wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 09:47 PM EDT

PDB ID	:	4AJ5
Title	:	Crystal structure of the Ska core complex
Authors	:	Jeyaprakash, A.A.; Santamaria, A.; Jayachandran, U.; Chan, Y.W.; Benda, C.; Nigg, E.A.; Conti, E.
Deposited on	:	2012-02-15
Resolution	:	3.32 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

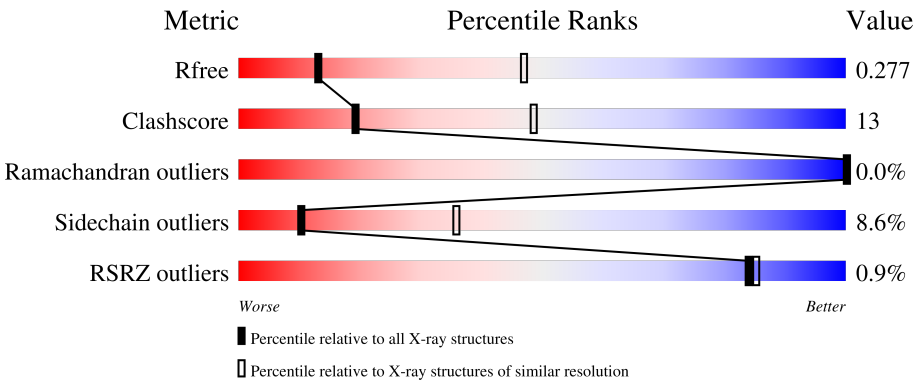
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 <=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	1	101	69% 25% • •
1	2	101	% 64% 30% 5% •
1	3	101	71% 24% • •
1	4	101	67% 25% 5% •
1	U	101	63% 33% • •

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Mol	Chain	Length	Quality of chain
1	V	101	%, 68%, 28%
1	W	101	67%, 28%
1	X	101	%, 74%, 21%
1	Y	101	65%, 26%, 7%
1	Z	101	%, 54%, 40%
2	A	91	%, 59%, 24%, 13%
2	B	91	%, 71%, 19%, 5%
2	C	91	64%, 18%, 5%, 13%
2	D	91	2%, 66%, 26%, 5%
2	E	91	68%, 23%, 5%
2	F	91	62%, 27%, 10%
2	G	91	76%, 16%, 5%
2	H	91	%, 63%, 24%, 9%
2	I	91	%, 75%, 15%, 5%
2	J	91	66%, 25%, 5%
3	K	123	%, 60%, 23%, 5%, 12%
3	L	123	3%, 63%, 21%, 14%
3	M	123	%, 59%, 25%, 5%, 11%
3	N	123	2%, 63%, 18%, 15%
3	O	123	54%, 32%, 11%
3	P	123	%, 57%, 25%, 15%
3	Q	123	63%, 19%, 17%
3	R	123	2%, 54%, 30%, 12%
3	S	123	2%, 57%, 27%, 13%
3	T	123	%, 58%, 28%, 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21691 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 SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	99	740	458	128	151	3	0	0	0
1	2	100	787	491	135	156	5	0	0	0
1	3	98	738	459	126	149	4	0	0	0
1	4	98	775	484	134	151	6	0	0	0
1	U	100	773	484	131	152	6	0	0	0
1	V	98	725	448	126	148	3	0	0	0
1	W	98	727	449	128	146	4	0	0	0
1	X	98	729	453	126	147	3	0	0	0
1	Y	99	763	479	133	146	5	0	0	0
1	Z	97	723	446	127	146	4	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	58	ILE	VAL	engineered mutation	UNP Q8IX90
2	58	ILE	VAL	engineered mutation	UNP Q8IX90
3	58	ILE	VAL	engineered mutation	UNP Q8IX90
4	58	ILE	VAL	engineered mutation	UNP Q8IX90
U	58	ILE	VAL	engineered mutation	UNP Q8IX90
V	58	ILE	VAL	engineered mutation	UNP Q8IX90
W	58	ILE	VAL	engineered mutation	UNP Q8IX90
X	58	ILE	VAL	engineered mutation	UNP Q8IX90

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	58	ILE	VAL	engineered mutation	UNP Q8IX90
Z	58	ILE	VAL	engineered mutation	UNP Q8IX90

- Molecule 2 is a protein called SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	79	588	363	99	123	3	0	0	0
2	B	87	656	406	109	138	3	0	0	0
2	C	79	595	369	100	123	3	0	0	0
2	D	86	646	399	108	136	3	0	0	0
2	E	86	630	387	108	132	3	0	0	0
2	F	82	585	362	102	118	3	0	0	0
2	G	86	637	392	108	134	3	0	0	0
2	H	83	633	391	104	135	3	0	0	0
2	I	86	645	398	109	135	3	0	0	0
2	J	86	639	396	105	135	3	0	0	0

- Molecule 3 is a protein called SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	K	108	813	511	132	166	4	0	0	0
3	L	106	779	491	130	155	3	0	0	0
3	M	109	800	505	133	158	4	0	0	0
3	N	104	770	485	129	152	4	0	0	0
3	O	109	840	528	140	168	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	P	105	776	491	125	155	5	0	0	0
			Total	C	N	O	S			
3	Q	102	729	457	123	145	4	0	0	0
			Total	C	N	O	S			
3	R	108	826	520	138	163	5	0	0	0
			Total	C	N	O	S			
3	S	107	785	495	129	157	4	0	0	0
			Total	C	N	O	S			
3	T	110	839	534	137	163	5	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	expression tag	UNP Q8WVK7
K	0	HIS	-	expression tag	UNP Q8WVK7
L	-1	GLY	-	expression tag	UNP Q8WVK7
L	0	HIS	-	expression tag	UNP Q8WVK7
M	-1	GLY	-	expression tag	UNP Q8WVK7
M	0	HIS	-	expression tag	UNP Q8WVK7
N	-1	GLY	-	expression tag	UNP Q8WVK7
N	0	HIS	-	expression tag	UNP Q8WVK7
O	-1	GLY	-	expression tag	UNP Q8WVK7
O	0	HIS	-	expression tag	UNP Q8WVK7
P	-1	GLY	-	expression tag	UNP Q8WVK7
P	0	HIS	-	expression tag	UNP Q8WVK7
Q	-1	GLY	-	expression tag	UNP Q8WVK7
Q	0	HIS	-	expression tag	UNP Q8WVK7
R	-1	GLY	-	expression tag	UNP Q8WVK7
R	0	HIS	-	expression tag	UNP Q8WVK7
S	-1	GLY	-	expression tag	UNP Q8WVK7
S	0	HIS	-	expression tag	UNP Q8WVK7
T	-1	GLY	-	expression tag	UNP Q8WVK7
T	0	HIS	-	expression tag	UNP Q8WVK7

3 Residue-property plots (i)

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: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

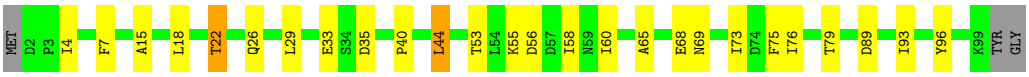
Chain 1:

• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain 2:

• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain 3:



• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

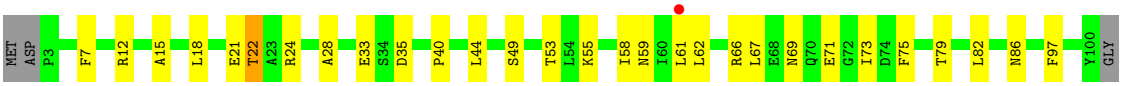
Chain 4:

• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain U:

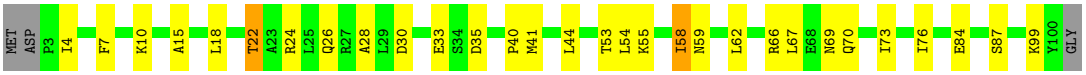
• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain V:



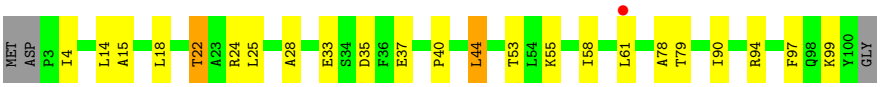
• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain W:



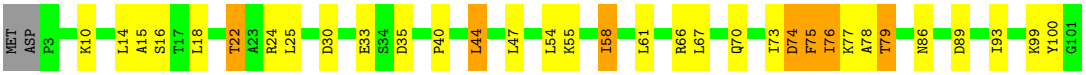
• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain X:



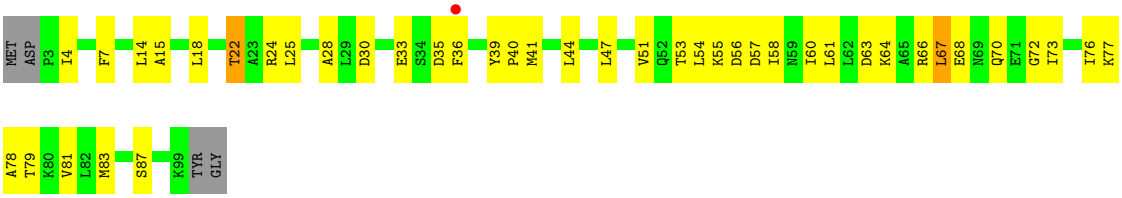
• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain Y:



• Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 3

Chain Z:

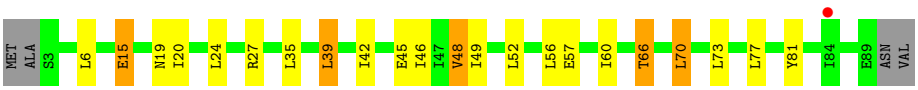


• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain A:

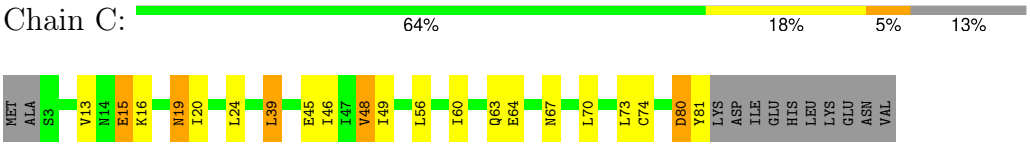
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain B:



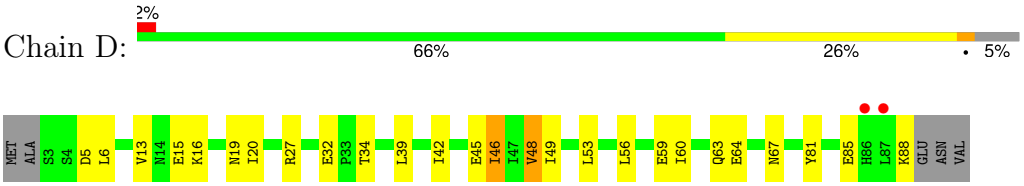
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain C:



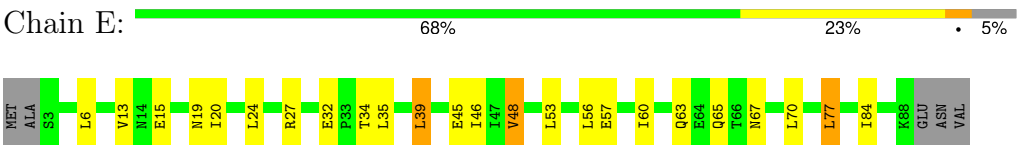
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain D:



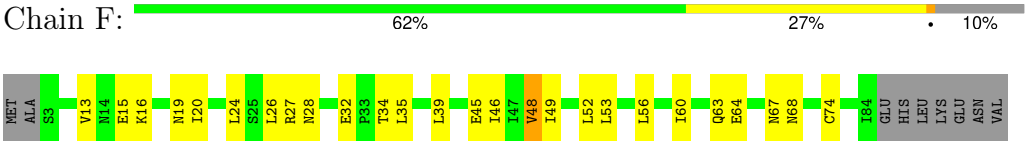
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain E:



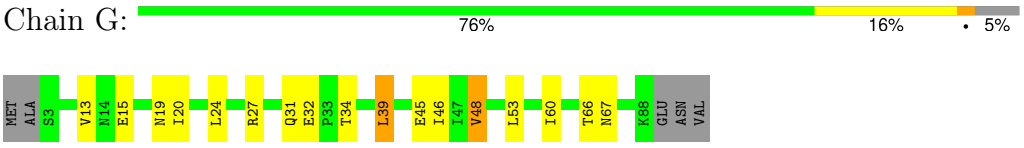
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain F:



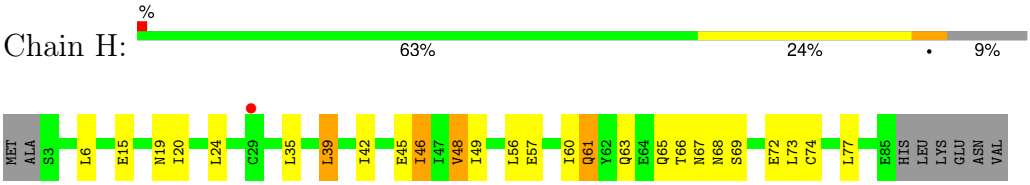
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain G:



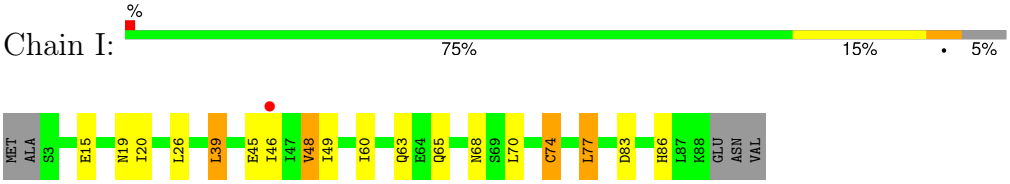
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain H:



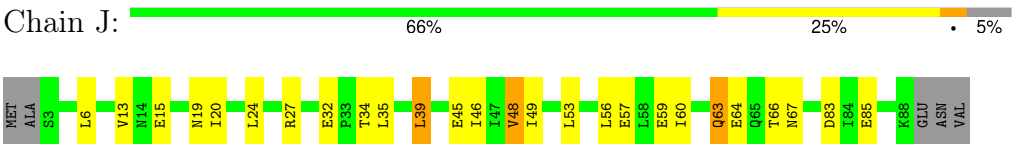
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain I:



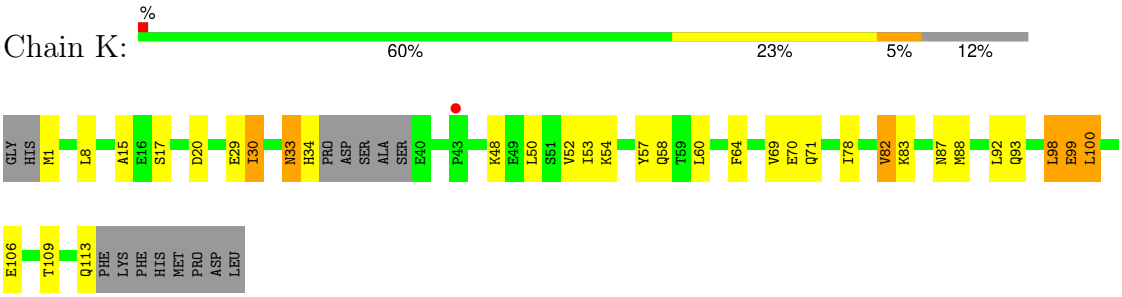
• Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 1

Chain J:



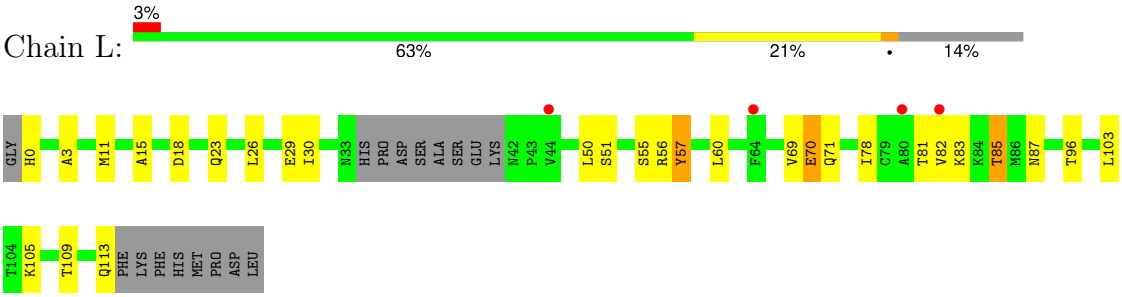
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain K:



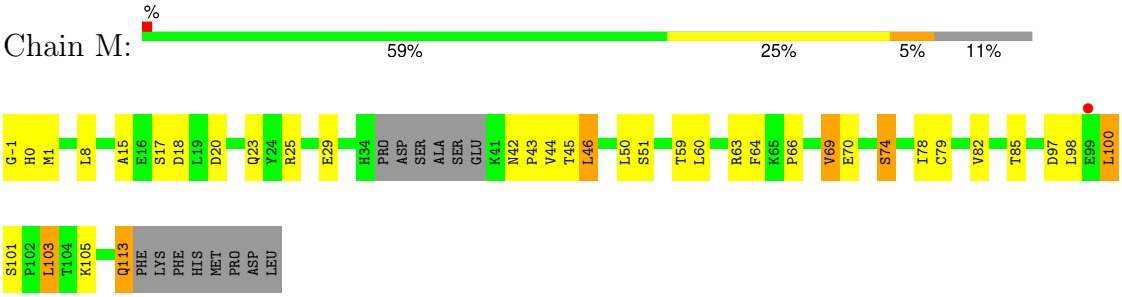
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain L:



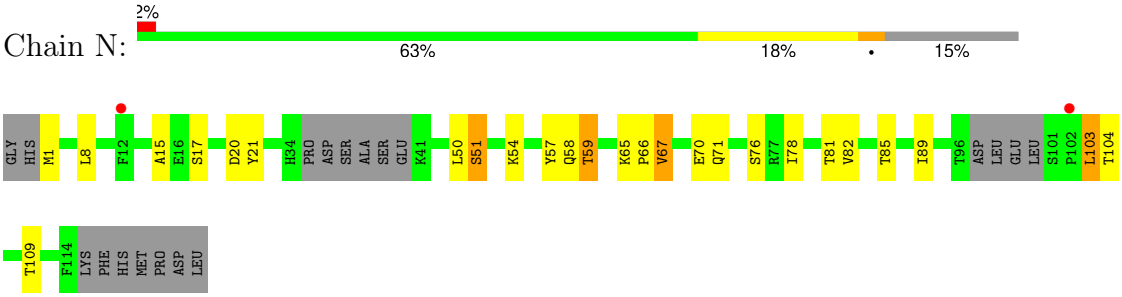
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain M:



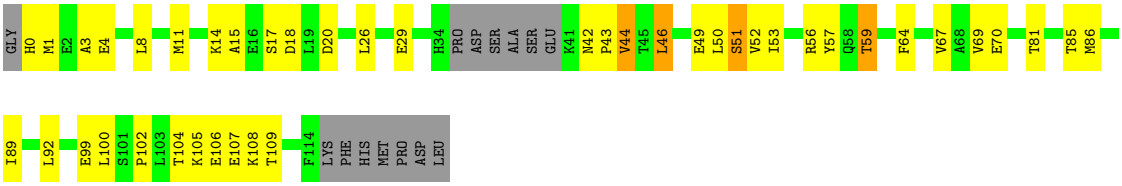
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain N:



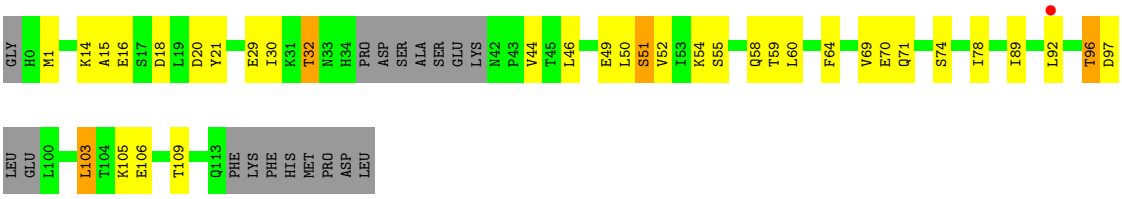
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain O:



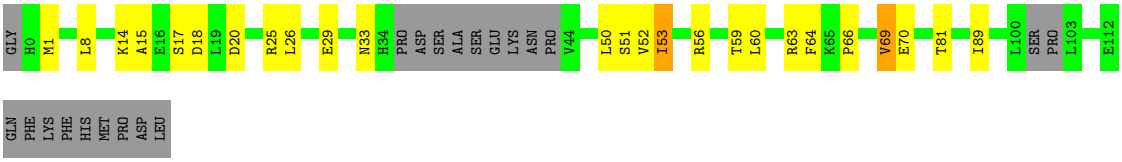
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain P:



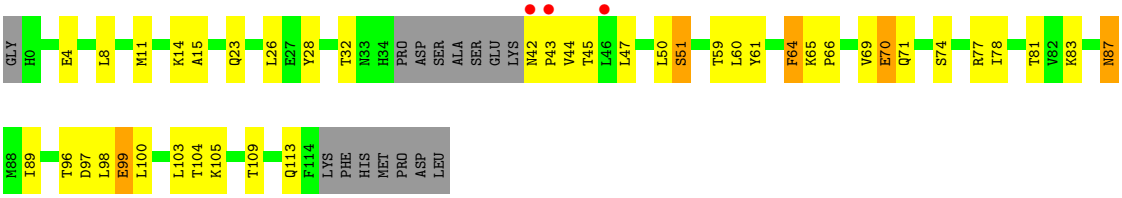
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain Q:



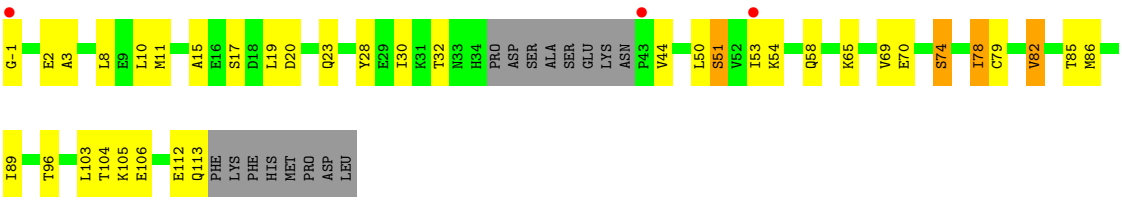
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain R:



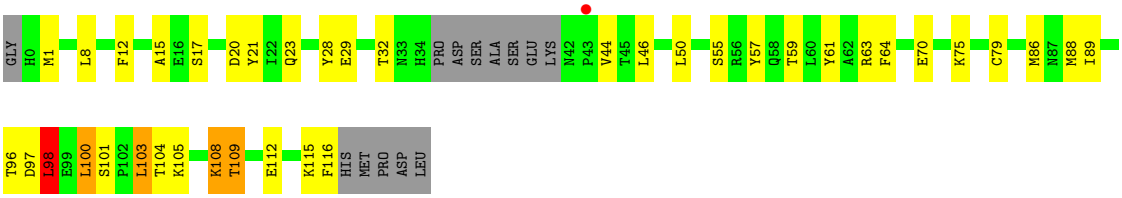
• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain S:



• Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATED PROTEIN 2

Chain T:


GLY
HO
M1
L8
F12
A15
E16
S17
D20
Y21
I22
Q23
Y28
E29
T32
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H34
PRO
ASP
SER
ALA
SER
GLU
LYS
N42
P43
V44
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L46
L50
S55
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D97
L98
E99
L100
S101
P102
L103
T104
K105
K108
T109
E112
K115
F116
HIS
MET
PRO
ASP
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.40Å 193.12Å 198.27Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	69.03 – 3.32 81.12 – 3.32	Depositor EDS
% Data completeness (in resolution range)	94.2 (69.03-3.32) 94.4 (81.12-3.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.234 , 0.280 0.233 , 0.277	Depositor DCC
R_{free} test set	4579 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	104.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 96.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21691	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1	0.39	0/747	0.64	0/1012
1	2	0.46	0/796	0.70	0/1071
1	3	0.38	0/745	0.65	0/1008
1	4	0.42	0/783	0.65	0/1050
1	U	0.41	0/782	0.69	0/1055
1	V	0.40	0/733	0.64	0/993
1	W	0.41	0/734	0.68	1/991 (0.1%)
1	X	0.42	0/738	0.64	0/1000
1	Y	0.48	0/772	0.75	1/1039 (0.1%)
1	Z	0.42	0/729	0.71	1/984 (0.1%)
2	A	0.37	0/590	0.52	0/800
2	B	0.37	0/659	0.53	0/894
2	C	0.38	0/598	0.51	0/811
2	D	0.45	0/649	0.54	0/879
2	E	0.38	0/632	0.53	0/858
2	F	0.40	0/587	0.53	0/799
2	G	0.40	0/639	0.51	0/867
2	H	0.47	0/636	0.61	0/862
2	I	0.40	0/648	0.47	0/879
2	J	0.39	0/642	0.50	0/873
3	K	0.40	0/822	0.63	1/1117 (0.1%)
3	L	0.42	0/788	0.58	0/1074
3	M	0.40	0/809	0.59	0/1101
3	N	0.40	0/778	0.57	1/1056 (0.1%)
3	O	0.50	0/850	0.70	0/1152
3	P	0.42	0/785	0.61	0/1070
3	Q	0.43	0/736	0.58	0/1001
3	R	0.46	0/836	0.69	0/1134
3	S	0.42	0/794	0.63	0/1081
3	T	0.42	0/851	0.67	2/1155 (0.2%)
All	All	0.42	0/21888	0.62	7/29666 (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
3	K	0	1
3	R	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	67	LEU	CA-CB-CG	5.96	129.02	115.30
3	T	98	LEU	CA-CB-CG	5.89	128.86	115.30
3	K	98	LEU	CA-CB-CG	5.69	128.39	115.30
3	T	103	LEU	CA-CB-CG	5.37	127.64	115.30
1	W	67	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	99	GLU	Peptide
3	R	99	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	1	740	0	677	20	0
1	2	787	0	758	32	0
1	3	738	0	691	18	0
1	4	775	0	763	29	0
1	U	773	0	737	33	0
1	V	725	0	643	24	0
1	W	727	0	663	26	0
1	X	729	0	648	18	0
1	Y	763	0	737	35	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	723	0	672	32	0
2	A	588	0	568	21	0
2	B	656	0	627	19	0
2	C	595	0	577	20	0
2	D	646	0	614	26	0
2	E	630	0	592	24	0
2	F	585	0	545	26	0
2	G	637	0	605	15	0
2	H	633	0	608	24	1
2	I	645	0	617	14	0
2	J	639	0	602	19	0
3	K	813	0	749	26	0
3	L	779	0	707	24	0
3	M	800	0	724	29	0
3	N	770	0	701	24	0
3	O	840	0	793	41	0
3	P	776	0	705	36	0
3	Q	729	0	621	23	0
3	R	826	0	779	43	0
3	S	785	0	715	31	0
3	T	839	0	784	34	0
All	All	21691	0	20222	540	1

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 13.

The worst 5 of 540 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)
2:B:52:LEU:HB3	1:W:58:ILE:HD11	1.45	0.98
3:M:25:ARG:HH12	3:P:59:THR:HG21	1.36	0.91
1:2:61:LEU:HD23	2:H:56:LEU:HD21	1.54	0.88
2:D:53:LEU:HD21	1:Y:58:ILE:HD11	1.57	0.87
2:F:49:ILE:HD11	1:Z:54:LEU:HD22	1.56	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:GLN:OE1	1:Y:70:GLN:NE2[3_445]	2.04	0.16

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	97/101 (96%)	89 (92%)	8 (8%)	0	100	100
1	2	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
1	3	96/101 (95%)	86 (90%)	10 (10%)	0	100	100
1	4	96/101 (95%)	85 (88%)	11 (12%)	0	100	100
1	U	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
1	V	96/101 (95%)	85 (88%)	11 (12%)	0	100	100
1	W	96/101 (95%)	89 (93%)	7 (7%)	0	100	100
1	X	96/101 (95%)	87 (91%)	9 (9%)	0	100	100
1	Y	97/101 (96%)	85 (88%)	12 (12%)	0	100	100
1	Z	95/101 (94%)	86 (90%)	9 (10%)	0	100	100
2	A	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
2	B	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
2	C	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
2	D	84/91 (92%)	82 (98%)	2 (2%)	0	100	100
2	E	84/91 (92%)	83 (99%)	1 (1%)	0	100	100
2	F	80/91 (88%)	78 (98%)	2 (2%)	0	100	100
2	G	84/91 (92%)	83 (99%)	1 (1%)	0	100	100
2	H	81/91 (89%)	77 (95%)	4 (5%)	0	100	100
2	I	84/91 (92%)	83 (99%)	1 (1%)	0	100	100
2	J	84/91 (92%)	82 (98%)	2 (2%)	0	100	100
3	K	104/123 (85%)	95 (91%)	8 (8%)	1 (1%)	15	47
3	L	102/123 (83%)	96 (94%)	6 (6%)	0	100	100
3	M	103/123 (84%)	96 (93%)	7 (7%)	0	100	100
3	N	98/123 (80%)	96 (98%)	2 (2%)	0	100	100
3	O	105/123 (85%)	90 (86%)	15 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	99/123 (80%)	93 (94%)	6 (6%)	0	100	100
3	Q	96/123 (78%)	93 (97%)	3 (3%)	0	100	100
3	R	104/123 (85%)	94 (90%)	10 (10%)	0	100	100
3	S	103/123 (84%)	96 (93%)	7 (7%)	0	100	100
3	T	106/123 (86%)	96 (91%)	10 (9%)	0	100	100
All	All	2805/3150 (89%)	2614 (93%)	190 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	30	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	74/92 (80%)	67 (90%)	7 (10%)	8	30
1	2	84/92 (91%)	77 (92%)	7 (8%)	11	37
1	3	76/92 (83%)	69 (91%)	7 (9%)	9	32
1	4	84/92 (91%)	78 (93%)	6 (7%)	14	44
1	U	81/92 (88%)	77 (95%)	4 (5%)	25	57
1	V	70/92 (76%)	67 (96%)	3 (4%)	29	61
1	W	71/92 (77%)	65 (92%)	6 (8%)	10	36
1	X	70/92 (76%)	65 (93%)	5 (7%)	14	44
1	Y	79/92 (86%)	72 (91%)	7 (9%)	9	33
1	Z	73/92 (79%)	68 (93%)	5 (7%)	16	46
2	A	66/87 (76%)	60 (91%)	6 (9%)	9	32
2	B	73/87 (84%)	66 (90%)	7 (10%)	8	30
2	C	67/87 (77%)	61 (91%)	6 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	71/87 (82%)	68 (96%)	3 (4%)	30	61
2	E	68/87 (78%)	62 (91%)	6 (9%)	10	34
2	F	60/87 (69%)	55 (92%)	5 (8%)	11	37
2	G	70/87 (80%)	66 (94%)	4 (6%)	20	52
2	H	72/87 (83%)	64 (89%)	8 (11%)	6	24
2	I	72/87 (83%)	65 (90%)	7 (10%)	8	30
2	J	70/87 (80%)	64 (91%)	6 (9%)	10	36
3	K	81/114 (71%)	70 (86%)	11 (14%)	3	16
3	L	74/114 (65%)	67 (90%)	7 (10%)	8	30
3	M	76/114 (67%)	66 (87%)	10 (13%)	4	17
3	N	73/114 (64%)	68 (93%)	5 (7%)	16	46
3	O	86/114 (75%)	78 (91%)	8 (9%)	9	31
3	P	76/114 (67%)	69 (91%)	7 (9%)	9	32
3	Q	63/114 (55%)	58 (92%)	5 (8%)	12	39
3	R	84/114 (74%)	77 (92%)	7 (8%)	11	37
3	S	75/114 (66%)	67 (89%)	8 (11%)	6	25
3	T	84/114 (74%)	76 (90%)	8 (10%)	8	30
All	All	2223/2930 (76%)	2032 (91%)	191 (9%)	10	36

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	67	VAL
3	R	100	LEU
3	O	46	LEU
3	P	69	VAL
3	S	82	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	23	GLN
3	T	23	GLN
3	Q	33	ASN
3	R	93	GLN

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Mol	Chain	Res	Type
2	G	40	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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
3	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	96:THR	C	97:ASP	N	3.27

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	1	99/101 (98%)	-0.19	0 100 100	78, 143, 198, 211	0
1	2	100/101 (99%)	-0.20	1 (1%) 82 83	88, 122, 176, 211	0
1	3	98/101 (97%)	-0.27	0 100 100	79, 143, 196, 243	0
1	4	98/101 (97%)	-0.12	0 100 100	82, 125, 196, 242	0
1	U	100/101 (99%)	-0.37	0 100 100	77, 136, 173, 194	0
1	V	98/101 (97%)	-0.03	1 (1%) 82 83	79, 155, 211, 241	0
1	W	98/101 (97%)	-0.32	0 100 100	76, 147, 187, 203	0
1	X	98/101 (97%)	-0.24	1 (1%) 82 83	82, 148, 196, 239	0
1	Y	99/101 (98%)	-0.24	0 100 100	75, 115, 161, 195	0
1	Z	97/101 (96%)	-0.05	1 (1%) 82 83	81, 151, 207, 236	0
2	A	79/91 (86%)	-0.11	1 (1%) 77 77	99, 142, 224, 229	0
2	B	87/91 (95%)	-0.34	1 (1%) 80 81	90, 142, 207, 223	0
2	C	79/91 (86%)	-0.22	0 100 100	93, 137, 222, 250	0
2	D	86/91 (94%)	-0.09	2 (2%) 60 59	84, 129, 190, 263	0
2	E	86/91 (94%)	-0.41	0 100 100	95, 140, 191, 245	0
2	F	82/91 (90%)	-0.26	0 100 100	98, 142, 194, 224	0
2	G	86/91 (94%)	-0.02	0 100 100	91, 140, 248, 277	0
2	H	83/91 (91%)	-0.24	1 (1%) 79 79	73, 127, 165, 227	0
2	I	86/91 (94%)	-0.16	1 (1%) 79 79	90, 144, 210, 281	0
2	J	86/91 (94%)	-0.24	0 100 100	84, 136, 207, 272	0
3	K	108/123 (87%)	-0.46	1 (0%) 84 85	81, 144, 199, 224	0
3	L	106/123 (86%)	-0.02	4 (3%) 40 39	85, 163, 229, 248	0
3	M	109/123 (88%)	-0.31	1 (0%) 84 85	85, 139, 223, 292	0
3	N	104/123 (84%)	-0.27	2 (1%) 66 65	83, 139, 224, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	O	109/123 (88%)	-0.38	0 100 100	83, 118, 159, 186	0
3	P	105/123 (85%)	-0.23	1 (0%) 82 83	79, 140, 217, 250	0
3	Q	102/123 (82%)	-0.33	0 100 100	81, 133, 214, 275	0
3	R	108/123 (87%)	-0.25	3 (2%) 53 51	75, 117, 176, 199	0
3	S	107/123 (86%)	-0.28	3 (2%) 53 51	89, 141, 211, 218	0
3	T	110/123 (89%)	-0.40	1 (0%) 84 85	81, 123, 187, 203	0
All	All	2893/3150 (91%)	-0.24	26 (0%) 84 85	73, 136, 206, 292	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	43	PRO	4.2
3	P	92	LEU	3.6
3	S	-1	GLY	3.5
2	A	73	LEU	2.9
3	S	53	ILE	2.8

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.