



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:23 PM UTC

PDB ID : 4D10 / pdb_00004d10
Title : Crystal structure of the COP9 signalosome
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Deposited on : 2014-04-30
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<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

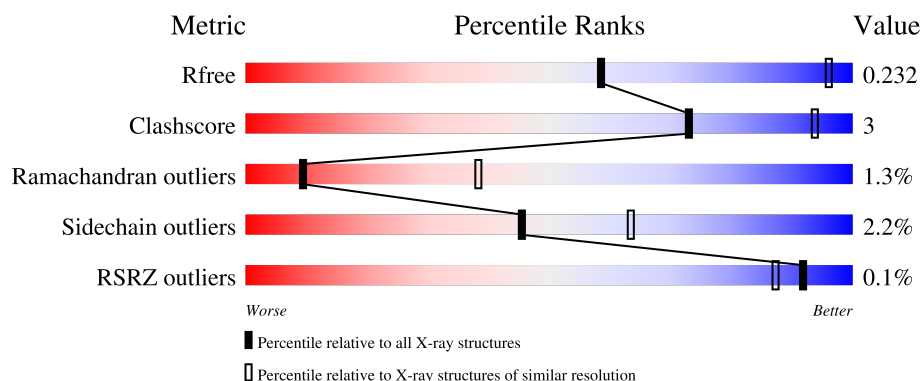
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



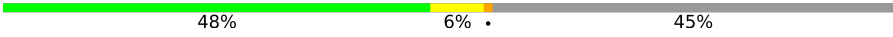
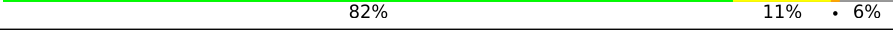
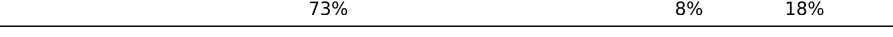
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	
2	B	447	
2	J	447	
3	C	423	

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Mol	Chain	Length	Quality of chain
3	K	423	 83%11%5%
4	D	410	 89%10%1%
4	L	410	 48%6%45%
5	E	334	 81%9%11%
5	M	334	 79%9%11%
6	F	331	 76%9%15%
6	N	331	 74%11%15%
7	G	222	 84%9%6%
7	O	222	 82%11%6%
8	H	212	 73%8%18%
8	P	212	 73%8%18%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 39976 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 4 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	L	225	Total	C	N	O	S	0	0	0
			1805	1137	319	337	12			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 6 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	281	Total	C	N	O	S	0	0	0
			2236	1429	371	421	15			
6	N	281	Total	C	N	O	S	0	0	0
			2236	1429	371	421	15			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLY	-	expression tag	UNP Q99627
H	-1	GLY	-	expression tag	UNP Q99627
H	0	GLY	-	expression tag	UNP Q99627
H	1	ARG	-	expression tag	UNP Q99627
P	-2	GLY	-	expression tag	UNP Q99627
P	-1	GLY	-	expression tag	UNP Q99627
P	0	GLY	-	expression tag	UNP Q99627
P	1	ARG	-	expression tag	UNP Q99627

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

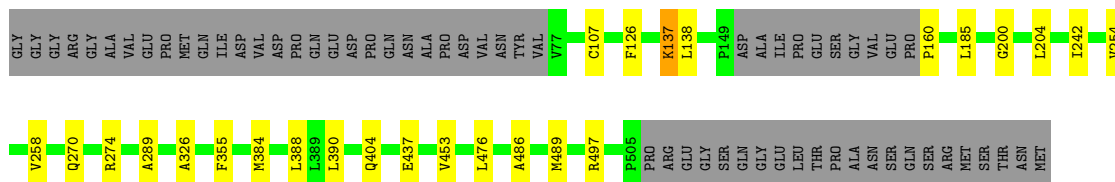
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total	Zn	0	0
			1	1		
9	M	1	Total	Zn	0	0
			1	1		

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.

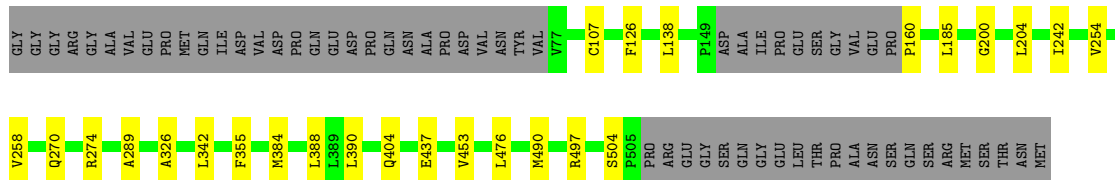
- Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain A:  82% 5% 13%



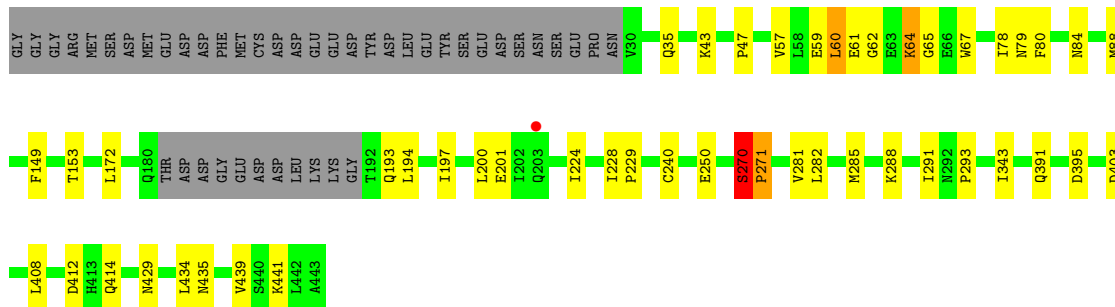
- Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

Chain I: 82% 5% 13%



● Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

Chain B:  79% 10% 10%

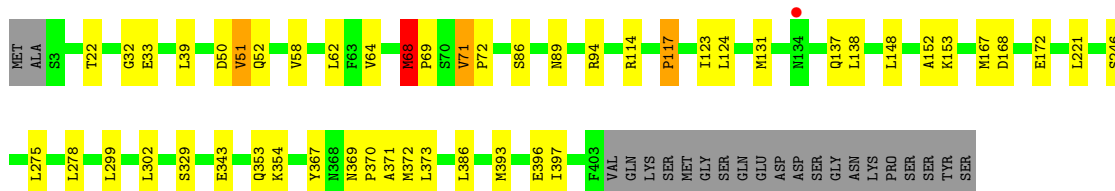


● Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

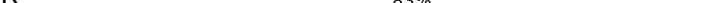
Chain J:  80% 9% 10%

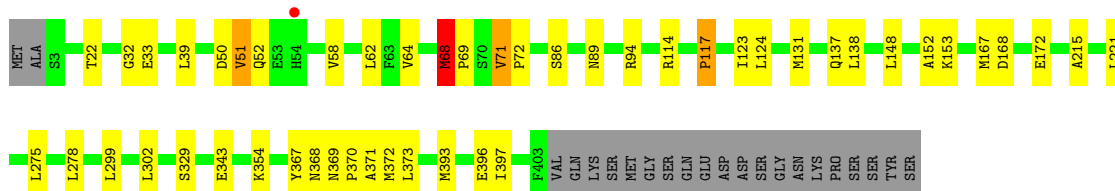
- Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain C: 83% 11% 5%

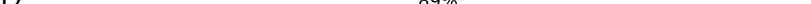


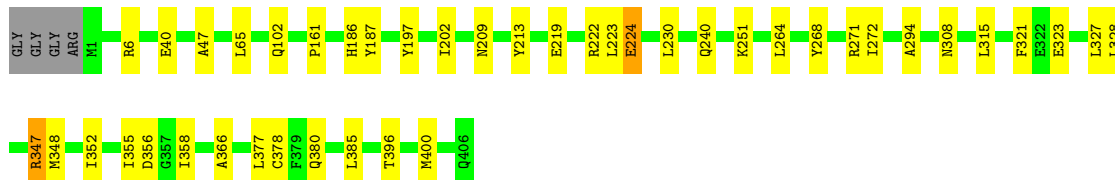
- Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain K:  83% 11% 5%



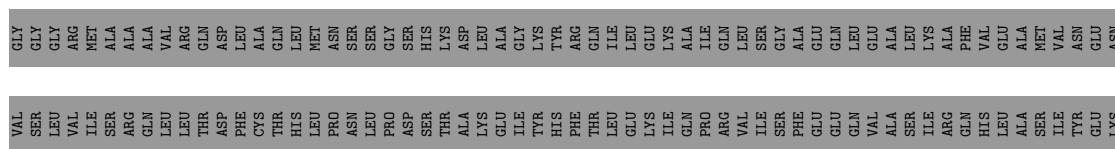
- Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

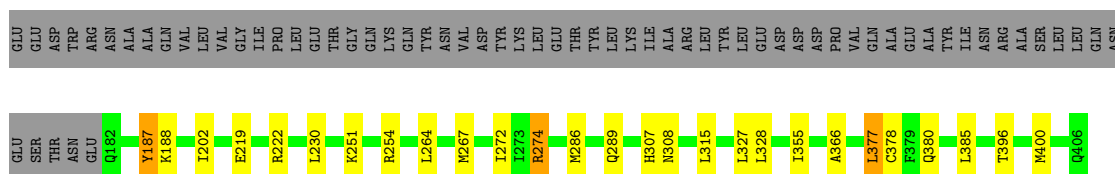
Chain D:  89% 10%



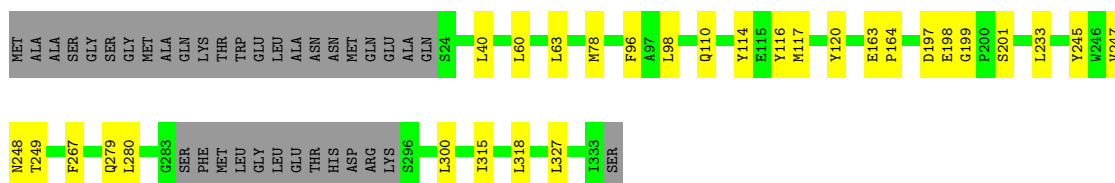
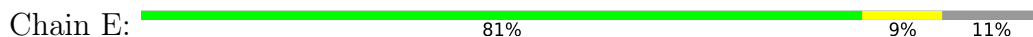
- Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

Chain L: 48% 6% • 45%

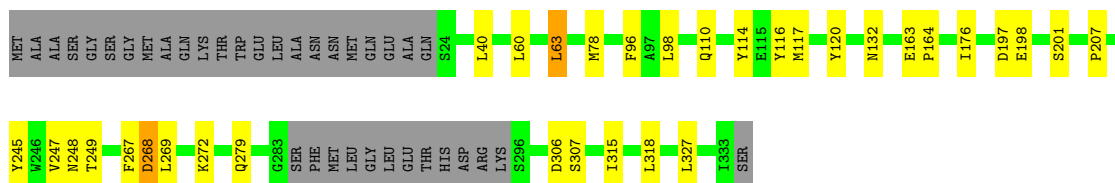
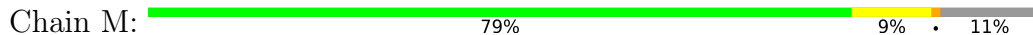




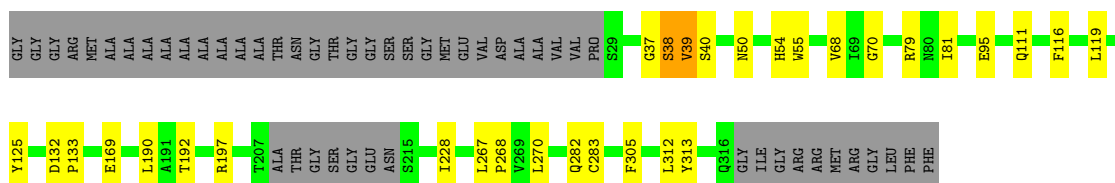
- Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5



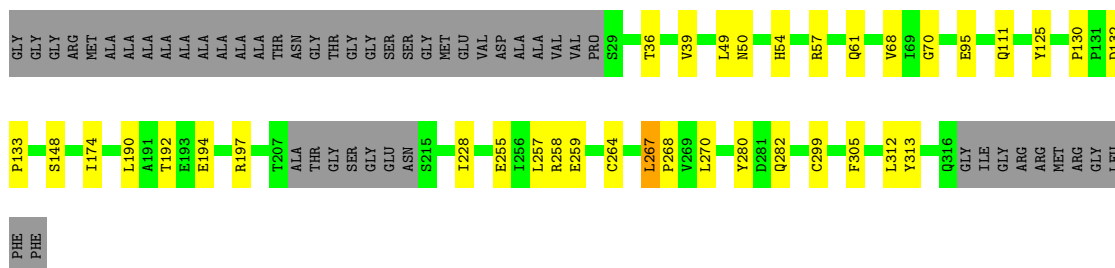
- Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5



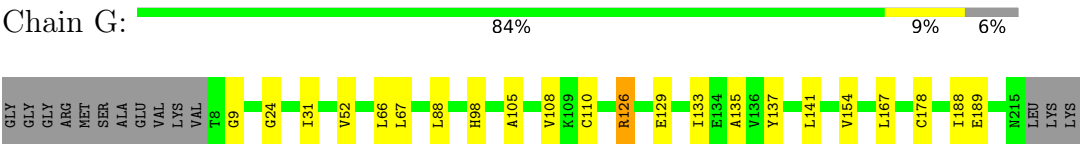
- Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6



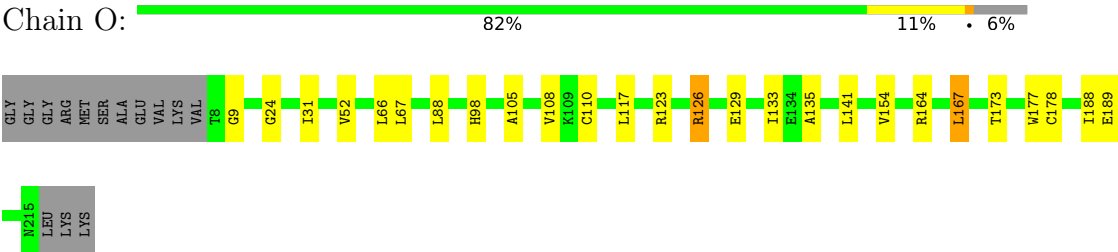
- Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6



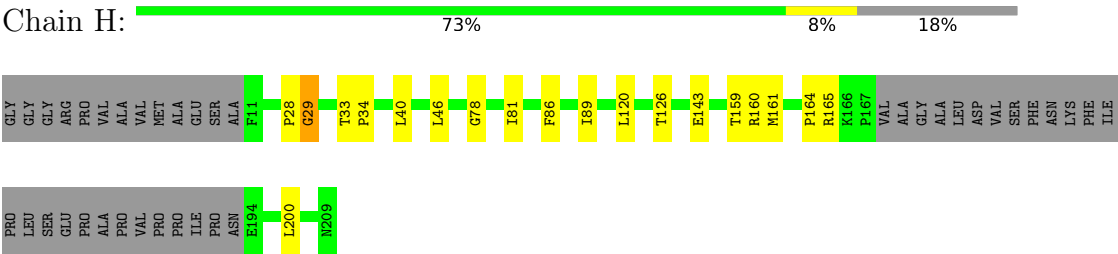
- Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



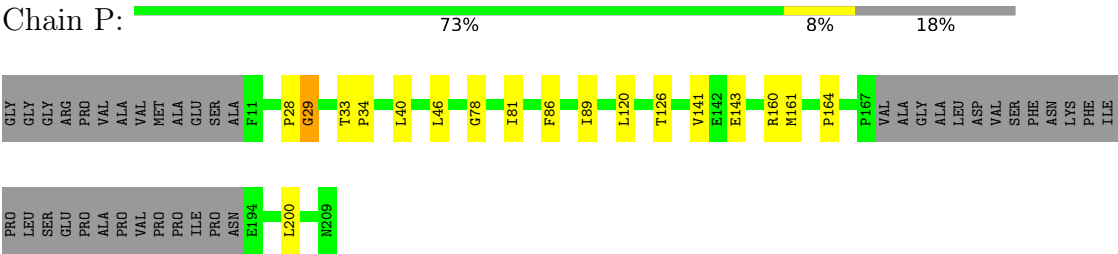
• Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



• Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	151.62Å 151.62Å 343.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.87 – 3.80 50.87 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.87-3.80) 100.0 (50.87-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.199 , 0.228 0.200 , 0.232	Depositor DCC
R_{free} test set	1656 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	156.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 136.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.096 for -h,-k,l 0.277 for h,-h-k,-l 0.097 for -k,-h,-l	Xtriage
Reported twinning fraction	0.636 for H, K, L 0.364 for K, H, -L	Depositor
Outliers	0 of 86819 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	39976	wwPDB-VP
Average B, all atoms (Å ²)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.84	1/3404 (0.0%)	0.86	3/4588 (0.1%)
1	I	0.64	0/3404	0.83	0/4588
2	B	0.62	0/3360	0.84	3/4519 (0.1%)
2	J	0.61	0/3361	0.85	4/4522 (0.1%)
3	C	0.61	0/3250	0.86	5/4390 (0.1%)
3	K	0.61	0/3250	0.86	6/4390 (0.1%)
4	D	0.84	4/3303 (0.1%)	0.82	2/4460 (0.0%)
4	L	0.57	0/1834	0.78	0/2470
5	E	0.57	0/2417	0.77	0/3266
5	M	0.59	0/2417	0.78	0/3266
6	F	0.64	0/2282	0.81	3/3092 (0.1%)
6	N	0.63	1/2282 (0.0%)	0.78	1/3092 (0.0%)
7	G	0.58	0/1652	0.83	0/2239
7	O	0.59	0/1652	0.82	0/2239
8	H	0.65	0/1416	0.89	2/1924 (0.1%)
8	P	0.64	0/1416	0.89	2/1924 (0.1%)
All	All	0.66	6/40700 (0.0%)	0.83	31/54969 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	6
2	J	0	6
3	C	0	2
3	K	0	2
5	E	0	2
5	M	0	2
6	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	N	0	2
8	H	0	2
8	P	0	2
All	All	0	27

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	LYS	C-N	31.40	1.77	1.34
4	D	347	ARG	C-N	29.75	1.76	1.33
4	D	187	TYR	C-N	-14.00	1.16	1.33
4	D	224	GLU	N-CA	-5.75	1.39	1.46
4	D	186	HIS	C-N	5.29	1.40	1.33
6	N	130	PRO	CA-C	5.20	1.54	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	187	TYR	CA-C-N	8.98	132.67	120.54
4	D	187	TYR	C-N-CA	8.98	132.67	120.54
8	P	29	GLY	N-CA-C	8.91	134.30	113.18
8	H	29	GLY	N-CA-C	8.85	134.16	113.18
2	J	60	LEU	N-CA-C	-7.85	98.85	110.23
3	K	68	MET	CA-C-N	7.84	129.64	119.84
3	K	68	MET	C-N-CA	7.84	129.64	119.84
3	C	68	MET	CA-C-N	7.79	129.57	119.84
3	C	68	MET	C-N-CA	7.79	129.57	119.84
1	A	137	LYS	O-C-N	-7.51	114.15	122.12
6	F	38	SER	CB-CA-C	-7.10	108.38	116.54
8	P	34	PRO	N-CA-C	6.50	118.63	110.70
8	H	34	PRO	N-CA-C	6.33	118.42	110.70
6	F	39	VAL	N-CA-C	6.21	118.57	109.63
1	A	137	LYS	CA-C-N	6.20	129.74	120.31
1	A	137	LYS	C-N-CA	6.20	129.74	120.31
3	K	69	PRO	N-CA-C	5.83	124.48	112.47
3	C	69	PRO	N-CA-C	5.81	124.43	112.47
6	F	268	PRO	N-CA-C	5.39	123.57	112.47
2	J	79	ASN	N-CA-C	5.29	116.73	111.07
2	B	79	ASN	N-CA-C	5.26	116.70	111.07
3	C	369	ASN	CA-C-N	-5.20	113.68	119.19
3	C	369	ASN	C-N-CA	-5.20	113.68	119.19
6	N	268	PRO	N-CA-C	5.18	123.15	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	270	SER	CA-C-N	5.09	126.20	119.84
2	B	270	SER	C-N-CA	5.09	126.20	119.84
2	J	270	SER	CA-C-N	5.06	126.17	119.84
2	J	270	SER	C-N-CA	5.06	126.17	119.84
3	K	369	ASN	CA-C-N	-5.06	113.83	119.19
3	K	369	ASN	C-N-CA	-5.06	113.83	119.19
3	K	68	MET	N-CA-C	5.04	120.94	109.81

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	270	SER	Peptide,Mainchain
2	B	288	LYS	Peptide,Mainchain
2	B	64	LYS	Peptide,Mainchain
3	C	68	MET	Peptide,Mainchain
5	E	163	GLU	Peptide,Mainchain
6	F	267	LEU	Peptide
8	H	28	PRO	Peptide,Mainchain
2	J	270	SER	Peptide,Mainchain
2	J	288	LYS	Peptide,Mainchain
2	J	64	LYS	Peptide,Mainchain
3	K	68	MET	Peptide,Mainchain
5	M	163	GLU	Peptide,Mainchain
6	N	267	LEU	Peptide,Mainchain
8	P	28	PRO	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3348	0	3384	19	0
1	I	3348	0	3385	17	0
2	B	3304	0	3350	23	0
2	J	3304	0	3351	18	0
3	C	3191	0	3208	20	0
3	K	3191	0	3208	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3251	0	3251	26	0
4	L	1805	0	1812	22	0
5	E	2366	0	2340	25	0
5	M	2366	0	2340	30	0
6	F	2236	0	2227	30	0
6	N	2236	0	2227	26	0
7	G	1631	0	1654	12	0
7	O	1631	0	1654	17	0
8	H	1383	0	1366	8	0
8	P	1383	0	1366	8	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
All	All	39976	0	40123	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:347:ARG:C	4:D:348:MET:N	1.76	1.42
1:A:137:LYS:C	1:A:138:LEU:N	1.77	1.40
1:A:200:GLY:O	1:A:204:LEU:HD13	1.45	1.15
1:I:200:GLY:O	1:I:204:LEU:HD13	1.45	1.14
2:B:60:LEU:O	2:B:61:GLU:O	1.68	1.12
5:M:96:PHE:CD2	5:M:120:TYR:CE2	2.40	1.09
4:L:274:ARG:NH2	4:L:327:LEU:HD12	1.81	0.95
5:E:96:PHE:CD2	5:E:120:TYR:CE2	2.57	0.92
1:I:200:GLY:O	1:I:204:LEU:CD1	2.20	0.89
1:A:200:GLY:O	1:A:204:LEU:CD1	2.21	0.88
2:B:61:GLU:C	2:B:62:GLY:N	2.35	0.84
6:F:39:VAL:HG11	6:F:81:ILE:HD11	1.60	0.83
5:M:96:PHE:CE2	5:M:120:TYR:CE2	2.67	0.82
1:I:185:LEU:HD22	1:I:204:LEU:HD21	1.62	0.80
1:A:185:LEU:HD22	1:A:204:LEU:HD21	1.62	0.80
7:G:126:ARG:NH2	7:G:129:GLU:HB3	1.97	0.79
4:D:251:LYS:NZ	6:F:38:SER:HB2	1.97	0.77
7:O:126:ARG:NH2	7:O:129:GLU:HB3	1.99	0.77
6:F:39:VAL:HG11	6:F:81:ILE:CD1	2.15	0.76
2:B:60:LEU:C	2:B:61:GLU:O	2.31	0.74
4:D:251:LYS:HZ2	6:F:38:SER:HB2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:96:PHE:CD2	5:M:120:TYR:HE2	2.00	0.73
6:F:39:VAL:HG21	6:F:81:ILE:HD12	1.72	0.72
7:G:126:ARG:NH2	7:G:129:GLU:CB	2.53	0.71
7:O:126:ARG:NH2	7:O:129:GLU:CB	2.54	0.70
4:L:274:ARG:HH22	4:L:327:LEU:HD12	1.56	0.69
6:F:116:PHE:HB3	6:F:119:LEU:HD13	1.74	0.69
1:I:200:GLY:C	1:I:204:LEU:HD13	2.17	0.69
1:A:138:LEU:HD21	1:A:160:PRO:HG3	1.75	0.68
1:I:490:MET:SD	3:K:167:MET:SD	2.92	0.68
1:A:200:GLY:C	1:A:204:LEU:HD13	2.18	0.67
2:J:64:LYS:HB3	2:J:65:GLY:HA2	1.76	0.67
5:M:198:GLU:OE1	5:M:198:GLU:HA	1.95	0.66
5:M:96:PHE:CE2	5:M:120:TYR:CD2	2.83	0.66
2:B:64:LYS:HB3	2:B:65:GLY:HA2	1.77	0.64
4:D:315:LEU:HD13	7:G:133:ILE:HG12	1.79	0.64
1:I:138:LEU:HD21	1:I:160:PRO:HG3	1.79	0.63
5:E:96:PHE:CE2	5:E:120:TYR:CE2	2.87	0.63
3:K:370:PRO:O	3:K:373:LEU:N	2.32	0.63
5:E:249:THR:HG23	6:F:197:ARG:NH1	2.14	0.62
3:C:353:GLN:O	7:O:123:ARG:NH1	2.33	0.62
3:C:370:PRO:O	3:C:373:LEU:N	2.32	0.62
4:D:268:TYR:OH	6:F:38:SER:HA	2.00	0.61
3:C:343:GLU:HG3	8:H:120:LEU:HD13	1.82	0.61
6:F:38:SER:OG	6:F:39:VAL:HG13	2.01	0.61
2:B:391:GLN:NE2	2:B:395:ASP:OD2	2.30	0.60
4:L:286:MET:HB2	4:L:289:GLN:OE1	2.02	0.60
2:J:34:ASN:OD1	2:J:60:LEU:HD12	2.01	0.60
3:C:367:TYR:CE1	3:C:372:MET:HE3	2.37	0.59
3:K:367:TYR:CE1	3:K:372:MET:HE3	2.38	0.59
4:L:378:CYS:HB3	5:M:247:VAL:HG22	1.84	0.59
8:P:126:THR:O	8:P:164:PRO:HD2	2.02	0.59
2:J:153:THR:HG23	2:J:200:LEU:HD11	1.85	0.58
5:E:78:MET:HE1	5:E:110:GLN:HB3	1.84	0.58
5:M:78:MET:HE1	5:M:110:GLN:HB3	1.85	0.58
5:E:96:PHE:CD2	5:E:120:TYR:HE2	2.17	0.58
1:A:138:LEU:CD2	1:A:160:PRO:HG3	2.34	0.58
2:B:153:THR:HG23	2:B:200:LEU:HD11	1.86	0.57
4:L:187:TYR:CD1	4:L:188:LYS:N	2.72	0.57
5:M:96:PHE:CE2	5:M:120:TYR:HE2	2.17	0.57
6:F:38:SER:OG	6:F:39:VAL:N	2.37	0.57
8:H:126:THR:O	8:H:164:PRO:HD2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:393:MET:HE3	6:N:305:PHE:CZ	2.39	0.57
4:D:219:GLU:O	4:D:223:LEU:HD13	2.04	0.57
3:K:71:VAL:HB	3:K:72:PRO:CD	2.35	0.57
5:M:96:PHE:CZ	5:M:120:TYR:CD2	2.92	0.57
4:D:321:PHE:HZ	4:D:352:ILE:HG23	1.69	0.57
1:I:497:ARG:HG3	6:N:313:TYR:CE1	2.39	0.57
4:D:323:GLU:OE2	7:G:126:ARG:HB2	2.04	0.57
5:M:60:LEU:HD11	6:N:50:ASN:OD1	2.05	0.57
1:I:185:LEU:HD22	1:I:204:LEU:CD2	2.33	0.56
3:C:71:VAL:HB	3:C:72:PRO:CD	2.35	0.56
2:B:434:LEU:HD21	5:E:300:LEU:HD11	1.87	0.56
3:C:354:LYS:HB2	8:H:161:MET:HE2	1.87	0.56
3:K:354:LYS:HB2	8:P:161:MET:HE2	1.88	0.56
6:N:264:CYS:HG	7:O:173:THR:HG1	1.51	0.56
1:A:185:LEU:HD22	1:A:204:LEU:CD2	2.33	0.56
5:M:315:ILE:HG23	8:P:200:LEU:HD22	1.87	0.55
4:L:308:ASN:HB3	4:L:328:LEU:HD22	1.88	0.55
4:D:251:LYS:NZ	6:F:38:SER:CB	2.68	0.55
4:L:315:LEU:HD13	7:O:133:ILE:HG12	1.89	0.55
6:N:255:GLU:OE1	6:N:258:ARG:NE	2.40	0.55
2:J:194:LEU:HA	2:J:197:ILE:HD12	1.88	0.55
5:M:116:TYR:CD1	5:M:116:TYR:C	2.85	0.55
3:K:343:GLU:HG3	8:P:120:LEU:HD13	1.88	0.54
1:I:138:LEU:CD2	1:I:160:PRO:HG3	2.38	0.54
5:M:248:ASN:OD1	6:N:192:THR:HG22	2.08	0.54
5:M:249:THR:HG23	6:N:197:ARG:NH1	2.23	0.54
4:D:308:ASN:HB3	4:D:328:LEU:HD22	1.89	0.54
4:L:251:LYS:NZ	6:N:148:SER:OG	2.41	0.54
2:B:194:LEU:HA	2:B:197:ILE:HD12	1.88	0.54
5:M:120:TYR:N	6:N:111:GLN:HE22	2.05	0.54
4:D:378:CYS:HB3	5:E:247:VAL:HG22	1.89	0.53
5:E:60:LEU:HD11	6:F:50:ASN:OD1	2.08	0.53
6:N:255:GLU:OE2	6:N:259:GLU:OE2	2.26	0.53
3:K:275:LEU:HD23	3:K:299:LEU:HD12	1.90	0.53
4:D:161:PRO:HB3	4:D:197:TYR:HB3	1.91	0.52
5:M:272:LYS:NZ	5:M:306:ASP:OD2	2.26	0.52
4:D:271:ARG:HB3	7:G:137:TYR:CE2	2.44	0.52
4:D:219:GLU:HA	4:D:222:ARG:HE	1.75	0.52
7:G:126:ARG:NH2	7:G:129:GLU:HB2	2.24	0.52
5:E:327:LEU:HD11	6:F:228:ILE:HG12	1.91	0.52
2:J:434:LEU:HD23	6:N:299:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:MET:HE2	5:E:98:LEU:HD12	1.92	0.51
4:L:219:GLU:HA	4:L:222:ARG:HE	1.76	0.51
4:L:254:ARG:HD3	6:N:174:ILE:HD12	1.92	0.51
6:N:255:GLU:OE1	6:N:255:GLU:HA	2.10	0.51
6:F:37:GLY:HA3	6:F:169:GLU:OE2	2.10	0.51
2:J:282:LEU:HD13	2:J:343:ILE:HG23	1.92	0.51
6:N:267:LEU:HD11	7:O:177:TRP:CE3	2.45	0.51
4:D:347:ARG:C	4:D:348:MET:CA	2.76	0.51
2:B:282:LEU:HD13	2:B:343:ILE:HG23	1.92	0.51
4:L:267:MET:HA	4:L:307:HIS:CE1	2.46	0.51
3:C:275:LEU:HD23	3:C:299:LEU:HD12	1.91	0.51
5:M:78:MET:HE2	5:M:98:LEU:HD12	1.92	0.51
2:B:270:SER:HB2	2:B:271:PRO:HA	1.93	0.51
5:E:116:TYR:CD1	5:E:116:TYR:C	2.89	0.50
5:M:96:PHE:CG	5:M:120:TYR:CE2	2.96	0.50
7:O:188:ILE:O	7:O:189:GLU:C	2.54	0.50
7:G:188:ILE:O	7:G:189:GLU:C	2.53	0.50
2:J:270:SER:HB2	2:J:271:PRO:HA	1.93	0.50
5:M:114:TYR:HA	5:M:117:MET:HE3	1.92	0.50
7:O:126:ARG:NH2	7:O:129:GLU:HB2	2.25	0.50
5:M:63:LEU:HD12	6:N:49:LEU:HD12	1.92	0.50
3:K:370:PRO:O	3:K:371:ALA:C	2.54	0.50
1:A:326:ALA:HB2	1:A:355:PHE:HB3	1.93	0.50
5:E:114:TYR:HA	5:E:117:MET:HE3	1.92	0.50
3:K:117:PRO:HD2	3:K:152:ALA:HB2	1.93	0.50
1:I:326:ALA:HB2	1:I:355:PHE:HB3	1.94	0.49
7:O:126:ARG:HH22	7:O:129:GLU:HB3	1.75	0.49
4:L:187:TYR:CD1	4:L:187:TYR:C	2.90	0.49
3:C:117:PRO:HD2	3:C:152:ALA:HB2	1.93	0.49
1:A:384:MET:HE3	1:A:388:LEU:HD11	1.95	0.49
7:G:126:ARG:HH22	7:G:129:GLU:HB3	1.73	0.49
1:I:384:MET:HE3	1:I:388:LEU:HD11	1.95	0.49
1:A:497:ARG:HG3	6:F:313:TYR:CE1	2.48	0.48
5:M:176:ILE:HG23	6:N:194:GLU:HG2	1.94	0.48
2:B:441:LYS:HE3	5:E:280:LEU:HD22	1.94	0.48
4:L:187:TYR:HE1	4:L:188:LYS:HD3	1.78	0.48
5:E:96:PHE:CE2	5:E:120:TYR:CD2	3.02	0.48
8:H:159:THR:HA	7:O:117:LEU:HD13	1.95	0.48
3:C:370:PRO:O	3:C:371:ALA:C	2.56	0.47
2:J:423:ALA:HB2	5:M:267:PHE:CE2	2.49	0.47
1:A:486:ALA:CB	3:C:386:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:96:PHE:CZ	5:M:120:TYR:HD2	2.32	0.47
7:O:105:ALA:HB1	7:O:154:VAL:HG11	1.97	0.47
5:E:233:LEU:HD22	6:F:55:TRP:CE3	2.49	0.47
1:I:437:GLU:HG3	1:I:453:VAL:HG11	1.96	0.47
4:D:6:ARG:HG2	4:D:47:ALA:HB1	1.97	0.46
7:G:105:ALA:HB1	7:G:154:VAL:HG11	1.97	0.46
2:B:172:LEU:HD22	2:B:201:GLU:HG3	1.95	0.46
5:E:245:TYR:HD1	6:F:190:LEU:HD13	1.80	0.46
5:E:318:LEU:HD11	6:F:283:CYS:HA	1.97	0.46
1:A:437:GLU:HG3	1:A:453:VAL:HG11	1.96	0.46
4:D:347:ARG:CA	4:D:348:MET:N	2.72	0.46
2:J:172:LEU:HD22	2:J:201:GLU:HG3	1.96	0.46
3:K:368:ASN:O	6:N:280:TYR:HB3	2.16	0.46
2:B:281:VAL:HG12	2:B:285:MET:HE2	1.98	0.46
3:C:117:PRO:HB2	3:C:148:LEU:HD22	1.98	0.46
2:J:281:VAL:HG12	2:J:285:MET:HE2	1.98	0.46
5:E:248:ASN:OD1	6:F:192:THR:HG22	2.16	0.46
2:B:408:LEU:HD22	4:D:355:ILE:HG12	1.97	0.46
1:I:107:CYS:HB2	1:I:390:LEU:HD22	1.97	0.46
3:K:117:PRO:HB2	3:K:148:LEU:HD22	1.98	0.46
1:A:107:CYS:HB2	1:A:390:LEU:HD22	1.97	0.45
2:B:149:PHE:CZ	2:B:193:GLN:HB2	2.51	0.45
2:J:149:PHE:CZ	2:J:193:GLN:HB2	2.52	0.45
5:M:318:LEU:HD23	8:P:200:LEU:HD21	1.98	0.45
8:P:86:PHE:HA	8:P:89:ILE:HD12	1.98	0.45
3:C:370:PRO:O	3:C:373:LEU:HB3	2.15	0.45
3:K:397:ILE:HG23	6:N:312:LEU:HD12	1.98	0.45
8:P:141:VAL:HG11	8:P:160:ARG:NH2	2.31	0.45
4:D:378:CYS:HB2	5:E:247:VAL:HG13	1.98	0.45
4:D:268:TYR:CE2	6:F:79:ARG:HD3	2.52	0.45
3:K:370:PRO:O	3:K:373:LEU:HB3	2.16	0.45
5:M:269:LEU:HD21	5:M:307:SER:HB3	1.99	0.45
3:C:393:MET:HE3	6:F:305:PHE:CZ	2.52	0.45
3:C:397:ILE:HG23	6:F:312:LEU:HD12	1.98	0.45
5:M:207:PRO:HB3	5:M:268:ASP:OD2	2.17	0.45
3:C:39:LEU:HD22	3:C:58:VAL:HG22	1.98	0.45
1:A:138:LEU:CD2	1:A:160:PRO:CG	2.95	0.44
2:B:59:GLU:O	2:B:61:GLU:N	2.48	0.44
5:E:318:LEU:HD11	6:F:283:CYS:SG	2.56	0.44
8:H:86:PHE:HA	8:H:89:ILE:HD12	1.98	0.44
4:L:187:TYR:CE1	4:L:188:LYS:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:HB3	2:B:78:ILE:HG21	2.00	0.44
2:B:57:VAL:HA	2:B:60:LEU:HD12	1.99	0.44
1:I:242:ILE:HG23	1:I:254:VAL:HG13	1.99	0.44
2:J:391:GLN:CD	2:J:391:GLN:C	2.85	0.44
2:J:47:PRO:HB3	2:J:78:ILE:HG21	1.99	0.44
3:K:39:LEU:HD22	3:K:58:VAL:HG22	1.98	0.44
1:A:242:ILE:HG23	1:A:254:VAL:HG13	2.00	0.44
4:D:272:ILE:CD1	4:D:327:LEU:HD21	2.48	0.44
7:G:66:LEU:HD21	7:G:88:LEU:HD21	2.00	0.44
1:I:504:SER:HA	3:K:215:ALA:HB2	1.99	0.44
3:K:71:VAL:HB	3:K:72:PRO:HD2	1.98	0.44
2:J:80:PHE:HB3	2:J:88:MET:HE2	2.00	0.44
3:C:71:VAL:HB	3:C:72:PRO:HD2	1.98	0.44
4:D:356:ASP:HB3	4:D:358:ILE:HD12	1.99	0.43
3:K:94:ARG:HH22	3:K:137:GLN:HE22	1.66	0.43
7:O:66:LEU:HD21	7:O:88:LEU:HD21	2.01	0.43
6:F:39:VAL:CG2	6:F:81:ILE:HD12	2.44	0.43
4:L:230:LEU:HD11	4:L:264:LEU:HB2	2.01	0.43
4:L:378:CYS:HB2	5:M:247:VAL:HG13	1.99	0.43
6:N:54:HIS:CE1	6:N:68:VAL:HB	2.54	0.43
7:O:31:ILE:HG23	7:O:67:LEU:HD13	1.99	0.43
1:A:486:ALA:HB1	3:C:386:LEU:HD21	1.99	0.43
4:D:396:THR:O	4:D:400:MET:HB2	2.18	0.43
5:E:318:LEU:HD23	8:H:200:LEU:HD21	2.01	0.43
6:F:132:ASP:HB2	6:F:133:PRO:CD	2.49	0.43
2:J:403:ASP:HB3	2:J:408:LEU:HG	2.00	0.43
2:B:80:PHE:HB3	2:B:88:MET:HE2	2.00	0.43
2:B:403:ASP:HB3	2:B:408:LEU:HG	2.00	0.43
7:G:31:ILE:HG23	7:G:67:LEU:HD13	2.00	0.43
4:L:377:LEU:HD21	7:O:177:TRP:CH2	2.53	0.43
4:L:396:THR:O	4:L:400:MET:HB2	2.18	0.43
6:N:132:ASP:HB2	6:N:133:PRO:CD	2.48	0.43
6:F:54:HIS:CE1	6:F:68:VAL:HB	2.54	0.43
4:L:272:ILE:CD1	4:L:327:LEU:HD21	2.49	0.43
4:L:274:ARG:NH2	4:L:327:LEU:CD1	2.68	0.43
3:C:50:ASP:C	3:C:52:GLN:H	2.27	0.42
2:B:391:GLN:C	2:B:391:GLN:CD	2.87	0.42
3:C:94:ARG:HH22	3:C:137:GLN:HE22	1.67	0.42
4:D:230:LEU:HD11	4:D:264:LEU:HB2	2.01	0.42
1:I:258:VAL:HG11	1:I:289:ALA:HB2	2.01	0.42
6:F:39:VAL:HA	6:F:79:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:275:LEU:HD22	3:K:302:LEU:HD22	2.01	0.42
1:A:258:VAL:HG11	1:A:289:ALA:HB2	2.01	0.42
5:E:96:PHE:CE2	5:E:120:TYR:HE2	2.37	0.42
6:N:257:LEU:HD22	7:O:167:LEU:HD21	2.02	0.42
1:A:489:MET:HB3	2:B:439:VAL:HG13	2.01	0.41
7:G:98:HIS:HD2	7:G:135:ALA:HB2	1.85	0.41
2:J:408:LEU:HD22	4:L:355:ILE:HG12	2.02	0.41
3:K:50:ASP:C	3:K:52:GLN:H	2.28	0.41
4:L:187:TYR:HD1	4:L:188:LYS:N	2.15	0.41
3:C:275:LEU:HD22	3:C:302:LEU:HD22	2.01	0.41
6:N:36:THR:HB	6:N:39:VAL:HG21	2.02	0.41
7:O:98:HIS:HD2	7:O:135:ALA:HB2	1.85	0.41
1:I:138:LEU:CD2	1:I:160:PRO:CG	2.98	0.41
2:J:35:GLN:HG2	2:J:67:TRP:CZ2	2.56	0.41
4:D:209:ASN:O	4:D:213:TYR:CD2	2.74	0.41
5:E:96:PHE:CG	5:E:120:TYR:CE2	3.07	0.41
6:F:70:GLY:HA3	6:F:125:TYR:CE2	2.55	0.41
5:M:245:TYR:HD1	6:N:190:LEU:HD13	1.84	0.41
5:E:120:TYR:N	6:F:111:GLN:HE22	2.19	0.41
8:H:78:GLY:HA2	8:H:81:ILE:HD12	2.03	0.41
5:M:327:LEU:HD11	6:N:228:ILE:HG12	2.02	0.41
6:N:70:GLY:HA3	6:N:125:TYR:CE2	2.55	0.41
2:B:35:GLN:HG2	2:B:67:TRP:CZ2	2.56	0.40
7:O:164:ARG:HA	7:O:167:LEU:HD12	2.03	0.40
5:E:315:ILE:HG23	8:H:200:LEU:HD22	2.03	0.40
8:P:78:GLY:HA2	8:P:81:ILE:HD12	2.04	0.40
4:D:223:LEU:O	4:D:224:GLU:C	2.63	0.40
6:F:132:ASP:HB2	6:F:133:PRO:HD2	2.02	0.40
2:J:152:ASN:HB3	2:J:175:LEU:HD21	2.03	0.40
5:M:96:PHE:CD2	5:M:120:TYR:CD2	3.01	0.40
6:N:57:ARG:HG2	6:N:61:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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%)	394 (95%)	18 (4%)	3 (1%)	18	51
1	I	415/480 (86%)	394 (95%)	18 (4%)	3 (1%)	18	51
2	B	397/447 (89%)	366 (92%)	23 (6%)	8 (2%)	6	32
2	J	399/447 (89%)	369 (92%)	23 (6%)	7 (2%)	6	33
3	C	399/423 (94%)	362 (91%)	24 (6%)	13 (3%)	3	24
3	K	399/423 (94%)	362 (91%)	24 (6%)	13 (3%)	3	24
4	D	404/410 (98%)	399 (99%)	3 (1%)	2 (0%)	24	57
4	L	223/410 (54%)	219 (98%)	3 (1%)	1 (0%)	30	62
5	E	294/334 (88%)	281 (96%)	10 (3%)	3 (1%)	12	43
5	M	294/334 (88%)	281 (96%)	11 (4%)	2 (1%)	18	51
6	F	277/331 (84%)	266 (96%)	9 (3%)	2 (1%)	18	51
6	N	277/331 (84%)	265 (96%)	10 (4%)	2 (1%)	18	51
7	G	206/222 (93%)	194 (94%)	10 (5%)	2 (1%)	12	43
7	O	206/222 (93%)	194 (94%)	10 (5%)	2 (1%)	12	43
8	H	169/212 (80%)	161 (95%)	7 (4%)	1 (1%)	21	54
8	P	169/212 (80%)	161 (95%)	7 (4%)	1 (1%)	21	54
All	All	4943/5718 (86%)	4668 (94%)	210 (4%)	65 (1%)	9	38

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	51	VAL
3	C	68	MET
8	H	29	GLY
3	K	51	VAL
3	K	68	MET
8	P	29	GLY
1	A	274	ARG
3	C	71	VAL
3	C	153	LYS
3	C	172	GLU
7	G	24	GLY
1	I	274	ARG
2	J	414	GLN
3	K	71	VAL

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Mol	Chain	Res	Type
3	K	153	LYS
3	K	172	GLU
7	O	24	GLY
2	B	43	LYS
2	B	271	PRO
2	B	414	GLN
3	C	33	GLU
3	C	89	ASN
3	C	114	ARG
3	C	168	ASP
4	D	294	ALA
1	I	270	GLN
2	J	43	LYS
2	J	271	PRO
3	K	33	GLU
3	K	89	ASN
3	K	114	ARG
3	K	168	ASP
1	A	126	PHE
1	A	270	GLN
2	B	84	ASN
3	C	86	SER
3	C	117	PRO
4	D	366	ALA
6	F	95	GLU
6	F	270	LEU
7	G	9	GLY
1	I	126	PHE
2	J	84	ASN
3	K	86	SER
3	K	117	PRO
4	L	366	ALA
6	N	95	GLU
6	N	270	LEU
7	O	9	GLY
2	B	60	LEU
2	B	229	PRO
2	B	291	ILE
3	C	329	SER
5	E	164	PRO
5	E	201	SER
2	J	229	PRO

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Mol	Chain	Res	Type
2	J	291	ILE
3	K	329	SER
5	M	164	PRO
5	M	201	SER
5	E	199	GLY
3	K	32	GLY
3	C	32	GLY
2	J	293	PRO
2	B	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%)	363 (100%)	2 (0%)	81	81
1	I	365/415 (88%)	362 (99%)	3 (1%)	73	76
2	B	367/406 (90%)	360 (98%)	7 (2%)	50	66
2	J	367/406 (90%)	360 (98%)	7 (2%)	50	66
3	C	358/377 (95%)	345 (96%)	13 (4%)	31	54
3	K	358/377 (95%)	347 (97%)	11 (3%)	35	57
4	D	347/348 (100%)	339 (98%)	8 (2%)	44	63
4	L	190/348 (55%)	184 (97%)	6 (3%)	34	56
5	E	255/283 (90%)	249 (98%)	6 (2%)	43	62
5	M	255/283 (90%)	249 (98%)	6 (2%)	43	62
6	F	251/277 (91%)	249 (99%)	2 (1%)	73	76
6	N	251/277 (91%)	250 (100%)	1 (0%)	84	83
7	G	174/184 (95%)	167 (96%)	7 (4%)	28	52
7	O	174/184 (95%)	167 (96%)	7 (4%)	28	52
8	H	144/173 (83%)	138 (96%)	6 (4%)	26	50
8	P	144/173 (83%)	140 (97%)	4 (3%)	38	58
All	All	4365/4926 (89%)	4269 (98%)	96 (2%)	45	63

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	GLN
1	A	476	LEU
2	B	224	ILE
2	B	228	ILE
2	B	240	CYS
2	B	250	GLU
2	B	412	ASP
2	B	429	ASN
2	B	435	ASN
3	C	22	THR
3	C	51	VAL
3	C	62	LEU
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	396	GLU
4	D	40	GLU
4	D	65	LEU
4	D	102	GLN
4	D	202	ILE
4	D	240	GLN
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	267	PHE
5	E	279	GLN
6	F	40	SER
6	F	282	GLN
7	G	52	VAL
7	G	108	VAL
7	G	110	CYS
7	G	126	ARG

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Mol	Chain	Res	Type
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
8	H	165	ARG
1	I	342	LEU
1	I	404	GLN
1	I	476	LEU
2	J	224	ILE
2	J	228	ILE
2	J	240	CYS
2	J	250	GLU
2	J	412	ASP
2	J	429	ASN
2	J	435	ASN
3	K	22	THR
3	K	51	VAL
3	K	62	LEU
3	K	64	VAL
3	K	123	ILE
3	K	124	LEU
3	K	131	MET
3	K	138	LEU
3	K	221	LEU
3	K	278	LEU
3	K	396	GLU
4	L	187	TYR
4	L	202	ILE
4	L	274	ARG
4	L	377	LEU
4	L	380	GLN
4	L	385	LEU
5	M	40	LEU
5	M	63	LEU
5	M	132	ASN
5	M	197	ASP
5	M	268	ASP
5	M	279	GLN

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Mol	Chain	Res	Type
6	N	282	GLN
7	O	52	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	250	ASN
1	A	483	GLN
1	A	501	HIS
2	B	34	ASN
2	B	90	ASN
2	B	174	GLN
2	B	208	GLN
2	B	210	ASN
2	B	297	GLN
2	B	319	GLN
2	B	321	ASN
2	B	333	ASN
2	B	436	GLN
3	C	89	ASN
3	C	106	GLN
3	C	126	GLN
3	C	147	GLN
3	C	239	GLN
3	C	270	ASN
3	C	327	GLN
3	C	369	ASN
3	C	375	ASN
4	D	380	GLN
5	E	126	GLN
5	E	132	ASN

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Mol	Chain	Res	Type
5	E	162	GLN
5	E	321	GLN
6	F	61	GLN
6	F	80	ASN
6	F	111	GLN
6	F	224	GLN
6	F	300	ASN
6	F	316	GLN
7	G	202	GLN
8	H	103	GLN
8	H	196	GLN
1	I	101	GLN
1	I	250	ASN
1	I	313	HIS
1	I	387	ASN
1	I	483	GLN
2	J	124	GLN
2	J	174	GLN
2	J	208	GLN
2	J	210	ASN
2	J	319	GLN
2	J	321	ASN
2	J	334	HIS
3	K	41	HIS
3	K	89	ASN
3	K	106	GLN
3	K	147	GLN
3	K	239	GLN
3	K	270	ASN
3	K	271	ASN
3	K	306	ASN
3	K	327	GLN
3	K	363	ASN
3	K	375	ASN
4	L	186	HIS
5	M	162	GLN
5	M	321	GLN
6	N	61	GLN
6	N	111	GLN
6	N	202	HIS
6	N	224	GLN
6	N	284	ASN

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Mol	Chain	Res	Type
6	N	316	GLN
7	O	10	GLN
7	O	202	GLN
8	P	103	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	D	2
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	61:GLU	C	62:GLY	N	2.35
1	A	137:LYS	C	138:LEU	N	1.77
1	D	347:ARG	C	348:MET	N	1.76
1	D	187:TYR	C	188:LYS	N	1.16

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%)	-0.92	0	100	100	130, 224, 265, 285	0
1	I	419/480 (87%)	-1.04	0	100	100	127, 198, 253, 268	0
2	B	403/447 (90%)	-0.93	1 (0%)	91	81	132, 224, 253, 270	0
2	J	403/447 (90%)	-0.93	1 (0%)	91	81	121, 208, 243, 263	0
3	C	401/423 (94%)	-0.93	1 (0%)	91	81	129, 172, 261, 280	0
3	K	401/423 (94%)	-0.86	1 (0%)	91	81	133, 186, 261, 276	0
4	D	406/410 (99%)	-1.02	0	100	100	133, 191, 268, 297	0
4	L	225/410 (54%)	-1.05	0	100	100	136, 189, 232, 249	0
5	E	298/334 (89%)	-0.99	0	100	100	142, 176, 217, 258	0
5	M	298/334 (89%)	-1.05	0	100	100	128, 156, 187, 222	0
6	F	281/331 (84%)	-1.00	0	100	100	133, 180, 208, 224	0
6	N	281/331 (84%)	-0.93	0	100	100	130, 177, 212, 221	0
7	G	208/222 (93%)	-0.84	0	100	100	140, 194, 247, 256	0
7	O	208/222 (93%)	-1.07	0	100	100	133, 186, 238, 250	0
8	H	173/212 (81%)	-1.07	0	100	100	135, 175, 215, 232	0
8	P	173/212 (81%)	-0.98	0	100	100	162, 198, 230, 240	0
All	All	4997/5718 (87%)	-0.97	4 (0%)	92	87	121, 187, 253, 297	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	54	HIS	3.9
2	J	203	GLN	3.6
2	B	203	GLN	3.4
3	C	134	ASN	2.2

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($\text{\AA}^2$)	Q<0.9
9	ZN	E	999	1/1	1.00	0.03	149,149,149,149	0
9	ZN	M	999	1/1	1.00	0.01	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.