



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:37 AM UTC

PDB ID : 5VJX / pdb_00005vjx
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

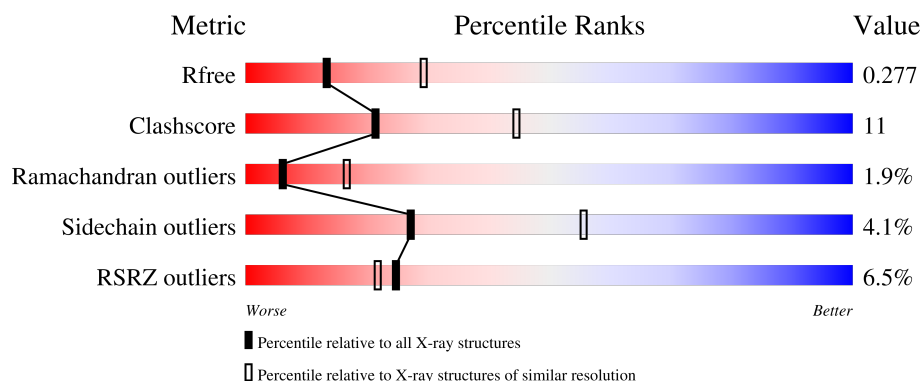
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	64	16% 61%25%14%
1	D	64	62%33% ..
1	G	64	3% 73%20%5% .
1	J	64	80%19% .
1	M	64	5% 66%28%6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	R	64	
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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

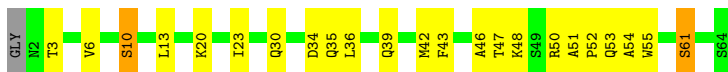
3 Residue-property plots [i](#)

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.

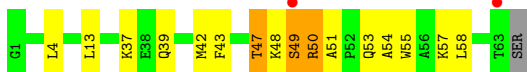
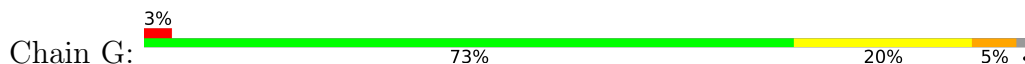
- Molecule 1: CLOCK-interacting pacemaker



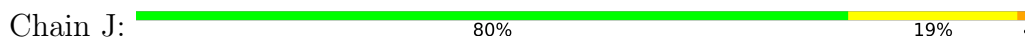
- Molecule 1: CLOCK-interacting pacemaker



- Molecule 1: CLOCK-interacting pacemaker



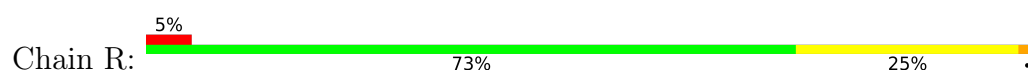
- Molecule 1: CLOCK-interacting pacemaker



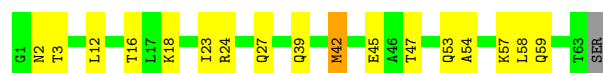
- Molecule 1: CLOCK-interacting pacemaker



- Molecule 1: CLOCK-interacting pacemaker



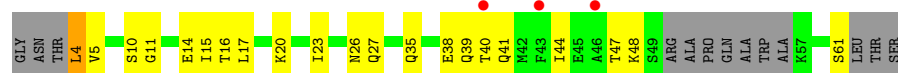
- Molecule 1: CLOCK-interacting pacemaker



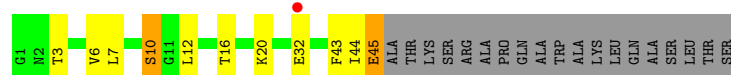
- Molecule 1: CLOCK-interacting pacemaker



- Molecule 1: CLOCK-interacting pacemaker



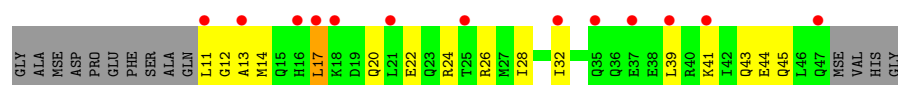
- Molecule 1: CLOCK-interacting pacemaker



- Molecule 2: Circadian locomotor output cycles protein kaput



- Molecule 2: Circadian locomotor output cycles protein kaput



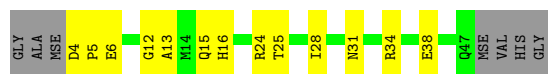
- Molecule 2: Circadian locomotor output cycles protein kaput

Chain E:  75% 20% . .



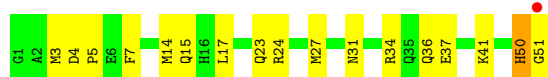
- Molecule 2: Circadian locomotor output cycles protein kaput

Chain F:  61% 25% 14%



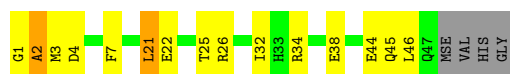
- Molecule 2: Circadian locomotor output cycles protein kaput

Chain H:  2% 67% 31% .



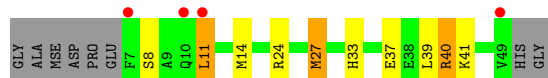
- Molecule 2: Circadian locomotor output cycles protein kaput

Chain I:  63% 25% . 8%



- Molecule 2: Circadian locomotor output cycles protein kaput

Chain K:  8% 65% 14% 6% 16%



- Molecule 2: Circadian locomotor output cycles protein kaput

Chain L:  2% 84% 12% .



- Molecule 2: Circadian locomotor output cycles protein kaput

Chain N:  10% 57% 22% . 18%

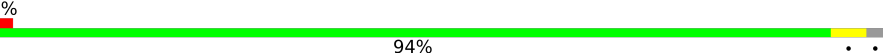


- Molecule 2: Circadian locomotor output cycles protein kaput

Chain O:  84% 10% 6%



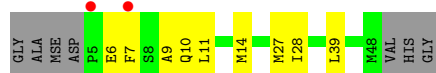
- Molecule 2: Circadian locomoter output cycles protein kaput

Chain S:  2% 94% . .



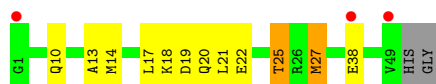
- Molecule 2: Circadian locomoter output cycles protein kaput

Chain T:  4% 69% 18% 14%



- Molecule 2: Circadian locomoter output cycles protein kaput

Chain V:  6% 73% 20% . .



- Molecule 2: Circadian locomoter output cycles protein kaput

Chain W:  4% 75% 20% . .

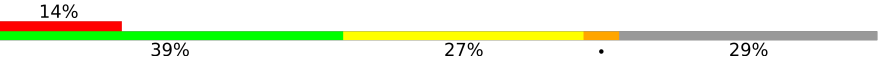


- Molecule 2: Circadian locomoter output cycles protein kaput

Chain Y:  4% 57% 29% . 10%

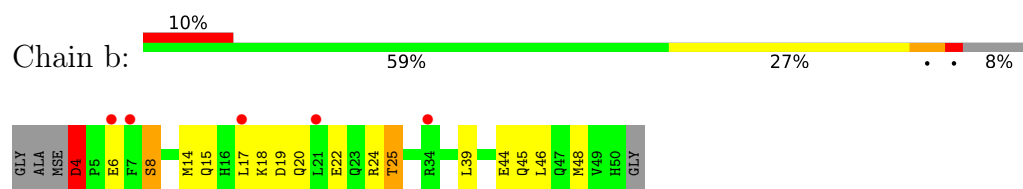


- Molecule 2: Circadian locomoter output cycles protein kaput

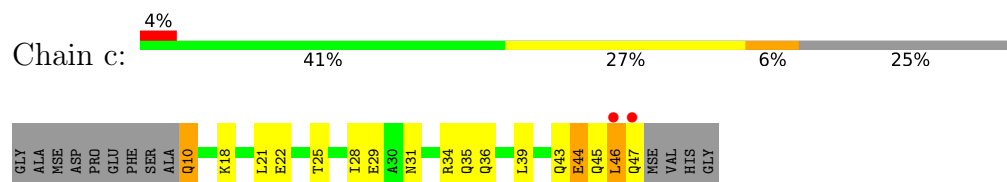
Chain Z:  14% 39% 27% . 29%



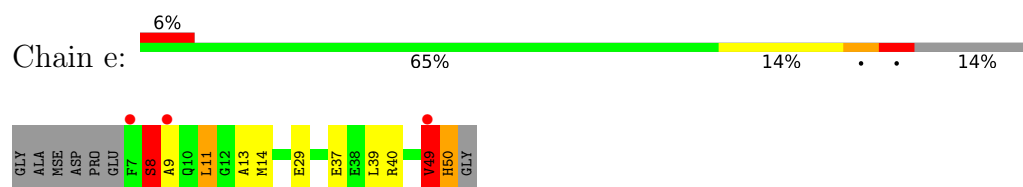
- Molecule 2: Circadian locomoter output cycles protein kaput



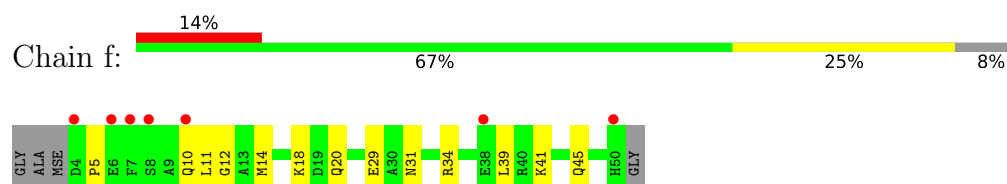
- Molecule 2: Circadian locomoter output cycles protein kaput



- Molecule 2: Circadian locomoter output cycles protein kaput



- Molecule 2: Circadian locomoter output cycles protein kaput



4 Data and refinement statistics

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 47.31 – 2.69	Depositor EDS
% Data completeness (in resolution range)	89.3 (47.31-2.69) 89.3 (47.31-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.218 , 0.275 0.222 , 0.277	Depositor DCC
R_{free} test set	2722 reflections (4.57%)	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 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.47	0/437	0.96	0/586
1	D	0.92	0/500	0.94	1/672 (0.1%)
1	G	0.86	0/498	1.20	5/669 (0.7%)
1	J	0.83	0/504	0.94	0/677
1	M	0.93	0/504	1.10	2/677 (0.3%)
1	R	0.98	0/515	1.03	2/691 (0.3%)
1	U	0.83	0/498	0.91	0/669
1	X	0.81	0/488	1.00	0/656
1	a	0.57	0/404	0.95	1/537 (0.2%)
1	d	0.87	0/360	1.07	1/481 (0.2%)
2	B	0.59	0/326	1.06	0/429
2	C	0.54	0/315	1.04	1/414 (0.2%)
2	E	0.87	0/402	0.87	0/528
2	F	0.95	0/372	0.94	0/492
2	H	0.79	0/417	0.99	2/548 (0.4%)
2	I	0.90	0/388	1.12	3/511 (0.6%)
2	K	0.80	0/369	0.90	0/484
2	L	0.95	0/409	0.92	2/538 (0.4%)
2	N	0.84	0/373	0.95	0/488
2	O	0.76	0/398	0.79	0/523
2	S	0.84	0/413	0.77	0/543
2	T	0.81	0/371	0.89	0/487
2	V	0.74	0/410	0.91	0/538
2	W	0.77	0/413	0.90	1/543 (0.2%)
2	Y	0.82	0/384	0.96	3/506 (0.6%)
2	Z	0.66	0/322	1.03	1/423 (0.2%)
2	b	0.49	0/397	0.99	3/524 (0.6%)
2	c	0.63	0/324	0.93	0/426
2	e	0.79	0/372	0.91	1/489 (0.2%)
2	f	0.64	0/397	0.92	0/524
All	All	0.80	0/12280	0.97	29/16273 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
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

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	49	SER	CA-C-N	10.39	140.41	121.70
1	G	49	SER	C-N-CA	10.39	140.41	121.70
1	d	10	SER	N-CA-C	9.76	121.99	111.36
1	R	48	LYS	N-CA-C	-7.80	98.67	110.14
2	W	7	PHE	N-CA-C	7.65	119.62	111.28
2	b	8	SER	N-CA-C	-7.42	104.23	113.28
2	I	4	ASP	CA-C-N	-7.26	112.39	120.45
2	I	4	ASP	C-N-CA	-7.26	112.39	120.45
2	C	12	GLY	N-CA-C	-7.25	105.38	114.16
1	a	40	THR	N-CA-C	-6.41	102.52	110.41
1	M	44	ILE	N-CA-C	-6.35	100.56	110.09
1	M	53	GLN	N-CA-C	5.65	119.91	113.19
2	H	50	HIS	N-CA-C	-5.59	98.88	110.80
2	Z	20	GLN	N-CA-C	-5.46	105.32	111.28
2	Y	6	GLU	N-CA-C	-5.46	104.86	112.45
1	G	53	GLN	N-CA-C	-5.44	102.23	110.28
2	b	4	ASP	CA-C-N	-5.43	115.17	120.98
2	b	4	ASP	C-N-CA	-5.43	115.17	120.98
2	L	4	ASP	CA-C-N	5.42	124.93	119.19
2	L	4	ASP	C-N-CA	5.42	124.93	119.19
1	D	13	LEU	N-CA-C	5.40	116.97	111.14
2	Y	4	ASP	CA-C-N	-5.32	114.54	120.45
2	Y	4	ASP	C-N-CA	-5.32	114.54	120.45
1	R	11	GLY	N-CA-C	5.28	125.69	113.18
1	G	47	THR	N-CA-C	-5.24	106.57	113.17
2	e	8	SER	N-CA-C	-5.20	106.93	113.28
2	H	7	PHE	N-CA-C	5.19	116.93	111.28
2	I	7	PHE	N-CA-C	5.16	116.91	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	49	SER	O-C-N	-5.12	117.55	123.33

There are no chirality outliers.

All (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
2	e	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	436	0	460	18	0
1	D	497	0	523	19	0
1	G	495	0	524	18	0
1	J	501	0	529	9	0
1	M	501	0	529	16	0
1	R	509	0	542	10	0
1	U	495	0	524	14	0
1	X	485	0	511	16	0
1	a	405	0	433	19	0
1	d	360	0	381	13	0
2	B	327	0	331	27	0
2	C	316	0	321	14	0
2	E	403	0	403	11	0
2	F	371	0	365	14	0
2	H	417	0	413	14	0
2	I	388	0	385	7	0
2	K	367	0	375	8	0
2	L	409	0	404	4	0
2	N	368	0	379	13	0
2	O	399	0	397	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	413	0	410	1	0
2	T	371	0	371	8	0
2	V	408	0	412	10	0
2	W	413	0	410	8	0
2	Y	384	0	379	16	0
2	Z	320	0	328	13	0
2	b	396	0	390	14	0
2	c	325	0	329	18	0
2	e	372	0	373	7	0
2	f	396	0	390	11	0
3	A	8	0	0	1	0
3	B	3	0	0	2	0
3	C	1	0	0	1	0
3	D	15	0	0	2	0
3	E	14	0	0	1	0
3	F	12	0	0	2	0
3	G	17	0	0	1	0
3	H	13	0	0	0	0
3	I	14	0	0	0	0
3	J	18	0	0	1	0
3	K	11	0	0	2	0
3	L	12	0	0	1	0
3	M	21	0	0	0	0
3	N	14	0	0	0	0
3	O	21	0	0	0	0
3	R	21	0	0	1	0
3	S	13	0	0	0	0
3	T	15	0	0	0	0
3	U	13	0	0	2	0
3	V	7	0	0	1	0
3	W	7	0	0	1	0
3	X	15	0	0	0	0
3	Y	8	0	0	1	0
3	Z	7	0	0	0	0
3	a	6	0	0	1	0
3	b	5	0	0	0	0
3	c	4	0	0	1	0
3	d	12	0	0	0	0
3	e	6	0	0	0	0
3	f	5	0	0	0	0
All	All	12585	0	12521	271	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 11.

All (271) 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)
1:J:45:GLU:OE1	3:J:101:HOH:O	1.96	0.83
2:F:4:ASP:O	1:G:50:ARG:NH1	2.15	0.80
1:G:49:SER:HA	1:G:50:ARG:HG2	1.66	0.78
2:E:43:GLN:HA	2:E:48:MSE:HE3	1.64	0.78
2:B:36:GLN:HG2	2:B:40:ARG:HH12	1.52	0.75
1:d:12:LEU:HD12	2:e:14:MSE:HE3	1.68	0.75
1:U:59:GLN:NE2	3:U:101:HOH:O	2.19	0.74
2:E:20:GLN:OE1	3:E:101:HOH:O	2.05	0.73
1:A:20:LYS:NZ	1:a:61:SER:O	2.22	0.73
1:X:21:GLU:OE2	1:X:24:ARG:NH2	2.19	0.71
2:F:15:GLN:OE1	2:H:15:GLN:NE2	2.24	0.71
2:O:31:ASN:OD1	2:O:34:ARG:NH2	2.23	0.71
1:G:50:ARG:H	1:G:55:TRP:HE1	1.37	0.70
2:B:29:GLU:HB2	2:C:39:LEU:HD21	1.72	0.70
1:a:41:GLN:OE1	2:c:45:GLN:NE2	2.24	0.70
1:A:54:ALA:N	3:A:101:HOH:O	2.24	0.69
1:G:48:LYS:O	1:G:50:ARG:NH1	2.26	0.69
2:c:44:GLU:C	2:c:46:LEU:H	2.01	0.69
2:H:37:GLU:OE1	2:H:41:LYS:NZ	2.25	0.69
1:R:23:ILE:HG13	2:T:28:ILE:HD11	1.75	0.68
1:D:50:ARG:NH2	2:H:3:MSE:O	2.25	0.68
2:Y:25:THR:HG21	2:Z:43[B]:GLN:HG2	1.75	0.68
1:G:48:LYS:NZ	3:G:101:HOH:O	2.26	0.67
1:X:24:ARG:NH1	1:d:32:GLU:OE2	2.28	0.67
1:G:42:MSE:HE2	1:G:57:LYS:HE2	1.76	0.67
2:N:8:SER:HA	2:N:10:GLN:H	1.58	0.66
1:J:62:LEU:HD21	2:L:17:LEU:HD22	1.76	0.66
2:B:19:ASP:O	2:B:22:GLU:HG2	1.94	0.66
2:B:31:ASN:OD1	2:B:34:ARG:NH2	2.28	0.66
2:L:37:GLU:OE1	3:L:101:HOH:O	2.14	0.65
1:D:55:TRP:CE3	2:H:3:MSE:HE1	2.31	0.65
2:F:38:GLU:OE1	3:F:101:HOH:O	2.13	0.65
2:K:37:GLU:OE2	2:K:40:ARG:NH1	2.30	0.65
2:f:10:GLN:HG3	2:f:11:LEU:H	1.62	0.65
1:G:49:SER:CA	1:G:50:ARG:HG2	2.27	0.64
1:D:35:GLN:NE2	3:D:102:HOH:O	2.30	0.64
1:R:12:LEU:HD12	2:T:14:MSE:HE3	1.79	0.64
2:b:4:ASP:N	2:b:4:ASP:OD1	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:GLU:OE1	3:F:102:HOH:O	2.14	0.64
1:D:34:ASP:OD2	2:N:26:ARG:NH1	2.30	0.64
2:B:44:GLU:O	2:B:46:LEU:N	2.31	0.63
1:D:39:GLN:OE1	2:F:24:ARG:NH1	2.31	0.63
1:A:17:LEU:HD11	2:b:17:LEU:HD23	1.81	0.62
1:R:7:LEU:HD23	2:T:14:MSE:HE1	1.81	0.62
2:F:31:ASN:OD1	2:F:34:ARG:NH2	2.33	0.62
1:a:15:ILE:HG21	2:b:46:LEU:HD13	1.81	0.62
2:C:20:GLN:HE21	2:C:24:ARG:HD2	1.64	0.62
2:N:8:SER:HA	2:N:10:GLN:N	2.15	0.62
2:I:34:ARG:HD2	2:Z:41:LYS:HE2	1.82	0.62
1:M:50:ARG:H	1:M:51:ALA:HA	1.64	0.61
1:U:23:ILE:HG13	2:W:28:ILE:HD11	1.81	0.61
2:N:24:ARG:HG3	2:N:24:ARG:HH11	1.66	0.61
1:X:43:PHE:HZ	2:Y:14:MSE:HE3	1.64	0.61
2:b:18:LYS:NZ	2:b:22:GLU:OE2	2.26	0.61
2:B:20:GLN:OE1	1:a:17:LEU:HB3	2.00	0.61
2:B:20:GLN:NE2	3:B:101:HOH:O	2.33	0.61
1:U:18:LYS:NZ	2:V:38:GLU:OE1	2.32	0.61
1:G:47:THR:HG22	2:H:14:MSE:SE	2.51	0.60
2:e:49:VAL:HG13	2:e:50:HIS:H	1.66	0.60
2:S:31:ASN:OD1	2:S:34:ARG:NH2	2.34	0.59
2:f:10:GLN:O	2:f:12:GLY:N	2.32	0.59
2:I:1:GLY:HA2	2:I:2:ALA:HB3	1.85	0.59
2:N:10:GLN:HG2	2:N:13:ALA:HB3	1.84	0.58
2:B:33:HIS:O	2:B:36:GLN:HB3	2.03	0.58
1:a:39:GLN:OE1	2:b:24:ARG:NH1	2.36	0.58
1:X:17:LEU:HD23	2:f:20:GLN:HG3	1.86	0.57
2:B:40:ARG:HA	2:B:43:GLN:HG2	1.87	0.57
2:B:8:SER:N	3:B:102:HOH:O	2.36	0.57
2:B:22:GLU:HG3	2:B:26:ARG:NH2	2.19	0.57
2:B:36:GLN:CG	2:B:40:ARG:HH12	2.16	0.57
2:K:33:HIS:ND1	3:K:101:HOH:O	2.23	0.57
1:a:26:ASN:OD1	2:c:35:GLN:NE2	2.35	0.57
2:F:4:ASP:C	2:F:6:GLU:H	2.13	0.57
1:J:39:GLN:OE1	2:L:24:ARG:NH2	2.28	0.57
2:W:1:GLY:N	3:W:101:HOH:O	2.28	0.56
2:E:22:GLU:O	2:E:25:THR:HG22	2.04	0.56
1:d:10:SER:HB2	1:d:12:LEU:H	1.70	0.56
2:c:44:GLU:O	2:c:46:LEU:N	2.35	0.56
1:U:39:GLN:HA	1:U:42:MSE:HE3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:43:PHE:O	1:J:47:THR:HG23	2.06	0.55
1:G:49:SER:HB3	1:G:51:ALA:H	1.71	0.55
1:R:7:LEU:HA	2:T:14:MSE:HE1	1.89	0.55
2:c:31:ASN:OD1	2:c:34:ARG:NH2	2.26	0.55
1:M:44:ILE:O	1:M:45:GLU:HB3	2.06	0.55
2:Y:44:GLU:O	2:Y:46:LEU:N	2.39	0.55
1:A:39:GLN:OE1	2:B:24:ARG:NH1	2.40	0.55
2:H:36:GLN:HG3	2:I:32:ILE:HG21	1.89	0.54
1:A:23:ILE:HD12	2:C:24:ARG:HH21	1.72	0.54
1:G:49:SER:CB	1:G:50:ARG:HG2	2.37	0.54
1:X:7:LEU:O	1:X:12:LEU:N	2.40	0.54
1:G:43:PHE:O	1:G:47:THR:HG23	2.08	0.54
2:Z:23:GLN:OE1	2:Z:26:ARG:NH2	2.41	0.54
2:N:43:GLN:HG2	2:O:25:THR:HG21	1.90	0.53
1:M:49:SER:OG	1:M:50:ARG:HB2	2.08	0.53
2:W:19:ASP:OD1	2:W:20:GLN:N	2.41	0.53
2:V:18:LYS:HE3	2:V:22:GLU:OE2	2.09	0.53
2:H:23:GLN:HG3	2:H:27:MSE:HE2	1.90	0.53
2:V:20:GLN:HG3	3:V:107:HOH:O	2.09	0.53
1:X:16:THR:HG22	2:Z:21:LEU:HD13	1.90	0.53
2:B:22:GLU:HG3	2:B:26:ARG:HH22	1.74	0.53
1:X:61:SER:O	1:d:20:LYS:NZ	2.40	0.53
1:M:23:ILE:HG13	2:N:28:ILE:HD11	1.91	0.53
1:U:3:THR:HG23	2:W:17:LEU:HD11	1.91	0.53
1:G:39:GLN:OE1	2:H:24:ARG:NH1	2.38	0.52
1:A:4:LEU:HD23	1:A:7:LEU:HD12	1.91	0.52
2:V:25:THR:HG23	2:W:39:LEU:HD21	1.91	0.52
1:A:23:ILE:HG13	2:C:28:ILE:HD11	1.91	0.52
1:M:49:SER:HB2	1:M:50:ARG:HD2	1.92	0.52
2:W:2:ALA:O	2:W:3:MSE:HG3	2.10	0.52
1:A:41:GLN:OE1	2:C:45:GLN:NE2	2.40	0.52
1:X:15:ILE:HG23	2:Y:42:ILE:HG23	1.92	0.52
1:a:44:ILE:HD11	2:c:46:LEU:HD23	1.91	0.52
1:a:23:ILE:HG13	2:c:28:ILE:HD11	1.92	0.52
2:c:10:GLN:N	3:c:101:HOH:O	2.43	0.51
2:F:4:ASP:HB3	2:F:5:PRO:HD2	1.91	0.51
1:X:15:ILE:HB	2:Z:21:LEU:HD21	1.92	0.51
1:M:12:LEU:HD12	2:N:14:MSE:HE3	1.93	0.51
2:B:11:LEU:O	2:B:15:GLN:HG2	2.09	0.51
1:R:52:PRO:O	3:R:101:HOH:O	2.20	0.51
2:c:18:LYS:NZ	2:c:22:GLU:OE2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ILE:HG13	2:E:28:ILE:HD11	1.92	0.50
1:D:46:ALA:O	2:H:3:MSE:HE3	2.10	0.50
2:B:42:ILE:O	2:B:45:GLN:HB2	2.12	0.50
1:D:6:VAL:O	1:D:10:SER:OG	2.25	0.50
2:V:27[A]:MSE:HA	2:V:27[A]:MSE:HE3	1.92	0.50
2:Y:18:LYS:NZ	2:Z:49:VAL:O	2.43	0.50
2:Y:3:MSE:O	3:Y:101:HOH:O	2.19	0.49
2:B:29:GLU:CB	2:C:39:LEU:HD21	2.42	0.49
2:T:6:GLU:HG3	2:T:9:ALA:HB3	1.94	0.49
1:U:39:GLN:HG2	2:V:21:LEU:HD21	1.95	0.49
1:X:59:GLN:HE22	1:d:3:THR:HG22	1.77	0.49
1:a:35:GLN:O	1:a:38:GLU:HG2	2.13	0.49
1:A:17:LEU:HB3	2:b:20:GLN:HE22	1.78	0.49
2:B:44:GLU:C	2:B:46:LEU:H	2.21	0.49
1:D:51:ALA:HB1	1:D:53:GLN:NE2	2.28	0.49
1:M:13:LEU:O	1:M:16:THR:HG22	2.12	0.49
1:M:51:ALA:H	1:M:52:PRO:HA	1.78	0.49
2:T:10:GLN:O	2:T:14:MSE:HG2	2.12	0.49
2:c:39:LEU:O	2:c:43:GLN:N	2.40	0.49
2:Y:14:MSE:HE2	2:Y:15:GLN:HA	1.95	0.49
1:A:20:LYS:HG2	2:C:24:ARG:HH22	1.78	0.48
2:B:41:LYS:O	2:B:45:GLN:HG3	2.14	0.48
1:d:43:PHE:CZ	2:f:18:LYS:HB2	2.48	0.48
1:D:30:GLN:OE1	2:E:34:ARG:NH2	2.44	0.48
2:Z:17:LEU:C	2:Z:19:ASP:H	2.22	0.48
1:U:12:LEU:O	1:U:16:THR:HG23	2.13	0.48
1:A:17:LEU:HB3	2:b:20:GLN:NE2	2.28	0.48
1:U:45:GLU:CD	1:U:57:LYS:HZ1	2.21	0.48
1:U:16:THR:HG22	2:W:21:LEU:HD11	1.95	0.48
2:b:15:GLN:NE2	2:b:19:ASP:OD1	2.47	0.48
1:A:61:SER:O	1:a:20:LYS:NZ	2.40	0.47
2:B:14:MSE:HE2	2:B:14:MSE:HA	1.95	0.47
2:T:39:LEU:HD23	2:T:39:LEU:HA	1.76	0.47
2:c:31:ASN:HB3	2:c:35:GLN:HE21	1.78	0.47
1:D:50:ARG:HA	1:D:50:ARG:NE	2.29	0.47
2:E:20:GLN:O	2:E:23:GLN:HG2	2.14	0.47
2:Y:43:GLN:HG2	2:Z:25:THR:HG21	1.97	0.47
2:W:20:GLN:O	2:W:23:GLN:HG2	2.14	0.47
2:B:10:GLN:HG3	1:a:5:VAL:HG13	1.97	0.47
1:D:3:THR:HG23	2:E:17:LEU:HD11	1.97	0.47
2:E:46:LEU:HB2	2:E:48:MSE:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:8:SER:HA	2:K:11:LEU:HB2	1.97	0.47
2:T:7:PHE:O	2:T:10:GLN:HB2	2.15	0.47
1:D:20:LYS:HE3	1:J:61:SER:O	2.14	0.47
1:D:61:SER:O	1:J:20:LYS:NZ	2.38	0.46
1:X:62:LEU:O	1:d:16:THR:HG21	2.15	0.46
1:U:53:GLN:HG3	1:U:54:ALA:N	2.31	0.46
2:Y:18:LYS:HE3	2:Z:46:LEU:O	2.14	0.46
1:A:55:TRP:HH2	1:a:4:LEU:HD22	1.81	0.46
2:B:14:MSE:HE2	2:B:17:LEU:HD12	1.96	0.46
1:R:44:ILE:HG23	1:R:48:LYS:HE2	1.98	0.46
2:B:44:GLU:C	2:B:46:LEU:N	2.73	0.46
2:f:10:GLN:O	2:f:11:LEU:HB2	2.14	0.46
1:X:44:ILE:HG22	1:X:48:LYS:HE2	1.96	0.46
2:Y:40:ARG:NH1	2:Y:44:GLU:OE2	2.48	0.46
2:N:8:SER:HA	2:N:9:ALA:HB3	1.97	0.46
2:e:39:LEU:HD21	2:f:29:GLU:HB2	1.96	0.46
1:M:44:ILE:O	1:M:45:GLU:CB	2.64	0.46
1:G:13:LEU:HD21	2:V:13:ALA:HA	1.98	0.45
2:K:41:LYS:NZ	3:K:102:HOH:O	2.38	0.45
1:U:45:GLU:OE1	1:U:57:LYS:NZ	2.46	0.45
2:K:33:HIS:HE1	2:b:44:GLU:HG2	1.81	0.45
2:F:4:ASP:HB3	2:F:5:PRO:CD	2.47	0.45
1:M:39:GLN:OE1	2:O:24:ARG:NH1	2.37	0.45
1:X:59:GLN:HE22	1:d:3:THR:CG2	2.29	0.45
1:A:55:TRP:HZ3	2:B:14:MSE:SE	2.49	0.45
2:b:25:THR:HG21	2:c:43:GLN:HG2	1.99	0.45
2:c:36:GLN:O	2:c:39:LEU:HB2	2.17	0.44
1:d:43:PHE:O	1:d:45:GLU:HG3	2.18	0.44
1:M:49:SER:CB	1:M:50:ARG:HD2	2.47	0.44
1:U:58:LEU:HD11	2:V:17:LEU:HD11	1.98	0.44
1:D:36:LEU:HD22	2:F:28:ILE:HD12	1.99	0.44
1:a:41:GLN:NE2	3:a:101:HOH:O	2.50	0.44
2:F:12:GLY:O	2:F:16:HIS:ND1	2.43	0.44
1:a:26:ASN:CG	2:c:35:GLN:HE22	2.24	0.44
1:G:37:LYS:NZ	2:I:38:GLU:OE2	2.37	0.44
2:I:44:GLU:O	2:I:46:LEU:N	2.51	0.44
2:K:39:LEU:HD12	2:K:39:LEU:HA	1.84	0.44
2:e:11:LEU:C	2:e:13:ALA:H	2.26	0.44
1:R:35:GLN:O	1:R:38:GLU:HG2	2.17	0.43
1:R:43:PHE:O	1:R:47:THR:HG23	2.18	0.43
2:Z:18:LYS:O	2:Z:18:LYS:HG2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:ARG:N	1:G:55:TRP:HE1	2.10	0.43
2:C:13:ALA:O	2:C:17:LEU:HD22	2.18	0.43
2:C:22:GLU:HB3	2:C:26:ARG:NH2	2.33	0.43
2:H:4:ASP:HA	2:H:5:PRO:HD3	1.89	0.43
2:K:24:ARG:O	2:K:27[A]:MSE:HG3	2.18	0.43
1:M:15:ILE:HG22	2:N:21:LEU:HD13	2.00	0.43
1:a:47:THR:HG22	2:b:14:MSE:HE2	2.00	0.43
2:b:6:GLU:O	2:b:8:SER:N	2.50	0.43
2:H:50:HIS:HB2	2:H:51:GLY:HA3	1.99	0.43
1:X:24:ARG:HD2	1:d:32:GLU:OE2	2.18	0.43
1:a:48:LYS:O	1:a:48:LYS:HG2	2.18	0.43
2:Y:11:LEU:HD23	2:Y:11:LEU:HA	1.89	0.43
1:A:36:LEU:HD22	2:B:28:ILE:HD12	2.00	0.43
1:D:55:TRP:HB2	2:H:3:MSE:CE	2.49	0.43
2:e:37:GLU:HG3	2:e:40:ARG:HH21	1.83	0.43
1:A:40:THR:O	1:A:43:PHE:HB3	2.19	0.43
2:b:39:LEU:HD21	2:c:29:GLU:HB2	2.01	0.43
2:E:43:GLN:HG2	2:F:25:THR:HG21	2.01	0.42
2:F:4:ASP:C	2:F:6:GLU:N	2.74	0.42
1:G:58:LEU:HD11	2:H:17:LEU:HD11	2.01	0.42
1:M:44:ILE:HG23	1:M:48:LYS:HE2	2.01	0.42
1:d:43:PHE:C	1:d:45:GLU:H	2.27	0.42
2:C:41:LYS:O	2:C:44:GLU:HB2	2.18	0.42
2:Y:46:LEU:HA	2:Y:47:GLN:HA	1.71	0.42
2:c:22:GLU:O	2:c:25:THR:OG1	2.31	0.42
1:M:43:PHE:C	1:M:44:ILE:O	2.57	0.42
1:a:14:GLU:CD	2:b:45:GLN:HE22	2.27	0.42
2:H:31:ASN:OD1	2:H:34:ARG:NH2	2.48	0.42
1:U:24:ARG:NH1	3:U:102:HOH:O	2.31	0.42
2:Y:44:GLU:C	2:Y:46:LEU:N	2.78	0.42
2:f:41:LYS:HE3	2:f:41:LYS:HB2	1.85	0.42
1:D:43:PHE:O	1:D:47:THR:HG23	2.19	0.42
2:I:22:GLU:O	2:I:26:ARG:HG2	2.20	0.42
1:R:4:LEU:HD23	1:R:4:LEU:HA	1.90	0.42
1:X:32:GLU:HG2	2:Y:24:ARG:HH22	1.85	0.42
2:Z:26:ARG:O	2:Z:29:GLU:HG2	2.20	0.42
2:V:10:GLN:O	2:V:14:MSE:HG2	2.20	0.41
1:X:11:GLY:O	1:X:15:ILE:HD12	2.20	0.41
2:B:25:THR:HG21	2:C:43:GLN:HG2	2.02	0.41
2:I:21:LEU:HD12	2:I:21:LEU:HA	1.76	0.41
1:J:6:VAL:HG13	2:K:14:MSE:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:9:ALA:C	2:N:11:LEU:H	2.28	0.41
2:B:25:THR:HG21	2:C:43:GLN:CG	2.50	0.41
2:Y:14:MSE:HE2	2:Y:14:MSE:C	2.45	0.41
2:c:21:LEU:HD23	2:c:21:LEU:HA	1.89	0.41
2:f:31:ASN:HA	2:f:34:ARG:NH1	2.35	0.41
1:U:27:GLN:NE2	2:Z:27:MSE:HA	2.35	0.41
1:R:53:GLN:H	1:R:53:GLN:CD	2.27	0.41
1:G:49:SER:HA	1:G:50:ARG:CG	2.44	0.41
2:L:40:ARG:NE	2:c:29:GLU:OE1	2.44	0.41
1:M:7:LEU:HD23	2:N:14:MSE:HE1	2.02	0.41
2:e:29:GLU:HB2	2:f:39:LEU:HD21	2.02	0.41
2:f:10:GLN:NE2	2:f:14:MSE:HG3	2.35	0.41
2:E:27:MSE:HG3	2:E:28:ILE:N	2.36	0.41
1:J:51:ALA:HB1	1:J:53:GLN:OE1	2.20	0.41
2:F:13:ALA:HB2	1:J:13:LEU:HD21	2.02	0.41
1:d:10:SER:OG	2:e:14:MSE:HE2	2.20	0.41
2:f:10:GLN:C	2:f:12:GLY:N	2.79	0.41
2:C:11:LEU:HD12	2:C:11:LEU:HA	1.83	0.41
1:D:52:PRO:O	3:D:101:HOH:O	2.21	0.41
1:G:4:LEU:HD11	2:V:13:ALA:HB2	2.02	0.41
2:Y:46:LEU:HD13	2:Z:22:GLU:HG2	2.03	0.41
2:C:11:LEU:N	3:C:101:HOH:O	2.54	0.40
1:M:44:ILE:HG13	2:N:45:GLN:HB3	2.03	0.40
2:E:17:LEU:HD23	2:E:17:LEU:HA	1.85	0.40
1:A:55:TRP:CH2	1:a:4:LEU:HD22	2.56	0.40
1:d:6:VAL:O	1:d:10:SER:OG	2.39	0.40
1:D:48:LYS:O	1:D:48:LYS:HG2	2.21	0.40
1:A:62:LEU:O	1:a:16:THR:HG21	2.21	0.40

There are no symmetry-related clashes.

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%)	6	16
1	D	61/64 (95%)	57 (93%)	3 (5%)	1 (2%)	7	20
1	G	61/64 (95%)	57 (93%)	2 (3%)	2 (3%)	3	7
1	J	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	7	20
1	M	62/64 (97%)	53 (86%)	7 (11%)	2 (3%)	3	7
1	R	63/64 (98%)	55 (87%)	5 (8%)	3 (5%)	2	3
1	U	61/64 (95%)	58 (95%)	2 (3%)	1 (2%)	7	20
1	X	60/64 (94%)	56 (93%)	4 (7%)	0	100	100
1	a	47/64 (73%)	43 (92%)	3 (6%)	1 (2%)	5	15
1	d	43/64 (67%)	38 (88%)	4 (9%)	1 (2%)	5	13
2	B	37/51 (72%)	34 (92%)	2 (5%)	1 (3%)	4	10
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	4
2	K	42/51 (82%)	40 (95%)	2 (5%)	0	100	100
2	L	47/51 (92%)	43 (92%)	3 (6%)	1 (2%)	5	15
2	N	42/51 (82%)	39 (93%)	1 (2%)	2 (5%)	2	3
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%)	5	15
2	Y	44/51 (86%)	42 (96%)	1 (2%)	1 (2%)	5	13
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%)	4	9
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	4
All	All	1436/1660 (86%)	1338 (93%)	71 (5%)	27 (2%)	6	17

All (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
2	Y	45	GLN
2	e	9	ALA
2	e	11	LEU
1	D	54	ALA
1	G	50	ARG
1	G	54	ALA
2	L	3	MSE
2	e	49	VAL
2	f	5	PRO
2	f	45	GLN
1	M	51	ALA
2	N	9	ALA
1	R	49	SER
2	N	10	GLN
2	c	44	GLU
2	I	2	ALA
2	W	49	VAL
1	R	3	THR
1	A	11	GLY
1	M	11	GLY
1	d	44	ILE
1	a	11	GLY

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	48/54 (89%)	47 (98%)	1 (2%)	47	75
1	D	55/54 (102%)	53 (96%)	2 (4%)	31	60
1	G	54/54 (100%)	54 (100%)	0	100	100
1	J	55/54 (102%)	53 (96%)	2 (4%)	31	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	55/54 (102%)	49 (89%)	6 (11%)	6	16
1	R	56/54 (104%)	56 (100%)	0	100	100
1	U	54/54 (100%)	52 (96%)	2 (4%)	30	59
1	X	53/54 (98%)	51 (96%)	2 (4%)	29	58
1	a	46/54 (85%)	44 (96%)	2 (4%)	26	54
1	d	41/54 (76%)	39 (95%)	2 (5%)	22	49
2	B	35/40 (88%)	34 (97%)	1 (3%)	37	67
2	C	34/40 (85%)	31 (91%)	3 (9%)	9	23
2	E	43/40 (108%)	42 (98%)	1 (2%)	44	73
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%)	38 (93%)	3 (7%)	13	32
2	K	40/40 (100%)	36 (90%)	4 (10%)	7	19
2	L	44/40 (110%)	44 (100%)	0	100	100
2	N	40/40 (100%)	39 (98%)	1 (2%)	42	71
2	O	43/40 (108%)	42 (98%)	1 (2%)	44	73
2	S	44/40 (110%)	44 (100%)	0	100	100
2	T	40/40 (100%)	38 (95%)	2 (5%)	22	48
2	V	44/40 (110%)	40 (91%)	4 (9%)	9	22
2	W	44/40 (110%)	42 (96%)	2 (4%)	24	52
2	Y	41/40 (102%)	38 (93%)	3 (7%)	13	32
2	Z	36/40 (90%)	33 (92%)	3 (8%)	10	26
2	b	43/40 (108%)	40 (93%)	3 (7%)	14	34
2	c	35/40 (88%)	32 (91%)	3 (9%)	10	25
2	e	40/40 (100%)	37 (92%)	3 (8%)	12	31
2	f	43/40 (108%)	43 (100%)	0	100	100
All	All	1331/1340 (99%)	1275 (96%)	56 (4%)	27	55

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
2	B	25	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	14	MSE
2	C	17	LEU
2	C	32	ILE
1	D	42	MSE
1	D	61	SER
2	E	48	MSE
2	I	3	MSE
2	I	21	LEU
2	I	25	THR
1	J	50	ARG
1	J	53	GLN
2	K	11	LEU
2	K	27[A]	MSE
2	K	27[B]	MSE
2	K	40	ARG
1	M	2	ASN
1	M	16	THR
1	M	47	THR
1	M	50	ARG
1	M	63	THR
1	M	64	SER
2	N	23	GLN
2	O	48	MSE
2	T	11	LEU
2	T	27	MSE
1	U	42	MSE
1	U	47	THR
2	V	19	ASP
2	V	25	THR
2	V	27[A]	MSE
2	V	27[B]	MSE
2	W	19	ASP
2	W	39	LEU
1	X	17	LEU
1	X	42	MSE
2	Y	14	MSE
2	Y	25	THR
2	Y	41	LYS
2	Z	25	THR
2	Z	27	MSE
2	Z	34	ARG
1	a	4	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	27	GLN
2	b	4	ASP
2	b	25	THR
2	b	48	MSE
2	c	10	GLN
2	c	46	LEU
2	c	47	GLN
1	d	7	LEU
1	d	45	GLU
2	e	8	SER
2	e	49	VAL
2	e	50	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	33	HIS
2	C	20	GLN
1	D	53	GLN
2	E	47	GLN
2	F	20	GLN
2	F	45	GLN
1	G	26	ASN
1	G	35	GLN
2	H	36	GLN
2	H	47	GLN
1	J	35	GLN
2	K	16	HIS
2	K	36	GLN
2	L	20	GLN
2	L	36	GLN
2	L	47	GLN
2	L	50	HIS
2	N	43	GLN
2	O	36	GLN
2	O	47	GLN
2	S	50	HIS
2	T	16	HIS
2	T	20	GLN
1	U	27	GLN
2	V	47	GLN
2	W	20	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	W	45	GLN
1	X	39	GLN
2	Y	16	HIS
2	Z	16	HIS
2	Z	35	GLN
2	Z	36	GLN
1	a	30	GLN
2	e	16	HIS
2	e	35	GLN
2	e	45	GLN
2	f	16	HIS

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](#)

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](#)

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, 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	54/64 (84%)	1.38	10 (18%) 3 3	60, 81, 98, 110	0
1	D	62/64 (96%)	-0.44	0 100 100	5, 15, 34, 43	0
1	G	62/64 (96%)	0.08	2 (3%) 50 46	5, 25, 53, 66	0
1	J	63/64 (98%)	-0.29	0 100 100	6, 20, 45, 57	0
1	M	63/64 (98%)	-0.06	3 (4%) 35 32	5, 17, 54, 74	0
1	R	63/64 (98%)	-0.16	3 (4%) 35 32	5, 15, 43, 52	1 (1%)
1	U	62/64 (96%)	0.18	0 100 100	12, 30, 45, 68	0
1	X	61/64 (95%)	0.31	3 (4%) 35 31	6, 28, 69, 75	0
1	a	50/64 (78%)	0.84	3 (6%) 27 24	24, 58, 85, 92	0
1	d	44/64 (68%)	-0.06	1 (2%) 61 58	6, 24, 51, 63	0
2	B	37/51 (72%)	1.57	10 (27%) 1 1	55, 79, 103, 107	0
2	C	35/51 (68%)	1.83	13 (37%) 1 0	70, 96, 112, 117	0
2	E	45/51 (88%)	-0.27	0 100 100	8, 23, 43, 46	0
2	F	42/51 (82%)	-0.44	0 100 100	5, 19, 40, 51	0
2	H	47/51 (92%)	-0.12	1 (2%) 63 61	7, 26, 40, 47	0
2	I	44/51 (86%)	-0.35	0 100 100	5, 20, 40, 53	0
2	K	40/51 (78%)	0.20	4 (10%) 12 10	6, 27, 78, 97	0
2	L	45/51 (88%)	-0.32	1 (2%) 62 59	5, 18, 43, 58	0
2	N	39/51 (76%)	0.54	5 (12%) 7 6	14, 30, 65, 78	1 (2%)
2	O	44/51 (86%)	-0.39	0 100 100	6, 20, 35, 49	0
2	S	46/51 (90%)	-0.31	1 (2%) 62 59	5, 13, 36, 60	0
2	T	41/51 (80%)	0.02	2 (4%) 35 31	6, 23, 62, 88	0
2	V	45/51 (88%)	0.05	3 (6%) 24 21	6, 29, 64, 74	0
2	W	46/51 (90%)	0.18	2 (4%) 40 36	10, 34, 55, 61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	43/51 (84%)	-0.01	2 (4%) 36 33	7, 26, 63, 68	0
2	Z	33/51 (64%)	1.19	7 (21%) 2 2	27, 51, 88, 91	1 (3%)
2	b	44/51 (86%)	1.07	5 (11%) 10 8	33, 67, 85, 90	0
2	c	36/51 (70%)	0.72	2 (5%) 30 26	28, 51, 87, 93	0
2	e	41/51 (80%)	0.32	3 (7%) 21 18	12, 31, 55, 67	0
2	f	44/51 (86%)	0.86	7 (15%) 5 4	20, 43, 68, 87	0
All	All	1421/1660 (85%)	0.22	93 (6%) 25 22	5, 29, 87, 117	3 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	4	LEU	6.1
2	Z	43[A]	GLN	5.4
2	N	7	PHE	4.6
2	K	7	PHE	4.5
2	H	51	GLY	4.4
2	e	7	PHE	4.2
2	Y	45	GLN	4.2
1	M	51	ALA	4.0
2	T	7	PHE	3.7
2	f	6	GLU	3.6
2	C	21	LEU	3.6
2	B	42	ILE	3.5
2	N	34[A]	ARG	3.5
1	G	49	SER	3.3
2	B	9	ALA	3.3
2	N	12	GLY	3.2
1	X	5	VAL	3.2
2	f	4	ASP	3.1
2	B	46	LEU	3.1
2	Z	24	ARG	3.1
1	A	4	LEU	3.0
2	C	17	LEU	3.0
2	b	21	LEU	2.9
2	T	5	PRO	2.9
2	f	10	GLN	2.9
2	C	32	ILE	2.9
2	f	50	HIS	2.9
2	W	50	HIS	2.9
2	f	8	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3	THR	2.8
2	Z	26	ARG	2.7
1	R	48	LYS	2.7
2	B	13	ALA	2.7
1	A	55	TRP	2.6
2	V	49	VAL	2.6
2	b	6	GLU	2.6
2	b	17	LEU	2.6
1	R	53	GLN	2.5
2	B	15	GLN	2.5
2	C	11	LEU	2.5
2	C	18	LYS	2.5
2	S	50	HIS	2.5
1	A	54	ALA	2.5
2	C	39	LEU	2.5
1	a	40	THR	2.5
1	a	43	PHE	2.5
2	B	38	GLU	2.4
2	B	39	LEU	2.4
2	Z	20	GLN	2.4
2	B	10	GLN	2.4
1	A	63	THR	2.4
2	Z	25	THR	2.4
2	V	38	GLU	2.4
1	R	50[A]	ARG	2.4
2	b	7	PHE	2.4
2	C	37	GLU	2.3
2	C	47	GLN	2.3
2	L	40	ARG	2.3
2	V	1	GLY	2.3
1	A	46	ALA	2.3
2	B	11	LEU	2.3
1	A	6	VAL	2.3
2	W	49	VAL	2.3
1	M	52	PRO	2.3
2	C	35	GLN	2.2
2	N	8	SER	2.2
2	B	23	GLN	2.2
2	K	49	VAL	2.2
1	M	54	ALA	2.2
2	Y	38	GLU	2.2
2	C	13	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	25	THR	2.2
2	c	47	GLN	2.2
2	C	41	LYS	2.2
2	K	11	LEU	2.2
1	A	45	GLU	2.1
1	X	3	THR	2.1
2	e	49	VAL	2.1
1	d	32	GLU	2.1
2	C	16	HIS	2.1
2	f	7	PHE	2.1
1	a	46	ALA	2.1
2	N	10	GLN	2.1
2	f	38	GLU	2.0
1	G	63	THR	2.0
2	Z	33	HIS	2.0
1	A	15	ILE	2.0
2	e	9	ALA	2.0
1	A	17	LEU	2.0
2	K	10	GLN	2.0
2	Z	21	LEU	2.0
2	c	46	LEU	2.0
2	b	34	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.