



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 05:38 am BST

PDB ID : 2Q4P  
Title : Ensemble refinement of the crystal structure of protein from Mus musculus Mm.29898  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.32 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

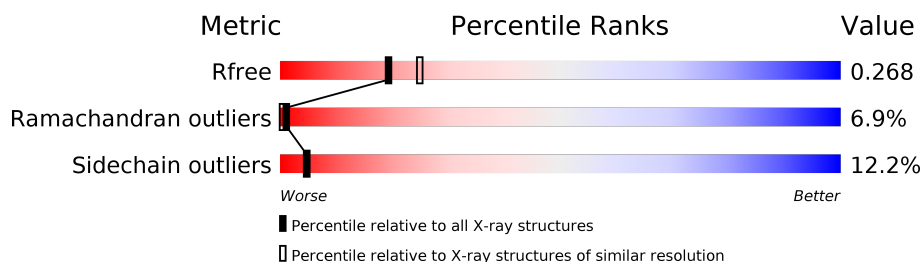
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 Å.

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





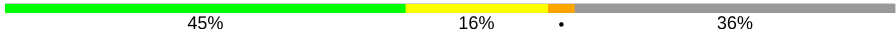

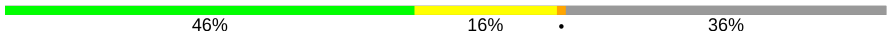
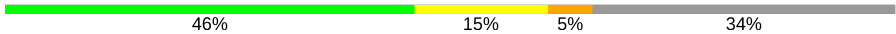
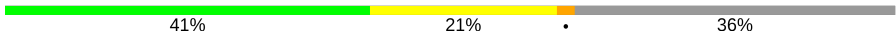
















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5974 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1-A	170	
1	1-B	170	
1	10-A	170	
1	10-B	170	
1	11-A	170	
1	11-B	170	
1	12-A	170	
1	12-B	170	
1	13-A	170	

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Mol	Chain	Length	Quality of chain
1	13-B	170	
1	14-A	170	
1	14-B	170	
1	15-A	170	
1	15-B	170	
1	16-A	170	
1	16-B	170	
1	2-A	170	
1	2-B	170	
1	3-A	170	
1	3-B	170	
1	4-A	170	
1	4-B	170	
1	5-A	170	
1	5-B	170	
1	6-A	170	
1	6-B	170	
1	7-A	170	
1	7-B	170	
1	8-A	170	
1	8-B	170	
1	9-A	170	
1	9-B	170	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 29392 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 Protein RS21-C6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	2-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	3-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	4-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	5-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	6-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	7-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	8-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	9-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	10-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	11-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	12-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	13-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	14-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	15-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			
1	16-A	113	Total	C	N	O	S	Se	0	0	0
			922	589	163	168	1	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	2-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	3-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	4-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	5-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	6-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	7-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	8-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	9-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	10-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	11-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	12-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	13-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	14-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	15-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			
1	16-B	109	Total	C	N	O	S	Se	0	0	0
			891	569	157	163	1	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9QY93
A	122	MSE	MET	MODIFIED RESIDUE	UNP Q9QY93
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9QY93
B	122	MSE	MET	MODIFIED RESIDUE	UNP Q9QY93

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	12	Total O 12 12	0	0
2	2-A	11	Total O 11 11	0	0
2	3-A	12	Total O 12 12	0	0
2	4-A	11	Total O 11 11	0	0
2	5-A	12	Total O 12 12	0	0
2	6-A	11	Total O 11 11	0	0
2	7-A	12	Total O 12 12	0	0
2	8-A	13	Total O 13 13	0	0
2	9-A	11	Total O 11 11	0	0
2	10-A	10	Total O 10 10	0	0
2	11-A	12	Total O 12 12	0	0
2	12-A	12	Total O 12 12	0	0
2	13-A	13	Total O 13 13	0	0
2	14-A	12	Total O 12 12	0	0
2	15-A	12	Total O 12 12	0	0
2	16-A	13	Total O 13 13	0	0
2	1-B	12	Total O 12 12	0	0
2	2-B	13	Total O 13 13	0	0
2	3-B	12	Total O 12 12	0	0
2	4-B	13	Total O 13 13	0	0
2	5-B	12	Total O 12 12	0	0
2	6-B	13	Total O 13 13	0	0

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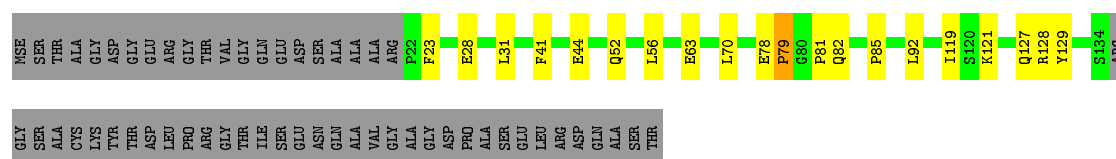
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-B	12	Total 12	O 12	0	0
2	8-B	11	Total 11	O 11	0	0
2	9-B	13	Total 13	O 13	0	0
2	10-B	14	Total 14	O 14	0	0
2	11-B	12	Total 12	O 12	0	0
2	12-B	12	Total 12	O 12	0	0
2	13-B	11	Total 11	O 11	0	0
2	14-B	12	Total 12	O 12	0	0
2	15-B	12	Total 12	O 12	0	0
2	16-B	11	Total 11	O 11	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

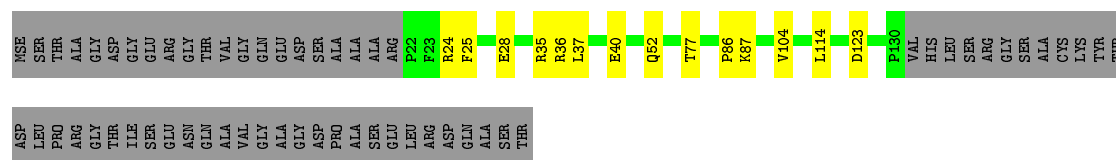
#### • Molecule 1: Protein RS21-C6

Chain 1-A: 



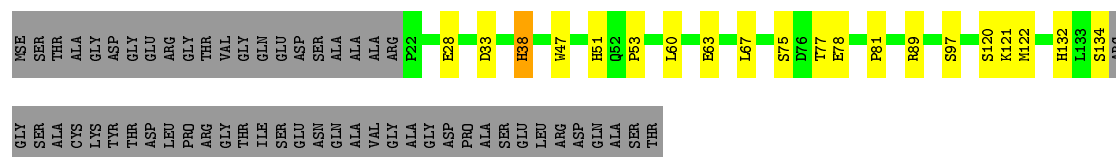
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Chain 1-B: 



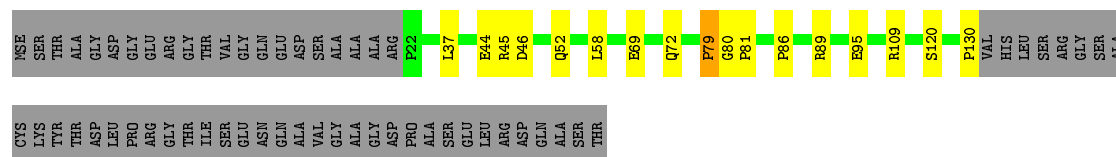
#### • Molecule 1: Protein RS21-C6

Chain 2-A: 



#### • Molecule 1: Protein RS21-C6

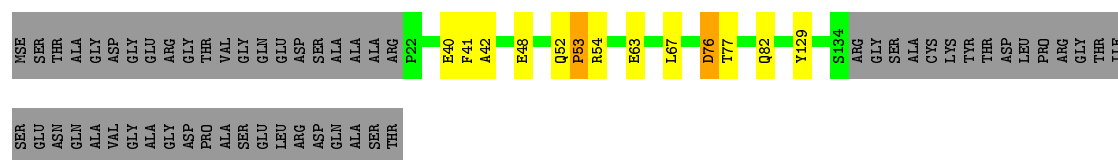
Chain 2-B: 



#### • Molecule 1: Protein RS21-C6

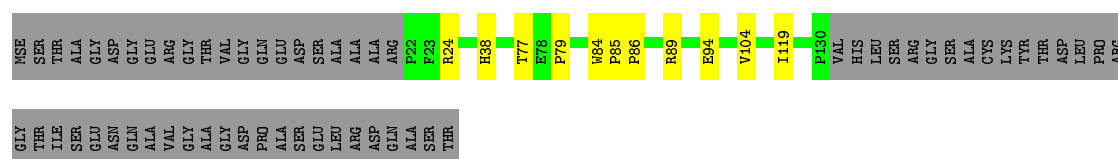


Chain 3-A:  59% 6% 34%



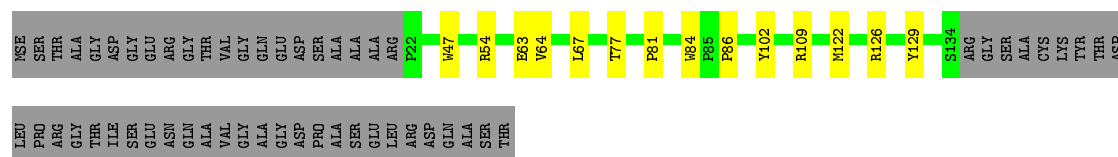
• Molecule 1: Protein RS21-C6

Chain 3-B:  58% 6% 36%



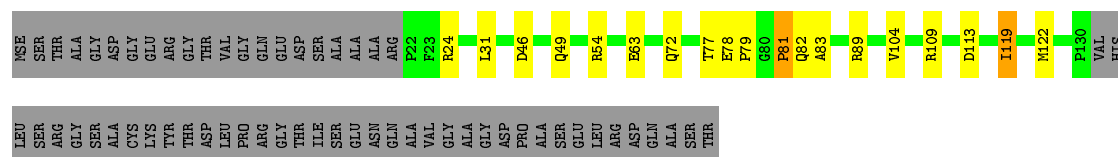
• Molecule 1: Protein RS21-C6

Chain 4-A:  58% 8% 34%



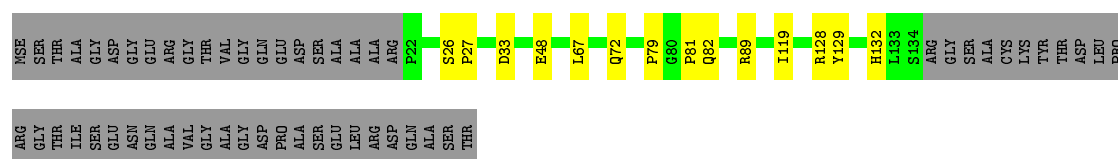
• Molecule 1: Protein RS21-C6

Chain 4-B:  53% 10% 36%



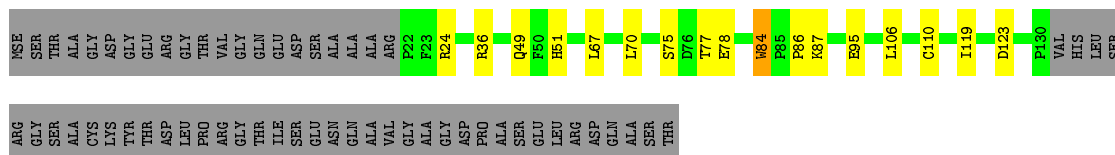
• Molecule 1: Protein RS21-C6

Chain 5-A:  58% 8% 34%

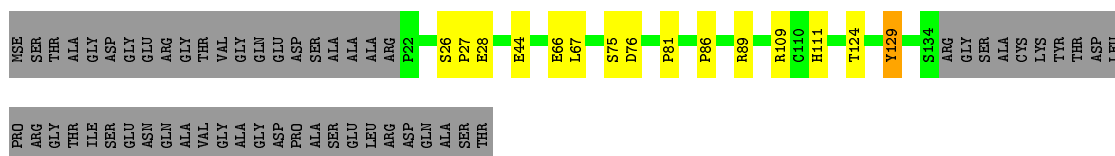


• Molecule 1: Protein RS21-C6

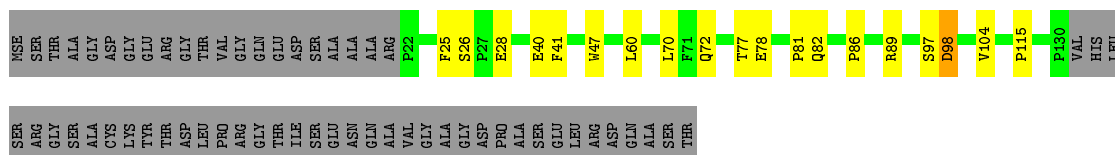
Chain 5-B:  54% 9% 36%



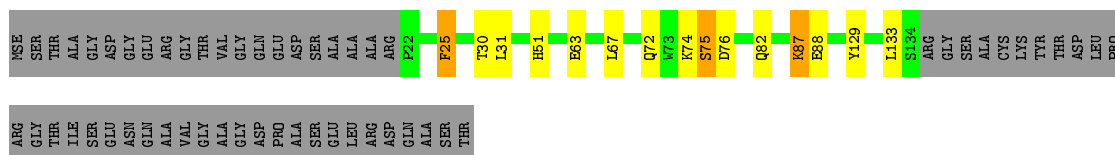
- Molecule 1: Protein RS21-C6



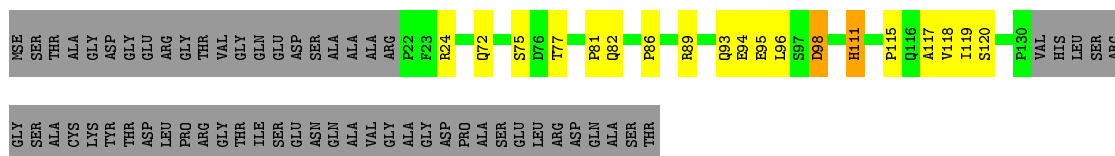
- Molecule 1: Protein RS21-C6



- Molecule 1: Protein RS21-C6



- Molecule 1: Protein RS21-C6



- Molecule 1: Protein RS21-C6



GLY  
THR  
SER  
ILE  
SER  
ALA  
GLY  
GLU  
ASN  
GLN  
VAL  
ALA  
VAL  
ALA  
GLY  
ASP  
PRO  
ALA  
SER  
SER  
GLU  
LEU  
ALA  
ARG  
ASP  
GLN  
SER  
THR

• Molecule 1: Protein RS21-C6

Chain 8-B:  52% 11% 36%

MSE  
SER  
THR  
THR  
GLY  
ALA  
SER  
LEU  
SER  
ASP  
GLY  
GLY  
GLU  
ARG  
GLY  
GLY  
ALA  
THR  
CYS  
GLY  
TYR  
THR  
GLN  
GLU  
ASP  
LEU  
PRO  
SER  
ALA  
ALA  
ALA  
THR  
ILE  
SER  
GLN  
ASN  
GLN  
ALA  
VAL  
GLY  
GLY  
ALA  
GLY  
GLY  
ASP  
PRO  
ASP  
LEU  
ARG  
GLN  
SER  
THR

• Molecule 1: Protein RS21-C6

Chain 9-A:  54% 11% 34%

MSE  
SER  
THR  
THR  
ALA  
LYS  
TYR  
THR  
ASP  
LEU  
PRO  
GLY  
GLY  
GLU  
ARG  
GLY  
GLY  
THR  
THR  
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SER  
GLY  
ASN  
GLU  
GLY  
CYS  
THR  
THR  
GLY  
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D46  
F23  
D46  
E47  
E48  
F71  
Q72  
E78  
Q82  
P86  
K87  
E88  
Q93  
E94  
E95  
D98  
Y99  
L100  
P115  
I119  
M122  
D123  
Y129  
S134  
ARG  
GLY  
SER

• Molecule 1: Protein RS21-C6

Chain 9-B:  57% 6% 36%

MSE  
SER  
THR  
THR  
ALA  
LYS  
TYR  
THR  
ASP  
LEU  
PRO  
GLY  
GLY  
GLU  
ARG  
GLY  
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THR  
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ALA  
ALA  
ALA  
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SER  
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THR  
GLY  
VAL  
D46  
F23  
R36  
D46  
Q49  
L67  
Q72  
S75  
E78  
P85  
R89  
A90  
Q93  
Y129  
P130  
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HIS  
LEU  
SER  
SER  
ARG  
GLY  
SER  
ALA  
CYS  
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THR  
THR  
LEU

• Molecule 1: Protein RS21-C6

Chain 10-A:  55% 9% 34%

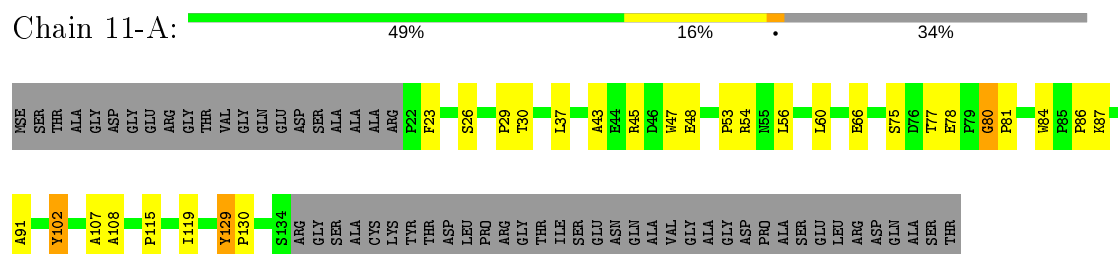
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ARG  
GLY  
GLY  
THR  
THR  
VAL  
GLY  
GLY  
GLN  
GLU  
ASP  
GLN  
SER  
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F23  
R24  
E28  
L37  
D46  
V47  
E48  
V64  
Q72  
S75  
E78  
P81  
Q82  
A83  
W84  
P85  
P86  
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E95  
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Y129  
H132  
L133  
S134  
ARG

• Molecule 1: Protein RS21-C6

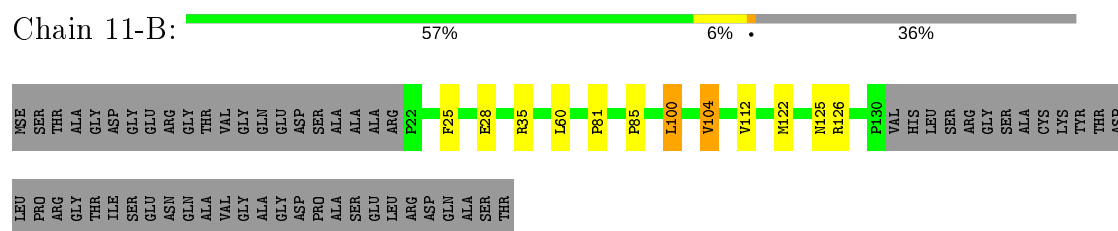
Chain 10-B:  54% 10% 36%

MSE  
SER  
THR  
THR  
ALA  
LYS  
TYR  
THR  
ASP  
LEU  
PRO  
GLY  
GLY  
GLU  
ARG  
GLY  
GLY  
THR  
THR  
VAL  
GLY  
GLY  
GLN  
GLU  
ASP  
GLN  
SER  
ALA  
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D46  
F23  
F25  
S26  
F27  
E28  
P29  
T30  
D33  
W73  
K74  
S75  
T77  
E78  
P86  
D98  
V104  
Q116  
M122  
D123  
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SER  
ARG  
GLY

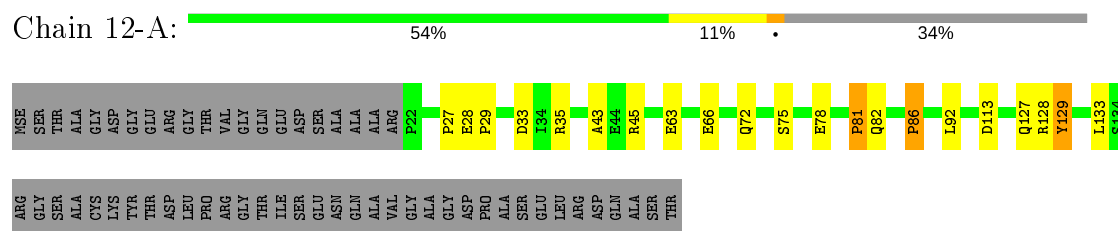
- Molecule 1: Protein RS21-C6



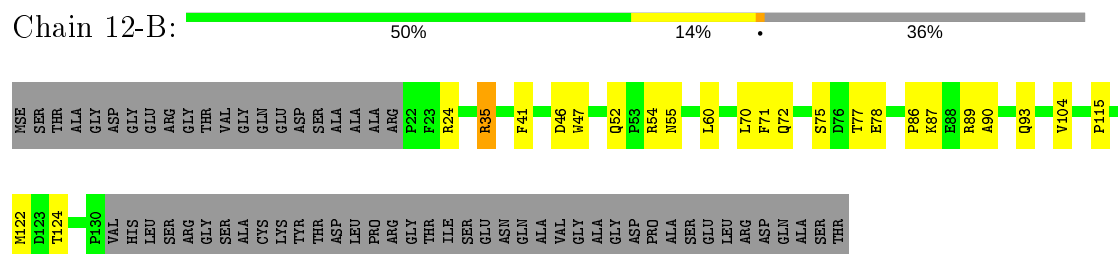
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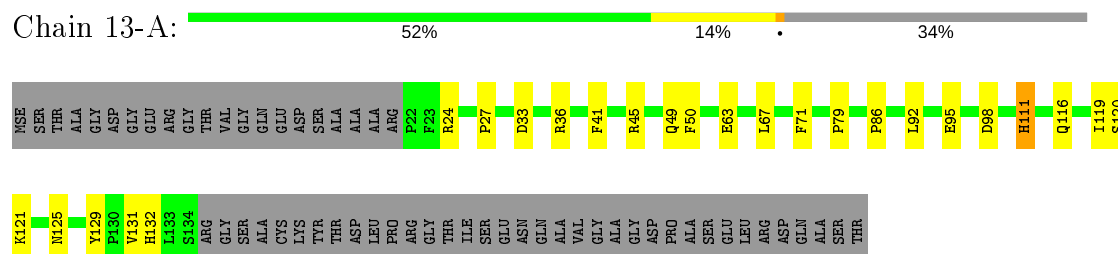
- Molecule 1: Protein RS21-C6



- Molecule 1: Protein RS21-C6

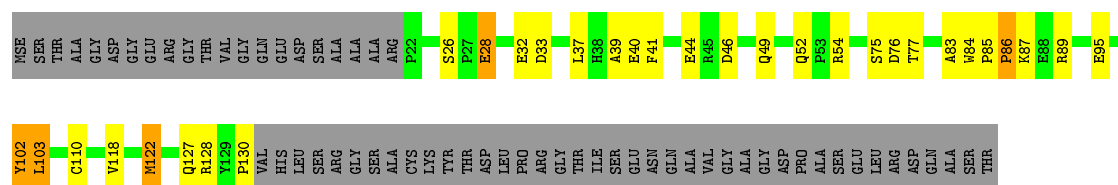


- Molecule 1: Protein RS21-C6



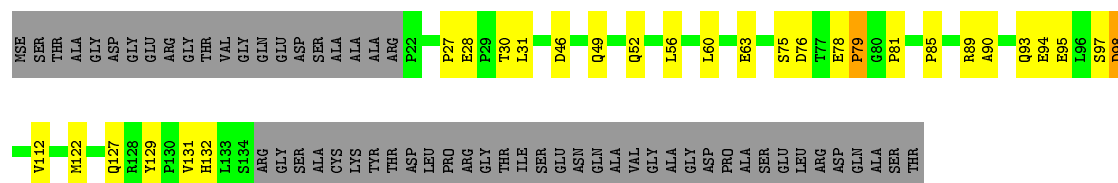
- Molecule 1: Protein RS21-C6

Chain 13-B: 



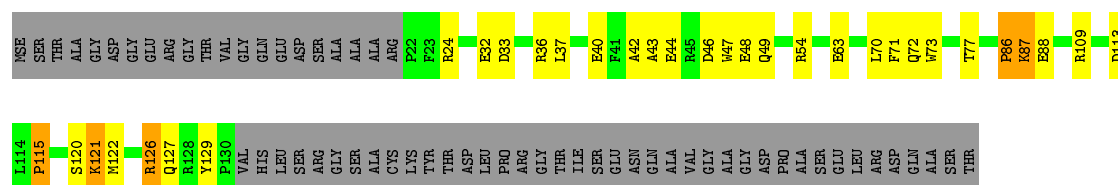
- Molecule 1: Protein RS21-C6

Chain 14-A: 



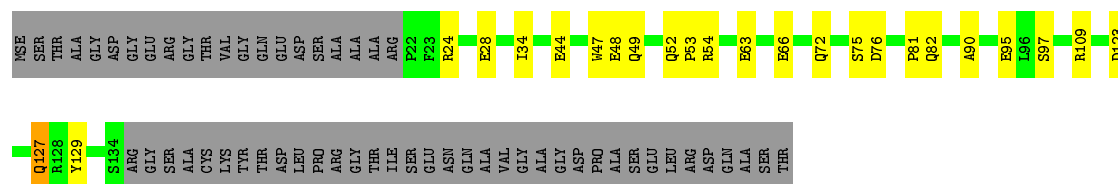
- Molecule 1: Protein RS21-C6

Chain 14-B: 



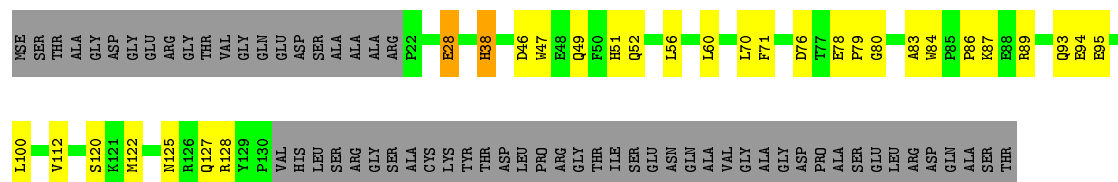
- Molecule 1: Protein RS21-C6

Chain 15-A: 



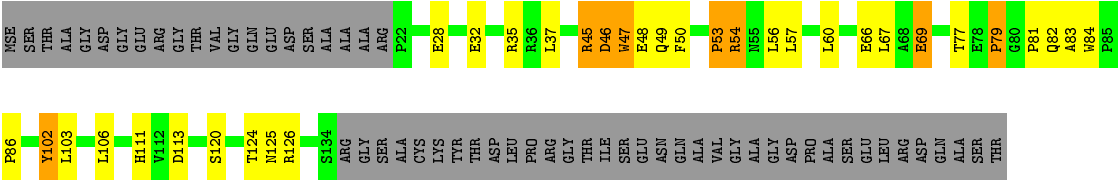
- Molecule 1: Protein RS21-C6

Chain 15-B: 



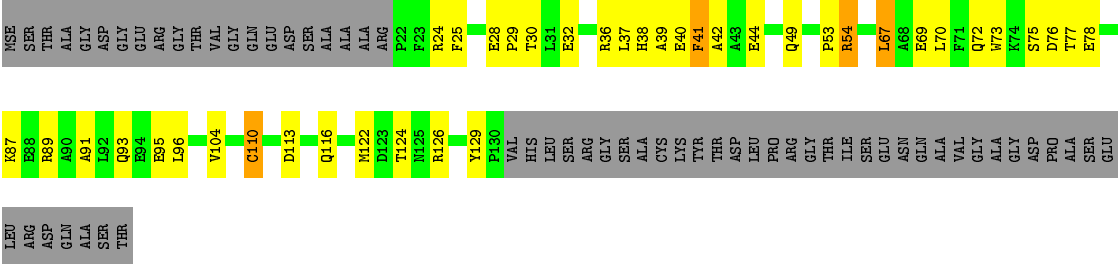
- Molecule 1: Protein RS21-C6

Chain 16-A:  46% 15% 5% 34%



● Molecule 1: Protein RS21-C6

Chain 16-B:  41% 21% • 36%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.54Å 73.54Å 236.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.93 – 2.32 43.29 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.93-2.32) 98.5 (43.29-2.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.138 , 0.233 0.192 , 0.268	Depositor DCC
$R_{free}$ test set	858 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 652.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29392	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1-A	0.83	0/947	1.09	1/1288 (0.1%)
1	1-B	0.93	0/915	1.02	2/1244 (0.2%)
1	2-A	0.92	0/947	1.08	2/1288 (0.2%)
1	2-B	0.94	1/915 (0.1%)	1.01	1/1244 (0.1%)
1	3-A	0.87	0/947	0.94	0/1288
1	3-B	0.99	0/915	0.95	0/1244
1	4-A	0.94	0/947	0.98	0/1288
1	4-B	1.01	0/915	1.11	3/1244 (0.2%)
1	5-A	0.89	0/947	0.91	0/1288
1	5-B	0.93	1/915 (0.1%)	0.98	3/1244 (0.2%)
1	6-A	0.87	0/947	0.98	0/1288
1	6-B	1.05	2/915 (0.2%)	1.11	4/1244 (0.3%)
1	7-A	0.90	0/947	0.99	2/1288 (0.2%)
1	7-B	0.92	0/915	0.98	1/1244 (0.1%)
1	8-A	0.86	0/947	0.99	1/1288 (0.1%)
1	8-B	0.99	2/915 (0.2%)	1.09	2/1244 (0.2%)
1	9-A	0.94	2/947 (0.2%)	0.98	0/1288
1	9-B	0.90	0/915	0.94	1/1244 (0.1%)
1	10-A	0.93	1/947 (0.1%)	1.01	2/1288 (0.2%)
1	10-B	0.98	0/915	1.04	4/1244 (0.3%)
1	11-A	0.95	1/947 (0.1%)	1.12	7/1288 (0.5%)
1	11-B	0.99	1/915 (0.1%)	1.22	4/1244 (0.3%)
1	12-A	0.96	1/947 (0.1%)	1.02	2/1288 (0.2%)
1	12-B	0.91	1/915 (0.1%)	1.07	3/1244 (0.2%)
1	13-A	1.05	0/947	1.15	2/1288 (0.2%)
1	13-B	1.28	5/915 (0.5%)	1.26	7/1244 (0.6%)
1	14-A	1.05	1/947 (0.1%)	1.23	4/1288 (0.3%)
1	14-B	1.10	2/915 (0.2%)	1.13	3/1244 (0.2%)
1	15-A	0.98	1/947 (0.1%)	1.10	2/1288 (0.2%)
1	15-B	1.16	2/915 (0.2%)	1.16	4/1244 (0.3%)
1	16-A	1.11	2/947 (0.2%)	1.31	10/1288 (0.8%)
1	16-B	1.39	9/915 (1.0%)	1.41	13/1244 (1.0%)
All	All	0.99	35/29792 (0.1%)	1.08	90/40512 (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	5-B	0	1
1	9-A	0	1
1	11-A	0	1
1	12-A	0	1
1	13-B	0	2
1	16-A	0	1
1	16-B	0	1
All	All	0	8

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-B	42	ALA	CA-CB	13.50	1.80	1.52
1	16-B	28	GLU	CD-OE1	-8.05	1.16	1.25
1	16-B	28	GLU	CG-CD	7.98	1.64	1.51
1	13-B	39	ALA	CA-CB	-7.26	1.37	1.52
1	14-A	94	GLU	CG-CD	7.26	1.62	1.51

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-B	35	ARG	NE-CZ-NH1	15.25	127.92	120.30
1	11-B	35	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	12-B	35	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	6-B	89	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	5-B	36	ARG	NE-CZ-NH1	8.12	124.36	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	11-A	102	TYR	Sidechain
1	12-A	129	TYR	Sidechain
1	13-B	41	PHE	Sidechain
1	5-B	51	HIS	Sidechain
1	9-A	71	PHE	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	1-A	922	0	901	0	0
1	1-B	891	0	869	0	0
1	2-A	922	0	901	0	0
1	2-B	891	0	869	0	0
1	3-A	922	0	901	0	0
1	3-B	891	0	869	0	0
1	4-A	922	0	901	0	0
1	4-B	891	0	869	0	0
1	5-A	922	0	901	0	0
1	5-B	891	0	869	0	0
1	6-A	922	0	901	0	0
1	6-B	891	0	869	0	0
1	7-A	922	0	901	0	0
1	7-B	891	0	869	0	0
1	8-A	922	0	901	0	0
1	8-B	891	0	869	0	0
1	9-A	922	0	901	0	0
1	9-B	891	0	869	0	0
1	10-A	922	0	901	0	0
1	10-B	891	0	869	0	0
1	11-A	922	0	901	0	0
1	11-B	891	0	869	0	0
1	12-A	922	0	901	0	0
1	12-B	891	0	869	0	0
1	13-A	922	0	901	0	0
1	13-B	891	0	869	0	0
1	14-A	922	0	901	0	0
1	14-B	891	0	869	0	0
1	15-A	922	0	901	0	0
1	15-B	891	0	869	0	0
1	16-A	922	0	901	0	0
1	16-B	891	0	869	0	0
2	1-A	12	0	0	0	0
2	1-B	12	0	0	0	0
2	2-A	11	0	0	0	0
2	2-B	13	0	0	0	0
2	3-A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-B	12	0	0	0	0
2	4-A	11	0	0	0	0
2	4-B	13	0	0	0	0
2	5-A	12	0	0	0	0
2	5-B	12	0	0	0	0
2	6-A	11	0	0	0	0
2	6-B	13	0	0	0	0
2	7-A	12	0	0	0	0
2	7-B	12	0	0	0	0
2	8-A	13	0	0	0	0
2	8-B	11	0	0	0	0
2	9-A	11	0	0	0	0
2	9-B	13	0	0	0	0
2	10-A	10	0	0	0	0
2	10-B	14	0	0	0	0
2	11-A	12	0	0	0	0
2	11-B	12	0	0	0	0
2	12-A	12	0	0	0	0
2	12-B	12	0	0	0	0
2	13-A	13	0	0	0	0
2	13-B	11	0	0	0	0
2	14-A	12	0	0	0	0
2	14-B	12	0	0	0	0
2	15-A	12	0	0	0	0
2	15-B	12	0	0	0	0
2	16-A	13	0	0	0	0
2	16-B	11	0	0	0	0
All	All	29392	0	28320	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	111/170 (65%)	83 (75%)	23 (21%)	5 (4%)	2	1
1	1-B	107/170 (63%)	83 (78%)	22 (21%)	2 (2%)	8	6
1	2-A	111/170 (65%)	89 (80%)	18 (16%)	4 (4%)	3	2
1	2-B	107/170 (63%)	90 (84%)	10 (9%)	7 (6%)	1	0
1	3-A	111/170 (65%)	97 (87%)	9 (8%)	5 (4%)	2	1
1	3-B	107/170 (63%)	98 (92%)	6 (6%)	3 (3%)	5	3
1	4-A	111/170 (65%)	92 (83%)	14 (13%)	5 (4%)	2	1
1	4-B	107/170 (63%)	85 (79%)	14 (13%)	8 (8%)	1	0
1	5-A	111/170 (65%)	95 (86%)	12 (11%)	4 (4%)	3	2
1	5-B	107/170 (63%)	98 (92%)	6 (6%)	3 (3%)	5	3
1	6-A	111/170 (65%)	91 (82%)	13 (12%)	7 (6%)	1	0
1	6-B	107/170 (63%)	85 (79%)	16 (15%)	6 (6%)	2	0
1	7-A	111/170 (65%)	85 (77%)	18 (16%)	8 (7%)	1	0
1	7-B	107/170 (63%)	85 (79%)	10 (9%)	12 (11%)	0	0
1	8-A	111/170 (65%)	96 (86%)	12 (11%)	3 (3%)	5	3
1	8-B	107/170 (63%)	80 (75%)	18 (17%)	9 (8%)	1	0
1	9-A	111/170 (65%)	80 (72%)	22 (20%)	9 (8%)	1	0
1	9-B	107/170 (63%)	92 (86%)	11 (10%)	4 (4%)	3	1
1	10-A	111/170 (65%)	90 (81%)	16 (14%)	5 (4%)	2	1
1	10-B	107/170 (63%)	85 (79%)	15 (14%)	7 (6%)	1	0
1	11-A	111/170 (65%)	79 (71%)	17 (15%)	15 (14%)	0	0
1	11-B	107/170 (63%)	87 (81%)	14 (13%)	6 (6%)	2	0
1	12-A	111/170 (65%)	82 (74%)	19 (17%)	10 (9%)	1	0
1	12-B	107/170 (63%)	75 (70%)	22 (21%)	10 (9%)	0	0
1	13-A	111/170 (65%)	85 (77%)	19 (17%)	7 (6%)	1	0
1	13-B	107/170 (63%)	82 (77%)	16 (15%)	9 (8%)	1	0
1	14-A	111/170 (65%)	77 (69%)	21 (19%)	13 (12%)	0	0
1	14-B	107/170 (63%)	81 (76%)	14 (13%)	12 (11%)	0	0
1	15-A	111/170 (65%)	80 (72%)	20 (18%)	11 (10%)	0	0
1	15-B	107/170 (63%)	84 (78%)	16 (15%)	7 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	16-A	111/170 (65%)	75 (68%)	23 (21%)	13 (12%)	0	0
1	16-B	107/170 (63%)	76 (71%)	19 (18%)	12 (11%)	0	0
All	All	3488/5440 (64%)	2742 (79%)	505 (14%)	241 (7%)	1	0

5 of 241 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	78	GLU
1	1-A	128	ARG
1	1-B	86	PRO
1	2-A	81	PRO
1	2-B	72	GLN

### 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	1-A	98/136 (72%)	83 (85%)	15 (15%)	2	2
1	1-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	2-A	98/136 (72%)	83 (85%)	15 (15%)	2	2
1	2-B	94/136 (69%)	85 (90%)	9 (10%)	8	9
1	3-A	98/136 (72%)	88 (90%)	10 (10%)	7	8
1	3-B	94/136 (69%)	86 (92%)	8 (8%)	10	12
1	4-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	4-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	5-A	98/136 (72%)	88 (90%)	10 (10%)	7	8
1	5-B	94/136 (69%)	82 (87%)	12 (13%)	4	4
1	6-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	6-B	94/136 (69%)	85 (90%)	9 (10%)	8	9
1	7-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	7-B	94/136 (69%)	86 (92%)	8 (8%)	10	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	8-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	9-A	98/136 (72%)	87 (89%)	11 (11%)	6	6
1	9-B	94/136 (69%)	86 (92%)	8 (8%)	10	12
1	10-A	98/136 (72%)	84 (86%)	14 (14%)	3	3
1	10-B	94/136 (69%)	86 (92%)	8 (8%)	10	12
1	11-A	98/136 (72%)	88 (90%)	10 (10%)	7	8
1	11-B	94/136 (69%)	90 (96%)	4 (4%)	29	40
1	12-A	98/136 (72%)	87 (89%)	11 (11%)	6	6
1	12-B	94/136 (69%)	82 (87%)	12 (13%)	4	4
1	13-A	98/136 (72%)	80 (82%)	18 (18%)	1	1
1	13-B	94/136 (69%)	79 (84%)	15 (16%)	2	2
1	14-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	14-B	94/136 (69%)	74 (79%)	20 (21%)	1	1
1	15-A	98/136 (72%)	86 (88%)	12 (12%)	5	5
1	15-B	94/136 (69%)	75 (80%)	19 (20%)	1	1
1	16-A	98/136 (72%)	79 (81%)	19 (19%)	1	1
1	16-B	94/136 (69%)	76 (81%)	18 (19%)	1	1
All	All	3072/4352 (71%)	2698 (88%)	374 (12%)	5	5

5 of 374 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9-A	119	ILE
1	11-A	78	GLU
1	16-A	66	GLU
1	9-B	46	ASP
1	10-A	86	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	8-B	51	HIS
1	10-B	125	ASN
1	15-B	38	HIS

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Mol	Chain	Res	Type
1	8-B	93	GLN
1	9-B	52	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.