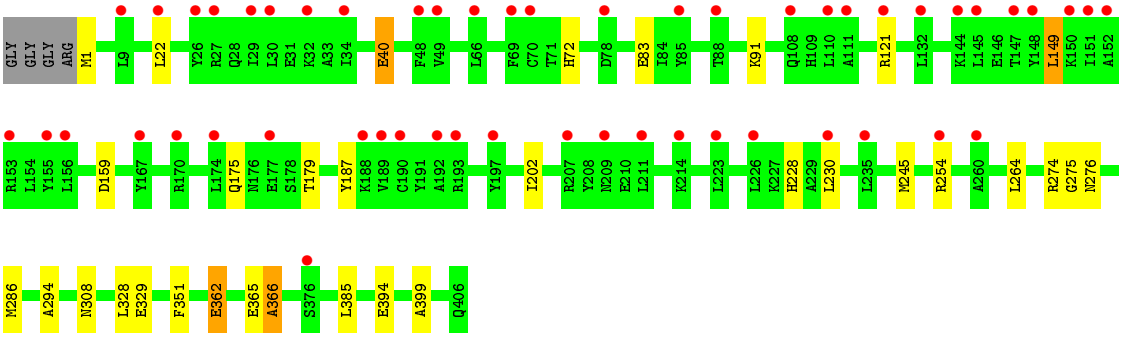
Chain D:





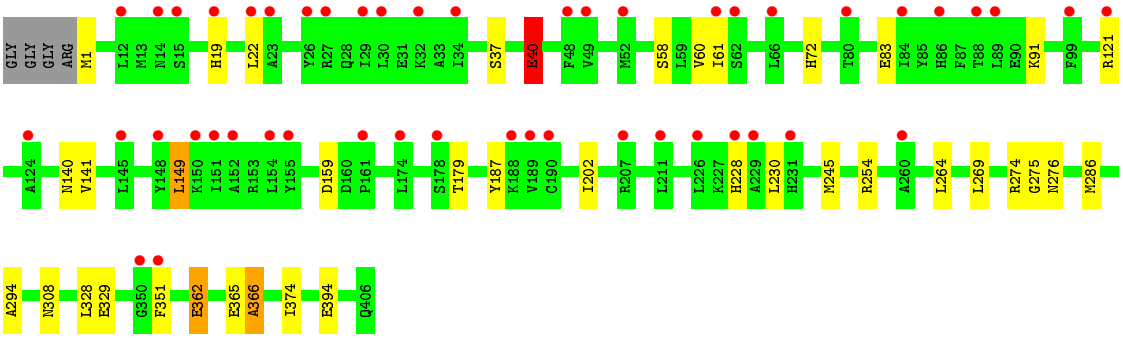
• Molecule 4: COP9 signalosome complex subunit 4

Chain L:



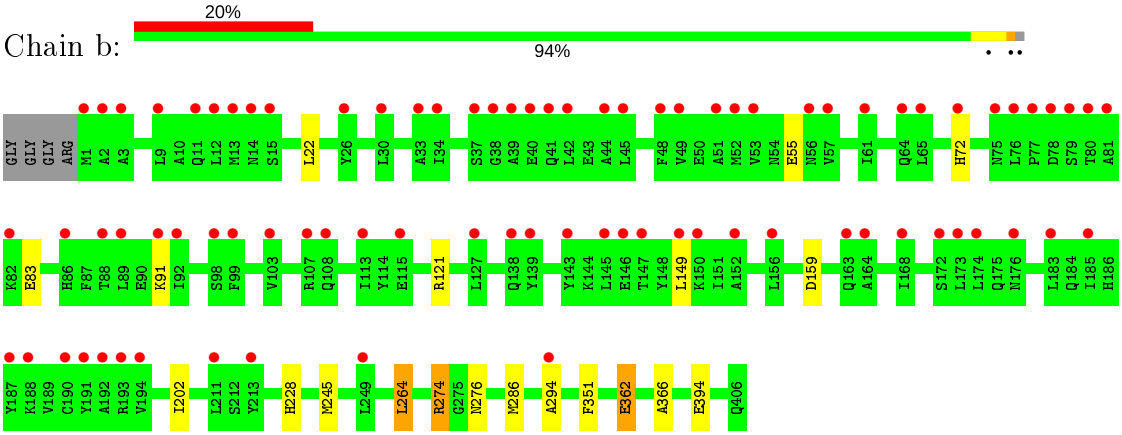
• Molecule 4: COP9 signalosome complex subunit 4

Chain T:



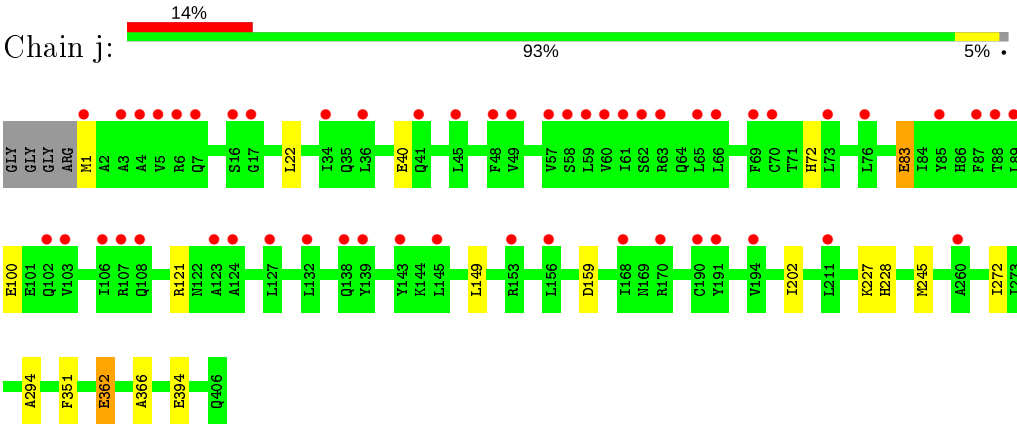
• Molecule 4: COP9 signalosome complex subunit 4

Chain b:



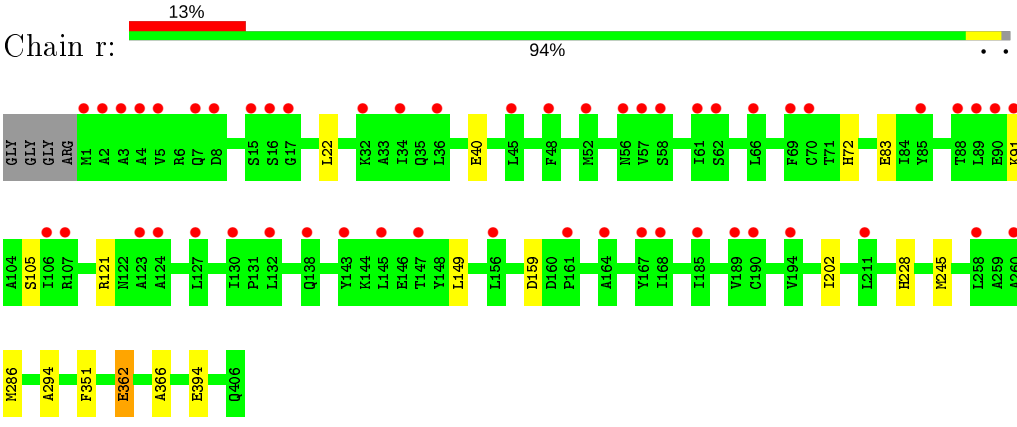
• Molecule 4: COP9 signalosome complex subunit 4

Chain j:



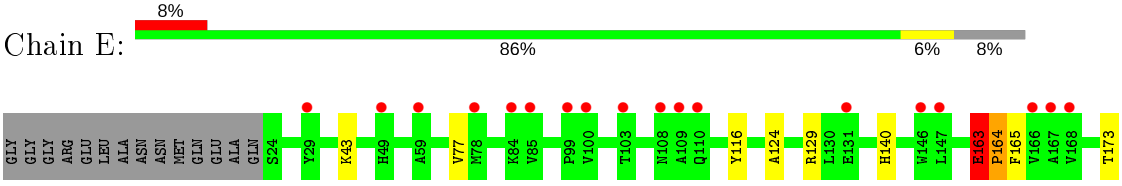
• Molecule 4: COP9 signalosome complex subunit 4

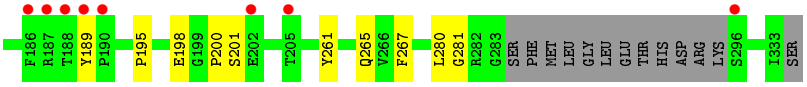
Chain r:



• Molecule 5: COP9 signalosome complex subunit 5

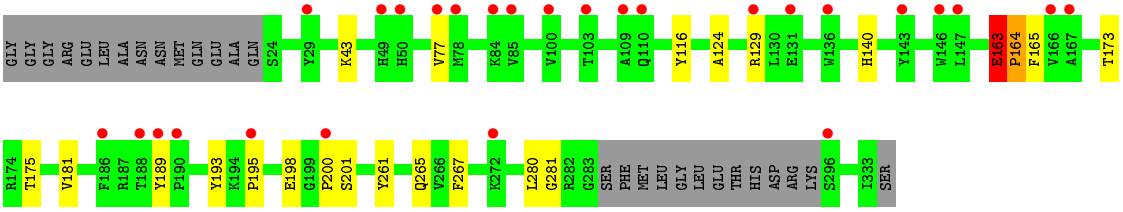
Chain E:





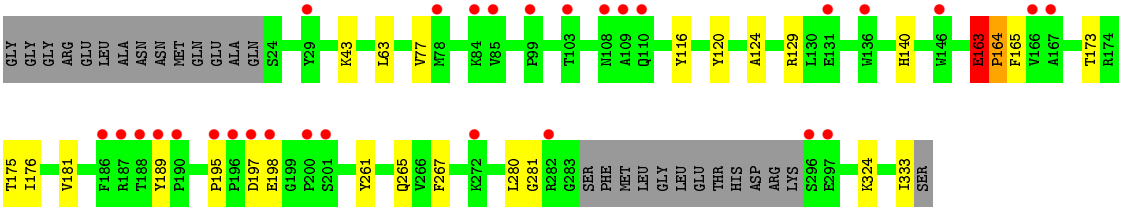
• Molecule 5: COP9 signalosome complex subunit 5

Chain M:



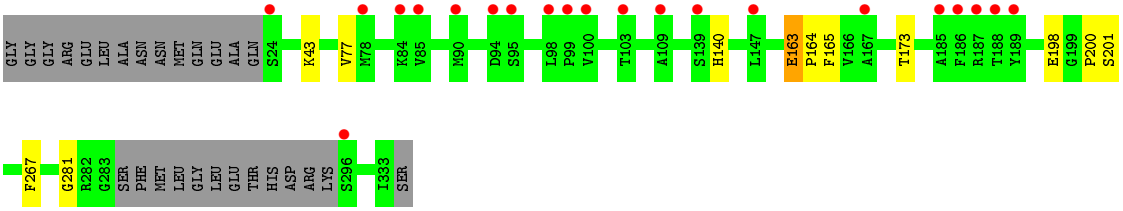
• Molecule 5: COP9 signalosome complex subunit 5

Chain U:



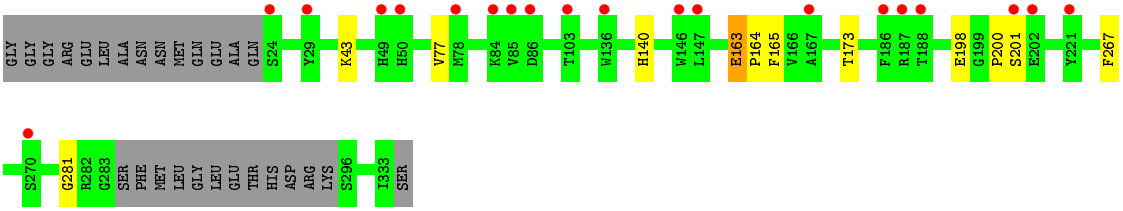
• Molecule 5: COP9 signalosome complex subunit 5

Chain c:



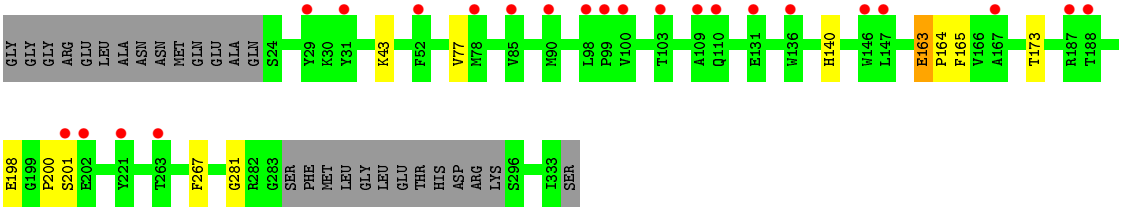
• Molecule 5: COP9 signalosome complex subunit 5

Chain k:



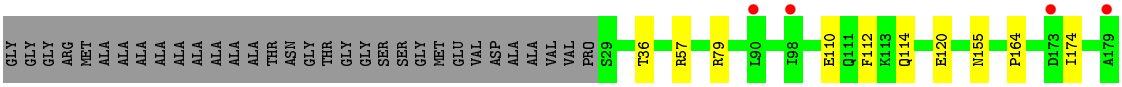
• Molecule 5: COP9 signalosome complex subunit 5

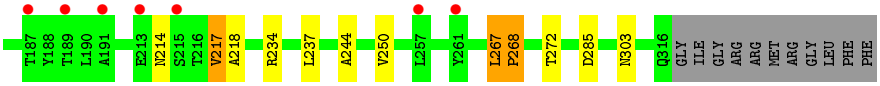
Chain s:



• Molecule 6: COP9 signalosome complex subunit 6

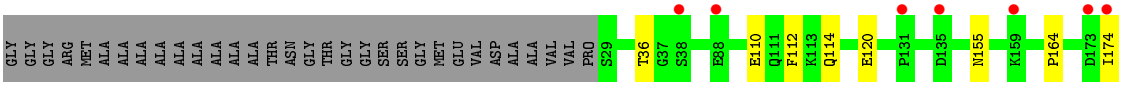
Chain F:

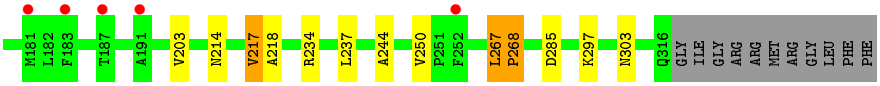




• Molecule 6: COP9 signalosome complex subunit 6

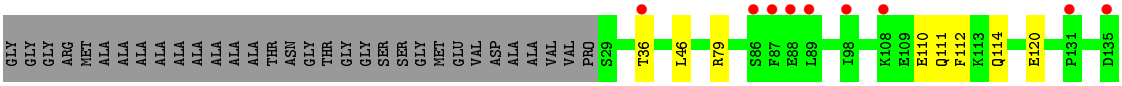
Chain N:

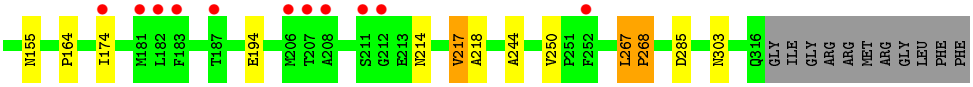




• Molecule 6: COP9 signalosome complex subunit 6

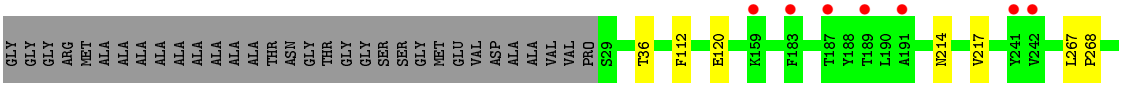
Chain V:





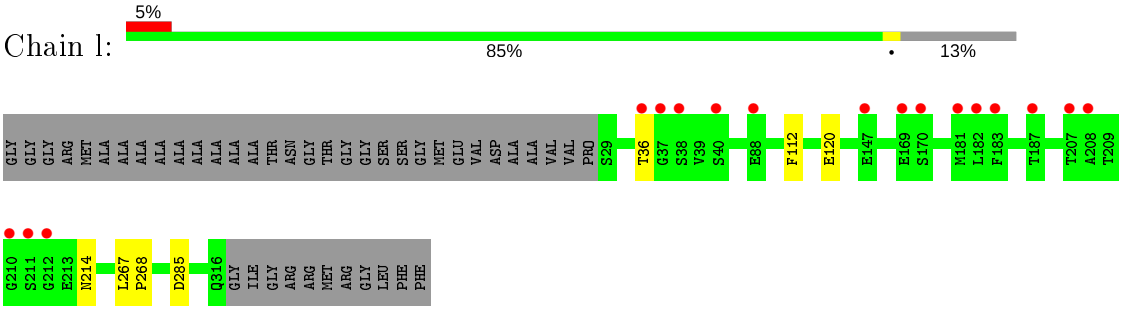
• Molecule 6: COP9 signalosome complex subunit 6

Chain d:



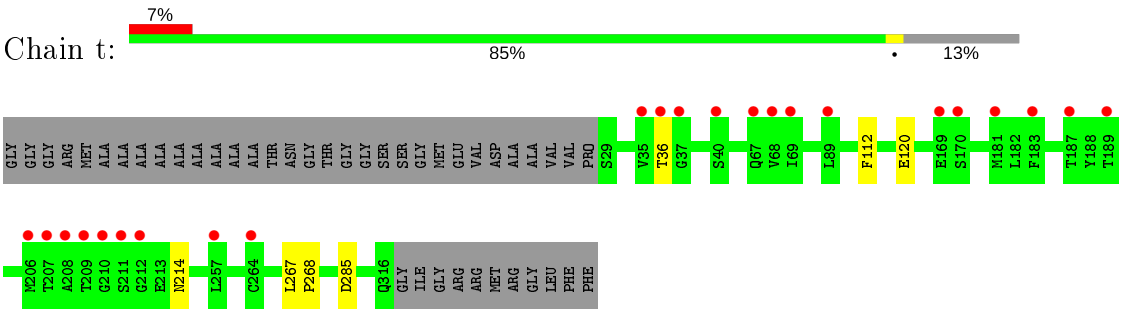
• Molecule 6: COP9 signalosome complex subunit 6

Chain l:



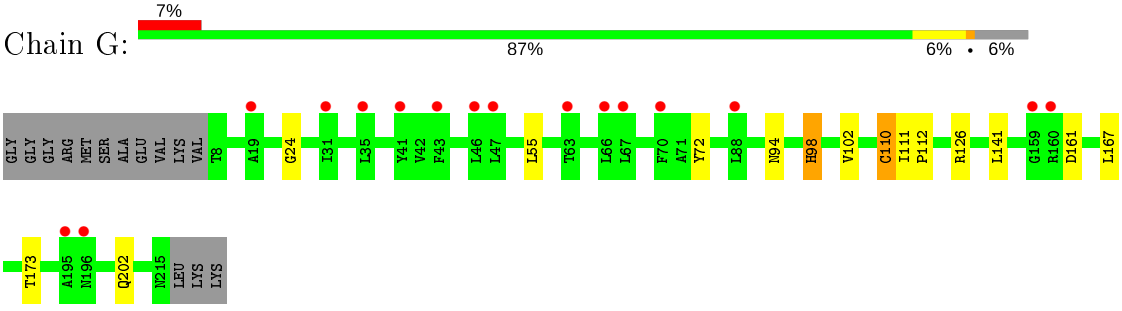
• Molecule 6: COP9 signalosome complex subunit 6

Chain t:



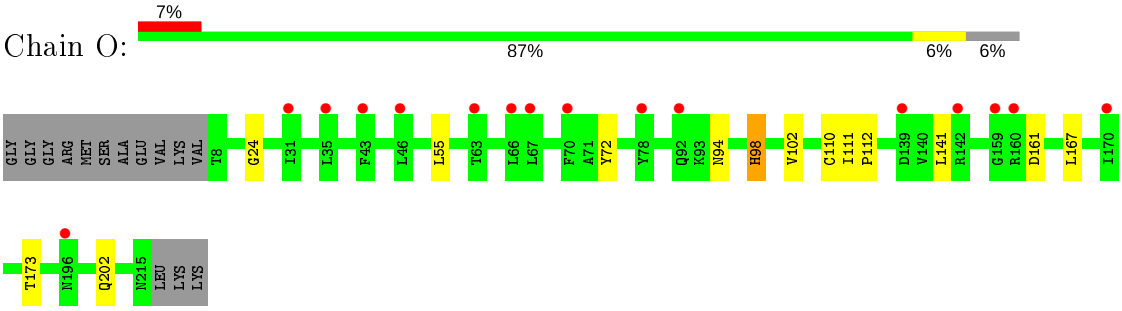
• Molecule 7: COP9 signalosome complex subunit 7a

Chain G:



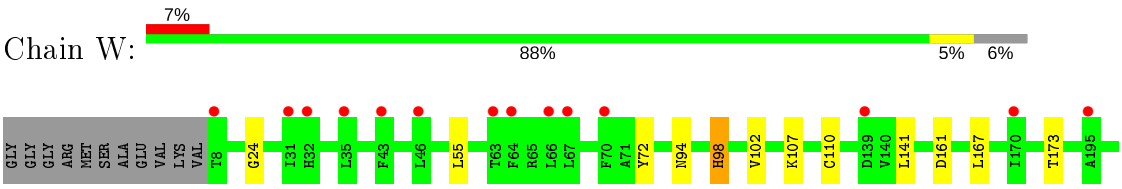
• Molecule 7: COP9 signalosome complex subunit 7a

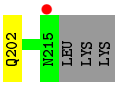
Chain O:



• Molecule 7: COP9 signalosome complex subunit 7a

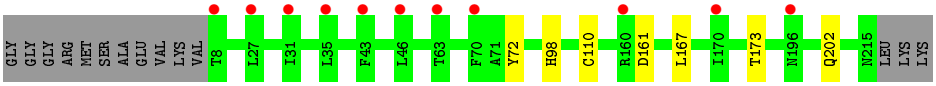
Chain W:





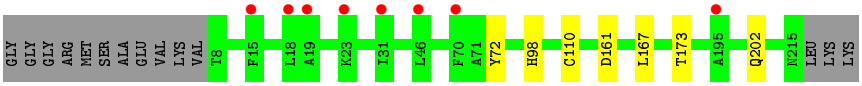
• Molecule 7: COP9 signalosome complex subunit 7a

Chain e:



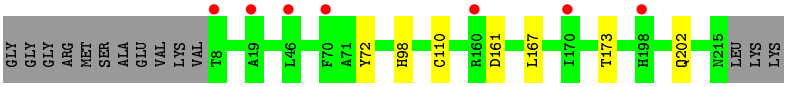
• Molecule 7: COP9 signalosome complex subunit 7a

Chain m:



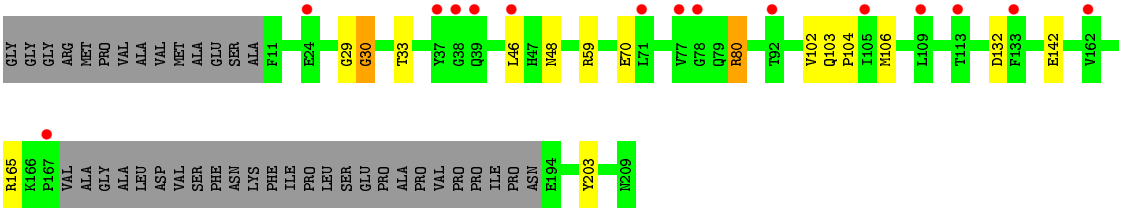
• Molecule 7: COP9 signalosome complex subunit 7a

Chain u:



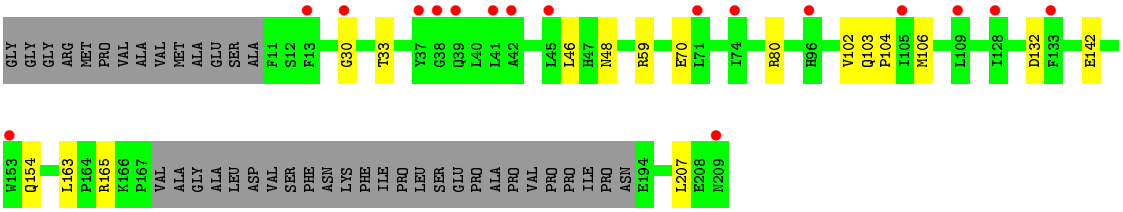
• Molecule 8: COP9 signalosome complex subunit 8

Chain H:



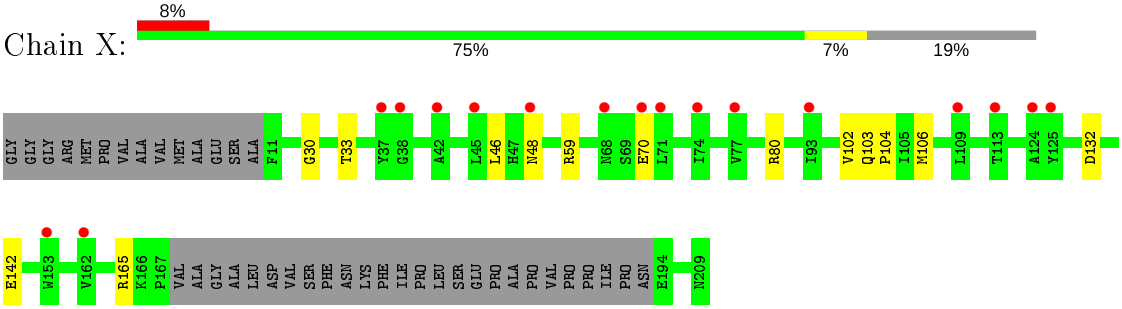
• Molecule 8: COP9 signalosome complex subunit 8

Chain P:



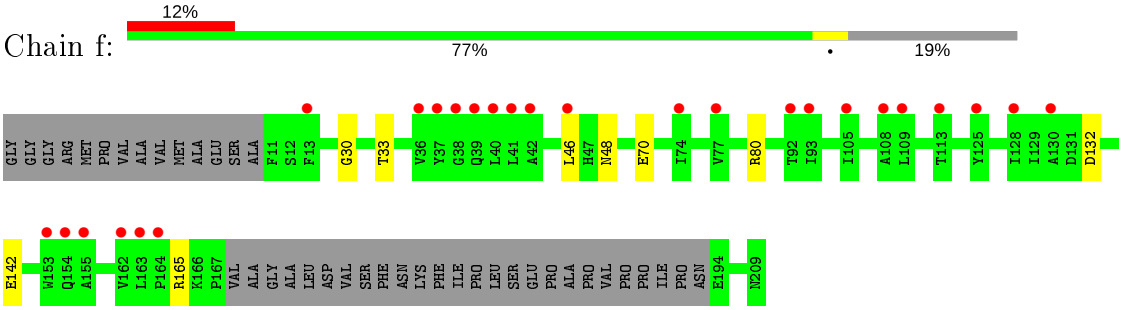
• Molecule 8: COP9 signalosome complex subunit 8

Chain X:



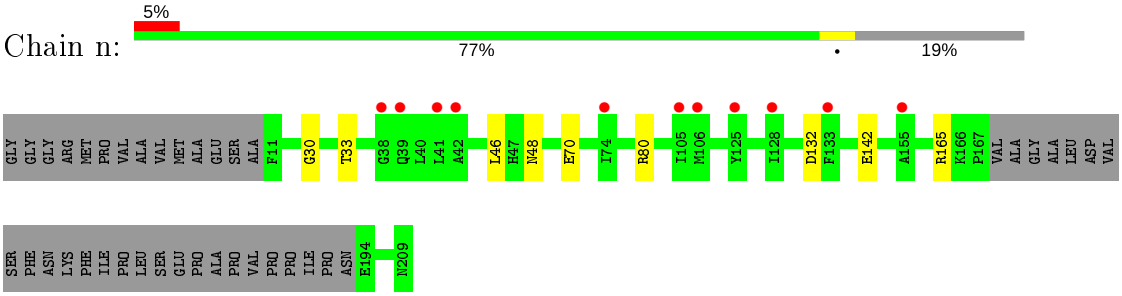
- Molecule 8: COP9 signalosome complex subunit 8

Chain f:



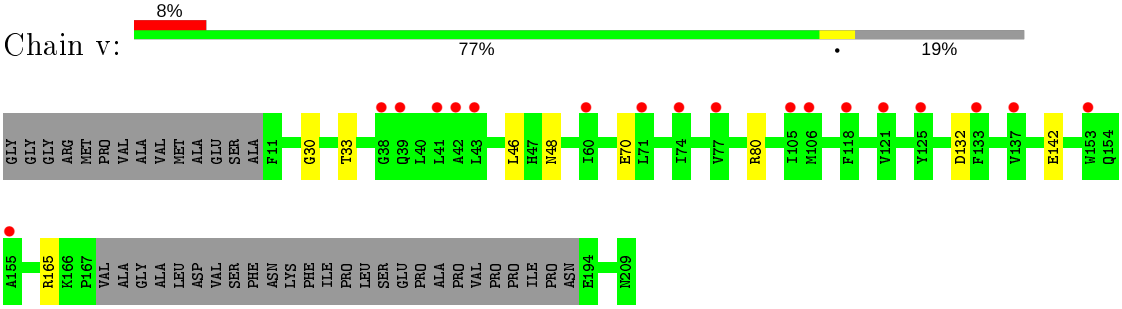
- Molecule 8: COP9 signalosome complex subunit 8

Chain n:



- Molecule 8: COP9 signalosome complex subunit 8

Chain v:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	150.64Å 150.98Å 336.72Å 92.34° 92.62° 119.88°	Depositor
Resolution (Å)	49.64 – 5.50 49.63 – 5.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.64-5.50) 83.8 (49.63-5.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.56 (at 5.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.254 , 0.282 0.293 , 0.325	Depositor DCC
R_{free} test set	1948 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å^2)	264.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 123.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	124428	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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

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	0.30	0/3404	0.46	0/4588
1	I	0.30	0/3404	0.47	0/4588
1	Q	0.30	0/3404	0.47	0/4588
1	Y	0.30	0/3404	0.47	0/4588
1	g	0.30	0/3404	0.47	0/4588
1	o	0.30	0/3404	0.47	0/4588
2	B	0.30	0/3360	0.45	0/4519
2	J	0.30	0/3360	0.45	0/4519
2	R	0.31	0/3360	0.45	0/4519
2	Z	0.30	0/3360	0.44	0/4519
2	h	0.30	0/3360	0.45	0/4519
2	p	0.30	0/3360	0.45	0/4519
3	C	0.29	0/3250	0.45	0/4390
3	K	0.29	0/3250	0.45	0/4390
3	S	0.29	0/3250	0.45	0/4390
3	a	0.29	0/3250	0.45	0/4390
3	i	0.29	0/3250	0.45	0/4390
3	q	0.29	0/3250	0.45	0/4390
4	D	0.33	0/3303	0.50	1/4460 (0.0%)
4	L	0.34	0/3303	0.49	0/4460
4	T	0.35	0/3303	0.51	1/4460 (0.0%)
4	b	0.34	0/3303	0.51	2/4460 (0.0%)
4	j	0.34	0/3302	0.52	1/4457 (0.0%)
4	r	0.35	0/3302	0.51	1/4457 (0.0%)
5	E	0.29	0/2417	0.44	0/3266
5	M	0.29	0/2417	0.44	0/3266
5	U	0.29	0/2417	0.45	0/3266
5	c	0.29	0/2417	0.44	0/3266
5	k	0.30	0/2417	0.45	0/3266
5	s	0.29	0/2417	0.45	0/3266
6	F	0.51	1/2310 (0.0%)	0.46	1/3133 (0.0%)
6	N	0.51	1/2310 (0.0%)	0.47	1/3133 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	V	0.48	1/2310 (0.0%)	0.47	1/3133 (0.0%)
6	d	0.50	1/2310 (0.0%)	0.46	1/3133 (0.0%)
6	l	0.31	0/2310	0.45	0/3133
6	t	0.30	0/2310	0.45	0/3133
7	G	0.31	0/1652	0.46	0/2239
7	O	0.30	0/1652	0.46	0/2239
7	W	0.30	0/1652	0.46	0/2239
7	e	0.31	0/1652	0.46	0/2239
7	m	0.31	0/1652	0.46	0/2239
7	u	0.31	0/1652	0.46	0/2239
8	H	0.30	0/1416	0.44	0/1924
8	P	0.30	0/1416	0.45	0/1924
8	X	0.30	0/1416	0.45	0/1924
8	f	0.29	0/1416	0.44	0/1924
8	n	0.30	0/1416	0.45	0/1924
8	v	0.30	0/1416	0.45	0/1924
All	All	0.32	4/126670 (0.0%)	0.46	10/171108 (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
5	E	0	1
5	M	0	1
5	U	0	1
5	c	0	1
5	k	0	1
5	s	0	1
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	217	VAL	C-N	20.09	1.80	1.34
6	N	217	VAL	C-N	19.82	1.79	1.34
6	d	217	VAL	C-N	19.29	1.78	1.34
6	V	217	VAL	C-N	17.96	1.75	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	217	VAL	O-C-N	-7.51	110.69	122.70
4	b	264	LEU	CB-CG-CD1	6.28	121.67	111.00
4	r	274	ARG	NE-CZ-NH1	6.18	123.39	120.30
4	T	40	GLU	CB-CA-C	6.08	122.56	110.40
4	D	364	ARG	NE-CZ-NH1	6.00	123.30	120.30
4	b	274	ARG	NE-CZ-NH1	5.85	123.22	120.30
6	d	217	VAL	O-C-N	-5.66	113.64	122.70
6	F	217	VAL	O-C-N	-5.57	113.79	122.70
4	j	83	GLU	CG-CD-OE2	5.55	129.41	118.30
6	N	217	VAL	O-C-N	-5.40	114.06	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	163	GLU	Peptide
5	M	163	GLU	Peptide
5	U	163	GLU	Peptide
5	c	163	GLU	Peptide
5	k	163	GLU	Peptide
5	s	163	GLU	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	3385	16	0
1	I	3348	0	3385	14	0
1	Q	3348	0	3385	14	0
1	Y	3348	0	3385	12	0
1	g	3348	0	3385	0	0
1	o	3348	0	3385	0	0
2	B	3304	0	3350	9	0
2	J	3304	0	3350	10	0
2	R	3304	0	3350	9	0
2	Z	3304	0	3350	9	0
2	h	3304	0	3350	0	0
2	p	3304	0	3350	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3191	0	3208	19	0
3	K	3191	0	3208	12	0
3	S	3191	0	3208	15	0
3	a	3191	0	3208	0	0
3	i	3191	0	3208	0	0
3	q	3191	0	3208	0	0
4	D	3251	0	3253	15	0
4	L	3251	0	3253	9	0
4	T	3251	0	3253	12	0
4	b	3251	0	3253	0	0
4	j	3251	0	3252	0	0
4	r	3251	0	3252	0	0
5	E	2366	0	2340	8	0
5	M	2366	0	2340	11	0
5	U	2366	0	2340	15	0
5	c	2366	0	2340	0	0
5	k	2366	0	2340	0	0
5	s	2366	0	2340	0	0
6	F	2263	0	2235	14	0
6	N	2263	0	2235	11	0
6	V	2263	0	2235	14	0
6	d	2263	0	2235	0	0
6	l	2263	0	2236	0	0
6	t	2263	0	2236	0	0
7	G	1631	0	1654	7	0
7	O	1631	0	1654	4	0
7	W	1631	0	1654	5	0
7	e	1631	0	1654	0	0
7	m	1631	0	1654	0	0
7	u	1631	0	1654	0	0
8	H	1383	0	1366	7	0
8	P	1383	0	1366	5	0
8	X	1383	0	1366	3	0
8	f	1383	0	1366	0	0
8	n	1383	0	1366	0	0
8	v	1383	0	1366	0	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
9	U	1	0	0	0	0
9	c	1	0	0	0	0
9	k	1	0	0	0	0
9	s	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	124428	0	124746	232	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 2.

All (232) 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:V:217:VAL:C	6:V:218:ALA:N	1.75	1.39
6:N:217:VAL:C	6:N:218:ALA:N	1.79	1.35
6:F:217:VAL:C	6:F:218:ALA:N	1.80	1.32
5:U:116:TYR:CE2	6:V:114:GLN:HG3	2.32	0.65
4:T:37:SER:O	4:T:40:GLU:OE1	2.17	0.61
3:C:153:LYS:O	8:H:59:ARG:NH1	2.33	0.61
3:K:88:CYS:O	3:K:90:GLY:N	2.35	0.59
3:C:88:CYS:O	3:C:90:GLY:N	2.36	0.58
4:D:254:ARG:HD3	6:F:174:ILE:HG13	1.85	0.58
7:W:24:GLY:HA2	7:W:55:LEU:HD21	1.86	0.58
7:O:24:GLY:HA2	7:O:55:LEU:HD21	1.86	0.58
3:S:88:CYS:O	3:S:90:GLY:N	2.36	0.58
4:D:140:ASN:HA	5:M:193:TYR:HD1	1.68	0.57
7:G:24:GLY:HA2	7:G:55:LEU:HD21	1.86	0.57
4:T:140:ASN:OD1	4:T:141:VAL:N	2.37	0.57
6:V:267:LEU:O	6:V:268:PRO:C	2.43	0.57
6:F:267:LEU:O	6:F:268:PRO:C	2.42	0.57
6:N:267:LEU:O	6:N:268:PRO:C	2.42	0.56
3:K:64:VAL:HG12	3:K:64:VAL:O	2.06	0.55
4:L:254:ARG:HD3	6:N:174:ILE:HG13	1.88	0.55
6:F:272:THR:HG22	7:G:110:CYS:SG	2.46	0.55
3:C:64:VAL:O	3:C:64:VAL:HG12	2.06	0.55
3:S:64:VAL:HG12	3:S:64:VAL:O	2.07	0.55
5:U:63:LEU:HB3	6:V:46:LEU:HD13	1.89	0.53
1:Y:496:LEU:HD11	2:Z:443:ALA:HB2	1.89	0.53
5:M:116:TYR:CE2	6:N:114:GLN:HG3	2.44	0.53
5:M:280:LEU:HD21	6:N:303:ASN:HD21	1.74	0.52
2:J:441:LYS:HE3	5:M:280:LEU:HD22	1.91	0.52
5:U:280:LEU:HD21	6:V:303:ASN:HD21	1.75	0.52
2:Z:283:ALA:O	2:Z:287:MET:N	2.43	0.52
2:B:272:ARG:O	2:B:276:CYS:N	2.44	0.51
2:J:272:ARG:O	2:J:276:CYS:N	2.44	0.51
4:D:385:LEU:HD22	6:F:234:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:283:ALA:O	2:R:287:MET:N	2.43	0.51
3:K:367:TYR:HA	3:K:372:MET:HG3	1.92	0.50
2:R:272:ARG:O	2:R:276:CYS:N	2.44	0.50
4:T:254:ARG:HD3	6:V:174:ILE:HG13	1.93	0.50
3:C:367:TYR:HA	3:C:372:MET:HG3	1.92	0.50
5:E:116:TYR:CE2	6:F:114:GLN:HG3	2.46	0.50
2:B:283:ALA:O	2:B:287:MET:N	2.42	0.50
2:J:283:ALA:O	2:J:287:MET:N	2.42	0.50
1:A:486:ALA:HB3	3:C:386:LEU:HD21	1.94	0.50
3:S:367:TYR:HA	3:S:372:MET:HG3	1.93	0.49
1:I:209:LEU:HG	1:I:217:ALA:HB1	1.94	0.49
1:I:486:ALA:HB3	3:K:386:LEU:HD21	1.94	0.49
1:Y:209:LEU:HG	1:Y:217:ALA:HB1	1.94	0.49
1:A:209:LEU:HG	1:A:217:ALA:HB1	1.95	0.49
1:Q:209:LEU:HG	1:Q:217:ALA:HB1	1.94	0.49
2:Z:272:ARG:O	2:Z:276:CYS:N	2.44	0.49
1:A:504:SER:HA	3:C:215:ALA:HB2	1.95	0.49
1:A:496:LEU:HD11	2:B:443:ALA:HB2	1.94	0.49
1:Q:486:ALA:HB3	3:S:386:LEU:HD21	1.95	0.48
4:L:275:GLY:N	4:L:329:GLU:OE2	2.45	0.48
3:K:153:LYS:O	8:P:59:ARG:NH1	2.44	0.48
1:Q:381:LEU:HG	1:Q:402:TYR:CE2	2.49	0.48
4:D:275:GLY:N	4:D:329:GLU:OE2	2.46	0.48
1:A:242:ILE:HG23	1:A:254:VAL:HG13	1.96	0.48
1:A:264:THR:HB	1:A:265:PRO:HD3	1.96	0.48
1:I:242:ILE:HG23	1:I:254:VAL:HG13	1.96	0.48
1:Q:264:THR:HB	1:Q:265:PRO:HD3	1.96	0.48
1:I:264:THR:HB	1:I:265:PRO:HD3	1.96	0.47
1:Q:242:ILE:HG23	1:Q:254:VAL:HG13	1.96	0.47
3:S:70:SER:O	3:S:71:VAL:HG22	2.14	0.47
8:X:103:GLN:N	8:X:104:PRO:HD2	2.29	0.47
1:Y:242:ILE:HG23	1:Y:254:VAL:HG13	1.97	0.47
1:A:381:LEU:HG	1:A:402:TYR:CE2	2.48	0.47
5:U:333:ILE:HG21	7:W:107:LYS:HA	1.95	0.47
1:Y:264:THR:HB	1:Y:265:PRO:HD3	1.96	0.47
3:C:70:SER:O	3:C:71:VAL:HG22	2.14	0.47
3:S:152:ALA:O	3:S:154:CYS:N	2.47	0.47
4:T:19:HIS:CE1	4:T:61:ILE:HD13	2.49	0.47
3:C:152:ALA:O	3:C:154:CYS:N	2.47	0.47
8:H:103:GLN:N	8:H:104:PRO:HD2	2.30	0.47
3:K:152:ALA:O	3:K:154:CYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:399:ALA:HB1	6:N:237:LEU:HD22	1.95	0.47
3:K:70:SER:O	3:K:71:VAL:HG22	2.14	0.47
4:L:385:LEU:HD22	6:N:234:ARG:HD2	1.97	0.47
5:E:163:GLU:HG3	5:E:164:PRO:HD3	1.97	0.47
6:N:297:LYS:HD3	8:P:207:LEU:HD23	1.98	0.46
1:Q:444:ILE:HG21	3:S:313:THR:HA	1.98	0.46
1:I:381:LEU:HG	1:I:402:TYR:CE2	2.49	0.46
8:P:103:GLN:N	8:P:104:PRO:HD2	2.30	0.46
6:V:217:VAL:CA	6:V:218:ALA:N	2.74	0.46
1:Y:381:LEU:HG	1:Y:402:TYR:CE2	2.49	0.46
1:A:468:ARG:NH2	3:C:367:TYR:O	2.46	0.46
5:M:163:GLU:HG3	5:M:164:PRO:HD3	1.98	0.46
3:K:9:VAL:HG21	3:K:42:LEU:HD22	1.98	0.46
1:Y:395:ALA:N	1:Y:396:PRO:CD	2.79	0.46
3:C:9:VAL:HG21	3:C:42:LEU:HD22	1.98	0.46
4:D:399:ALA:HB1	6:F:237:LEU:HD22	1.98	0.46
6:F:272:THR:CG2	7:G:110:CYS:SG	3.03	0.46
4:D:269:LEU:HA	6:F:79:ARG:HD3	1.98	0.45
5:E:163:GLU:HG3	5:E:164:PRO:CD	2.46	0.45
3:S:9:VAL:HG21	3:S:42:LEU:HD22	1.98	0.45
5:U:163:GLU:HG3	5:U:164:PRO:HD3	1.97	0.45
4:T:275:GLY:N	4:T:329:GLU:OE2	2.47	0.45
4:D:274:ARG:HD3	4:D:274:ARG:HA	1.82	0.45
5:U:163:GLU:HG3	5:U:164:PRO:CD	2.46	0.45
5:M:163:GLU:HG3	5:M:164:PRO:CD	2.47	0.45
1:Q:395:ALA:N	1:Q:396:PRO:CD	2.80	0.45
3:C:119:ARG:HD3	8:H:29:GLY:HA2	1.99	0.45
6:F:244:ALA:HB1	6:F:250:VAL:HG21	1.99	0.45
5:U:124:ALA:HB1	5:U:129:ARG:HB2	1.99	0.45
4:L:230:LEU:CD1	4:L:264:LEU:HD22	2.47	0.45
3:S:341:MET:HB3	3:S:347:ILE:HG22	1.99	0.45
4:T:269:LEU:HA	6:V:79:ARG:HD3	1.99	0.45
4:D:230:LEU:CD1	4:D:264:LEU:HD22	2.48	0.44
2:R:293:PRO:CG	2:R:315:VAL:HG21	2.47	0.44
4:T:230:LEU:CD1	4:T:264:LEU:HD22	2.47	0.44
1:I:94:LEU:HD22	1:I:98:GLU:HG3	1.99	0.44
6:N:244:ALA:HB1	6:N:250:VAL:HG21	2.00	0.44
6:V:244:ALA:HB1	6:V:250:VAL:HG21	2.00	0.44
2:Z:413:HIS:O	2:Z:415:LYS:N	2.51	0.44
3:C:118:LEU:HD23	8:H:30:GLY:O	2.18	0.44
3:C:341:MET:HB3	3:C:347:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ALA:HB2	1:A:312:ASP:HB3	1.99	0.44
1:A:395:ALA:N	1:A:396:PRO:CD	2.80	0.44
1:A:94:LEU:HD22	1:A:98:GLU:HG3	2.00	0.44
1:I:280:ALA:HB2	1:I:312:ASP:HB3	1.99	0.44
2:J:293:PRO:CG	2:J:315:VAL:HG21	2.47	0.44
1:Y:280:ALA:HB2	1:Y:312:ASP:HB3	1.99	0.44
1:I:395:ALA:N	1:I:396:PRO:CD	2.81	0.44
2:Z:293:PRO:CG	2:Z:315:VAL:HG21	2.48	0.44
2:R:85:PHE:CZ	2:R:123:LYS:HG3	2.53	0.44
2:B:413:HIS:O	2:B:415:LYS:N	2.51	0.44
5:E:124:ALA:HB1	5:E:129:ARG:HB2	1.99	0.44
6:V:110:GLU:O	6:V:114:GLN:HG2	2.18	0.44
1:Y:108:PRO:O	1:Y:109:THR:OG1	2.31	0.44
1:Y:94:LEU:HD22	1:Y:98:GLU:HG3	2.00	0.44
2:Z:85:PHE:CZ	2:Z:123:LYS:HG3	2.52	0.44
1:A:486:ALA:CB	3:C:386:LEU:HD21	2.47	0.43
2:B:293:PRO:CG	2:B:315:VAL:HG21	2.48	0.43
3:K:341:MET:HB3	3:K:347:ILE:HG22	2.00	0.43
5:M:124:ALA:HB1	5:M:129:ARG:HB2	1.99	0.43
6:N:110:GLU:O	6:N:114:GLN:HG2	2.18	0.43
8:P:102:VAL:HG12	8:P:106:MET:HG2	2.00	0.43
2:J:85:PHE:CZ	2:J:123:LYS:HG3	2.53	0.43
4:T:365:GLU:O	4:T:366:ALA:HB3	2.18	0.43
6:F:110:GLU:O	6:F:114:GLN:HG2	2.18	0.43
7:O:102:VAL:HG22	7:O:141:LEU:HD21	2.00	0.43
1:Q:280:ALA:HB2	1:Q:312:ASP:HB3	1.99	0.43
1:Q:94:LEU:HD22	1:Q:98:GLU:HG3	1.99	0.43
7:W:102:VAL:HG22	7:W:141:LEU:HD21	2.00	0.43
2:B:85:PHE:CZ	2:B:123:LYS:HG3	2.53	0.43
3:S:153:LYS:O	8:X:59:ARG:NH1	2.50	0.43
1:Q:415:SER:N	1:Q:416:PRO:HD2	2.33	0.43
8:H:102:VAL:HG12	8:H:106:MET:HG2	2.00	0.43
3:S:138:LEU:HB2	3:S:166:MET:HG3	2.01	0.43
1:Q:486:ALA:CB	3:S:386:LEU:HD21	2.49	0.43
5:U:120:TYR:HA	6:V:111:GLN:OE1	2.19	0.43
5:U:333:ILE:CG2	7:W:107:LYS:HA	2.48	0.43
4:D:327:LEU:HD13	7:G:126:ARG:NH1	2.33	0.43
1:A:477:LEU:O	1:A:481:GLU:HG2	2.19	0.43
5:E:261:TYR:CZ	5:E:265:GLN:HG3	2.54	0.43
1:I:128:VAL:HG11	1:I:171:ARG:HD3	2.01	0.43
2:J:413:HIS:O	2:J:415:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:189:TYR:CE2	5:U:195:PRO:HB3	2.54	0.42
8:X:102:VAL:HG12	8:X:106:MET:HG2	2.00	0.42
7:G:102:VAL:HG22	7:G:141:LEU:HD21	2.00	0.42
4:L:365:GLU:O	4:L:366:ALA:HB3	2.19	0.42
1:Q:477:LEU:O	1:Q:481:GLU:HG2	2.18	0.42
2:R:413:HIS:O	2:R:415:LYS:N	2.52	0.42
2:Z:101:SER:O	2:Z:102:ALA:HB3	2.19	0.42
2:B:101:SER:O	2:B:102:ALA:HB3	2.19	0.42
2:J:101:SER:O	2:J:102:ALA:HB3	2.19	0.42
3:S:94:ARG:NH1	3:S:137:GLN:OE1	2.52	0.42
3:C:94:ARG:NH1	3:C:137:GLN:OE1	2.52	0.42
1:I:477:LEU:O	1:I:481:GLU:HG2	2.19	0.42
3:K:94:ARG:NH1	3:K:137:GLN:OE1	2.53	0.42
1:Q:128:VAL:HG11	1:Q:171:ARG:HD3	2.01	0.42
1:Y:477:LEU:O	1:Y:481:GLU:HG2	2.19	0.42
4:D:365:GLU:O	4:D:366:ALA:HB3	2.19	0.42
6:V:155:ASN:HB3	6:V:164:PRO:HB2	2.01	0.42
5:M:261:TYR:CZ	5:M:265:GLN:HG3	2.55	0.42
1:Y:128:VAL:HG11	1:Y:171:ARG:HD3	2.01	0.42
1:A:128:VAL:HG11	1:A:171:ARG:HD3	2.02	0.42
4:D:274:ARG:NH1	4:D:327:LEU:HD11	2.35	0.42
6:N:155:ASN:HB3	6:N:164:PRO:HB2	2.00	0.42
2:Z:192:THR:HA	2:Z:228:ILE:HG13	2.02	0.42
6:F:155:ASN:HB3	6:F:164:PRO:HB2	2.01	0.42
5:M:189:TYR:CE2	5:M:195:PRO:HB3	2.55	0.42
1:Y:415:SER:N	1:Y:416:PRO:HD2	2.35	0.42
5:E:189:TYR:CE2	5:E:195:PRO:HB3	2.55	0.41
4:T:149:LEU:HD21	4:T:187:TYR:HA	2.02	0.41
1:A:415:SER:N	1:A:416:PRO:HD2	2.34	0.41
7:G:94:ASN:O	7:G:98:HIS:ND1	2.53	0.41
1:I:415:SER:N	1:I:416:PRO:HD2	2.34	0.41
3:C:138:LEU:HB2	3:C:166:MET:HG3	2.01	0.41
2:R:101:SER:O	2:R:102:ALA:HB3	2.19	0.41
4:T:58:SER:OG	4:T:60:VAL:HG22	2.20	0.41
3:C:377:ASP:OD1	8:H:203:TYR:OH	2.37	0.41
4:D:149:LEU:HD21	4:D:187:TYR:HA	2.02	0.41
2:J:192:THR:HA	2:J:228:ILE:HG13	2.02	0.41
5:U:176:ILE:HG23	6:V:194:GLU:HG2	2.02	0.41
3:K:138:LEU:HB2	3:K:166:MET:HG3	2.01	0.41
2:B:192:THR:HA	2:B:228:ILE:HG13	2.03	0.41
3:C:292:MET:HA	3:C:295:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:80:ARG:N	8:H:80:ARG:HD2	2.36	0.41
1:I:482:PHE:CD1	2:J:435:ASN:HB2	2.55	0.41
2:R:141:ASP:OD2	2:R:144:ASN:ND2	2.53	0.41
4:L:308:ASN:HB3	4:L:328:LEU:HD22	2.03	0.41
5:E:129:ARG:HG3	6:F:57:ARG:NH2	2.35	0.41
2:R:192:THR:HA	2:R:228:ILE:HG13	2.03	0.41
4:T:308:ASN:HB3	4:T:328:LEU:HD22	2.02	0.41
4:D:308:ASN:HB3	4:D:328:LEU:HD22	2.03	0.41
4:L:149:LEU:HD21	4:L:187:TYR:HA	2.02	0.41
5:M:175:THR:HG23	5:M:181:VAL:HA	2.02	0.41
5:U:261:TYR:CZ	5:U:265:GLN:HG3	2.55	0.41
2:Z:141:ASP:OD2	2:Z:144:ASN:ND2	2.54	0.41
4:D:140:ASN:HA	5:M:193:TYR:CD1	2.52	0.41
3:K:292:MET:HA	3:K:295:VAL:HG12	2.02	0.41
4:L:1:MET:N	4:L:40:GLU:OE1	2.54	0.41
7:O:111:ILE:HG22	7:O:112:PRO:O	2.21	0.41
5:U:120:TYR:N	6:V:111:GLN:HE22	2.19	0.41
1:A:258:VAL:HG11	1:A:289:ALA:HB2	2.03	0.40
3:C:46:LEU:O	3:C:48:ALA:N	2.54	0.40
4:T:374:ILE:HD13	5:U:324:LYS:HD2	2.03	0.40
7:W:94:ASN:O	7:W:98:HIS:ND1	2.54	0.40
2:B:141:ASP:OD2	2:B:144:ASN:ND2	2.54	0.40
4:D:1:MET:N	4:D:40:GLU:OE1	2.55	0.40
2:R:303:LYS:HA	2:R:308:ILE:HD11	2.04	0.40
2:J:141:ASP:OD2	2:J:144:ASN:ND2	2.54	0.40
3:S:292:MET:HA	3:S:295:VAL:HG12	2.02	0.40
5:E:280:LEU:HD21	6:F:303:ASN:HD21	1.87	0.40
7:G:111:ILE:HG22	7:G:112:PRO:O	2.21	0.40
1:I:148:ALA:HB3	1:I:149:PRO:HD3	2.03	0.40
1:I:258:VAL:HG11	1:I:289:ALA:HB2	2.03	0.40
7:O:94:ASN:O	7:O:98:HIS:ND1	2.54	0.40
8:P:154:GLN:HB3	8:P:163:LEU:HB2	2.04	0.40
1:Q:148:ALA:HB3	1:Q:149:PRO:HD3	2.03	0.40
3:S:249:VAL:HA	3:S:253:ILE:HB	2.04	0.40
5:U:175:THR:HG23	5:U:181:VAL:HA	2.03	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%)	374 (90%)	37 (9%)	4 (1%)	15	53
1	I	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	15	53
1	Q	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	15	53
1	Y	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	15	53
1	g	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	15	53
1	o	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	15	53
2	B	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	4	28
2	J	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	4	28
2	R	397/447 (89%)	353 (89%)	32 (8%)	12 (3%)	4	28
2	Z	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	4	28
2	h	397/447 (89%)	351 (88%)	36 (9%)	10 (2%)	5	32
2	p	397/447 (89%)	351 (88%)	35 (9%)	11 (3%)	5	30
3	C	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	3	24
3	K	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	3	25
3	S	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	3	25
3	a	399/427 (93%)	341 (86%)	43 (11%)	15 (4%)	3	24
3	i	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	3	24
3	q	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	3	24
4	D	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	15	53
4	L	404/410 (98%)	373 (92%)	27 (7%)	4 (1%)	15	53
4	T	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	15	53
4	b	404/410 (98%)	374 (93%)	26 (6%)	4 (1%)	15	53
4	j	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	15	53
4	r	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	15	53
5	E	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	M	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	7 37
5	U	294/325 (90%)	262 (89%)	28 (10%)	4 (1%)	11 45
5	c	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	7 37
5	k	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	7 37
5	s	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	7 37
6	F	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	11 45
6	N	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	11 45
6	V	286/331 (86%)	258 (90%)	24 (8%)	4 (1%)	11 45
6	d	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	11 45
6	l	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	11 45
6	t	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	11 45
7	G	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	29 69
7	O	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	29 69
7	W	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	29 69
7	e	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	29 69
7	m	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	29 69
7	u	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	29 69
8	H	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	13 49
8	P	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	13 49
8	X	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	13 49
8	f	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	13 49
8	n	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	13 49
8	v	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	13 49
All	All	15416/17130 (90%)	13844 (90%)	1291 (8%)	281 (2%)	8 40

All (281) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	229	PRO
2	B	414	GLN
3	C	51	VAL
3	C	89	ASN
3	C	364	PRO
3	C	401	PRO

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Mol	Chain	Res	Type
5	E	164	PRO
6	F	267	LEU
6	F	268	PRO
2	J	414	GLN
3	K	51	VAL
3	K	89	ASN
3	K	364	PRO
3	K	401	PRO
5	M	164	PRO
6	N	267	LEU
6	N	268	PRO
2	R	414	GLN
3	S	51	VAL
3	S	89	ASN
3	S	364	PRO
3	S	401	PRO
5	U	164	PRO
6	V	267	LEU
6	V	268	PRO
2	Z	414	GLN
3	a	51	VAL
3	a	89	ASN
3	a	364	PRO
3	a	401	PRO
5	c	164	PRO
6	d	267	LEU
6	d	268	PRO
2	h	229	PRO
2	h	414	GLN
3	i	51	VAL
3	i	89	ASN
3	i	364	PRO
3	i	401	PRO
5	k	164	PRO
6	l	267	LEU
6	l	268	PRO
2	p	229	PRO
2	p	414	GLN
3	q	51	VAL
3	q	89	ASN
3	q	364	PRO
3	q	401	PRO

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Mol	Chain	Res	Type
5	s	164	PRO
6	t	267	LEU
6	t	268	PRO
2	B	61	GLU
2	B	289	SER
2	B	413	HIS
3	C	47	GLY
3	C	86	SER
3	C	91	GLU
3	C	136	ASN
4	D	362	GLU
6	F	214	ASN
8	H	48	ASN
2	J	61	GLU
2	J	229	PRO
2	J	289	SER
2	J	413	HIS
3	K	47	GLY
3	K	86	SER
3	K	91	GLU
3	K	136	ASN
4	L	362	GLU
6	N	214	ASN
8	P	48	ASN
2	R	61	GLU
2	R	229	PRO
2	R	289	SER
2	R	413	HIS
3	S	47	GLY
3	S	86	SER
3	S	91	GLU
3	S	136	ASN
4	T	362	GLU
5	U	198	GLU
6	V	214	ASN
8	X	48	ASN
2	Z	61	GLU
2	Z	229	PRO
2	Z	289	SER
2	Z	413	HIS
3	a	47	GLY
3	a	86	SER

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Mol	Chain	Res	Type
3	a	91	GLU
3	a	136	ASN
4	b	362	GLU
6	d	214	ASN
8	f	48	ASN
2	h	61	GLU
2	h	289	SER
2	h	413	HIS
3	i	47	GLY
3	i	86	SER
3	i	91	GLU
3	i	136	ASN
4	j	362	GLU
6	l	214	ASN
8	n	48	ASN
2	p	61	GLU
2	p	289	SER
2	p	413	HIS
3	q	47	GLY
3	q	86	SER
3	q	91	GLU
3	q	136	ASN
4	r	362	GLU
6	t	214	ASN
8	v	48	ASN
2	B	43	LYS
2	B	293	PRO
2	B	296	SER
3	C	33	GLU
3	C	114	ARG
3	C	172	GLU
4	D	294	ALA
4	D	366	ALA
5	E	198	GLU
5	E	201	SER
8	H	30	GLY
2	J	43	LYS
2	J	293	PRO
2	J	296	SER
3	K	33	GLU
3	K	114	ARG
3	K	172	GLU

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Mol	Chain	Res	Type
4	L	294	ALA
4	L	366	ALA
5	M	198	GLU
5	M	201	SER
6	N	36	THR
8	P	30	GLY
2	R	43	LYS
2	R	293	PRO
2	R	296	SER
3	S	33	GLU
3	S	114	ARG
3	S	172	GLU
4	T	294	ALA
4	T	366	ALA
8	X	30	GLY
2	Z	43	LYS
2	Z	293	PRO
2	Z	296	SER
3	a	33	GLU
3	a	114	ARG
3	a	172	GLU
4	b	294	ALA
4	b	366	ALA
5	c	198	GLU
5	c	201	SER
8	f	30	GLY
2	h	43	LYS
2	h	293	PRO
2	h	296	SER
3	i	33	GLU
3	i	114	ARG
3	i	172	GLU
4	j	294	ALA
4	j	366	ALA
5	k	198	GLU
6	l	36	THR
8	n	30	GLY
2	p	43	LYS
2	p	293	PRO
2	p	296	SER
3	q	33	GLU
3	q	114	ARG

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Mol	Chain	Res	Type
3	q	172	GLU
4	r	294	ALA
4	r	366	ALA
5	s	198	GLU
5	s	201	SER
8	v	30	GLY
2	B	396	ASN
6	F	36	THR
2	J	396	ASN
2	R	396	ASN
6	V	36	THR
2	Z	396	ASN
6	d	36	THR
2	h	396	ASN
5	k	201	SER
2	p	396	ASN
6	t	36	THR
1	A	275	ASP
1	A	276	SER
1	A	314	CYS
3	C	71	VAL
3	C	117	PRO
3	C	329	SER
5	E	200	PRO
1	I	275	ASP
1	I	276	SER
1	I	314	CYS
3	K	71	VAL
3	K	117	PRO
3	K	329	SER
5	M	200	PRO
1	Q	275	ASP
1	Q	276	SER
1	Q	314	CYS
2	R	44	GLU
3	S	71	VAL
3	S	117	PRO
3	S	329	SER
5	U	281	GLY
1	Y	275	ASP
1	Y	276	SER
1	Y	314	CYS

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Mol	Chain	Res	Type
3	a	71	VAL
3	a	117	PRO
3	a	329	SER
4	b	159	ASP
5	c	200	PRO
5	c	281	GLY
1	g	275	ASP
1	g	276	SER
1	g	314	CYS
3	i	71	VAL
3	i	117	PRO
3	i	175	ALA
3	i	329	SER
4	j	159	ASP
1	o	275	ASP
1	o	276	SER
1	o	314	CYS
3	q	71	VAL
3	q	117	PRO
3	q	329	SER
4	r	159	ASP
5	s	200	PRO
2	B	44	GLU
2	B	231	PRO
3	C	175	ALA
4	D	159	ASP
5	E	281	GLY
7	G	72	TYR
2	J	44	GLU
2	J	231	PRO
4	L	159	ASP
5	M	281	GLY
7	O	72	TYR
2	R	231	PRO
4	T	159	ASP
7	W	72	TYR
2	Z	44	GLU
2	Z	231	PRO
3	a	175	ALA
7	e	72	TYR
2	h	231	PRO
5	k	200	PRO

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Mol	Chain	Res	Type
7	m	72	TYR
2	p	44	GLU
2	p	231	PRO
3	q	175	ALA
7	u	72	TYR
5	E	43	LYS
5	M	43	LYS
5	U	43	LYS
5	c	43	LYS
5	k	43	LYS
5	k	281	GLY
5	s	43	LYS
5	s	281	GLY
2	Z	417	GLY
1	A	264	THR
2	B	417	GLY
2	J	417	GLY
1	Q	264	THR
2	R	417	GLY
1	g	264	THR
1	o	264	THR
1	I	264	THR
1	Y	264	THR

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%)	354 (97%)	11 (3%)	41	63
1	I	365/415 (88%)	354 (97%)	11 (3%)	41	63
1	Q	365/415 (88%)	355 (97%)	10 (3%)	44	65
1	Y	365/415 (88%)	355 (97%)	10 (3%)	44	65
1	g	365/415 (88%)	354 (97%)	11 (3%)	41	63
1	o	365/415 (88%)	355 (97%)	10 (3%)	44	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/406 (90%)	360 (98%)	7 (2%)	57	75
2	J	367/406 (90%)	360 (98%)	7 (2%)	57	75
2	R	367/406 (90%)	360 (98%)	7 (2%)	57	75
2	Z	367/406 (90%)	360 (98%)	7 (2%)	57	75
2	h	367/406 (90%)	360 (98%)	7 (2%)	57	75
2	p	367/406 (90%)	360 (98%)	7 (2%)	57	75
3	C	358/378 (95%)	351 (98%)	7 (2%)	55	73
3	K	358/378 (95%)	352 (98%)	6 (2%)	60	78
3	S	358/378 (95%)	352 (98%)	6 (2%)	60	78
3	a	358/378 (95%)	351 (98%)	7 (2%)	55	73
3	i	358/378 (95%)	351 (98%)	7 (2%)	55	73
3	q	358/378 (95%)	352 (98%)	6 (2%)	60	78
4	D	347/348 (100%)	328 (94%)	19 (6%)	21	48
4	L	347/348 (100%)	329 (95%)	18 (5%)	23	49
4	T	347/348 (100%)	329 (95%)	18 (5%)	23	49
4	b	347/348 (100%)	330 (95%)	17 (5%)	25	51
4	j	347/348 (100%)	327 (94%)	20 (6%)	20	46
4	r	347/348 (100%)	330 (95%)	17 (5%)	25	51
5	E	255/276 (92%)	249 (98%)	6 (2%)	49	69
5	M	255/276 (92%)	249 (98%)	6 (2%)	49	69
5	U	255/276 (92%)	248 (97%)	7 (3%)	44	65
5	c	255/276 (92%)	249 (98%)	6 (2%)	49	69
5	k	255/276 (92%)	249 (98%)	6 (2%)	49	69
5	s	255/276 (92%)	249 (98%)	6 (2%)	49	69
6	F	250/277 (90%)	247 (99%)	3 (1%)	71	84
6	N	250/277 (90%)	246 (98%)	4 (2%)	62	79
6	V	250/277 (90%)	247 (99%)	3 (1%)	71	84
6	d	250/277 (90%)	247 (99%)	3 (1%)	71	84
6	l	250/277 (90%)	247 (99%)	3 (1%)	71	84
6	t	250/277 (90%)	247 (99%)	3 (1%)	71	84
7	G	174/184 (95%)	168 (97%)	6 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	O	174/184 (95%)	168 (97%)	6 (3%)	37	60
7	W	174/184 (95%)	168 (97%)	6 (3%)	37	60
7	e	174/184 (95%)	168 (97%)	6 (3%)	37	60
7	m	174/184 (95%)	168 (97%)	6 (3%)	37	60
7	u	174/184 (95%)	168 (97%)	6 (3%)	37	60
8	H	144/174 (83%)	137 (95%)	7 (5%)	25	51
8	P	144/174 (83%)	137 (95%)	7 (5%)	25	51
8	X	144/174 (83%)	137 (95%)	7 (5%)	25	51
8	f	144/174 (83%)	137 (95%)	7 (5%)	25	51
8	n	144/174 (83%)	137 (95%)	7 (5%)	25	51
8	v	144/174 (83%)	137 (95%)	7 (5%)	25	51
All	All	13560/14748 (92%)	13173 (97%)	387 (3%)	42	64

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	106	HIS
1	A	182	ASP
1	A	208	TYR
1	A	226	ASP
1	A	287	CYS
1	A	294	LEU
1	A	315	ASP
1	A	342	LEU
1	A	408	ARG
1	A	498	ASN
2	B	84	ASN
2	B	162	ARG
2	B	193	GLN
2	B	208	GLN
2	B	239	GLU
2	B	247	ARG
2	B	342	PHE
3	C	52	GLN
3	C	124	LEU
3	C	167	MET
3	C	221	LEU

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Mol	Chain	Res	Type
3	C	362	ASP
3	C	365	GLU
3	C	370	PRO
4	D	1	MET
4	D	22	LEU
4	D	40	GLU
4	D	55	GLU
4	D	72	HIS
4	D	83	GLU
4	D	91	LYS
4	D	100	GLU
4	D	121	ARG
4	D	149	LEU
4	D	179	THR
4	D	202	ILE
4	D	228	HIS
4	D	245	MET
4	D	276	ASN
4	D	286	MET
4	D	351	PHE
4	D	362	GLU
4	D	394	GLU
5	E	77	VAL
5	E	140	HIS
5	E	163	GLU
5	E	165	PHE
5	E	173	THR
5	E	267	PHE
6	F	112	PHE
6	F	120	GLU
6	F	285	ASP
7	G	98	HIS
7	G	110	CYS
7	G	161	ASP
7	G	167	LEU
7	G	173	THR
7	G	202	GLN
8	H	33	THR
8	H	46	LEU
8	H	70	GLU
8	H	80	ARG
8	H	132	ASP

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Mol	Chain	Res	Type
8	H	142	GLU
8	H	165	ARG
1	I	94	LEU
1	I	106	HIS
1	I	182	ASP
1	I	208	TYR
1	I	226	ASP
1	I	287	CYS
1	I	294	LEU
1	I	315	ASP
1	I	342	LEU
1	I	408	ARG
1	I	498	ASN
2	J	84	ASN
2	J	162	ARG
2	J	193	GLN
2	J	208	GLN
2	J	239	GLU
2	J	247	ARG
2	J	342	PHE
3	K	52	GLN
3	K	124	LEU
3	K	167	MET
3	K	221	LEU
3	K	362	ASP
3	K	365	GLU
4	L	22	LEU
4	L	40	GLU
4	L	72	HIS
4	L	83	GLU
4	L	91	LYS
4	L	121	ARG
4	L	149	LEU
4	L	175	GLN
4	L	179	THR
4	L	202	ILE
4	L	228	HIS
4	L	245	MET
4	L	274	ARG
4	L	276	ASN
4	L	286	MET
4	L	351	PHE

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Mol	Chain	Res	Type
4	L	362	GLU
4	L	394	GLU
5	M	77	VAL
5	M	140	HIS
5	M	163	GLU
5	M	165	PHE
5	M	173	THR
5	M	267	PHE
6	N	112	PHE
6	N	120	GLU
6	N	203	VAL
6	N	285	ASP
7	O	98	HIS
7	O	110	CYS
7	O	161	ASP
7	O	167	LEU
7	O	173	THR
7	O	202	GLN
8	P	33	THR
8	P	46	LEU
8	P	70	GLU
8	P	80	ARG
8	P	132	ASP
8	P	142	GLU
8	P	165	ARG
1	Q	94	LEU
1	Q	182	ASP
1	Q	208	TYR
1	Q	226	ASP
1	Q	287	CYS
1	Q	294	LEU
1	Q	315	ASP
1	Q	342	LEU
1	Q	408	ARG
1	Q	498	ASN
2	R	84	ASN
2	R	162	ARG
2	R	193	GLN
2	R	208	GLN
2	R	239	GLU
2	R	247	ARG
2	R	342	PHE

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Mol	Chain	Res	Type
3	S	52	GLN
3	S	124	LEU
3	S	167	MET
3	S	221	LEU
3	S	362	ASP
3	S	365	GLU
4	T	1	MET
4	T	22	LEU
4	T	40	GLU
4	T	72	HIS
4	T	83	GLU
4	T	91	LYS
4	T	121	ARG
4	T	149	LEU
4	T	179	THR
4	T	202	ILE
4	T	228	HIS
4	T	245	MET
4	T	274	ARG
4	T	276	ASN
4	T	286	MET
4	T	351	PHE
4	T	362	GLU
4	T	394	GLU
5	U	77	VAL
5	U	140	HIS
5	U	163	GLU
5	U	165	PHE
5	U	173	THR
5	U	197	ASP
5	U	267	PHE
6	V	112	PHE
6	V	120	GLU
6	V	285	ASP
7	W	98	HIS
7	W	110	CYS
7	W	161	ASP
7	W	167	LEU
7	W	173	THR
7	W	202	GLN
8	X	33	THR
8	X	46	LEU

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Mol	Chain	Res	Type
8	X	70	GLU
8	X	80	ARG
8	X	132	ASP
8	X	142	GLU
8	X	165	ARG
1	Y	94	LEU
1	Y	182	ASP
1	Y	208	TYR
1	Y	226	ASP
1	Y	287	CYS
1	Y	294	LEU
1	Y	315	ASP
1	Y	342	LEU
1	Y	408	ARG
1	Y	498	ASN
2	Z	84	ASN
2	Z	162	ARG
2	Z	193	GLN
2	Z	208	GLN
2	Z	239	GLU
2	Z	247	ARG
2	Z	342	PHE
3	a	52	GLN
3	a	124	LEU
3	a	167	MET
3	a	212	PRO
3	a	221	LEU
3	a	362	ASP
3	a	365	GLU
4	b	22	LEU
4	b	55	GLU
4	b	72	HIS
4	b	83	GLU
4	b	91	LYS
4	b	121	ARG
4	b	149	LEU
4	b	202	ILE
4	b	228	HIS
4	b	245	MET
4	b	264	LEU
4	b	274	ARG
4	b	276	ASN

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Mol	Chain	Res	Type
4	b	286	MET
4	b	351	PHE
4	b	362	GLU
4	b	394	GLU
5	c	77	VAL
5	c	140	HIS
5	c	163	GLU
5	c	165	PHE
5	c	173	THR
5	c	267	PHE
6	d	112	PHE
6	d	120	GLU
6	d	285	ASP
7	e	98	HIS
7	e	110	CYS
7	e	161	ASP
7	e	167	LEU
7	e	173	THR
7	e	202	GLN
8	f	33	THR
8	f	46	LEU
8	f	70	GLU
8	f	80	ARG
8	f	132	ASP
8	f	142	GLU
8	f	165	ARG
1	g	94	LEU
1	g	106	HIS
1	g	182	ASP
1	g	208	TYR
1	g	226	ASP
1	g	287	CYS
1	g	294	LEU
1	g	315	ASP
1	g	342	LEU
1	g	408	ARG
1	g	498	ASN
2	h	84	ASN
2	h	162	ARG
2	h	193	GLN
2	h	208	GLN
2	h	239	GLU

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Mol	Chain	Res	Type
2	h	247	ARG
2	h	342	PHE
3	i	52	GLN
3	i	124	LEU
3	i	167	MET
3	i	221	LEU
3	i	362	ASP
3	i	365	GLU
3	i	370	PRO
4	j	1	MET
4	j	22	LEU
4	j	40	GLU
4	j	72	HIS
4	j	83	GLU
4	j	91	LYS
4	j	100	GLU
4	j	121	ARG
4	j	149	LEU
4	j	202	ILE
4	j	227	LYS
4	j	228	HIS
4	j	245	MET
4	j	272	ILE
4	j	274	ARG
4	j	276	ASN
4	j	286	MET
4	j	351	PHE
4	j	362	GLU
4	j	394	GLU
5	k	77	VAL
5	k	140	HIS
5	k	163	GLU
5	k	165	PHE
5	k	173	THR
5	k	267	PHE
6	l	112	PHE
6	l	120	GLU
6	l	285	ASP
7	m	98	HIS
7	m	110	CYS
7	m	161	ASP
7	m	167	LEU

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Mol	Chain	Res	Type
7	m	173	THR
7	m	202	GLN
8	n	33	THR
8	n	46	LEU
8	n	70	GLU
8	n	80	ARG
8	n	132	ASP
8	n	142	GLU
8	n	165	ARG
1	o	94	LEU
1	o	182	ASP
1	o	208	TYR
1	o	226	ASP
1	o	287	CYS
1	o	294	LEU
1	o	315	ASP
1	o	342	LEU
1	o	408	ARG
1	o	498	ASN
2	p	84	ASN
2	p	162	ARG
2	p	193	GLN
2	p	208	GLN
2	p	239	GLU
2	p	247	ARG
2	p	342	PHE
3	q	52	GLN
3	q	124	LEU
3	q	167	MET
3	q	221	LEU
3	q	362	ASP
3	q	365	GLU
4	r	22	LEU
4	r	40	GLU
4	r	72	HIS
4	r	83	GLU
4	r	91	LYS
4	r	105	SER
4	r	121	ARG
4	r	149	LEU
4	r	202	ILE
4	r	228	HIS

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Mol	Chain	Res	Type
4	r	245	MET
4	r	274	ARG
4	r	276	ASN
4	r	286	MET
4	r	351	PHE
4	r	362	GLU
4	r	394	GLU
5	s	77	VAL
5	s	140	HIS
5	s	163	GLU
5	s	165	PHE
5	s	173	THR
5	s	267	PHE
6	t	112	PHE
6	t	120	GLU
6	t	285	ASP
7	u	98	HIS
7	u	110	CYS
7	u	161	ASP
7	u	167	LEU
7	u	173	THR
7	u	202	GLN
8	v	33	THR
8	v	46	LEU
8	v	70	GLU
8	v	80	ARG
8	v	132	ASP
8	v	142	GLU
8	v	165	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	ASN
2	B	35	GLN
2	B	84	ASN
6	F	284	ASN
1	I	324	ASN
1	I	467	GLN
1	I	483	GLN
2	J	35	GLN
2	J	84	ASN

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Mol	Chain	Res	Type
6	N	284	ASN
7	O	196	ASN
1	Q	106	HIS
1	Q	324	ASN
2	R	35	GLN
2	R	84	ASN
6	V	284	ASN
1	Y	324	ASN
2	Z	35	GLN
2	Z	84	ASN
4	b	125	GLN
5	c	321	GLN
6	d	284	ASN
1	g	106	HIS
1	g	324	ASN
2	h	35	GLN
2	h	84	ASN
4	j	240	GLN
4	j	375	GLN
5	k	321	GLN
1	o	324	ASN
2	p	35	GLN
2	p	84	ASN
4	r	19	HIS
4	r	240	GLN
4	r	277	GLN
4	r	375	GLN
5	s	321	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 6 ligands modelled in this entry, 6 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	p	1
2	J	1
6	d	1
2	h	1
2	B	1
4	j	1
6	V	1
2	Z	1
6	N	1
4	r	1
2	R	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	290:LYS	C	291:ALA	N	3.62
1	J	193:GLN	C	194:LEU	N	2.88
1	B	193:GLN	C	194:LEU	N	2.87
1	R	193:GLN	C	194:LEU	N	2.86
1	p	193:GLN	C	194:LEU	N	2.85

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	193:GLN	C	194:LEU	N	2.83
1	h	193:GLN	C	194:LEU	N	2.81
1	j	290:LYS	C	291:ALA	N	2.53
1	F	217:VAL	C	218:ALA	N	1.80
1	N	217:VAL	C	218:ALA	N	1.79
1	d	217:VAL	C	218:ALA	N	1.78
1	V	217:VAL	C	218:ALA	N	1.75

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%)	0.41	21 (5%)	28	26	60, 128, 170, 185	0
1	I	419/480 (87%)	0.48	33 (7%)	12	13	67, 120, 169, 191	0
1	Q	419/480 (87%)	0.48	31 (7%)	14	14	81, 121, 167, 197	0
1	Y	419/480 (87%)	0.31	18 (4%)	35	31	68, 108, 148, 176	0
1	g	419/480 (87%)	0.40	24 (5%)	23	22	80, 111, 161, 190	0
1	o	419/480 (87%)	0.29	16 (3%)	40	34	75, 109, 168, 189	0
2	B	403/447 (90%)	0.42	25 (6%)	20	18	65, 127, 155, 189	0
2	J	403/447 (90%)	0.34	21 (5%)	27	26	70, 125, 159, 172	0
2	R	403/447 (90%)	0.30	20 (4%)	28	26	75, 108, 139, 163	0
2	Z	403/447 (90%)	0.46	29 (7%)	15	15	68, 139, 167, 189	0
2	h	403/447 (90%)	0.43	25 (6%)	20	18	85, 135, 176, 202	0
2	p	403/447 (90%)	0.38	24 (5%)	21	20	81, 126, 165, 179	0
3	C	401/427 (93%)	0.32	14 (3%)	44	37	58, 118, 219, 260	0
3	K	401/427 (93%)	0.34	15 (3%)	41	35	69, 118, 201, 220	0
3	S	401/427 (93%)	0.28	15 (3%)	41	35	68, 99, 195, 216	0
3	a	401/427 (93%)	0.42	22 (5%)	25	24	69, 134, 218, 238	0
3	i	401/427 (93%)	0.30	14 (3%)	44	37	81, 114, 207, 257	0
3	q	401/427 (93%)	0.25	12 (2%)	50	41	77, 116, 208, 249	0
4	D	406/410 (99%)	0.86	61 (15%)	2	4	68, 145, 251, 272	0
4	L	406/410 (99%)	0.70	52 (12%)	3	6	80, 152, 188, 216	0
4	T	406/410 (99%)	0.72	48 (11%)	4	7	88, 131, 183, 209	0
4	b	406/410 (99%)	1.12	83 (20%)	1	2	73, 166, 243, 253	0
4	j	406/410 (99%)	0.76	56 (13%)	2	5	86, 132, 269, 285	0
4	r	406/410 (99%)	0.83	55 (13%)	3	5	81, 162, 253, 272	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	E	298/325 (91%)	0.53	26 (8%) 10 11	73, 112, 148, 170	0
5	M	298/325 (91%)	0.59	27 (9%) 9 10	78, 107, 159, 185	0
5	U	298/325 (91%)	0.60	29 (9%) 7 9	89, 121, 174, 198	0
5	c	298/325 (91%)	0.43	21 (7%) 16 15	61, 88, 126, 144	0
5	k	298/325 (91%)	0.46	20 (6%) 17 16	85, 107, 145, 166	0
5	s	298/325 (91%)	0.52	23 (7%) 13 13	84, 108, 148, 170	0
6	F	288/331 (87%)	0.36	11 (3%) 40 34	62, 114, 153, 184	0
6	N	288/331 (87%)	0.41	12 (4%) 36 31	73, 113, 165, 193	0
6	V	288/331 (87%)	0.45	20 (6%) 16 15	84, 120, 160, 194	0
6	d	288/331 (87%)	0.33	7 (2%) 59 50	63, 97, 150, 185	0
6	l	288/331 (87%)	0.45	17 (5%) 22 21	84, 116, 156, 182	0
6	t	288/331 (87%)	0.44	23 (7%) 12 13	77, 116, 160, 190	0
7	G	208/222 (93%)	0.37	16 (7%) 13 13	92, 114, 162, 187	0
7	O	208/222 (93%)	0.32	16 (7%) 13 13	68, 115, 160, 181	0
7	W	208/222 (93%)	0.34	15 (7%) 15 15	111, 135, 161, 174	0
7	e	208/222 (93%)	0.32	11 (5%) 26 25	84, 106, 145, 168	0
7	m	208/222 (93%)	0.19	8 (3%) 40 34	72, 98, 143, 188	0
7	u	208/222 (93%)	0.27	7 (3%) 45 38	73, 111, 149, 164	0
8	H	173/213 (81%)	0.45	15 (8%) 10 11	82, 123, 154, 168	0
8	P	173/213 (81%)	0.46	17 (9%) 7 9	91, 121, 147, 161	0
8	X	173/213 (81%)	0.49	17 (9%) 7 9	91, 114, 142, 150	0
8	f	173/213 (81%)	0.60	26 (15%) 2 4	81, 169, 190, 196	0
8	n	173/213 (81%)	0.42	11 (6%) 19 17	98, 129, 164, 181	0
8	v	173/213 (81%)	0.53	18 (10%) 6 8	94, 139, 175, 187	0
All	All	15576/17130 (90%)	0.47	1147 (7%) 14 14	58, 119, 209, 285	0

All (1147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	b	78	ASP	14.6
1	I	160	PRO	8.9
4	b	2	ALA	8.0
4	r	1	MET	7.4
5	U	189	TYR	7.3

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Mol	Chain	Res	Type	RSRZ
3	C	54	HIS	7.2
4	r	16	SER	7.2
5	U	188	THR	7.0
1	Y	160	PRO	6.4
1	Q	160	PRO	6.4
4	b	77	PRO	6.4
6	l	170	SER	6.2
4	b	51	ALA	6.0
4	D	12	LEU	6.0
4	j	69	PHE	6.0
1	I	161	ALA	5.8
8	f	39	GLN	5.8
4	r	2	ALA	5.7
4	b	76	LEU	5.6
4	D	88	THR	5.4
5	E	110	GLN	5.4
5	M	146	TRP	5.3
4	b	14	ASN	5.3
4	D	11	GLN	5.3
4	D	151	ILE	5.3
4	b	41	GLN	5.3
4	D	8	ASP	5.2
4	b	79	SER	5.2
4	b	146	GLU	5.2
4	b	40	GLU	5.2
8	f	162	VAL	5.2
3	C	53	GLU	5.1
6	V	183	PHE	5.1
1	I	309	ALA	5.0
5	M	167	ALA	5.0
5	k	85	VAL	5.0
6	F	187	THR	5.0
4	T	350	GLY	5.0
5	M	189	TYR	5.0
8	f	37	TYR	4.9
8	X	71	LEU	4.9
4	D	9	LEU	4.9
5	s	103	THR	4.8
2	J	298	GLU	4.8
4	b	13	MET	4.8
4	D	148	TYR	4.8
4	L	148	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
4	r	99	PHE	4.7
5	M	110	GLN	4.7
4	D	34	ILE	4.7
4	r	62	SER	4.7
8	f	155	ALA	4.6
5	U	85	VAL	4.6
4	r	69	PHE	4.6
2	h	143	LYS	4.6
6	t	170	SER	4.6
2	p	71	ALA	4.5
1	Q	128	VAL	4.5
5	E	109	ALA	4.5
1	I	224	ALA	4.5
2	B	311	MET	4.5
8	f	154	GLN	4.5
4	D	16	SER	4.5
3	S	54	HIS	4.5
5	k	136	TRP	4.5
4	L	30	LEU	4.4
4	L	26	TYR	4.4
4	T	26	TYR	4.4
2	B	259	PHE	4.4
4	b	34	ILE	4.4
4	b	52	MET	4.4
4	T	152	ALA	4.4
2	h	293	PRO	4.4
5	U	167	ALA	4.4
5	s	29	TYR	4.3
5	s	78	MET	4.3
2	B	298	GLU	4.3
4	j	106	ILE	4.3
5	c	103	THR	4.3
8	P	37	TYR	4.3
4	T	30	LEU	4.3
4	D	7	GLN	4.3
1	A	309	ALA	4.3
1	g	420	ALA	4.3
8	P	38	GLY	4.2
6	t	211	SER	4.2
4	b	15	SER	4.2
3	a	28	ILE	4.2
5	E	167	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
4	j	58	SER	4.2
4	b	99	PHE	4.2
4	j	102	GLN	4.2
4	r	127	LEU	4.2
5	M	85	VAL	4.2
7	e	8	THR	4.2
5	s	221	TYR	4.1
2	B	293	PRO	4.1
1	I	114	ALA	4.1
4	b	168	ILE	4.1
4	j	16	SER	4.1
7	O	67	LEU	4.1
4	j	99	PHE	4.1
5	E	108	ASN	4.1
4	j	45	LEU	4.1
5	k	29	TYR	4.1
1	I	227	TYR	4.1
2	Z	308	ILE	4.1
4	D	152	ALA	4.1
1	A	82	LEU	4.1
4	b	11	GLN	4.1
5	s	90	MET	4.1
7	G	70	PHE	4.1
2	B	51	LEU	4.0
3	K	53	GLU	4.0
1	Y	78	GLU	4.0
4	b	80	THR	4.0
4	D	147	THR	4.0
8	f	92	THR	4.0
6	t	187	THR	4.0
4	b	48	PHE	4.0
1	Y	309	ALA	4.0
2	Z	298	GLU	4.0
2	J	308	ILE	4.0
3	a	54	HIS	4.0
1	o	160	PRO	4.0
1	o	78	GLU	4.0
4	D	127	LEU	4.0
2	p	143	LYS	4.0
5	M	84	LYS	4.0
7	u	8	THR	4.0
2	Z	293	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
3	a	53	GLU	3.9
2	h	67	TRP	3.9
7	m	195	ALA	3.9
4	L	29	ILE	3.9
4	j	127	LEU	3.9
3	C	170	CYS	3.9
5	k	78	MET	3.9
1	g	82	LEU	3.9
2	Z	311	MET	3.9
8	v	74	ILE	3.9
4	D	91	LYS	3.9
2	p	293	PRO	3.9
4	r	52	MET	3.9
5	M	186	PHE	3.8
4	r	5	VAL	3.8
4	D	124	ALA	3.8
6	t	37	GLY	3.8
8	f	38	GLY	3.8
4	b	139	TYR	3.8
5	s	52	PHE	3.8
3	S	92	HIS	3.8
4	L	188	LYS	3.8
2	Z	51	LEU	3.8
5	U	166	VAL	3.8
1	Q	117	MET	3.8
4	T	151	ILE	3.8
4	j	4	ALA	3.8
3	S	53	GLU	3.8
4	D	4	ALA	3.8
3	a	139	THR	3.8
4	b	12	LEU	3.7
7	O	70	PHE	3.7
8	v	38	GLY	3.7
3	a	140	SER	3.7
2	B	280	LEU	3.7
4	b	1	MET	3.7
2	Z	259	PHE	3.7
4	b	115	GLU	3.7
4	T	88	THR	3.7
4	b	150	LYS	3.7
4	r	123	ALA	3.7
4	L	207	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
4	b	81	ALA	3.7
4	D	193	ARG	3.7
4	b	49	VAL	3.7
6	N	187	THR	3.7
8	n	105	ILE	3.6
4	D	66	LEU	3.6
7	W	31	ILE	3.6
4	L	167	TYR	3.6
8	H	105	ILE	3.6
7	u	19	ALA	3.6
8	n	155	ALA	3.6
8	X	93	ILE	3.6
5	s	131	GLU	3.6
4	b	194	VAL	3.6
4	r	56	ASN	3.6
5	U	187	ARG	3.6
4	j	1	MET	3.6
4	T	48	PHE	3.6
8	n	39	GLN	3.6
4	T	22	LEU	3.6
4	r	66	LEU	3.6
4	r	3	ALA	3.6
7	m	70	PHE	3.6
4	r	4	ALA	3.6
7	O	63	THR	3.6
2	p	298	GLU	3.5
4	b	191	TYR	3.5
5	E	147	LEU	3.5
5	M	100	VAL	3.5
4	b	26	TYR	3.5
4	b	145	LEU	3.5
1	I	225	ARG	3.5
4	b	156	LEU	3.5
4	r	7	GLN	3.5
8	n	74	ILE	3.5
7	O	66	LEU	3.5
1	I	162	LEU	3.5
6	l	207	THR	3.5
6	V	211	SER	3.5
5	s	136	TRP	3.5
6	N	181	MET	3.5
2	B	281	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
4	r	8	ASP	3.5
4	T	89	LEU	3.4
4	r	260	ALA	3.4
5	s	85	VAL	3.4
5	c	189	TYR	3.4
5	k	187	ARG	3.4
1	I	226	ASP	3.4
4	D	85	TYR	3.4
7	e	46	LEU	3.4
4	L	211	LEU	3.4
4	L	48	PHE	3.4
4	j	103	VAL	3.4
8	f	105	ILE	3.4
1	Y	82	LEU	3.4
4	r	143	TYR	3.4
6	t	36	THR	3.4
2	p	80	PHE	3.4
5	s	202	GLU	3.4
5	U	103	THR	3.4
4	r	91	LYS	3.4
4	j	91	LYS	3.4
5	k	167	ALA	3.4
7	G	63	THR	3.4
4	D	10	ALA	3.4
2	J	311	MET	3.4
4	j	73	LEU	3.4
2	p	142	ALA	3.4
4	j	70	CYS	3.3
6	V	212	GLY	3.3
4	r	34	ILE	3.3
4	D	86	HIS	3.3
4	b	75	ASN	3.3
5	E	84	LYS	3.3
1	I	87	TYR	3.3
3	i	139	THR	3.3
6	F	215	SER	3.3
3	q	54	HIS	3.3
3	K	54	HIS	3.3
5	M	78	MET	3.3
6	t	209	THR	3.3
4	L	152	ALA	3.3
4	D	17	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	J	277	LEU	3.3
7	W	35	LEU	3.3
7	u	46	LEU	3.3
2	J	278	LYS	3.3
4	b	172	SER	3.3
1	I	320	LEU	3.3
7	O	31	ILE	3.3
1	Q	82	LEU	3.3
6	V	98	ILE	3.3
4	D	26	TYR	3.3
4	j	107	ARG	3.3
5	E	131	GLU	3.3
1	A	160	PRO	3.3
6	t	210	GLY	3.3
8	f	40	LEU	3.3
1	I	319	LEU	3.3
4	j	5	VAL	3.3
2	R	311	MET	3.3
2	p	34	ASN	3.3
3	K	303	TYR	3.3
8	H	37	TYR	3.3
4	b	53	VAL	3.3
6	l	210	GLY	3.3
8	n	125	TYR	3.2
4	j	88	THR	3.2
1	Q	227	TYR	3.2
6	t	208	ALA	3.2
8	f	153	TRP	3.2
4	b	98	SER	3.2
7	W	32	HIS	3.2
1	g	100	LEU	3.2
2	h	82	LEU	3.2
2	Z	281	VAL	3.2
1	I	111	ARG	3.2
7	W	63	THR	3.2
2	h	239	GLU	3.2
4	T	84	ILE	3.2
4	j	3	ALA	3.2
5	c	185	ALA	3.2
5	s	146	TRP	3.2
4	j	57	VAL	3.2
6	l	211	SER	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	189	VAL	3.2
2	h	81	LYS	3.2
6	N	174	ILE	3.2
4	D	226	LEU	3.2
8	f	93	ILE	3.2
4	L	193	ARG	3.2
1	Q	114	ALA	3.2
4	D	49	VAL	3.2
3	a	349	ALA	3.2
4	b	37	SER	3.2
7	G	31	ILE	3.2
5	U	282	ARG	3.2
8	v	155	ALA	3.2
7	G	35	LEU	3.2
5	E	205	THR	3.2
4	r	161	PRO	3.2
4	j	89	LEU	3.1
6	t	212	GLY	3.1
8	v	41	LEU	3.1
1	Q	207	HIS	3.1
1	Q	111	ARG	3.1
2	Z	54	PHE	3.1
5	c	187	ARG	3.1
7	e	160	ARG	3.1
5	E	187	ARG	3.1
5	s	188	THR	3.1
2	h	54	PHE	3.1
5	s	147	LEU	3.1
6	d	187	THR	3.1
1	Q	319	LEU	3.1
4	j	139	TYR	3.1
4	r	138	GLN	3.1
8	n	38	GLY	3.1
4	b	103	VAL	3.1
7	W	67	LEU	3.1
2	p	131	PHE	3.1
4	b	56	ASN	3.1
4	r	45	LEU	3.1
4	j	62	SER	3.1
8	P	105	ILE	3.1
1	A	126	PHE	3.1
5	U	131	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
6	t	207	THR	3.1
1	o	319	LEU	3.1
6	t	68	VAL	3.1
3	C	31	SER	3.1
4	j	138	GLN	3.1
4	r	32	LYS	3.1
4	j	66	LEU	3.1
4	b	107	ARG	3.1
5	M	195	PRO	3.1
7	G	43	PHE	3.1
2	h	298	GLU	3.1
3	i	272	PRO	3.1
4	j	6	ARG	3.1
2	p	92	TYR	3.1
5	U	108	ASN	3.1
8	X	45	LEU	3.1
4	b	88	THR	3.1
4	b	192	ALA	3.1
5	E	103	THR	3.1
5	c	94	ASP	3.1
2	Z	131	PHE	3.0
5	M	166	VAL	3.0
1	g	126	PHE	3.0
2	R	274	THR	3.0
5	U	200	PRO	3.0
4	T	23	ALA	3.0
4	b	187	TYR	3.0
2	B	292	ASN	3.0
4	j	61	ILE	3.0
1	I	103	ILE	3.0
2	p	119	ILE	3.0
4	b	188	LYS	3.0
4	r	145	LEU	3.0
8	f	42	ALA	3.0
7	G	67	LEU	3.0
4	T	150	LYS	3.0
6	l	182	LEU	3.0
4	L	88	THR	3.0
1	Q	161	ALA	3.0
3	S	91	GLU	3.0
1	g	309	ALA	3.0
4	j	156	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
8	H	39	GLN	3.0
4	b	89	LEU	3.0
1	Y	126	PHE	3.0
8	v	125	TYR	3.0
5	c	84	LYS	3.0
4	L	177	GLU	3.0
1	Y	79	ASN	3.0
4	L	226	LEU	3.0
2	Z	262	PHE	3.0
1	A	128	VAL	2.9
4	T	351	PHE	2.9
4	T	12	LEU	2.9
6	l	37	GLY	2.9
3	C	260	TYR	2.9
4	L	69	PHE	2.9
5	c	85	VAL	2.9
4	D	150	LYS	2.9
4	T	52	MET	2.9
2	B	282	LEU	2.9
5	c	186	PHE	2.9
4	j	190	CYS	2.9
2	Z	75	MET	2.9
1	I	100	LEU	2.9
4	b	45	LEU	2.9
7	G	46	LEU	2.9
8	f	77	VAL	2.9
2	B	294	PHE	2.9
2	B	296	SER	2.9
5	M	296	SER	2.9
1	A	319	LEU	2.9
3	C	28	ILE	2.9
4	D	145	LEU	2.9
6	l	88	GLU	2.9
7	O	46	LEU	2.9
4	r	103	VAL	2.9
5	U	146	TRP	2.9
5	U	196	PRO	2.9
8	f	41	LEU	2.9
3	K	12	VAL	2.9
4	b	108	GLN	2.9
4	r	124	ALA	2.9
4	b	9	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
6	l	212	GLY	2.9
7	W	70	PHE	2.9
8	H	113	THR	2.9
4	L	189	VAL	2.9
5	E	188	THR	2.9
4	D	15	SER	2.9
5	E	146	TRP	2.9
4	D	190	CYS	2.9
4	D	197	TYR	2.9
1	Q	115	LEU	2.9
2	Z	201	GLU	2.9
6	l	40	SER	2.9
3	a	27	LEU	2.9
4	j	87	PHE	2.9
2	R	293	PRO	2.9
5	E	85	VAL	2.9
5	k	188	THR	2.9
5	U	272	LYS	2.9
4	D	194	VAL	2.9
3	S	303	TYR	2.9
4	D	69	PHE	2.9
7	m	19	ALA	2.9
1	Q	309	ALA	2.9
6	l	187	THR	2.9
4	T	161	PRO	2.9
4	b	176	ASN	2.9
2	R	80	PHE	2.9
2	B	92	TYR	2.9
3	i	53	GLU	2.9
4	T	148	TYR	2.9
8	P	42	ALA	2.9
7	e	35	LEU	2.9
1	A	320	LEU	2.9
6	N	88	GLU	2.9
8	f	109	LEU	2.9
2	J	259	PHE	2.9
2	h	259	PHE	2.9
2	Z	92	TYR	2.8
1	o	269	GLU	2.8
7	W	66	LEU	2.8
1	g	505	PRO	2.8
4	b	190	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
4	L	144	LYS	2.8
7	e	70	PHE	2.8
1	o	109	THR	2.8
2	h	294	PHE	2.8
3	K	92	HIS	2.8
4	b	3	ALA	2.8
6	d	241	TYR	2.8
5	U	78	MET	2.8
6	l	36	THR	2.8
4	L	111	ALA	2.8
4	r	107	ARG	2.8
8	P	41	LEU	2.8
2	Z	144	ASN	2.8
8	f	128	ILE	2.8
1	A	227	TYR	2.8
5	c	147	LEU	2.8
4	T	207	ARG	2.8
4	L	190	CYS	2.8
5	M	49	HIS	2.8
7	G	47	LEU	2.8
1	A	221	TYR	2.8
6	V	252	PHE	2.8
1	g	319	LEU	2.8
5	E	49	HIS	2.8
4	b	152	ALA	2.8
5	c	109	ALA	2.8
1	g	84	LEU	2.8
6	V	207	THR	2.8
8	X	74	ILE	2.8
5	U	190	PRO	2.8
6	t	257	LEU	2.8
4	T	189	VAL	2.8
5	M	136	TRP	2.8
4	r	90	GLU	2.8
5	k	84	LYS	2.8
5	c	188	THR	2.8
7	O	35	LEU	2.8
2	J	293	PRO	2.8
2	R	298	GLU	2.8
4	T	61	ILE	2.8
1	Y	231	ALA	2.7
4	j	60	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
8	P	30	GLY	2.7
4	D	156	LEU	2.7
5	E	166	VAL	2.7
1	I	82	LEU	2.7
3	q	181	PHE	2.7
6	l	183	PHE	2.7
2	h	209	LYS	2.7
2	h	299	ALA	2.7
4	b	92	ILE	2.7
5	E	189	TYR	2.7
8	f	113	THR	2.7
4	D	123	ALA	2.7
8	H	109	LEU	2.7
5	c	24	SER	2.7
8	P	74	ILE	2.7
6	t	181	MET	2.7
4	L	85	TYR	2.7
4	j	108	GLN	2.7
4	r	89	LEU	2.7
5	k	186	PHE	2.7
1	I	115	LEU	2.7
5	E	78	MET	2.7
2	B	123	LYS	2.7
4	j	41	GLN	2.7
4	j	49	VAL	2.7
8	f	130	ALA	2.7
3	i	303	TYR	2.7
5	k	221	TYR	2.7
4	b	65	LEU	2.7
6	F	173	ASP	2.7
3	q	260	TYR	2.7
1	A	390	LEU	2.7
2	Z	30	VAL	2.7
2	p	442	LEU	2.7
4	b	143	TYR	2.7
4	j	143	TYR	2.7
1	Q	238	CYS	2.7
1	Q	307	LEU	2.7
4	T	190	CYS	2.7
1	o	126	PHE	2.7
5	M	147	LEU	2.7
7	W	43	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	h	119	ILE	2.7
5	c	99	PRO	2.7
2	B	308	ILE	2.7
3	K	39	LEU	2.7
4	j	124	ALA	2.7
5	U	296	SER	2.7
6	d	189	THR	2.7
5	M	103	THR	2.7
5	M	131	GLU	2.7
6	t	206	MET	2.7
4	j	260	ALA	2.7
3	K	307	ILE	2.7
4	D	231	HIS	2.7
4	L	151	ILE	2.7
4	b	82	LYS	2.7
3	S	139	THR	2.7
4	r	190	CYS	2.7
2	p	81	LYS	2.6
3	C	131	MET	2.6
1	I	196	SER	2.6
2	h	221	SER	2.6
6	d	242	VAL	2.6
5	U	29	TYR	2.6
4	j	191	TYR	2.6
4	b	149	LEU	2.6
5	U	110	GLN	2.6
6	l	181	MET	2.6
3	q	53	GLU	2.6
6	F	213	GLU	2.6
6	N	173	ASP	2.6
4	D	110	LEU	2.6
5	U	198	GLU	2.6
4	b	147	THR	2.6
4	r	147	THR	2.6
1	Q	87	TYR	2.6
1	Y	221	TYR	2.6
1	A	107	CYS	2.6
2	p	54	PHE	2.6
3	a	39	LEU	2.6
5	k	146	TRP	2.6
6	d	159	LYS	2.6
6	t	169	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
8	v	106	MET	2.6
5	M	200	PRO	2.6
6	V	174	ILE	2.6
4	L	153	ARG	2.6
4	r	70	CYS	2.6
7	O	43	PHE	2.6
4	T	66	LEU	2.6
4	T	29	ILE	2.6
4	r	98	SER	2.6
1	Q	223	ARG	2.6
2	Z	55	GLN	2.6
2	B	240	CYS	2.6
2	J	237	ILE	2.6
8	X	37	TYR	2.6
6	F	191	ALA	2.6
1	Q	118	ALA	2.6
6	V	87	PHE	2.6
4	b	61	ILE	2.6
4	r	168	ILE	2.6
3	S	138	LEU	2.6
4	L	214	LYS	2.6
4	b	211	LEU	2.6
4	L	197	TYR	2.6
4	T	121	ARG	2.6
1	I	121	PHE	2.6
3	K	95	TYR	2.6
3	C	358	VAL	2.6
4	j	145	LEU	2.6
8	H	38	GLY	2.6
7	e	43	PHE	2.6
2	Z	240	CYS	2.6
2	p	75	MET	2.6
3	K	131	MET	2.6
5	c	296	SER	2.6
4	D	6	ARG	2.6
4	L	174	LEU	2.6
1	Q	194	LYS	2.6
3	C	127	ALA	2.6
4	L	209	ASN	2.6
3	a	260	TYR	2.6
7	u	170	ILE	2.6
3	i	8	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	197	ILE	2.5
1	Q	121	PHE	2.5
2	Z	239	GLU	2.5
8	P	39	GLN	2.5
8	f	125	TYR	2.5
4	L	66	LEU	2.5
4	T	211	LEU	2.5
3	C	178	ALA	2.5
3	a	347	ILE	2.5
4	D	254	ARG	2.5
5	c	167	ALA	2.5
1	g	87	TYR	2.5
6	N	252	PHE	2.5
8	P	71	LEU	2.5
5	M	129	ARG	2.5
2	h	47	PRO	2.5
4	j	123	ALA	2.5
1	I	390	LEU	2.5
1	Q	320	LEU	2.5
3	i	138	LEU	2.5
1	A	287	CYS	2.5
3	a	58	VAL	2.5
4	b	91	LYS	2.5
5	U	84	LYS	2.5
3	a	131	MET	2.5
4	j	59	LEU	2.5
6	V	36	THR	2.5
6	l	38	SER	2.5
1	Q	234	VAL	2.5
6	t	69	ILE	2.5
3	i	54	HIS	2.5
5	U	136	TRP	2.5
3	S	131	MET	2.5
8	P	133	PHE	2.5
3	i	349	ALA	2.5
4	b	185	ILE	2.5
1	I	128	VAL	2.5
2	Z	277	LEU	2.5
5	M	190	PRO	2.5
3	q	94	ARG	2.5
4	b	193	ARG	2.5
6	N	159	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
7	W	139	ASP	2.5
8	H	167	PRO	2.5
8	v	77	VAL	2.5
2	Z	111	SER	2.5
2	Z	258	PHE	2.5
1	I	110	LEU	2.5
4	j	7	GLN	2.5
6	t	89	LEU	2.5
2	B	241	GLY	2.5
3	C	55	SER	2.5
6	l	208	ALA	2.5
5	E	100	VAL	2.5
8	n	41	LEU	2.5
5	E	202	GLU	2.5
5	k	24	SER	2.5
7	m	23	LYS	2.5
4	T	34	ILE	2.5
4	D	144	LYS	2.5
4	b	42	LEU	2.5
4	r	132	LEU	2.5
8	v	42	ALA	2.5
4	D	161	PRO	2.5
1	g	185	LEU	2.5
2	p	279	TYR	2.5
3	C	317	LEU	2.5
4	L	110	LEU	2.5
4	D	188	LYS	2.4
6	V	88	GLU	2.4
1	Q	390	LEU	2.4
4	D	154	LEU	2.4
4	b	127	LEU	2.4
1	I	78	GLU	2.4
4	b	38	GLY	2.4
8	H	77	VAL	2.4
4	j	63	ARG	2.4
5	s	110	GLN	2.4
4	D	13	MET	2.4
4	T	80	THR	2.4
6	N	135	ASP	2.4
6	d	191	ALA	2.4
2	R	175	LEU	2.4
5	E	296	SER	2.4

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Mol	Chain	Res	Type	RSRZ
7	O	92	GLN	2.4
4	T	154	LEU	2.4
6	N	191	ALA	2.4
8	X	38	GLY	2.4
8	f	164	PRO	2.4
2	J	296	SER	2.4
3	a	85	ILE	2.4
3	q	326	VAL	2.4
1	Y	227	TYR	2.4
4	j	85	TYR	2.4
2	B	277	LEU	2.4
8	v	137	VAL	2.4
2	J	299	ALA	2.4
4	T	27	ARG	2.4
4	r	167	TYR	2.4
8	H	133	PHE	2.4
1	g	504	SER	2.4
1	Y	114	ALA	2.4
4	b	39	ALA	2.4
2	h	237	ILE	2.4
4	r	185	ILE	2.4
8	X	125	TYR	2.4
3	K	299	LEU	2.4
8	X	109	LEU	2.4
4	D	72	HIS	2.4
4	L	27	ARG	2.4
4	j	76	LEU	2.4
4	j	211	LEU	2.4
8	P	45	LEU	2.4
4	b	44	ALA	2.4
1	g	188	TYR	2.4
6	F	189	THR	2.4
6	V	187	THR	2.4
8	n	133	PHE	2.4
5	c	98	LEU	2.4
5	k	202	GLU	2.4
7	G	196	ASN	2.4
8	X	124	ALA	2.4
2	R	278	LYS	2.4
4	r	106	ILE	2.4
5	M	109	ALA	2.4
5	s	167	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	246	LEU	2.4
8	H	24	GLU	2.4
2	R	292	ASN	2.4
8	P	13	PHE	2.4
4	L	108	GLN	2.4
4	b	138	GLN	2.4
4	b	163	GLN	2.4
5	k	147	LEU	2.4
1	Y	420	ALA	2.4
2	Z	442	LEU	2.4
4	r	48	PHE	2.4
5	U	297	GLU	2.4
1	I	107	CYS	2.4
1	Q	287	CYS	2.4
8	v	153	TRP	2.4
2	B	131	PHE	2.4
3	S	5	LEU	2.4
3	a	181	PHE	2.4
7	G	159	GLY	2.4
1	Q	196	SER	2.4
1	I	223	ARG	2.4
1	o	194	LYS	2.4
5	E	186	PHE	2.4
5	M	272	LYS	2.4
5	c	139	SER	2.4
1	A	87	TYR	2.4
5	U	197	ASP	2.4
2	B	239	GLU	2.4
6	t	35	VAL	2.4
2	p	311	MET	2.4
4	T	174	LEU	2.4
5	U	186	PHE	2.4
3	a	170	CYS	2.4
4	r	194	VAL	2.4
2	R	277	LEU	2.3
2	Z	202	ILE	2.3
8	P	109	LEU	2.3
5	s	100	VAL	2.3
2	R	201	GLU	2.3
8	n	106	MET	2.3
4	r	88	THR	2.3
2	J	410	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	T	178	SER	2.3
2	h	194	LEU	2.3
1	g	269	GLU	2.3
4	j	34	ILE	2.3
6	l	147	GLU	2.3
1	I	131	TYR	2.3
2	R	281	VAL	2.3
4	D	174	LEU	2.3
8	v	133	PHE	2.3
7	O	159	GLY	2.3
2	p	194	LEU	2.3
7	W	46	LEU	2.3
8	v	105	ILE	2.3
4	T	155	TYR	2.3
4	T	226	LEU	2.3
4	b	164	ALA	2.3
3	q	131	MET	2.3
1	I	346	VAL	2.3
2	J	67	TRP	2.3
5	U	109	ALA	2.3
8	v	43	LEU	2.3
3	K	28	ILE	2.3
6	V	181	MET	2.3
8	X	68	ASN	2.3
4	L	121	ARG	2.3
3	a	9	VAL	2.3
4	D	126	VAL	2.3
4	b	174	LEU	2.3
5	M	77	VAL	2.3
7	m	46	LEU	2.3
2	B	299	ALA	2.3
8	P	209	ASN	2.3
4	D	84	ILE	2.3
4	L	49	VAL	2.3
6	t	40	SER	2.3
3	S	170	CYS	2.3
8	v	118	PHE	2.3
7	e	170	ILE	2.3
8	f	74	ILE	2.3
2	J	280	LEU	2.3
2	R	131	PHE	2.3
7	O	196	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	o	287	CYS	2.3
6	F	98	ILE	2.3
7	e	31	ILE	2.3
7	G	88	LEU	2.3
1	Y	198	ARG	2.3
2	B	71	ALA	2.3
4	L	78	ASP	2.3
4	T	228	HIS	2.3
8	v	121	VAL	2.3
4	L	22	LEU	2.3
4	L	156	LEU	2.3
3	a	33	GLU	2.3
1	A	315	ASP	2.3
2	h	51	LEU	2.3
4	T	124	ALA	2.3
4	b	183	LEU	2.3
8	f	108	ALA	2.3
2	Z	180	GLN	2.3
4	T	14	ASN	2.3
4	L	34	ILE	2.3
5	M	143	TYR	2.3
5	s	201	SER	2.3
2	J	30	VAL	2.3
3	S	118	LEU	2.3
6	F	90	LEU	2.3
6	V	206	MET	2.3
5	c	100	VAL	2.3
8	f	36	VAL	2.3
2	p	79	ASN	2.3
8	H	46	LEU	2.3
2	R	259	PHE	2.3
2	h	80	PHE	2.3
5	U	195	PRO	2.3
2	R	237	ILE	2.3
2	R	279	TYR	2.3
4	D	216	ILE	2.3
4	b	113	ILE	2.3
8	v	39	GLN	2.3
1	I	118	ALA	2.3
4	T	32	LYS	2.3
5	U	201	SER	2.3
4	D	70	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
4	L	145	LEU	2.3
4	T	145	LEU	2.3
4	T	231	HIS	2.3
1	A	207	HIS	2.2
3	K	260	TYR	2.2
3	a	217	SER	2.2
2	h	71	ALA	2.2
8	n	42	ALA	2.2
1	Q	77	VAL	2.2
1	Y	225	ARG	2.2
1	g	225	ARG	2.2
2	J	282	LEU	2.2
3	C	181	PHE	2.2
1	g	127	ASN	2.2
1	o	320	LEU	2.2
2	B	210	ASN	2.2
2	Z	292	ASN	2.2
1	Q	237	MET	2.2
1	o	489	MET	2.2
7	O	170	ILE	2.2
2	p	258	PHE	2.2
4	r	58	SER	2.2
1	Y	134	ILE	2.2
2	R	77	LYS	2.2
7	u	160	ARG	2.2
5	c	95	SER	2.2
4	j	36	LEU	2.2
2	B	278	LYS	2.2
4	L	147	THR	2.2
6	F	261	TYR	2.2
4	r	15	SER	2.2
5	E	29	TYR	2.2
4	L	150	LYS	2.2
5	M	188	THR	2.2
1	o	118	ALA	2.2
4	T	86	HIS	2.2
5	s	109	ALA	2.2
8	X	48	ASN	2.2
5	s	187	ARG	2.2
2	R	72	LEU	2.2
4	j	194	VAL	2.2
4	r	258	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
6	V	182	LEU	2.2
7	G	195	ALA	2.2
8	H	162	VAL	2.2
3	a	142	HIS	2.2
1	Q	162	LEU	2.2
4	T	188	LYS	2.2
8	P	153	TRP	2.2
1	o	192	SER	2.2
2	p	400	GLY	2.2
4	D	111	ALA	2.2
3	S	260	TYR	2.2
4	L	376	SER	2.2
7	e	196	ASN	2.2
2	J	309	LEU	2.2
4	r	17	GLY	2.2
8	f	46	LEU	2.2
8	X	153	TRP	2.2
3	q	272	PRO	2.2
4	T	49	VAL	2.2
4	b	294	ALA	2.2
4	b	249	LEU	2.2
7	W	64	PHE	2.2
1	A	225	ARG	2.2
5	E	190	PRO	2.2
6	l	169	GLU	2.2
1	Q	119	LEU	2.2
1	g	135	HIS	2.2
1	g	238	CYS	2.2
2	p	176	HIS	2.2
4	L	70	CYS	2.2
6	F	179	ALA	2.2
4	D	233	THR	2.2
5	k	103	THR	2.2
3	C	12	VAL	2.2
3	i	99	THR	2.2
7	m	31	ILE	2.2
2	Z	310	ALA	2.2
3	i	181	PHE	2.2
4	L	32	LYS	2.2
7	O	139	ASP	2.2
7	e	63	THR	2.2
8	X	113	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	80	PHE	2.2
4	L	132	LEU	2.2
4	r	211	LEU	2.2
4	L	170	ARG	2.2
4	b	64	GLN	2.2
4	r	189	VAL	2.2
8	v	60	ILE	2.2
4	b	33	ALA	2.2
4	j	48	PHE	2.2
6	d	183	PHE	2.2
4	j	17	GLY	2.2
6	t	67	GLN	2.2
2	J	292	ASN	2.2
4	D	143	TYR	2.2
4	b	213	TYR	2.2
6	t	183	PHE	2.2
2	J	54	PHE	2.2
2	Z	309	LEU	2.2
1	g	291	LEU	2.1
4	L	9	LEU	2.1
4	b	173	LEU	2.1
1	o	87	TYR	2.1
8	H	92	THR	2.1
4	r	130	ILE	2.1
5	M	50	HIS	2.1
5	k	50	HIS	2.1
4	T	99	PHE	2.1
7	O	160	ARG	2.1
8	v	71	LEU	2.1
7	W	8	THR	2.1
7	W	170	ILE	2.1
4	D	318	ASN	2.1
4	L	254	ARG	2.1
6	V	89	LEU	2.1
5	c	78	MET	2.1
1	I	189	LYS	2.1
1	o	110	LEU	2.1
1	I	127	ASN	2.1
3	K	65	LYS	2.1
5	E	168	VAL	2.1
3	a	96	ALA	2.1
3	a	270	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
4	T	260	ALA	2.1
3	S	181	PHE	2.1
7	m	18	LEU	2.1
5	k	201	SER	2.1
6	t	264	CYS	2.1
8	X	42	ALA	2.1
6	V	108	LYS	2.1
6	t	189	THR	2.1
4	b	86	HIS	2.1
4	j	98	SER	2.1
4	j	132	LEU	2.1
1	I	287	CYS	2.1
2	Z	237	ILE	2.1
4	T	19	HIS	2.1
4	b	72	HIS	2.1
7	u	198	HIS	2.1
4	T	229	ALA	2.1
7	u	70	PHE	2.1
8	f	163	LEU	2.1
1	o	189	LYS	2.1
3	i	176	TYR	2.1
5	c	90	MET	2.1
5	U	99	PRO	2.1
6	F	257	LEU	2.1
1	I	126	PHE	2.1
1	g	141	ALA	2.1
4	L	260	ALA	2.1
4	T	15	SER	2.1
4	L	230	LEU	2.1
4	j	168	ILE	2.1
6	N	131	PRO	2.1
3	i	260	TYR	2.1
6	N	183	PHE	2.1
8	f	13	PHE	2.1
6	V	86	SER	2.1
5	s	31	TYR	2.1
2	h	258	PHE	2.1
6	V	131	PRO	2.1
8	H	71	LEU	2.1
2	h	262	PHE	2.1
5	E	59	ALA	2.1
1	g	138	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	q	56	LEU	2.1
5	k	270	SER	2.1
7	G	66	LEU	2.1
7	G	160	ARG	2.1
5	s	99	PRO	2.1
2	p	239	GLU	2.1
6	V	208	ALA	2.1
8	X	77	VAL	2.1
1	o	227	TYR	2.1
3	a	307	ILE	2.1
5	E	99	PRO	2.1
1	Q	226	ASP	2.1
1	Y	315	ASP	2.1
4	r	57	VAL	2.1
4	D	230	LEU	2.1
5	k	86	ASP	2.1
7	G	19	ALA	2.1
4	D	92	ILE	2.1
2	J	143	LYS	2.1
2	p	277	LEU	2.1
4	r	85	TYR	2.1
8	n	128	ILE	2.1
4	j	65	LEU	2.1
2	h	176	HIS	2.1
4	j	170	ARG	2.1
2	R	81	LYS	2.1
2	R	400	GLY	2.1
3	K	52	GLN	2.1
3	i	226	LYS	2.1
5	s	263	THR	2.1
4	r	164	ALA	2.1
6	N	38	SER	2.1
1	Y	87	TYR	2.0
2	J	302	TYR	2.0
2	h	131	PHE	2.1
8	P	128	ILE	2.1
2	R	312	THR	2.0
4	r	36	LEU	2.0
4	r	156	LEU	2.0
6	V	135	ASP	2.0
1	A	449	ILE	2.0
7	W	215	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
4	L	223	LEU	2.0
4	b	30	LEU	2.0
8	X	162	VAL	2.0
1	g	97	ILE	2.0
2	B	237	ILE	2.0
2	Z	241	GLY	2.0
5	k	49	HIS	2.0
8	P	96	HIS	2.0
4	T	62	SER	2.0
4	D	139	TYR	2.0
1	g	346	VAL	2.0
2	h	115	ILE	2.0
8	H	78	GLY	2.0
1	A	460	LEU	2.0
1	g	115	LEU	2.0
4	L	155	TYR	2.0
1	Q	329	GLY	2.0
1	A	115	LEU	2.0
1	Y	207	HIS	2.0
1	g	189	LYS	2.0
5	M	29	TYR	2.0
7	W	195	ALA	2.0
3	i	12	VAL	2.0
4	j	153	ARG	2.0
7	m	15	PHE	2.0
2	p	82	LEU	2.0
3	q	211	THR	2.0
4	L	235	LEU	2.0
1	Y	101	GLN	2.0
1	A	223	ARG	2.0
4	D	165	GLU	2.0
3	S	24	LEU	2.0
7	e	27	LEU	2.0
1	A	78	GLU	2.0
3	q	307	ILE	2.0
4	L	192	ALA	2.0
3	q	69	PRO	2.0
4	D	125	GLN	2.0
4	r	61	ILE	2.0
5	s	98	LEU	2.0
8	X	70	GLU	2.0
4	b	57	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	S	353	GLN	2.0
4	D	196	ASP	2.0
1	Q	225	ARG	2.0
2	J	212	LYS	2.0
3	K	399	VAL	2.0
7	G	41	TYR	2.0
7	O	78	TYR	2.0
7	O	142	ARG	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
9	ZN	s	401	1/1	0.80	0.10	130,130,130,130	0
9	ZN	M	401	1/1	0.93	0.15	130,130,130,130	0
9	ZN	U	401	1/1	0.94	0.08	130,130,130,130	0
9	ZN	k	401	1/1	0.97	0.10	130,130,130,130	0
9	ZN	c	401	1/1	0.98	0.08	130,130,130,130	0
9	ZN	E	401	1/1	0.99	0.17	130,130,130,130	0

6.5 Other polymers (i)

There are no such residues in this entry.