



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:45 AM UTC

PDB ID : 2Q4P / pdb_00002q4p
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

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

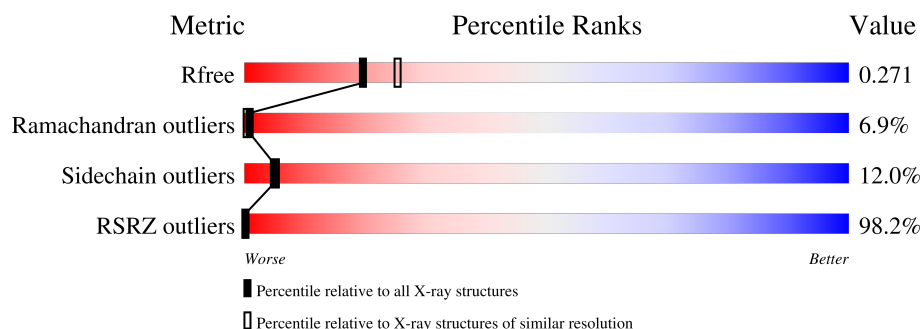
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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.



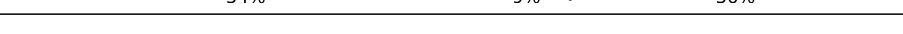
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 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	1-A	170	65% 56% 9% 34%
1	1-B	170	62% 57% 7% 36%
1	10-A	170	56% 9% 34%
1	10-B	170	55% 9% 36%
1	11-A	170	50% 16% 34%
1	11-B	170	55% 9% 36%
1	12-A	170	54% 12% 34%

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

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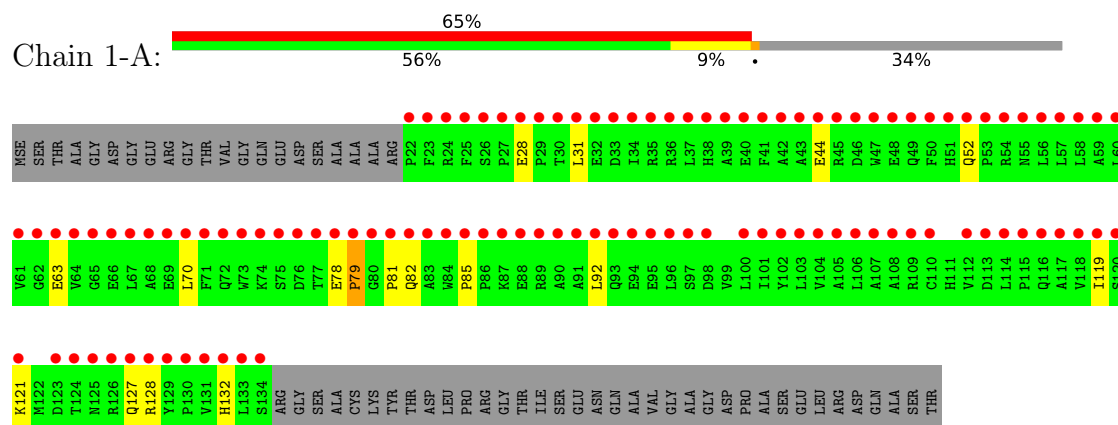
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-B	12	Total 12	O 12	0	0
2	8-B	11	Total 11	O 11	0	0
2	9-B	13	Total 13	O 13	0	0
2	10-B	14	Total 14	O 14	0	0
2	11-B	12	Total 12	O 12	0	0
2	12-B	12	Total 12	O 12	0	0
2	13-B	11	Total 11	O 11	0	0
2	14-B	12	Total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

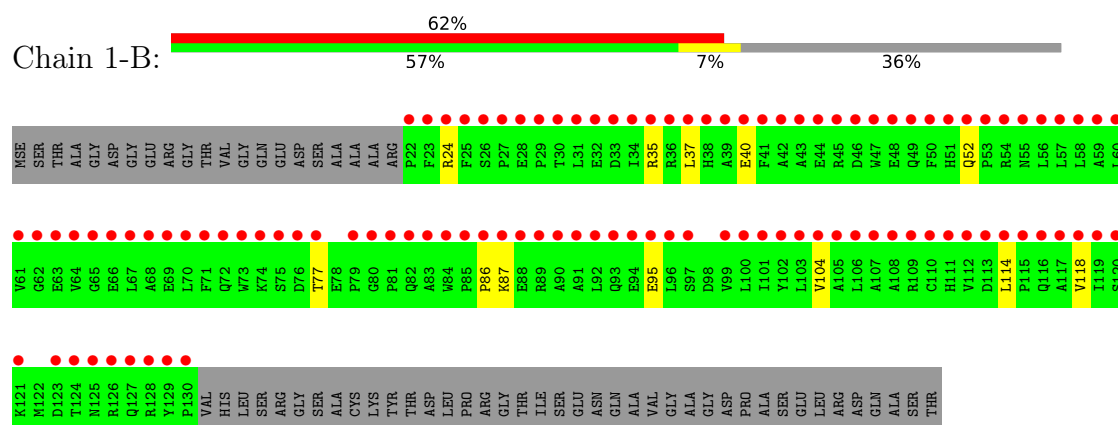
3 Residue-property plots

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.

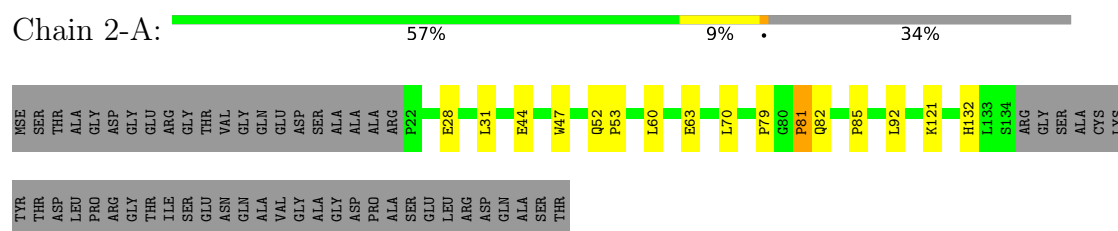
• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6

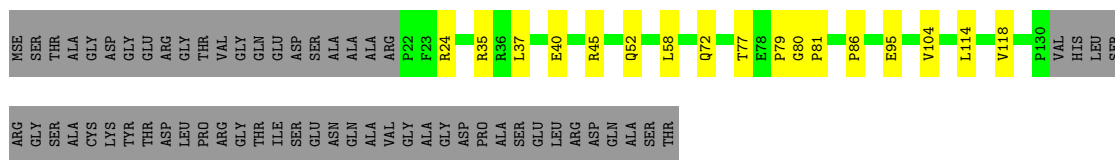


• Molecule 1: Protein RS21-C6



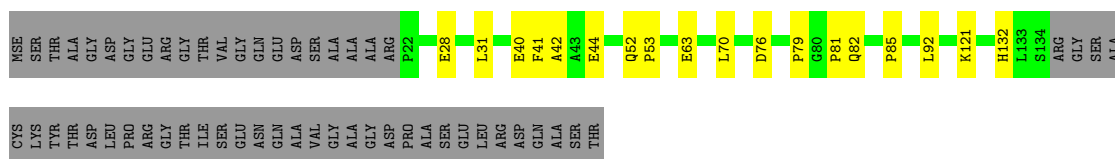
• Molecule 1: Protein RS21-C6

Chain 2-B:  54% 10% 36%



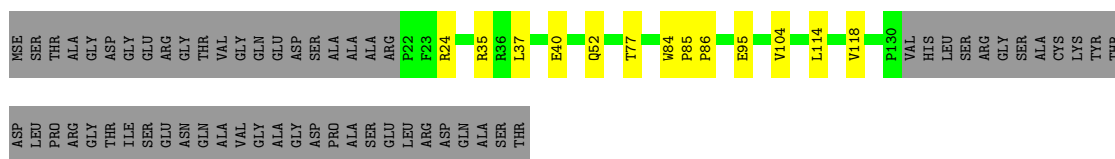
• Molecule 1: Protein RS21-C6

Chain 3-A:  56% 11% 34%



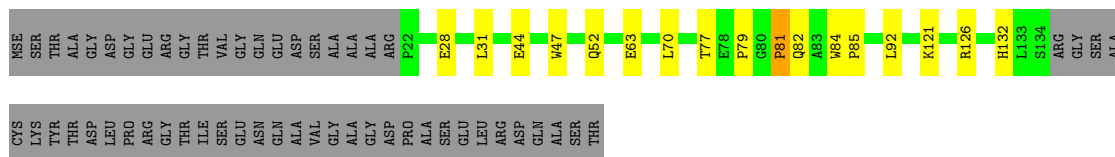
• Molecule 1: Protein RS21-C6

Chain 3-B:  56% 8% 36%



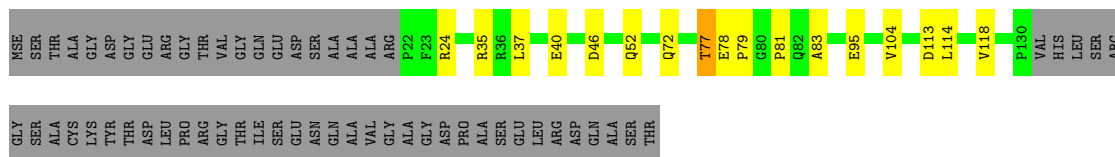
• Molecule 1: Protein RS21-C6

Chain 4-A:  56% 9% 34%



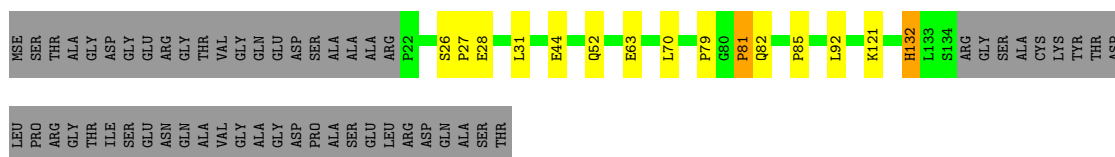
• Molecule 1: Protein RS21-C6

Chain 4-B:  54% 9% 36%



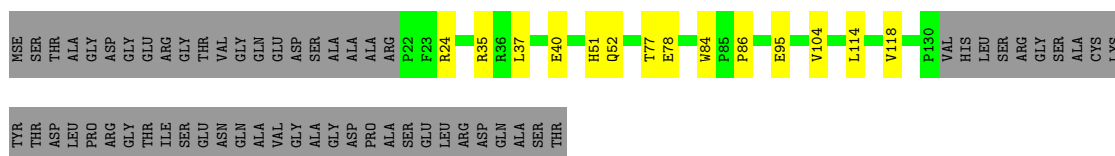
• Molecule 1: Protein RS21-C6

Chain 5-A:  58% 8% 34%



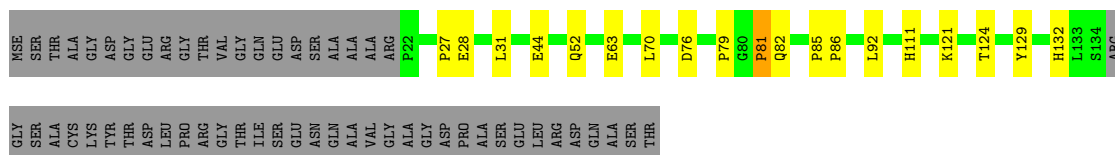
- Molecule 1: Protein RS21-C6

Chain 5-B: 56% 8% 36%



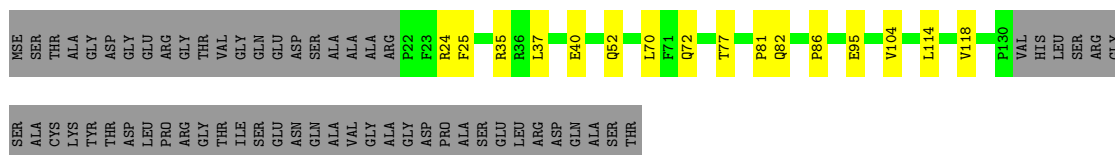
- Molecule 1: Protein RS21-C6

Chain 6-A: 55% 11% 34%



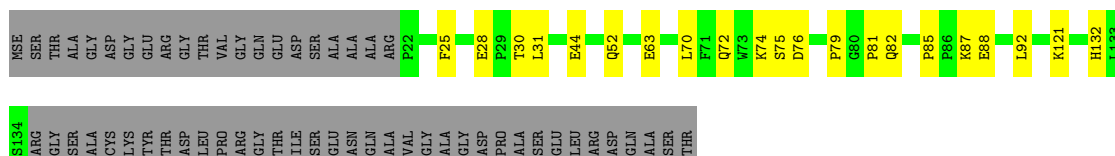
- Molecule 1: Protein RS21-C6

Chain 6-B: 55% 9% 36%



- Molecule 1: Protein RS21-C6

Chain 7-A: 54% 12% 34%



- Molecule 1: Protein RS21-C6

Chain 7-B: 52% 11% 36%



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

- Molecule 1: Protein RS21-C6

Chain 8-A: 57% 9% 34%

MSE THR SER THR
SER ARG ALA
ALA ALA
GLY ASP
GLY ASP
GLY GLY
GLU ARG
GLY THR
THR THR
ASP ASP
LEU LEU
VAL VAL
GLY GLY
GLN GLN
GLU GLY
ASP ASP
SER SER
ALA ALA
ALA ALA
ALA ALA
ARG ARG
P22
E28
L31
E44
W47
Q52
G62
E63
L70
P79
G80
P81
Q82
P85
P86
L92
K121
H132
L133
S134
ARG
GLY
SER
ALA
CYS
LYS
TYR

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

- Molecule 1: Protein RS21-C6

Chain 8-B: 54% 9% 36%

MSE SER SER THR
SER THR
ALA ALA
GLY GLY
ASP ASP
GLY GLY
GLU GLY
ARG ARG
GLY THR
THR THR
VAL VAL
GLY GLY
GLN GLN
GLU GLY
ASP ASP
SER SER
ALA ALA
ALA ALA
ALA ALA
ARG ARG
P22
F23
R24
R35
R36
L37
E40
R45
F50
H51
Q52
Q72
T77
P85
P86
K87
E95
V104
H111
L114
V118
P130
VAL
HIS
LEU
SER

ARG GLY
SER SER
ALA ALA
CYS CYS
LYS TYR
THR THR
ASP ASP
PRO PRO
ARG ARG
GLY GLY
THR THR
ILE ILE
SER SER
ASN ASN
ALA ALA
ALA ALA
VAL VAL
GLY GLY
ALA ALA
GLY GLY
ASP ASP
PRO PRO
ALA ALA
SER SER
THR THR

- Molecule 1: Protein RS21-C6

Chain 9-A: 54% 12% 34%

MSE SER SER THR
SER THR
ALA ALA
CYS CYS
LYS TYR
THR THR
GLU GLY
ARG ARG
GLY THR
THR THR
VAL VAL
GLY GLY
GLN GLN
GLU GLY
ASP ASP
SER SER
ALA ALA
ALA ALA
ALA ALA
ARG ARG
P22
F23
E28
L31
E44
W47
Q52
E63
L70
F71
P79
G80
P81
Q82
P85
P86
K87
E88
L92
Q93
E94
P115
K121
H132
L133
S134

ARG GLY
SER SER
ALA ALA
CYS CYS
LYS TYR
THR THR
ASP ASP
PRO PRO
ARG ARG
GLY GLY
THR THR
ILE ILE
SER SER
ASN ASN
ALA ALA
ALA ALA
VAL VAL
GLY GLY
ALA ALA
GLY GLY
ASP ASP
PRO PRO
ALA ALA
SER SER
THR THR

- Molecule 1: Protein RS21-C6

Chain 9-B: 56% 8% 36%

MSE SER SER THR
SER THR
ALA ALA
CYS CYS
LYS TYR
THR THR
GLU GLY
ARG ARG
GLY THR
THR THR
VAL VAL
GLY GLY
GLN GLN
GLU GLY
ASP ASP
SER SER
ALA ALA
ALA ALA
ALA ALA
ARG ARG
P22
F23
R24
R35
R36
L37
E40
Q52
Q72
T77
P85
R89
A90
E95
V104
L114
V118
F130
VAL
HIS
LEU
SER
ARG
GLY
SER
ALA
CYS

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

- Molecule 1: Protein RS21-C6

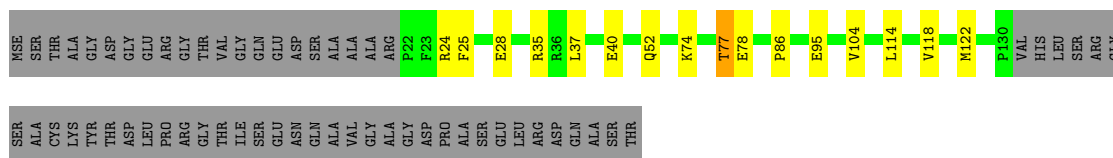
Chain 10-A: 56% 9% 34%

MSE SER SER THR
SER THR
ALA ALA
CYS CYS
LYS TYR
THR THR
GLU GLY
ARG ARG
GLY GLY
GLU GLY
ARG ARG
GLY THR
THR THR
VAL VAL
GLY GLY
GLN GLN
GLU GLY
ASP ASP
SER SER
ALA ALA
ALA ALA
ALA ALA
ARG ARG
P22
E28
L31
E44
Q52
E63
L70
F71
Q72
P79
G80
P81
Q82
W84
P85
P86
L92
Q93
K121
H132
L133
S134
ARG
GLY
SER
SER
ALA
CYS
LYS

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

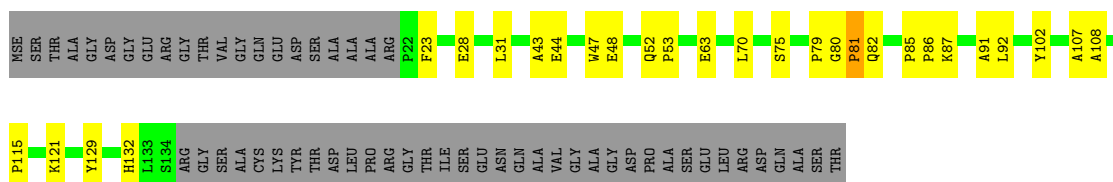
- Molecule 1: Protein RS21-C6

Chain 10-B:  55% 9% 36%



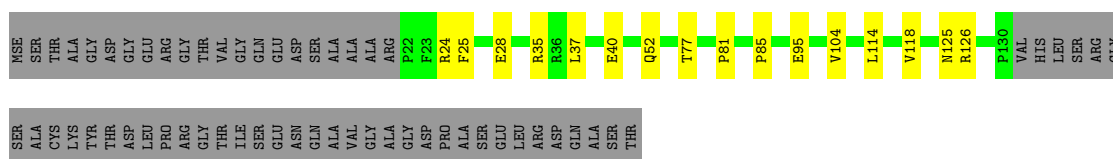
• Molecule 1: Protein RS21-C6

Chain 11-A:  50% 16% 34%



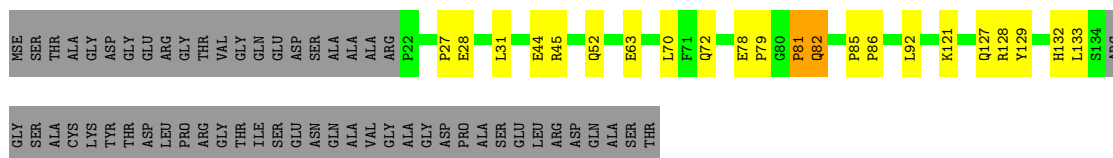
• Molecule 1: Protein RS21-C6

Chain 11-B:  55% 9% 36%



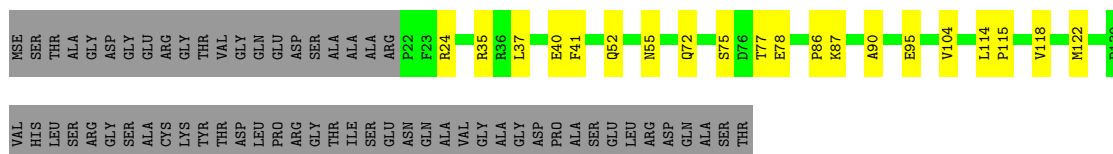
• Molecule 1: Protein RS21-C6

Chain 12-A:  54% 12% 34%



• Molecule 1: Protein RS21-C6

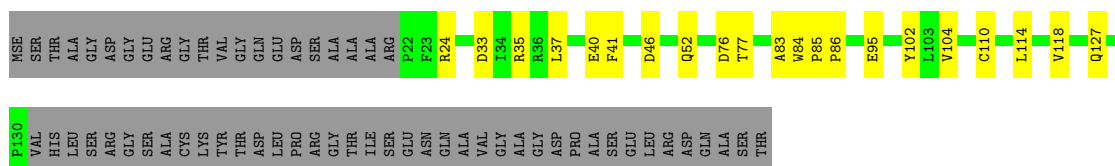
Chain 12-B:  52% 12% 36%



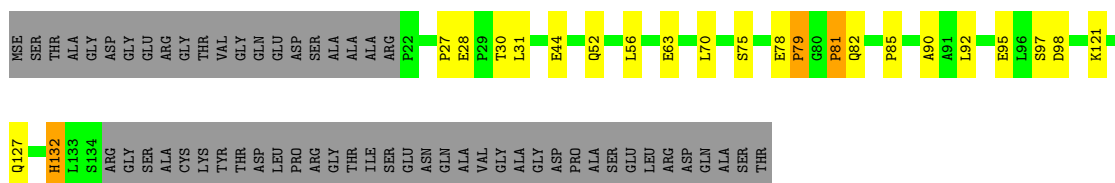
• Molecule 1: Protein RS21-C6

Chain 13-A:  55% 11% 34%

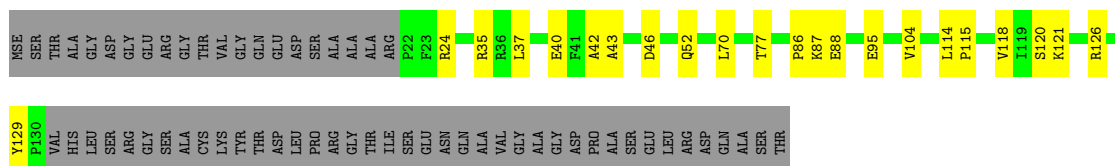
- Molecule 1: Protein RS21-C6



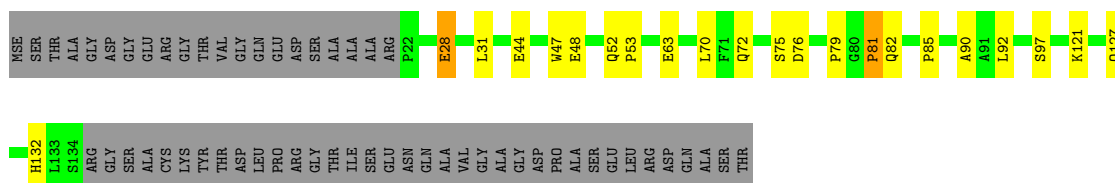
- Molecule 1: Protein RS21-C6



- Molecule 1: Protein RS21-C6

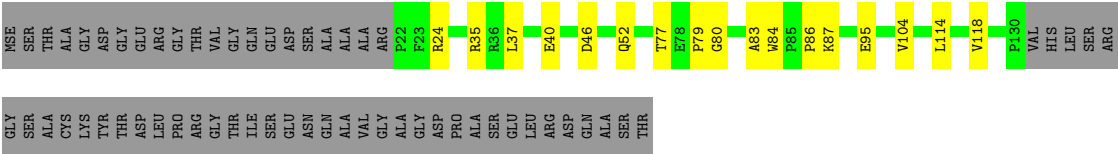


- Molecule 1: Protein RS21-C6

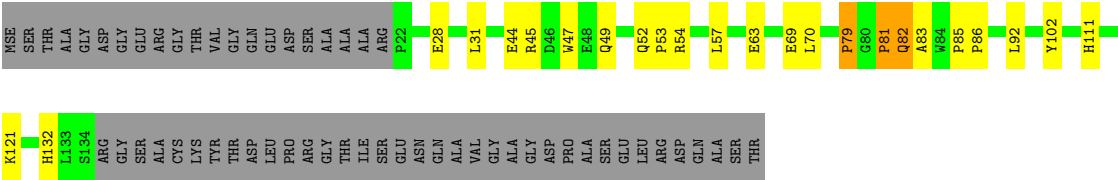


- Molecule 1: Protein RS21-C6

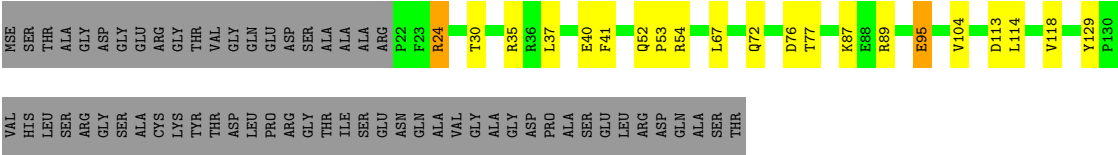




• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	73.54Å 73.54Å 236.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.93 – 2.32 37.93 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.93-2.32) 98.4 (37.93-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.138 , 0.233 0.196 , 0.271	Depositor DCC
R_{free} test set	858 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	29392	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	1-A	0.17	0/947	0.23	0/1288
1	1-B	0.21	0/915	0.22	0/1244
1	2-A	0.17	0/947	0.23	0/1288
1	2-B	0.21	0/915	0.22	0/1244
1	3-A	0.17	0/947	0.23	0/1288
1	3-B	0.21	0/915	0.22	0/1244
1	4-A	0.17	0/947	0.23	0/1288
1	4-B	0.21	0/915	0.22	0/1244
1	5-A	0.17	0/947	0.23	0/1288
1	5-B	0.21	0/915	0.22	0/1244
1	6-A	0.17	0/947	0.23	0/1288
1	6-B	0.21	0/915	0.22	0/1244
1	7-A	0.17	0/947	0.23	0/1288
1	7-B	0.21	0/915	0.22	0/1244
1	8-A	0.17	0/947	0.23	0/1288
1	8-B	0.21	0/915	0.22	0/1244
1	9-A	0.17	0/947	0.23	0/1288
1	9-B	0.21	0/915	0.22	0/1244
1	10-A	0.17	0/947	0.23	0/1288
1	10-B	0.21	0/915	0.22	0/1244
1	11-A	0.17	0/947	0.23	0/1288
1	11-B	0.21	0/915	0.22	0/1244
1	12-A	0.17	0/947	0.23	0/1288
1	12-B	0.21	0/915	0.22	0/1244
1	13-A	0.17	0/947	0.23	0/1288
1	13-B	0.21	0/915	0.22	0/1244
1	14-A	0.17	0/947	0.23	0/1288
1	14-B	0.21	0/915	0.22	0/1244
1	15-A	0.17	0/947	0.23	0/1288
1	15-B	0.21	0/915	0.22	0/1244
1	16-A	0.17	0/947	0.23	0/1288
1	16-B	0.21	0/915	0.22	0/1244
All	All	0.19	0/29792	0.23	0/40512

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

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	111/170 (65%)	83 (75%)	23 (21%)	5 (4%)	2	1
1	1-B	107/170 (63%)	83 (78%)	22 (21%)	2 (2%)	6	5
1	2-A	111/170 (65%)	89 (80%)	18 (16%)	4 (4%)	2	1
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-B	107/170 (63%)	98 (92%)	6 (6%)	3 (3%)	4	2
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%)	2	1
1	5-B	107/170 (63%)	98 (92%)	6 (6%)	3 (3%)	4	2
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%)	1	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%)	4	2
1	8-B	107/170 (63%)	80 (75%)	18 (17%)	9 (8%)	0	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%)	2	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%)	1	0
1	12-A	111/170 (65%)	82 (74%)	19 (17%)	10 (9%)	0	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%)	0	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
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

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Mol	Chain	Res	Type
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%)	85 (87%)	13 (13%)	4	4
1	1-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	2-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	2-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	3-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	3-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	4-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	4-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	5-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	5-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	6-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	6-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	7-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	7-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	8-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	8-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	9-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	9-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	10-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	10-B	94/136 (69%)	84 (89%)	10 (11%)	6	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	11-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	12-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	12-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	13-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	13-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	14-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	14-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	15-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	15-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	16-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	16-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
All	All	3072/4352 (71%)	2704 (88%)	368 (12%)	5	5

5 of 368 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	11-A	31	LEU
1	13-A	92	LEU
1	11-A	82	GLN
1	12-A	81	PRO
1	14-A	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
1	13-A	111	HIS
1	13-B	72	GLN
1	14-B	55	ASN
1	6-B	127	GLN
1	6-B	93	GLN

5.3.3 RNA ⓘ

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	1-A	112/170 (65%)	4.78	110 (98%) 0 0	2, 3, 3, 4	112 (100%)
1	1-B	108/170 (63%)	4.54	106 (98%) 0 0	2, 3, 3, 4	108 (100%)
1	2-A	0/170	-	-	-	-
1	2-B	0/170	-	-	-	-
1	3-A	0/170	-	-	-	-
1	3-B	0/170	-	-	-	-
1	4-A	0/170	-	-	-	-
1	4-B	0/170	-	-	-	-
1	5-A	0/170	-	-	-	-
1	5-B	0/170	-	-	-	-
1	6-A	0/170	-	-	-	-
1	6-B	0/170	-	-	-	-
1	7-A	0/170	-	-	-	-
1	7-B	0/170	-	-	-	-
1	8-A	0/170	-	-	-	-
1	8-B	0/170	-	-	-	-
1	9-A	0/170	-	-	-	-
1	9-B	0/170	-	-	-	-
1	10-A	0/170	-	-	-	-
1	10-B	0/170	-	-	-	-
1	11-A	0/170	-	-	-	-
1	11-B	0/170	-	-	-	-
1	12-A	0/170	-	-	-	-
1	12-B	0/170	-	-	-	-
1	13-A	0/170	-	-	-	-
1	13-B	0/170	-	-	-	-
1	14-A	0/170	-	-	-	-
1	14-B	0/170	-	-	-	-
1	15-A	0/170	-	-	-	-
1	15-B	0/170	-	-	-	-
1	16-A	0/170	-	-	-	-
1	16-B	0/170	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	220/5440 (4%)	4.66	216 (98%) 0 0	2, 3, 3, 4	220 (100%)

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	40	GLU	10.8
1	1-A	76	ASP	10.5
1	1-A	56	LEU	10.4
1	1-B	119	ILE	10.4
1	1-B	124	THR	10.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.