



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2016 – 11:59 AM EDT

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

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

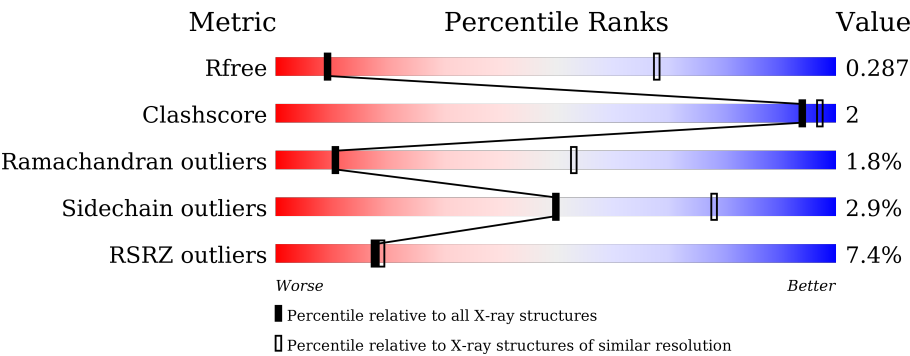
1 Overall quality at a glance i

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}	91344	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	<div><div>5%</div><div><div></div><div>79%</div><div>8%</div><div>13%</div></div></div>
1	I	480	<div><div>7%</div><div><div></div><div>79%</div><div>8%</div><div>13%</div></div></div>
1	Q	480	<div><div>6%</div><div><div></div><div>80%</div><div>7%</div><div>13%</div></div></div>
1	Y	480	<div><div>4%</div><div><div></div><div>80%</div><div>7%</div><div>13%</div></div></div>
1	g	480	<div><div>5%</div><div><div></div><div>84%</div><div>•</div><div>13%</div></div></div>
1	o	480	<div><div>4%</div><div><div></div><div>84%</div><div>•</div><div>13%</div></div></div>

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	N	331	
6	V	331	
6	d	331	
6	l	331	
6	t	331	
7	G	222	
7	O	222	
7	W	222	
7	e	222	
7	m	222	
7	u	222	
8	H	213	
8	P	213	
8	X	213	
8	f	213	
8	n	213	
8	v	213	

2 Entry composition [i](#)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

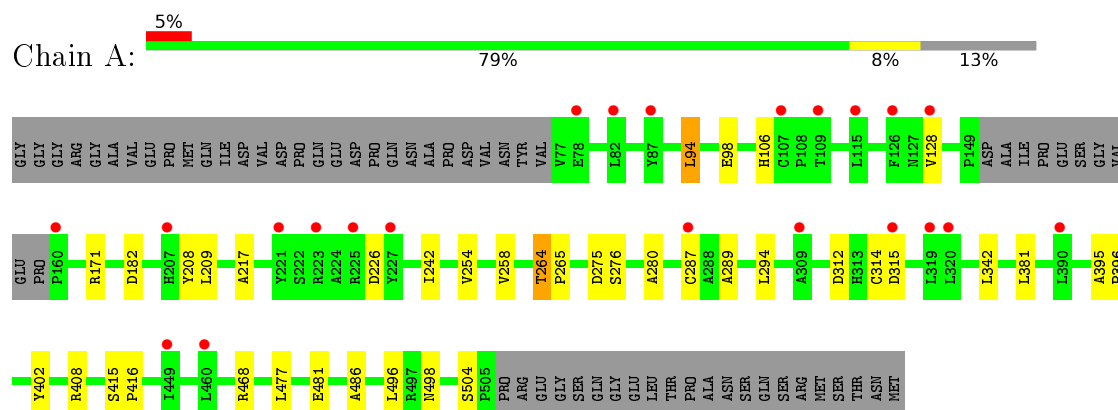
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

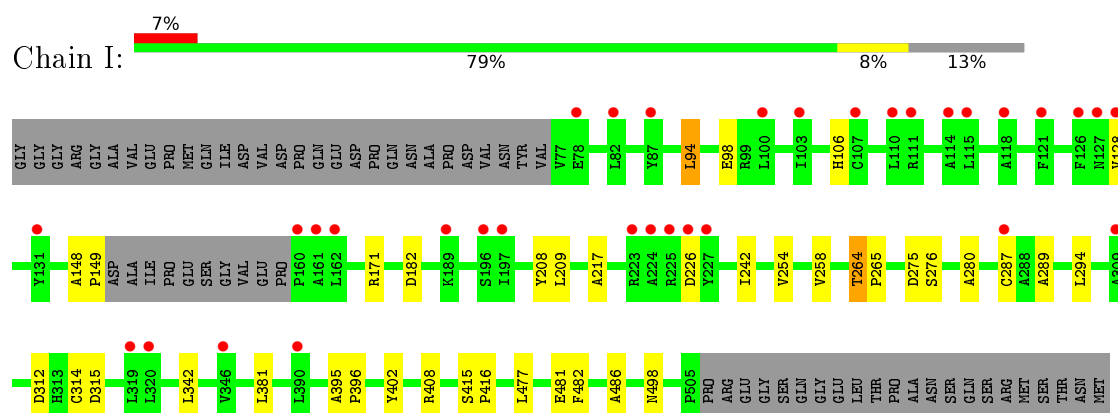
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

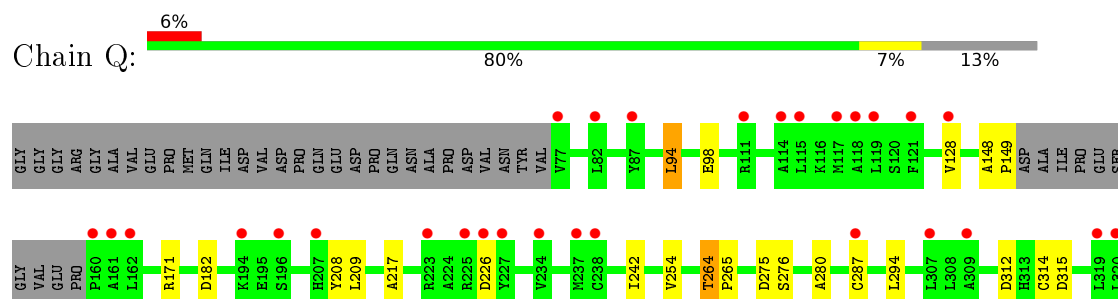
- Molecule 1: COP9 signalosome complex subunit 1



- Molecule 1: COP9 signalosome complex subunit 1

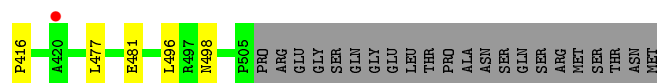
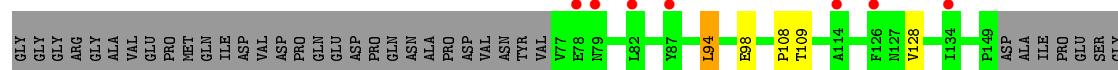
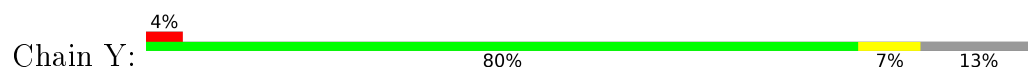


- Molecule 1: COP9 signalosome complex subunit 1

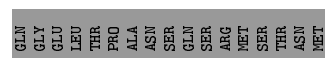
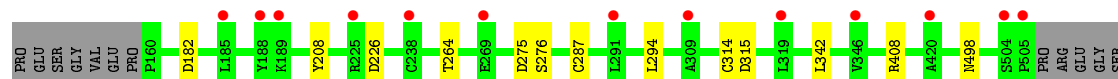
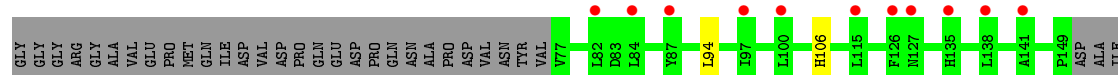
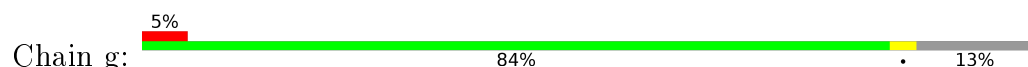




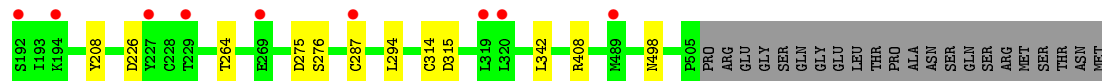
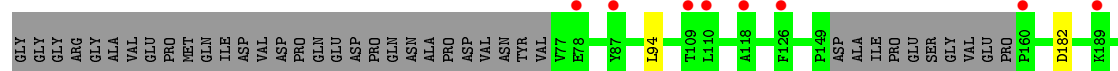
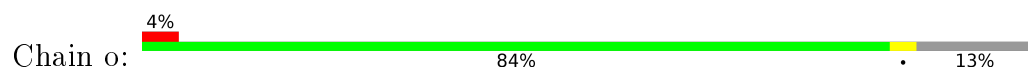
- Molecule 1: COP9 signalosome complex subunit 1



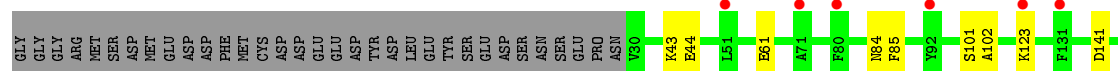
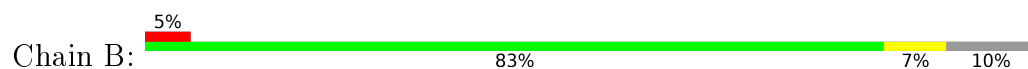
- Molecule 1: COP9 signalosome complex subunit 1

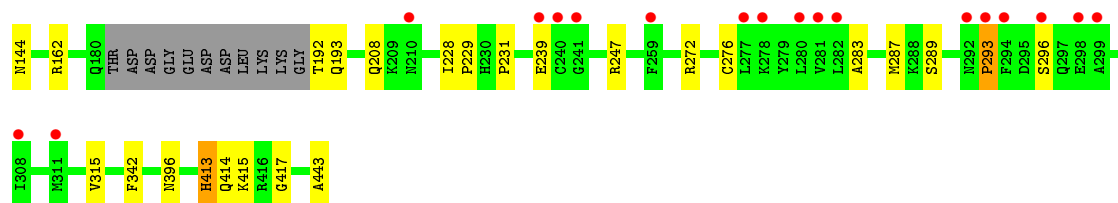


- Molecule 1: COP9 signalosome complex subunit 1

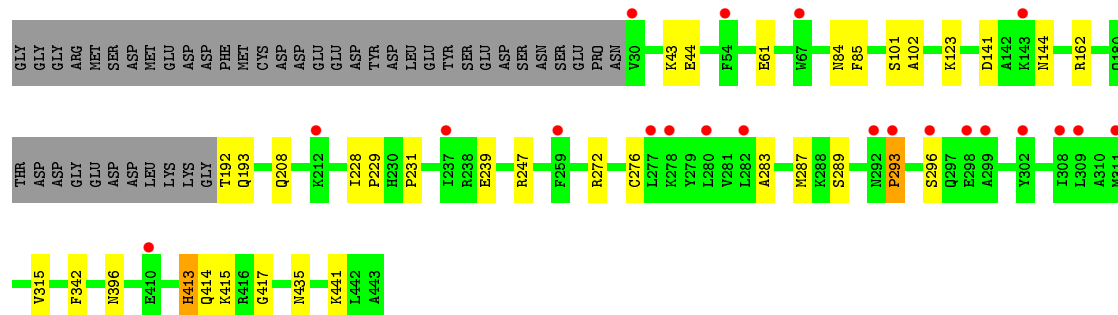
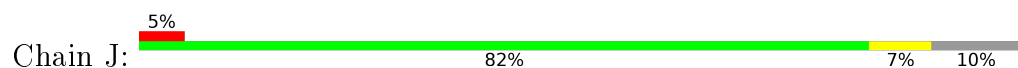


- Molecule 2: COP9 signalosome complex subunit 2

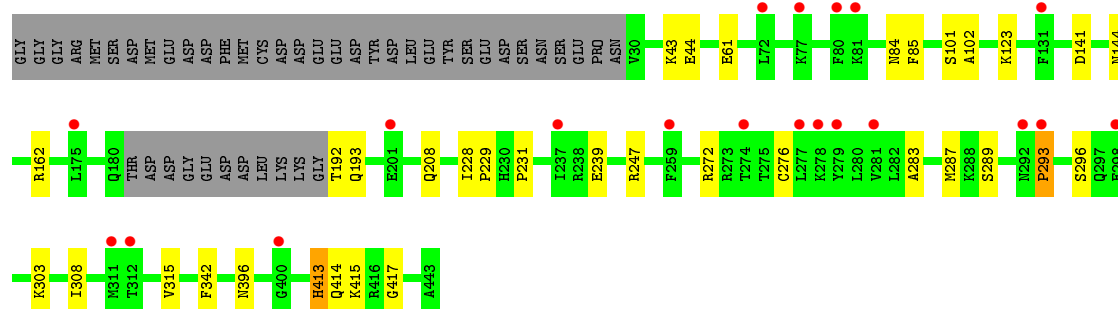
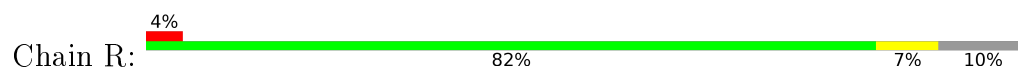




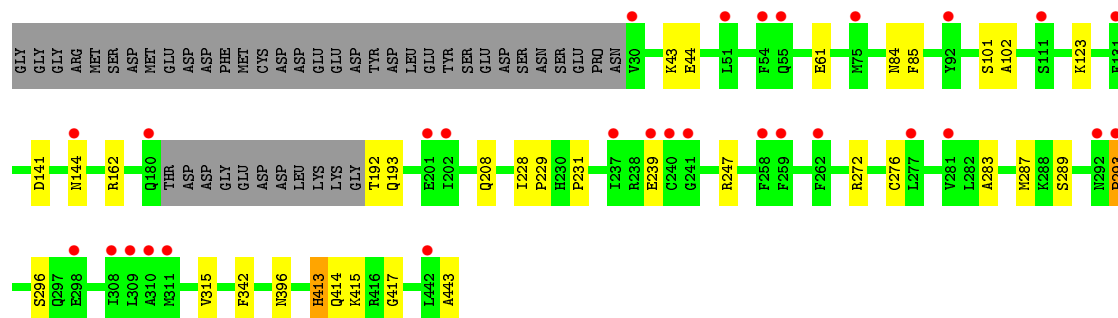
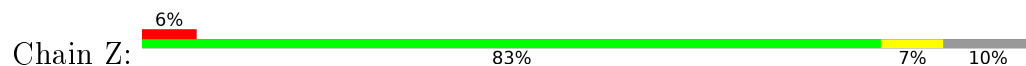
- Molecule 2: COP9 signalosome complex subunit 2



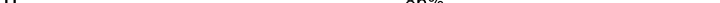
- Molecule 2: COP9 signalosome complex subunit 2

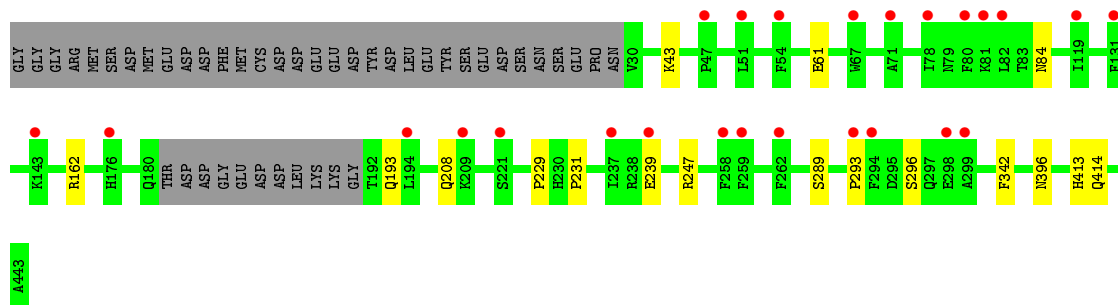


- Molecule 2: COP9 signalosome complex subunit 2

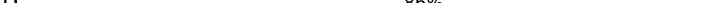


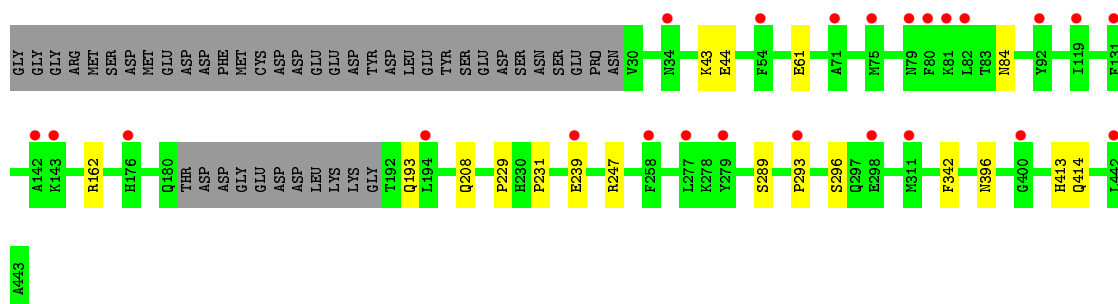
- Molecule 2: COP9 signalosome complex subunit 2

Chain h:  6% 86% 10%




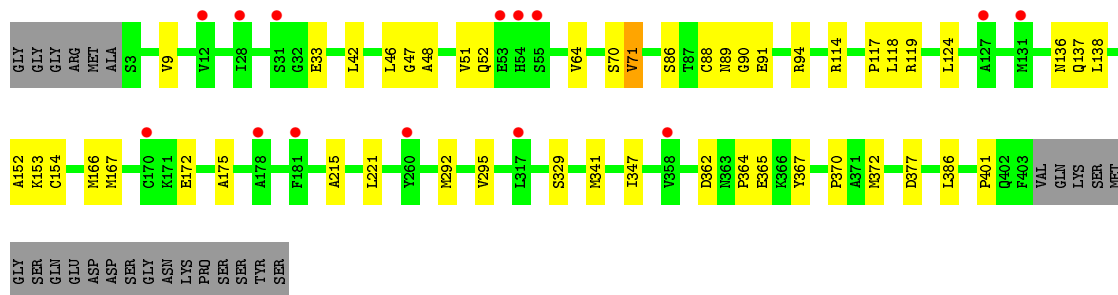
- Molecule 2: COP9 signalosome complex subunit 2

Chain p:  5% 86% 10%




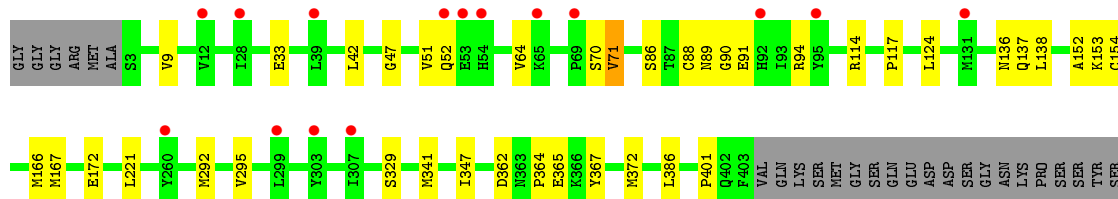
- Molecule 3: COP9 signalosome complex subunit 3

Chain C: 

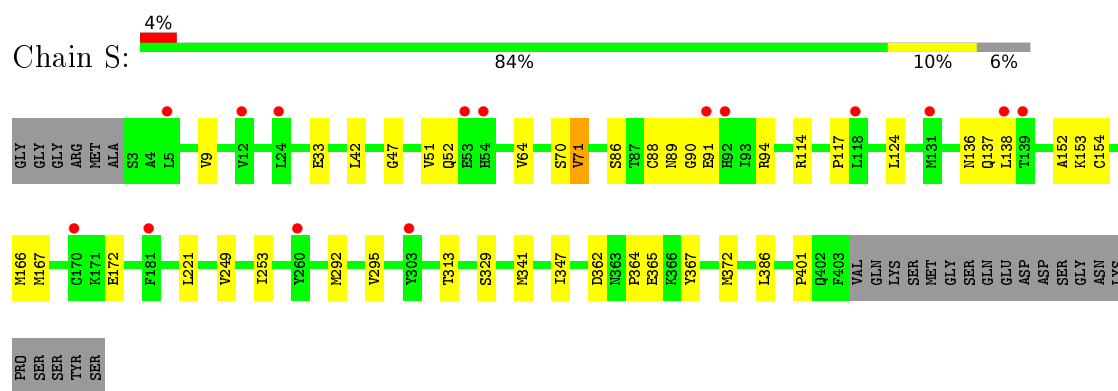


- Molecule 3: COP9 signalosome complex subunit 3

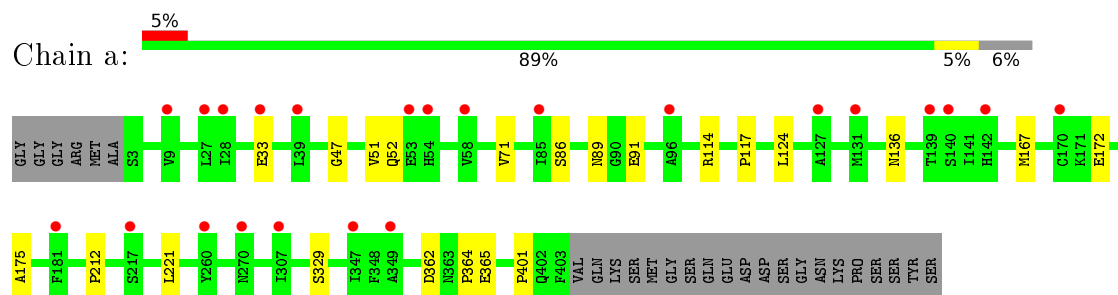
Chain K:  4% 85% 9% 6%



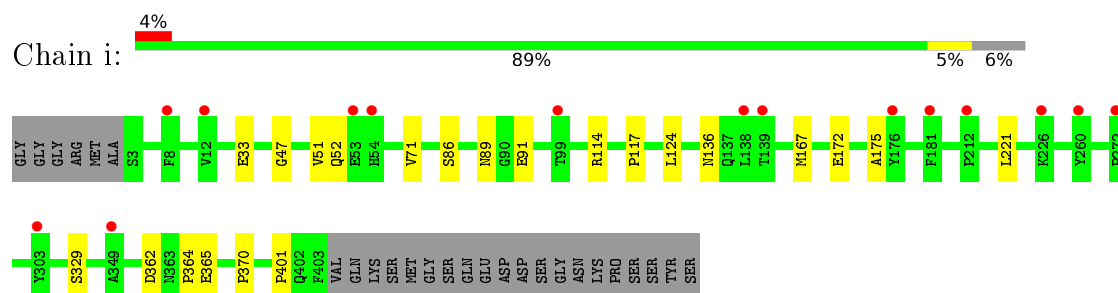
- Molecule 3: COP9 signalosome complex subunit 3



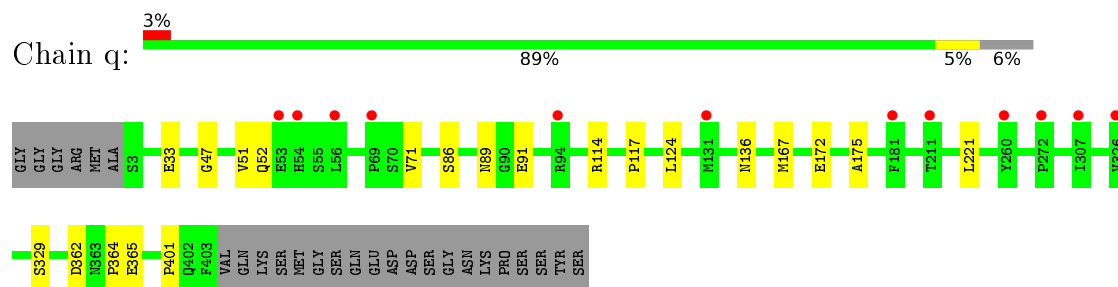
• Molecule 3: COP9 signalosome complex subunit 3



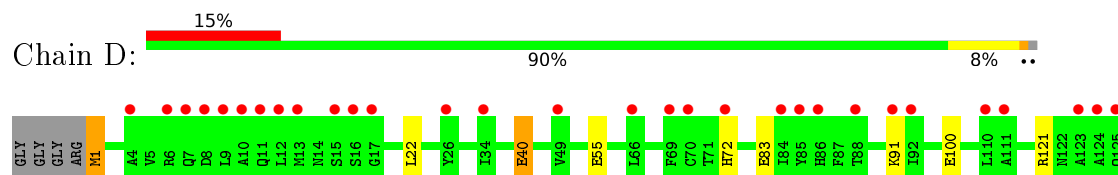
• Molecule 3: COP9 signalosome complex subunit 3

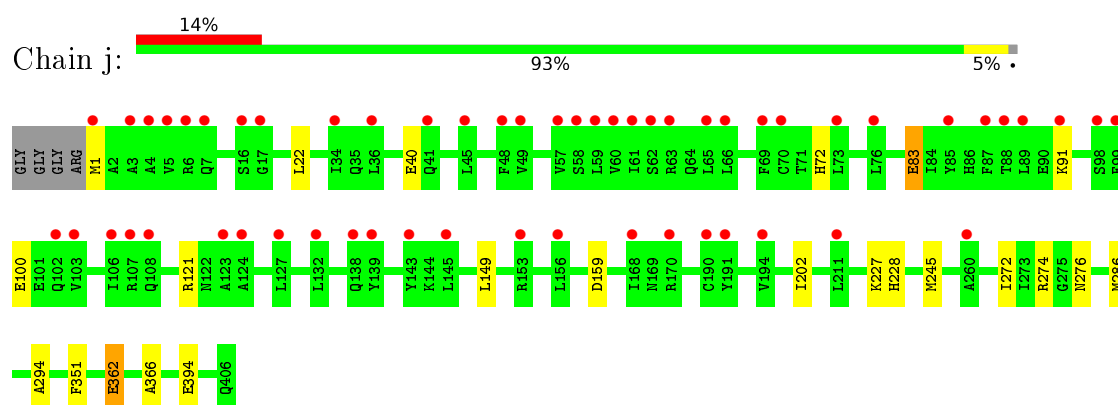


• Molecule 3: COP9 signalosome complex subunit 3

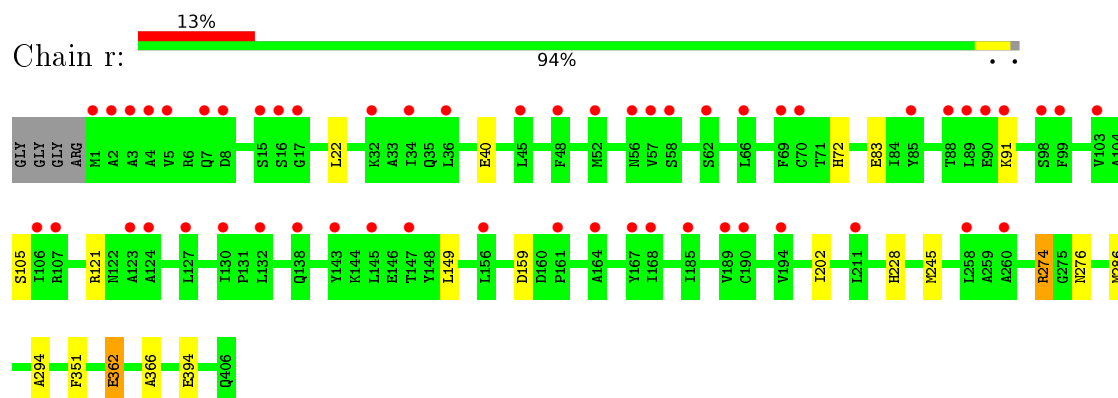


• Molecule 4: COP9 signalosome complex subunit 4

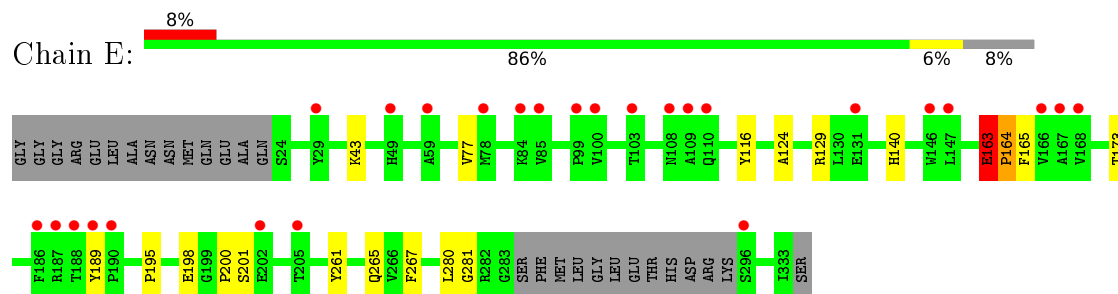




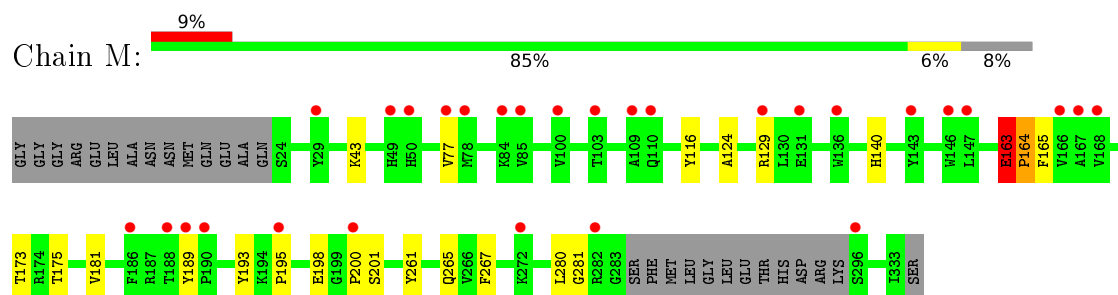
- Molecule 4: COP9 signalosome complex subunit 4



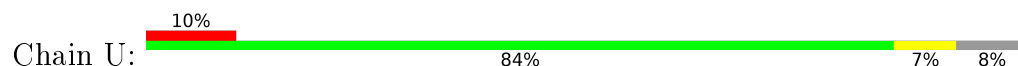
- Molecule 5: COP9 signalosome complex subunit 5

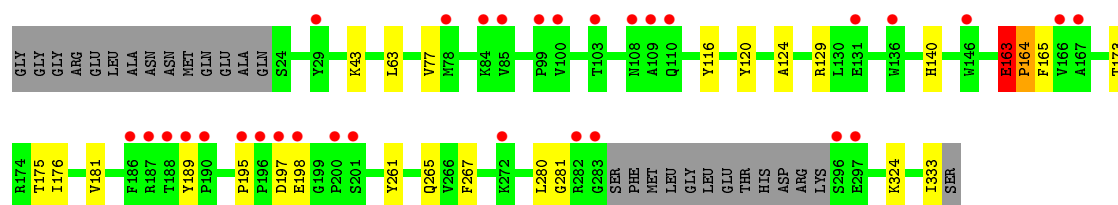


- Molecule 5: COP9 signalosome complex subunit 5

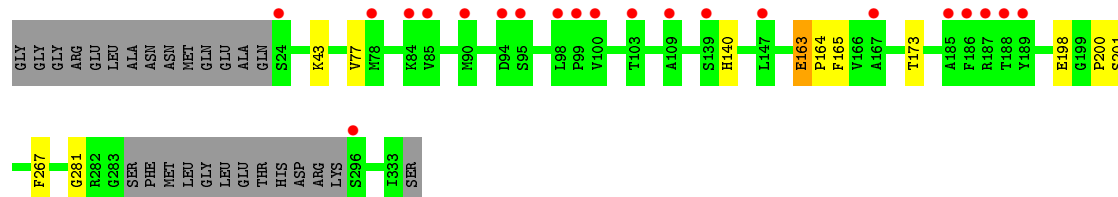
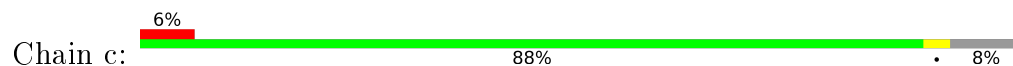


- Molecule 5: COP9 signalosome complex subunit 5

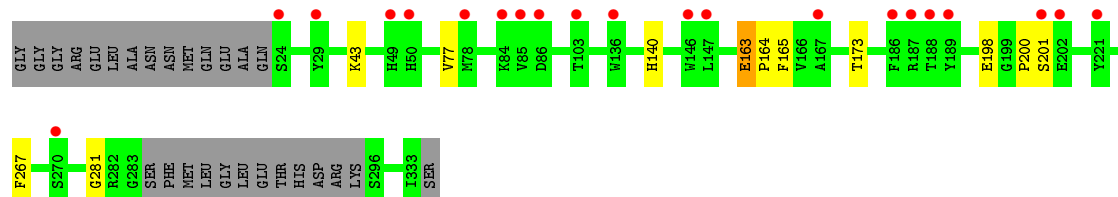
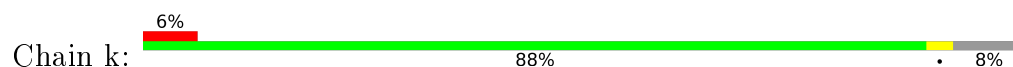




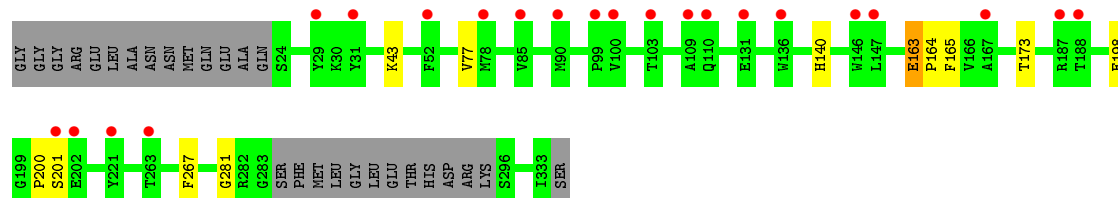
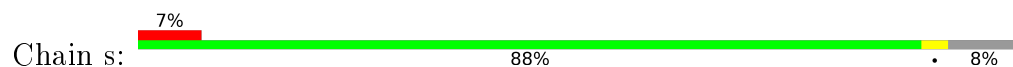
• Molecule 5: COP9 signalosome complex subunit 5



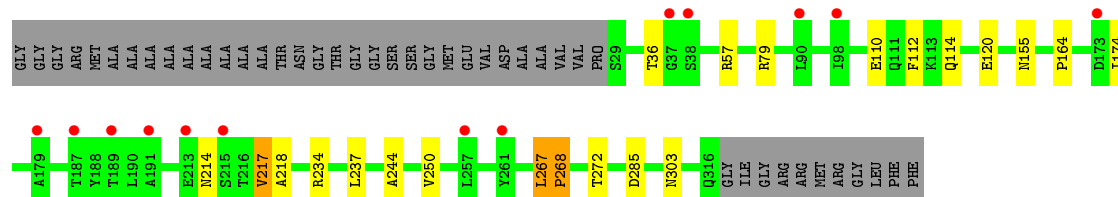
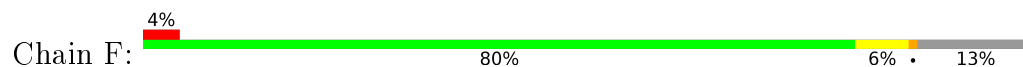
• Molecule 5: COP9 signalosome complex subunit 5



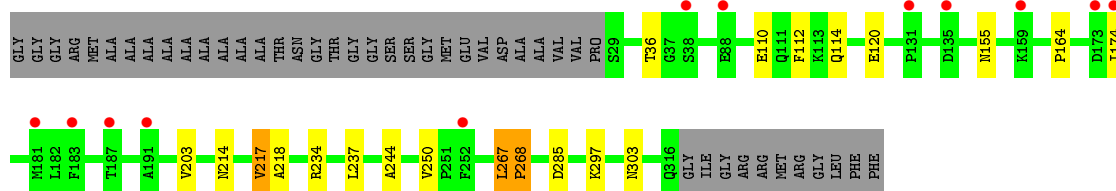
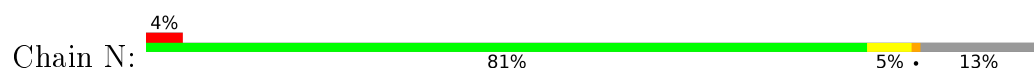
• Molecule 5: COP9 signalosome complex subunit 5



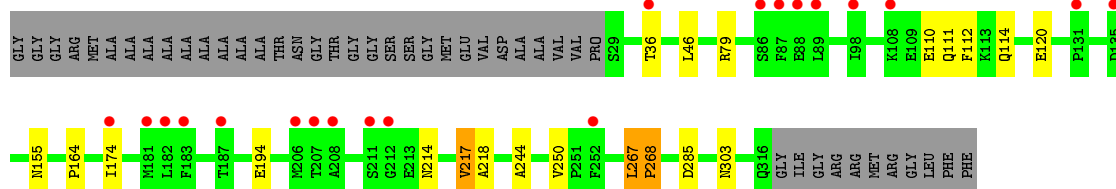
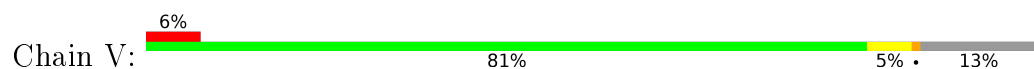
• Molecule 6: COP9 signalosome complex subunit 6



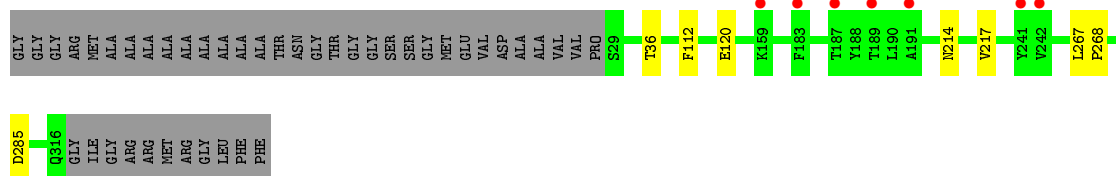
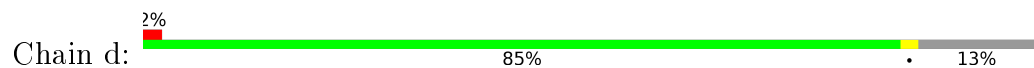
• Molecule 6: COP9 signalosome complex subunit 6



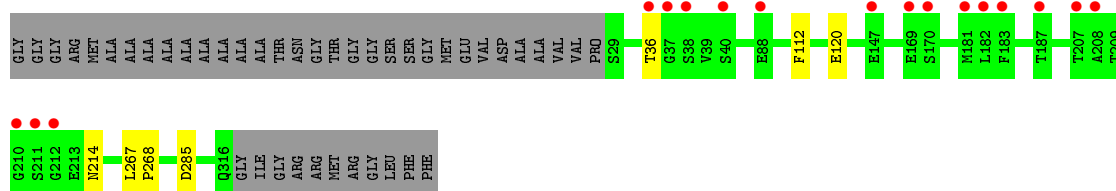
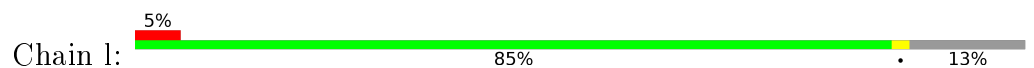
- Molecule 6: COP9 signalosome complex subunit 6



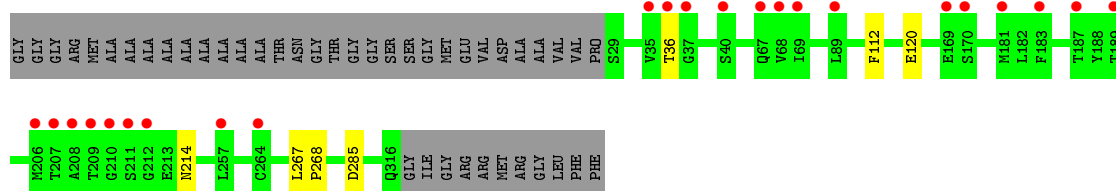
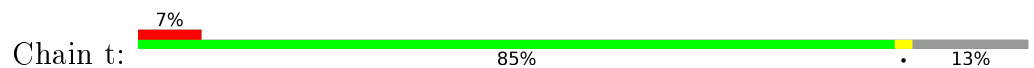
- Molecule 6: COP9 signalosome complex subunit 6



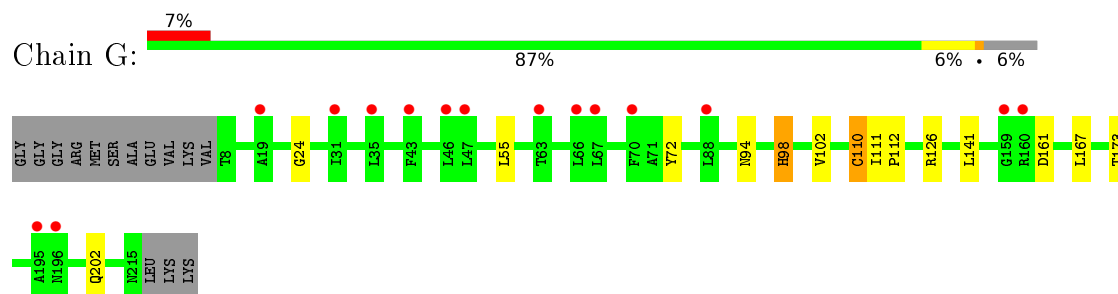
- Molecule 6: COP9 signalosome complex subunit 6



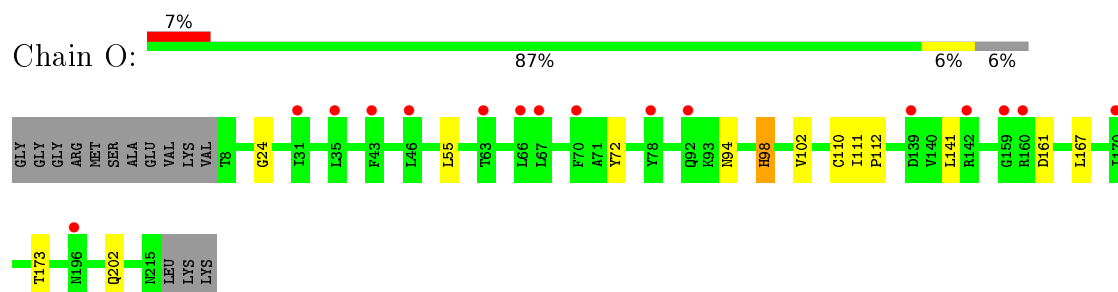
- Molecule 6: COP9 signalosome complex subunit 6



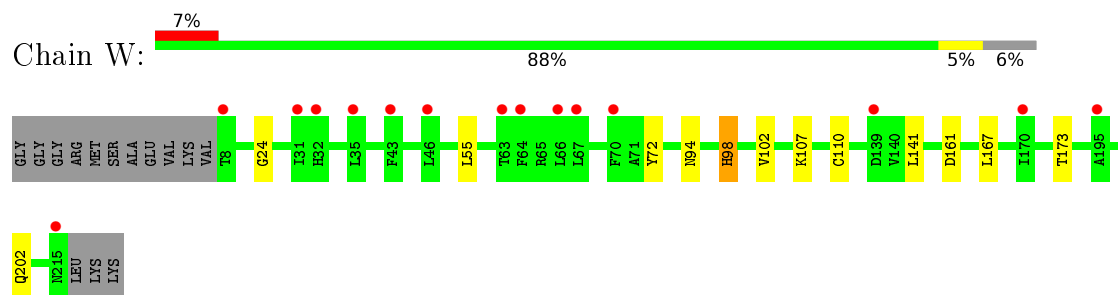
- Molecule 7: COP9 signalosome complex subunit 7a



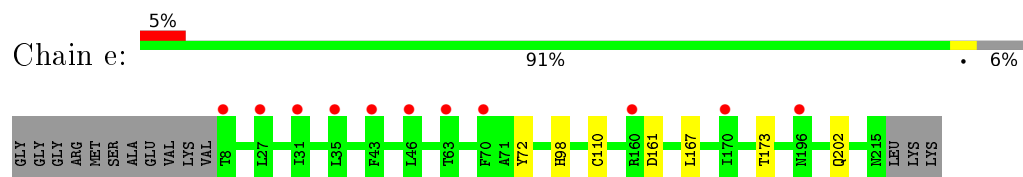
- Molecule 7: COP9 signalosome complex subunit 7a



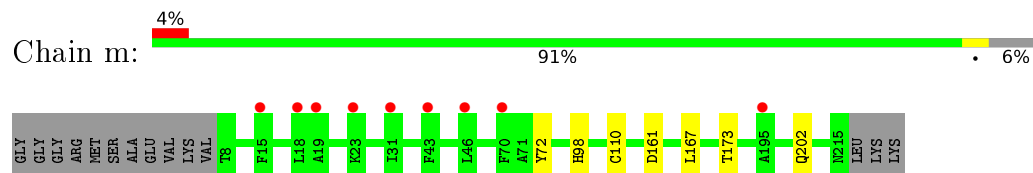
- Molecule 7: COP9 signalosome complex subunit 7a



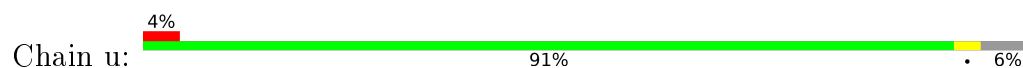
- Molecule 7: COP9 signalosome complex subunit 7a

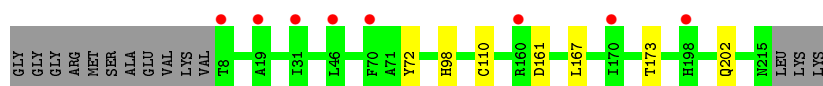


- Molecule 7: COP9 signalosome complex subunit 7a

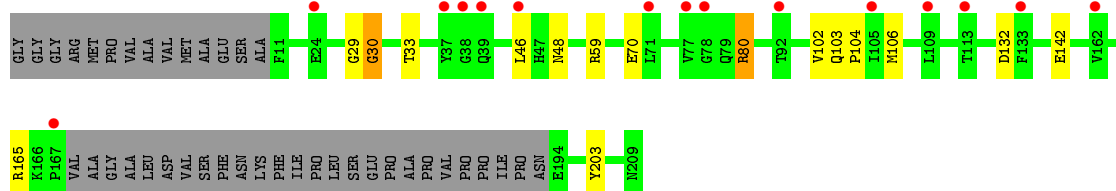
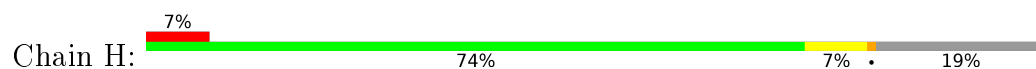


- Molecule 7: COP9 signalosome complex subunit 7a

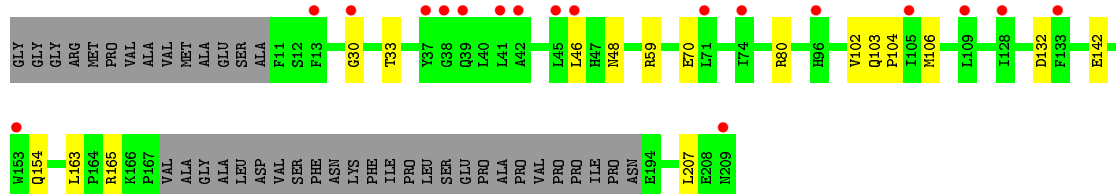
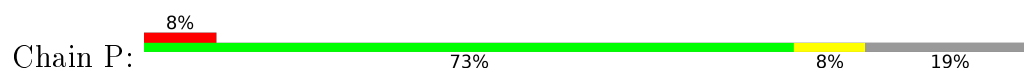




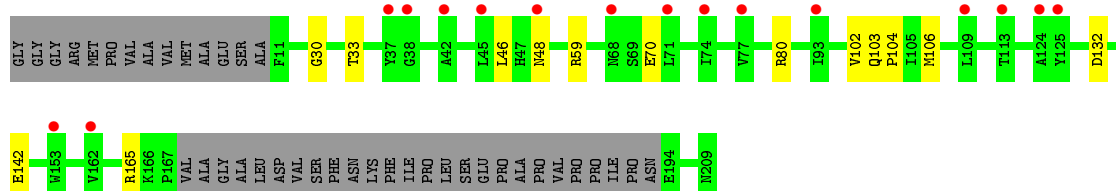
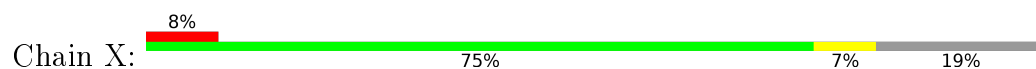
- Molecule 8: COP9 signalosome complex subunit 8



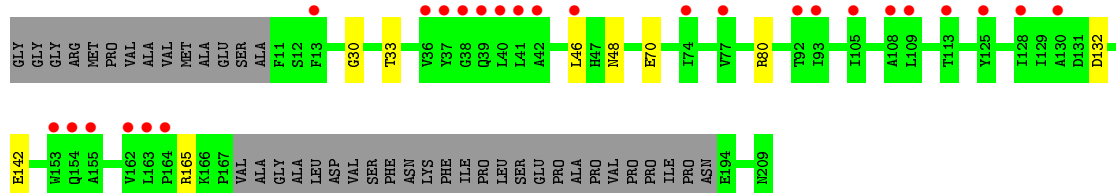
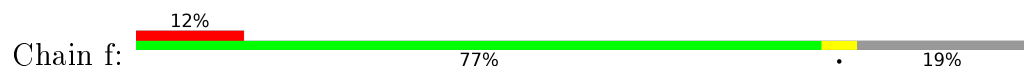
- Molecule 8: COP9 signalosome complex subunit 8



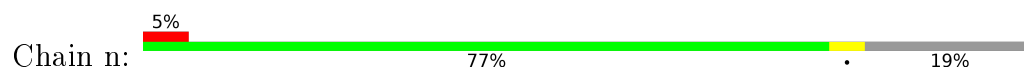
- Molecule 8: COP9 signalosome complex subunit 8

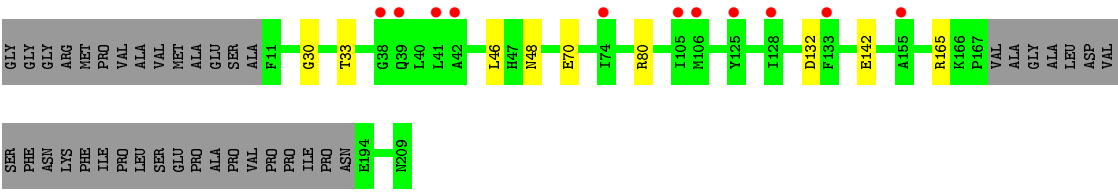


- Molecule 8: COP9 signalosome complex subunit 8

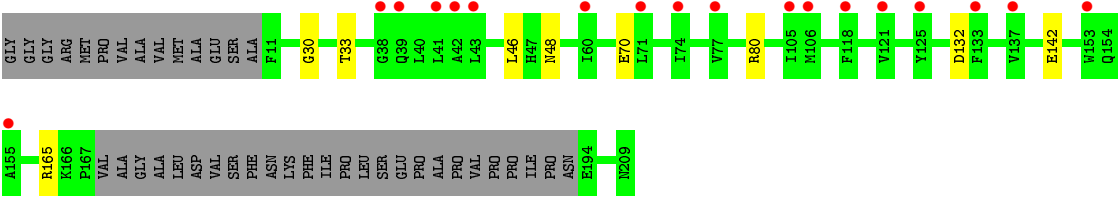
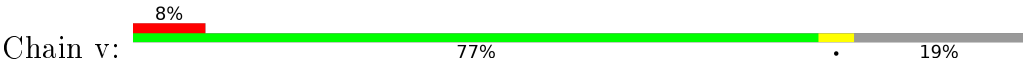


- Molecule 8: COP9 signalosome complex subunit 8





● Molecule 8: COP9 signalosome complex subunit 8



4 Data and refinement statistics

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) 82.0 (49.63-5.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 5.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.254 , 0.282 0.250 , 0.287	Depositor DCC
R_{free} test set	3398 reflections (2.45%)	DCC
Wilson B-factor (Å ²)	258.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 123.7	EDS
Estimated twinning fraction	0.084 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 79094 reflections	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 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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(°)	Ideal(°)
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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
6:F:244:ALA:HB1	6:F:250:VAL:HG21	1.99	0.45
3:C:119:ARG:HD3	8:H:29:GLY:HA2	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:341:MET:HB3	3:C:347:ILE:HG22	1.99	0.44
3:C:118:LEU:HD23	8:H:30:GLY:O	2.18	0.44

Continued on next page...

Continued from previous page...

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:333:ILE:CG2	7:W:107:LYS:HA	2.48	0.43
5:U:120:TYR:HA	6:V:111:GLN:OE1	2.19	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	19	64
1	I	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	19	64
1	Q	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	19	64
1	Y	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	19	64
1	g	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	19	64
1	o	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	19	64
2	B	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	5	42
2	J	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	5	42
2	R	397/447 (89%)	353 (89%)	32 (8%)	12 (3%)	5	42
2	Z	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	5	42
2	h	397/447 (89%)	351 (88%)	36 (9%)	10 (2%)	7	46
2	p	397/447 (89%)	351 (88%)	35 (9%)	11 (3%)	6	44
3	C	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	4	37
3	K	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	4	39
3	S	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	4	39
3	a	399/427 (93%)	341 (86%)	43 (11%)	15 (4%)	4	37
3	i	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	4	37
3	q	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	4	37
4	D	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	19	64
4	L	404/410 (98%)	373 (92%)	27 (7%)	4 (1%)	19	64
4	T	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	19	64
4	b	404/410 (98%)	374 (93%)	26 (6%)	4 (1%)	19	64
4	j	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	19	64
4	r	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	19	64
5	E	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	9	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	9	51
5	U	294/325 (90%)	262 (89%)	28 (10%)	4 (1%)	14	58
5	c	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	9	51
5	k	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	9	51
5	s	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	9	51
6	F	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	N	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	V	286/331 (86%)	258 (90%)	24 (8%)	4 (1%)	14	58
6	d	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	l	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
6	t	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	14	58
7	G	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
7	O	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	34	77
7	W	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	34	77
7	e	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
7	m	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
7	u	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	34	77
8	H	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	P	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	X	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	f	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	n	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
8	v	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	16	61
All	All	15416/17130 (90%)	13844 (90%)	1291 (8%)	281 (2%)	11	53

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	48	77
1	I	365/415 (88%)	354 (97%)	11 (3%)	48	77
1	Q	365/415 (88%)	355 (97%)	10 (3%)	52	79
1	Y	365/415 (88%)	355 (97%)	10 (3%)	52	79
1	g	365/415 (88%)	354 (97%)	11 (3%)	48	77
1	o	365/415 (88%)	355 (97%)	10 (3%)	52	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	J	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	R	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	Z	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	h	367/406 (90%)	360 (98%)	7 (2%)	65	86
2	p	367/406 (90%)	360 (98%)	7 (2%)	65	86
3	C	358/378 (95%)	351 (98%)	7 (2%)	63	85
3	K	358/378 (95%)	352 (98%)	6 (2%)	68	88
3	S	358/378 (95%)	352 (98%)	6 (2%)	68	88
3	a	358/378 (95%)	351 (98%)	7 (2%)	63	85
3	i	358/378 (95%)	351 (98%)	7 (2%)	63	85
3	q	358/378 (95%)	352 (98%)	6 (2%)	68	88
4	D	347/348 (100%)	328 (94%)	19 (6%)	27	64
4	L	347/348 (100%)	329 (95%)	18 (5%)	29	65
4	T	347/348 (100%)	329 (95%)	18 (5%)	29	65
4	b	347/348 (100%)	330 (95%)	17 (5%)	31	67
4	j	347/348 (100%)	327 (94%)	20 (6%)	25	62
4	r	347/348 (100%)	330 (95%)	17 (5%)	31	67
5	E	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	M	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	U	255/276 (92%)	248 (97%)	7 (3%)	52	79
5	c	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	k	255/276 (92%)	249 (98%)	6 (2%)	57	82
5	s	255/276 (92%)	249 (98%)	6 (2%)	57	82
6	F	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	N	250/277 (90%)	246 (98%)	4 (2%)	70	88
6	V	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	d	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	l	250/277 (90%)	247 (99%)	3 (1%)	78	90
6	t	250/277 (90%)	247 (99%)	3 (1%)	78	90
7	G	174/184 (95%)	168 (97%)	6 (3%)	44	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	O	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	W	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	e	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	m	174/184 (95%)	168 (97%)	6 (3%)	44	76
7	u	174/184 (95%)	168 (97%)	6 (3%)	44	76
8	H	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	P	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	X	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	f	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	n	144/174 (83%)	137 (95%)	7 (5%)	31	67
8	v	144/174 (83%)	137 (95%)	7 (5%)	31	67
All	All	13560/14748 (92%)	13173 (97%)	387 (3%)	50	78

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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

Continued on next page...

Continued from previous page...

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	419/480 (87%)	0.42	22 (5%) 30 29	60, 128, 170, 185	0
1	I	419/480 (87%)	0.49	33 (7%) 15 17	67, 120, 169, 191	0
1	Q	419/480 (87%)	0.48	31 (7%) 17 19	81, 121, 167, 197	0
1	Y	419/480 (87%)	0.31	17 (4%) 41 37	68, 108, 148, 176	0
1	g	419/480 (87%)	0.40	24 (5%) 27 26	80, 111, 161, 190	0
1	o	419/480 (87%)	0.29	17 (4%) 41 37	75, 109, 168, 189	0
2	B	403/447 (90%)	0.42	24 (5%) 25 24	65, 127, 155, 189	0
2	J	403/447 (90%)	0.34	21 (5%) 31 29	70, 125, 159, 172	0
2	R	403/447 (90%)	0.30	20 (4%) 32 30	75, 108, 139, 163	0
2	Z	403/447 (90%)	0.46	29 (7%) 18 19	68, 139, 167, 189	0
2	h	403/447 (90%)	0.43	25 (6%) 24 23	85, 135, 176, 202	0
2	p	403/447 (90%)	0.38	24 (5%) 25 24	81, 126, 165, 179	0
3	C	401/427 (93%)	0.32	14 (3%) 48 43	58, 118, 219, 260	0
3	K	401/427 (93%)	0.34	15 (3%) 45 41	69, 118, 201, 220	0
3	S	401/427 (93%)	0.28	15 (3%) 45 41	68, 99, 195, 216	0
3	a	401/427 (93%)	0.43	23 (5%) 27 26	69, 134, 218, 238	0
3	i	401/427 (93%)	0.30	15 (3%) 45 41	81, 114, 207, 257	0
3	q	401/427 (93%)	0.25	12 (2%) 54 47	77, 116, 208, 249	0
4	D	406/410 (99%)	0.86	60 (14%) 3 7	68, 145, 251, 272	0
4	L	406/410 (99%)	0.70	53 (13%) 5 8	80, 152, 188, 216	0
4	T	406/410 (99%)	0.72	50 (12%) 5 9	88, 131, 183, 209	0
4	b	406/410 (99%)	1.13	84 (20%) 1 5	73, 166, 243, 253	0
4	j	406/410 (99%)	0.76	56 (13%) 4 8	86, 132, 269, 285	0
4	r	406/410 (99%)	0.82	54 (13%) 4 8	81, 162, 253, 272	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
5	E	298/325 (91%)	0.54	26 (8%)	13 15	73, 112, 148, 170	0
5	M	298/325 (91%)	0.59	29 (9%)	10 13	78, 107, 159, 185	0
5	U	298/325 (91%)	0.60	31 (10%)	8 12	89, 121, 174, 198	0
5	c	298/325 (91%)	0.43	21 (7%)	19 20	61, 88, 126, 144	0
5	k	298/325 (91%)	0.46	21 (7%)	19 20	85, 107, 145, 166	0
5	s	298/325 (91%)	0.52	22 (7%)	17 19	84, 108, 148, 170	0
6	F	288/331 (87%)	0.37	13 (4%)	37 34	62, 114, 153, 184	0
6	N	288/331 (87%)	0.41	12 (4%)	40 36	73, 113, 165, 193	0
6	V	288/331 (87%)	0.46	20 (6%)	20 20	84, 120, 160, 194	0
6	d	288/331 (87%)	0.33	7 (2%)	62 57	63, 97, 150, 185	0
6	l	288/331 (87%)	0.45	17 (5%)	26 25	84, 116, 156, 182	0
6	t	288/331 (87%)	0.45	23 (7%)	15 17	77, 116, 160, 190	0
7	G	208/222 (93%)	0.37	15 (7%)	18 19	92, 114, 162, 187	0
7	O	208/222 (93%)	0.32	16 (7%)	16 17	68, 115, 160, 181	0
7	W	208/222 (93%)	0.33	15 (7%)	18 19	111, 135, 161, 174	0
7	e	208/222 (93%)	0.32	11 (5%)	30 29	84, 106, 145, 168	0
7	m	208/222 (93%)	0.19	9 (4%)	39 35	72, 98, 143, 188	0
7	u	208/222 (93%)	0.27	8 (3%)	44 40	73, 111, 149, 164	0
8	H	173/213 (81%)	0.45	15 (8%)	13 15	82, 123, 154, 168	0
8	P	173/213 (81%)	0.46	18 (10%)	8 12	91, 121, 147, 161	0
8	X	173/213 (81%)	0.49	16 (9%)	11 14	91, 114, 142, 150	0
8	f	173/213 (81%)	0.60	26 (15%)	3 7	81, 169, 190, 196	0
8	n	173/213 (81%)	0.42	11 (6%)	23 22	98, 129, 164, 181	0
8	v	173/213 (81%)	0.53	18 (10%)	8 12	94, 139, 175, 187	0
All	All	15576/17130 (90%)	0.47	1158 (7%)	17 19	58, 119, 209, 285	0

All (1158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	b	78	ASP	15.2
1	I	160	PRO	8.6
4	b	2	ALA	8.2
5	U	189	TYR	7.3
3	C	54	HIS	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	r	1	MET	7.2
4	r	16	SER	7.2
5	U	188	THR	7.2
4	b	77	PRO	6.5
1	Q	160	PRO	6.4
6	l	170	SER	6.3
1	Y	160	PRO	6.2
4	b	51	ALA	6.0
4	D	12	LEU	5.9
4	j	69	PHE	5.9
8	f	39	GLN	5.8
1	I	161	ALA	5.8
4	r	2	ALA	5.7
4	b	76	LEU	5.6
4	D	88	THR	5.5
5	E	110	GLN	5.4
4	b	14	ASN	5.3
4	D	8	ASP	5.3
4	D	11	GLN	5.3
4	b	41	GLN	5.3
4	b	79	SER	5.2
4	D	151	ILE	5.2
4	b	40	GLU	5.2
5	M	146	TRP	5.2
8	f	162	VAL	5.2
3	C	53	GLU	5.2
1	I	309	ALA	5.1
4	b	146	GLU	5.1
6	V	183	PHE	5.1
5	M	189	TYR	5.1
5	M	167	ALA	5.0
5	k	85	VAL	5.0
6	F	187	THR	5.0
4	D	9	LEU	4.9
8	X	71	LEU	4.9
8	f	37	TYR	4.9
4	T	350	GLY	4.9
5	s	103	THR	4.8
4	L	148	TYR	4.8
4	r	99	PHE	4.8
4	b	13	MET	4.8
4	D	148	TYR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	r	62	SER	4.8
2	J	298	GLU	4.7
4	D	34	ILE	4.7
5	M	110	GLN	4.7
8	f	155	ALA	4.7
6	t	170	SER	4.7
5	U	85	VAL	4.6
4	r	69	PHE	4.6
4	D	16	SER	4.6
1	Q	128	VAL	4.6
2	B	311	MET	4.5
2	h	143	LYS	4.5
1	A	309	ALA	4.5
3	S	54	HIS	4.5
1	I	224	ALA	4.5
5	E	109	ALA	4.5
2	p	71	ALA	4.4
8	f	154	GLN	4.4
5	k	136	TRP	4.4
2	B	259	PHE	4.4
4	b	52	MET	4.4
4	T	152	ALA	4.4
8	P	37	TYR	4.4
4	T	26	TYR	4.4
4	L	30	LEU	4.4
4	b	34	ILE	4.4
5	U	167	ALA	4.4
4	L	26	TYR	4.4
2	h	293	PRO	4.4
5	s	78	MET	4.4
1	g	420	ALA	4.3
5	c	103	THR	4.3
2	B	298	GLU	4.3
3	a	28	ILE	4.3
4	b	15	SER	4.3
4	j	16	SER	4.3
4	j	106	ILE	4.3
4	T	30	LEU	4.3
8	P	38	GLY	4.3
6	t	211	SER	4.2
5	s	29	TYR	4.2
4	D	7	GLN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	b	99	PHE	4.2
4	j	58	SER	4.2
5	E	167	ALA	4.2
5	s	221	TYR	4.2
5	E	108	ASN	4.2
5	M	85	VAL	4.2
4	D	152	ALA	4.2
4	b	168	ILE	4.2
4	r	127	LEU	4.2
7	O	67	LEU	4.2
4	j	45	LEU	4.1
2	Z	308	ILE	4.1
1	I	114	ALA	4.1
1	I	227	TYR	4.1
4	D	147	THR	4.1
4	j	102	GLN	4.1
5	s	90	MET	4.1
2	B	293	PRO	4.1
5	k	29	TYR	4.1
4	j	99	PHE	4.1
8	f	92	THR	4.1
6	t	187	THR	4.1
4	b	11	GLN	4.0
7	e	8	THR	4.0
3	K	53	GLU	4.0
7	u	8	THR	4.0
2	h	67	TRP	4.0
1	A	82	LEU	4.0
2	B	51	LEU	4.0
7	G	70	PHE	4.0
7	m	195	ALA	4.0
2	J	308	ILE	4.0
4	b	48	PHE	4.0
1	Y	309	ALA	4.0
2	p	143	LYS	4.0
3	a	54	HIS	4.0
1	Y	78	GLU	4.0
4	b	80	THR	4.0
5	M	84	LYS	4.0
2	Z	298	GLU	4.0
4	D	127	LEU	4.0
1	o	78	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	a	53	GLU	3.9
4	L	29	ILE	3.9
4	j	127	LEU	3.9
8	v	74	ILE	3.9
1	o	160	PRO	3.9
5	k	78	MET	3.9
3	C	170	CYS	3.9
2	Z	293	PRO	3.9
4	r	52	MET	3.9
1	g	82	LEU	3.9
5	s	52	PHE	3.9
2	Z	311	MET	3.9
3	a	140	SER	3.9
4	D	91	LYS	3.9
4	L	188	LYS	3.9
2	p	293	PRO	3.8
5	M	186	PHE	3.8
4	D	124	ALA	3.8
4	b	139	TYR	3.8
8	f	38	GLY	3.8
4	j	4	ALA	3.8
4	b	1	MET	3.8
2	Z	51	LEU	3.8
4	T	151	ILE	3.8
3	S	92	HIS	3.8
3	a	139	THR	3.8
4	r	5	VAL	3.8
6	t	37	GLY	3.8
8	v	38	GLY	3.8
4	b	12	LEU	3.8
1	Q	117	MET	3.8
3	S	53	GLU	3.8
5	U	166	VAL	3.8
4	D	4	ALA	3.8
4	b	115	GLU	3.7
2	B	280	LEU	3.7
2	Z	259	PHE	3.7
7	O	70	PHE	3.7
4	T	88	THR	3.7
4	D	193	ARG	3.7
4	L	207	ARG	3.7
4	b	150	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	n	155	ALA	3.7
6	N	187	THR	3.7
5	s	131	GLU	3.7
4	b	49	VAL	3.7
4	L	167	TYR	3.7
4	r	123	ALA	3.6
4	b	194	VAL	3.6
7	W	31	ILE	3.6
8	n	105	ILE	3.6
4	j	1	MET	3.6
7	u	19	ALA	3.6
4	b	81	ALA	3.6
8	X	93	ILE	3.6
4	D	66	LEU	3.6
5	M	100	VAL	3.6
4	r	3	ALA	3.6
5	U	187	ARG	3.6
4	r	66	LEU	3.6
8	H	105	ILE	3.6
4	T	48	PHE	3.6
4	T	22	LEU	3.6
7	O	63	THR	3.6
8	n	39	GLN	3.6
5	E	147	LEU	3.6
7	m	70	PHE	3.6
4	r	4	ALA	3.6
4	r	56	ASN	3.5
4	r	7	GLN	3.5
2	p	298	GLU	3.5
4	b	26	TYR	3.5
8	n	74	ILE	3.5
4	b	145	LEU	3.5
2	B	281	VAL	3.5
6	l	207	THR	3.5
1	I	162	LEU	3.5
4	r	8	ASP	3.5
4	b	191	TYR	3.5
7	O	66	LEU	3.5
1	I	226	ASP	3.5
6	V	211	SER	3.5
1	I	225	ARG	3.5
7	e	46	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	s	202	GLU	3.5
6	t	36	THR	3.5
1	Y	82	LEU	3.5
5	s	85	VAL	3.5
4	D	85	TYR	3.5
5	c	189	TYR	3.5
5	U	103	THR	3.4
7	G	63	THR	3.4
4	T	89	LEU	3.4
5	k	167	ALA	3.4
4	r	260	ALA	3.4
5	E	84	LYS	3.4
5	s	136	TRP	3.4
6	V	212	GLY	3.4
2	p	80	PHE	3.4
4	L	48	PHE	3.4
8	f	105	ILE	3.4
4	D	10	ALA	3.4
5	k	187	ARG	3.4
4	j	103	VAL	3.4
4	D	17	GLY	3.4
4	b	156	LEU	3.4
6	N	181	MET	3.4
4	L	211	LEU	3.4
2	p	142	ALA	3.4
4	r	143	TYR	3.4
3	q	54	HIS	3.4
4	j	91	LYS	3.4
3	i	139	THR	3.4
4	r	34	ILE	3.4
4	b	172	SER	3.4
4	j	107	ARG	3.3
2	J	311	MET	3.3
1	Q	82	LEU	3.3
1	I	320	LEU	3.3
4	j	73	LEU	3.3
1	I	87	TYR	3.3
7	u	46	LEU	3.3
4	r	91	LYS	3.3
2	J	277	LEU	3.3
6	F	215	SER	3.3
7	O	31	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	54	HIS	3.3
5	M	78	MET	3.3
6	t	210	GLY	3.3
4	L	152	ALA	3.3
4	D	86	HIS	3.3
5	E	131	GLU	3.3
6	V	98	ILE	3.3
1	A	160	PRO	3.3
6	t	209	THR	3.3
8	H	37	TYR	3.3
4	j	5	VAL	3.3
4	b	75	ASN	3.3
6	t	208	ALA	3.3
4	j	88	THR	3.3
2	Z	281	VAL	3.3
2	R	311	MET	3.3
1	Q	227	TYR	3.3
2	h	82	LEU	3.3
4	j	70	CYS	3.3
8	f	40	LEU	3.3
6	N	174	ILE	3.3
7	W	35	LEU	3.3
7	e	160	ARG	3.3
1	I	319	LEU	3.3
4	D	26	TYR	3.2
1	Q	114	ALA	3.2
3	K	303	TYR	3.2
1	g	100	LEU	3.2
2	J	278	LYS	3.2
8	f	153	TRP	3.2
8	n	125	TYR	3.2
4	j	3	ALA	3.2
5	U	282	ARG	3.2
6	l	210	GLY	3.2
4	L	193	ARG	3.2
1	I	111	ARG	3.2
5	c	185	ALA	3.2
7	W	63	THR	3.2
6	t	212	GLY	3.2
5	E	205	THR	3.2
4	b	53	VAL	3.2
8	f	93	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	T	84	ILE	3.2
2	p	34	ASN	3.2
6	t	207	THR	3.2
7	W	32	HIS	3.2
4	D	49	VAL	3.2
2	h	81	LYS	3.2
4	b	98	SER	3.2
6	l	211	SER	3.2
4	j	57	VAL	3.2
3	a	349	ALA	3.2
4	D	189	VAL	3.2
4	D	226	LEU	3.2
7	G	31	ILE	3.2
4	b	37	SER	3.2
1	Q	319	LEU	3.2
5	s	146	TRP	3.2
7	G	35	LEU	3.2
2	h	239	GLU	3.2
2	Z	54	PHE	3.2
8	v	155	ALA	3.2
8	v	41	LEU	3.1
4	b	103	VAL	3.1
4	j	62	SER	3.1
2	p	131	PHE	3.1
6	d	187	THR	3.1
6	t	68	VAL	3.1
1	Q	111	ARG	3.1
4	r	32	LYS	3.1
7	W	67	LEU	3.1
5	E	187	ARG	3.1
5	c	187	ARG	3.1
2	h	54	PHE	3.1
4	j	138	GLN	3.1
4	r	45	LEU	3.1
4	b	107	ARG	3.1
1	o	319	LEU	3.1
8	n	38	GLY	3.1
5	U	131	GLU	3.1
3	i	272	PRO	3.1
7	G	43	PHE	3.1
4	T	23	ALA	3.1
4	j	89	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	s	147	LEU	3.1
1	A	126	PHE	3.1
1	Q	207	HIS	3.1
3	C	31	SER	3.1
2	h	298	GLU	3.1
4	j	139	TYR	3.1
4	j	66	LEU	3.1
5	s	188	THR	3.1
8	X	45	LEU	3.1
4	b	188	LYS	3.1
4	b	56	ASN	3.1
4	r	161	PRO	3.1
2	Z	131	PHE	3.1
2	p	119	ILE	3.1
2	p	92	TYR	3.1
4	L	88	THR	3.1
8	P	105	ILE	3.1
4	r	138	GLN	3.1
5	E	103	THR	3.1
4	b	192	ALA	3.1
4	T	150	LYS	3.1
6	l	182	LEU	3.1
4	b	88	THR	3.0
5	c	94	ASP	3.0
2	B	292	ASN	3.0
4	b	187	TYR	3.0
5	U	200	PRO	3.0
1	I	103	ILE	3.0
2	R	274	THR	3.0
4	r	145	LEU	3.0
1	g	126	PHE	3.0
6	l	212	GLY	3.0
4	j	61	ILE	3.0
5	M	166	VAL	3.0
6	l	37	GLY	3.0
1	g	309	ALA	3.0
5	U	108	ASN	3.0
5	M	195	PRO	3.0
8	H	39	GLN	3.0
4	j	6	ARG	3.0
8	v	125	TYR	3.0
7	G	67	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	T	351	PHE	3.0
3	S	91	GLU	3.0
1	A	128	VAL	3.0
5	c	84	LYS	3.0
6	l	36	THR	3.0
4	D	15	SER	3.0
7	O	46	LEU	3.0
8	f	41	LEU	3.0
2	Z	262	PHE	2.9
4	L	69	PHE	2.9
2	Z	75	MET	2.9
4	L	226	LEU	2.9
4	T	12	LEU	2.9
4	b	45	LEU	2.9
3	a	27	LEU	2.9
4	b	9	LEU	2.9
5	c	186	PHE	2.9
8	f	42	ALA	2.9
1	I	100	LEU	2.9
4	j	190	CYS	2.9
5	M	296	SER	2.9
2	B	282	LEU	2.9
5	c	85	VAL	2.9
6	l	88	GLU	2.9
3	C	260	TYR	2.9
3	S	303	TYR	2.9
4	T	52	MET	2.9
4	b	89	LEU	2.9
5	U	196	PRO	2.9
1	Y	126	PHE	2.9
4	D	197	TYR	2.9
4	b	108	GLN	2.9
3	C	28	ILE	2.9
7	G	46	LEU	2.9
1	Q	309	ALA	2.9
8	f	77	VAL	2.9
2	B	296	SER	2.9
1	A	319	LEU	2.9
2	Z	201	GLU	2.9
4	r	103	VAL	2.9
4	D	69	PHE	2.9
7	W	70	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	85	VAL	2.9
4	j	156	LEU	2.9
6	l	40	SER	2.9
1	A	320	LEU	2.9
4	D	194	VAL	2.9
5	U	272	LYS	2.9
1	Q	161	ALA	2.9
1	Q	115	LEU	2.9
2	B	294	PHE	2.9
2	R	293	PRO	2.9
4	j	87	PHE	2.9
8	f	128	ILE	2.9
5	E	188	THR	2.9
4	D	150	LYS	2.9
4	r	124	ALA	2.9
7	W	66	LEU	2.9
2	R	80	PHE	2.9
4	D	145	LEU	2.9
5	U	146	TRP	2.9
7	m	19	ALA	2.9
3	K	12	VAL	2.9
4	D	190	CYS	2.9
4	L	144	LYS	2.9
7	e	35	LEU	2.9
1	A	227	TYR	2.9
4	L	177	GLU	2.9
8	P	41	LEU	2.9
1	Y	79	ASN	2.9
8	f	109	LEU	2.9
4	T	161	PRO	2.9
5	M	49	HIS	2.9
1	g	84	LEU	2.9
1	o	269	GLU	2.9
5	U	78	MET	2.9
2	J	259	PHE	2.9
1	o	109	THR	2.8
6	V	207	THR	2.8
5	k	188	THR	2.8
6	l	187	THR	2.8
1	g	505	PRO	2.8
2	Z	92	TYR	2.8
6	d	241	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	P	30	GLY	2.8
2	Z	144	ASN	2.8
8	H	113	THR	2.8
2	h	259	PHE	2.8
2	B	92	TYR	2.8
4	L	189	VAL	2.8
4	T	207	ARG	2.8
4	b	3	ALA	2.8
3	i	53	GLU	2.8
4	r	107	ARG	2.8
5	c	109	ALA	2.8
3	K	92	HIS	2.8
4	T	189	VAL	2.8
6	V	252	PHE	2.8
4	L	111	ALA	2.8
4	T	148	TYR	2.8
5	c	147	LEU	2.8
6	N	88	GLU	2.8
5	E	146	TRP	2.8
4	b	190	CYS	2.8
8	P	74	ILE	2.8
1	g	319	LEU	2.8
6	t	257	LEU	2.8
7	G	47	LEU	2.8
7	e	70	PHE	2.8
8	X	74	ILE	2.8
4	L	190	CYS	2.8
6	l	183	PHE	2.8
5	E	49	HIS	2.8
4	j	60	VAL	2.8
2	h	294	PHE	2.8
5	k	84	LYS	2.8
8	P	42	ALA	2.8
5	c	188	THR	2.8
2	J	293	PRO	2.8
1	Y	231	ALA	2.8
1	I	82	LEU	2.8
1	A	221	TYR	2.8
4	b	176	ASN	2.8
5	E	189	TYR	2.8
5	U	190	PRO	2.8
8	H	109	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	b	152	ALA	2.8
2	R	298	GLU	2.7
4	D	123	ALA	2.7
6	t	181	MET	2.8
3	q	181	PHE	2.7
4	j	41	GLN	2.7
7	O	35	LEU	2.7
4	T	61	ILE	2.7
4	r	90	GLU	2.7
5	k	186	PHE	2.7
2	h	209	LYS	2.7
6	F	173	ASP	2.7
2	p	81	LYS	2.7
4	D	156	LEU	2.7
8	f	113	THR	2.7
4	j	260	ALA	2.7
5	M	131	GLU	2.7
5	U	296	SER	2.7
2	h	299	ALA	2.7
4	b	92	ILE	2.7
1	A	390	LEU	2.7
6	l	181	MET	2.7
2	Z	30	VAL	2.7
5	M	136	TRP	2.7
4	j	49	VAL	2.7
4	b	65	LEU	2.7
5	c	24	SER	2.7
2	B	123	LYS	2.7
4	j	143	TYR	2.7
5	k	221	TYR	2.7
3	S	139	THR	2.7
3	i	303	TYR	2.7
1	I	115	LEU	2.7
5	M	147	LEU	2.7
5	E	78	MET	2.7
4	L	85	TYR	2.7
4	T	190	CYS	2.7
6	d	189	THR	2.7
2	h	119	ILE	2.7
5	U	110	GLN	2.7
4	b	143	TYR	2.7
1	Q	307	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	166	VAL	2.7
5	U	198	GLU	2.7
3	q	260	TYR	2.7
1	Q	238	CYS	2.7
5	M	103	THR	2.7
7	W	43	PHE	2.7
4	j	108	GLN	2.7
2	p	442	LEU	2.7
3	K	39	LEU	2.7
3	K	307	ILE	2.7
6	t	206	MET	2.7
1	Q	87	TYR	2.7
8	f	130	ALA	2.7
2	h	221	SER	2.7
4	D	231	HIS	2.7
4	L	151	ILE	2.7
2	p	54	PHE	2.6
4	b	147	THR	2.7
4	j	124	ALA	2.6
3	C	131	MET	2.6
6	N	173	ASP	2.6
2	B	308	ILE	2.6
4	r	147	THR	2.6
5	M	200	PRO	2.6
4	r	89	LEU	2.6
5	c	99	PRO	2.6
4	j	191	TYR	2.6
6	d	159	LYS	2.6
2	Z	240	CYS	2.6
6	d	242	VAL	2.6
4	T	29	ILE	2.6
1	o	126	PHE	2.6
1	A	107	CYS	2.6
6	V	174	ILE	2.6
5	U	29	TYR	2.6
3	C	127	ALA	2.6
4	b	38	GLY	2.6
4	r	70	CYS	2.6
8	H	38	GLY	2.6
3	K	131	MET	2.6
4	b	149	LEU	2.6
3	i	8	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	153	ARG	2.6
4	L	174	LEU	2.6
4	b	211	LEU	2.6
4	r	98	SER	2.6
1	Q	118	ALA	2.6
4	r	168	ILE	2.6
1	Q	121	PHE	2.6
7	O	43	PHE	2.6
1	I	196	SER	2.6
2	B	240	CYS	2.6
4	D	110	LEU	2.6
4	b	82	LYS	2.6
5	k	146	TRP	2.6
1	Q	223	ARG	2.6
4	T	66	LEU	2.6
1	I	197	ILE	2.6
8	X	37	TYR	2.6
4	L	214	LYS	2.6
3	S	138	LEU	2.6
2	J	237	ILE	2.6
6	V	87	PHE	2.6
3	q	53	GLU	2.6
2	Z	55	GLN	2.6
7	u	170	ILE	2.6
1	I	121	PHE	2.6
4	j	59	LEU	2.6
4	r	190	CYS	2.6
6	F	191	ALA	2.6
6	t	169	GLU	2.6
1	Y	221	TYR	2.6
4	L	197	TYR	2.6
4	j	145	LEU	2.6
3	a	131	MET	2.6
1	g	87	TYR	2.6
4	L	209	ASN	2.6
5	M	129	ARG	2.6
3	a	260	TYR	2.6
8	v	106	MET	2.6
4	D	254	ARG	2.6
1	Q	194	LYS	2.6
2	p	75	MET	2.6
4	j	7	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	j	123	ALA	2.6
5	U	84	LYS	2.6
6	F	213	GLU	2.6
5	c	296	SER	2.6
3	C	358	VAL	2.5
4	b	185	ILE	2.5
6	l	208	ALA	2.5
1	A	287	CYS	2.5
1	I	128	VAL	2.5
3	q	94	ARG	2.5
2	Z	239	GLU	2.5
1	Q	234	VAL	2.5
6	l	38	SER	2.5
3	a	347	ILE	2.5
4	b	39	ALA	2.5
6	t	69	ILE	2.5
8	f	125	TYR	2.5
5	M	190	PRO	2.5
4	L	66	LEU	2.5
4	T	121	ARG	2.5
4	b	61	ILE	2.5
8	P	39	GLN	2.5
8	P	71	LEU	2.5
8	v	77	VAL	2.5
3	a	39	LEU	2.5
6	N	252	PHE	2.5
4	T	34	ILE	2.5
7	e	43	PHE	2.5
6	N	159	LYS	2.5
3	i	138	LEU	2.5
3	a	58	VAL	2.5
7	W	139	ASP	2.5
2	Z	277	LEU	2.5
4	T	211	LEU	2.5
1	Q	320	LEU	2.5
3	i	54	HIS	2.5
8	P	133	PHE	2.5
4	b	91	LYS	2.5
4	r	132	LEU	2.5
3	i	349	ALA	2.5
5	c	167	ALA	2.5
3	C	178	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	d	191	ALA	2.5
1	I	390	LEU	2.5
3	K	95	TYR	2.5
6	V	88	GLU	2.5
8	H	167	PRO	2.5
8	n	41	LEU	2.5
5	E	202	GLU	2.5
2	Z	111	SER	2.5
4	D	6	ARG	2.5
4	b	193	ARG	2.5
4	j	63	ARG	2.5
1	I	110	LEU	2.5
2	h	47	PRO	2.5
5	E	100	VAL	2.5
6	N	191	ALA	2.5
4	D	144	LYS	2.5
4	T	80	THR	2.5
2	B	241	GLY	2.5
3	C	55	SER	2.5
3	S	131	MET	2.5
8	v	42	ALA	2.5
5	U	136	TRP	2.5
1	Y	227	TYR	2.5
4	D	188	LYS	2.5
5	k	24	SER	2.5
1	g	185	LEU	2.5
2	p	279	TYR	2.5
4	b	42	LEU	2.5
6	t	89	LEU	2.5
8	X	38	GLY	2.5
1	Q	390	LEU	2.5
4	T	27	ARG	2.4
4	b	127	LEU	2.4
6	V	36	THR	2.4
2	Z	258	PHE	2.4
6	V	187	THR	2.4
2	J	299	ALA	2.4
8	f	164	PRO	2.4
2	B	277	LEU	2.4
5	s	110	GLN	2.4
4	r	167	TYR	2.4
6	N	135	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	T	174	LEU	2.4
4	b	163	GLN	2.4
4	j	85	TYR	2.4
4	L	110	LEU	2.4
1	g	504	SER	2.4
5	k	147	LEU	2.4
7	m	23	LYS	2.4
8	P	45	LEU	2.4
5	k	202	GLU	2.4
4	r	48	PHE	2.4
8	H	77	VAL	2.4
8	v	137	VAL	2.4
1	Y	114	ALA	2.4
3	a	85	ILE	2.4
4	b	138	GLN	2.4
4	r	185	ILE	2.4
4	D	154	LEU	2.4
4	T	154	LEU	2.4
6	F	189	THR	2.4
3	C	317	LEU	2.4
4	D	13	MET	2.4
4	L	27	ARG	2.4
5	U	297	GLU	2.4
2	J	296	SER	2.4
7	O	92	GLN	2.4
1	o	194	LYS	2.4
3	K	299	LEU	2.4
3	q	326	VAL	2.4
7	G	196	ASN	2.4
5	s	167	ALA	2.4
2	R	175	LEU	2.4
1	Y	420	ALA	2.4
4	L	34	ILE	2.4
8	H	133	PHE	2.4
8	n	133	PHE	2.4
1	I	223	ARG	2.4
4	D	126	VAL	2.4
8	X	109	LEU	2.4
1	g	188	TYR	2.4
2	p	194	LEU	2.4
8	v	153	TRP	2.4
3	a	170	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	j	211	LEU	2.4
1	Q	287	CYS	2.4
4	D	72	HIS	2.4
2	B	131	PHE	2.4
1	A	87	TYR	2.4
2	h	237	ILE	2.4
5	E	186	PHE	2.4
5	M	109	ALA	2.4
4	T	178	SER	2.4
4	D	246	LEU	2.4
5	s	100	VAL	2.4
1	I	107	CYS	2.4
4	D	161	PRO	2.4
1	I	78	GLU	2.4
8	P	109	LEU	2.4
6	t	35	VAL	2.4
8	X	125	TYR	2.4
1	Q	196	SER	2.4
2	R	292	ASN	2.4
4	L	108	GLN	2.4
4	T	226	LEU	2.4
4	r	106	ILE	2.4
5	E	296	SER	2.4
6	V	181	MET	2.4
2	Z	442	LEU	2.4
3	S	5	LEU	2.4
3	a	181	PHE	2.4
8	P	13	PHE	2.4
4	r	194	VAL	2.4
4	b	174	LEU	2.4
5	c	98	LEU	2.4
5	c	139	SER	2.4
3	S	170	CYS	2.4
4	r	88	THR	2.4
2	p	311	MET	2.4
5	U	186	PHE	2.3
8	H	24	GLU	2.4
2	Z	202	ILE	2.3
1	I	118	ALA	2.3
3	a	9	VAL	2.3
8	X	124	ALA	2.3
3	q	131	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	278	LYS	2.3
2	B	239	GLU	2.3
2	R	201	GLU	2.3
7	G	159	GLY	2.3
7	W	46	LEU	2.3
8	v	121	VAL	2.3
8	n	106	MET	2.3
1	I	346	VAL	2.3
2	J	280	LEU	2.3
4	j	76	LEU	2.3
7	m	46	LEU	2.3
6	F	98	ILE	2.3
7	O	196	ASN	2.3
2	h	194	LEU	2.3
4	T	155	TYR	2.3
4	b	164	ALA	2.3
8	v	133	PHE	2.3
1	I	131	TYR	2.3
4	b	44	ALA	2.3
5	M	272	LYS	2.3
8	v	118	PHE	2.3
4	L	121	ARG	2.3
4	j	17	GLY	2.3
2	R	277	LEU	2.3
4	D	174	LEU	2.3
8	v	43	LEU	2.3
3	K	28	ILE	2.3
2	J	67	TRP	2.3
4	b	113	ILE	2.3
5	U	197	ASP	2.3
4	b	183	LEU	2.3
8	f	36	VAL	2.3
1	g	269	GLU	2.3
1	A	315	ASP	2.3
4	D	84	ILE	2.3
3	a	217	SER	2.3
2	R	279	TYR	2.3
2	J	410	GLU	2.3
7	e	170	ILE	2.3
8	f	74	ILE	2.3
1	Q	77	VAL	2.3
2	R	281	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	h	51	LEU	2.3
4	L	22	LEU	2.3
2	B	299	ALA	2.3
4	D	216	ILE	2.3
7	O	170	ILE	2.3
1	Y	198	ARG	2.3
5	s	201	SER	2.3
6	t	40	SER	2.3
4	j	34	ILE	2.3
8	v	39	GLN	2.3
5	U	109	ALA	2.3
6	V	206	MET	2.3
3	a	33	GLU	2.3
7	G	88	LEU	2.3
5	c	100	VAL	2.3
4	r	58	SER	2.3
7	e	31	ILE	2.3
8	v	105	ILE	2.3
1	o	287	CYS	2.3
8	H	46	LEU	2.3
8	P	209	ASN	2.3
4	L	49	VAL	2.3
6	l	147	GLU	2.3
4	T	124	ALA	2.3
2	R	131	PHE	2.3
4	T	228	HIS	2.3
5	M	143	TYR	2.3
1	Q	237	MET	2.3
3	S	118	LEU	2.3
4	L	156	LEU	2.3
4	L	147	THR	2.3
1	o	320	LEU	2.3
6	F	90	LEU	2.3
4	L	78	ASP	2.3
4	T	231	HIS	2.3
5	M	77	VAL	2.3
2	R	237	ILE	2.3
2	Z	309	LEU	2.3
2	B	71	ALA	2.3
7	G	195	ALA	2.3
8	X	68	ASN	2.3
5	E	190	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	n	42	ALA	2.3
2	R	77	LYS	2.3
4	T	32	LYS	2.3
1	A	207	HIS	2.3
4	D	70	CYS	2.3
6	F	261	TYR	2.3
2	R	259	PHE	2.3
4	T	14	ASN	2.3
5	U	195	PRO	2.3
6	l	169	GLU	2.2
1	Y	225	ARG	2.2
2	p	79	ASN	2.2
3	K	260	TYR	2.2
4	L	150	LYS	2.2
4	T	145	LEU	2.2
5	U	201	SER	2.2
2	p	258	PHE	2.2
1	g	225	ARG	2.2
2	B	210	ASN	2.2
2	Z	292	ASN	2.2
4	T	188	LYS	2.2
4	j	36	LEU	2.2
2	h	80	PHE	2.2
1	g	127	ASN	2.2
1	o	489	MET	2.2
3	C	181	PHE	2.2
2	Z	180	GLN	2.2
5	M	188	THR	2.2
7	W	8	THR	2.2
2	J	282	LEU	2.2
8	P	153	TRP	2.2
4	L	70	CYS	2.2
7	O	159	GLY	2.2
7	e	196	ASN	2.2
8	f	108	ALA	2.2
1	o	118	ALA	2.2
2	J	309	LEU	2.2
4	b	294	ALA	2.2
5	E	29	TYR	2.2
1	Q	162	LEU	2.2
3	q	272	PRO	2.2
6	t	183	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	u	160	ARG	2.2
4	j	194	VAL	2.2
8	f	46	LEU	2.2
2	J	292	ASN	2.2
3	S	260	TYR	2.2
4	L	376	SER	2.2
8	v	60	ILE	2.2
1	g	291	LEU	2.2
2	Z	310	ALA	2.2
2	p	400	GLY	2.2
1	g	135	HIS	2.2
2	p	176	HIS	2.2
3	a	142	HIS	2.2
8	X	153	TRP	2.2
3	C	12	VAL	2.2
4	T	49	VAL	2.2
5	c	95	SER	2.2
6	V	182	LEU	2.2
1	Y	134	ILE	2.2
3	i	99	THR	2.2
5	s	187	ARG	2.2
5	k	50	HIS	2.2
2	B	278	LYS	2.2
4	r	189	VAL	2.2
1	Q	119	LEU	2.2
2	B	80	PHE	2.2
2	R	72	LEU	2.2
4	L	145	LEU	2.2
6	d	183	PHE	2.2
1	A	225	ARG	2.2
8	H	162	VAL	2.2
4	D	111	ALA	2.2
4	D	143	TYR	2.2
4	L	9	LEU	2.2
4	b	249	LEU	2.2
5	k	103	THR	2.2
8	X	48	ASN	2.2
4	L	132	LEU	2.2
4	j	48	PHE	2.2
4	r	211	LEU	2.2
7	W	64	PHE	2.2
8	X	113	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	T	86	HIS	2.2
4	D	233	THR	2.2
7	m	31	ILE	2.2
1	g	238	CYS	2.2
1	o	192	SER	2.2
2	h	71	ALA	2.2
4	b	173	LEU	2.2
4	b	213	TYR	2.2
8	v	71	LEU	2.2
4	T	99	PHE	2.2
4	r	258	LEU	2.2
5	s	109	ALA	2.2
4	L	170	ARG	2.2
1	I	127	ASN	2.2
3	K	65	LYS	2.2
4	b	72	HIS	2.2
4	D	318	ASN	2.2
4	L	32	LYS	2.2
4	T	260	ALA	2.2
3	i	181	PHE	2.1
5	E	168	VAL	2.1
5	c	90	MET	2.1
7	m	18	LEU	2.1
1	o	87	TYR	2.1
4	r	15	SER	2.1
1	o	110	LEU	2.1
6	t	67	GLN	2.1
7	O	139	ASP	2.1
4	j	132	LEU	2.1
4	b	33	ALA	2.1
4	b	64	GLN	2.1
4	r	130	ILE	2.1
5	s	263	THR	2.1
8	X	42	ALA	2.1
3	S	181	PHE	2.1
4	T	19	HIS	2.1
4	b	86	HIS	2.1
5	k	201	SER	2.1
7	W	170	ILE	2.1
1	I	287	CYS	2.1
4	j	98	SER	2.1
5	c	78	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	s	31	TYR	2.1
7	O	160	ARG	2.1
2	Z	237	ILE	2.1
6	F	179	ALA	2.1
2	J	30	VAL	2.1
6	N	183	PHE	2.1
6	t	189	THR	2.1
8	H	92	THR	2.1
5	M	50	HIS	2.1
3	a	270	ASN	2.1
2	J	54	PHE	2.1
6	V	89	LEU	2.1
6	V	108	LYS	2.1
8	f	163	LEU	2.1
7	W	215	ASN	2.1
7	e	63	THR	2.1
4	L	254	ARG	2.1
4	T	229	ALA	2.1
1	o	189	LYS	2.1
4	L	230	LEU	2.1
2	R	81	LYS	2.1
3	a	307	ILE	2.1
4	r	36	LEU	2.1
8	n	128	ILE	2.1
1	Q	226	ASP	2.1
3	a	96	ALA	2.1
4	j	168	ILE	2.1
8	P	128	ILE	2.1
4	j	170	ARG	2.1
5	U	99	PRO	2.1
3	i	176	TYR	2.1
4	D	92	ILE	2.1
6	F	257	LEU	2.1
1	g	141	ALA	2.1
2	h	262	PHE	2.1
6	t	264	CYS	2.1
5	k	86	ASP	2.1
6	N	131	PRO	2.1
2	h	258	PHE	2.1
7	u	70	PHE	2.1
3	q	56	LEU	2.1
8	H	71	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	f	13	PHE	2.1
3	i	212	PRO	2.1
6	V	131	PRO	2.1
2	R	400	GLY	2.1
2	h	131	PHE	2.1
4	r	57	VAL	2.1
7	W	195	ALA	2.1
1	I	126	PHE	2.1
1	Y	87	TYR	2.1
1	o	227	TYR	2.1
1	Q	329	GLY	2.1
1	Y	315	ASP	2.1
2	R	312	THR	2.1
4	D	230	LEU	2.1
4	L	223	LEU	2.1
4	L	260	ALA	2.1
6	V	208	ALA	2.1
2	h	176	HIS	2.1
1	I	189	LYS	2.1
1	g	138	LEU	2.1
1	A	449	ILE	2.1
3	K	52	GLN	2.1
3	i	260	TYR	2.1
5	s	99	PRO	2.1
4	r	164	ALA	2.1
5	E	59	ALA	2.1
1	A	223	ARG	2.1
1	g	97	ILE	2.1
7	u	198	HIS	2.1
2	Z	241	GLY	2.1
2	p	277	LEU	2.1
4	r	17	GLY	2.1
6	F	37	GLY	2.1
8	H	78	GLY	2.1
8	X	77	VAL	2.1
2	p	239	GLU	2.1
5	k	49	HIS	2.1
4	T	15	SER	2.1
5	k	270	SER	2.1
6	F	38	SER	2.1
4	r	85	TYR	2.0
1	A	115	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	460	LEU	2.0
3	q	211	THR	2.0
6	V	135	ASP	2.0
4	L	192	ALA	2.0
5	E	99	PRO	2.0
7	G	19	ALA	2.0
2	p	82	LEU	2.0
3	i	226	LYS	2.0
1	g	346	VAL	2.0
2	J	212	LYS	2.0
7	G	160	ARG	2.0
3	q	69	PRO	2.0
4	T	62	SER	2.0
1	A	78	GLU	2.0
1	g	115	LEU	2.0
5	M	168	VAL	2.0
7	G	66	LEU	2.0
8	X	162	VAL	2.0
1	Q	225	ARG	2.0
4	j	153	ARG	2.0
2	J	302	TYR	2.0
3	S	24	LEU	2.0
4	D	125	GLN	2.0
4	L	155	TYR	2.0
4	T	78	ASP	2.0
5	M	29	TYR	2.0
6	V	86	SER	2.0
4	b	57	VAL	2.0
7	e	27	LEU	2.0
4	T	69	PHE	2.0
7	m	15	PHE	2.0
7	O	78	TYR	2.0
8	P	96	HIS	2.0
1	g	189	LYS	2.0
4	r	156	LEU	2.0
3	q	307	ILE	2.0
1	Y	207	HIS	2.0
3	a	127	ALA	2.0
4	D	139	TYR	2.0
4	b	30	LEU	2.0
3	S	12	VAL	2.0
4	L	19	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	U	283	GLY	2.0
5	k	189	TYR	2.0
4	b	151	ILE	2.0
6	N	38	SER	2.0
4	D	165	GLU	2.0
1	o	229	THR	2.0
2	h	78	ILE	2.0
4	L	235	LEU	2.0
4	j	65	LEU	2.0
8	P	46	LEU	2.0
1	A	109	THR	2.0
3	K	69	PRO	2.0
3	i	12	VAL	2.0
5	U	100	VAL	2.0
7	m	43	PHE	2.0
7	u	31	ILE	2.0
2	J	143	LYS	2.0
5	M	282	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	ZN	M	401	1/1	0.92	0.16	-0.82	130,130,130,130	0
9	ZN	E	401	1/1	0.98	0.17	-1.06	130,130,130,130	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	ZN	s	401	1/1	0.80	0.09	-1.31	130,130,130,130	0
9	ZN	k	401	1/1	0.98	0.09	-1.51	130,130,130,130	0
9	ZN	c	401	1/1	0.97	0.09	-1.72	130,130,130,130	0
9	ZN	U	401	1/1	0.94	0.08	-1.93	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.