



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:12 AM EDT

PDB ID : 4WSN / pdb_00004wsn
Title : Crystal structure of the COP9 signalosome, a P1 crystal form
Authors : Bunker, R.D.; Lingaraju, G.M.; Thoma, N.H.
Deposited on : 2014-10-28
Resolution : 5.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

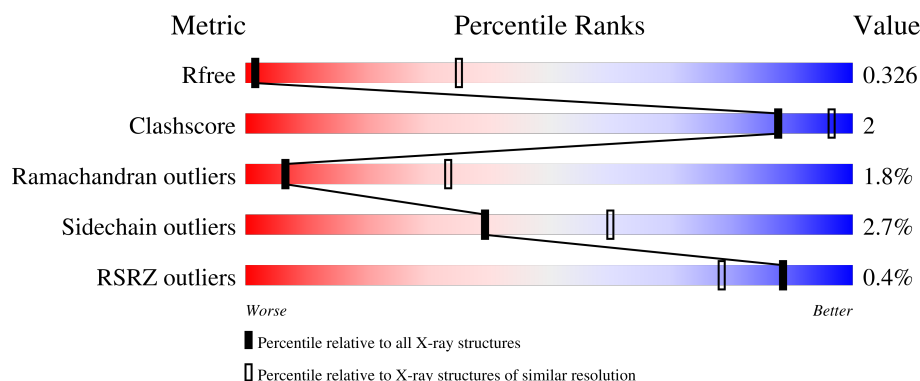
1 Overall quality at a glance

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}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	I	480	
1	Q	480	
1	Y	480	
1	g	480	

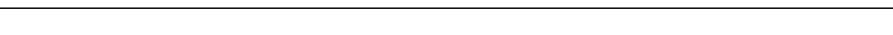
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Mol	Chain	Length	Quality of chain
1	o	480	
2	B	447	
2	J	447	
2	R	447	
2	Z	447	
2	h	447	
2	p	447	
3	C	427	
3	K	427	
3	S	427	
3	a	427	
3	i	427	
3	q	427	
4	D	410	
4	L	410	
4	T	410	
4	b	410	
4	j	410	
4	r	410	
5	E	325	
5	M	325	
5	U	325	
5	c	325	
5	k	325	
5	s	325	

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Mol	Chain	Length	Quality of chain
6	F	331	 80%6% • 13%
6	N	331	 80%6% • 13%
6	V	331	 %79%7% • 13%
6	d	331	 82%• • 13%
6	l	331	 79%8% • 13%
6	t	331	 %80%6% • 13%
7	G	222	 %86%8%6%
7	O	222	 %86%8%6%
7	W	222	 86%8%6%
7	e	222	 85%9%6%
7	m	222	 %84%10%6%
7	u	222	 85%9%6%
8	H	213	 73%7% • 19%
8	P	213	 74%7% 19%
8	X	213	 75%6% 19%
8	f	213	 75%6% • 19%
8	n	213	 73%8% 19%
8	v	213	 73%8% 19%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 124428 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	I	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	Q	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	Y	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	g	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	o	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP Q13098
A	49	GLY	-	expression tag	UNP Q13098
A	50	GLY	-	expression tag	UNP Q13098
A	51	ARG	-	expression tag	UNP Q13098
I	48	GLY	-	expression tag	UNP Q13098
I	49	GLY	-	expression tag	UNP Q13098
I	50	GLY	-	expression tag	UNP Q13098
I	51	ARG	-	expression tag	UNP Q13098
Q	48	GLY	-	expression tag	UNP Q13098
Q	49	GLY	-	expression tag	UNP Q13098
Q	50	GLY	-	expression tag	UNP Q13098
Q	51	ARG	-	expression tag	UNP Q13098
Y	48	GLY	-	expression tag	UNP Q13098
Y	49	GLY	-	expression tag	UNP Q13098
Y	50	GLY	-	expression tag	UNP Q13098
Y	51	ARG	-	expression tag	UNP Q13098
g	48	GLY	-	expression tag	UNP Q13098

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Chain	Residue	Modelled	Actual	Comment	Reference
g	49	GLY	-	expression tag	UNP Q13098
g	50	GLY	-	expression tag	UNP Q13098
g	51	ARG	-	expression tag	UNP Q13098
o	48	GLY	-	expression tag	UNP Q13098
o	49	GLY	-	expression tag	UNP Q13098
o	50	GLY	-	expression tag	UNP Q13098
o	51	ARG	-	expression tag	UNP Q13098

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	J	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	R	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	Z	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	h	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	p	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P61201
B	-2	GLY	-	expression tag	UNP P61201
B	-1	GLY	-	expression tag	UNP P61201
B	0	ARG	-	expression tag	UNP P61201
J	-3	GLY	-	expression tag	UNP P61201
J	-2	GLY	-	expression tag	UNP P61201
J	-1	GLY	-	expression tag	UNP P61201
J	0	ARG	-	expression tag	UNP P61201
R	-3	GLY	-	expression tag	UNP P61201
R	-2	GLY	-	expression tag	UNP P61201
R	-1	GLY	-	expression tag	UNP P61201
R	0	ARG	-	expression tag	UNP P61201
Z	-3	GLY	-	expression tag	UNP P61201
Z	-2	GLY	-	expression tag	UNP P61201
Z	-1	GLY	-	expression tag	UNP P61201

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	ARG	-	expression tag	UNP P61201
h	-3	GLY	-	expression tag	UNP P61201
h	-2	GLY	-	expression tag	UNP P61201
h	-1	GLY	-	expression tag	UNP P61201
h	0	ARG	-	expression tag	UNP P61201
p	-3	GLY	-	expression tag	UNP P61201
p	-2	GLY	-	expression tag	UNP P61201
p	-1	GLY	-	expression tag	UNP P61201
p	0	ARG	-	expression tag	UNP P61201

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	K	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	S	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	a	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	i	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	q	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9UNS2
C	-2	GLY	-	expression tag	UNP Q9UNS2
C	-1	GLY	-	expression tag	UNP Q9UNS2
C	0	ARG	-	expression tag	UNP Q9UNS2
K	-3	GLY	-	expression tag	UNP Q9UNS2
K	-2	GLY	-	expression tag	UNP Q9UNS2
K	-1	GLY	-	expression tag	UNP Q9UNS2
K	0	ARG	-	expression tag	UNP Q9UNS2
S	-3	GLY	-	expression tag	UNP Q9UNS2
S	-2	GLY	-	expression tag	UNP Q9UNS2
S	-1	GLY	-	expression tag	UNP Q9UNS2
S	0	ARG	-	expression tag	UNP Q9UNS2
a	-3	GLY	-	expression tag	UNP Q9UNS2

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-2	GLY	-	expression tag	UNP Q9UNS2
a	-1	GLY	-	expression tag	UNP Q9UNS2
a	0	ARG	-	expression tag	UNP Q9UNS2
i	-3	GLY	-	expression tag	UNP Q9UNS2
i	-2	GLY	-	expression tag	UNP Q9UNS2
i	-1	GLY	-	expression tag	UNP Q9UNS2
i	0	ARG	-	expression tag	UNP Q9UNS2
q	-3	GLY	-	expression tag	UNP Q9UNS2
q	-2	GLY	-	expression tag	UNP Q9UNS2
q	-1	GLY	-	expression tag	UNP Q9UNS2
q	0	ARG	-	expression tag	UNP Q9UNS2

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	L	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	T	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	b	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	j	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	r	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q9BT78
D	-2	GLY	-	expression tag	UNP Q9BT78
D	-1	GLY	-	expression tag	UNP Q9BT78
D	0	ARG	-	expression tag	UNP Q9BT78
L	-3	GLY	-	expression tag	UNP Q9BT78
L	-2	GLY	-	expression tag	UNP Q9BT78
L	-1	GLY	-	expression tag	UNP Q9BT78
L	0	ARG	-	expression tag	UNP Q9BT78
T	-3	GLY	-	expression tag	UNP Q9BT78
T	-2	GLY	-	expression tag	UNP Q9BT78
T	-1	GLY	-	expression tag	UNP Q9BT78

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Chain	Residue	Modelled	Actual	Comment	Reference
T	0	ARG	-	expression tag	UNP Q9BT78
b	-3	GLY	-	expression tag	UNP Q9BT78
b	-2	GLY	-	expression tag	UNP Q9BT78
b	-1	GLY	-	expression tag	UNP Q9BT78
b	0	ARG	-	expression tag	UNP Q9BT78
j	-3	GLY	-	expression tag	UNP Q9BT78
j	-2	GLY	-	expression tag	UNP Q9BT78
j	-1	GLY	-	expression tag	UNP Q9BT78
j	0	ARG	-	expression tag	UNP Q9BT78
r	-3	GLY	-	expression tag	UNP Q9BT78
r	-2	GLY	-	expression tag	UNP Q9BT78
r	-1	GLY	-	expression tag	UNP Q9BT78
r	0	ARG	-	expression tag	UNP Q9BT78

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	M	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	U	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	c	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	k	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			
5	s	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			

There are 24 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
U	11	GLY	-	expression tag	UNP Q92905
U	12	GLY	-	expression tag	UNP Q92905
U	13	ARG	-	expression tag	UNP Q92905
c	10	GLY	-	expression tag	UNP Q92905
c	11	GLY	-	expression tag	UNP Q92905
c	12	GLY	-	expression tag	UNP Q92905
c	13	ARG	-	expression tag	UNP Q92905
k	10	GLY	-	expression tag	UNP Q92905
k	11	GLY	-	expression tag	UNP Q92905
k	12	GLY	-	expression tag	UNP Q92905
k	13	ARG	-	expression tag	UNP Q92905
s	10	GLY	-	expression tag	UNP Q92905
s	11	GLY	-	expression tag	UNP Q92905
s	12	GLY	-	expression tag	UNP Q92905
s	13	ARG	-	expression tag	UNP Q92905

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	N	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	V	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	d	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	l	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			
6	t	288	Total	C	N	O	S	0	0	0
			2263	1445	375	428	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP Q7L5N1
F	-2	GLY	-	expression tag	UNP Q7L5N1
F	-1	GLY	-	expression tag	UNP Q7L5N1
F	0	ARG	-	expression tag	UNP Q7L5N1
N	-3	GLY	-	expression tag	UNP Q7L5N1
N	-2	GLY	-	expression tag	UNP Q7L5N1
N	-1	GLY	-	expression tag	UNP Q7L5N1

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Chain	Residue	Modelled	Actual	Comment	Reference
N	0	ARG	-	expression tag	UNP Q7L5N1
V	-3	GLY	-	expression tag	UNP Q7L5N1
V	-2	GLY	-	expression tag	UNP Q7L5N1
V	-1	GLY	-	expression tag	UNP Q7L5N1
V	0	ARG	-	expression tag	UNP Q7L5N1
d	-3	GLY	-	expression tag	UNP Q7L5N1
d	-2	GLY	-	expression tag	UNP Q7L5N1
d	-1	GLY	-	expression tag	UNP Q7L5N1
d	0	ARG	-	expression tag	UNP Q7L5N1
l	-3	GLY	-	expression tag	UNP Q7L5N1
l	-2	GLY	-	expression tag	UNP Q7L5N1
l	-1	GLY	-	expression tag	UNP Q7L5N1
l	0	ARG	-	expression tag	UNP Q7L5N1
t	-3	GLY	-	expression tag	UNP Q7L5N1
t	-2	GLY	-	expression tag	UNP Q7L5N1
t	-1	GLY	-	expression tag	UNP Q7L5N1
t	0	ARG	-	expression tag	UNP Q7L5N1

- Molecule 7 is a protein called COP9 signalosome complex subunit 7a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	O	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	W	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	e	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	m	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	u	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q9UBW8
G	-2	GLY	-	expression tag	UNP Q9UBW8
G	-1	GLY	-	expression tag	UNP Q9UBW8
G	0	ARG	-	expression tag	UNP Q9UBW8
O	-3	GLY	-	expression tag	UNP Q9UBW8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	expression tag	UNP Q9UBW8
O	-1	GLY	-	expression tag	UNP Q9UBW8
O	0	ARG	-	expression tag	UNP Q9UBW8
W	-3	GLY	-	expression tag	UNP Q9UBW8
W	-2	GLY	-	expression tag	UNP Q9UBW8
W	-1	GLY	-	expression tag	UNP Q9UBW8
W	0	ARG	-	expression tag	UNP Q9UBW8
e	-3	GLY	-	expression tag	UNP Q9UBW8
e	-2	GLY	-	expression tag	UNP Q9UBW8
e	-1	GLY	-	expression tag	UNP Q9UBW8
e	0	ARG	-	expression tag	UNP Q9UBW8
m	-3	GLY	-	expression tag	UNP Q9UBW8
m	-2	GLY	-	expression tag	UNP Q9UBW8
m	-1	GLY	-	expression tag	UNP Q9UBW8
m	0	ARG	-	expression tag	UNP Q9UBW8
u	-3	GLY	-	expression tag	UNP Q9UBW8
u	-2	GLY	-	expression tag	UNP Q9UBW8
u	-1	GLY	-	expression tag	UNP Q9UBW8
u	0	ARG	-	expression tag	UNP Q9UBW8

- Molecule 8 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	173	Total 1383	C 885	N 240	O 254	S 4	0	0	0
8	P	173	Total 1383	C 885	N 240	O 254	S 4	0	0	0
8	X	173	Total 1383	C 885	N 240	O 254	S 4	0	0	0
8	f	173	Total 1383	C 885	N 240	O 254	S 4	0	0	0
8	n	173	Total 1383	C 885	N 240	O 254	S 4	0	0	0
8	v	173	Total 1383	C 885	N 240	O 254	S 4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP Q99627
H	-2	GLY	-	expression tag	UNP Q99627
H	-1	GLY	-	expression tag	UNP Q99627

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

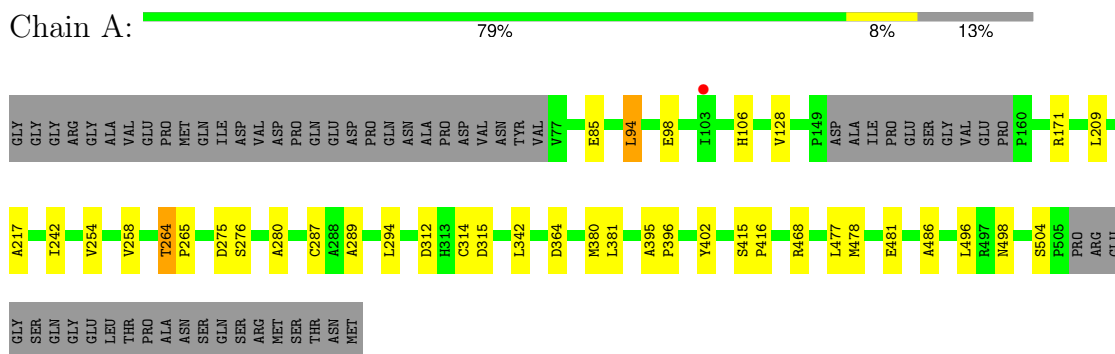
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

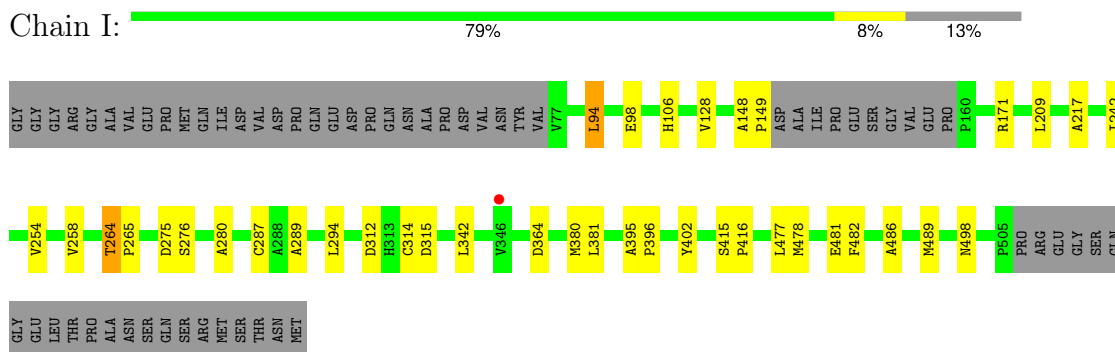
3 Residue-property plots

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

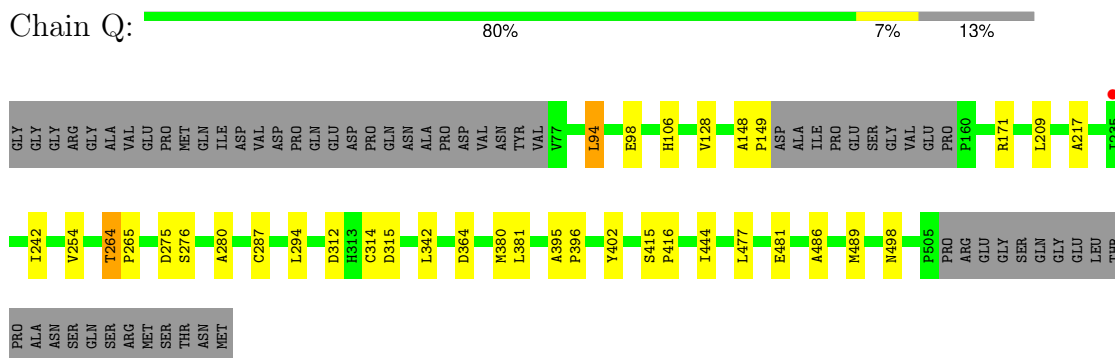
• Molecule 1: COP9 signalosome complex subunit 1



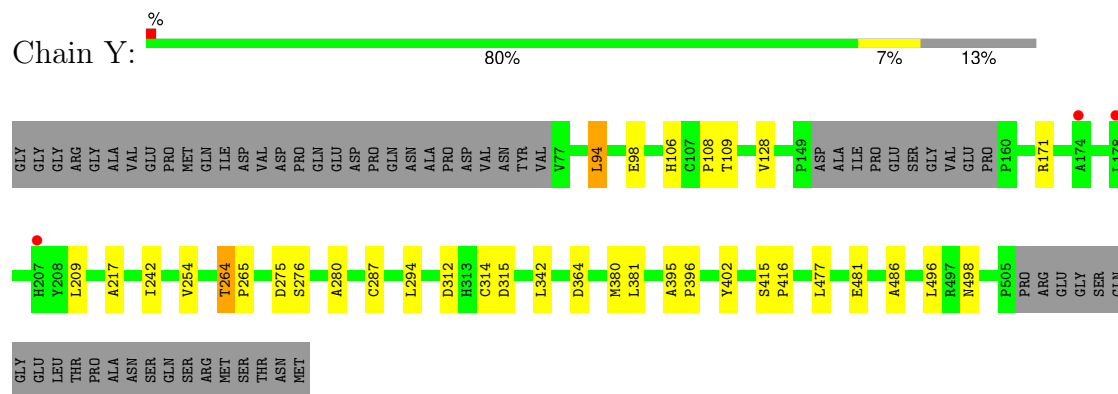
• Molecule 1: COP9 signalosome complex subunit 1



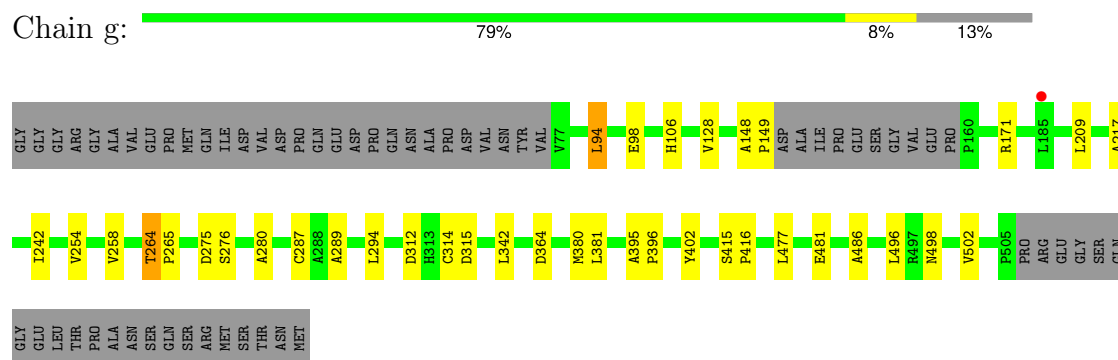
• Molecule 1: COP9 signalosome complex subunit 1



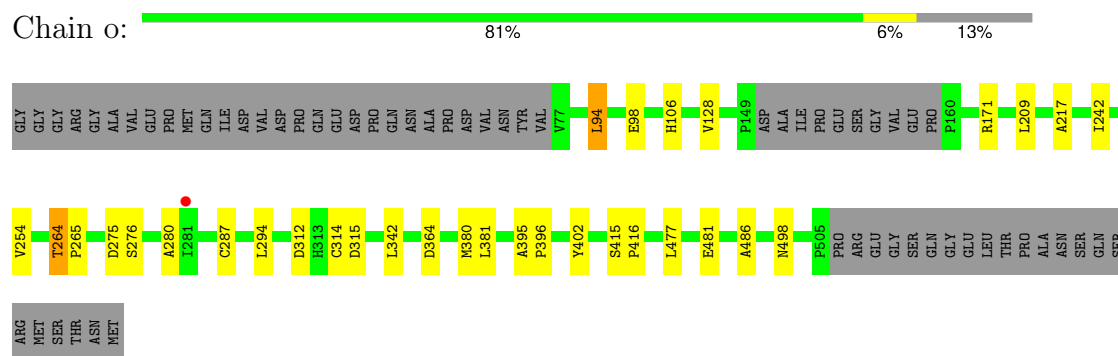
- Molecule 1: COP9 signalosome complex subunit 1



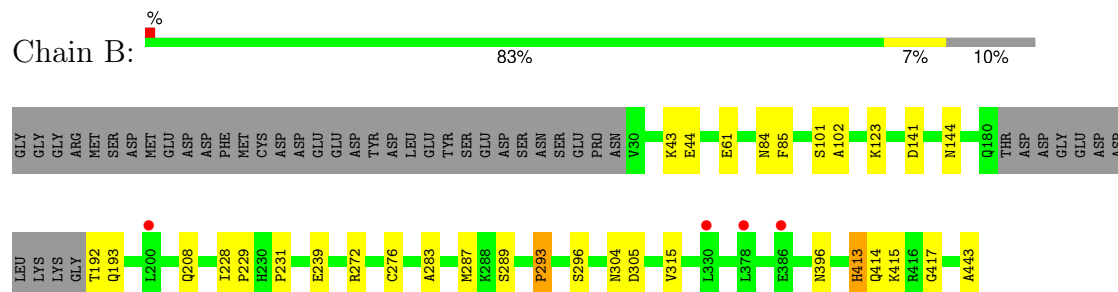
- Molecule 1: COP9 signalosome complex subunit 1



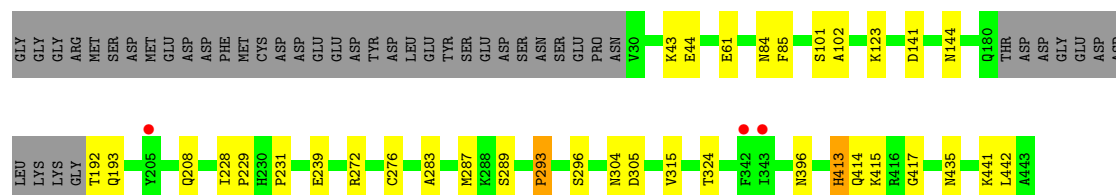
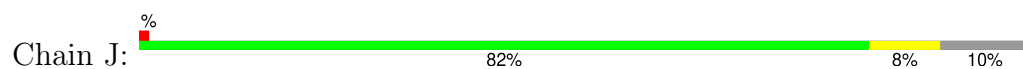
- Molecule 1: COP9 signalosome complex subunit 1



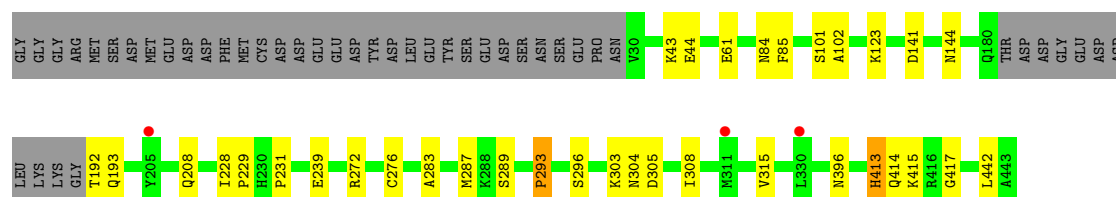
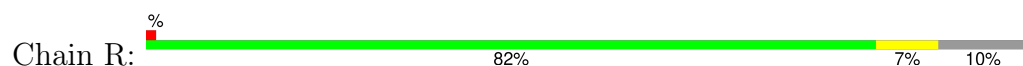
- Molecule 2: COP9 signalosome complex subunit 2



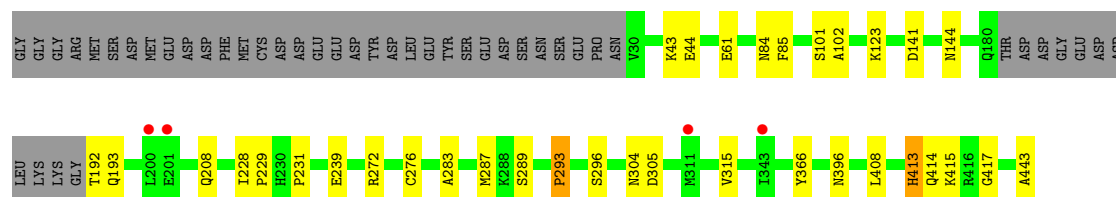
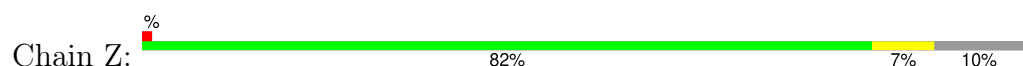
- Molecule 2: COP9 signalosome complex subunit 2



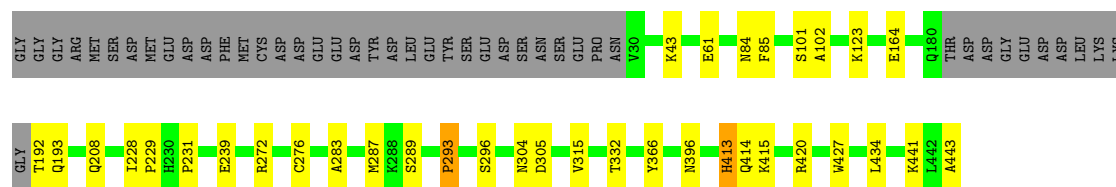
- Molecule 2: COP9 signalosome complex subunit 2



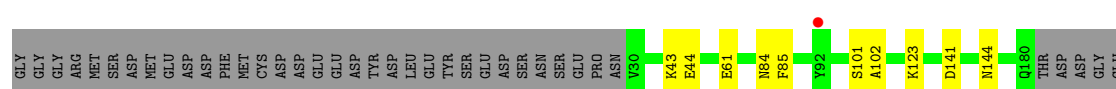
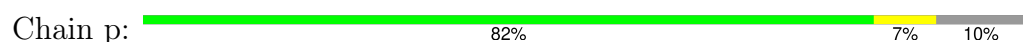
- Molecule 2: COP9 signalosome complex subunit 2



- Molecule 2: COP9 signalosome complex subunit 2

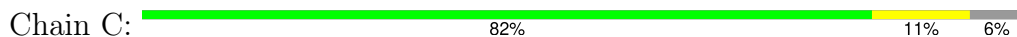


- Molecule 2: COP9 signalosome complex subunit 2

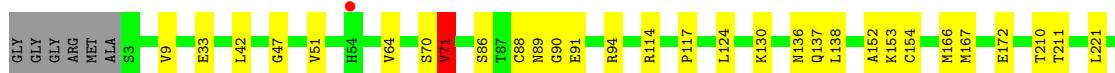
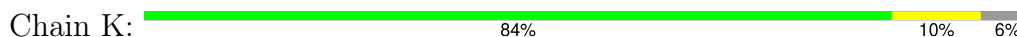




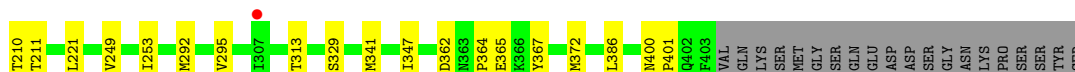
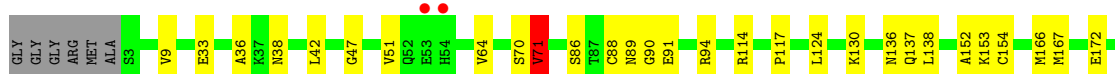
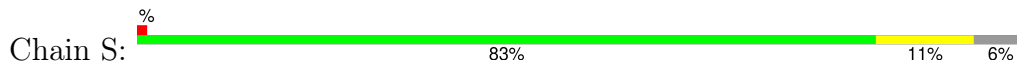
- Molecule 3: COP9 signalosome complex subunit 3



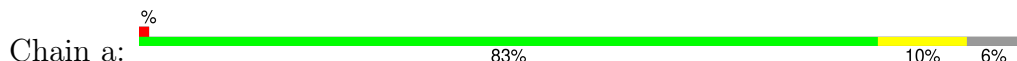
- Molecule 3: COP9 signalosome complex subunit 3



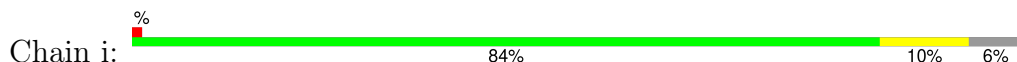
- Molecule 3: COP9 signalosome complex subunit 3

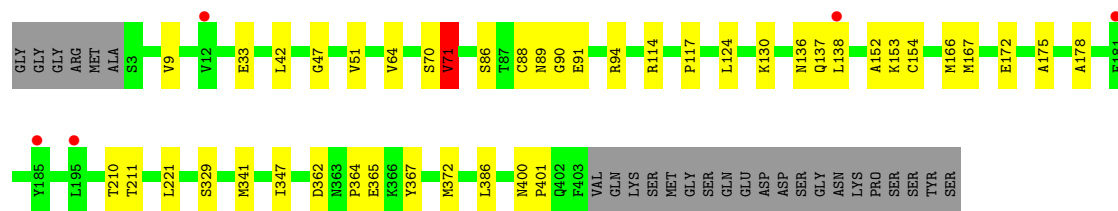


- Molecule 3: COP9 signalosome complex subunit 3



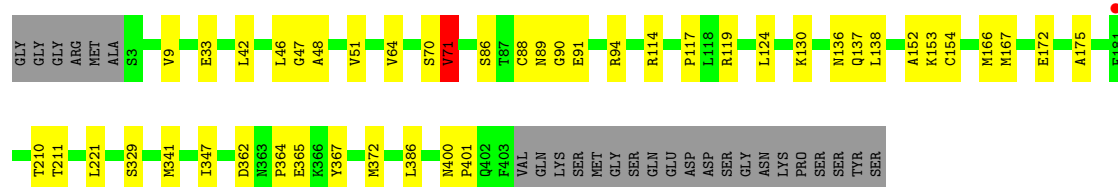
- Molecule 3: COP9 signalosome complex subunit 3





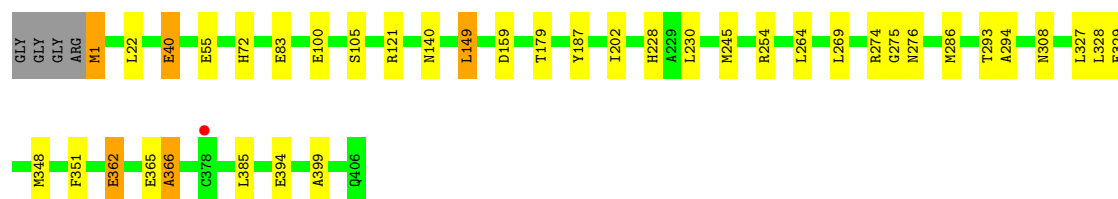
• Molecule 3: COP9 signalosome complex subunit 3

Chain q: 83% 10% 6%



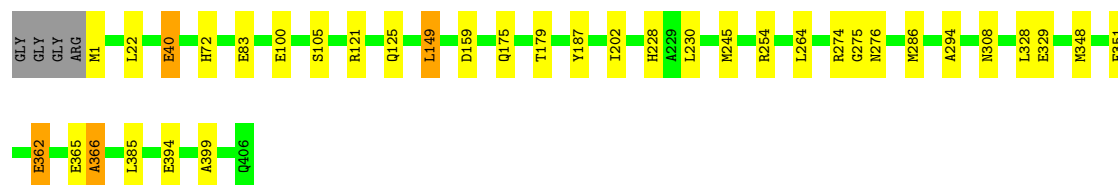
• Molecule 4: COP9 signalosome complex subunit 4

Chain D: 90% 8% ..



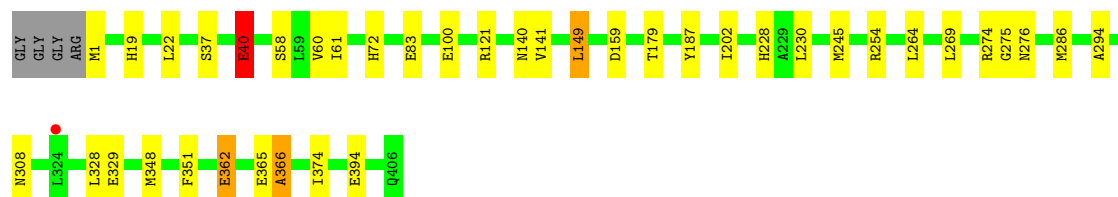
• Molecule 4: COP9 signalosome complex subunit 4

Chain L: 90% 8% ..



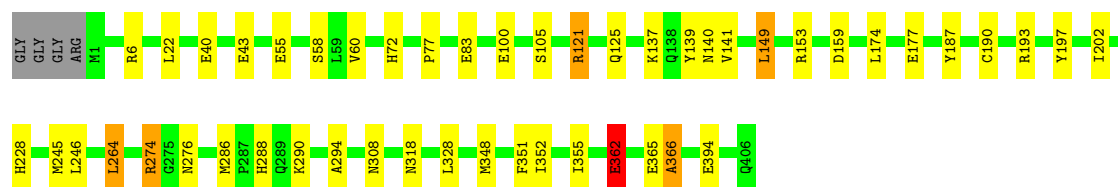
• Molecule 4: COP9 signalosome complex subunit 4

Chain T: 89% 9% ..



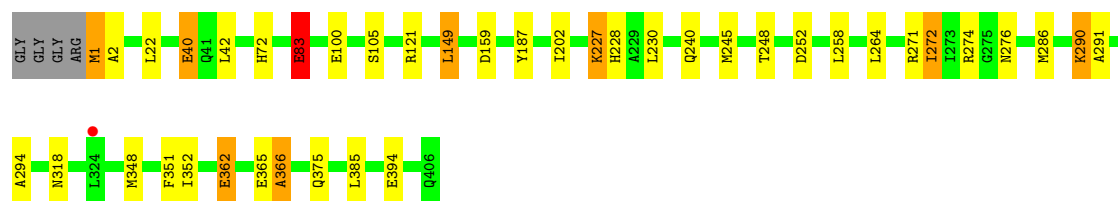
• Molecule 4: COP9 signalosome complex subunit 4

Chain b:  87% 10% ..



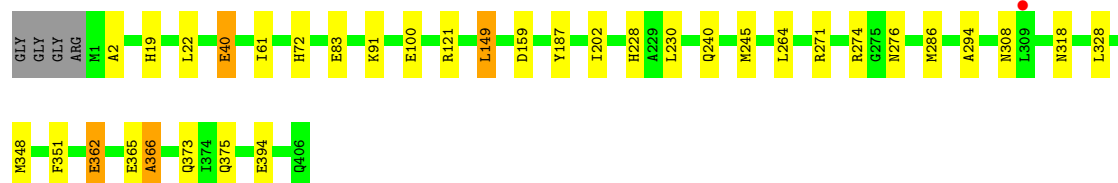
- Molecule 4: COP9 signalosome complex subunit 4

Chain j:  89% 8% ..



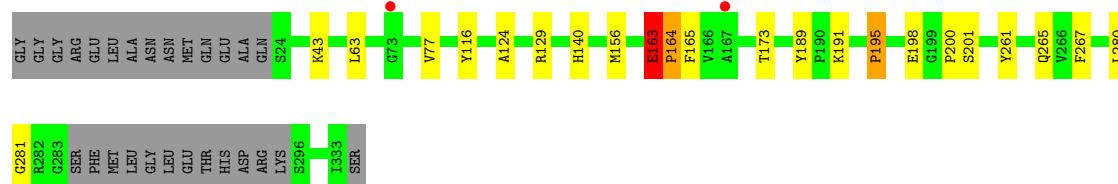
- Molecule 4: COP9 signalosome complex subunit 4

Chain r:  90% 8% ..



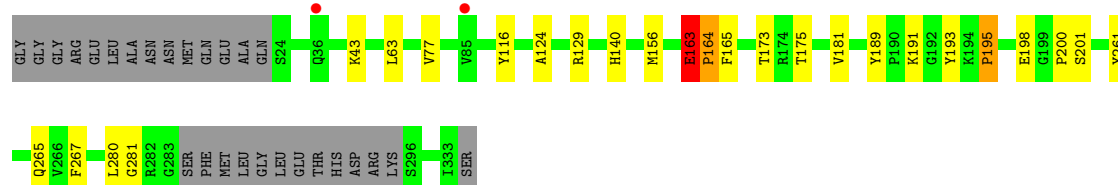
- Molecule 5: COP9 signalosome complex subunit 5

Chain E:  85% 6% • 8%

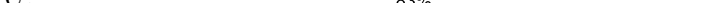


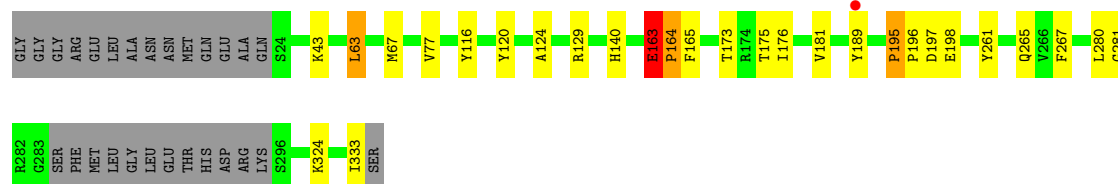
- Molecule 5: COP9 signalosome complex subunit 5

Chain M:  84% 7% • 8%

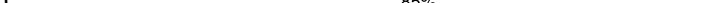


- Molecule 5: COP9 signalosome complex subunit 5

Chain U:  83% 7% • 8%



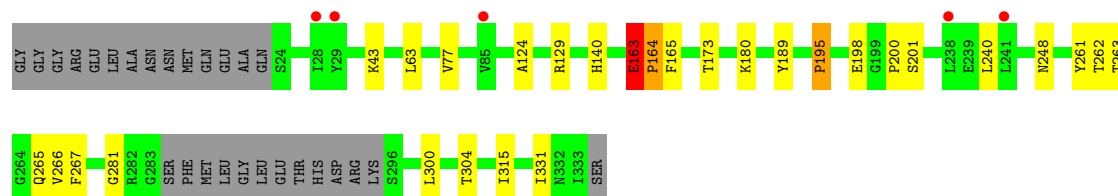
- Molecule 5: COP9 signalosome complex subunit 5

Chain c:  85% 6% 8%



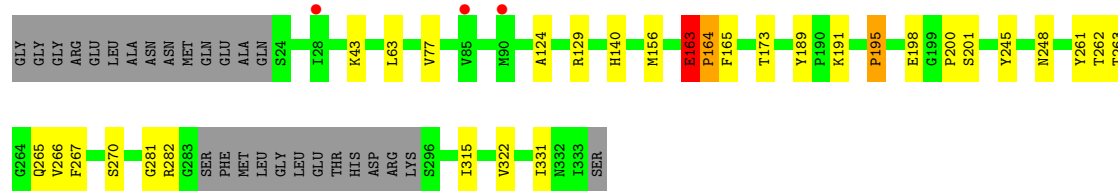
- Molecule 5: COP9 signalosome complex subunit 5

Chain k:  2% 83% 8% 8%

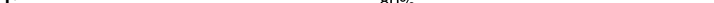


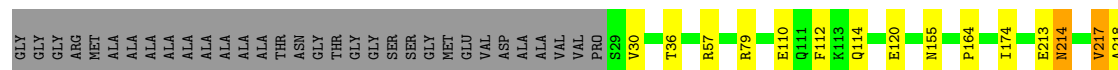
- Molecule 5: COP9 signalosome complex subunit 5

Chain s: 



- Molecule 6: COP9 signalosome complex subunit 6

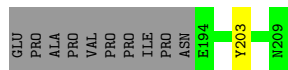
Chain F:  80% 6% • 13%



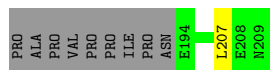




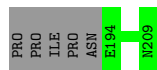
• Molecule 8: COP9 signalosome complex subunit 8



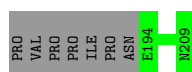
• Molecule 8: COP9 signalosome complex subunit 8



• Molecule 8: COP9 signalosome complex subunit 8

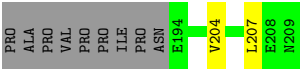
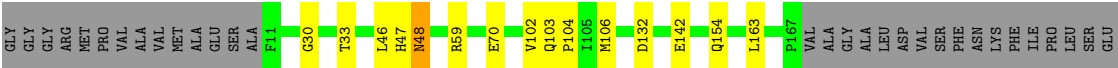


• Molecule 8: COP9 signalosome complex subunit 8

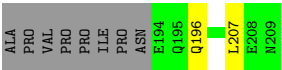


• Molecule 8: COP9 signalosome complex subunit 8





● 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 49.64 – 5.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.64-5.50) 83.7 (49.64-5.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 5.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.254 , 0.282 0.293 , 0.326	Depositor DCC
R_{free} test set	1948 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	264.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 203.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	124428	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/3404	0.73	0/4588
1	I	0.44	0/3404	0.72	0/4588
1	Q	0.43	0/3404	0.72	0/4588
1	Y	0.44	0/3404	0.73	0/4588
1	g	0.43	0/3404	0.72	0/4588
1	o	0.43	0/3404	0.72	0/4588
2	B	0.43	0/3360	0.72	0/4519
2	J	0.43	0/3360	0.72	0/4519
2	R	0.44	0/3360	0.72	0/4519
2	Z	0.43	0/3360	0.72	0/4519
2	h	0.43	0/3360	0.72	0/4519
2	p	0.44	0/3360	0.72	0/4519
3	C	0.42	0/3250	0.74	2/4390 (0.0%)
3	K	0.41	0/3250	0.73	2/4390 (0.0%)
3	S	0.42	0/3250	0.73	2/4390 (0.0%)
3	a	0.41	0/3250	0.73	2/4390 (0.0%)
3	i	0.41	0/3250	0.74	2/4390 (0.0%)
3	q	0.41	0/3250	0.74	2/4390 (0.0%)
4	D	0.48	0/3303	0.74	0/4460
4	L	0.48	0/3303	0.74	1/4460 (0.0%)
4	T	0.51	1/3303 (0.0%)	0.76	2/4460 (0.0%)
4	b	0.49	0/3303	0.76	1/4460 (0.0%)
4	j	0.48	1/3302 (0.0%)	0.75	2/4457 (0.0%)
4	r	0.48	0/3302	0.74	0/4457
5	E	0.42	0/2417	0.69	1/3266 (0.0%)
5	M	0.42	0/2417	0.69	1/3266 (0.0%)
5	U	0.42	0/2417	0.71	1/3266 (0.0%)
5	c	0.42	0/2417	0.69	0/3266
5	k	0.43	0/2417	0.69	1/3266 (0.0%)
5	s	0.42	0/2417	0.69	1/3266 (0.0%)
6	F	0.86	1/2310 (0.0%)	0.72	1/3133 (0.0%)
6	N	0.85	1/2310 (0.0%)	0.72	1/3133 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	V	0.77	1/2310 (0.0%)	0.73	1/3133 (0.0%)
6	d	0.83	1/2310 (0.0%)	0.72	1/3133 (0.0%)
6	l	0.46	0/2310	0.72	1/3133 (0.0%)
6	t	0.46	0/2310	0.71	1/3133 (0.0%)
7	G	0.45	0/1652	0.76	0/2239
7	O	0.45	0/1652	0.76	0/2239
7	W	0.45	0/1652	0.76	1/2239 (0.0%)
7	e	0.45	0/1652	0.76	0/2239
7	m	0.46	0/1652	0.76	1/2239 (0.0%)
7	u	0.46	0/1652	0.76	0/2239
8	H	0.44	0/1416	0.75	0/1924
8	P	0.44	0/1416	0.75	0/1924
8	X	0.44	0/1416	0.75	0/1924
8	f	0.43	0/1416	0.75	0/1924
8	n	0.44	0/1416	0.75	0/1924
8	v	0.44	0/1416	0.75	0/1924
All	All	0.48	6/126670 (0.0%)	0.73	31/171108 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	217	VAL	C-N	35.36	1.80	1.33
6	N	217	VAL	C-N	34.88	1.79	1.33
6	d	217	VAL	C-N	33.95	1.78	1.33
6	V	217	VAL	C-N	30.47	1.75	1.33
4	j	272	ILE	CB-CG1	5.53	1.64	1.53
4	T	40	GLU	CA-CB	5.27	1.62	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	217	VAL	O-C-N	-9.83	110.69	121.80
4	T	40	GLU	CB-CA-C	7.29	122.56	109.29
6	d	217	VAL	O-C-N	-7.22	113.64	121.80
4	b	290	LYS	N-CA-C	-7.10	104.54	112.57
6	F	217	VAL	O-C-N	-7.09	113.79	121.80
6	N	217	VAL	O-C-N	-6.85	114.06	121.80
4	j	290	LYS	CB-CA-C	-6.40	100.72	111.02
5	U	195	PRO	N-CA-C	6.31	118.40	110.70
3	q	400	ASN	CA-C-N	5.63	126.88	119.84
3	q	400	ASN	C-N-CA	5.63	126.88	119.84
4	L	175	GLN	CB-CA-C	5.29	118.91	109.29
3	S	400	ASN	CA-C-N	5.28	126.44	119.84
3	S	400	ASN	C-N-CA	5.28	126.44	119.84
3	K	400	ASN	CA-C-N	5.19	126.33	119.84
3	K	400	ASN	C-N-CA	5.19	126.33	119.84
3	i	400	ASN	CA-C-N	5.19	126.33	119.84
3	i	400	ASN	C-N-CA	5.19	126.33	119.84
6	l	217	VAL	N-CA-C	-5.17	105.50	110.72
6	t	217	VAL	N-CA-C	-5.16	105.51	110.72
5	k	195	PRO	N-CA-C	5.15	116.99	110.70
3	a	400	ASN	CA-C-N	5.12	126.25	119.84
3	a	400	ASN	C-N-CA	5.12	126.25	119.84
7	m	162	ILE	N-CA-C	-5.12	106.81	111.67
5	E	195	PRO	N-CA-C	5.10	116.92	110.70
4	T	40	GLU	CA-CB-CG	5.08	124.26	114.10
4	j	83	GLU	CB-CG-CD	5.02	121.14	112.60
5	M	195	PRO	N-CA-C	5.02	116.82	110.70
5	s	195	PRO	N-CA-C	5.01	116.81	110.70
7	W	143	GLY	N-CA-C	5.00	116.69	110.29
3	C	400	ASN	CA-C-N	5.00	126.09	119.84
3	C	400	ASN	C-N-CA	5.00	126.09	119.84

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

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Mol	Chain	Res	Type	Group
5	s	163	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3348	0	3385	19	0
1	I	3348	0	3385	17	0
1	Q	3348	0	3385	16	0
1	Y	3348	0	3385	14	0
1	g	3348	0	3385	17	0
1	o	3348	0	3385	12	0
2	B	3304	0	3350	10	0
2	J	3304	0	3350	13	0
2	R	3304	0	3350	11	0
2	Z	3304	0	3350	13	0
2	h	3304	0	3350	17	0
2	p	3304	0	3350	14	0
3	C	3191	0	3208	20	0
3	K	3191	0	3208	14	0
3	S	3191	0	3208	17	0
3	a	3191	0	3208	14	0
3	i	3191	0	3208	14	0
3	q	3191	0	3208	14	0
4	D	3251	0	3253	15	0
4	L	3251	0	3253	10	0
4	T	3251	0	3253	12	0
4	b	3251	0	3253	29	0
4	j	3251	0	3252	20	0
4	r	3251	0	3252	11	0
5	E	2366	0	2340	9	0
5	M	2366	0	2340	12	0
5	U	2366	0	2340	23	0
5	c	2366	0	2340	8	0
5	k	2366	0	2340	15	0
5	s	2366	0	2340	19	0
6	F	2263	0	2235	15	0
6	N	2263	0	2235	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	V	2263	0	2235	16	0
6	d	2263	0	2235	9	0
6	l	2263	0	2236	19	0
6	t	2263	0	2236	13	0
7	G	1631	0	1654	8	0
7	O	1631	0	1654	5	0
7	W	1631	0	1654	6	0
7	e	1631	0	1654	7	0
7	m	1631	0	1654	9	0
7	u	1631	0	1654	8	0
8	H	1383	0	1366	9	0
8	P	1383	0	1366	6	0
8	X	1383	0	1366	4	0
8	f	1383	0	1366	6	0
8	n	1383	0	1366	7	0
8	v	1383	0	1366	9	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
All	All	124428	0	124746	499	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 (499) 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	1.44
6:N:217:VAL:C	6:N:218:ALA:N	1.79	1.40
6:d:217:VAL:C	6:d:218:ALA:N	1.78	1.40
6:F:217:VAL:C	6:F:218:ALA:N	1.80	1.37
5:U:196:PRO:HA	4:b:140:ASN:CG	2.03	0.81
5:k:248:ASN:ND2	6:l:191:ALA:O	2.19	0.75
5:s:248:ASN:ND2	6:t:191:ALA:O	2.20	0.75
3:q:153:LYS:O	8:v:59:ARG:NH1	2.25	0.70
4:j:290:LYS:C	4:j:291:ALA:N	2.53	0.67
4:r:240:GLN:OE1	6:t:76:GLN:O	2.14	0.65
8:H:158:THR:HG21	7:e:150:GLN:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:116:TYR:CE2	6:V:114:GLN:HG3	2.32	0.65
6:l:267:LEU:O	6:l:268:PRO:C	2.42	0.62
6:F:267:LEU:O	6:F:268:PRO:C	2.42	0.62
6:V:267:LEU:O	6:V:268:PRO:C	2.43	0.62
4:T:37:SER:O	4:T:40:GLU:OE1	2.17	0.61
6:t:267:LEU:O	6:t:268:PRO:C	2.42	0.61
4:j:42:LEU:HD11	4:j:83:GLU:CG	2.30	0.61
6:N:267:LEU:O	6:N:268:PRO:C	2.42	0.61
3:C:153:LYS:O	8:H:59:ARG:NH1	2.33	0.61
3:i:153:LYS:O	8:n:59:ARG:NH1	2.34	0.60
5:U:197:ASP:H	4:b:140:ASN:HA	1.67	0.60
4:j:318:ASN:OD1	7:m:147:GLN:N	2.33	0.60
4:j:271:ARG:NH1	7:m:137:TYR:O	2.35	0.60
6:d:267:LEU:O	6:d:268:PRO:C	2.43	0.60
1:g:486:ALA:HB3	3:i:386:LEU:HD21	1.83	0.60
3:i:88:CYS:O	3:i:90:GLY:N	2.35	0.59
3:K:88:CYS:O	3:K:90:GLY:N	2.35	0.59
3:q:88:CYS:O	3:q:90:GLY:N	2.35	0.59
3:C:88:CYS:O	3:C:90:GLY:N	2.36	0.58
4:b:121:ARG:HG3	4:b:125:GLN:HE21	1.67	0.58
4:b:140:ASN:OD1	4:b:141:VAL:N	2.36	0.58
7:u:24:GLY:HA2	7:u:55:LEU:HD21	1.85	0.58
3:a:88:CYS:O	3:a:90:GLY:N	2.35	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
7:e:24:GLY:HA2	7:e:55:LEU:HD21	1.85	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:m:24:GLY:HA2	7:m:55:LEU:HD21	1.85	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
4:j:42:LEU:HD11	4:j:83:GLU:HG2	1.85	0.57
2:h:420:ARG:CD	5:k:263:THR:HG22	2.35	0.57
3:a:64:VAL:HG12	3:a:64:VAL:O	2.06	0.56
3:q:119:ARG:HD3	8:v:29:GLY:HA2	1.89	0.55
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
4:j:240:GLN:OE1	6:l:76:GLN:O	2.25	0.55
1:g:496:LEU:HD11	2:h:443:ALA:HB2	1.87	0.55
6:F:272:THR:HG22	7:G:110:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:64:VAL:HG12	3:i:64:VAL:O	2.06	0.55
3:C:64:VAL:HG12	3:C:64:VAL:O	2.06	0.55
3:S:64:VAL:HG12	3:S:64:VAL:O	2.07	0.55
5:U:197:ASP:N	4:b:140:ASN:HA	2.22	0.55
3:a:153:LYS:O	8:f:59:ARG:NH1	2.37	0.55
4:L:125:GLN:NE2	2:h:164:GLU:OE2	2.39	0.54
3:q:64:VAL:HG12	3:q:64:VAL:O	2.07	0.54
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
4:b:197:TYR:O	4:b:288:HIS:CE1	2.62	0.53
5:M:116:TYR:CE2	6:N:114:GLN:HG3	2.44	0.53
4:r:271:ARG:NH1	7:u:137:TYR:O	2.41	0.53
5:M:280:LEU:HD21	6:N:303:ASN:HD21	1.74	0.52
1:Q:489:MET:HE3	2:R:442:LEU:HD23	1.91	0.52
4:r:318:ASN:OD1	7:u:147:GLN:N	2.43	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:h:283:ALA:O	2:h:287:MET:N	2.42	0.52
2:Z:283:ALA:O	2:Z:287:MET:N	2.43	0.52
2:p:420:ARG:CD	5:s:263:THR:HG22	2.40	0.52
4:j:375:GLN:HE22	6:l:192:THR:HG21	1.75	0.52
2:B:272:ARG:O	2:B:276:CYS:N	2.44	0.51
3:a:367:TYR:HA	3:a:372:MET:HG3	1.92	0.51
2:p:272:ARG:O	2:p:276:CYS:N	2.43	0.51
3:q:367:TYR:HA	3:q:372:MET:HG3	1.92	0.51
2:J:272:ARG:O	2:J:276:CYS:N	2.44	0.51
3:i:367:TYR:HA	3:i:372:MET:HG3	1.93	0.51
2:p:283:ALA:O	2:p:287:MET:N	2.42	0.51
4:D:385:LEU:HD22	6:F:234:ARG:HD2	1.93	0.51
2:R:283:ALA:O	2:R:287:MET:N	2.43	0.51
5:k:180:LYS:NZ	6:l:207:THR:OG1	2.40	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:U:197:ASP:OD1	4:b:141:VAL:HG23	2.11	0.50
5:E:116:TYR:CE2	6:F:114:GLN:HG3	2.46	0.50
4:j:290:LYS:C	4:j:291:ALA:C	2.80	0.50
4:r:373:GLN:HG3	6:t:270:LEU:HD21	1.94	0.50
4:b:153:ARG:HG3	4:b:193:ARG:NH2	2.26	0.50
2:B:283:ALA:O	2:B:287:MET:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:272:ARG:O	2:h:276:CYS:N	2.43	0.50
1:o:486:ALA:HB3	3:q:386:LEU:HD21	1.94	0.50
2:J:283:ALA:O	2:J:287:MET:N	2.42	0.50
5:U:197:ASP:HB2	4:b:139:TYR:O	2.12	0.50
2:p:427:TRP:HB2	5:s:266:VAL:HG13	1.93	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
4:b:153:ARG:HG3	4:b:193:ARG:HH22	1.75	0.49
2:h:420:ARG:HD2	5:k:263:THR:HG22	1.94	0.49
4:j:248:THR:OG1	6:l:147:GLU:O	2.29	0.49
1:I:209:LEU:HG	1:I:217:ALA:HB1	1.94	0.49
1:g:209:LEU:HG	1:g: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
4:b:362:GLU:OE1	4:b:362:GLU:HA	2.11	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:o:209:LEU:HG	1:o:217:ALA:HB1	1.94	0.49
1:Q:486:ALA:HB3	3:S:386:LEU:HD21	1.95	0.48
5:c:280:LEU:HD21	6:d:303:ASN:HD21	1.77	0.48
5:s:331:ILE:HG21	6:t:267:LEU:HD13	1.94	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
1:o:264:THR:HB	1:o:265:PRO:HD3	1.96	0.48
4:D:275:GLY:N	4:D:329:GLU:OE2	2.46	0.48
4:j:252:ASP:HA	6:l:172:ILE:HG23	1.94	0.48
4:j:290:LYS:C	4:j:291:ALA:CA	2.86	0.48
1:o:381:LEU:HG	1:o:402:TYR:CE2	2.49	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
4:b:190:CYS:HA	4:b:193:ARG:NH1	2.29	0.48
4:j:42:LEU:HD11	4:j:83:GLU:HG3	1.95	0.48
1:Q:264:THR:HB	1:Q:265:PRO:HD3	1.96	0.48
1:g:242:ILE:HG23	1:g:254:VAL:HG13	1.96	0.48
1:g:264:THR:HB	1:g:265:PRO:HD3	1.96	0.47
1:I:264:THR:HB	1:I:265:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:19:HIS:CE1	4:r:61:ILE:HD13	2.49	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
3:a:70:SER:O	3:a:71:VAL:HG22	2.14	0.47
1:o:242:ILE:HG23	1:o:254:VAL:HG13	1.96	0.47
1:Y:242:ILE:HG23	1:Y:254:VAL:HG13	1.97	0.47
3:a:152:ALA:O	3:a:154:CYS:N	2.48	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
6:t:258:ARG:HB2	7:u:162:ILE:HD12	1.95	0.47
3:C:70:SER:O	3:C:71:VAL:HG22	2.14	0.47
3:K:353:GLN:O	7:m:123:ARG:NH1	2.47	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
8:n:103:GLN:N	8:n:104:PRO:HD2	2.30	0.47
3:C:152:ALA:O	3:C:154:CYS:N	2.47	0.47
3:a:118:LEU:HD23	8:f:30:GLY:O	2.15	0.47
8:f:103:GLN:N	8:f:104:PRO:HD2	2.30	0.47
3:i:70:SER:O	3:i:71:VAL:HG22	2.14	0.47
3:i:152:ALA:O	3:i:154:CYS:N	2.47	0.47
3:q:152:ALA:O	3:q: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
4:L:399:ALA:HB1	6:N:237:LEU:HD22	1.95	0.47
4:j:385:LEU:HD22	6:l:234:ARG:HD2	1.97	0.47
2:J:324:THR:HB	2:h:332:THR:HG23	1.97	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
4:j:1:MET:SD	4:j:1:MET:N	2.84	0.47
8:v:103:GLN:N	8:v:104:PRO:HD2	2.30	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
2:Z:366:TYR:CE2	4:b:352:ILE:HG21	2.50	0.46
3:q:70:SER:O	3:q:71:VAL:HG22	2.14	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
1:g:502:VAL:HG22	3:i:178:ALA:HB1	1.98	0.46
2:h:427:TRP:HB2	5:k:266:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:381:LEU:HG	1:Y:402:TYR:CE2	2.49	0.46
1:g:486:ALA:CB	3:i:386:LEU:HD21	2.45	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
5:c:163:GLU:HG3	5:c:164:PRO:HD3	1.98	0.46
3:i:9:VAL:HG21	3:i:42:LEU:HD22	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
4:b:362:GLU:OE1	4:b:362:GLU:CA	2.64	0.46
5:k:331:ILE:HG21	6:l:267:LEU:HD13	1.98	0.46
2:p:420:ARG:HD2	5:s:263:THR:HG22	1.97	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
1:o:395:ALA:N	1:o:396:PRO:CD	2.79	0.46
3:q:9:VAL:HG21	3:q:42:LEU:HD22	1.98	0.46
4:D:269:LEU:HA	6:F:79:ARG:HD3	1.98	0.45
1:g:381:LEU:HG	1:g:402:TYR:CE2	2.49	0.45
4:j:227:LYS:HE2	4:j:258:LEU:HD22	1.97	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
3:a:9:VAL:HG21	3:a:42:LEU:HD22	1.98	0.45
4:T:275:GLY:N	4:T:329:GLU:OE2	2.47	0.45
5:s:163:GLU:HG3	5:s:164:PRO:HD3	1.97	0.45
5:s:124:ALA:HB1	5:s:129:ARG:HB2	1.99	0.45
4:D:274:ARG:HA	4:D:274:ARG:HD3	1.82	0.45
5:U:163:GLU:HG3	5:U:164:PRO:CD	2.46	0.45
5:k:163:GLU:HG3	5:k:164:PRO:HD3	1.97	0.45
6:l:297:LYS:HD3	8:n:207:LEU:HD23	1.98	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
1:g:395:ALA:N	1:g:396:PRO:CD	2.80	0.45
3:i:341:MET:HB3	3:i:347:ILE:HG22	1.99	0.45
5:c:163:GLU:HG3	5:c:164:PRO:CD	2.47	0.45
3:C:119:ARG:HD3	8:H:29:GLY:HA2	1.99	0.45
6:F:244:ALA:HB1	6:F:250:VAL:HG21	1.99	0.45
1:I:489:MET:HE3	2:J:442:LEU:HD23	1.97	0.45
5:U:124:ALA:HB1	5:U:129:ARG:HB2	1.99	0.45
3:a:341:MET:HB3	3:a:347:ILE:HG22	1.99	0.45
5:k:163:GLU:HG3	5:k:164:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s:163:GLU:HG3	5:s:164:PRO:CD	2.46	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
5:k:124:ALA:HB1	5:k:129:ARG:HB2	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
8:H:47:HIS:O	8:H:48:ASN:C	2.61	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:g:280:ALA:HB2	1:g:312:ASP:HB3	1.99	0.44
2:p:85:PHE:CZ	2:p:123:LYS:HG3	2.52	0.44
6:t:244:ALA:HB1	6:t:250:VAL:HG21	2.00	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
2:R:304:ASN:O	2:R:305:ASP:C	2.61	0.44
6:V:244:ALA:HB1	6:V:250:VAL:HG21	2.00	0.44
2:Z:413:HIS:O	2:Z:415:LYS:N	2.51	0.44
3:C:118:LEU:HD23	8:H:30:GLY:O	2.18	0.44
3:C:341:MET:HB3	3:C:347:ILE:HG22	1.99	0.44
5:U:197:ASP:OD2	4:b:141:VAL:N	2.50	0.44
2:h:293:PRO:CG	2:h:315:VAL:HG21	2.48	0.44
5:s:322:VAL:HG11	8:v:196:GLN:CB	2.46	0.44
1:A:94:LEU:HD22	1:A:98:GLU:HG3	2.00	0.44
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:I:280:ALA:HB2	1:I:312:ASP:HB3	1.99	0.44
2:Z:408:LEU:HD22	4:b:355:ILE:HG12	2.00	0.44
8:f:102:VAL:HG12	8:f:106:MET:HG2	2.00	0.44
1:o:280:ALA:HB2	1:o: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
6:l:155:ASN:HB3	6:l:164:PRO:HB2	2.00	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
4:r:230:LEU:CD1	4:r:264:LEU:HD22	2.48	0.44
2:R:85:PHE:CZ	2:R:123:LYS:HG3	2.53	0.44
2:h:85:PHE:CZ	2:h:123:LYS:HG3	2.52	0.44
4:j:230:LEU:CD1	4:j:264:LEU:HD22	2.48	0.44
6:l:110:GLU:O	6:l:114:GLN:HG2	2.18	0.44
2:p:304:ASN:O	2:p:305:ASP:C	2.61	0.44
7:u:102:VAL:HG22	7:u:141:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:c:124:ALA:HB1	5:c:129:ARG:HB2	1.99	0.44
1:g:94:LEU:HD22	1:g:98:GLU:HG3	2.00	0.44
2:h:366:TYR:CD2	4:j:352:ILE:HB	2.53	0.44
3:q:341:MET:HB3	3:q:347:ILE:HG22	1.99	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
5:k:261:TYR:CZ	5:k:265:GLN:HG3	2.53	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
6:l:244:ALA:HB1	6:l:250:VAL:HG21	1.99	0.43
8:n:102:VAL:HG12	8:n: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
1:Y:486:ALA:HB3	3:a:386:LEU:HD21	2.00	0.43
4:b:141:VAL:HG22	4:b:177:GLU:OE2	2.18	0.43
2:h:413:HIS:O	2:h:415:LYS:N	2.51	0.43
8:v:102:VAL:HG12	8:v:106:MET:HG2	2.00	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:94:LEU:HD22	1:Q:98:GLU:HG3	1.99	0.43
1:Q:280:ALA:HB2	1:Q:312:ASP:HB3	1.99	0.43
7:W:102:VAL:HG22	7:W:141:LEU:HD21	2.00	0.43
4:b:149:LEU:HD21	4:b:187:TYR:HA	1.99	0.43
4:b:274:ARG:HA	4:b:274:ARG:HD3	1.84	0.43
8:f:47:HIS:O	8:f:48:ASN:C	2.61	0.43
2:p:293:PRO:CG	2:p:315:VAL:HG21	2.48	0.43
2:p:413:HIS:O	2:p:415:LYS:N	2.51	0.43
5:s:245:TYR:OH	6:t:197:ARG:HA	2.19	0.43
6:t:110:GLU:O	6:t:114:GLN:HG2	2.18	0.43
2:B:85:PHE:CZ	2:B:123:LYS:HG3	2.53	0.43
6:d:110:GLU:O	6:d:114:GLN:HG2	2.18	0.43
6:d:213:GLU:O	6:d:214:ASN:C	2.61	0.43
6:d:244:ALA:HB1	6:d:250:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:102:VAL:HG22	7:e:141:LEU:HD21	2.00	0.43
6:F:213:GLU:O	6:F:214:ASN:C	2.61	0.43
3:S:153:LYS:O	8:X:59:ARG:NH1	2.50	0.43
8:v:47:HIS:O	8:v:48:ASN:C	2.62	0.43
1:Q:415:SER:N	1:Q:416:PRO:HD2	2.33	0.43
8:X:47:HIS:O	8:X:48:ASN:C	2.61	0.43
4:r:365:GLU:O	4:r:366:ALA:HB3	2.19	0.43
6:t:213:GLU:O	6:t:214:ASN:C	2.62	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
6:l:103:GLU:HG2	5:s:282:ARG:HD2	2.00	0.43
7:m:102:VAL:HG22	7:m:141:LEU:HD21	2.00	0.43
6:N:213:GLU:O	6:N:214:ASN:C	2.62	0.43
8:P:47:HIS:O	8:P:48:ASN:C	2.62	0.43
1:Q:486:ALA:CB	3:S:386:LEU:HD21	2.49	0.43
5:U:120:TYR:HA	6:V:111:GLN:OE1	2.19	0.43
5:U:333:ILE:CG2	7:W:107:LYS:HA	2.48	0.43
4:j:149:LEU:HD21	4:j:187:TYR:HA	2.00	0.43
5:s:322:VAL:HG11	8:v:196:GLN:HB3	2.01	0.43
4:D:327:LEU:HD13	7:G:126:ARG:NH1	2.33	0.43
7:G:127:GLN:O	7:G:128:LEU:C	2.62	0.43
4:b:318:ASN:OD1	7:e:147:GLN:N	2.52	0.43
1:o:94:LEU:HD22	1:o:98:GLU:HG3	2.00	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
6:V:213:GLU:O	6:V:214:ASN:C	2.61	0.43
4:b:365:GLU:O	4:b:366:ALA:HB3	2.19	0.43
8:n:47:HIS:O	8:n:48:ASN:C	2.62	0.43
1:o:415:SER:N	1:o:416:PRO:HD2	2.34	0.43
4:r:149:LEU:HD21	4:r:187:TYR:HA	2.00	0.43
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
5:c:261:TYR:CZ	5:c:265:GLN:HG3	2.54	0.42
6:d:155:ASN:HB3	6:d:164:PRO:HB2	2.01	0.42
1:g:477:LEU:O	1:g:481:GLU:HG2	2.19	0.42
1:o:128:VAL:HG11	1:o:171:ARG:HD3	2.01	0.42
2:p:101:SER:O	2:p:102:ALA:HB3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:o:477:LEU:O	1:o:481:GLU:HG2	2.19	0.42
5:s:261:TYR:CZ	5:s:265:GLN:HG3	2.54	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
7:O:127:GLN:O	7:O:128:LEU:C	2.62	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
1:g:128:VAL:HG11	1:g:171:ARG:HD3	2.01	0.42
4:j:365:GLU:O	4:j:366:ALA:HB3	2.19	0.42
6:t:155:ASN:HB3	6:t:164:PRO:HB2	2.00	0.42
4:D:365:GLU:O	4:D:366:ALA:HB3	2.19	0.42
2:J:304:ASN:O	2:J:305:ASP:C	2.61	0.42
6:V:155:ASN:HB3	6:V:164:PRO:HB2	2.01	0.42
3:a:94:ARG:NH1	3:a:137:GLN:OE1	2.52	0.42
2:h:101:SER:O	2:h:102:ALA:HB3	2.19	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
4:b:246:LEU:HD23	4:b:264:LEU:HD21	2.01	0.42
5:s:262:THR:HB	6:t:289:MET:HE1	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:304:ASN:O	2:Z:305:ASP:C	2.62	0.42
3:i:138:LEU:HB2	3:i:166:MET:HG3	2.01	0.42
6:l:213:GLU:O	6:l:214:ASN:C	2.62	0.42
2:B:304:ASN:O	2:B:305:ASP:C	2.62	0.42
2:Z:192:THR:HA	2:Z:228:ILE:HG13	2.02	0.42
3:q:94:ARG:NH1	3:q:137:GLN:OE1	2.53	0.42
3:C:210:THR:O	3:C:211:THR:C	2.63	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
3:a:138:LEU:HB2	3:a:166:MET:HG3	2.01	0.42
5:E:189:TYR:CE2	5:E:195:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:149:LEU:HD21	4:T:187:TYR:HA	2.02	0.41
7:e:94:ASN:O	7:e:98:HIS:ND1	2.53	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
4:b:174:LEU:HA	4:b:177:GLU:HG2	2.02	0.41
1:g:364:ASP:HB2	1:g:380:MET:HE2	2.03	0.41
1:g:415:SER:N	1:g:416:PRO:HD2	2.35	0.41
5:k:262:THR:HB	6:l:289:MET:HE1	2.01	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:i:210:THR:O	3:i:211:THR:C	2.63	0.41
4:r:308:ASN:HB3	4:r:328:LEU:HD22	2.01	0.41
1:A:85:GLU:HG2	4:b:77:PRO:HB3	2.02	0.41
1:A:364:ASP:HB2	1:A:380:MET:HE2	2.03	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
1:Q:364:ASP:HB2	1:Q:380:MET:HE2	2.03	0.41
7:W:127:GLN:O	7:W:128:LEU:C	2.63	0.41
3:a:292:MET:HA	3:a:295:VAL:HG12	2.02	0.41
3:q:138:LEU:HB2	3:q:166:MET:HG3	2.01	0.41
5:U:176:ILE:HG23	6:V:194:GLU:HG2	2.02	0.41
6:V:215:SER:O	6:V:216:THR:OG1	2.38	0.41
2:h:304:ASN:O	2:h:305:ASP:C	2.62	0.41
3:i:94:ARG:NH1	3:i:137:GLN:OE1	2.53	0.41
1:I:364:ASP:HB2	1:I:380:MET:HE2	2.03	0.41
3:K:138:LEU:HB2	3:K:166:MET:HG3	2.01	0.41
3:S:210:THR:O	3:S:211:THR:C	2.64	0.41
2:Z:366:TYR:CD2	4:b:352:ILE:HB	2.55	0.41
5:c:189:TYR:CE2	5:c:195:PRO:HB3	2.56	0.41
2:h:434:LEU:HG	6:l:299:CYS:SG	2.59	0.41
5:s:156:MET:HE1	5:s:191:LYS:HB2	2.03	0.41
7:u:127:GLN:O	7:u:128:LEU:C	2.63	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
5:E:156:MET:HE1	5:E:191:LYS:HB2	2.02	0.41
8:H:80:ARG:HD2	8:H:80:ARG:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:364:ASP:HB2	1:Y:380:MET:HE2	2.03	0.41
3:a:210:THR:O	3:a:211:THR:C	2.62	0.41
5:k:189:TYR:CE2	5:k:195:PRO:HB3	2.56	0.41
7:m:111:ILE:HG22	7:m:112:PRO:O	2.21	0.41
2:p:141:ASP:OD2	2:p:144:ASN:ND2	2.54	0.41
7:u:94:ASN:O	7:u:98:HIS:ND1	2.54	0.41
4:L:308:ASN:HB3	4:L:328:LEU:HD22	2.03	0.41
4:b:58:SER:OG	4:b:60:VAL:HG12	2.21	0.41
4:b:308:ASN:HB3	4:b:328:LEU:HD22	2.01	0.41
2:h:192:THR:HA	2:h:228:ILE:HG13	2.03	0.41
4:r:375:GLN:HE22	6:t:192:THR:HG21	1.86	0.41
4:D:308:ASN:HB3	4:D:328:LEU:HD22	2.03	0.41
5:E:129:ARG:HG3	6:F:57:ARG:NH2	2.35	0.41
3:K:210:THR:O	3:K:211:THR:C	2.64	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
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
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
7:m:94:ASN:O	7:m:98:HIS:ND1	2.54	0.41
3:q:46:LEU:O	3:q:48:ALA:N	2.54	0.41
3:q:210:THR:O	3:q:211:THR:C	2.64	0.41
5:s:189:TYR:CE2	5:s:195:PRO:HB3	2.55	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
5:M:156:MET:HE1	5:M:191:LYS:HB2	2.03	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
4:b:6:ARG:HH22	4:b:43:GLU:HG2	1.86	0.41
5:c:156:MET:HE1	5:c:191:LYS:HB2	2.02	0.41
5:k:240:LEU:HD13	6:l:164:PRO:HD3	2.02	0.41
7:u:111:ILE:HG22	7:u:112:PRO:O	2.21	0.41
8:v:80:ARG:HD2	8:v:80:ARG:N	2.36	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
5:U:67:MET:HE1	6:V:84:MET:HE3	2.02	0.40
7:W:94:ASN:O	7:W:98:HIS:ND1	2.54	0.40
7:e:111:ILE:HG22	7:e:112:PRO:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:315:ILE:HG21	8:n:204:VAL:HG23	2.03	0.40
1:o:364:ASP:HB2	1:o:380:MET:HE2	2.03	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
5:c:331:ILE:HG21	6:d:267:LEU:HD13	2.03	0.40
6:d:112:PHE:CD1	6:d:112:PHE:C	2.99	0.40
7:e:116:LEU:HD13	7:e:128:LEU:HD11	2.04	0.40
1:A:478:MET:SD	1:A:478:MET:C	3.04	0.40
1:I:478:MET:SD	1:I:478:MET:C	3.04	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:U:197:ASP:OD2	4:b:140:ASN:C	2.64	0.40
1:g:258:VAL:HG11	1:g:289:ALA:HB2	2.03	0.40
2:h:441:LYS:O	6:l:310:ASN:ND2	2.54	0.40
8:n:154:GLN:HB3	8:n:163:LEU:HB2	2.04	0.40
2:p:424:LEU:HA	5:s:266:VAL:HG11	2.04	0.40
5:s:315:ILE:HD11	8:v:207:LEU:HD12	2.03	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
4:j:2:ALA:HB2	4:j:40:GLU:HG3	2.03	0.40
5:k:300:LEU:O	5:k:304:THR:OG1	2.35	0.40
7:m:116:LEU:HD13	7:m:128:LEU:HD11	2.04	0.40
7:m:127:GLN:O	7:m:128:LEU:C	2.63	0.40
2:p:430:GLN:HG3	5:s:270:SER:OG	2.21	0.40
1:Q:148:ALA:HB3	1:Q:149:PRO:HD3	2.03	0.40
3:S:36:ALA:C	3:S:38:ASN:H	2.30	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
8:f:98:TRP:HB3	8:f:102:VAL:HB	2.04	0.40
1:g:148:ALA:HB3	1:g:149:PRO:HD3	2.03	0.40
2:p:192:THR:HA	2:p:228:ILE:HG13	2.03	0.40
4:r:2:ALA:HB2	4:r:40:GLU:HG3	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%)	12	48
1	I	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	12	48
1	Q	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	12	48
1	Y	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	12	48
1	g	415/480 (86%)	374 (90%)	37 (9%)	4 (1%)	12	48
1	o	415/480 (86%)	373 (90%)	38 (9%)	4 (1%)	12	48
2	B	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	3	22
2	J	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	3	22
2	R	397/447 (89%)	353 (89%)	32 (8%)	12 (3%)	3	22
2	Z	397/447 (89%)	351 (88%)	34 (9%)	12 (3%)	3	22
2	h	397/447 (89%)	351 (88%)	36 (9%)	10 (2%)	4	25
2	p	397/447 (89%)	351 (88%)	35 (9%)	11 (3%)	4	24
3	C	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	2	19
3	K	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	3	20
3	S	399/427 (93%)	342 (86%)	43 (11%)	14 (4%)	3	20
3	a	399/427 (93%)	341 (86%)	43 (11%)	15 (4%)	2	19
3	i	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	2	19
3	q	399/427 (93%)	342 (86%)	42 (10%)	15 (4%)	2	19
4	D	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	12	48
4	L	404/410 (98%)	373 (92%)	27 (7%)	4 (1%)	12	48
4	T	404/410 (98%)	372 (92%)	28 (7%)	4 (1%)	12	48
4	b	404/410 (98%)	374 (93%)	26 (6%)	4 (1%)	12	48
4	j	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	12	48
4	r	402/410 (98%)	372 (92%)	26 (6%)	4 (1%)	12	48
5	E	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	6	30
5	U	294/325 (90%)	262 (89%)	28 (10%)	4 (1%)	9	39
5	c	294/325 (90%)	262 (89%)	26 (9%)	6 (2%)	6	30
5	k	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	6	30
5	s	294/325 (90%)	261 (89%)	27 (9%)	6 (2%)	6	30
6	F	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	9	39
6	N	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	9	39
6	V	286/331 (86%)	258 (90%)	24 (8%)	4 (1%)	9	39
6	d	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	9	39
6	l	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	9	39
6	t	286/331 (86%)	257 (90%)	25 (9%)	4 (1%)	9	39
7	G	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	24	64
7	O	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	24	64
7	W	206/222 (93%)	194 (94%)	11 (5%)	1 (0%)	24	64
7	e	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	24	64
7	m	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	24	64
7	u	206/222 (93%)	193 (94%)	12 (6%)	1 (0%)	24	64
8	H	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	10	43
8	P	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	10	43
8	X	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	10	43
8	f	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	10	43
8	n	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	10	43
8	v	169/213 (79%)	156 (92%)	11 (6%)	2 (1%)	10	43
All	All	15416/17130 (90%)	13844 (90%)	1291 (8%)	281 (2%)	6	33

All (281) Ramachandran outliers are listed below:

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

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

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

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

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

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

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

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

5.3.2 Protein sidechains ⓘ

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%)	358 (98%)	7 (2%)	50	66
1	I	365/415 (88%)	358 (98%)	7 (2%)	50	66
1	Q	365/415 (88%)	358 (98%)	7 (2%)	50	66
1	Y	365/415 (88%)	358 (98%)	7 (2%)	50	66
1	g	365/415 (88%)	358 (98%)	7 (2%)	50	66
1	o	365/415 (88%)	358 (98%)	7 (2%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/406 (90%)	363 (99%)	4 (1%)	65	75
2	J	367/406 (90%)	363 (99%)	4 (1%)	65	75
2	R	367/406 (90%)	363 (99%)	4 (1%)	65	75
2	Z	367/406 (90%)	363 (99%)	4 (1%)	65	75
2	h	367/406 (90%)	363 (99%)	4 (1%)	65	75
2	p	367/406 (90%)	363 (99%)	4 (1%)	65	75
3	C	358/378 (95%)	351 (98%)	7 (2%)	48	66
3	K	358/378 (95%)	351 (98%)	7 (2%)	48	66
3	S	358/378 (95%)	351 (98%)	7 (2%)	48	66
3	a	358/378 (95%)	351 (98%)	7 (2%)	48	66
3	i	358/378 (95%)	351 (98%)	7 (2%)	48	66
3	q	358/378 (95%)	351 (98%)	7 (2%)	48	66
4	D	347/348 (100%)	326 (94%)	21 (6%)	17	38
4	L	347/348 (100%)	328 (94%)	19 (6%)	19	41
4	T	347/348 (100%)	328 (94%)	19 (6%)	19	41
4	b	347/348 (100%)	326 (94%)	21 (6%)	17	38
4	j	347/348 (100%)	326 (94%)	21 (6%)	17	38
4	r	347/348 (100%)	329 (95%)	18 (5%)	21	42
5	E	255/276 (92%)	248 (97%)	7 (3%)	39	60
5	M	255/276 (92%)	248 (97%)	7 (3%)	39	60
5	U	255/276 (92%)	248 (97%)	7 (3%)	39	60
5	c	255/276 (92%)	248 (97%)	7 (3%)	39	60
5	k	255/276 (92%)	248 (97%)	7 (3%)	39	60
5	s	255/276 (92%)	248 (97%)	7 (3%)	39	60
6	F	250/277 (90%)	246 (98%)	4 (2%)	55	69
6	N	250/277 (90%)	245 (98%)	5 (2%)	48	66
6	V	250/277 (90%)	246 (98%)	4 (2%)	55	69
6	d	250/277 (90%)	246 (98%)	4 (2%)	55	69
6	l	250/277 (90%)	246 (98%)	4 (2%)	55	69
6	t	250/277 (90%)	246 (98%)	4 (2%)	55	69
7	G	174/184 (95%)	168 (97%)	6 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	O	174/184 (95%)	168 (97%)	6 (3%)	32	54
7	W	174/184 (95%)	168 (97%)	6 (3%)	32	54
7	e	174/184 (95%)	168 (97%)	6 (3%)	32	54
7	m	174/184 (95%)	168 (97%)	6 (3%)	32	54
7	u	174/184 (95%)	168 (97%)	6 (3%)	32	54
8	H	144/174 (83%)	139 (96%)	5 (4%)	32	53
8	P	144/174 (83%)	139 (96%)	5 (4%)	32	53
8	X	144/174 (83%)	139 (96%)	5 (4%)	32	53
8	f	144/174 (83%)	139 (96%)	5 (4%)	32	53
8	n	144/174 (83%)	139 (96%)	5 (4%)	32	53
8	v	144/174 (83%)	139 (96%)	5 (4%)	32	53
All	All	13560/14748 (92%)	13200 (97%)	360 (3%)	39	60

All (360) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	106	HIS
1	A	287	CYS
1	A	294	LEU
1	A	315	ASP
1	A	342	LEU
1	A	498	ASN
2	B	84	ASN
2	B	193	GLN
2	B	208	GLN
2	B	239	GLU
3	C	71	VAL
3	C	124	LEU
3	C	130	LYS
3	C	167	MET
3	C	221	LEU
3	C	362	ASP
3	C	365	GLU
4	D	1	MET
4	D	22	LEU
4	D	40	GLU
4	D	55	GLU

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Mol	Chain	Res	Type
4	D	72	HIS
4	D	83	GLU
4	D	100	GLU
4	D	105	SER
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	293	THR
4	D	348	MET
4	D	351	PHE
4	D	362	GLU
4	D	394	GLU
5	E	63	LEU
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	30	VAL
6	F	112	PHE
6	F	120	GLU
6	F	285	ASP
7	G	110	CYS
7	G	161	ASP
7	G	167	LEU
7	G	173	THR
7	G	174	LEU
7	G	202	GLN
8	H	33	THR
8	H	46	LEU
8	H	70	GLU
8	H	132	ASP
8	H	142	GLU
1	I	94	LEU
1	I	106	HIS
1	I	287	CYS

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Mol	Chain	Res	Type
1	I	294	LEU
1	I	315	ASP
1	I	342	LEU
1	I	498	ASN
2	J	84	ASN
2	J	193	GLN
2	J	208	GLN
2	J	239	GLU
3	K	71	VAL
3	K	124	LEU
3	K	130	LYS
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	100	GLU
4	L	105	SER
4	L	121	ARG
4	L	149	LEU
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	348	MET
4	L	351	PHE
4	L	362	GLU
4	L	394	GLU
5	M	63	LEU
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	30	VAL

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Mol	Chain	Res	Type
6	N	112	PHE
6	N	120	GLU
6	N	203	VAL
6	N	285	ASP
7	O	110	CYS
7	O	161	ASP
7	O	167	LEU
7	O	173	THR
7	O	174	LEU
7	O	202	GLN
8	P	33	THR
8	P	46	LEU
8	P	70	GLU
8	P	132	ASP
8	P	142	GLU
1	Q	94	LEU
1	Q	106	HIS
1	Q	287	CYS
1	Q	294	LEU
1	Q	315	ASP
1	Q	342	LEU
1	Q	498	ASN
2	R	84	ASN
2	R	193	GLN
2	R	208	GLN
2	R	239	GLU
3	S	71	VAL
3	S	124	LEU
3	S	130	LYS
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	100	GLU
4	T	121	ARG
4	T	149	LEU
4	T	179	THR

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Mol	Chain	Res	Type
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	348	MET
4	T	351	PHE
4	T	362	GLU
4	T	394	GLU
5	U	63	LEU
5	U	77	VAL
5	U	140	HIS
5	U	163	GLU
5	U	165	PHE
5	U	173	THR
5	U	267	PHE
6	V	30	VAL
6	V	112	PHE
6	V	120	GLU
6	V	285	ASP
7	W	110	CYS
7	W	161	ASP
7	W	167	LEU
7	W	173	THR
7	W	174	LEU
7	W	202	GLN
8	X	33	THR
8	X	46	LEU
8	X	70	GLU
8	X	132	ASP
8	X	142	GLU
1	Y	94	LEU
1	Y	106	HIS
1	Y	287	CYS
1	Y	294	LEU
1	Y	315	ASP
1	Y	342	LEU
1	Y	498	ASN
2	Z	84	ASN
2	Z	193	GLN
2	Z	208	GLN

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Mol	Chain	Res	Type
2	Z	239	GLU
3	a	71	VAL
3	a	124	LEU
3	a	130	LYS
3	a	167	MET
3	a	221	LEU
3	a	362	ASP
3	a	365	GLU
4	b	22	LEU
4	b	40	GLU
4	b	55	GLU
4	b	72	HIS
4	b	83	GLU
4	b	100	GLU
4	b	105	SER
4	b	121	ARG
4	b	137	LYS
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
4	b	286	MET
4	b	348	MET
4	b	351	PHE
4	b	362	GLU
4	b	394	GLU
5	c	63	LEU
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	30	VAL
6	d	112	PHE
6	d	120	GLU
6	d	285	ASP
7	e	110	CYS
7	e	161	ASP

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Mol	Chain	Res	Type
7	e	167	LEU
7	e	173	THR
7	e	174	LEU
7	e	202	GLN
8	f	33	THR
8	f	46	LEU
8	f	70	GLU
8	f	132	ASP
8	f	142	GLU
1	g	94	LEU
1	g	106	HIS
1	g	287	CYS
1	g	294	LEU
1	g	315	ASP
1	g	342	LEU
1	g	498	ASN
2	h	84	ASN
2	h	193	GLN
2	h	208	GLN
2	h	239	GLU
3	i	71	VAL
3	i	124	LEU
3	i	130	LYS
3	i	167	MET
3	i	221	LEU
3	i	362	ASP
3	i	365	GLU
4	j	1	MET
4	j	22	LEU
4	j	40	GLU
4	j	72	HIS
4	j	83	GLU
4	j	100	GLU
4	j	105	SER
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

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Mol	Chain	Res	Type
4	j	276	ASN
4	j	286	MET
4	j	348	MET
4	j	351	PHE
4	j	362	GLU
4	j	394	GLU
5	k	63	LEU
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	30	VAL
6	l	112	PHE
6	l	120	GLU
6	l	285	ASP
7	m	110	CYS
7	m	161	ASP
7	m	167	LEU
7	m	173	THR
7	m	174	LEU
7	m	202	GLN
8	n	33	THR
8	n	46	LEU
8	n	70	GLU
8	n	132	ASP
8	n	142	GLU
1	o	94	LEU
1	o	106	HIS
1	o	287	CYS
1	o	294	LEU
1	o	315	ASP
1	o	342	LEU
1	o	498	ASN
2	p	84	ASN
2	p	193	GLN
2	p	208	GLN
2	p	239	GLU
3	q	71	VAL
3	q	124	LEU
3	q	130	LYS

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Mol	Chain	Res	Type
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	100	GLU
4	r	121	ARG
4	r	149	LEU
4	r	202	ILE
4	r	228	HIS
4	r	245	MET
4	r	274	ARG
4	r	276	ASN
4	r	286	MET
4	r	348	MET
4	r	351	PHE
4	r	362	GLU
4	r	394	GLU
5	s	63	LEU
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	30	VAL
6	t	112	PHE
6	t	120	GLU
6	t	285	ASP
7	u	110	CYS
7	u	161	ASP
7	u	167	LEU
7	u	173	THR
7	u	174	LEU
7	u	202	GLN
8	v	33	THR
8	v	46	LEU
8	v	70	GLU

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Mol	Chain	Res	Type
8	v	132	ASP
8	v	142	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	324	ASN
2	B	34	ASN
2	B	84	ASN
2	B	94	GLN
2	B	113	ASN
2	B	255	HIS
2	B	284	ASN
2	B	297	GLN
2	B	304	ASN
2	B	321	ASN
2	B	413	HIS
2	B	436	GLN
3	C	52	GLN
3	C	89	ASN
3	C	340	HIS
3	C	353	GLN
4	D	72	HIS
4	D	125	GLN
4	D	276	ASN
5	E	204	GLN
5	E	275	GLN
5	E	321	GLN
6	F	61	GLN
6	F	284	ASN
6	F	300	ASN
6	F	303	ASN
7	G	12	GLN
7	G	32	HIS
7	G	201	GLN
8	H	68	ASN
8	H	195	GLN
1	I	106	HIS
1	I	233	HIS
1	I	324	ASN
1	I	467	GLN

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Mol	Chain	Res	Type
2	J	34	ASN
2	J	84	ASN
2	J	94	GLN
2	J	113	ASN
2	J	220	GLN
2	J	255	HIS
2	J	284	ASN
2	J	297	GLN
2	J	304	ASN
2	J	321	ASN
2	J	436	GLN
3	K	52	GLN
3	K	82	GLN
3	K	89	ASN
3	K	353	GLN
4	L	72	HIS
4	L	136	GLN
4	L	276	ASN
5	M	126	GLN
5	M	321	GLN
6	N	61	GLN
6	N	284	ASN
6	N	300	ASN
7	O	12	GLN
7	O	32	HIS
7	O	196	ASN
8	P	68	ASN
8	P	195	GLN
1	Q	106	HIS
1	Q	233	HIS
1	Q	324	ASN
2	R	34	ASN
2	R	84	ASN
2	R	94	GLN
2	R	113	ASN
2	R	255	HIS
2	R	284	ASN
2	R	297	GLN
2	R	304	ASN
2	R	321	ASN
2	R	436	GLN
3	S	52	GLN

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Mol	Chain	Res	Type
3	S	89	ASN
3	S	353	GLN
4	T	19	HIS
4	T	72	HIS
4	T	136	GLN
4	T	276	ASN
5	U	126	GLN
5	U	204	GLN
5	U	258	ASN
5	U	275	GLN
5	U	321	GLN
6	V	61	GLN
6	V	282	GLN
6	V	284	ASN
6	V	300	ASN
6	V	303	ASN
7	W	11	ASN
7	W	12	GLN
7	W	32	HIS
7	W	196	ASN
8	X	68	ASN
8	X	195	GLN
1	Y	233	HIS
1	Y	324	ASN
2	Z	34	ASN
2	Z	84	ASN
2	Z	94	GLN
2	Z	113	ASN
2	Z	255	HIS
2	Z	284	ASN
2	Z	297	GLN
2	Z	304	ASN
2	Z	321	ASN
2	Z	370	HIS
2	Z	436	GLN
3	a	52	GLN
3	a	82	GLN
3	a	89	ASN
4	b	72	HIS
4	b	125	GLN
4	b	136	GLN
4	b	276	ASN

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Mol	Chain	Res	Type
5	c	204	GLN
5	c	258	ASN
5	c	275	GLN
5	c	321	GLN
6	d	282	GLN
6	d	284	ASN
7	e	11	ASN
7	e	12	GLN
7	e	32	HIS
7	e	198	HIS
8	f	68	ASN
1	g	106	HIS
1	g	233	HIS
1	g	324	ASN
2	h	34	ASN
2	h	84	ASN
2	h	94	GLN
2	h	113	ASN
2	h	255	HIS
2	h	284	ASN
2	h	297	GLN
2	h	304	ASN
2	h	321	ASN
2	h	370	HIS
2	h	436	GLN
3	i	52	GLN
3	i	89	ASN
3	i	353	GLN
3	i	361	HIS
4	j	72	HIS
4	j	136	GLN
4	j	240	GLN
4	j	276	ASN
4	j	375	GLN
5	k	204	GLN
5	k	258	ASN
5	k	321	GLN
6	l	61	GLN
6	l	220	HIS
7	m	11	ASN
7	m	12	GLN
7	m	32	HIS

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Mol	Chain	Res	Type
8	n	68	ASN
8	n	195	GLN
1	o	233	HIS
1	o	324	ASN
1	o	483	GLN
2	p	34	ASN
2	p	84	ASN
2	p	94	GLN
2	p	113	ASN
2	p	174	GLN
2	p	255	HIS
2	p	284	ASN
2	p	297	GLN
2	p	304	ASN
2	p	321	ASN
2	p	370	HIS
2	p	436	GLN
3	q	52	GLN
3	q	89	ASN
3	q	353	GLN
4	r	19	HIS
4	r	72	HIS
4	r	136	GLN
4	r	240	GLN
4	r	276	ASN
4	r	288	HIS
4	r	373	GLN
4	r	375	GLN
5	s	204	GLN
5	s	321	GLN
6	t	61	GLN
6	t	220	HIS
6	t	284	ASN
7	u	12	GLN
7	u	32	HIS
7	u	163	GLN
7	u	201	GLN
8	v	68	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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
4	r	1
2	J	1
2	B	1
2	R	1
2	p	1
2	Z	1
2	h	1
4	j	1
6	F	1
6	N	1
6	d	1
6	V	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
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%)	-0.53	1 (0%) 91 84	60, 128, 170, 185	0
1	I	419/480 (87%)	-0.46	1 (0%) 91 84	67, 120, 169, 191	0
1	Q	419/480 (87%)	-0.45	1 (0%) 91 84	81, 121, 167, 197	0
1	Y	419/480 (87%)	-0.51	3 (0%) 84 73	68, 108, 148, 176	0
1	g	419/480 (87%)	-0.49	1 (0%) 91 84	80, 111, 161, 190	0
1	o	419/480 (87%)	-0.55	1 (0%) 91 84	75, 109, 168, 189	0
2	B	403/447 (90%)	-0.40	4 (0%) 79 67	65, 127, 155, 189	0
2	J	403/447 (90%)	-0.49	3 (0%) 84 73	70, 125, 159, 172	0
2	R	403/447 (90%)	-0.41	3 (0%) 84 73	75, 108, 139, 162	0
2	Z	403/447 (90%)	-0.45	4 (0%) 79 67	68, 139, 167, 189	0
2	h	403/447 (90%)	-0.47	0 100 100	85, 135, 176, 202	0
2	p	403/447 (90%)	-0.51	1 (0%) 91 84	81, 126, 165, 179	0
3	C	401/427 (93%)	-0.46	1 (0%) 91 84	58, 118, 219, 260	0
3	K	401/427 (93%)	-0.42	2 (0%) 87 77	69, 118, 201, 220	0
3	S	401/427 (93%)	-0.45	3 (0%) 84 73	68, 99, 195, 216	0
3	a	401/427 (93%)	-0.40	3 (0%) 84 73	69, 134, 218, 238	0
3	i	401/427 (93%)	-0.47	5 (1%) 76 64	81, 114, 207, 257	0
3	q	401/427 (93%)	-0.47	1 (0%) 91 84	77, 116, 208, 249	0
4	D	406/410 (99%)	-0.53	1 (0%) 91 84	68, 145, 251, 272	0
4	L	406/410 (99%)	-0.54	0 100 100	80, 152, 188, 216	0
4	T	406/410 (99%)	-0.53	1 (0%) 91 84	88, 131, 183, 209	0
4	b	406/410 (99%)	-0.41	0 100 100	73, 166, 243, 253	0
4	j	406/410 (99%)	-0.42	1 (0%) 91 84	86, 132, 269, 285	0
4	r	406/410 (99%)	-0.44	1 (0%) 91 84	81, 162, 253, 272	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	E	298/325 (91%)	-0.37	2 (0%) 84 73	73, 112, 148, 170	0
5	M	298/325 (91%)	-0.38	2 (0%) 84 73	78, 107, 159, 185	0
5	U	298/325 (91%)	-0.47	1 (0%) 90 81	89, 121, 174, 198	0
5	c	298/325 (91%)	-0.42	0 100 100	61, 88, 126, 144	0
5	k	298/325 (91%)	-0.43	5 (1%) 69 58	85, 107, 145, 166	0
5	s	298/325 (91%)	-0.42	3 (1%) 79 67	84, 108, 148, 170	0
6	F	288/331 (87%)	-0.57	0 100 100	62, 114, 153, 184	0
6	N	288/331 (87%)	-0.54	1 (0%) 90 81	73, 113, 165, 193	0
6	V	288/331 (87%)	-0.46	2 (0%) 84 73	84, 120, 160, 194	0
6	d	288/331 (87%)	-0.54	0 100 100	63, 97, 150, 185	0
6	l	288/331 (87%)	-0.41	0 100 100	84, 116, 156, 182	0
6	t	288/331 (87%)	-0.49	2 (0%) 84 73	77, 116, 160, 190	0
7	G	208/222 (93%)	-0.50	2 (0%) 79 67	92, 114, 162, 187	0
7	O	208/222 (93%)	-0.52	3 (1%) 73 61	68, 115, 160, 181	0
7	W	208/222 (93%)	-0.50	1 (0%) 87 77	111, 135, 161, 174	0
7	e	208/222 (93%)	-0.55	0 100 100	84, 106, 145, 168	0
7	m	208/222 (93%)	-0.44	3 (1%) 73 61	72, 98, 143, 188	0
7	u	208/222 (93%)	-0.48	1 (0%) 87 77	73, 111, 149, 164	0
8	H	173/213 (81%)	-0.48	0 100 100	82, 123, 154, 168	0
8	P	173/213 (81%)	-0.55	0 100 100	91, 121, 147, 161	0
8	X	173/213 (81%)	-0.59	0 100 100	91, 114, 142, 150	0
8	f	173/213 (81%)	-0.57	0 100 100	81, 169, 190, 196	0
8	n	173/213 (81%)	-0.57	0 100 100	98, 129, 164, 181	0
8	v	173/213 (81%)	-0.64	0 100 100	94, 139, 175, 187	0
All	All	15576/17130 (90%)	-0.48	70 (0%) 88 78	58, 119, 209, 285	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	i	181	PHE	7.5
3	S	54	HIS	4.2
7	O	66	LEU	4.0
3	C	54	HIS	4.0
3	K	54	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
7	O	46	LEU	3.7
5	k	28	ILE	3.7
6	V	183	PHE	3.3
7	u	46	LEU	3.3
2	B	200	LEU	3.3
5	k	241	LEU	3.1
3	i	138	LEU	3.1
2	B	330	LEU	3.0
2	B	386	GLU	3.0
5	s	28	ILE	3.0
5	k	29	TYR	3.0
1	Y	174	ALA	3.0
5	s	85	VAL	2.9
7	W	177	TRP	2.9
5	k	238	LEU	2.9
5	k	85	VAL	2.8
7	m	195	ALA	2.8
3	S	53	GLU	2.7
4	j	324	LEU	2.7
6	N	195	ALA	2.7
5	M	85	VAL	2.7
3	q	181	PHE	2.6
1	I	346	VAL	2.6
1	Y	207	HIS	2.6
7	m	70	PHE	2.6
6	V	195	ALA	2.6
2	R	205	TYR	2.5
6	t	169	GLU	2.5
7	O	152	LEU	2.5
2	Z	311	MET	2.5
5	M	36	GLN	2.5
2	Z	200	LEU	2.4
5	U	189	TYR	2.4
3	S	307	ILE	2.4
2	J	205	TYR	2.4
2	p	92	TYR	2.4
3	a	224	TYR	2.3
1	Q	235	ILE	2.3
3	i	195	LEU	2.3
4	D	378	CYS	2.3
2	Z	343	ILE	2.3
5	E	167	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
5	s	90	MET	2.2
1	A	103	ILE	2.2
3	a	260	TYR	2.2
1	g	185	LEU	2.2
4	T	324	LEU	2.2
2	J	343	ILE	2.2
7	G	46	LEU	2.2
3	i	12	VAL	2.1
3	i	185	TYR	2.1
2	B	378	LEU	2.1
7	G	209	ILE	2.1
2	R	311	MET	2.1
5	E	73	GLY	2.1
7	m	19	ALA	2.1
2	Z	201	GLU	2.1
2	J	342	PHE	2.1
3	K	307	ILE	2.1
3	a	220	MET	2.0
1	o	281	ILE	2.0
2	R	330	LEU	2.0
4	r	309	LEU	2.0
6	t	60	SER	2.0
1	Y	178	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ZN	s	401	1/1	0.96	0.10	130,130,130,130	0
9	ZN	M	401	1/1	0.99	0.05	130,130,130,130	0
9	ZN	U	401	1/1	0.99	0.05	130,130,130,130	0
9	ZN	c	401	1/1	0.99	0.12	130,130,130,130	0
9	ZN	E	401	1/1	0.99	0.06	130,130,130,130	0
9	ZN	k	401	1/1	1.00	0.05	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.