



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:17 PM UTC

PDB ID : 8P24 / pdb_00008p24
Title : The crystal structure of the C-terminal domain of Mengla nucleoprotein
Authors : Ferrero, D.S.; Tomas Gilabert, O.; Verdaguer, N.
Deposited on : 2023-05-14
Resolution : 3.73 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

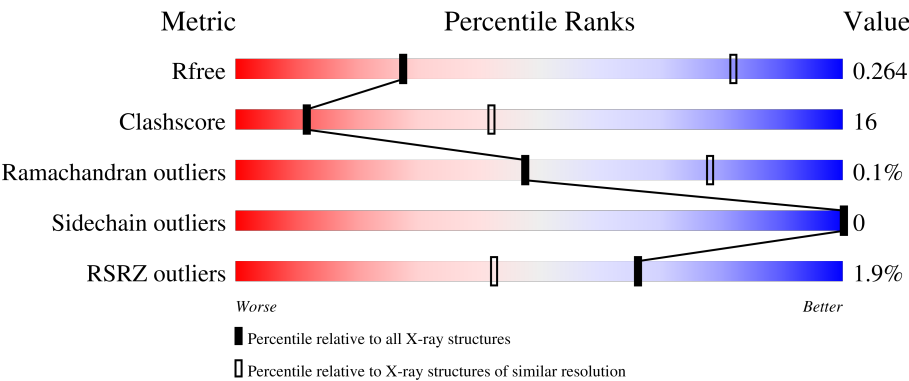
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.73 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	1234 (3.88-3.60)
Clashscore	190562	1274 (3.88-3.60)
Ramachandran outliers	187476	1226 (3.88-3.60)
Sidechain outliers	187428	1221 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)

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	130	% 41%10%49%
1	B	130	% 29%20%51%
1	C	130	% 31%18%51%
1	D	130	% 38%12%51%
1	E	130	% 30%20%50%

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Mol	Chain	Length	Quality of chain
1	F	130	29% 20% 51%
1	G	130	32% 16% 52%
1	H	130	2% 29% 19% 52%
1	I	130	30% 20% 50%
1	J	130	2% 32% 18% 49%
1	K	130	3% 30% 20% 49%
1	L	130	2% 38% 10% 51%
1	M	130	34% 18% 48%
1	N	130	2% 32% 18% 49%
1	O	130	37% 13% 50%
1	P	130	2% 26% 22% 52%
1	Q	130	32% 18% 50%
1	R	130	2% 25% 23% 52%
1	S	130	24% 24% 52%
1	T	130	33% 16% 51%
1	U	130	2% 32% 18% 51%
1	V	130	35% 15% 49%
1	W	130	33% 15% 52%
1	X	130	33% 17% 49%
1	Y	130	34% 16% 50%
1	Z	130	38% 12% 50%
1	a	130	2% 34% 15% 51%
1	b	130	30% 19% 51%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15048 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	Z	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	Y	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	T	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	P	62	Total	C	N	O	S	0	0	0
			514	325	88	99	2			
1	S	62	Total	C	N	O	S	0	0	0
			514	325	88	99	2			
1	X	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	W	63	Total	C	N	O	S	0	0	0
			521	330	89	100	2			
1	Q	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	R	63	Total	C	N	O	S	0	0	0
			521	330	89	100	2			
1	U	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	a	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	O	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	A	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	E	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	L	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	H	63	Total	C	N	O	S	0	0	0
			521	330	89	100	2			
1	B	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	G	62	Total	C	N	O	S	0	0	0
			514	325	88	99	2			
1	C	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	M	67	Total	C	N	O	S	0	0	0
			558	353	95	108	2			
1	N	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	I	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	D	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	J	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	F	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	b	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	568	GLY	-	expression tag	UNP A0A1Q1NMU1
V	569	PRO	-	expression tag	UNP A0A1Q1NMU1
V	570	LEU	-	expression tag	UNP A0A1Q1NMU1
V	571	GLY	-	expression tag	UNP A0A1Q1NMU1
V	572	SER	-	expression tag	UNP A0A1Q1NMU1
Z	568	GLY	-	expression tag	UNP A0A1Q1NMU1
Z	569	PRO	-	expression tag	UNP A0A1Q1NMU1
Z	570	LEU	-	expression tag	UNP A0A1Q1NMU1
Z	571	GLY	-	expression tag	UNP A0A1Q1NMU1
Z	572	SER	-	expression tag	UNP A0A1Q1NMU1
Y	568	GLY	-	expression tag	UNP A0A1Q1NMU1
Y	569	PRO	-	expression tag	UNP A0A1Q1NMU1
Y	570	LEU	-	expression tag	UNP A0A1Q1NMU1
Y	571	GLY	-	expression tag	UNP A0A1Q1NMU1
Y	572	SER	-	expression tag	UNP A0A1Q1NMU1

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Chain	Residue	Modelled	Actual	Comment	Reference
T	568	GLY	-	expression tag	UNP A0A1Q1NMU1
T	569	PRO	-	expression tag	UNP A0A1Q1NMU1
T	570	LEU	-	expression tag	UNP A0A1Q1NMU1
T	571	GLY	-	expression tag	UNP A0A1Q1NMU1
T	572	SER	-	expression tag	UNP A0A1Q1NMU1
P	568	GLY	-	expression tag	UNP A0A1Q1NMU1
P	569	PRO	-	expression tag	UNP A0A1Q1NMU1
P	570	LEU	-	expression tag	UNP A0A1Q1NMU1
P	571	GLY	-	expression tag	UNP A0A1Q1NMU1
P	572	SER	-	expression tag	UNP A0A1Q1NMU1
S	568	GLY	-	expression tag	UNP A0A1Q1NMU1
S	569	PRO	-	expression tag	UNP A0A1Q1NMU1
S	570	LEU	-	expression tag	UNP A0A1Q1NMU1
S	571	GLY	-	expression tag	UNP A0A1Q1NMU1
S	572	SER	-	expression tag	UNP A0A1Q1NMU1
X	568	GLY	-	expression tag	UNP A0A1Q1NMU1
X	569	PRO	-	expression tag	UNP A0A1Q1NMU1
X	570	LEU	-	expression tag	UNP A0A1Q1NMU1
X	571	GLY	-	expression tag	UNP A0A1Q1NMU1
X	572	SER	-	expression tag	UNP A0A1Q1NMU1
W	568	GLY	-	expression tag	UNP A0A1Q1NMU1
W	569	PRO	-	expression tag	UNP A0A1Q1NMU1
W	570	LEU	-	expression tag	UNP A0A1Q1NMU1
W	571	GLY	-	expression tag	UNP A0A1Q1NMU1
W	572	SER	-	expression tag	UNP A0A1Q1NMU1
Q	568	GLY	-	expression tag	UNP A0A1Q1NMU1
Q	569	PRO	-	expression tag	UNP A0A1Q1NMU1
Q	570	LEU	-	expression tag	UNP A0A1Q1NMU1
Q	571	GLY	-	expression tag	UNP A0A1Q1NMU1
Q	572	SER	-	expression tag	UNP A0A1Q1NMU1
R	568	GLY	-	expression tag	UNP A0A1Q1NMU1
R	569	PRO	-	expression tag	UNP A0A1Q1NMU1
R	570	LEU	-	expression tag	UNP A0A1Q1NMU1
R	571	GLY	-	expression tag	UNP A0A1Q1NMU1
R	572	SER	-	expression tag	UNP A0A1Q1NMU1
U	568	GLY	-	expression tag	UNP A0A1Q1NMU1
U	569	PRO	-	expression tag	UNP A0A1Q1NMU1
U	570	LEU	-	expression tag	UNP A0A1Q1NMU1
U	571	GLY	-	expression tag	UNP A0A1Q1NMU1
U	572	SER	-	expression tag	UNP A0A1Q1NMU1
a	568	GLY	-	expression tag	UNP A0A1Q1NMU1
a	569	PRO	-	expression tag	UNP A0A1Q1NMU1

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Chain	Residue	Modelled	Actual	Comment	Reference
a	570	LEU	-	expression tag	UNP A0A1Q1NMU1
a	571	GLY	-	expression tag	UNP A0A1Q1NMU1
a	572	SER	-	expression tag	UNP A0A1Q1NMU1
O	568	GLY	-	expression tag	UNP A0A1Q1NMU1
O	569	PRO	-	expression tag	UNP A0A1Q1NMU1
O	570	LEU	-	expression tag	UNP A0A1Q1NMU1
O	571	GLY	-	expression tag	UNP A0A1Q1NMU1
O	572	SER	-	expression tag	UNP A0A1Q1NMU1
A	568	GLY	-	expression tag	UNP A0A1Q1NMU1
A	569	PRO	-	expression tag	UNP A0A1Q1NMU1
A	570	LEU	-	expression tag	UNP A0A1Q1NMU1
A	571	GLY	-	expression tag	UNP A0A1Q1NMU1
A	572	SER	-	expression tag	UNP A0A1Q1NMU1
E	568	GLY	-	expression tag	UNP A0A1Q1NMU1
E	569	PRO	-	expression tag	UNP A0A1Q1NMU1
E	570	LEU	-	expression tag	UNP A0A1Q1NMU1
E	571	GLY	-	expression tag	UNP A0A1Q1NMU1
E	572	SER	-	expression tag	UNP A0A1Q1NMU1
L	568	GLY	-	expression tag	UNP A0A1Q1NMU1
L	569	PRO	-	expression tag	UNP A0A1Q1NMU1
L	570	LEU	-	expression tag	UNP A0A1Q1NMU1
L	571	GLY	-	expression tag	UNP A0A1Q1NMU1
L	572	SER	-	expression tag	UNP A0A1Q1NMU1
K	568	GLY	-	expression tag	UNP A0A1Q1NMU1
K	569	PRO	-	expression tag	UNP A0A1Q1NMU1
K	570	LEU	-	expression tag	UNP A0A1Q1NMU1
K	571	GLY	-	expression tag	UNP A0A1Q1NMU1
K	572	SER	-	expression tag	UNP A0A1Q1NMU1
H	568	GLY	-	expression tag	UNP A0A1Q1NMU1
H	569	PRO	-	expression tag	UNP A0A1Q1NMU1
H	570	LEU	-	expression tag	UNP A0A1Q1NMU1
H	571	GLY	-	expression tag	UNP A0A1Q1NMU1
H	572	SER	-	expression tag	UNP A0A1Q1NMU1
B	568	GLY	-	expression tag	UNP A0A1Q1NMU1
B	569	PRO	-	expression tag	UNP A0A1Q1NMU1
B	570	LEU	-	expression tag	UNP A0A1Q1NMU1
B	571	GLY	-	expression tag	UNP A0A1Q1NMU1
B	572	SER	-	expression tag	UNP A0A1Q1NMU1
G	568	GLY	-	expression tag	UNP A0A1Q1NMU1
G	569	PRO	-	expression tag	UNP A0A1Q1NMU1
G	570	LEU	-	expression tag	UNP A0A1Q1NMU1
G	571	GLY	-	expression tag	UNP A0A1Q1NMU1

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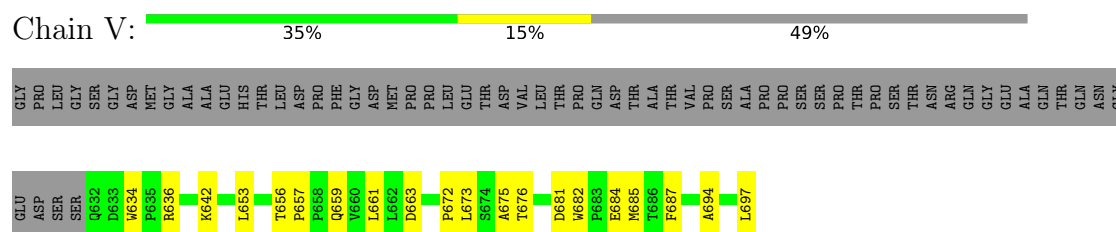
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Chain	Residue	Modelled	Actual	Comment	Reference
G	572	SER	-	expression tag	UNP A0A1Q1NMU1
C	568	GLY	-	expression tag	UNP A0A1Q1NMU1
C	569	PRO	-	expression tag	UNP A0A1Q1NMU1
C	570	LEU	-	expression tag	UNP A0A1Q1NMU1
C	571	GLY	-	expression tag	UNP A0A1Q1NMU1
C	572	SER	-	expression tag	UNP A0A1Q1NMU1
M	568	GLY	-	expression tag	UNP A0A1Q1NMU1
M	569	PRO	-	expression tag	UNP A0A1Q1NMU1
M	570	LEU	-	expression tag	UNP A0A1Q1NMU1
M	571	GLY	-	expression tag	UNP A0A1Q1NMU1
M	572	SER	-	expression tag	UNP A0A1Q1NMU1
N	568	GLY	-	expression tag	UNP A0A1Q1NMU1
N	569	PRO	-	expression tag	UNP A0A1Q1NMU1
N	570	LEU	-	expression tag	UNP A0A1Q1NMU1
N	571	GLY	-	expression tag	UNP A0A1Q1NMU1
N	572	SER	-	expression tag	UNP A0A1Q1NMU1
I	568	GLY	-	expression tag	UNP A0A1Q1NMU1
I	569	PRO	-	expression tag	UNP A0A1Q1NMU1
I	570	LEU	-	expression tag	UNP A0A1Q1NMU1
I	571	GLY	-	expression tag	UNP A0A1Q1NMU1
I	572	SER	-	expression tag	UNP A0A1Q1NMU1
D	568	GLY	-	expression tag	UNP A0A1Q1NMU1
D	569	PRO	-	expression tag	UNP A0A1Q1NMU1
D	570	LEU	-	expression tag	UNP A0A1Q1NMU1
D	571	GLY	-	expression tag	UNP A0A1Q1NMU1
D	572	SER	-	expression tag	UNP A0A1Q1NMU1
J	568	GLY	-	expression tag	UNP A0A1Q1NMU1
J	569	PRO	-	expression tag	UNP A0A1Q1NMU1
J	570	LEU	-	expression tag	UNP A0A1Q1NMU1
J	571	GLY	-	expression tag	UNP A0A1Q1NMU1
J	572	SER	-	expression tag	UNP A0A1Q1NMU1
F	568	GLY	-	expression tag	UNP A0A1Q1NMU1
F	569	PRO	-	expression tag	UNP A0A1Q1NMU1
F	570	LEU	-	expression tag	UNP A0A1Q1NMU1
F	571	GLY	-	expression tag	UNP A0A1Q1NMU1
F	572	SER	-	expression tag	UNP A0A1Q1NMU1
b	568	GLY	-	expression tag	UNP A0A1Q1NMU1
b	569	PRO	-	expression tag	UNP A0A1Q1NMU1
b	570	LEU	-	expression tag	UNP A0A1Q1NMU1
b	571	GLY	-	expression tag	UNP A0A1Q1NMU1
b	572	SER	-	expression tag	UNP A0A1Q1NMU1

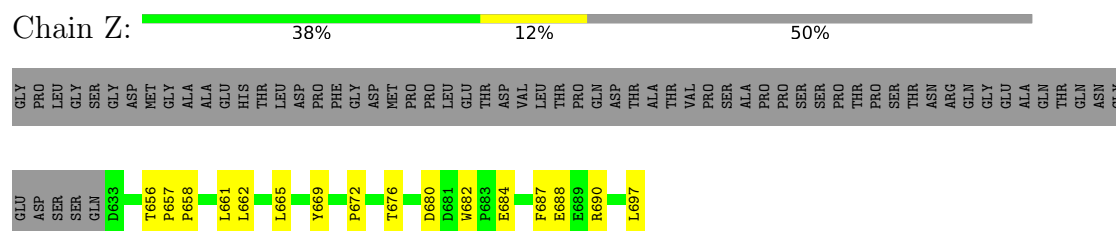
3 Residue-property plots [i](#)

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.

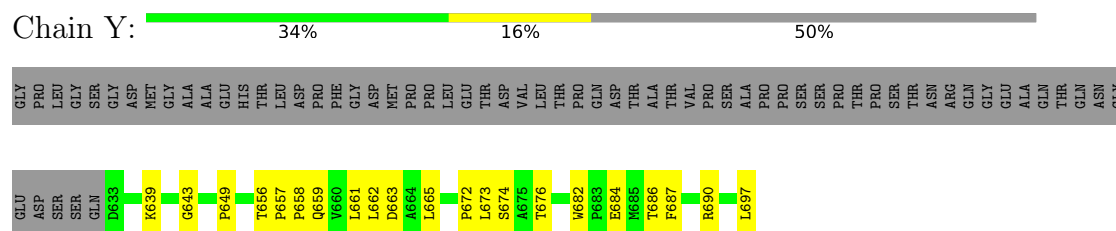
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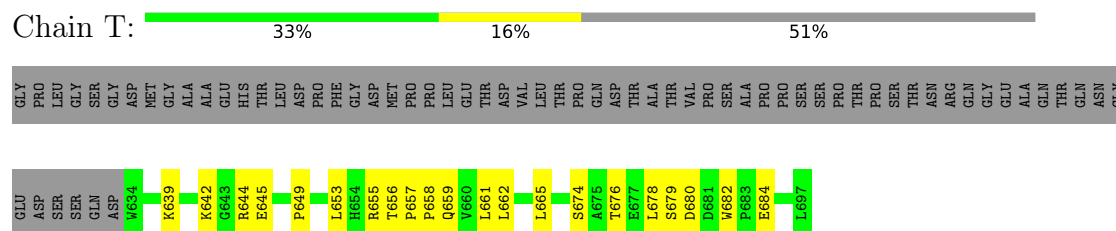
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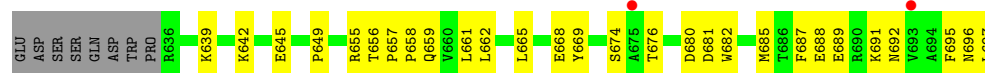
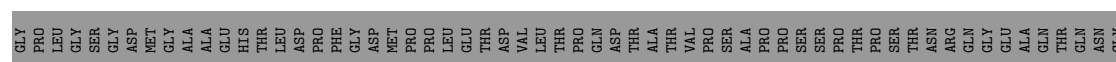
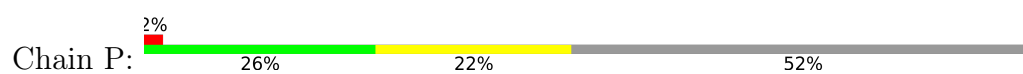
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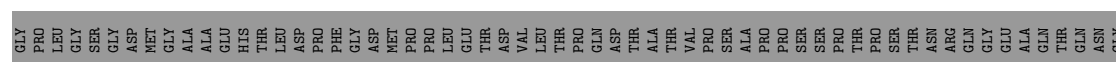
- Molecule 1: Nucleoprotein



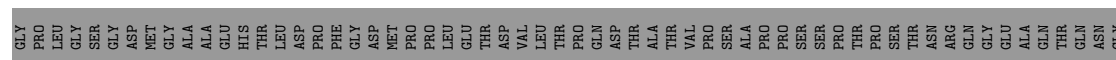
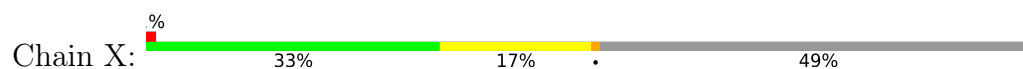
- Molecule 1: Nucleoprotein



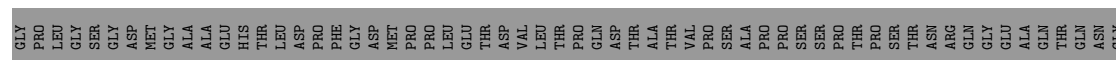
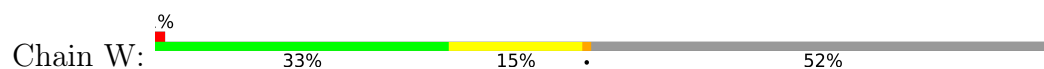
• Molecule 1: Nucleoprotein



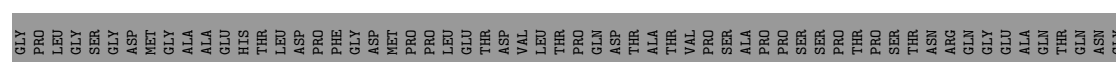
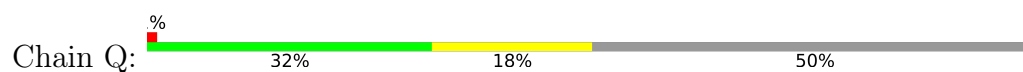
• Molecule 1: Nucleoprotein



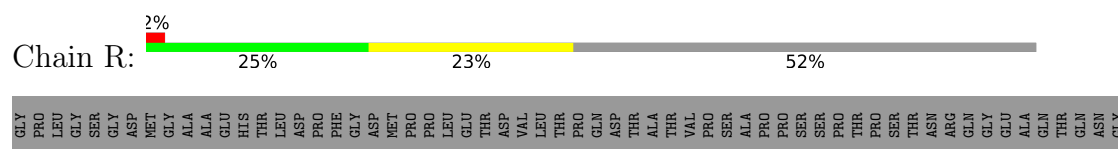
• Molecule 1: Nucleoprotein



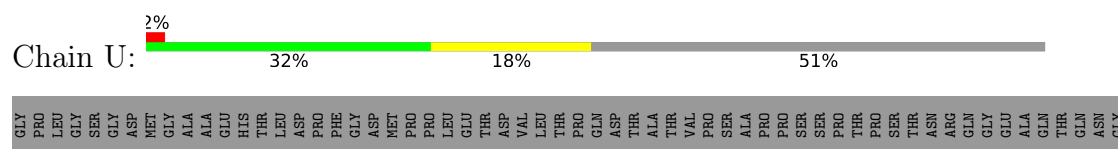
• Molecule 1: Nucleoprotein



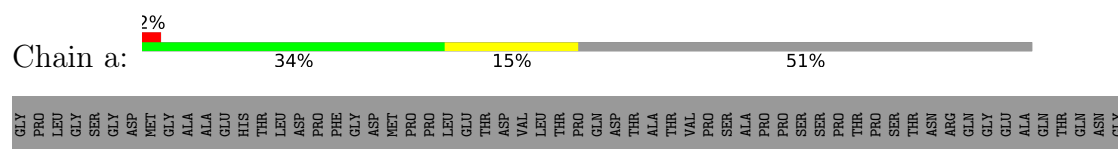
• Molecule 1: Nucleoprotein



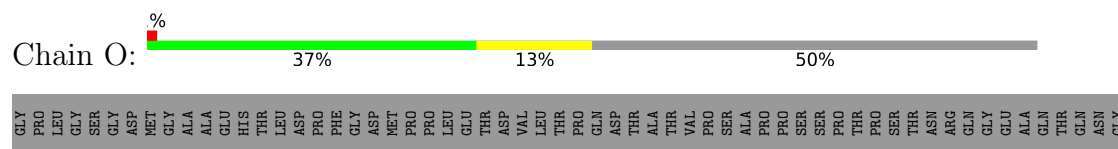
- Molecule 1: Nucleoprotein



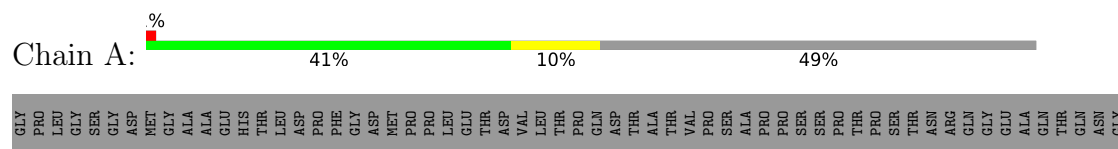
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein

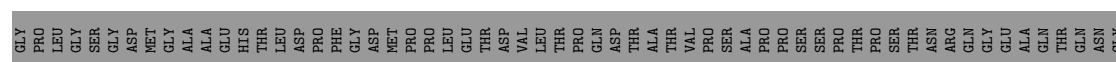
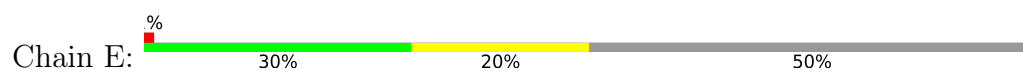


- Molecule 1: Nucleoprotein

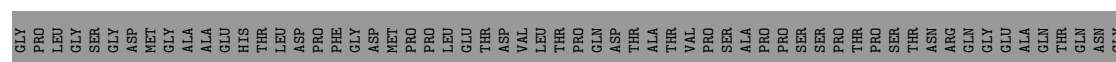
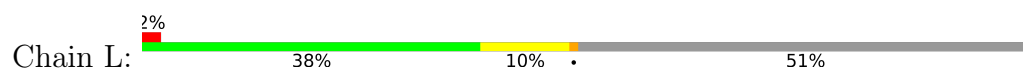


- Molecule 1: Nucleoprotein

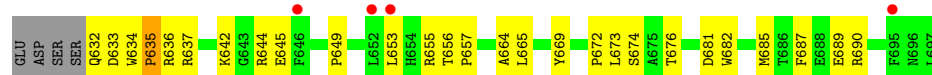
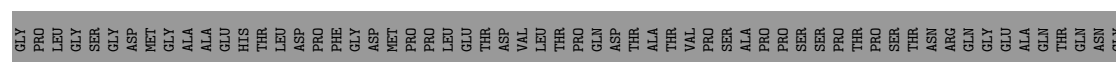
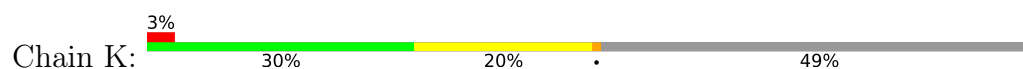




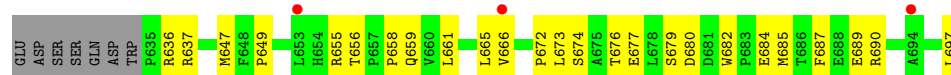
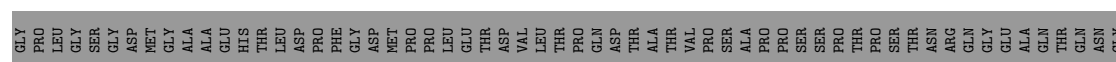
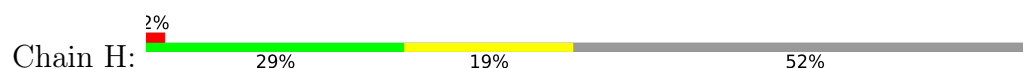
• Molecule 1: Nucleoprotein



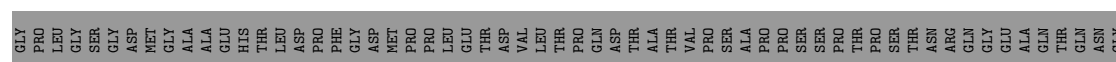
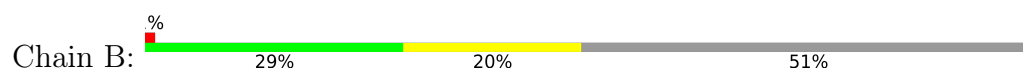
• Molecule 1: Nucleoprotein



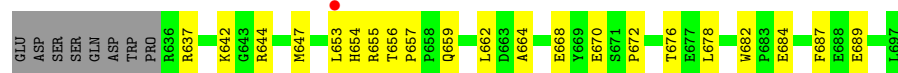
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



Chain C:

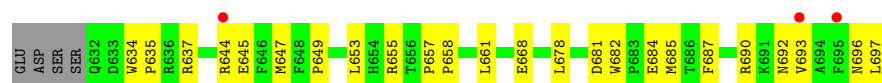


Chain M: 34% 18% 48%

Amino Acid	Count
GLY	1
PRO	1
LEU	1
GLY	1
SER	1
GLY	1
ASP	1
MET	1
GLY	1
ALA	1
ALA	1
GLU	1
HIS	1
THR	1
LEU	1
ASP	1
PRO	1
PHE	1
GLY	1
ASP	1
MET	1
PRO	1
PRO	1
LEU	1
GLU	1
THR	1
ASP	1
VAL	1
LEU	1
THR	1
THR	1
ALA	1
THR	1
VAL	1
PRO	1
SER	1
SER	1
ALA	1
PRO	1
PRO	1
SER	1
SER	1
PRO	1
THR	1
PRO	1
SER	1
THR	1
ASN	1
ARG	1
GLN	1
GLY	1
GLU	1
ALA	1
GLN	1
THR	1
GLN	1
ASN	1



Chain N:

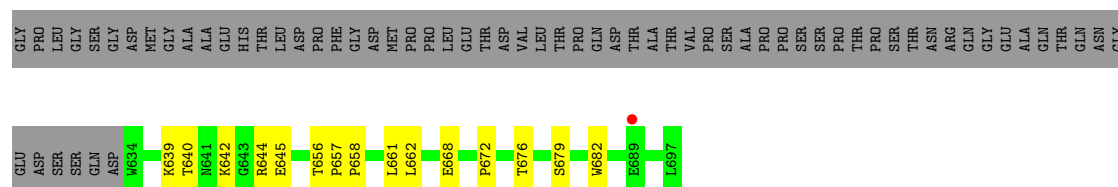


Chain I:

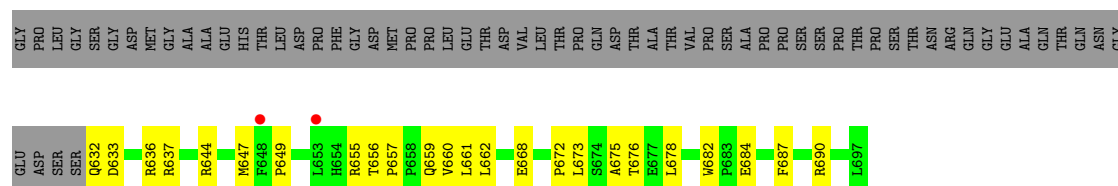
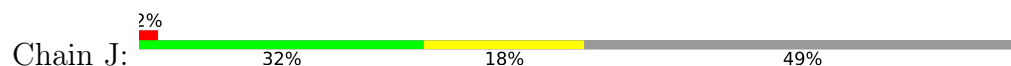
Amino Acid	Percentage
GLY	30%
PRO	30%
LEU	30%
GLY	20%
SER	20%
GLY	20%
ASP	20%
MET	20%
GLY	20%
ALA	20%
ALA	20%
GLU	20%
HIS	20%
THR	20%
LEU	20%
ASP	20%
PRO	20%
PHE	20%
GLY	20%
ASP	20%
MET	20%
PRO	20%
LEU	20%
GLU	20%
THR	20%
VAL	20%
LEU	20%
THR	20%
PRO	20%
GLN	20%
ASP	20%
THR	20%
ALA	20%
ALA	20%
SER	20%
SER	20%
PRO	20%
THR	20%
PRO	20%
SER	20%
THR	20%
ASN	20%
ARG	20%
GLN	20%
GLY	20%
GLU	20%
ALA	20%
GLN	20%
THR	20%
GLN	20%
ASN	20%



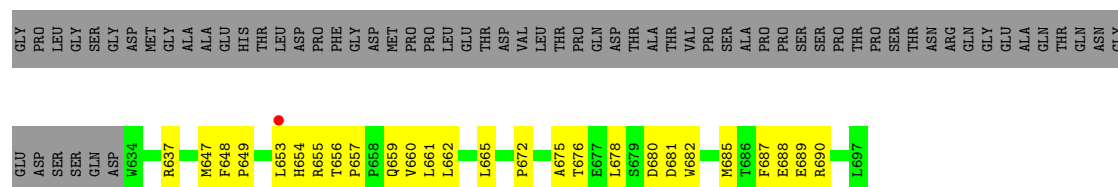
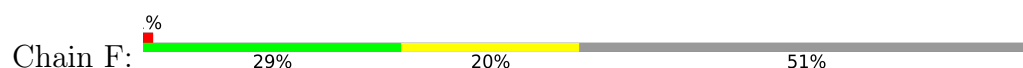
Chain D: %



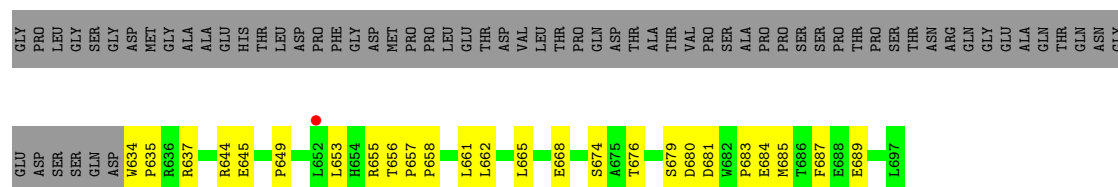
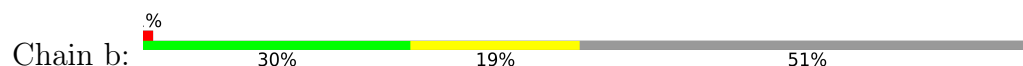
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.75Å 162.94Å 175.36Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	173.13 – 3.73 173.13 – 3.73	Depositor EDS
% Data completeness (in resolution range)	25.1 (173.13-3.73) 25.0 (173.13-3.73)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.78Å)	Xtriage
Refinement program	REFMAC dev_4788, PHENIX dev_4788	Depositor
R, R_{free}	0.248 , 0.265 0.264 , 0.264	Depositor DCC
R_{free} test set	435 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	108.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 95.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15048	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.18% 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	0.12	0/567	0.28	0/770
1	B	0.13	0/550	0.34	0/747
1	C	0.12	0/550	0.31	0/747
1	D	0.12	0/550	0.27	0/747
1	E	0.14	0/558	0.34	0/758
1	F	0.12	0/550	0.30	0/747
1	G	0.14	0/526	0.31	0/712
1	H	0.19	0/534	0.40	0/723
1	I	0.13	0/558	0.29	0/758
1	J	0.13	0/567	0.30	0/770
1	K	0.29	0/567	0.51	1/770 (0.1%)
1	L	0.24	0/550	0.70	1/747 (0.1%)
1	M	0.16	0/573	0.35	0/778
1	N	0.13	0/567	0.34	0/770
1	O	0.15	0/558	0.32	0/758
1	P	0.11	0/526	0.26	0/712
1	Q	0.13	0/558	0.34	0/758
1	R	0.15	0/534	0.34	0/723
1	S	0.13	0/526	0.28	0/712
1	T	0.12	0/550	0.32	0/747
1	U	0.13	0/550	0.30	0/747
1	V	0.12	0/567	0.31	0/770
1	W	0.27	0/534	0.41	0/723
1	X	0.16	0/567	0.35	0/770
1	Y	0.14	0/558	0.34	0/758
1	Z	0.12	0/558	0.27	0/758
1	a	0.15	0/550	0.37	0/747
1	b	0.12	0/550	0.30	0/747
All	All	0.16	0/15453	0.35	2/20974 (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	K	0	2
1	L	0	2
1	W	0	2
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	L	637	ARG	N-CA-C	-14.57	85.32	108.63
1	K	635	PRO	N-CA-C	-5.83	100.46	112.47

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	636	ARG	Sidechain
1	K	637	ARG	Sidechain
1	L	636	ARG	Sidechain
1	L	637	ARG	Sidechain
1	W	636	ARG	Sidechain
1	W	637	ARG	Sidechain

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	552	0	529	8	0
1	B	535	0	517	22	0
1	C	535	0	517	20	0
1	D	535	0	517	15	0
1	E	543	0	521	21	0
1	F	535	0	517	26	0
1	G	514	0	500	28	0
1	H	521	0	508	38	0
1	I	543	0	521	37	0
1	J	552	0	529	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	552	0	529	29	0
1	L	535	0	517	10	0
1	M	558	0	534	19	0
1	N	552	0	529	17	1
1	O	543	0	521	15	1
1	P	514	0	500	24	0
1	Q	543	0	521	24	0
1	R	521	0	508	28	0
1	S	514	0	500	33	0
1	T	535	0	517	27	0
1	U	535	0	517	23	0
1	V	552	0	529	17	0
1	W	521	0	508	24	0
1	X	552	0	529	26	0
1	Y	543	0	521	22	0
1	Z	543	0	521	16	0
1	a	535	0	517	17	0
1	b	535	0	517	21	0
All	All	15048	0	14511	469	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 16.

All (469) 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:X:672:PRO:HB2	1:W:649:PRO:HG2	1.32	1.12
1:T:655:ARG:HB2	1:U:659:GLN:HG2	1.55	0.88
1:Y:656:THR:HB	1:X:684:GLU:HA	1.56	0.87
1:I:659:GLN:HG2	1:J:655:ARG:HB2	1.57	0.85
1:W:635:PRO:HD2	1:W:649:PRO:HD3	1.60	0.83
1:I:656:THR:HB	1:J:684:GLU:HA	1.62	0.82
1:H:684:GLU:HA	1:G:656:THR:OG1	1.79	0.82
1:T:680:ASP:HA	1:S:686:THR:OG1	1.81	0.81
1:H:659:GLN:HG2	1:I:655:ARG:HB2	1.63	0.81
1:T:684:GLU:HA	1:U:656:THR:HB	1.64	0.80
1:X:659:GLN:HG2	1:W:655:ARG:HB2	1.62	0.80
1:H:684:GLU:OE2	1:G:654:HIS:ND1	2.15	0.79
1:X:676:THR:HG23	1:W:687:PHE:CD1	2.16	0.79
1:G:653:LEU:HB3	1:F:662:LEU:HD21	1.63	0.79
1:T:659:GLN:HG2	1:S:655:ARG:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:655:ARG:HB2	1:R:659:GLN:HG2	1.66	0.77
1:B:634:TRP:HD1	1:D:672:PRO:HG2	1.46	0.77
1:V:672:PRO:HB2	1:U:649:PRO:HG2	1.66	0.77
1:H:666:VAL:HG21	1:I:653:LEU:HD13	1.66	0.77
1:B:684:GLU:HA	1:D:656:THR:HB	1.67	0.77
1:a:669:TYR:OH	1:a:697:LEU:O	2.02	0.77
1:T:642:LYS:NZ	1:G:670:GLU:HG3	2.01	0.76
1:K:632:GLN:O	1:K:632:GLN:HG2	1.87	0.73
1:S:639:LYS:HG2	1:S:645:GLU:HG2	1.69	0.73
1:X:676:THR:HG23	1:W:687:PHE:CG	2.25	0.72
1:Z:656:THR:HB	1:Y:684:GLU:HA	1.70	0.72
1:Z:672:PRO:HB2	1:Y:649:PRO:HG2	1.71	0.72
1:K:649:PRO:HG2	1:J:672:PRO:HB2	1.72	0.72
1:H:676:THR:HG23	1:I:687:PHE:CD2	2.25	0.71
1:E:688:GLU:N	1:b:680:ASP:OD1	2.23	0.71
1:V:684:GLU:HA	1:W:656:THR:HB	1.72	0.70
1:Y:672:PRO:HB2	1:X:649:PRO:HG2	1.72	0.70
1:M:636:ARG:O	1:M:648:PHE:N	2.25	0.70
1:S:676:THR:HG23	1:R:687:PHE:CD2	2.27	0.70
1:O:637:ARG:HD2	1:O:638:VAL:H	1.56	0.70
1:E:689:GLU:OE2	1:b:655:ARG:NH2	2.24	0.70
1:Y:676:THR:HG23	1:X:687:PHE:CD2	2.27	0.69
1:Z:676:THR:HG23	1:Y:687:PHE:CD2	2.27	0.69
1:E:676:THR:HG23	1:F:687:PHE:CD2	2.28	0.69
1:T:676:THR:HG23	1:S:687:PHE:CG	2.27	0.69
1:B:692:ASN:OD1	1:B:696:ASN:ND2	2.27	0.68
1:W:635:PRO:CD	1:W:649:PRO:HD3	2.24	0.68
1:Q:684:GLU:HA	1:R:656:THR:HB	1.76	0.68
1:B:665:LEU:HG	1:B:697:LEU:HD21	1.76	0.68
1:P:656:THR:HB	1:O:684:GLU:HA	1.76	0.67
1:I:637:ARG:HG2	1:I:647:MET:HG2	1.77	0.66
1:S:637:ARG:HA	1:S:647:MET:HA	1.78	0.66
1:K:645:GLU:N	1:K:645:GLU:OE1	2.29	0.66
1:H:656:THR:HG22	1:I:684:GLU:HG2	1.78	0.65
1:D:640:THR:HG22	1:D:642:LYS:H	1.60	0.65
1:I:656:THR:HG22	1:J:684:GLU:HG2	1.77	0.65
1:H:637:ARG:HG2	1:H:647:MET:HG2	1.79	0.65
1:T:676:THR:HG23	1:S:687:PHE:CD1	2.31	0.65
1:F:662:LEU:HG	1:F:675:ALA:HB1	1.80	0.64
1:S:672:PRO:HB2	1:R:649:PRO:HG2	1.79	0.64
1:V:672:PRO:HG3	1:U:635:PRO:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:639:LYS:HG2	1:I:645:GLU:HG2	1.79	0.63
1:B:687:PHE:CD2	1:D:676:THR:HG23	2.33	0.63
1:E:666:VAL:HG21	1:F:653:LEU:HD13	1.81	0.63
1:E:672:PRO:HB2	1:F:649:PRO:HG2	1.78	0.63
1:B:642:LYS:O	1:B:644:ARG:NH1	2.31	0.63
1:a:682:TRP:O	1:a:690:ARG:NH2	2.33	0.62
1:Y:665:LEU:HG	1:Y:697:LEU:HD21	1.81	0.62
1:H:680:ASP:HA	1:I:686:THR:CG2	2.29	0.62
1:a:644:ARG:HH12	1:a:668:GLU:HG3	1.65	0.62
1:C:659:GLN:HG2	1:b:655:ARG:HB2	1.80	0.62
1:R:673:LEU:O	1:R:677:GLU:HG2	2.00	0.61
1:K:644:ARG:HH21	1:K:664:ALA:HB1	1.64	0.61
1:Z:665:LEU:HG	1:Z:697:LEU:HD21	1.82	0.61
1:S:692:ASN:OD1	1:S:696:ASN:ND2	2.33	0.61
1:Y:659:GLN:HG2	1:X:655:ARG:HB2	1.82	0.61
1:T:642:LYS:HZ3	1:G:670:GLU:HG3	1.65	0.61
1:P:649:PRO:HG2	1:Q:672:PRO:HB2	1.81	0.61
1:S:680:ASP:HA	1:R:686:THR:CG2	2.30	0.61
1:H:637:ARG:HG2	1:H:647:MET:CG	2.30	0.61
1:L:684:GLU:HA	1:K:656:THR:OG1	2.00	0.61
1:V:676:THR:HG23	1:U:687:PHE:CD2	2.36	0.60
1:H:656:THR:CG2	1:I:684:GLU:HG2	2.32	0.60
1:H:656:THR:HB	1:I:684:GLU:HA	1.83	0.60
1:M:685:MET:HE3	1:M:689:GLU:HG3	1.84	0.60
1:X:665:LEU:HD11	1:X:697:LEU:HD21	1.82	0.60
1:E:687:PHE:N	1:b:679:SER:OG	2.34	0.59
1:Y:657:PRO:HG2	1:Y:662:LEU:HD11	1.83	0.59
1:J:632:GLN:HA	1:J:636:ARG:HH12	1.67	0.59
1:O:637:ARG:HH21	1:O:645:GLU:HG3	1.67	0.59
1:b:637:ARG:NH1	1:b:645:GLU:OE2	2.35	0.59
1:X:672:PRO:HB2	1:W:649:PRO:CG	2.19	0.59
1:C:665:LEU:HG	1:C:697:LEU:HD21	1.84	0.58
1:J:637:ARG:HA	1:J:647:MET:HA	1.85	0.58
1:V:653:LEU:HD21	1:W:676:THR:HG22	1.84	0.58
1:Z:680:ASP:HA	1:Y:686:THR:CG2	2.34	0.58
1:G:659:GLN:HA	1:G:662:LEU:HD12	1.86	0.58
1:H:680:ASP:OD1	1:I:686:THR:HG22	2.03	0.58
1:Y:656:THR:CB	1:X:684:GLU:HA	2.31	0.58
1:M:644:ARG:HH22	1:M:668:GLU:CD	2.10	0.58
1:I:656:THR:CB	1:J:684:GLU:HA	2.32	0.58
1:T:657:PRO:HG3	1:T:678:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:639:LYS:HB3	1:P:645:GLU:HG2	1.86	0.58
1:S:659:GLN:HG2	1:R:655:ARG:HB2	1.85	0.57
1:T:642:LYS:HZ2	1:G:670:GLU:HG3	1.69	0.57
1:R:639:LYS:HB3	1:R:645:GLU:HG2	1.86	0.57
1:B:676:THR:HG23	1:C:687:PHE:CD2	2.39	0.57
1:M:665:LEU:HG	1:M:697:LEU:HD21	1.86	0.57
1:H:637:ARG:CG	1:H:647:MET:HG2	2.35	0.57
1:H:656:THR:CB	1:I:684:GLU:HA	2.34	0.57
1:K:655:ARG:HB2	1:J:659:GLN:HG2	1.87	0.56
1:b:665:LEU:HD22	1:b:674:SER:HB3	1.87	0.56
1:T:684:GLU:HA	1:U:656:THR:CB	2.33	0.56
1:W:637:ARG:HA	1:W:647:MET:HA	1.87	0.56
1:H:649:PRO:HG2	1:G:672:PRO:HB2	1.87	0.56
1:I:658:PRO:HD2	1:I:661:LEU:HD12	1.88	0.56
1:V:673:LEU:HD21	1:U:634:TRP:CD2	2.40	0.56
1:Z:658:PRO:HD2	1:Z:661:LEU:HD12	1.87	0.56
1:S:680:ASP:OD1	1:R:686:THR:HG22	2.05	0.56
1:a:637:ARG:NH1	1:a:645:GLU:OE2	2.35	0.56
1:H:673:LEU:O	1:H:677:GLU:HG2	2.06	0.56
1:G:657:PRO:HG3	1:G:678:LEU:HD23	1.87	0.56
1:I:676:THR:HG23	1:J:687:PHE:CD2	2.41	0.56
1:b:634:TRP:HD1	1:b:635:PRO:HD2	1.71	0.56
1:M:672:PRO:HB2	1:N:649:PRO:HG2	1.88	0.55
1:K:672:PRO:HG2	1:K:673:LEU:HD22	1.87	0.55
1:B:634:TRP:CD1	1:D:672:PRO:HG2	2.36	0.55
1:E:665:LEU:HG	1:E:697:LEU:HD21	1.88	0.55
1:G:644:ARG:NH2	1:G:668:GLU:OE1	2.40	0.55
1:A:665:LEU:HD22	1:A:674:SER:HB3	1.88	0.54
1:H:665:LEU:HG	1:H:697:LEU:HD21	1.88	0.54
1:B:649:PRO:HG2	1:D:672:PRO:HB2	1.88	0.54
1:D:644:ARG:NH2	1:D:668:GLU:OE1	2.40	0.54
1:H:689:GLU:OE2	1:G:655:ARG:NH2	2.40	0.54
1:N:634:TRP:CD2	1:N:635:PRO:HD2	2.43	0.54
1:F:637:ARG:HA	1:F:647:MET:HA	1.88	0.54
1:X:656:THR:HB	1:W:684:GLU:HA	1.89	0.54
1:A:685:MET:HE3	1:A:689:GLU:HG3	1.89	0.54
1:F:685:MET:HE2	1:F:689:GLU:HB3	1.90	0.54
1:W:658:PRO:HD2	1:W:661:LEU:HD12	1.89	0.54
1:G:637:ARG:HA	1:G:647:MET:HA	1.88	0.54
1:T:656:THR:HG23	1:T:657:PRO:HD2	1.90	0.54
1:J:673:LEU:O	1:J:676:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:666:VAL:HG11	1:I:653:LEU:CD1	2.37	0.53
1:N:682:TRP:O	1:N:690:ARG:NH2	2.40	0.53
1:M:658:PRO:HD2	1:M:661:LEU:HD12	1.89	0.53
1:E:692:ASN:OD1	1:E:696:ASN:ND2	2.40	0.53
1:F:665:LEU:HD11	1:F:678:LEU:HD13	1.90	0.53
1:P:676:THR:HG23	1:O:687:PHE:CD2	2.43	0.53
1:S:665:LEU:HG	1:S:697:LEU:HD21	1.89	0.53
1:H:655:ARG:H	1:G:659:GLN:NE2	2.07	0.53
1:B:659:GLN:HA	1:B:662:LEU:HD12	1.90	0.53
1:G:689:GLU:OE2	1:F:655:ARG:NH2	2.42	0.53
1:G:687:PHE:HB3	1:F:680:ASP:OD1	2.07	0.53
1:T:644:ARG:H	1:T:644:ARG:HD2	1.74	0.53
1:U:685:MET:HE2	1:U:689:GLU:HG3	1.90	0.53
1:M:659:GLN:HG2	1:N:655:ARG:HB2	1.91	0.53
1:T:657:PRO:HD3	1:T:682:TRP:CB	2.38	0.53
1:V:684:GLU:HG2	1:W:656:THR:HG22	1.91	0.53
1:N:637:ARG:HE	1:N:645:GLU:HG2	1.73	0.53
1:X:656:THR:HG22	1:W:684:GLU:HG2	1.90	0.52
1:E:684:GLU:HA	1:b:656:THR:HB	1.91	0.52
1:K:644:ARG:HE	1:K:664:ALA:HB2	1.73	0.52
1:S:658:PRO:HD2	1:S:661:LEU:HD12	1.91	0.52
1:R:681:ASP:O	1:R:685:MET:HG3	2.08	0.52
1:D:640:THR:N	1:D:644:ARG:O	2.28	0.52
1:Y:659:GLN:NE2	1:Y:663:ASP:OD1	2.42	0.52
1:T:639:LYS:HA	1:T:645:GLU:HA	1.92	0.52
1:S:644:ARG:HH12	1:S:668:GLU:HG3	1.74	0.52
1:B:665:LEU:HD22	1:B:674:SER:HB3	1.91	0.52
1:R:637:ARG:HB2	1:R:647:MET:HE2	1.92	0.52
1:H:679:SER:OG	1:I:686:THR:HA	2.09	0.52
1:P:680:ASP:HA	1:O:686:THR:CG2	2.40	0.52
1:U:658:PRO:HD2	1:U:661:LEU:HD12	1.91	0.52
1:D:657:PRO:HG2	1:D:662:LEU:HD11	1.92	0.52
1:P:688:GLU:HG2	1:Q:680:ASP:CG	2.35	0.52
1:U:665:LEU:HG	1:U:697:LEU:HD21	1.92	0.52
1:C:656:THR:HB	1:b:684:GLU:HA	1.93	0.52
1:A:682:TRP:O	1:A:690:ARG:NH2	2.42	0.51
1:X:676:THR:HG23	1:W:687:PHE:CE1	2.44	0.51
1:H:666:VAL:HG11	1:I:653:LEU:HD11	1.92	0.51
1:M:676:THR:HG23	1:N:687:PHE:CD2	2.45	0.51
1:K:642:LYS:CG	1:K:644:ARG:HH12	2.23	0.51
1:H:672:PRO:HB2	1:I:649:PRO:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ASN:N	1:C:641:ASN:OD1	2.44	0.51
1:H:687:PHE:CD2	1:G:676:THR:HG23	2.46	0.51
1:J:657:PRO:HG3	1:J:678:LEU:HD23	1.93	0.51
1:F:657:PRO:HG3	1:F:678:LEU:HD23	1.92	0.51
1:X:675:ALA:HB3	1:W:653:LEU:HD13	1.92	0.51
1:U:665:LEU:HD22	1:U:674:SER:HB3	1.92	0.51
1:H:636:ARG:HG2	1:H:637:ARG:N	2.25	0.51
1:Z:656:THR:HG22	1:Y:684:GLU:HG2	1.93	0.51
1:V:675:ALA:HB3	1:U:653:LEU:HD13	1.92	0.50
1:P:658:PRO:HD2	1:P:661:LEU:HD12	1.93	0.50
1:P:687:PHE:CE2	1:Q:676:THR:HG23	2.47	0.50
1:C:640:THR:OG1	1:C:644:ARG:HB2	2.12	0.50
1:M:642:LYS:NZ	1:M:668:GLU:OE2	2.39	0.50
1:N:658:PRO:HD2	1:N:661:LEU:HD12	1.93	0.50
1:P:665:LEU:HG	1:P:697:LEU:HD21	1.92	0.50
1:Q:684:GLU:HA	1:R:656:THR:CB	2.42	0.50
1:I:659:GLN:HA	1:I:662:LEU:HD12	1.92	0.50
1:H:656:THR:CG2	1:I:684:GLU:HA	2.42	0.50
1:B:637:ARG:HD3	1:B:647:MET:HG2	1.93	0.50
1:C:657:PRO:HG2	1:C:662:LEU:HD11	1.91	0.50
1:T:656:THR:CB	1:S:684:GLU:HA	2.42	0.50
1:F:657:PRO:HB3	1:F:682:TRP:CE3	2.46	0.50
1:V:661:LEU:HD21	1:V:694:ALA:HA	1.94	0.50
1:T:656:THR:HG21	1:S:683:PRO:O	2.10	0.50
1:P:692:ASN:OD1	1:P:696:ASN:ND2	2.45	0.50
1:N:657:PRO:HB3	1:N:682:TRP:CE3	2.46	0.50
1:S:681:ASP:O	1:S:685:MET:HG3	2.11	0.50
1:X:633:ASP:OD1	1:X:634:TRP:N	2.43	0.50
1:Q:665:LEU:HG	1:Q:697:LEU:HD21	1.94	0.50
1:U:681:ASP:O	1:U:685:MET:HG3	2.12	0.50
1:G:642:LYS:HB3	1:G:644:ARG:HH12	1.77	0.49
1:F:656:THR:HG23	1:F:657:PRO:HD2	1.93	0.49
1:F:657:PRO:HD3	1:F:682:TRP:CB	2.42	0.49
1:F:681:ASP:O	1:F:685:MET:HG3	2.11	0.49
1:L:681:ASP:O	1:L:685:MET:HG3	2.13	0.49
1:K:642:LYS:HG3	1:K:644:ARG:HH12	1.77	0.49
1:K:682:TRP:O	1:K:690:ARG:NH2	2.41	0.49
1:H:656:THR:HG21	1:I:684:GLU:HA	1.95	0.49
1:E:687:PHE:CD2	1:b:676:THR:HG23	2.48	0.49
1:S:656:THR:CB	1:R:684:GLU:HA	2.42	0.49
1:a:672:PRO:O	1:a:676:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:644:ARG:NH2	1:J:668:GLU:OE1	2.40	0.49
1:B:684:GLU:HA	1:D:656:THR:CB	2.38	0.49
1:B:687:PHE:N	1:D:679:SER:OG	2.46	0.49
1:Y:682:TRP:O	1:Y:690:ARG:NH2	2.45	0.49
1:W:635:PRO:N	1:W:649:PRO:HD3	2.28	0.49
1:U:657:PRO:HG2	1:U:662:LEU:HD11	1.94	0.49
1:O:657:PRO:HG2	1:O:662:LEU:HD11	1.95	0.49
1:A:659:GLN:HA	1:A:662:LEU:HD12	1.94	0.49
1:G:644:ARG:HH21	1:G:664:ALA:HB1	1.77	0.49
1:D:658:PRO:HD2	1:D:661:LEU:HD12	1.95	0.49
1:J:633:ASP:OD1	1:J:633:ASP:N	2.45	0.49
1:S:657:PRO:HD3	1:S:682:TRP:CB	2.43	0.49
1:R:658:PRO:HD2	1:R:661:LEU:HD12	1.95	0.49
1:R:685:MET:HE2	1:R:689:GLU:HG3	1.93	0.49
1:K:665:LEU:HD22	1:K:674:SER:HB3	1.95	0.49
1:J:657:PRO:HB3	1:J:682:TRP:CE3	2.48	0.49
1:Y:658:PRO:HD2	1:Y:661:LEU:HD12	1.94	0.48
1:M:659:GLN:HA	1:M:662:LEU:HD12	1.95	0.48
1:T:662:LEU:HD21	1:T:679:SER:HB2	1.94	0.48
1:B:672:PRO:HB2	1:C:649:PRO:HG2	1.94	0.48
1:G:684:GLU:CD	1:F:654:HIS:HB3	2.37	0.48
1:M:656:THR:HB	1:N:684:GLU:HA	1.95	0.48
1:Q:659:GLN:HA	1:Q:662:LEU:HD12	1.94	0.48
1:H:679:SER:O	1:I:686:THR:HG23	2.13	0.48
1:Y:657:PRO:HB3	1:Y:682:TRP:CE3	2.49	0.48
1:T:656:THR:HB	1:S:684:GLU:HA	1.94	0.48
1:J:659:GLN:HA	1:J:662:LEU:HD12	1.94	0.48
1:P:657:PRO:HG2	1:P:662:LEU:HD11	1.94	0.48
1:X:657:PRO:HG2	1:X:662:LEU:HD11	1.94	0.48
1:G:655:ARG:HB2	1:F:659:GLN:HG2	1.94	0.48
1:P:655:ARG:HB2	1:Q:659:GLN:HG2	1.94	0.48
1:K:665:LEU:HD23	1:K:669:TYR:HD2	1.79	0.48
1:K:681:ASP:O	1:K:685:MET:HG3	2.13	0.48
1:H:655:ARG:HB2	1:G:659:GLN:CD	2.38	0.48
1:Y:676:THR:HG23	1:X:687:PHE:CG	2.48	0.48
1:a:682:TRP:HA	1:a:685:MET:SD	2.53	0.48
1:Q:657:PRO:HB3	1:Q:682:TRP:CE3	2.48	0.48
1:R:665:LEU:HD22	1:R:674:SER:HB3	1.94	0.48
1:J:656:THR:HG23	1:J:657:PRO:HD2	1.95	0.48
1:O:637:ARG:HD2	1:O:646:PHE:O	2.14	0.48
1:J:660:VAL:HG23	1:J:661:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:682:TRP:O	1:X:690:ARG:NH2	2.45	0.47
1:C:658:PRO:HD2	1:C:661:LEU:HD12	1.96	0.47
1:b:657:PRO:HG2	1:b:662:LEU:HD11	1.96	0.47
1:Q:644:ARG:NH2	1:Q:668:GLU:OE1	2.47	0.47
1:X:658:PRO:HD2	1:X:661:LEU:HD12	1.96	0.47
1:Q:657:PRO:HD3	1:Q:682:TRP:CB	2.44	0.47
1:T:653:LEU:HD21	1:U:676:THR:HG22	1.96	0.47
1:S:680:ASP:HA	1:R:686:THR:HG23	1.96	0.47
1:O:658:PRO:HD2	1:O:661:LEU:HD12	1.97	0.47
1:Q:686:THR:HB	1:Q:689:GLU:HG2	1.97	0.47
1:a:657:PRO:HD3	1:a:682:TRP:CB	2.45	0.47
1:C:675:ALA:HB3	1:b:653:LEU:HD13	1.97	0.47
1:T:657:PRO:HB3	1:T:682:TRP:CE3	2.50	0.47
1:O:659:GLN:HG2	1:A:655:ARG:HB2	1.97	0.47
1:M:675:ALA:HB3	1:N:653:LEU:HD13	1.97	0.47
1:b:681:ASP:O	1:b:685:MET:HG3	2.14	0.47
1:Z:687:PHE:CD2	1:a:676:THR:HB	2.50	0.47
1:a:681:ASP:O	1:a:685:MET:HG3	2.14	0.47
1:a:693:VAL:O	1:a:697:LEU:HB2	2.15	0.47
1:K:633:ASP:HB2	1:K:634:TRP:CE3	2.50	0.47
1:M:657:PRO:HG2	1:M:662:LEU:HD11	1.97	0.47
1:b:662:LEU:HD21	1:b:679:SER:HB2	1.95	0.47
1:S:657:PRO:HG3	1:S:678:LEU:HD23	1.97	0.47
1:E:634:TRP:N	1:E:635:PRO:HD3	2.29	0.47
1:C:662:LEU:HD21	1:C:679:SER:HB2	1.96	0.47
1:P:668:GLU:HG2	1:P:669:TYR:CD1	2.49	0.46
1:Y:639:LYS:HE3	1:Y:643:GLY:HA2	1.98	0.46
1:O:634:TRP:HB3	1:O:636:ARG:HH21	1.80	0.46
1:E:680:ASP:OD1	1:F:688:GLU:N	2.47	0.46
1:B:665:LEU:HD23	1:B:669:TYR:HD2	1.81	0.46
1:F:682:TRP:O	1:F:690:ARG:NH2	2.47	0.46
1:P:656:THR:CB	1:O:684:GLU:HA	2.44	0.46
1:J:657:PRO:HD3	1:J:682:TRP:CB	2.45	0.46
1:J:672:PRO:O	1:J:676:THR:HG23	2.15	0.46
1:S:665:LEU:HD11	1:S:678:LEU:HD13	1.97	0.46
1:P:687:PHE:CD2	1:Q:676:THR:HG23	2.50	0.46
1:Z:682:TRP:O	1:Z:690:ARG:NH2	2.48	0.46
1:T:665:LEU:HD22	1:T:674:SER:HB3	1.97	0.46
1:T:649:PRO:HG2	1:U:672:PRO:HB2	1.97	0.46
1:K:632:GLN:N	1:K:632:GLN:OE1	2.48	0.45
1:Q:657:PRO:HG3	1:Q:678:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:672:PRO:O	1:U:676:THR:HG23	2.15	0.45
1:I:644:ARG:HH12	1:I:668:GLU:CD	2.25	0.45
1:X:676:THR:CG2	1:W:687:PHE:CD1	2.94	0.45
1:E:657:PRO:HD3	1:E:682:TRP:CB	2.46	0.45
1:J:682:TRP:O	1:J:690:ARG:NH2	2.49	0.45
1:a:658:PRO:HD2	1:a:661:LEU:HD12	1.98	0.45
1:N:681:ASP:O	1:N:685:MET:HG3	2.15	0.45
1:V:634:TRP:O	1:V:636:ARG:HG2	2.17	0.45
1:Y:665:LEU:HD22	1:Y:674:SER:HB3	1.99	0.45
1:E:681:ASP:O	1:E:685:MET:HG3	2.17	0.45
1:M:672:PRO:HG3	1:N:635:PRO:HD3	1.99	0.45
1:I:673:LEU:O	1:I:677:GLU:HG2	2.16	0.45
1:X:637:ARG:HA	1:X:647:MET:HA	1.97	0.45
1:Y:673:LEU:HD12	1:X:634:TRP:HZ2	1.82	0.45
1:R:637:ARG:HA	1:R:647:MET:HA	1.99	0.45
1:A:657:PRO:HB3	1:A:682:TRP:CE3	2.52	0.45
1:Z:665:LEU:HD23	1:Z:669:TYR:HD2	1.82	0.45
1:Q:662:LEU:HD21	1:Q:679:SER:HB2	1.99	0.45
1:R:693:VAL:O	1:R:697:LEU:HB3	2.17	0.45
1:U:659:GLN:HA	1:U:662:LEU:HD12	1.99	0.45
1:L:683:PRO:O	1:K:656:THR:HG21	2.17	0.45
1:K:657:PRO:HB3	1:K:682:TRP:CE3	2.52	0.45
1:B:657:PRO:HB3	1:B:682:TRP:CE3	2.52	0.45
1:C:682:TRP:O	1:C:690:ARG:NH2	2.48	0.45
1:E:639:LYS:HG2	1:E:640:THR:O	2.16	0.45
1:I:657:PRO:HG2	1:I:662:LEU:HD11	1.99	0.45
1:T:656:THR:OG1	1:S:684:GLU:HA	2.18	0.44
1:K:689:GLU:OE2	1:J:655:ARG:NH2	2.50	0.44
1:U:643:GLY:C	1:U:644:ARG:HD2	2.42	0.44
1:L:659:GLN:NE2	1:L:663:ASP:OD1	2.50	0.44
1:V:656:THR:HG23	1:V:657:PRO:HD2	1.98	0.44
1:V:657:PRO:HD3	1:V:682:TRP:CB	2.47	0.44
1:V:659:GLN:NE2	1:V:663:ASP:OD1	2.46	0.44
1:G:642:LYS:HB3	1:G:644:ARG:NH1	2.33	0.44
1:Z:657:PRO:HG2	1:Z:662:LEU:HD11	1.98	0.44
1:Z:680:ASP:HA	1:Y:686:THR:HG23	1.99	0.44
1:W:672:PRO:O	1:W:676:THR:HG23	2.17	0.44
1:T:657:PRO:HD3	1:T:682:TRP:CG	2.52	0.44
1:G:657:PRO:HB3	1:G:682:TRP:CE3	2.53	0.44
1:C:657:PRO:HB3	1:C:682:TRP:CE3	2.53	0.44
1:P:657:PRO:HB3	1:P:682:TRP:CE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:682:TRP:O	1:Q:690:ARG:NH2	2.49	0.44
1:E:656:THR:HG23	1:E:657:PRO:HD2	1.99	0.44
1:C:672:PRO:HG3	1:b:635:PRO:HG3	2.00	0.44
1:M:665:LEU:HD22	1:M:674:SER:HB3	1.99	0.44
1:Z:684:GLU:HA	1:a:656:THR:HB	1.98	0.44
1:V:681:ASP:O	1:V:685:MET:HG3	2.18	0.44
1:E:644:ARG:NH2	1:E:668:GLU:OE1	2.47	0.44
1:L:672:PRO:HB2	1:M:649:PRO:HG2	1.99	0.44
1:D:639:LYS:HA	1:D:645:GLU:HA	2.00	0.44
1:K:632:GLN:O	1:K:632:GLN:CG	2.62	0.43
1:H:659:GLN:OE1	1:I:655:ARG:HA	2.18	0.43
1:C:681:ASP:O	1:C:685:MET:HG3	2.17	0.43
1:S:691:LYS:HE3	1:S:695:PHE:CE2	2.53	0.43
1:Q:656:THR:HG23	1:Q:657:PRO:HD2	1.99	0.43
1:a:649:PRO:O	1:a:653:LEU:HG	2.18	0.43
1:G:644:ARG:HE	1:G:664:ALA:HB2	1.83	0.43
1:J:659:GLN:NE2	1:J:662:LEU:HB2	2.33	0.43
1:Z:688:GLU:HB2	1:a:680:ASP:OD2	2.18	0.43
1:T:658:PRO:HD2	1:T:661:LEU:HD12	2.00	0.43
1:O:659:GLN:HA	1:O:662:LEU:HD12	1.99	0.43
1:E:657:PRO:HB3	1:E:682:TRP:CE3	2.53	0.43
1:K:653:LEU:HD13	1:J:675:ALA:HB3	2.00	0.43
1:H:680:ASP:HA	1:I:686:THR:HG23	2.00	0.43
1:C:676:THR:HG23	1:b:687:PHE:CE2	2.52	0.43
1:R:657:PRO:HB3	1:R:682:TRP:CE3	2.53	0.43
1:b:644:ARG:HH12	1:b:668:GLU:HG3	1.83	0.43
1:Q:644:ARG:NH1	1:Q:697:LEU:O	2.51	0.43
1:H:637:ARG:HA	1:H:647:MET:HA	1.99	0.43
1:D:657:PRO:HB3	1:D:682:TRP:CE3	2.52	0.43
1:S:656:THR:HG23	1:S:657:PRO:HD2	1.99	0.43
1:S:657:PRO:HB3	1:S:682:TRP:CE3	2.53	0.43
1:S:686:THR:HG23	1:S:689:GLU:H	1.83	0.43
1:R:672:PRO:O	1:R:676:THR:HG23	2.19	0.43
1:E:676:THR:HG23	1:F:687:PHE:CE2	2.53	0.43
1:K:649:PRO:O	1:K:653:LEU:HG	2.19	0.43
1:N:657:PRO:HG3	1:N:678:LEU:HD23	1.99	0.43
1:W:657:PRO:HG2	1:W:662:LEU:HD11	2.00	0.43
1:K:634:TRP:O	1:K:635:PRO:C	2.62	0.43
1:X:634:TRP:N	1:X:635:PRO:HD3	2.33	0.43
1:H:637:ARG:HG2	1:H:647:MET:HG3	1.99	0.43
1:B:682:TRP:O	1:B:690:ARG:NH2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:LEU:HD22	1:C:674:SER:HB3	2.00	0.43
1:a:657:PRO:HB3	1:a:682:TRP:CE3	2.54	0.43
1:O:665:LEU:HD22	1:O:674:SER:HB3	2.01	0.43
1:S:656:THR:HB	1:R:684:GLU:HA	2.01	0.42
1:K:657:PRO:HD3	1:K:682:TRP:CB	2.49	0.42
1:H:685:MET:N	1:G:656:THR:HG21	2.34	0.42
1:F:648:PHE:HA	1:F:649:PRO:HA	1.85	0.42
1:V:673:LEU:HD21	1:U:634:TRP:CE2	2.54	0.42
1:U:644:ARG:HH21	1:U:664:ALA:HB1	1.84	0.42
1:L:657:PRO:HD3	1:L:682:TRP:CB	2.49	0.42
1:B:681:ASP:O	1:B:685:MET:HG3	2.19	0.42
1:C:656:THR:HG21	1:b:683:PRO:O	2.20	0.42
1:R:665:LEU:HD11	1:R:678:LEU:HD13	2.01	0.42
1:I:634:TRP:N	1:I:635:PRO:HD3	2.34	0.42
1:P:691:LYS:HG3	1:P:695:PHE:CE2	2.54	0.42
1:H:666:VAL:CG2	1:I:653:LEU:HD22	2.50	0.42
1:B:665:LEU:HD11	1:B:678:LEU:HD13	2.01	0.42
1:P:659:GLN:HA	1:P:662:LEU:HD12	2.00	0.42
1:Q:649:PRO:O	1:Q:653:LEU:HG	2.19	0.42
1:L:682:TRP:O	1:L:690:ARG:NH2	2.52	0.42
1:G:684:GLU:OE1	1:F:654:HIS:HB3	2.20	0.42
1:N:692:ASN:OD1	1:N:696:ASN:ND2	2.53	0.42
1:X:693:VAL:O	1:X:697:LEU:HB3	2.20	0.42
1:E:682:TRP:O	1:E:690:ARG:NH2	2.50	0.42
1:V:687:PHE:CD2	1:W:676:THR:HB	2.55	0.42
1:Q:634:TRP:CD1	1:Q:635:PRO:HD2	2.55	0.42
1:Y:659:GLN:HE21	1:Y:663:ASP:CG	2.28	0.42
1:P:688:GLU:HG2	1:Q:680:ASP:OD1	2.20	0.42
1:D:644:ARG:H	1:D:644:ARG:HG2	1.66	0.42
1:F:660:VAL:HG23	1:F:661:LEU:HD12	2.01	0.42
1:S:656:THR:OG1	1:R:684:GLU:HA	2.20	0.41
1:N:644:ARG:HH12	1:N:668:GLU:HG3	1.85	0.41
1:A:647:MET:HE3	1:A:647:MET:HB3	1.98	0.41
1:L:657:PRO:HB3	1:L:682:TRP:CE3	2.56	0.41
1:P:642:LYS:HD2	1:P:642:LYS:HA	1.73	0.41
1:A:648:PHE:HA	1:A:649:PRO:HA	1.86	0.41
1:Z:684:GLU:HA	1:a:656:THR:CB	2.50	0.41
1:P:681:ASP:O	1:P:685:MET:HG3	2.20	0.41
1:L:693:VAL:O	1:L:697:LEU:HB2	2.21	0.41
1:K:656:THR:HG22	1:K:657:PRO:O	2.19	0.41
1:K:656:THR:HG23	1:K:657:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:673:LEU:HD13	1:K:673:LEU:HA	1.80	0.41
1:H:658:PRO:HD2	1:H:661:LEU:HD12	2.03	0.41
1:B:658:PRO:HD2	1:B:661:LEU:HD12	2.03	0.41
1:F:672:PRO:O	1:F:676:THR:HG23	2.20	0.41
1:V:642:LYS:HD2	1:V:697:LEU:C	2.45	0.41
1:T:680:ASP:OD1	1:S:686:THR:OG1	2.31	0.41
1:H:682:TRP:O	1:H:690:ARG:NH2	2.54	0.41
1:Z:665:LEU:HD23	1:Z:665:LEU:HA	1.95	0.41
1:a:656:THR:HG23	1:a:657:PRO:HD2	2.02	0.41
1:H:665:LEU:HD22	1:H:674:SER:HB3	2.03	0.41
1:M:657:PRO:HB3	1:M:682:TRP:CE3	2.56	0.41
1:Q:684:GLU:HA	1:R:656:THR:CG2	2.51	0.41
1:U:644:ARG:NH2	1:U:664:ALA:HB1	2.36	0.41
1:G:653:LEU:HD13	1:F:675:ALA:HB3	2.02	0.41
1:I:656:THR:CG2	1:J:684:GLU:HG2	2.48	0.41
1:I:672:PRO:HB2	1:J:649:PRO:HG2	2.02	0.41
1:N:693:VAL:O	1:N:697:LEU:HB3	2.21	0.41
1:W:693:VAL:HG13	1:W:697:LEU:HD12	2.03	0.41
1:K:687:PHE:CD2	1:J:676:THR:HB	2.56	0.41
1:N:647:MET:HE2	1:N:647:MET:HB2	1.91	0.41
1:I:650:THR:HA	1:I:653:LEU:HD21	2.02	0.41
1:Q:686:THR:HG22	1:Q:688:GLU:H	1.85	0.41
1:R:657:PRO:HG2	1:R:662:LEU:HD11	2.03	0.41
1:b:658:PRO:HD2	1:b:661:LEU:HD12	2.03	0.41
1:L:659:GLN:HG2	1:M:655:ARG:HB2	2.03	0.40
1:M:668:GLU:HG2	1:M:669:TYR:CD1	2.56	0.40
1:I:656:THR:CG2	1:J:684:GLU:HA	2.51	0.40
1:b:685:MET:HE2	1:b:689:GLU:HG3	2.03	0.40
1:R:648:PHE:HA	1:R:649:PRO:HA	1.85	0.40
1:U:665:LEU:HD11	1:U:678:LEU:HD13	2.03	0.40
1:K:673:LEU:HA	1:K:676:THR:OG1	2.21	0.40
1:C:672:PRO:HB2	1:b:649:PRO:HG2	2.03	0.40
1:P:685:MET:HE3	1:P:689:GLU:HG3	2.03	0.40
1:S:666:VAL:HG22	1:R:653:LEU:HD13	2.04	0.40
1:O:637:ARG:HD2	1:O:638:VAL:N	2.31	0.40
1:B:657:PRO:HD3	1:B:682:TRP:CB	2.51	0.40
1:I:648:PHE:HA	1:I:649:PRO:HA	1.88	0.40
1:P:656:THR:CG2	1:O:684:GLU:HA	2.51	0.40
1:P:665:LEU:HD22	1:P:674:SER:HB3	2.03	0.40
1:X:656:THR:CB	1:W:684:GLU:HA	2.51	0.40
1:W:681:ASP:O	1:W:685:MET:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:659:GLN:HA	1:E:662:LEU:HD12	2.04	0.40
1:G:653:LEU:HD11	1:F:676:THR:HG23	2.04	0.40
1:C:634:TRP:HD1	1:C:636:ARG:HG3	1.86	0.40

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)
1:O:633:ASP:O	1:N:692:ASN:ND2[2_444]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	64/130 (49%)	60 (94%)	4 (6%)	0	100	100
1	B	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	C	62/130 (48%)	56 (90%)	6 (10%)	0	100	100
1	D	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	E	63/130 (48%)	60 (95%)	3 (5%)	0	100	100
1	F	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	G	60/130 (46%)	53 (88%)	7 (12%)	0	100	100
1	H	61/130 (47%)	59 (97%)	2 (3%)	0	100	100
1	I	63/130 (48%)	60 (95%)	3 (5%)	0	100	100
1	J	64/130 (49%)	61 (95%)	3 (5%)	0	100	100
1	K	64/130 (49%)	61 (95%)	3 (5%)	0	100	100
1	L	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	M	65/130 (50%)	59 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	64/130 (49%)	62 (97%)	2 (3%)	0	100	100
1	O	63/130 (48%)	59 (94%)	4 (6%)	0	100	100
1	P	60/130 (46%)	56 (93%)	4 (7%)	0	100	100
1	Q	63/130 (48%)	58 (92%)	5 (8%)	0	100	100
1	R	61/130 (47%)	53 (87%)	8 (13%)	0	100	100
1	S	60/130 (46%)	57 (95%)	3 (5%)	0	100	100
1	T	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	U	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	V	64/130 (49%)	59 (92%)	5 (8%)	0	100	100
1	W	61/130 (47%)	56 (92%)	5 (8%)	0	100	100
1	X	64/130 (49%)	59 (92%)	4 (6%)	1 (2%)	7	35
1	Y	63/130 (48%)	57 (90%)	6 (10%)	0	100	100
1	Z	63/130 (48%)	60 (95%)	3 (5%)	0	100	100
1	a	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	b	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
All	All	1748/3640 (48%)	1635 (94%)	112 (6%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	635	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/114 (54%)	62 (100%)	0	100	100
1	B	60/114 (53%)	60 (100%)	0	100	100
1	C	60/114 (53%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	60/114 (53%)	60 (100%)	0	100	100
1	E	61/114 (54%)	61 (100%)	0	100	100
1	F	60/114 (53%)	60 (100%)	0	100	100
1	G	58/114 (51%)	58 (100%)	0	100	100
1	H	59/114 (52%)	59 (100%)	0	100	100
1	I	61/114 (54%)	61 (100%)	0	100	100
1	J	62/114 (54%)	62 (100%)	0	100	100
1	K	62/114 (54%)	62 (100%)	0	100	100
1	L	60/114 (53%)	60 (100%)	0	100	100
1	M	63/114 (55%)	63 (100%)	0	100	100
1	N	62/114 (54%)	62 (100%)	0	100	100
1	O	61/114 (54%)	61 (100%)	0	100	100
1	P	58/114 (51%)	58 (100%)	0	100	100
1	Q	61/114 (54%)	61 (100%)	0	100	100
1	R	59/114 (52%)	59 (100%)	0	100	100
1	S	58/114 (51%)	58 (100%)	0	100	100
1	T	60/114 (53%)	60 (100%)	0	100	100
1	U	60/114 (53%)	60 (100%)	0	100	100
1	V	62/114 (54%)	62 (100%)	0	100	100
1	W	59/114 (52%)	59 (100%)	0	100	100
1	X	62/114 (54%)	62 (100%)	0	100	100
1	Y	61/114 (54%)	61 (100%)	0	100	100
1	Z	61/114 (54%)	61 (100%)	0	100	100
1	a	60/114 (53%)	60 (100%)	0	100	100
1	b	60/114 (53%)	60 (100%)	0	100	100
All	All	1692/3192 (53%)	1692 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	696	ASN

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Mol	Chain	Res	Type
1	T	641	ASN
1	P	667	ASN
1	S	667	ASN
1	X	632	GLN
1	W	654	HIS
1	W	659	GLN
1	U	641	ASN
1	E	659	GLN
1	E	696	ASN
1	M	654	HIS
1	N	659	GLN
1	N	667	ASN
1	N	696	ASN
1	I	659	GLN
1	I	667	ASN
1	J	659	GLN
1	J	696	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 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 ⓘ

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	66/130 (50%)	0.03	1 (1%) 72 47	80, 120, 151, 167	0
1	B	64/130 (49%)	-0.00	1 (1%) 70 45	95, 137, 169, 181	0
1	C	64/130 (49%)	-0.05	1 (1%) 70 45	82, 113, 135, 141	0
1	D	64/130 (49%)	-0.05	1 (1%) 70 45	77, 108, 129, 137	0
1	E	65/130 (50%)	-0.14	1 (1%) 72 47	122, 146, 169, 204	0
1	F	64/130 (49%)	-0.05	1 (1%) 70 45	116, 136, 164, 175	0
1	G	62/130 (47%)	0.06	1 (1%) 70 45	102, 123, 139, 148	0
1	H	63/130 (48%)	0.09	3 (4%) 35 24	96, 127, 142, 152	0
1	I	65/130 (50%)	0.11	0 100 100	74, 100, 137, 186	0
1	J	66/130 (50%)	0.15	2 (3%) 52 33	82, 111, 149, 174	0
1	K	66/130 (50%)	0.29	4 (6%) 27 19	30, 82, 122, 129	0
1	L	64/130 (49%)	0.07	2 (3%) 51 32	60, 83, 106, 132	0
1	M	67/130 (51%)	0.07	0 100 100	71, 96, 127, 192	0
1	N	66/130 (50%)	0.28	3 (4%) 38 25	56, 73, 139, 186	0
1	O	65/130 (50%)	0.19	1 (1%) 72 47	63, 85, 125, 157	0
1	P	62/130 (47%)	0.25	2 (3%) 50 32	58, 92, 143, 157	0
1	Q	65/130 (50%)	0.04	1 (1%) 72 47	62, 103, 147, 165	0
1	R	63/130 (48%)	0.14	2 (3%) 50 32	70, 99, 123, 134	0
1	S	62/130 (47%)	0.01	0 100 100	89, 121, 151, 173	0
1	T	64/130 (49%)	-0.02	0 100 100	90, 119, 136, 143	0
1	U	64/130 (49%)	-0.03	2 (3%) 51 32	94, 130, 155, 178	0
1	V	66/130 (50%)	-0.15	0 100 100	98, 131, 151, 159	0
1	W	63/130 (48%)	-0.08	1 (1%) 70 45	95, 130, 154, 166	0
1	X	66/130 (50%)	-0.07	1 (1%) 72 47	86, 116, 135, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	Y	65/130 (50%)	-0.16	0	100	100	90, 137, 186, 196	0
1	Z	65/130 (50%)	-0.19	0	100	100	80, 119, 147, 158	0
1	a	64/130 (49%)	0.28	2 (3%)	51	32	62, 92, 132, 162	0
1	b	64/130 (49%)	-0.18	1 (1%)	70	45	96, 134, 160, 177	0
All	All	1804/3640 (49%)	0.03	34 (1%)	66	42	30, 116, 157, 204	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	653	LEU	4.4
1	X	653	LEU	3.7
1	K	646	PHE	3.7
1	J	653	LEU	3.5
1	B	675	ALA	3.2
1	U	679	SER	3.2
1	G	653	LEU	3.1
1	Q	648	PHE	3.1
1	R	679	SER	3.0
1	N	644	ARG	3.0
1	R	687	PHE	2.8
1	H	653	LEU	2.8
1	C	653	LEU	2.7
1	P	675	ALA	2.7
1	H	694	ALA	2.5
1	K	652	LEU	2.4
1	O	653	LEU	2.4
1	K	653	LEU	2.4
1	N	693	VAL	2.4
1	a	684	GLU	2.4
1	H	666	VAL	2.3
1	K	695	PHE	2.3
1	J	648	PHE	2.2
1	P	693	VAL	2.2
1	a	680	ASP	2.2
1	L	653	LEU	2.2
1	b	652	LEU	2.2
1	L	687	PHE	2.2
1	F	653	LEU	2.1
1	D	689	GLU	2.1
1	E	675	ALA	2.1
1	N	695	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	653	LEU	2.0
1	W	653	LEU	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.