



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:12 AM EDT

PDB ID : 4D18 / pdb_00004d18
Title : Crystal structure of the COP9 signalosome
Authors : Bunker, R.D.; Lingaraju, G.M.; Thoma, N.H.
Deposited on : 2014-05-01
Resolution : 4.08 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

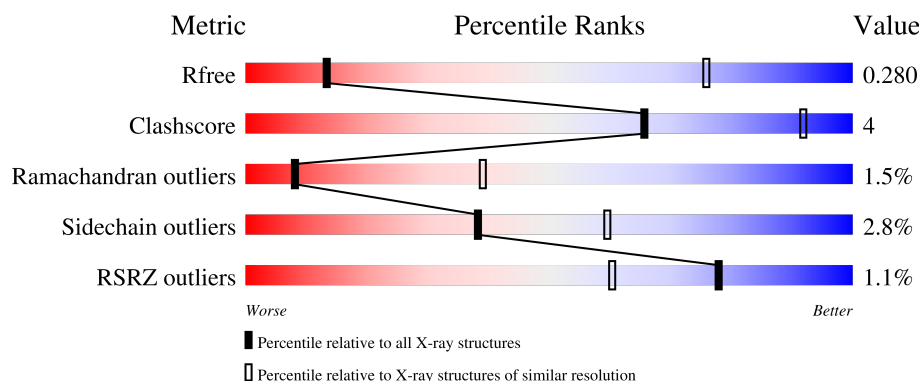
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.08 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	1200 (4.36-3.80)
Clashscore	190562	1249 (4.36-3.80)
Ramachandran outliers	187476	1169 (4.36-3.80)
Sidechain outliers	187428	1158 (4.36-3.80)
RSRZ outliers	180081	1199 (4.36-3.80)

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	79% 8% 13%
1	I	480	80% 7% 13%
2	B	447	78% 11% 10%
2	J	447	78% 11% 10%
3	C	427	78% 13% 6%

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Mol	Chain	Length	Quality of chain
3	K	427	
4	D	410	
4	L	410	
5	E	327	
5	M	327	
6	F	331	
6	N	331	
7	G	222	
7	O	222	
8	H	213	
8	P	213	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 41422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 1.

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 2.

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

- Molecule 3 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 3.

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

There are 8 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

- 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			

There are 8 discrepancies between the modelled and reference sequences:

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

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

- Molecule 5 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 5.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	GLY	-	expression tag	UNP Q92905
E	9	GLY	-	expression tag	UNP Q92905
E	10	GLY	-	expression tag	UNP Q92905
E	11	ARG	-	expression tag	UNP Q92905
M	8	GLY	-	expression tag	UNP Q92905
M	9	GLY	-	expression tag	UNP Q92905
M	10	GLY	-	expression tag	UNP Q92905
M	11	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	281	Total	C	N	O	S	0	0	0
			2236	1429	371	421	15			
6	N	281	Total	C	N	O	S	0	0	0
			2236	1429	371	421	15			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 7A.

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 8 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 8.

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

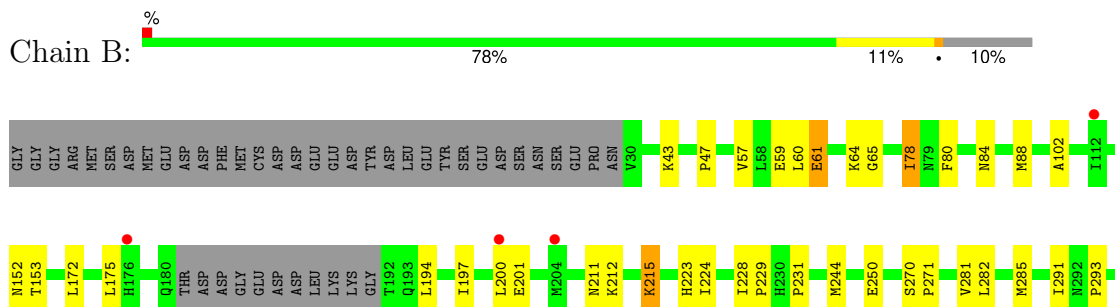
There are 8 discrepancies between the modelled and reference sequences:

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

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

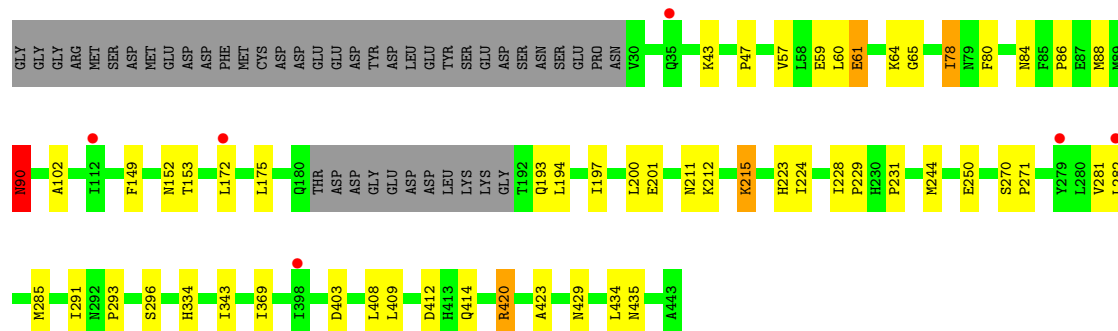
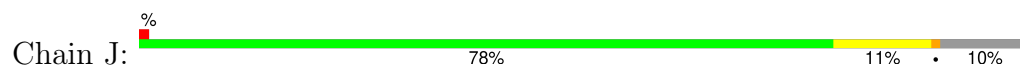
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total 1	Zn 1	0	0
9	M	1	Total 1	Zn 1	0	0

- Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

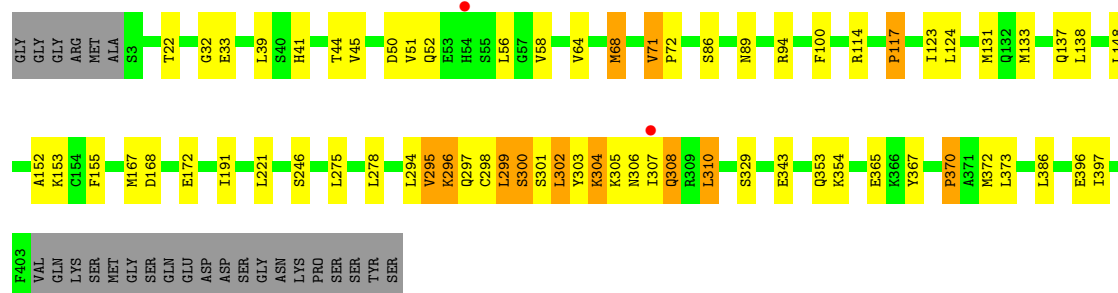
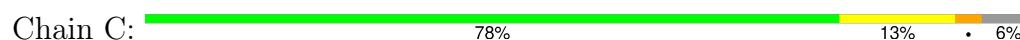




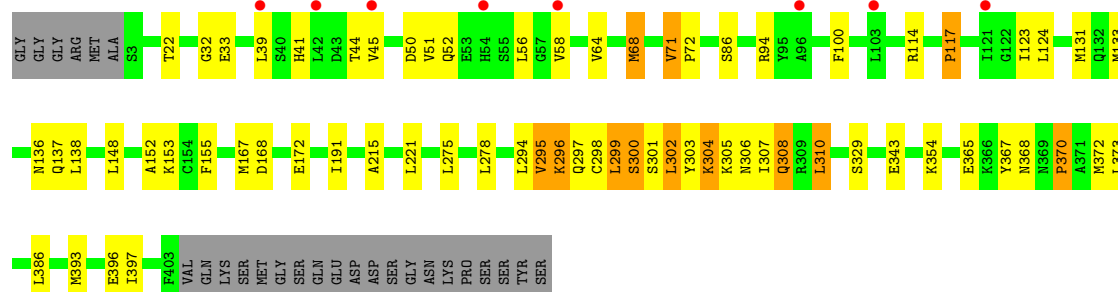
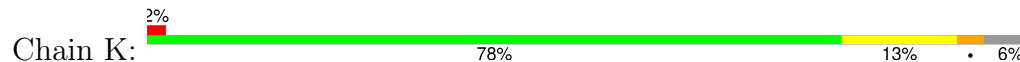
• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2



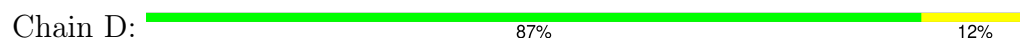
• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

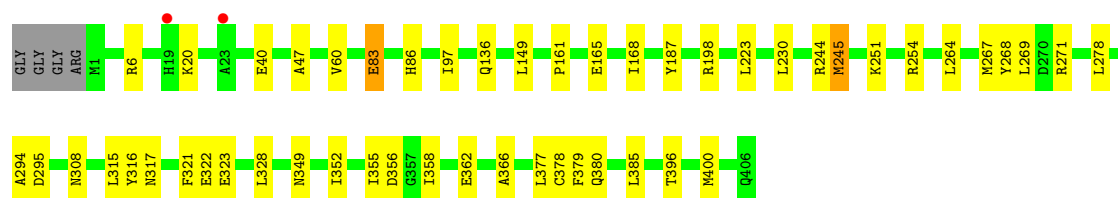


• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3



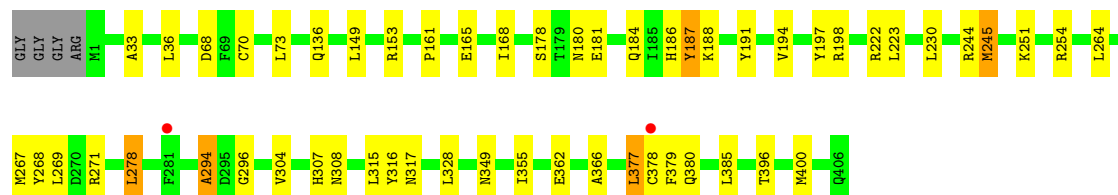
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4





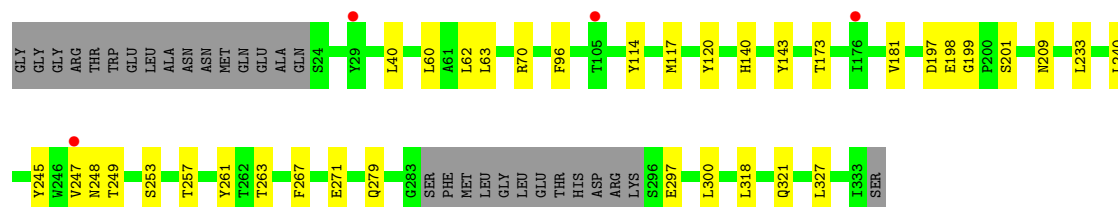
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

Chain L: 86% 12% ..



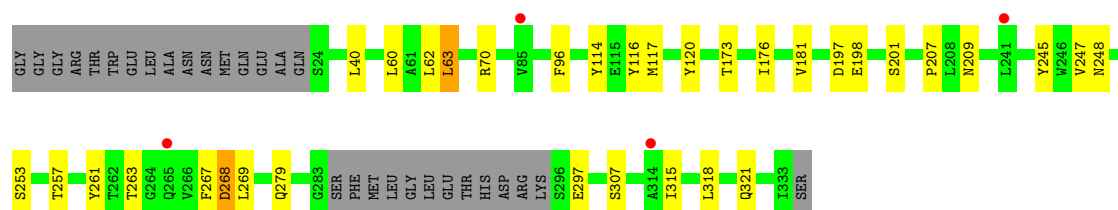
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain E: 80% 11% 9%



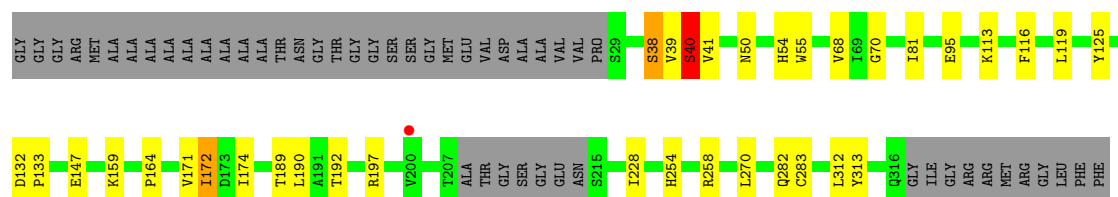
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain M: 81% 10% 9%

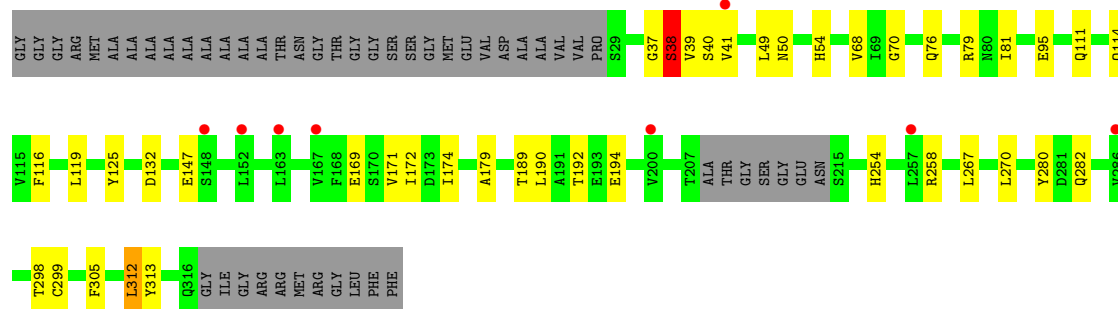
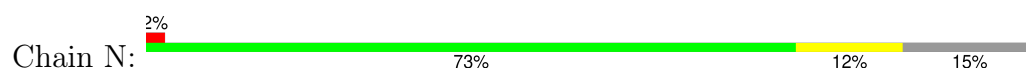


• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

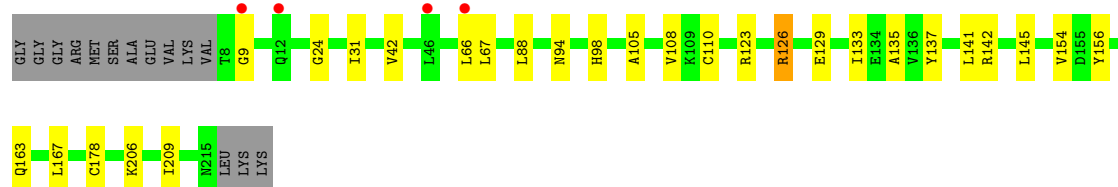
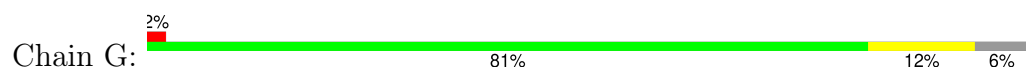
Chain F: 74% 10% 15%



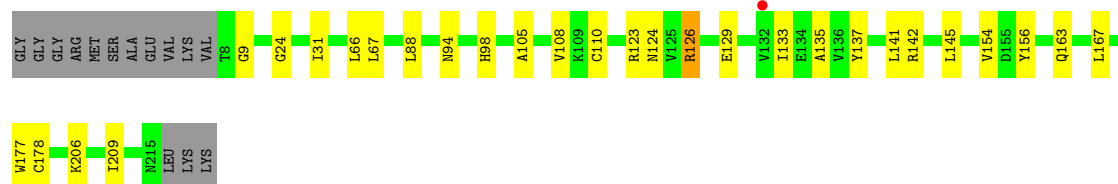
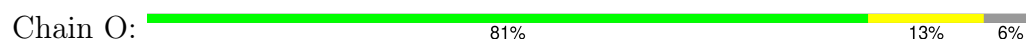
• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6



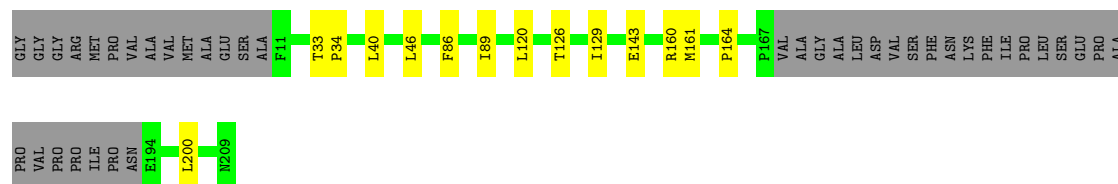
• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



PRO	PRO	ILE	PRO	ASN	E194	L200	N209
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	147.68Å 147.68Å 317.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.98 – 4.08 52.98 – 4.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.98-4.08) 99.9 (52.98-4.08)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.236 , 0.253 0.264 , 0.280	Depositor DCC
R_{free} test set	3085 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	175.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 194.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l 0.115 for h,-h-k,-l 0.067 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	41422	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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	0.67	1/3404 (0.0%)	1.12	2/4588 (0.0%)
1	I	0.64	0/3404	1.13	0/4588
2	B	0.71	0/3361	1.13	2/4522 (0.0%)
2	J	0.71	0/3361	1.14	3/4522 (0.1%)
3	C	0.94	19/3250 (0.6%)	1.35	46/4390 (1.0%)
3	K	0.94	19/3250 (0.6%)	1.35	45/4390 (1.0%)
4	D	0.70	0/3303	1.12	1/4460 (0.0%)
4	L	0.69	1/3303 (0.0%)	1.19	5/4460 (0.1%)
5	E	0.67	0/2417	1.07	0/3266
5	M	0.69	0/2417	1.06	0/3266
6	F	1.07	1/2282 (0.0%)	1.15	7/3092 (0.2%)
6	N	0.65	0/2281	1.12	5/3089 (0.2%)
7	G	0.65	0/1652	1.13	0/2239
7	O	0.65	0/1652	1.13	0/2239
8	H	0.67	0/1416	1.11	1/1924 (0.1%)
8	P	0.67	0/1416	1.10	1/1924 (0.1%)
All	All	0.75	41/42169 (0.1%)	1.16	118/56959 (0.2%)

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
3	C	0	6
3	K	0	6
All	All	0	12

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	40	SER	C-N	41.13	1.94	1.33
3	K	301	SER	C-O	-9.23	1.12	1.24
3	C	301	SER	C-O	-9.21	1.12	1.24
3	C	297	GLN	C-O	-8.73	1.13	1.24
3	K	297	GLN	C-O	-8.70	1.13	1.24
3	C	300	SER	C-O	-8.13	1.14	1.24
3	C	298	CYS	C-O	-7.84	1.14	1.24
3	K	300	SER	C-O	-7.79	1.14	1.24
3	C	305	LYS	C-O	-7.75	1.15	1.24
3	K	298	CYS	C-O	-7.75	1.14	1.24
3	K	305	LYS	C-O	-7.74	1.15	1.24
3	K	294	LEU	C-O	-7.64	1.14	1.24
3	C	294	LEU	C-O	-7.56	1.14	1.24
3	K	302	LEU	C-O	-7.27	1.15	1.24
3	C	302	LEU	C-O	-7.20	1.15	1.24
3	C	304	LYS	C-O	-6.96	1.16	1.24
3	K	304	LYS	C-O	-6.96	1.16	1.24
3	C	306	ASN	C-O	-6.92	1.15	1.24
3	K	306	ASN	C-O	-6.86	1.15	1.24
3	K	303	TYR	C-O	-6.74	1.16	1.24
3	C	295	VAL	C-O	-6.59	1.15	1.24
3	K	295	VAL	C-O	-6.57	1.15	1.24
3	C	303	TYR	C-O	-6.56	1.16	1.24
3	C	296	LYS	C-O	-6.56	1.16	1.24
3	K	296	LYS	C-O	-6.52	1.16	1.24
4	L	181	GLU	C-N	6.39	1.42	1.33
1	A	137	LYS	C-N	5.91	1.42	1.33
3	C	295	VAL	N-CA	-5.78	1.38	1.46
3	C	308	GLN	C-O	-5.76	1.17	1.24
3	K	295	VAL	N-CA	-5.74	1.38	1.46
3	K	307	ILE	C-O	-5.69	1.17	1.24
3	K	310	LEU	C-O	-5.68	1.16	1.24
3	K	294	LEU	N-CA	-5.66	1.38	1.46
3	C	307	ILE	C-O	-5.63	1.17	1.24
3	K	308	GLN	C-O	-5.63	1.17	1.24
3	C	294	LEU	N-CA	-5.61	1.39	1.46
3	C	310	LEU	C-O	-5.57	1.16	1.24
3	C	301	SER	N-CA	-5.51	1.39	1.46
3	K	301	SER	N-CA	-5.47	1.39	1.46
3	K	298	CYS	CA-C	-5.42	1.45	1.52
3	C	298	CYS	CA-C	-5.31	1.46	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	304	LYS	CA-C-O	-10.93	108.97	120.55
3	C	304	LYS	CA-C-O	-10.92	108.98	120.55
3	C	300	SER	CA-C-O	-10.46	109.47	120.55
3	K	300	SER	CA-C-O	-10.32	109.48	120.42
6	F	40	SER	O-C-N	-10.00	111.15	123.05
6	F	38	SER	CA-C-N	9.93	133.81	120.50
6	F	38	SER	C-N-CA	9.93	133.81	120.50
3	K	301	SER	CA-C-O	-9.54	109.00	119.97
3	C	301	SER	CA-C-O	-9.50	109.05	119.97
3	C	304	LYS	CA-C-N	9.22	132.63	120.28
3	C	304	LYS	C-N-CA	9.22	132.63	120.28
3	K	304	LYS	CA-C-N	9.21	132.63	120.28
3	K	304	LYS	C-N-CA	9.21	132.63	120.28
3	C	305	LYS	CA-C-O	-9.12	110.88	120.55
3	K	305	LYS	CA-C-O	-9.02	110.99	120.55
3	C	297	GLN	CA-C-O	-8.88	109.76	119.97
3	K	297	GLN	CA-C-O	-8.85	109.79	119.97
3	K	308	GLN	CA-C-O	-8.81	111.21	120.55
3	C	295	VAL	CA-C-O	-8.80	110.74	120.25
3	K	295	VAL	CA-C-O	-8.76	110.78	120.25
3	C	298	CYS	CA-C-O	-8.70	111.20	120.42
3	C	308	GLN	CA-C-O	-8.65	111.38	120.55
3	K	298	CYS	CA-C-O	-8.56	111.35	120.42
6	N	132	ASP	CA-CB-CG	8.27	120.87	112.60
2	J	90	ASN	CA-CB-CG	-8.26	104.34	112.60
3	C	302	LEU	CA-C-O	-8.20	111.73	120.42
3	K	302	LEU	CA-C-O	-8.10	111.84	120.42
3	K	296	LYS	CA-C-O	-7.88	111.49	120.24
3	C	296	LYS	CA-C-O	-7.87	111.51	120.24
3	C	303	TYR	CA-C-O	-7.79	112.64	120.82
3	K	303	TYR	CA-C-O	-7.62	112.82	120.82
3	C	299	LEU	CA-C-O	-7.50	112.98	120.70
3	K	299	LEU	CA-C-O	-7.48	112.99	120.70
6	F	40	SER	CA-C-N	-7.47	113.52	122.93
6	F	40	SER	C-N-CA	-7.47	113.52	122.93
3	C	307	ILE	CA-C-O	-7.18	113.03	120.71
3	K	307	ILE	CA-C-O	-7.17	113.04	120.71
3	C	294	LEU	CA-C-O	-6.97	111.56	119.79
6	N	37	GLY	CA-C-N	6.93	134.78	121.54
6	N	37	GLY	C-N-CA	6.93	134.78	121.54
3	K	294	LEU	CA-C-O	-6.92	111.63	119.79
3	C	310	LEU	CA-C-O	-6.89	111.67	119.79
3	K	296	LYS	CA-C-N	6.84	130.71	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	296	LYS	C-N-CA	6.84	130.71	120.31
3	C	296	LYS	CA-C-N	6.83	130.69	120.31
3	C	296	LYS	C-N-CA	6.83	130.69	120.31
3	K	310	LEU	CA-C-O	-6.76	111.81	119.79
3	K	298	CYS	CA-C-N	6.71	129.57	120.44
3	K	298	CYS	C-N-CA	6.71	129.57	120.44
3	C	306	ASN	CA-C-O	-6.70	112.26	119.97
3	C	298	CYS	CA-C-N	6.66	129.50	120.44
3	C	298	CYS	C-N-CA	6.66	129.50	120.44
3	K	297	GLN	CA-C-N	6.60	129.66	120.29
3	K	297	GLN	C-N-CA	6.60	129.66	120.29
3	K	306	ASN	CA-C-O	-6.60	112.38	119.97
3	C	297	GLN	CA-C-N	6.57	129.62	120.29
3	C	297	GLN	C-N-CA	6.57	129.62	120.29
3	C	299	LEU	CA-C-N	6.56	129.08	120.28
3	C	299	LEU	C-N-CA	6.56	129.08	120.28
3	C	303	TYR	CA-C-N	6.50	128.99	120.28
3	C	303	TYR	C-N-CA	6.50	128.99	120.28
3	K	301	SER	CA-C-N	6.46	129.47	120.29
3	K	301	SER	C-N-CA	6.46	129.47	120.29
3	K	303	TYR	CA-C-N	6.42	128.88	120.28
3	K	303	TYR	C-N-CA	6.42	128.88	120.28
4	L	181	GLU	CA-C-O	-6.42	114.08	120.82
3	C	301	SER	CA-C-N	6.39	129.37	120.29
3	C	301	SER	C-N-CA	6.39	129.37	120.29
3	C	294	LEU	N-CA-C	-6.28	104.31	112.23
3	K	294	LEU	N-CA-C	-6.25	104.36	112.23
3	C	300	SER	CA-C-N	6.13	129.62	120.31
3	C	300	SER	C-N-CA	6.13	129.62	120.31
4	L	181	GLU	N-CA-C	6.12	117.61	111.07
3	K	299	LEU	CA-C-N	6.11	128.97	120.29
3	K	299	LEU	C-N-CA	6.11	128.97	120.29
3	C	294	LEU	CA-C-N	6.04	130.68	120.29
3	C	294	LEU	C-N-CA	6.04	130.68	120.29
3	K	300	SER	CA-C-N	6.03	129.47	120.31
3	K	300	SER	C-N-CA	6.03	129.47	120.31
3	K	294	LEU	CA-C-N	5.96	130.54	120.29
3	K	294	LEU	C-N-CA	5.96	130.54	120.29
3	K	296	LYS	N-CA-C	-5.92	104.41	111.69
6	N	38	SER	CA-C-N	5.90	132.60	121.97
6	N	38	SER	C-N-CA	5.90	132.60	121.97
2	B	211	ASN	CA-C-N	5.83	128.41	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	ASN	C-N-CA	5.83	128.41	120.54
3	C	296	LYS	N-CA-C	-5.81	104.54	111.69
3	C	305	LYS	CA-C-N	5.79	129.12	120.31
3	C	305	LYS	C-N-CA	5.79	129.12	120.31
2	J	211	ASN	CA-C-N	5.77	128.33	120.54
2	J	211	ASN	C-N-CA	5.77	128.33	120.54
4	L	317	ASN	N-CA-C	-5.69	105.44	112.90
3	K	305	LYS	CA-C-N	5.67	128.94	120.31
3	K	305	LYS	C-N-CA	5.67	128.94	120.31
3	K	297	GLN	N-CA-C	-5.64	105.28	111.82
3	C	297	GLN	N-CA-C	-5.57	105.36	111.82
8	P	34	PRO	N-CA-C	5.56	117.48	110.70
3	K	370	PRO	N-CA-C	-5.55	106.30	113.57
3	C	370	PRO	N-CA-C	-5.52	106.34	113.57
4	D	317	ASN	N-CA-C	-5.52	105.67	112.90
3	C	307	ILE	CA-C-N	5.41	127.53	120.28
3	C	307	ILE	C-N-CA	5.41	127.53	120.28
8	H	34	PRO	N-CA-C	5.38	117.27	110.70
3	C	302	LEU	N-CA-C	-5.36	105.52	111.36
3	C	302	LEU	CA-C-N	5.35	127.40	120.44
3	C	302	LEU	C-N-CA	5.35	127.40	120.44
6	F	38	SER	N-CA-C	5.34	115.90	108.00
3	K	302	LEU	CA-C-N	5.32	127.36	120.44
3	K	302	LEU	C-N-CA	5.32	127.36	120.44
3	K	302	LEU	N-CA-C	-5.30	105.58	111.36
1	A	137	LYS	CA-C-N	5.28	127.79	120.29
1	A	137	LYS	C-N-CA	5.28	127.79	120.29
3	K	307	ILE	CA-C-N	5.23	127.28	120.28
3	K	307	ILE	C-N-CA	5.23	127.28	120.28
4	L	68	ASP	CA-C-N	5.16	127.20	120.28
4	L	68	ASP	C-N-CA	5.16	127.20	120.28
6	F	172	ILE	CB-CA-C	5.15	118.35	111.19
3	C	89	ASN	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	295	VAL	Mainchain
3	C	296	LYS	Mainchain
3	C	300	SER	Mainchain
3	C	304	LYS	Mainchain

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Mol	Chain	Res	Type	Group
3	C	308	GLN	Mainchain
3	C	310	LEU	Mainchain
3	K	295	VAL	Mainchain
3	K	296	LYS	Mainchain
3	K	300	SER	Mainchain
3	K	304	LYS	Mainchain
3	K	308	GLN	Mainchain
3	K	310	LEU	Mainchain

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	23	0
1	I	3348	0	3385	27	0
2	B	3304	0	3351	27	0
2	J	3304	0	3351	37	0
3	C	3191	0	3208	29	0
3	K	3191	0	3208	25	0
4	D	3251	0	3253	31	0
4	L	3251	0	3253	41	0
5	E	2366	0	2340	30	0
5	M	2366	0	2340	32	0
6	F	2236	0	2226	30	0
6	N	2236	0	2226	34	0
7	G	1631	0	1654	19	0
7	O	1631	0	1654	25	0
8	H	1383	0	1366	8	0
8	P	1383	0	1366	6	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
All	All	41422	0	41566	317	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 4.

All (317) 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:F:40:SER:C	6:F:41:VAL:N	1.94	1.25
1:A:200:GLY:O	1:A:204:LEU:HD13	1.63	0.98
1:I:200:GLY:O	1:I:204:LEU:HD13	1.64	0.98
5:M:70:ARG:NH2	5:M:257:THR:HG22	1.78	0.97
3:K:41:HIS:O	3:K:44:THR:HG22	1.63	0.96
3:C:41:HIS:O	3:C:44:THR:HG22	1.63	0.95
5:E:70:ARG:NH2	5:E:257:THR:HG22	1.83	0.94
5:M:173:THR:CG2	5:M:261:TYR:HB2	1.98	0.93
4:D:83:GLU:HG3	2:J:90:ASN:HB2	1.53	0.91
1:I:354:LEU:CD2	2:J:212:LYS:HB3	2.01	0.89
2:J:420:ARG:HD3	5:M:263:THR:HG22	1.58	0.86
5:E:173:THR:CG2	5:E:261:TYR:HB2	2.05	0.85
4:L:161:PRO:HB3	4:L:197:TYR:HB3	1.59	0.84
4:L:165:GLU:HA	4:L:194:VAL:HG11	1.61	0.83
4:D:254:ARG:HG2	6:F:174:ILE:HD11	1.61	0.81
5:M:173:THR:HG21	5:M:261:TYR:HB2	1.61	0.81
5:M:96:PHE:CD1	5:M:120:TYR:CE2	2.68	0.80
5:E:70:ARG:HH21	5:E:257:THR:HG22	1.44	0.80
5:E:96:PHE:CD1	5:E:120:TYR:CE2	2.70	0.79
6:N:40:SER:HA	6:N:41:VAL:N	1.99	0.78
1:I:275:ASP:HB3	2:J:223:HIS:CE1	2.19	0.76
2:B:420:ARG:HD3	5:E:263:THR:HG22	1.68	0.76
1:I:354:LEU:HD21	2:J:212:LYS:HB3	1.67	0.75
5:M:70:ARG:HH21	5:M:257:THR:HG22	1.49	0.74
1:A:275:ASP:HB3	2:B:223:HIS:CE1	2.22	0.74
4:L:178:SER:HB3	4:L:184:GLN:HE21	1.51	0.74
7:G:126:ARG:NH2	7:G:129:GLU:HB3	2.02	0.73
7:O:126:ARG:NH2	7:O:129:GLU:HB3	2.03	0.72
8:H:129:ILE:HD11	7:O:123:ARG:CZ	2.20	0.71
1:I:200:GLY:O	1:I:204:LEU:CD1	2.38	0.71
1:A:200:GLY:O	1:A:204:LEU:CD1	2.38	0.71
5:E:173:THR:HG21	5:E:261:TYR:HB2	1.74	0.69
4:L:180:ASN:O	4:L:184:GLN:HG3	1.92	0.69
1:A:354:LEU:HD21	2:B:212:LYS:HB3	1.74	0.69
3:C:353:GLN:HB3	7:O:123:ARG:HH12	1.58	0.69
1:A:185:LEU:HD22	1:A:204:LEU:HD21	1.74	0.68
1:I:185:LEU:HD22	1:I:204:LEU:HD21	1.74	0.68
4:D:315:LEU:HD13	7:G:133:ILE:HG12	1.76	0.68
3:C:353:GLN:HB3	7:O:123:ARG:HH22	1.59	0.67
4:L:268:TYR:OH	6:N:38:SER:HA	1.95	0.67
6:N:40:SER:CA	6:N:41:VAL:N	2.58	0.66
2:B:153:THR:HG23	2:B:200:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:116:PHE:HB3	6:F:119:LEU:HD13	1.79	0.65
4:D:268:TYR:OH	6:F:38:SER:HA	1.97	0.64
1:I:354:LEU:HD23	2:J:212:LYS:HB3	1.79	0.64
4:D:321:PHE:HZ	4:D:352:ILE:HG23	1.63	0.64
4:L:254:ARG:HG2	6:N:174:ILE:HD11	1.80	0.63
6:N:116:PHE:HB3	6:N:119:LEU:HD13	1.79	0.63
7:G:126:ARG:NH2	7:G:129:GLU:CB	2.61	0.63
2:J:153:THR:HG23	2:J:200:LEU:HD11	1.79	0.62
2:B:383:ALA:HB2	4:L:296:GLY:HA3	1.81	0.62
7:O:126:ARG:NH2	7:O:129:GLU:CB	2.62	0.62
8:H:126:THR:O	8:H:164:PRO:HD2	2.00	0.62
2:B:420:ARG:CD	5:E:263:THR:HG22	2.30	0.62
8:P:126:THR:O	8:P:164:PRO:HD2	2.00	0.62
3:C:117:PRO:HD2	3:C:152:ALA:HB2	1.81	0.61
3:K:117:PRO:HD2	3:K:152:ALA:HB2	1.81	0.61
1:A:115:LEU:HB3	1:A:138:LEU:HG	1.82	0.61
3:K:44:THR:HG23	3:K:45:VAL:HG23	1.83	0.61
1:A:275:ASP:HB3	2:B:223:HIS:HE1	1.65	0.60
6:F:39:VAL:HG11	6:F:81:ILE:HD11	1.82	0.60
3:C:397:ILE:CG2	6:F:312:LEU:HD23	2.30	0.60
6:N:40:SER:C	6:N:41:VAL:N	2.59	0.60
6:F:39:VAL:HG11	6:F:81:ILE:CD1	2.31	0.60
5:M:173:THR:HG22	5:M:261:TYR:HB2	1.82	0.59
4:D:83:GLU:HG3	2:J:90:ASN:CB	2.29	0.59
3:C:44:THR:HG23	3:C:45:VAL:HG23	1.84	0.59
4:L:269:LEU:HD13	4:L:271:ARG:HH21	1.67	0.59
4:D:251:LYS:O	6:F:171:VAL:HG13	2.03	0.59
5:M:63:LEU:HD22	6:N:49:LEU:HD12	1.83	0.59
2:J:270:SER:HB2	2:J:271:PRO:HA	1.85	0.58
2:J:420:ARG:CD	5:M:263:THR:HG22	2.33	0.58
2:B:270:SER:HB2	2:B:271:PRO:HA	1.84	0.57
4:L:244:ARG:HG2	6:N:76:GLN:HE22	1.69	0.57
4:L:251:LYS:O	6:N:171:VAL:HG13	2.05	0.56
4:L:245:MET:HG2	6:N:147:GLU:HG2	1.88	0.56
3:C:343:GLU:HG3	8:H:120:LEU:HD13	1.88	0.56
4:L:70:CYS:HA	4:L:73:LEU:HD12	1.88	0.56
4:D:245:MET:HG2	6:F:147:GLU:HG2	1.86	0.56
1:I:115:LEU:HB3	1:I:138:LEU:HG	1.87	0.56
1:I:275:ASP:HB3	2:J:223:HIS:HE1	1.67	0.56
3:K:354:LYS:HB2	8:P:161:MET:HE2	1.88	0.56
4:L:271:ARG:HD2	7:O:137:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:308:ASN:HB3	4:L:328:LEU:HD22	1.87	0.56
1:I:200:GLY:C	1:I:204:LEU:HD13	2.31	0.55
4:L:165:GLU:CA	4:L:194:VAL:HG11	2.35	0.55
4:L:168:ILE:HG12	4:L:191:TYR:HA	1.89	0.55
3:C:275:LEU:HD23	3:C:299:LEU:HD12	1.87	0.55
3:K:275:LEU:HD23	3:K:299:LEU:HD12	1.87	0.55
1:A:200:GLY:C	1:A:204:LEU:HD13	2.31	0.55
5:M:96:PHE:CE1	5:M:120:TYR:CE2	2.95	0.55
4:D:295:ASP:HB3	2:J:334:HIS:CE1	2.42	0.55
2:J:215:LYS:HE3	2:J:244:MET:SD	2.48	0.55
4:L:315:LEU:HD13	7:O:133:ILE:HG12	1.87	0.54
3:K:71:VAL:HB	3:K:72:PRO:CD	2.37	0.54
3:C:71:VAL:HB	3:C:72:PRO:CD	2.37	0.54
3:C:354:LYS:HB2	8:H:161:MET:HE2	1.88	0.54
6:F:39:VAL:HG21	6:F:81:ILE:HD12	1.89	0.54
4:D:379:PHE:CZ	6:F:189:THR:HB	2.43	0.54
1:A:486:ALA:HB1	3:C:386:LEU:HD21	1.88	0.54
4:L:180:ASN:O	4:L:184:GLN:CG	2.56	0.54
4:D:308:ASN:HB3	4:D:328:LEU:HD22	1.90	0.54
5:M:70:ARG:HH21	5:M:257:THR:CG2	2.17	0.53
3:K:343:GLU:HG3	8:P:120:LEU:HD13	1.90	0.53
3:K:397:ILE:CG2	6:N:312:LEU:HD23	2.38	0.53
2:B:215:LYS:HE3	2:B:244:MET:SD	2.49	0.53
5:E:96:PHE:CE1	5:E:120:TYR:CE2	2.97	0.53
4:L:178:SER:CB	4:L:184:GLN:HE21	2.19	0.53
1:A:384:MET:HE3	1:A:388:LEU:HD11	1.90	0.53
2:B:194:LEU:HA	2:B:197:ILE:HD12	1.91	0.53
1:I:384:MET:HE3	1:I:388:LEU:HD11	1.90	0.52
7:G:123:ARG:HD3	1:I:423:HIS:CG	2.44	0.52
3:C:397:ILE:HG23	6:F:312:LEU:HD23	1.90	0.52
3:K:393:MET:HE3	6:N:305:PHE:CZ	2.45	0.52
7:G:123:ARG:HH11	1:I:423:HIS:HB2	1.74	0.52
4:D:230:LEU:HD11	4:D:264:LEU:HB2	1.92	0.52
1:A:486:ALA:CB	3:C:386:LEU:HD21	2.40	0.51
2:B:47:PRO:HB3	2:B:78:ILE:HG21	1.92	0.51
2:B:59:GLU:C	2:B:61:GLU:H	2.19	0.51
1:I:107:CYS:HB2	1:I:390:LEU:HD22	1.92	0.51
5:M:315:ILE:HG23	8:P:200:LEU:HD22	1.93	0.51
5:E:173:THR:HG22	5:E:261:TYR:HB2	1.89	0.51
4:L:278:LEU:CD2	4:L:304:VAL:HG21	2.41	0.51
4:L:378:CYS:HB3	5:M:247:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD13	2:B:343:ILE:HG23	1.91	0.51
2:J:47:PRO:HB3	2:J:78:ILE:HG21	1.92	0.51
4:L:187:TYR:CD1	4:L:188:LYS:N	2.78	0.51
3:C:353:GLN:HB3	7:O:123:ARG:NH1	2.26	0.51
3:C:367:TYR:CE2	3:C:372:MET:HE3	2.45	0.51
1:A:107:CYS:HB2	1:A:390:LEU:HD22	1.93	0.51
4:D:378:CYS:HB3	5:E:247:VAL:HG22	1.92	0.51
4:L:379:PHE:CZ	6:N:189:THR:HB	2.46	0.51
2:J:282:LEU:HD13	2:J:343:ILE:HG23	1.92	0.51
3:K:367:TYR:CE2	3:K:372:MET:HE3	2.46	0.50
1:A:326:ALA:HB2	1:A:355:PHE:HB3	1.93	0.50
4:D:295:ASP:HA	2:J:334:HIS:CE1	2.46	0.50
5:E:249:THR:HG23	6:F:197:ARG:NH1	2.25	0.50
1:A:489:MET:HB3	2:B:439:VAL:HG13	1.94	0.50
2:J:194:LEU:HA	2:J:197:ILE:HD12	1.93	0.50
6:N:39:VAL:HG11	6:N:81:ILE:CD1	2.40	0.50
2:B:434:LEU:HD21	5:E:300:LEU:HD11	1.93	0.50
3:C:353:GLN:HB3	7:O:123:ARG:NH2	2.27	0.50
3:K:397:ILE:HG23	6:N:312:LEU:HD23	1.93	0.50
3:C:354:LYS:O	7:O:124:ASN:HB3	2.10	0.50
4:L:222:ARG:NH2	6:N:179:ALA:HB3	2.26	0.50
5:M:60:LEU:HD11	6:N:50:ASN:OD1	2.11	0.50
5:M:120:TYR:N	6:N:111:GLN:HE22	2.10	0.50
4:L:161:PRO:CB	4:L:197:TYR:HB3	2.38	0.50
1:I:326:ALA:HB2	1:I:355:PHE:HB3	1.93	0.49
2:B:420:ARG:HD3	5:E:263:THR:CG2	2.41	0.49
4:D:316:TYR:CD1	7:G:145:LEU:HB2	2.47	0.49
5:M:173:THR:HG22	5:M:261:TYR:CB	2.41	0.49
1:I:504:SER:HA	3:K:215:ALA:HB2	1.95	0.49
5:E:60:LEU:HD11	6:F:50:ASN:OD1	2.13	0.49
1:I:497:ARG:HG3	6:N:313:TYR:CE1	2.48	0.49
2:J:59:GLU:C	2:J:61:GLU:H	2.21	0.49
5:M:318:LEU:HD23	8:P:200:LEU:HD21	1.94	0.49
7:O:105:ALA:HB1	7:O:154:VAL:HG11	1.94	0.49
3:C:117:PRO:HB2	3:C:148:LEU:HD22	1.95	0.49
7:G:105:ALA:HB1	7:G:154:VAL:HG11	1.93	0.49
5:E:245:TYR:HD1	6:F:190:LEU:HD13	1.77	0.49
2:B:64:LYS:HB3	2:B:65:GLY:HA2	1.95	0.48
3:K:117:PRO:HB2	3:K:148:LEU:HD22	1.95	0.48
4:L:230:LEU:HD11	4:L:264:LEU:HB2	1.95	0.48
4:L:278:LEU:HD21	4:L:304:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:SER:C	6:F:41:VAL:CA	2.84	0.48
2:J:64:LYS:HB3	2:J:65:GLY:HA2	1.96	0.48
3:K:368:ASN:O	6:N:280:TYR:HB3	2.13	0.48
8:H:86:PHE:HA	8:H:89:ILE:HD12	1.95	0.48
7:O:66:LEU:HD21	7:O:88:LEU:HD21	1.96	0.48
5:M:114:TYR:HA	5:M:117:MET:HE3	1.95	0.47
5:M:207:PRO:HA	5:M:268:ASP:OD2	2.13	0.47
5:E:114:TYR:HA	5:E:117:MET:HE3	1.94	0.47
2:B:172:LEU:HD22	2:B:201:GLU:HG3	1.96	0.47
4:L:267:MET:HA	4:L:307:HIS:CE1	2.48	0.47
4:D:244:ARG:HB3	6:F:147:GLU:HB2	1.97	0.47
6:N:267:LEU:HD11	7:O:177:TRP:CE3	2.49	0.47
4:D:271:ARG:HD2	7:G:137:TYR:CD2	2.50	0.47
5:E:327:LEU:HD11	6:F:228:ILE:HG12	1.95	0.47
2:J:172:LEU:HD22	2:J:201:GLU:HG3	1.96	0.47
2:J:420:ARG:HD3	5:M:263:THR:CG2	2.39	0.47
2:B:408:LEU:HD22	4:D:355:ILE:HG12	1.96	0.47
2:B:403:ASP:HB3	2:B:408:LEU:HG	1.96	0.47
3:C:353:GLN:CB	7:O:123:ARG:HH12	2.27	0.47
4:D:295:ASP:HA	2:J:334:HIS:HE1	1.80	0.47
1:I:437:GLU:HG3	1:I:453:VAL:HG11	1.96	0.47
5:M:245:TYR:HD1	6:N:190:LEU:HD13	1.79	0.47
2:B:80:PHE:HB3	2:B:88:MET:HE2	1.97	0.46
4:D:6:ARG:HG2	4:D:47:ALA:HB1	1.97	0.46
4:D:295:ASP:CB	2:J:334:HIS:CE1	2.98	0.46
1:I:411:ILE:HA	1:I:449:ILE:HD11	1.97	0.46
8:H:129:ILE:CG1	7:O:123:ARG:NH2	2.79	0.46
8:P:86:PHE:HA	8:P:89:ILE:HD12	1.96	0.46
2:J:281:VAL:HG12	2:J:285:MET:HE2	1.96	0.46
2:B:281:VAL:HG12	2:B:285:MET:HE2	1.97	0.46
4:D:161:PRO:HB2	4:D:198:ARG:HG2	1.97	0.46
7:G:66:LEU:HD21	7:G:88:LEU:HD21	1.96	0.46
2:J:80:PHE:HB3	2:J:88:MET:HE2	1.97	0.46
1:A:437:GLU:HG3	1:A:453:VAL:HG11	1.96	0.46
1:I:283:THR:HG22	1:I:310:SER:H	1.80	0.46
2:J:403:ASP:HB3	2:J:408:LEU:HG	1.97	0.46
1:A:185:LEU:HD22	1:A:204:LEU:CD2	2.44	0.46
1:A:411:ILE:HA	1:A:449:ILE:HD11	1.98	0.46
5:E:70:ARG:HH21	5:E:257:THR:CG2	2.23	0.46
2:B:175:LEU:HB3	2:B:197:ILE:HG12	1.98	0.45
4:D:271:ARG:HD2	7:G:137:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:ARG:HH22	7:G:129:GLU:HB3	1.76	0.45
3:C:39:LEU:HD22	3:C:58:VAL:HG22	1.98	0.45
5:M:253:SER:HA	5:M:321:GLN:HE22	1.81	0.45
4:D:86:HIS:NE2	2:J:86:PRO:HG2	2.32	0.45
3:K:370:PRO:O	3:K:373:LEU:HB3	2.17	0.45
1:A:283:THR:HG22	1:A:310:SER:H	1.81	0.45
4:D:295:ASP:CB	2:J:334:HIS:HE1	2.30	0.45
1:I:185:LEU:HD22	1:I:204:LEU:CD2	2.45	0.45
3:K:39:LEU:HD22	3:K:58:VAL:HG22	1.98	0.45
3:C:370:PRO:O	3:C:373:LEU:HB3	2.16	0.45
2:J:175:LEU:HB3	2:J:197:ILE:HG12	1.99	0.45
7:O:126:ARG:HH22	7:O:129:GLU:HB3	1.77	0.45
1:A:134:ILE:HG22	1:A:138:LEU:HD12	1.98	0.45
1:A:497:ARG:HG3	6:F:313:TYR:CE1	2.52	0.44
5:E:253:SER:HA	5:E:321:GLN:HE22	1.82	0.44
3:K:68:MET:HB3	3:K:71:VAL:H	1.81	0.44
4:D:165:GLU:HA	4:D:168:ILE:HG22	1.99	0.44
5:E:233:LEU:HD22	6:F:55:TRP:CE3	2.52	0.44
1:I:258:VAL:HG11	1:I:289:ALA:HB2	1.99	0.44
4:L:187:TYR:HE1	4:L:188:LYS:HD3	1.82	0.44
6:F:38:SER:OG	6:F:39:VAL:HG13	2.17	0.44
5:M:116:TYR:HE2	6:N:114:GLN:HG3	1.83	0.44
3:K:94:ARG:HH22	3:K:137:GLN:HE22	1.64	0.44
3:C:68:MET:HB3	3:C:71:VAL:H	1.81	0.44
3:C:94:ARG:HH22	3:C:137:GLN:HE22	1.64	0.44
4:D:378:CYS:HB2	5:E:247:VAL:HG13	1.98	0.44
5:M:173:THR:HG22	5:M:261:TYR:CG	2.52	0.44
5:M:269:LEU:HD21	5:M:307:SER:HB3	2.00	0.44
4:L:316:TYR:CD1	7:O:145:LEU:HB2	2.53	0.44
3:K:155:PHE:HB3	3:K:191:ILE:HG23	2.00	0.44
3:C:155:PHE:HB3	3:C:191:ILE:HG23	2.00	0.44
4:D:269:LEU:HD13	4:D:271:ARG:HH21	1.81	0.43
5:E:248:ASN:OD1	6:F:192:THR:HG22	2.18	0.43
6:F:54:HIS:CE1	6:F:68:VAL:HB	2.53	0.43
5:M:248:ASN:OD1	6:N:192:THR:HG22	2.18	0.43
6:N:54:HIS:CE1	6:N:68:VAL:HB	2.53	0.43
2:J:434:LEU:HD23	6:N:299:CYS:SG	2.58	0.43
2:J:57:VAL:HA	2:J:60:LEU:HD12	1.99	0.43
5:E:318:LEU:HD11	6:F:283:CYS:SG	2.58	0.43
5:M:62:LEU:HD11	5:M:181:VAL:HG11	2.01	0.43
2:B:57:VAL:HA	2:B:60:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG11	1:A:289:ALA:HB2	2.00	0.43
2:J:149:PHE:CZ	2:J:193:GLN:HB2	2.53	0.43
2:B:152:ASN:HB3	2:B:175:LEU:HD21	2.00	0.43
4:L:187:TYR:CD1	4:L:187:TYR:C	2.96	0.43
5:E:318:LEU:HD23	8:H:200:LEU:HD21	2.01	0.43
7:G:142:ARG:HB2	7:G:156:TYR:HB3	2.00	0.43
4:L:244:ARG:HB3	6:N:147:GLU:HB2	2.01	0.43
7:O:126:ARG:NH2	7:O:129:GLU:HB2	2.34	0.43
7:O:142:ARG:HB2	7:O:156:TYR:HB3	2.00	0.43
2:J:152:ASN:HB3	2:J:175:LEU:HD21	2.01	0.43
4:D:356:ASP:HB3	4:D:358:ILE:HD12	2.00	0.42
5:E:173:THR:HG22	5:E:261:TYR:CG	2.53	0.42
7:O:31:ILE:HG23	7:O:67:LEU:HD13	2.01	0.42
5:E:173:THR:HG22	5:E:261:TYR:CB	2.49	0.42
3:K:386:LEU:HD23	6:N:298:THR:HG21	2.00	0.42
7:O:206:LYS:HA	7:O:209:ILE:HD12	2.01	0.42
7:G:126:ARG:NH2	7:G:129:GLU:HB2	2.35	0.42
5:E:62:LEU:HD11	5:E:181:VAL:HG11	2.02	0.42
1:I:134:ILE:HG22	1:I:138:LEU:HD12	2.01	0.42
5:M:96:PHE:CE1	5:M:120:TYR:CD2	3.08	0.42
3:K:56:LEU:HD11	3:K:100:PHE:HA	2.02	0.42
5:M:176:ILE:HG23	6:N:194:GLU:HG2	2.01	0.42
7:G:123:ARG:HD3	1:I:423:HIS:CD2	2.55	0.42
1:I:333:ALA:O	1:I:337:PHE:HB2	2.20	0.42
2:J:408:LEU:HD22	4:L:355:ILE:HG12	2.01	0.42
1:A:333:ALA:O	1:A:337:PHE:HB2	2.20	0.42
6:F:70:GLY:HA3	6:F:125:TYR:CE2	2.54	0.42
3:C:370:PRO:O	3:C:373:LEU:N	2.53	0.42
7:G:206:LYS:HA	7:G:209:ILE:HD12	2.01	0.42
4:L:33:ALA:HA	4:L:36:LEU:HD12	2.01	0.42
2:B:369:ILE:HG23	2:B:409:LEU:HB3	2.02	0.41
3:C:56:LEU:HD11	3:C:100:PHE:HA	2.02	0.41
4:D:396:THR:O	4:D:400:MET:HB2	2.20	0.41
6:F:258:ARG:HD2	7:G:42:VAL:HG21	2.02	0.41
6:N:70:GLY:HA3	6:N:125:TYR:CE2	2.54	0.41
7:G:31:ILE:HG23	7:G:67:LEU:HD13	2.00	0.41
2:J:369:ILE:HG23	2:J:409:LEU:HB3	2.02	0.41
5:M:173:THR:CG2	5:M:261:TYR:CB	2.83	0.41
3:K:370:PRO:O	3:K:373:LEU:N	2.53	0.41
4:L:378:CYS:HB2	5:M:247:VAL:HG13	2.01	0.41
2:B:381:ASP:OD2	4:L:294:ALA:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:129:ILE:HG13	7:O:123:ARG:NH2	2.35	0.41
4:L:165:GLU:CD	4:L:198:ARG:HE	2.29	0.41
3:K:275:LEU:HD22	3:K:302:LEU:HD22	2.02	0.41
3:C:39:LEU:HB3	3:C:58:VAL:HG13	2.02	0.41
3:C:275:LEU:HD22	3:C:302:LEU:HD22	2.02	0.41
4:D:321:PHE:CZ	4:D:352:ILE:HG23	2.51	0.41
7:G:98:HIS:HD2	7:G:135:ALA:HB2	1.86	0.41
3:K:39:LEU:HB3	3:K:58:VAL:HG13	2.02	0.41
3:K:50:ASP:C	3:K:52:GLN:H	2.28	0.41
7:O:98:HIS:HD2	7:O:135:ALA:HB2	1.86	0.41
5:E:240:LEU:HD13	6:F:164:PRO:HD3	2.03	0.41
1:I:242:ILE:HG23	1:I:254:VAL:HG13	2.02	0.41
4:L:222:ARG:HH22	6:N:179:ALA:HB3	1.86	0.41
4:L:396:THR:O	4:L:400:MET:HB2	2.21	0.41
6:N:254:HIS:O	6:N:258:ARG:HB2	2.21	0.41
4:L:153:ARG:NH2	4:L:186:HIS:HB3	2.36	0.40
6:N:38:SER:HB2	6:N:169:GLU:OE1	2.21	0.40
1:A:242:ILE:HG23	1:A:254:VAL:HG13	2.02	0.40
3:C:50:ASP:C	3:C:52:GLN:H	2.28	0.40
6:F:132:ASP:HB2	6:F:133:PRO:CD	2.51	0.40
6:F:254:HIS:O	6:F:258:ARG:HB2	2.22	0.40
2:J:423:ALA:HB2	5:M:267:PHE:CE2	2.56	0.40
6:N:39:VAL:HA	6:N:79:ARG:O	2.21	0.40
5:E:140:HIS:CG	5:E:143:TYR:CE1	3.10	0.40
5:E:318:LEU:HD11	6:F:283:CYS:HA	2.03	0.40
7:O:94:ASN:C	7:O:98:HIS:HD1	2.30	0.40
7:G:94:ASN:C	7:G:98:HIS:HD1	2.30	0.40
1:I:275:ASP:HB3	2:J:223:HIS:ND1	2.35	0.40
4:L:377:LEU:HD21	7:O:177:TRP:CH2	2.56	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%)	395 (95%)	16 (4%)	4 (1%)	12	46
1	I	415/480 (86%)	395 (95%)	17 (4%)	3 (1%)	18	55
2	B	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	4	29
2	J	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	4	29
3	C	399/427 (93%)	360 (90%)	26 (6%)	13 (3%)	3	24
3	K	399/427 (93%)	360 (90%)	25 (6%)	14 (4%)	3	23
4	D	404/410 (98%)	399 (99%)	2 (0%)	3 (1%)	18	55
4	L	404/410 (98%)	400 (99%)	1 (0%)	3 (1%)	18	55
5	E	294/327 (90%)	283 (96%)	8 (3%)	3 (1%)	12	46
5	M	294/327 (90%)	283 (96%)	9 (3%)	2 (1%)	18	55
6	F	277/331 (84%)	267 (96%)	8 (3%)	2 (1%)	18	55
6	N	275/331 (83%)	264 (96%)	8 (3%)	3 (1%)	11	44
7	G	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	8	39
7	O	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	8	39
8	H	169/213 (79%)	162 (96%)	7 (4%)	0	100	100
8	P	169/213 (79%)	162 (96%)	7 (4%)	0	100	100
All	All	5124/5714 (90%)	4850 (95%)	198 (4%)	76 (2%)	8	39

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	51	VAL
3	C	68	MET
3	C	153	LYS
4	D	294	ALA
5	E	297	GLU
3	K	51	VAL
3	K	68	MET
3	K	153	LYS
4	L	294	ALA
5	M	297	GLU
6	N	38	SER
1	A	274	ARG
2	B	61	GLU
2	B	414	GLN
3	C	86	SER
3	C	172	GLU

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Mol	Chain	Res	Type
7	G	24	GLY
2	J	61	GLU
2	J	414	GLN
3	K	86	SER
3	K	172	GLU
7	O	24	GLY
2	B	43	LYS
2	B	84	ASN
3	C	33	GLU
3	C	71	VAL
3	C	114	ARG
4	D	362	GLU
4	D	366	ALA
6	F	95	GLU
1	I	274	ARG
2	J	43	LYS
2	J	84	ASN
3	K	33	GLU
3	K	71	VAL
3	K	114	ARG
4	L	362	GLU
4	L	366	ALA
6	N	95	GLU
1	A	126	PHE
1	A	270	GLN
3	C	168	ASP
6	F	270	LEU
7	G	9	GLY
1	I	126	PHE
1	I	270	GLN
3	K	117	PRO
3	K	168	ASP
6	N	270	LEU
7	O	9	GLY
2	B	229	PRO
2	B	291	ILE
2	B	296	SER
3	C	117	PRO
3	C	133	MET
3	C	329	SER
5	E	199	GLY
5	E	201	SER

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Mol	Chain	Res	Type
2	J	229	PRO
2	J	291	ILE
2	J	296	SER
3	K	133	MET
3	K	329	SER
5	M	201	SER
7	O	163	GLN
2	B	102	ALA
3	C	32	GLY
7	G	163	GLN
2	J	102	ALA
3	K	32	GLY
3	K	136	ASN
2	B	231	PRO
2	B	293	PRO
2	J	231	PRO
1	A	267	ILE
2	J	293	PRO

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%)	360 (99%)	5 (1%)	59	71
1	I	365/415 (88%)	360 (99%)	5 (1%)	59	71
2	B	367/406 (90%)	358 (98%)	9 (2%)	42	62
2	J	367/406 (90%)	357 (97%)	10 (3%)	39	60
3	C	358/378 (95%)	346 (97%)	12 (3%)	32	55
3	K	358/378 (95%)	347 (97%)	11 (3%)	35	57
4	D	347/348 (100%)	329 (95%)	18 (5%)	21	45
4	L	347/348 (100%)	337 (97%)	10 (3%)	37	58
5	E	255/278 (92%)	247 (97%)	8 (3%)	35	57
5	M	255/278 (92%)	248 (97%)	7 (3%)	39	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	251/277 (91%)	246 (98%)	5 (2%)	48	66
6	N	251/277 (91%)	248 (99%)	3 (1%)	63	73
7	G	174/184 (95%)	168 (97%)	6 (3%)	32	55
7	O	174/184 (95%)	168 (97%)	6 (3%)	32	55
8	H	144/174 (83%)	139 (96%)	5 (4%)	32	54
8	P	144/174 (83%)	139 (96%)	5 (4%)	32	54
All	All	4522/4920 (92%)	4397 (97%)	125 (3%)	38	59

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	319	LEU
1	A	342	LEU
1	A	404	GLN
1	A	476	LEU
2	B	78	ILE
2	B	215	LYS
2	B	224	ILE
2	B	228	ILE
2	B	250	GLU
2	B	412	ASP
2	B	420	ARG
2	B	429	ASN
2	B	435	ASN
3	C	22	THR
3	C	64	VAL
3	C	123	ILE
3	C	124	LEU
3	C	131	MET
3	C	138	LEU
3	C	167	MET
3	C	221	LEU
3	C	246	SER
3	C	278	LEU
3	C	365	GLU
3	C	396	GLU
4	D	20	LYS
4	D	40	GLU
4	D	60	VAL

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Mol	Chain	Res	Type
4	D	83	GLU
4	D	97	ILE
4	D	136	GLN
4	D	149	LEU
4	D	187	TYR
4	D	223	LEU
4	D	245	MET
4	D	267	MET
4	D	278	LEU
4	D	322	GLU
4	D	323	GLU
4	D	349	ASN
4	D	377	LEU
4	D	380	GLN
4	D	385	LEU
5	E	40	LEU
5	E	63	LEU
5	E	197	ASP
5	E	198	GLU
5	E	209	ASN
5	E	267	PHE
5	E	271	GLU
5	E	279	GLN
6	F	40	SER
6	F	113	LYS
6	F	159	LYS
6	F	172	ILE
6	F	282	GLN
7	G	108	VAL
7	G	110	CYS
7	G	126	ARG
7	G	141	LEU
7	G	167	LEU
7	G	178	CYS
8	H	33	THR
8	H	40	LEU
8	H	46	LEU
8	H	143	GLU
8	H	160	ARG
1	I	138	LEU
1	I	319	LEU
1	I	342	LEU

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Mol	Chain	Res	Type
1	I	404	GLN
1	I	476	LEU
2	J	78	ILE
2	J	90	ASN
2	J	215	LYS
2	J	224	ILE
2	J	228	ILE
2	J	250	GLU
2	J	412	ASP
2	J	420	ARG
2	J	429	ASN
2	J	435	ASN
3	K	22	THR
3	K	64	VAL
3	K	123	ILE
3	K	124	LEU
3	K	131	MET
3	K	138	LEU
3	K	167	MET
3	K	221	LEU
3	K	278	LEU
3	K	365	GLU
3	K	396	GLU
4	L	136	GLN
4	L	149	LEU
4	L	187	TYR
4	L	223	LEU
4	L	245	MET
4	L	278	LEU
4	L	349	ASN
4	L	377	LEU
4	L	380	GLN
4	L	385	LEU
5	M	40	LEU
5	M	63	LEU
5	M	197	ASP
5	M	198	GLU
5	M	209	ASN
5	M	268	ASP
5	M	279	GLN
6	N	172	ILE
6	N	282	GLN

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Mol	Chain	Res	Type
6	N	312	LEU
7	O	108	VAL
7	O	110	CYS
7	O	126	ARG
7	O	141	LEU
7	O	167	LEU
7	O	178	CYS
8	P	33	THR
8	P	40	LEU
8	P	46	LEU
8	P	143	GLU
8	P	160	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	412	GLN
1	A	483	GLN
1	A	501	HIS
2	B	208	GLN
2	B	210	ASN
2	B	223	HIS
2	B	297	GLN
2	B	319	GLN
2	B	321	ASN
2	B	333	ASN
3	C	89	ASN
3	C	106	GLN
3	C	126	GLN
3	C	147	GLN
3	C	197	ASN
3	C	239	GLN
3	C	270	ASN
3	C	327	GLN
3	C	375	ASN
4	D	228	HIS
4	D	276	ASN
4	D	360	HIS
5	E	132	ASN
5	E	162	GLN
5	E	321	GLN

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Mol	Chain	Res	Type
6	F	61	GLN
6	F	76	GLN
6	F	80	ASN
6	F	111	GLN
6	F	202	HIS
6	F	300	ASN
6	F	303	ASN
6	F	316	GLN
7	G	202	GLN
8	H	39	GLN
8	H	103	GLN
8	H	196	GLN
1	I	101	GLN
1	I	313	HIS
1	I	412	GLN
1	I	483	GLN
1	I	501	HIS
2	J	38	ASN
2	J	174	GLN
2	J	208	GLN
2	J	210	ASN
2	J	223	HIS
2	J	255	HIS
2	J	297	GLN
2	J	319	GLN
2	J	321	ASN
2	J	333	ASN
2	J	334	HIS
3	K	41	HIS
3	K	89	ASN
3	K	106	GLN
3	K	116	GLN
3	K	126	GLN
3	K	147	GLN
3	K	197	ASN
3	K	239	GLN
3	K	270	ASN
3	K	306	ASN
3	K	327	GLN
3	K	375	ASN
4	L	35	GLN
4	L	184	GLN

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Mol	Chain	Res	Type
4	L	186	HIS
4	L	276	ASN
4	L	360	HIS
5	M	132	ASN
5	M	162	GLN
5	M	275	GLN
5	M	321	GLN
6	N	76	GLN
6	N	111	GLN
6	N	202	HIS
6	N	316	GLN
7	O	12	GLN
7	O	202	GLN
8	P	39	GLN
8	P	103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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
6	N	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	40:SER	C	41:VAL	N	2.59
1	F	40:SER	C	41:VAL	N	1.94

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%)	-0.00	4 (0%) 79 62	152, 242, 277, 283	0
1	I	419/480 (87%)	0.03	5 (1%) 76 59	140, 208, 264, 271	0
2	B	403/447 (90%)	0.05	5 (1%) 76 59	147, 264, 281, 288	0
2	J	403/447 (90%)	0.03	6 (1%) 72 54	134, 243, 264, 276	0
3	C	401/427 (93%)	0.09	2 (0%) 87 74	149, 205, 267, 276	0
3	K	401/427 (93%)	0.18	8 (1%) 65 48	121, 179, 260, 268	0
4	D	406/410 (99%)	0.04	2 (0%) 87 74	139, 227, 276, 281	0
4	L	406/410 (99%)	0.04	2 (0%) 87 74	162, 249, 287, 292	0
5	E	298/327 (91%)	0.02	4 (1%) 75 57	132, 172, 222, 242	0
5	M	298/327 (91%)	0.08	4 (1%) 75 57	148, 206, 242, 258	0
6	F	281/331 (84%)	0.15	1 (0%) 88 76	132, 181, 230, 244	0
6	N	281/331 (84%)	0.13	8 (2%) 55 41	132, 213, 247, 259	0
7	G	208/222 (93%)	0.08	4 (1%) 66 49	152, 211, 255, 264	0
7	O	208/222 (93%)	-0.05	1 (0%) 87 74	175, 226, 268, 272	0
8	H	173/213 (81%)	-0.07	0 100 100	165, 200, 231, 241	0
8	P	173/213 (81%)	-0.10	0 100 100	160, 193, 228, 239	0
All	All	5178/5714 (90%)	0.05	56 (1%) 78 60	121, 212, 275, 292	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	54	HIS	9.5
1	I	309	ALA	4.9
2	B	204	MET	4.1
2	J	172	LEU	3.6
1	A	331	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
5	M	85	VAL	3.5
3	K	121	ILE	3.2
2	B	112	ILE	3.1
7	G	66	LEU	2.9
2	J	398	ILE	2.9
4	L	378	CYS	2.9
1	I	322	PRO	2.9
3	C	54	HIS	2.9
1	A	334	LEU	2.8
7	G	46	LEU	2.7
5	M	241	LEU	2.6
1	I	390	LEU	2.5
6	N	200	VAL	2.5
5	M	314	ALA	2.5
2	J	112	ILE	2.4
6	N	163	LEU	2.4
3	K	58	VAL	2.4
7	O	132	VAL	2.4
2	B	200	LEU	2.4
7	G	12	GLN	2.4
3	K	45	VAL	2.4
5	E	105	THR	2.3
6	N	167	VAL	2.3
3	K	103	LEU	2.3
4	D	23	ALA	2.3
6	N	152	LEU	2.3
6	N	257	LEU	2.3
5	E	176	ILE	2.3
6	N	148	SER	2.2
5	E	247	VAL	2.2
4	D	19	HIS	2.2
2	J	35	GLN	2.2
4	L	281	PHE	2.2
6	F	200	VAL	2.2
7	G	9	GLY	2.2
3	C	307	ILE	2.2
1	I	88	ALA	2.2
3	K	39	LEU	2.2
1	A	94	LEU	2.2
6	N	286	VAL	2.2
6	N	41	VAL	2.1
2	J	282	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	176	HIS	2.1
3	K	96	ALA	2.1
5	E	29	TYR	2.1
1	A	500	ILE	2.1
2	J	279	TYR	2.1
1	I	323	SER	2.1
2	B	442	LEU	2.0
3	K	42	LEU	2.0
5	M	265	GLN	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	ZN	M	999	1/1	0.98	0.06	173,173,173,173	0
9	ZN	E	999	1/1	0.99	0.04	138,138,138,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.