wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 04:32 AM EDT

PDB ID	:	5VJX
Title	:	Crystal structure of the CLOCK Transcription Domain Exon19 in Complex with a Repressor
Authors	:	Hou, Z.; Su, L.; Pei, J.; Grishin, N.V.; Zhang, H.
Deposited on	:	2017-04-20
Resolution	:	2.69 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 (i)) were used in the production of this report:

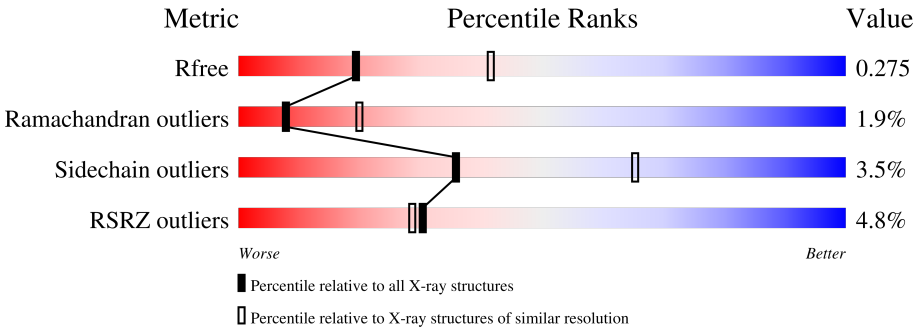
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.69 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	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	A	64	14%, 84%, ·, 14%
1	D	64	92%, 6%, ·
1	G	64	2%, 92%, 6%, ·
1	J	64	2%, 95%, 5%
1	M	64	2%, 84%, 16%
1	R	64	91%, 9%

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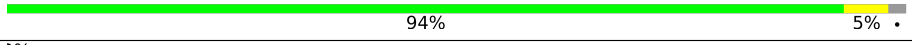
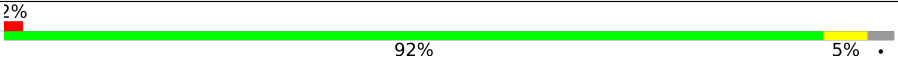
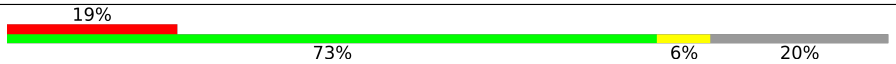
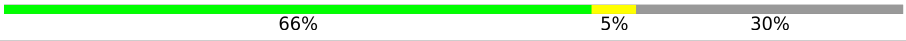
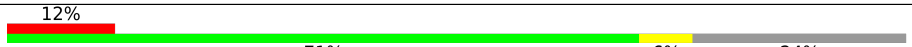
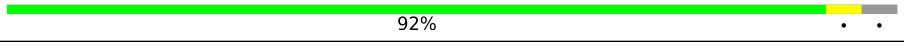
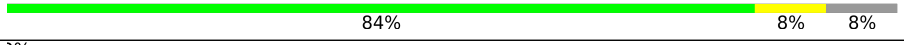
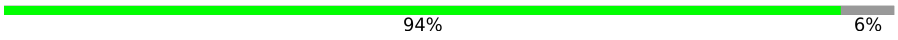
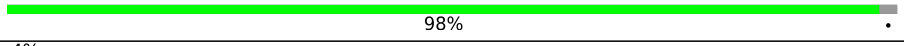
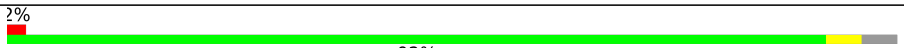
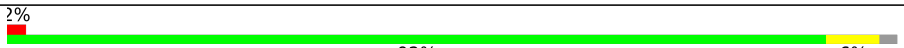
Mol	Chain	Length	Quality of chain
1	U	64	
1	X	64	
1	a	64	
1	d	64	
2	B	51	
2	C	51	
2	E	51	
2	F	51	
2	H	51	
2	I	51	
2	K	51	
2	L	51	
2	N	51	
2	O	51	
2	S	51	
2	T	51	
2	V	51	
2	W	51	
2	Y	51	
2	Z	51	
2	b	51	
2	c	51	
2	e	51	
2	f	51	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12585 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 CLOCK-interacting pacemaker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	55	Total	C	N	O	Se	0	0	0
			436	277	74	84	1			
1	D	63	Total	C	N	O	Se	0	0	0
			497	312	88	96	1			
1	G	63	Total	C	N	O	Se	0	0	0
			495	311	88	95	1			
1	J	64	Total	C	N	O	Se	0	0	0
			501	314	89	97	1			
1	M	64	Total	C	N	O	Se	0	0	0
			501	314	89	97	1			
1	R	64	Total	C	N	O	Se	0	1	0
			509	319	92	97	1			
1	U	63	Total	C	N	O	Se	0	0	0
			495	311	88	95	1			
1	X	62	Total	C	N	O	Se	0	0	0
			485	306	85	93	1			
1	a	51	Total	C	N	O	Se	0	0	0
			405	255	70	79	1			
1	d	45	Total	C	N	O	Se	0	0	0
			360	226	62	71	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8R0W1
D	1	GLY	-	expression tag	UNP Q8R0W1
G	1	GLY	-	expression tag	UNP Q8R0W1
J	1	GLY	-	expression tag	UNP Q8R0W1
M	1	GLY	-	expression tag	UNP Q8R0W1
R	1	GLY	-	expression tag	UNP Q8R0W1
U	1	GLY	-	expression tag	UNP Q8R0W1
X	1	GLY	-	expression tag	UNP Q8R0W1
a	1	GLY	-	expression tag	UNP Q8R0W1

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Chain	Residue	Modelled	Actual	Comment	Reference
d	1	GLY	-	expression tag	UNP Q8R0W1

- Molecule 2 is a protein called Circadian locomoter output cycles protein kaput.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	Se	0	0	0
			327	197	66	62	2			
2	C	37	Total	C	N	O	Se	0	0	0
			316	191	64	59	2			
2	E	49	Total	C	N	O	Se	0	0	0
			403	245	77	77	4			
2	F	44	Total	C	N	O	Se	0	0	0
			371	225	72	72	2			
2	H	51	Total	C	N	O	Se	0	0	0
			417	253	81	79	4			
2	I	47	Total	C	N	O	Se	0	0	0
			388	235	75	75	3			
2	K	43	Total	C	N	O	Se	0	1	0
			367	225	71	67	4			
2	L	49	Total	C	N	O	Se	0	0	0
			409	249	79	77	4			
2	N	42	Total	C	N	O	Se	0	2	0
			368	225	73	66	4			
2	O	48	Total	C	N	O	Se	0	0	0
			399	243	76	76	4			
2	S	50	Total	C	N	O	Se	0	0	0
			413	251	80	78	4			
2	T	44	Total	C	N	O	Se	0	0	0
			371	226	72	70	3			
2	V	49	Total	C	N	O	Se	0	1	0
			408	249	77	77	5			
2	W	50	Total	C	N	O	Se	0	0	0
			413	251	80	78	4			
2	Y	46	Total	C	N	O	Se	0	0	0
			384	233	74	74	3			
2	Z	36	Total	C	N	O	Se	0	1	0
			320	194	64	59	3			
2	b	47	Total	C	N	O	Se	0	0	0
			396	241	77	75	3			
2	c	38	Total	C	N	O	Se	0	0	0
			325	196	66	61	2			
2	e	44	Total	C	N	O	Se	0	0	0
			372	227	74	68	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	f	47	Total	C	N	O	Se	0	0	0
			396	241	77	75	3			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP O08785
B	2	ALA	-	expression tag	UNP O08785
B	3	MSE	-	expression tag	UNP O08785
B	4	ASP	-	expression tag	UNP O08785
B	5	PRO	-	expression tag	UNP O08785
B	6	GLU	GLN	conflict	UNP O08785
C	1	GLY	-	expression tag	UNP O08785
C	2	ALA	-	expression tag	UNP O08785
C	3	MSE	-	expression tag	UNP O08785
C	4	ASP	-	expression tag	UNP O08785
C	5	PRO	-	expression tag	UNP O08785
C	6	GLU	GLN	conflict	UNP O08785
E	1	GLY	-	expression tag	UNP O08785
E	2	ALA	-	expression tag	UNP O08785
E	3	MSE	-	expression tag	UNP O08785
E	4	ASP	-	expression tag	UNP O08785
E	5	PRO	-	expression tag	UNP O08785
E	6	GLU	GLN	conflict	UNP O08785
F	1	GLY	-	expression tag	UNP O08785
F	2	ALA	-	expression tag	UNP O08785
F	3	MSE	-	expression tag	UNP O08785
F	4	ASP	-	expression tag	UNP O08785
F	5	PRO	-	expression tag	UNP O08785
F	6	GLU	GLN	conflict	UNP O08785
H	1	GLY	-	expression tag	UNP O08785
H	2	ALA	-	expression tag	UNP O08785
H	3	MSE	-	expression tag	UNP O08785
H	4	ASP	-	expression tag	UNP O08785
H	5	PRO	-	expression tag	UNP O08785
H	6	GLU	GLN	conflict	UNP O08785
I	1	GLY	-	expression tag	UNP O08785
I	2	ALA	-	expression tag	UNP O08785
I	3	MSE	-	expression tag	UNP O08785
I	4	ASP	-	expression tag	UNP O08785
I	5	PRO	-	expression tag	UNP O08785
I	6	GLU	GLN	conflict	UNP O08785

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	GLY	-	expression tag	UNP O08785
K	2	ALA	-	expression tag	UNP O08785
K	3	MSE	-	expression tag	UNP O08785
K	4	ASP	-	expression tag	UNP O08785
K	5	PRO	-	expression tag	UNP O08785
K	6	GLU	GLN	conflict	UNP O08785
L	1	GLY	-	expression tag	UNP O08785
L	2	ALA	-	expression tag	UNP O08785
L	3	MSE	-	expression tag	UNP O08785
L	4	ASP	-	expression tag	UNP O08785
L	5	PRO	-	expression tag	UNP O08785
L	6	GLU	GLN	conflict	UNP O08785
N	1	GLY	-	expression tag	UNP O08785
N	2	ALA	-	expression tag	UNP O08785
N	3	MSE	-	expression tag	UNP O08785
N	4	ASP	-	expression tag	UNP O08785
N	5	PRO	-	expression tag	UNP O08785
N	6	GLU	GLN	conflict	UNP O08785
O	1	GLY	-	expression tag	UNP O08785
O	2	ALA	-	expression tag	UNP O08785
O	3	MSE	-	expression tag	UNP O08785
O	4	ASP	-	expression tag	UNP O08785
O	5	PRO	-	expression tag	UNP O08785
O	6	GLU	GLN	conflict	UNP O08785
S	1	GLY	-	expression tag	UNP O08785
S	2	ALA	-	expression tag	UNP O08785
S	3	MSE	-	expression tag	UNP O08785
S	4	ASP	-	expression tag	UNP O08785
S	5	PRO	-	expression tag	UNP O08785
S	6	GLU	GLN	conflict	UNP O08785
T	1	GLY	-	expression tag	UNP O08785
T	2	ALA	-	expression tag	UNP O08785
T	3	MSE	-	expression tag	UNP O08785
T	4	ASP	-	expression tag	UNP O08785
T	5	PRO	-	expression tag	UNP O08785
T	6	GLU	GLN	conflict	UNP O08785
V	1	GLY	-	expression tag	UNP O08785
V	2	ALA	-	expression tag	UNP O08785
V	3	MSE	-	expression tag	UNP O08785
V	4	ASP	-	expression tag	UNP O08785
V	5	PRO	-	expression tag	UNP O08785
V	6	GLU	GLN	conflict	UNP O08785

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Chain	Residue	Modelled	Actual	Comment	Reference
W	1	GLY	-	expression tag	UNP O08785
W	2	ALA	-	expression tag	UNP O08785
W	3	MSE	-	expression tag	UNP O08785
W	4	ASP	-	expression tag	UNP O08785
W	5	PRO	-	expression tag	UNP O08785
W	6	GLU	GLN	conflict	UNP O08785
Y	1	GLY	-	expression tag	UNP O08785
Y	2	ALA	-	expression tag	UNP O08785
Y	3	MSE	-	expression tag	UNP O08785
Y	4	ASP	-	expression tag	UNP O08785
Y	5	PRO	-	expression tag	UNP O08785
Y	6	GLU	GLN	conflict	UNP O08785
Z	1	GLY	-	expression tag	UNP O08785
Z	2	ALA	-	expression tag	UNP O08785
Z	3	MSE	-	expression tag	UNP O08785
Z	4	ASP	-	expression tag	UNP O08785
Z	5	PRO	-	expression tag	UNP O08785
Z	6	GLU	GLN	conflict	UNP O08785
b	1	GLY	-	expression tag	UNP O08785
b	2	ALA	-	expression tag	UNP O08785
b	3	MSE	-	expression tag	UNP O08785
b	4	ASP	-	expression tag	UNP O08785
b	5	PRO	-	expression tag	UNP O08785
b	6	GLU	GLN	conflict	UNP O08785
c	1	GLY	-	expression tag	UNP O08785
c	2	ALA	-	expression tag	UNP O08785
c	3	MSE	-	expression tag	UNP O08785
c	4	ASP	-	expression tag	UNP O08785
c	5	PRO	-	expression tag	UNP O08785
c	6	GLU	GLN	conflict	UNP O08785
e	1	GLY	-	expression tag	UNP O08785
e	2	ALA	-	expression tag	UNP O08785
e	3	MSE	-	expression tag	UNP O08785
e	4	ASP	-	expression tag	UNP O08785
e	5	PRO	-	expression tag	UNP O08785
e	6	GLU	GLN	conflict	UNP O08785
f	1	GLY	-	expression tag	UNP O08785
f	2	ALA	-	expression tag	UNP O08785
f	3	MSE	-	expression tag	UNP O08785
f	4	ASP	-	expression tag	UNP O08785
f	5	PRO	-	expression tag	UNP O08785
f	6	GLU	GLN	conflict	UNP O08785

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	3	Total O 3 3	0	0
3	C	1	Total O 1 1	0	0
3	D	15	Total O 15 15	0	0
3	E	14	Total O 14 14	0	0
3	F	12	Total O 12 12	0	0
3	G	17	Total O 17 17	0	0
3	H	13	Total O 13 13	0	0
3	I	14	Total O 14 14	0	0
3	J	18	Total O 18 18	0	0
3	K	11	Total O 11 11	0	0
3	L	12	Total O 12 12	0	0
3	M	21	Total O 21 21	0	0
3	N	14	Total O 14 14	0	0
3	O	21	Total O 21 21	0	0
3	R	21	Total O 21 21	0	0
3	S	13	Total O 13 13	0	0
3	T	15	Total O 15 15	0	0
3	U	13	Total O 13 13	0	0
3	V	7	Total O 7 7	0	0
3	W	7	Total O 7 7	0	0

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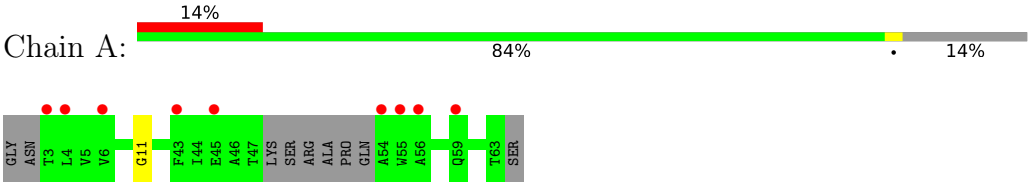
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	15	Total O 15 15	0	0
3	Y	8	Total O 8 8	0	0
3	Z	7	Total O 7 7	0	0
3	a	6	Total O 6 6	0	0
3	b	5	Total O 5 5	0	0
3	c	4	Total O 4 4	0	0
3	d	12	Total O 12 12	0	0
3	e	6	Total O 6 6	0	0
3	f	5	Total O 5 5	0	0

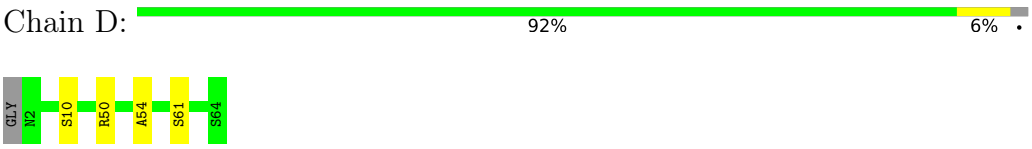
3 Residue-property plots (i)

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.

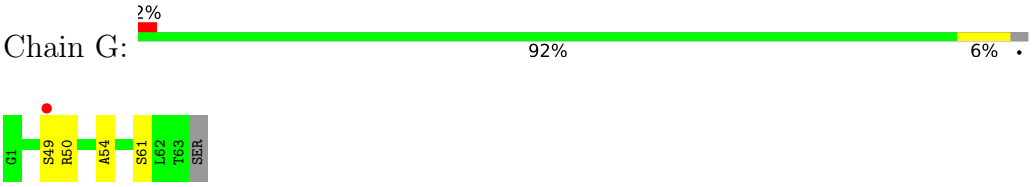
• Molecule 1: CLOCK-interacting pacemaker



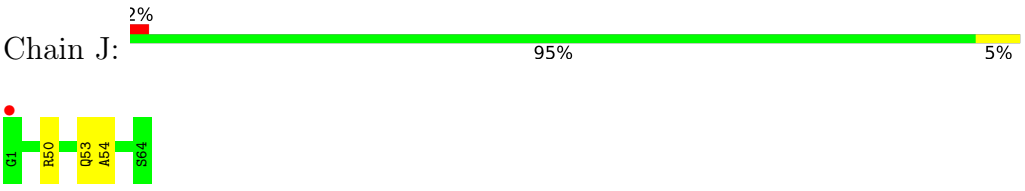
• Molecule 1: CLOCK-interacting pacemaker



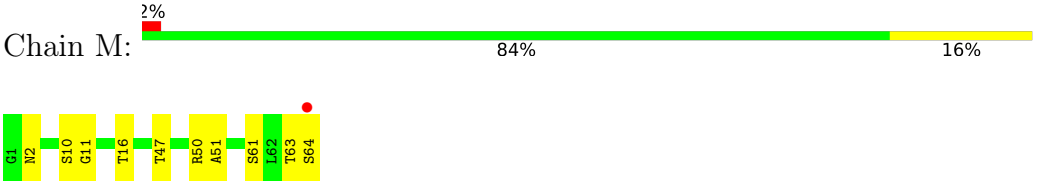
• Molecule 1: CLOCK-interacting pacemaker



• Molecule 1: CLOCK-interacting pacemaker

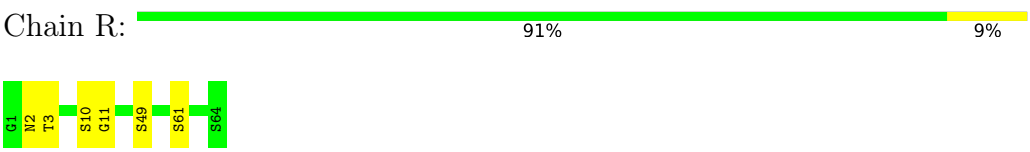


• Molecule 1: CLOCK-interacting pacemaker



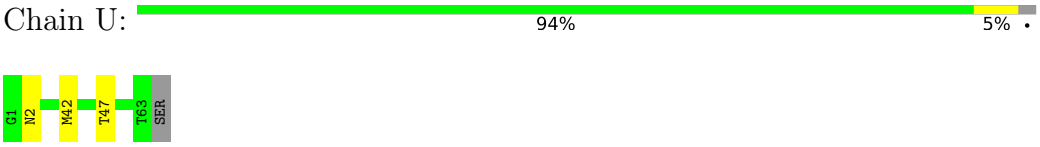
• Molecule 1: CLOCK-interacting pacemaker

Chain R:



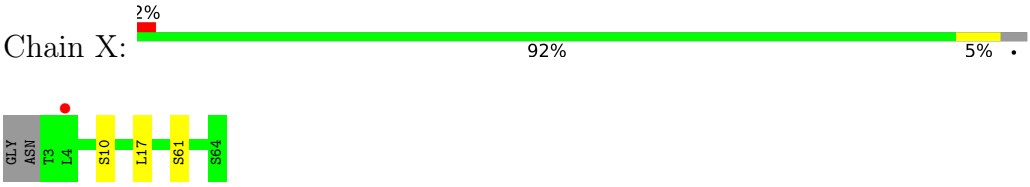
• Molecule 1: CLOCK-interacting pacemaker

Chain U:



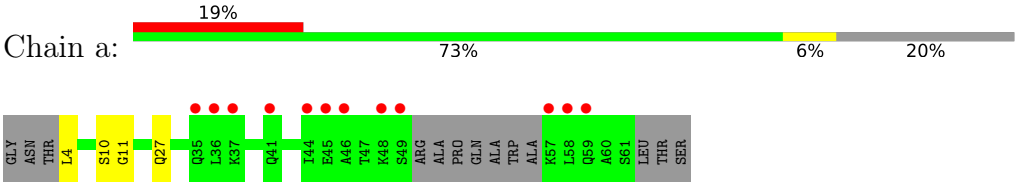
• Molecule 1: CLOCK-interacting pacemaker

Chain X:



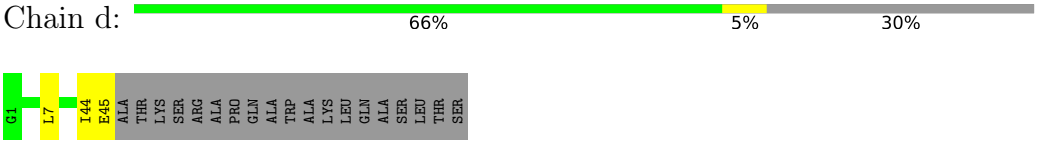
• Molecule 1: CLOCK-interacting pacemaker

Chain a:



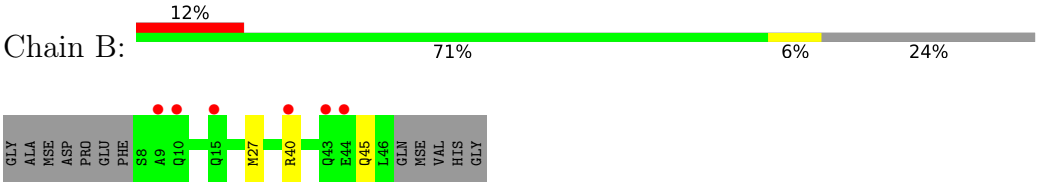
• Molecule 1: CLOCK-interacting pacemaker

Chain d:



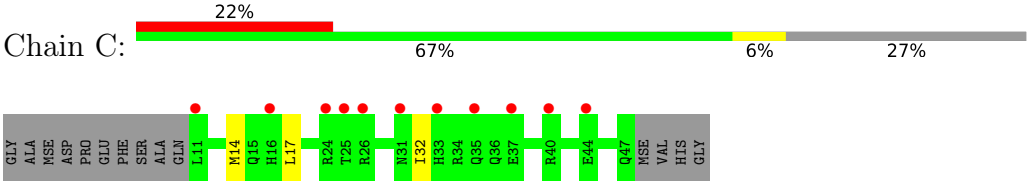
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain B:



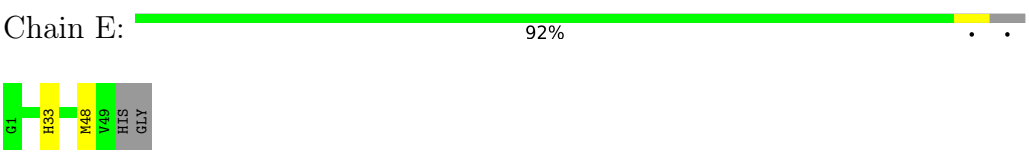
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain C:



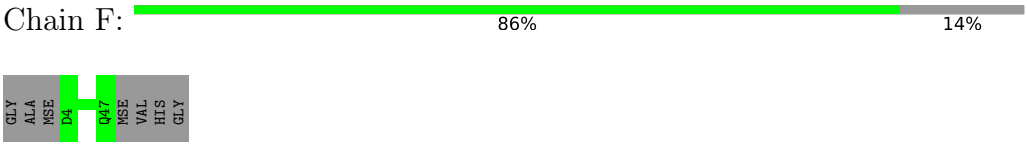
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain E:



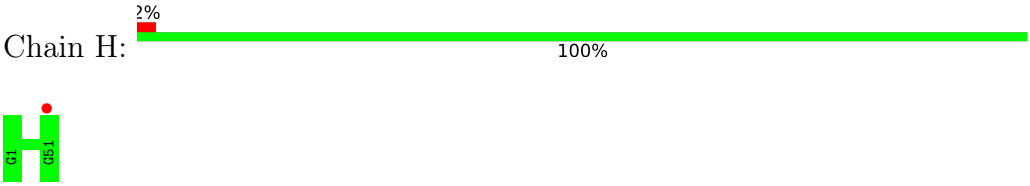
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain F:



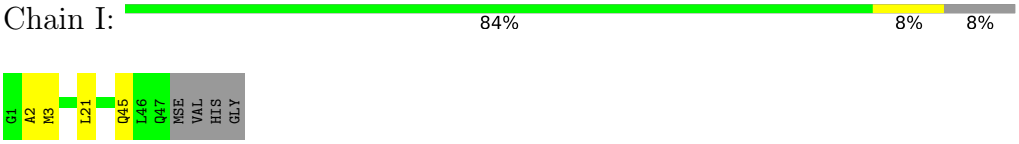
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain H:



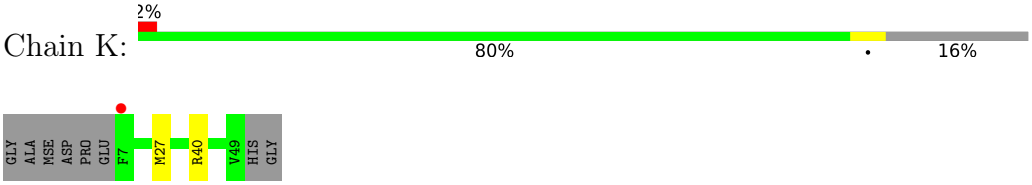
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain I:



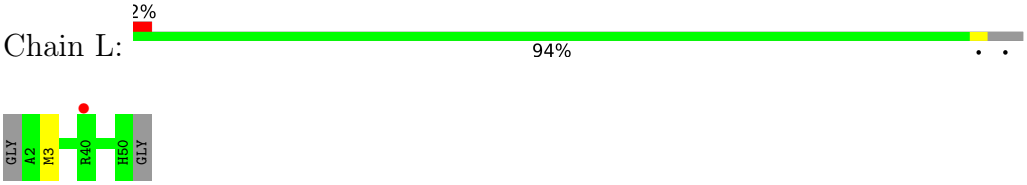
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain K:



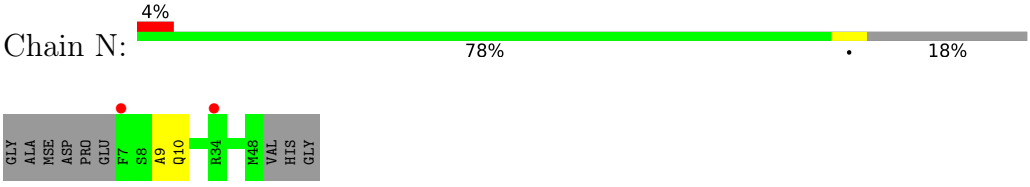
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain L:



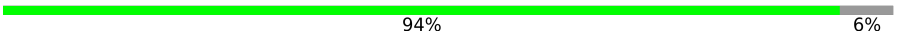
• Molecule 2: Circadian locomoter output cycles protein kaput

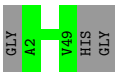
Chain N:



• Molecule 2: Circadian locomoter output cycles protein kaput

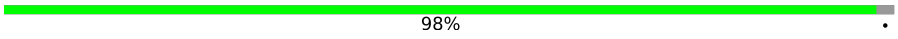
Chain O:





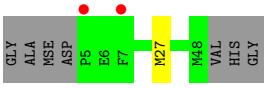
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain S:



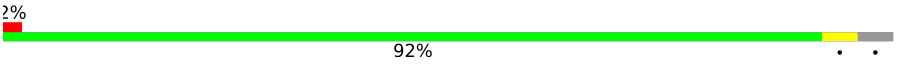
• Molecule 2: Circadian locomoter output cycles protein kaput

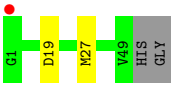
Chain T:



• Molecule 2: Circadian locomoter output cycles protein kaput

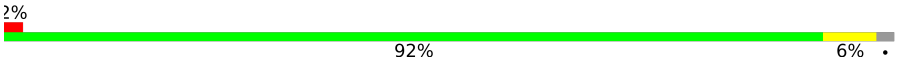
Chain V:

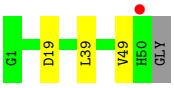




• Molecule 2: Circadian locomoter output cycles protein kaput

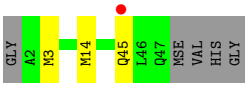
Chain W:





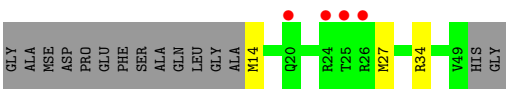
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain Y:



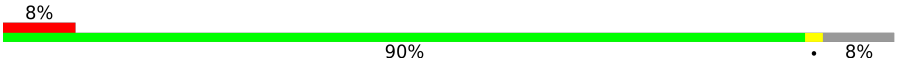
• Molecule 2: Circadian locomoter output cycles protein kaput

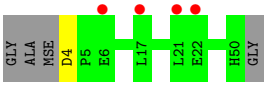
Chain Z:



• Molecule 2: Circadian locomoter output cycles protein kaput

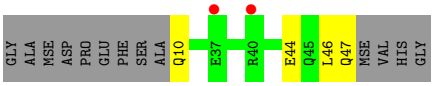
Chain b:





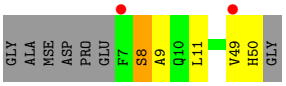
• Molecule 2: Circadian locomoter output cycles protein kaput

Chain c:



• Molecule 2: Circadian locomoter output cycles protein kaput

Chain e:



• Molecule 2: Circadian locomoter output cycles protein kaput

Chain f:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.54Å 116.84Å 132.93Å 90.00° 126.54° 90.00°	Depositor
Resolution (Å)	47.31 – 2.69 49.87 – 2.69	Depositor EDS
% Data completeness (in resolution range)	89.3 (47.31-2.69) 89.3 (49.87-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.218 , 0.275 0.220 , 0.275	Depositor DCC
R_{free} test set	2721 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12585	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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	A	0.34	0/437	0.64	0/586
1	D	0.65	0/500	0.71	0/672
1	G	0.61	0/498	0.81	1/669 (0.1%)
1	J	0.58	0/504	0.67	0/677
1	M	0.67	0/504	0.80	0/677
1	R	0.69	0/515	0.78	1/691 (0.1%)
1	U	0.58	0/498	0.70	0/669
1	X	0.59	0/488	0.67	0/656
1	a	0.38	0/404	0.64	0/537
1	d	0.73	1/360 (0.3%)	0.73	0/481
2	B	0.48	0/326	0.80	1/429 (0.2%)
2	C	0.39	0/315	0.73	0/414
2	E	0.61	0/402	0.62	0/528
2	F	0.73	0/372	0.70	0/492
2	H	0.57	0/417	0.75	0/548
2	I	0.63	0/388	0.73	0/511
2	K	0.62	0/369	0.70	0/484
2	L	0.68	0/409	0.67	0/538
2	N	0.54	0/373	0.68	0/488
2	O	0.56	0/398	0.59	0/523
2	S	0.64	0/413	0.58	0/543
2	T	0.56	0/371	0.68	0/487
2	V	0.57	0/410	0.67	0/538
2	W	0.53	0/413	0.64	0/543
2	Y	0.60	0/384	0.67	0/506
2	Z	0.55	0/322	0.74	0/423
2	b	0.39	0/397	0.63	0/524
2	c	0.42	0/324	0.63	0/426
2	e	0.52	0/372	0.65	0/489
2	f	0.47	0/397	0.67	0/524
All	All	0.58	1/12280 (0.0%)	0.69	3/16273 (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
1	D	0	1
1	M	0	1
1	R	0	1
1	X	0	1
1	a	0	1
2	e	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	45	GLU	CD-OE2	7.02	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	49	SER	C-N-CA	7.48	140.41	121.70
1	R	11	GLY	N-CA-C	5.04	125.69	113.10
2	B	40	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	10	SER	Peptide
1	M	10	SER	Peptide
1	R	10	SER	Peptide
1	X	10	SER	Peptide
1	a	10	SER	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A	51/64 (80%)	46 (90%)	4 (8%)	1 (2%)	7 19
1	D	61/64 (95%)	57 (93%)	3 (5%)	1 (2%)	9 24
1	G	61/64 (95%)	57 (93%)	2 (3%)	2 (3%)	4 8
1	J	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	9 24
1	M	62/64 (97%)	53 (86%)	7 (11%)	2 (3%)	4 9
1	R	63/64 (98%)	55 (87%)	5 (8%)	3 (5%)	2 4
1	U	61/64 (95%)	58 (95%)	2 (3%)	1 (2%)	9 24
1	X	60/64 (94%)	56 (93%)	4 (7%)	0	100 100
1	a	47/64 (73%)	43 (92%)	3 (6%)	1 (2%)	7 18
1	d	43/64 (67%)	38 (88%)	4 (9%)	1 (2%)	6 16
2	B	37/51 (72%)	34 (92%)	2 (5%)	1 (3%)	5 12
2	C	35/51 (69%)	32 (91%)	3 (9%)	0	100 100
2	E	47/51 (92%)	47 (100%)	0	0	100 100
2	F	42/51 (82%)	40 (95%)	2 (5%)	0	100 100
2	H	49/51 (96%)	46 (94%)	3 (6%)	0	100 100
2	I	45/51 (88%)	42 (93%)	1 (2%)	2 (4%)	2 5
2	K	42/51 (82%)	40 (95%)	2 (5%)	0	100 100
2	L	47/51 (92%)	43 (92%)	3 (6%)	1 (2%)	7 18
2	N	42/51 (82%)	39 (93%)	1 (2%)	2 (5%)	2 4
2	O	46/51 (90%)	46 (100%)	0	0	100 100
2	S	48/51 (94%)	47 (98%)	1 (2%)	0	100 100
2	T	42/51 (82%)	40 (95%)	2 (5%)	0	100 100
2	V	48/51 (94%)	48 (100%)	0	0	100 100
2	W	48/51 (94%)	47 (98%)	0	1 (2%)	7 18
2	Y	44/51 (86%)	42 (96%)	1 (2%)	1 (2%)	6 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Z	35/51 (69%)	33 (94%)	2 (6%)	0	100 100
2	b	45/51 (88%)	42 (93%)	3 (7%)	0	100 100
2	c	36/51 (71%)	32 (89%)	3 (8%)	1 (3%)	5 11
2	e	42/51 (82%)	36 (86%)	3 (7%)	3 (7%)	1 1
2	f	45/51 (88%)	41 (91%)	2 (4%)	2 (4%)	2 5
All	All	1436/1660 (86%)	1338 (93%)	71 (5%)	27 (2%)	8 20

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	45	GLN
2	I	45	GLN
1	J	54	ALA
1	R	2	ASN
1	U	2	ASN

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	A	48/54 (89%)	48 (100%)	0	100 100
1	D	55/54 (102%)	53 (96%)	2 (4%)	35 64
1	G	54/54 (100%)	53 (98%)	1 (2%)	57 82
1	J	55/54 (102%)	53 (96%)	2 (4%)	35 64
1	M	55/54 (102%)	48 (87%)	7 (13%)	4 10
1	R	56/54 (104%)	55 (98%)	1 (2%)	59 83
1	U	54/54 (100%)	52 (96%)	2 (4%)	34 63
1	X	53/54 (98%)	51 (96%)	2 (4%)	33 62
1	a	46/54 (85%)	44 (96%)	2 (4%)	29 57
1	d	41/54 (76%)	40 (98%)	1 (2%)	49 77
2	B	35/40 (88%)	34 (97%)	1 (3%)	42 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	34/40 (85%)	31 (91%)	3 (9%)	10 23
2	E	43/40 (108%)	41 (95%)	2 (5%)	26 54
2	F	40/40 (100%)	40 (100%)	0	100 100
2	H	44/40 (110%)	44 (100%)	0	100 100
2	I	41/40 (102%)	39 (95%)	2 (5%)	25 52
2	K	40/40 (100%)	37 (92%)	3 (8%)	13 31
2	L	44/40 (110%)	44 (100%)	0	100 100
2	N	40/40 (100%)	40 (100%)	0	100 100
2	O	43/40 (108%)	43 (100%)	0	100 100
2	S	44/40 (110%)	44 (100%)	0	100 100
2	T	40/40 (100%)	39 (98%)	1 (2%)	47 76
2	V	44/40 (110%)	41 (93%)	3 (7%)	16 36
2	W	44/40 (110%)	42 (96%)	2 (4%)	27 55
2	Y	41/40 (102%)	39 (95%)	2 (5%)	25 52
2	Z	36/40 (90%)	33 (92%)	3 (8%)	11 25
2	b	43/40 (108%)	42 (98%)	1 (2%)	50 78
2	c	35/40 (88%)	32 (91%)	3 (9%)	10 24
2	e	40/40 (100%)	38 (95%)	2 (5%)	24 51
2	f	43/40 (108%)	43 (100%)	0	100 100
All	All	1331/1340 (99%)	1283 (96%)	48 (4%)	36 64

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	27[A]	MSE
2	Y	14	MSE
2	V	27[B]	MSE
1	X	17	LEU
2	Z	27	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	43	GLN

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Mol	Chain	Res	Type
1	U	27	GLN
2	T	20	GLN
2	W	45	GLN
1	G	35	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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, 95^{th} 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	54/64 (84%)	1.10	9 (16%) 1 1	60, 81, 98, 110	0
1	D	62/64 (96%)	-0.35	0 100 100	5, 15, 34, 43	0
1	G	62/64 (96%)	0.02	1 (1%) 72 74	5, 25, 53, 66	0
1	J	63/64 (98%)	-0.22	1 (1%) 72 74	6, 20, 45, 57	0
1	M	63/64 (98%)	-0.18	1 (1%) 72 74	5, 17, 54, 74	0
1	R	63/64 (98%)	-0.17	0 100 100	5, 15, 45, 52	0
1	U	62/64 (96%)	-0.08	0 100 100	12, 30, 45, 68	0
1	X	61/64 (95%)	0.00	1 (1%) 72 74	6, 28, 69, 75	0
1	a	50/64 (78%)	1.05	12 (24%) 0 0	24, 58, 85, 92	0
1	d	44/64 (68%)	-0.32	0 100 100	6, 24, 51, 63	0
2	B	37/51 (72%)	1.18	6 (16%) 1 1	55, 79, 103, 107	0
2	C	35/51 (68%)	1.41	11 (31%) 0 0	70, 96, 112, 117	0
2	E	45/51 (88%)	-0.25	0 100 100	8, 23, 43, 46	0
2	F	42/51 (82%)	-0.41	0 100 100	5, 19, 40, 51	0
2	H	47/51 (92%)	-0.12	1 (2%) 63 65	7, 26, 40, 47	0
2	I	44/51 (86%)	-0.34	0 100 100	5, 20, 40, 53	0
2	K	40/51 (78%)	0.01	1 (2%) 57 59	6, 27, 78, 97	0
2	L	45/51 (88%)	-0.29	1 (2%) 62 63	5, 18, 43, 58	0
2	N	39/51 (76%)	0.13	2 (5%) 28 26	14, 30, 65, 78	0
2	O	44/51 (86%)	-0.29	0 100 100	6, 20, 35, 49	0
2	S	46/51 (90%)	-0.32	0 100 100	5, 13, 36, 60	0
2	T	41/51 (80%)	-0.10	2 (4%) 29 28	6, 23, 62, 88	0
2	V	45/51 (88%)	-0.03	1 (2%) 62 63	6, 29, 64, 74	0
2	W	46/51 (90%)	-0.11	1 (2%) 62 63	10, 34, 55, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	Y	43/51 (84%)	-0.20	1 (2%) 60 62	7, 26, 63, 68	0
2	Z	33/51 (64%)	0.47	4 (12%) 4 3	27, 53, 88, 91	0
2	b	44/51 (86%)	0.68	4 (9%) 9 7	33, 67, 85, 90	0
2	c	36/51 (70%)	0.43	2 (5%) 24 23	28, 51, 87, 93	0
2	e	41/51 (80%)	-0.23	2 (4%) 29 28	12, 31, 55, 67	0
2	f	44/51 (86%)	0.43	4 (9%) 9 7	20, 43, 68, 87	0
All	All	1421/1660 (85%)	0.07	68 (4%) 30 28	5, 29, 87, 117	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	TRP	5.9
1	A	54	ALA	5.3
2	B	9	ALA	4.9
2	b	21	LEU	4.5
1	X	4	LEU	4.5

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.