



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 05:50 pm GMT

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	(not set)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

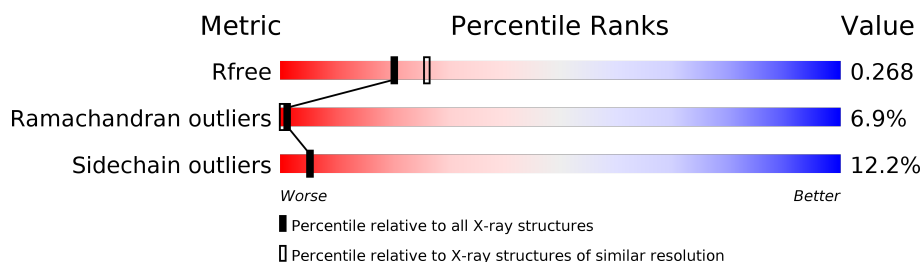
1 Overall quality at a glance

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.





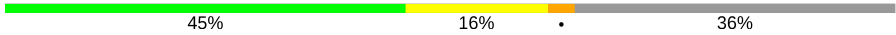

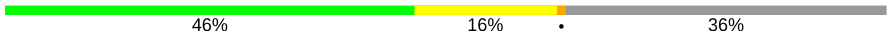
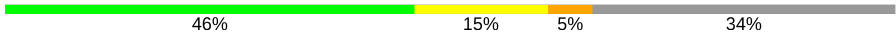
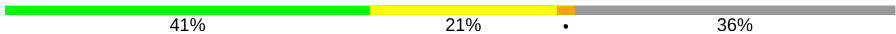
















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	5225 (2.34-2.30)
Ramachandran outliers	120053	5790 (2.34-2.30)
Sidechain outliers	120020	5789 (2.34-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

Continued on next page...

Continued from previous page...

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

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

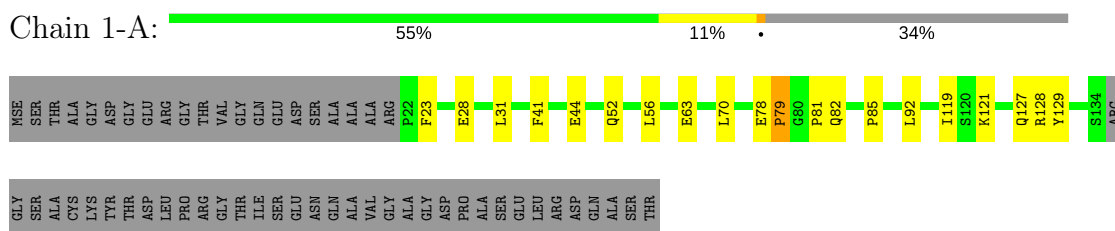
Continued from previous page...

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

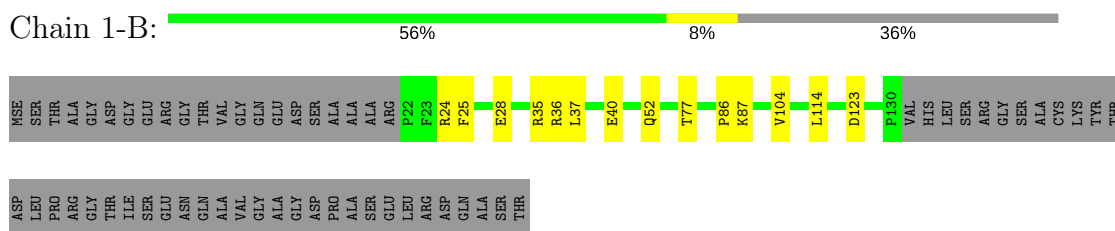
3 Residue-property plots [i](#)

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.

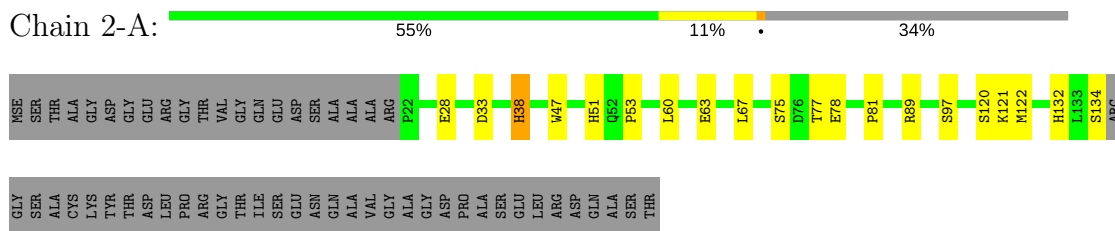
• Molecule 1: Protein RS21-C6



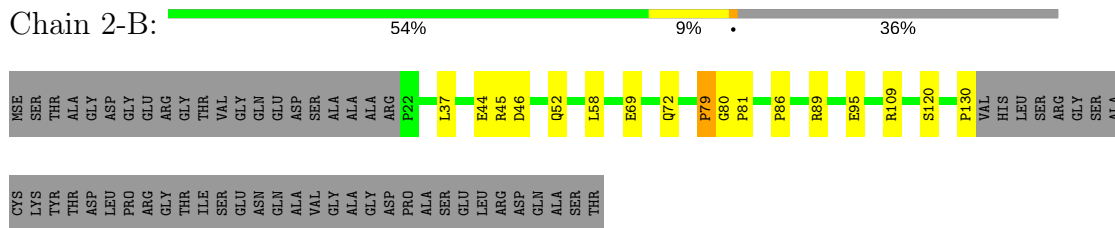
• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6

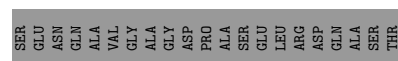
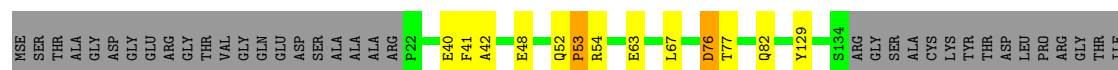


• Molecule 1: Protein RS21-C6



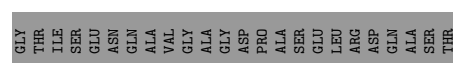
• Molecule 1: Protein RS21-C6

Chain 3-A:  59% 6% 34%



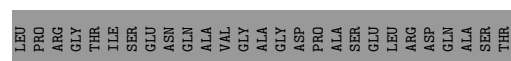
• Molecule 1: Protein RS21-C6

Chain 3-B:  58% 6% 36%



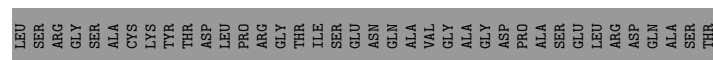
• Molecule 1: Protein RS21-C6

Chain 4-A:  58% 8% 34%



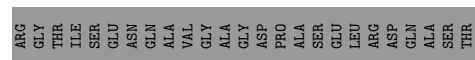
• Molecule 1: Protein RS21-C6

Chain 4-B:  53% 10% 36%



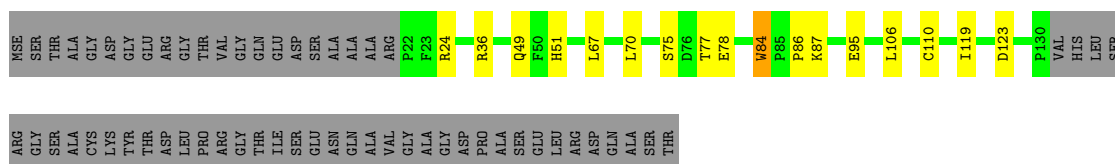
• Molecule 1: Protein RS21-C6

Chain 5-A:  58% 8% 34%



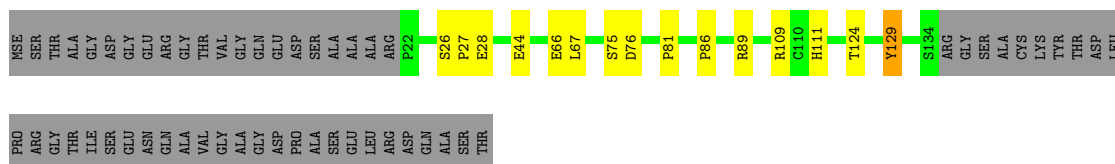
• Molecule 1: Protein RS21-C6

Chain 5-B:  54% 9% 36%



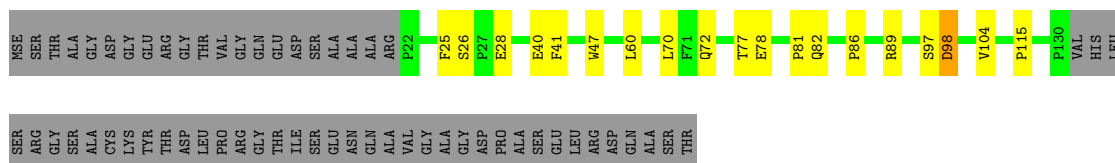
• Molecule 1: Protein RS21-C6

Chain 6-A: 58% 8% 34%



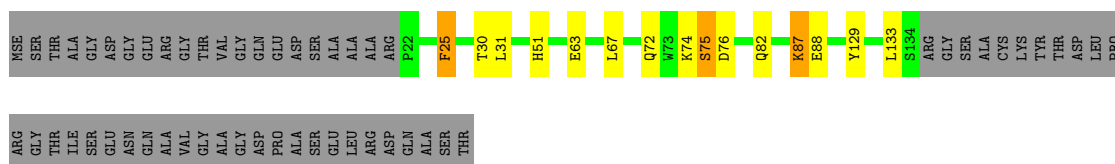
• Molecule 1: Protein RS21-C6

Chain 6-B: 53% 11% 36%



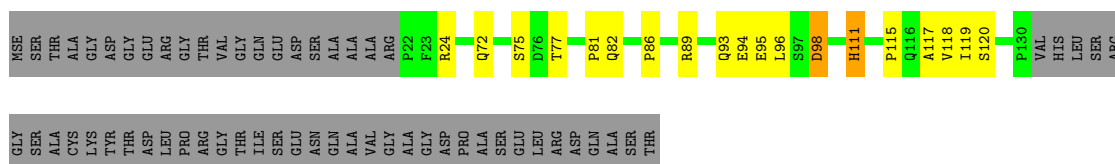
• Molecule 1: Protein RS21-C6

Chain 7-A: 58% 7% 34%



• Molecule 1: Protein RS21-C6

Chain 7-B: 53% 10% 36%



• Molecule 1: Protein RS21-C6

Chain 8-A: 59% 8% 34%



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

• Molecule 1: Protein RS21-C6

Chain 8-B: 52% 11% 36%

MSE
SER
THR
ALA
GLY
ASP
GLY
GLU
ARG
GLY
THR
VAL
GLY
GLN
ASP
SER
ALA
ALA
ARG
P22
D33
R36
L37
R45
F50
L56
L60
E63
L67
A69
E69
Q72
P85
P86
K87
Q93
E94
E95
H111
V112
D113
L114
D123
Q127

• Molecule 1: Protein RS21-C6

Chain 9-A: 54% 11% 34%

MSE
SER
THR
ALA
GLY
ASP
GLY
GLU
ARG
GLY
THR
VAL
GLY
GLN
ASP
SER
ALA
ALA
ARG
P22
F23
D46
W47
E48
F71
Q72
E78
Q82
P86
K87
E88
Q93
E94
E95
D98
V99
L100
P115
I119
M122
D123
Y129
S134
ARG
GLY
SER

• Molecule 1: Protein RS21-C6

Chain 9-B: 57% 6% 36%

MSE
SER
THR
ALA
GLY
ASP
GLY
GLU
ARG
GLY
THR
VAL
GLY
GLN
ASP
SER
ALA
ALA
ARG
P22
R36
D46
Q49
L67
Q72
S75
E78
P85
R89
A90
Q93
Y129
P130
VAL
HIS
LEU
SER
ARG
GLY
SER
SER
ALA
ALA
CYS
LYS
TYR
THR
LEU

• Molecule 1: Protein RS21-C6

Chain 10-A: 55% 9% 34%

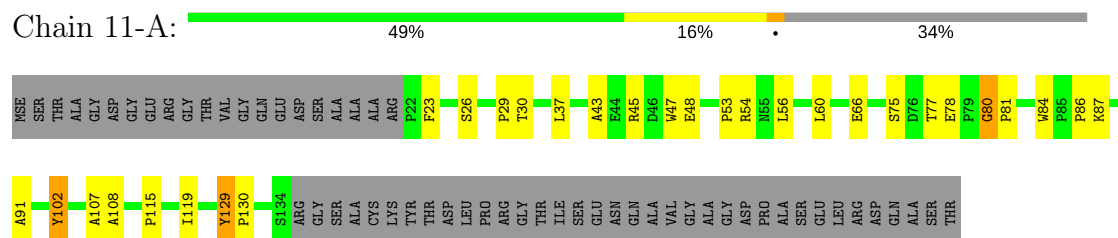
MSE
SER
THR
ALA
GLY
ASP
GLY
GLU
ARG
GLY
THR
VAL
GLY
GLN
ASP
SER
ALA
ALA
ARG
P22
F23
R24
E28
L37
D46
W47
E48
V64
Q72
S75
E78
P81
Q82
W84
P85
P86
Q93
E94
E95
Y102
Y129
H132
L133
S134
ARG

• Molecule 1: Protein RS21-C6

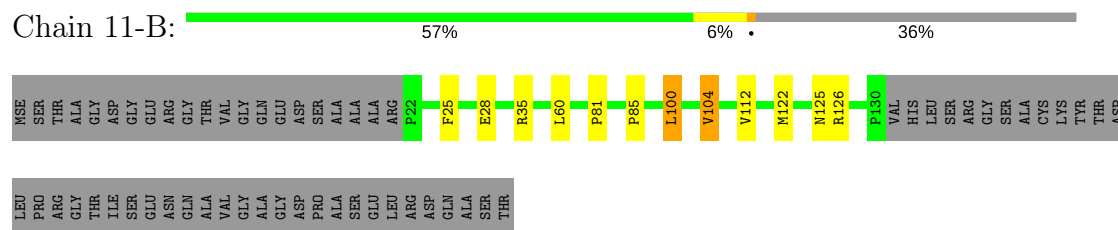
Chain 10-B: 54% 10% 36%

MSE
SER
THR
ALA
GLY
ASP
GLY
GLU
ARG
GLY
THR
VAL
GLY
GLN
ASP
SER
ALA
ALA
ARG
P22
F25
S26
P27
E28
P29
T30
D33
W73
K74
S75
D76
T77
E78
P86
D98
V104
Q116
M122
D123
T124
M125
R126
P130
VAL
HIS
LEU
SER
ARG
GLY

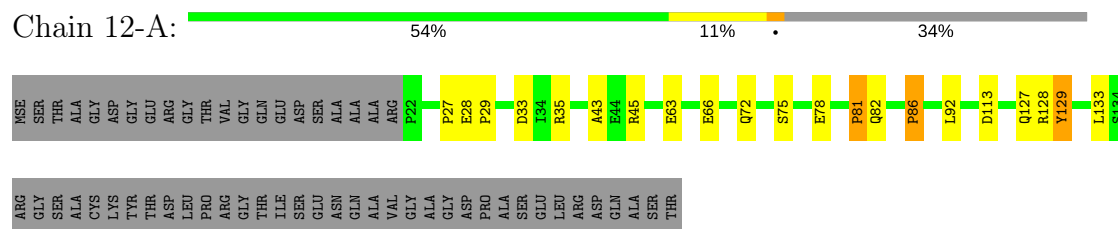
• Molecule 1: Protein RS21-C6



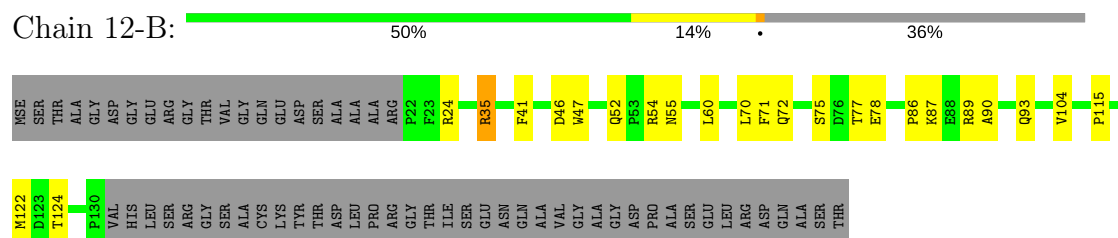
• Molecule 1: Protein RS21-C6



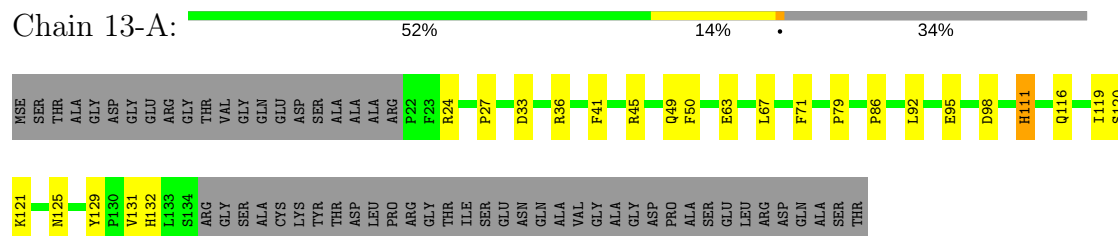
• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6

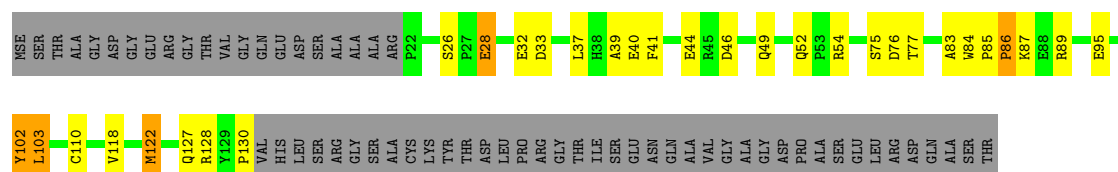


• Molecule 1: Protein RS21-C6



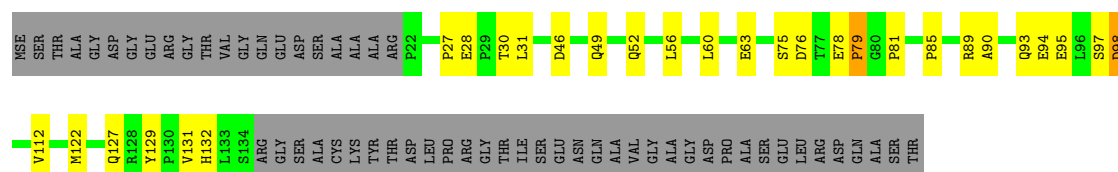
• Molecule 1: Protein RS21-C6





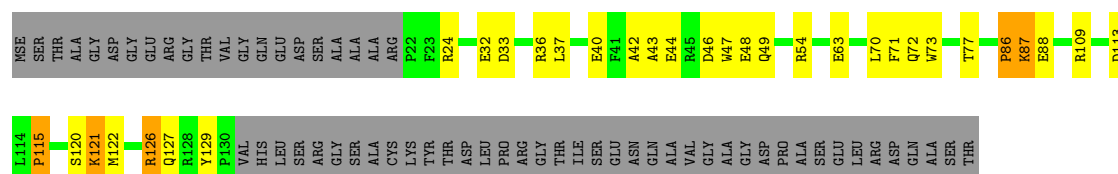
• Molecule 1: Protein RS21-C6

Chain 14-A: 49% 16% 34%



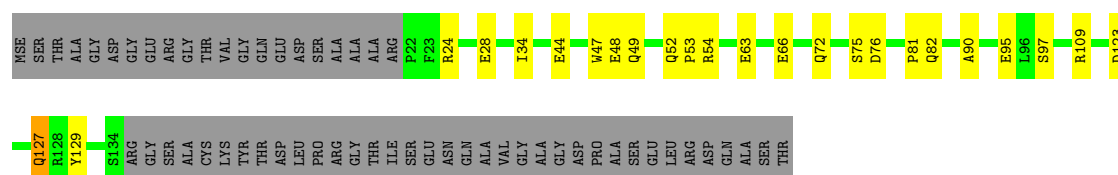
• Molecule 1: Protein RS21-C6

Chain 14-B: 45% 16% 36%



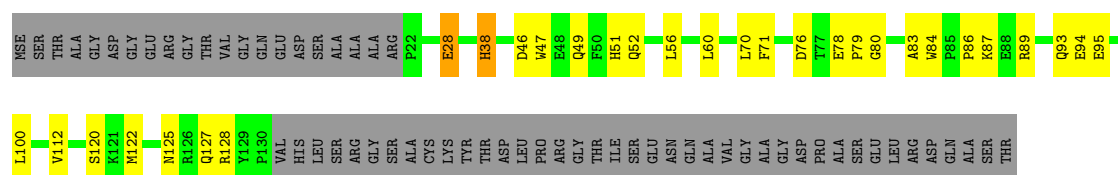
• Molecule 1: Protein RS21-C6

Chain 15-A: 52% 14% 34%



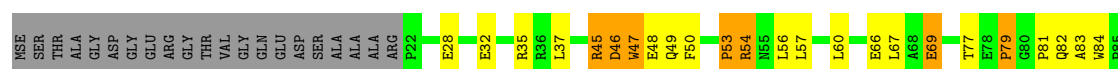
• Molecule 1: Protein RS21-C6

Chain 15-B: 46% 16% 36%



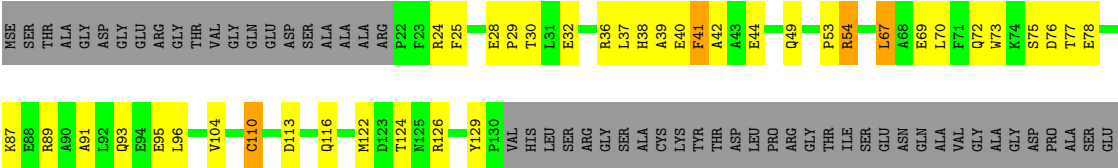
• Molecule 1: Protein RS21-C6

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





● 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 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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	55.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 652.5	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	0.93	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	0.83	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

All (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
1	9-A	78	GLU	CG-CD	7.16	1.62	1.51
1	12-A	113	ASP	CB-CG	7.02	1.66	1.51
1	16-B	69	GLU	CG-CD	6.97	1.62	1.51
1	16-B	69	GLU	CB-CG	6.86	1.65	1.52
1	13-B	102	TYR	CD2-CE2	6.27	1.48	1.39
1	14-B	47	TRP	CG-CD1	5.94	1.45	1.36
1	16-B	104	VAL	CB-CG1	-5.85	1.40	1.52
1	5-B	36	ARG	CG-CD	5.78	1.66	1.51
1	15-B	28	GLU	CG-CD	5.64	1.60	1.51
1	15-B	47	TRP	CG-CD1	5.61	1.44	1.36
1	11-A	102	TYR	CD1-CE1	5.59	1.47	1.39
1	13-B	28	GLU	CG-CD	5.57	1.60	1.51
1	16-A	69	GLU	CG-CD	5.47	1.60	1.51
1	15-A	109	ARG	CZ-NH2	5.46	1.40	1.33
1	16-B	28	GLU	CB-CG	5.42	1.62	1.52
1	13-B	44	GLU	CB-CG	5.42	1.62	1.52
1	6-B	41	PHE	CE2-CZ	5.41	1.47	1.37
1	13-B	102	TYR	CZ-OH	5.35	1.47	1.37
1	8-B	69	GLU	CG-CD	5.33	1.59	1.51
1	2-B	69	GLU	CG-CD	5.25	1.59	1.51
1	14-B	73	TRP	CE3-CZ3	5.25	1.47	1.38
1	8-B	33	ASP	CB-CG	5.24	1.62	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	32	GLU	CG-CD	5.23	1.59	1.51
1	10-A	95	GLU	CG-CD	5.18	1.59	1.51
1	12-B	47	TRP	CB-CG	-5.18	1.41	1.50
1	16-B	40	GLU	CB-CG	-5.17	1.42	1.52
1	16-B	104	VAL	CA-CB	5.16	1.65	1.54
1	9-A	94	GLU	CG-CD	5.06	1.59	1.51
1	11-B	104	VAL	CA-CB	5.05	1.65	1.54
1	6-B	47	TRP	CG-CD1	5.01	1.43	1.36

All (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
1	12-B	35	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	5-B	67	LEU	CA-CB-CG	7.83	133.32	115.30
1	11-A	56	LEU	CA-CB-CG	7.65	132.90	115.30
1	13-B	54	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	6-B	89	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	16-A	37	LEU	CA-CB-CG	-7.19	98.76	115.30
1	8-B	56	LEU	CA-CB-CG	7.17	131.79	115.30
1	7-A	31	LEU	N-CA-C	-7.14	91.72	111.00
1	15-A	109	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	11-A	37	LEU	CA-CB-CG	-7.03	99.14	115.30
1	2-A	38	HIS	N-CA-C	-7.00	92.11	111.00
1	16-B	39	ALA	C-N-CA	6.99	139.19	121.70
1	8-A	113	ASP	CB-CG-OD1	-6.96	112.04	118.30
1	4-B	109	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	12-B	46	ASP	CB-CG-OD1	6.89	124.50	118.30
1	7-A	31	LEU	CA-CB-CG	6.87	131.10	115.30
1	13-B	54	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	1-B	28	GLU	N-CA-C	-6.76	92.76	111.00
1	16-B	39	ALA	CA-C-N	-6.74	102.38	117.20
1	10-B	30	THR	N-CA-C	-6.67	92.99	111.00
1	16-A	47	TRP	N-CA-C	6.66	128.97	111.00
1	10-B	26	SER	C-N-CD	-6.65	105.96	120.60
1	14-B	54	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	16-A	45	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	16-B	91	ALA	N-CA-C	-6.45	93.60	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	54	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	13-B	49	GLN	N-CA-C	-6.40	93.73	111.00
1	16-B	39	ALA	N-CA-C	6.39	128.25	111.00
1	10-A	24	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	14-B	109	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	5-B	36	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	13-B	130	PRO	N-CA-C	6.30	128.48	112.10
1	11-B	100	LEU	CA-CB-CG	6.24	129.64	115.30
1	6-B	26	SER	C-N-CD	-6.18	107.00	120.60
1	13-A	36	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	10-B	26	SER	C-N-CA	6.14	147.77	122.00
1	16-A	103	LEU	CA-CB-CG	-6.07	101.34	115.30
1	16-A	54	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	2-B	109	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	16-A	45	ARG	CG-CD-NE	5.93	124.24	111.80
1	12-A	43	ALA	N-CA-C	-5.92	95.02	111.00
1	16-B	110	CYS	CA-CB-SG	-5.90	103.38	114.00
1	16-B	36	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	9-B	67	LEU	CA-CB-CG	5.84	128.73	115.30
1	14-A	49	GLN	N-CA-C	-5.84	95.24	111.00
1	1-B	25	PHE	N-CA-C	-5.83	95.26	111.00
1	12-A	113	ASP	CB-CG-OD2	5.76	123.48	118.30
1	16-B	39	ALA	O-C-N	5.69	131.80	122.70
1	2-A	33	ASP	CB-CG-OD1	5.67	123.41	118.30
1	14-A	76	ASP	CB-CG-OD1	5.62	123.36	118.30
1	16-A	113	ASP	N-CA-C	-5.61	95.85	111.00
1	11-A	80	GLY	N-CA-C	5.61	127.12	113.10
1	13-B	103	LEU	CA-CB-CG	-5.55	102.53	115.30
1	16-B	70	LEU	CB-CG-CD1	-5.55	101.57	111.00
1	13-A	36	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	16-A	46	ASP	CB-CG-OD2	5.52	123.27	118.30
1	11-A	84	TRP	N-CA-C	-5.45	96.29	111.00
1	11-A	45	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	16-B	70	LEU	C-N-CA	-5.42	108.14	121.70
1	16-B	96	LEU	CA-CB-CG	-5.39	102.90	115.30
1	16-B	69	GLU	OE1-CD-OE2	-5.36	116.86	123.30
1	16-B	25	PHE	CB-CA-C	-5.36	99.68	110.40
1	14-B	36	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	11-A	102	TYR	CA-CB-CG	5.33	123.53	113.40
1	13-B	26	SER	N-CA-C	-5.29	96.72	111.00
1	16-A	46	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	11-B	112	VAL	N-CA-C	-5.26	96.81	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	131	VAL	CB-CA-C	-5.25	101.42	111.40
1	15-B	56	LEU	CA-CB-CG	-5.24	103.24	115.30
1	1-A	56	LEU	CA-CB-CG	5.23	127.32	115.30
1	7-B	98	ASP	CB-CG-OD1	5.20	122.98	118.30
1	13-B	122	MSE	N-CA-C	-5.20	96.96	111.00
1	15-B	112	VAL	CB-CA-C	-5.19	101.54	111.40
1	8-B	36	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	10-A	37	LEU	CA-CB-CG	-5.17	103.42	115.30
1	4-B	31	LEU	N-CA-C	-5.16	97.08	111.00
1	15-B	70	LEU	CA-CB-CG	5.14	127.12	115.30
1	15-B	38	HIS	N-CA-C	5.14	124.87	111.00
1	16-B	38	HIS	N-CA-C	5.13	124.87	111.00
1	14-A	112	VAL	N-CA-C	-5.06	97.35	111.00
1	4-B	119	ILE	N-CA-C	-5.04	97.41	111.00
1	16-A	46	ASP	CB-CA-C	5.04	120.47	110.40
1	6-B	98	ASP	CB-CG-OD1	5.03	122.83	118.30
1	10-B	30	THR	CB-CA-C	-5.01	98.06	111.60
1	11-A	60	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (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	102	TYR	Sidechain
1	13-B	41	PHE	Sidechain
1	16-A	102	TYR	Sidechain
1	16-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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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 [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%)	3 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-B	107/170 (63%)	83 (78%)	22 (21%)	2 (2%)	9	7
1	2-A	111/170 (65%)	89 (80%)	18 (16%)	4 (4%)	4	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%)	3	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%)	3	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%)	4	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	1
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%)	4	2
1	10-A	111/170 (65%)	90 (81%)	16 (14%)	5 (4%)	3	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	1
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%)	1	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%)	1	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3488/5440 (64%)	2742 (79%)	505 (14%)	241 (7%)	1	0

All (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
1	2-B	81	PRO
1	2-B	86	PRO
1	3-A	41	PHE
1	4-A	47	TRP
1	4-B	72	GLN
1	4-B	79	PRO
1	4-B	81	PRO
1	5-A	26	SER
1	5-B	78	GLU
1	5-B	86	PRO
1	6-A	27	PRO
1	6-A	76	ASP
1	6-A	111	HIS
1	6-A	124	THR
1	6-A	129	TYR
1	6-B	72	GLN
1	6-B	82	GLN
1	6-B	86	PRO
1	7-A	30	THR
1	7-A	74	LYS
1	7-A	88	GLU
1	7-B	75	SER
1	7-B	81	PRO
1	7-B	95	GLU
1	7-B	96	LEU
1	7-B	111	HIS
1	7-B	118	VAL
1	7-B	119	ILE
1	7-B	120	SER
1	8-B	72	GLN
1	8-B	85	PRO
1	8-B	86	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	87	LYS
1	8-B	111	HIS
1	9-A	23	PHE
1	9-A	47	TRP
1	9-A	82	GLN
1	9-A	93	GLN
1	9-A	94	GLU
1	9-B	72	GLN
1	10-A	72	GLN
1	10-A	81	PRO
1	10-A	86	PRO
1	10-B	25	PHE
1	10-B	78	GLU
1	10-B	122	MSE
1	11-A	23	PHE
1	11-A	47	TRP
1	11-A	48	GLU
1	11-A	80	GLY
1	11-A	107	ALA
1	12-A	81	PRO
1	12-B	72	GLN
1	12-B	75	SER
1	12-B	86	PRO
1	12-B	87	LYS
1	13-A	49	GLN
1	13-A	111	HIS
1	13-B	76	ASP
1	13-B	83	ALA
1	13-B	110	CYS
1	14-A	30	THR
1	14-A	78	GLU
1	14-A	81	PRO
1	14-A	97	SER
1	14-A	98	ASP
1	14-B	42	ALA
1	14-B	43	ALA
1	14-B	70	LEU
1	14-B	121	LYS
1	14-B	126	ARG
1	14-B	129	TYR
1	15-A	28	GLU
1	15-A	47	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-A	48	GLU
1	15-A	75	SER
1	15-A	76	ASP
1	15-A	81	PRO
1	15-A	90	ALA
1	15-B	86	PRO
1	15-B	87	LYS
1	16-A	49	GLN
1	16-A	53	PRO
1	16-A	54	ARG
1	16-A	69	GLU
1	16-A	81	PRO
1	16-A	82	GLN
1	16-A	83	ALA
1	16-A	111	HIS
1	16-B	24	ARG
1	16-B	30	THR
1	16-B	129	TYR
1	1-A	119	ILE
1	1-A	127	GLN
1	2-A	47	TRP
1	4-B	78	GLU
1	4-B	83	ALA
1	6-B	81	PRO
1	7-A	87	LYS
1	7-B	117	ALA
1	8-A	47	TRP
1	8-A	62	GLY
1	8-B	37	LEU
1	9-A	87	LYS
1	9-B	89	ARG
1	10-B	74	LYS
1	10-B	86	PRO
1	11-A	81	PRO
1	11-A	87	LYS
1	11-A	108	ALA
1	11-B	25	PHE
1	11-B	85	PRO
1	12-A	45	ARG
1	12-A	86	PRO
1	12-A	127	GLN
1	12-A	128	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-B	41	PHE
1	12-B	122	MSE
1	13-A	50	PHE
1	13-B	127	GLN
1	14-A	132	HIS
1	14-B	120	SER
1	15-A	72	GLN
1	15-B	46	ASP
1	15-B	80	GLY
1	15-B	83	ALA
1	16-B	53	PRO
1	16-B	54	ARG
1	16-B	72	GLN
1	16-B	113	ASP
1	1-A	79	PRO
1	1-B	87	LYS
1	2-B	80	GLY
1	3-A	76	ASP
1	4-A	77	THR
1	4-A	81	PRO
1	4-B	46	ASP
1	5-A	132	HIS
1	6-B	25	PHE
1	7-A	75	SER
1	7-A	76	ASP
1	7-B	94	GLU
1	8-B	50	PHE
1	9-A	88	GLU
1	9-B	85	PRO
1	9-B	90	ALA
1	10-A	84	TRP
1	11-A	75	SER
1	11-B	81	PRO
1	12-A	72	GLN
1	12-B	90	ALA
1	13-A	27	PRO
1	14-A	79	PRO
1	14-A	95	GLU
1	14-A	127	GLN
1	14-B	46	ASP
1	14-B	87	LYS
1	15-B	79	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16-A	45	ARG
1	16-A	47	TRP
1	16-A	57	LEU
1	16-B	67	LEU
1	16-B	89	ARG
1	2-A	60	LEU
1	2-B	45	ARG
1	2-B	58	LEU
1	3-A	40	GLU
1	3-B	85	PRO
1	4-B	77	THR
1	4-B	113	ASP
1	6-B	70	LEU
1	7-A	25	PHE
1	7-B	72	GLN
1	7-B	115	PRO
1	8-B	45	ARG
1	10-B	28	GLU
1	10-B	77	THR
1	11-A	43	ALA
1	11-A	86	PRO
1	13-B	46	ASP
1	13-B	85	PRO
1	14-A	75	SER
1	14-A	90	ALA
1	14-B	88	GLU
1	14-B	115	PRO
1	15-A	53	PRO
1	15-A	97	SER
1	16-B	76	ASP
1	2-A	53	PRO
1	2-B	79	PRO
1	3-A	42	ALA
1	3-B	84	TRP
1	3-B	86	PRO
1	4-A	84	TRP
1	4-A	126	ARG
1	7-A	72	GLN
1	10-A	93	GLN
1	11-A	91	ALA
1	11-A	115	PRO
1	12-A	27	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-A	82	GLN
1	12-B	115	PRO
1	14-A	27	PRO
1	14-A	56	LEU
1	14-B	86	PRO
1	15-A	127	GLN
1	16-B	87	LYS
1	16-B	95	GLU
1	5-A	27	PRO
1	11-B	125	ASN
1	11-B	126	ARG
1	12-A	133	LEU
1	12-B	55	ASN
1	12-B	78	GLU
1	13-A	131	VAL
1	13-B	33	ASP
1	13-B	84	TRP
1	13-B	86	PRO
1	15-B	84	TRP
1	3-A	53	PRO
1	6-A	81	PRO
1	8-A	86	PRO
1	13-A	119	ILE
1	5-A	81	PRO
1	6-A	86	PRO
1	8-B	114	LEU
1	9-A	86	PRO
1	9-A	115	PRO
1	11-A	53	PRO
1	16-A	79	PRO
1	12-A	78	GLU
1	16-A	86	PRO
1	11-A	129	TYR
1	11-B	28	GLU
1	13-A	79	PRO
1	5-B	84	TRP

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%)	3	2
1	1-B	94/136 (69%)	84 (89%)	10 (11%)	7	8
1	2-A	98/136 (72%)	83 (85%)	15 (15%)	3	2
1	2-B	94/136 (69%)	85 (90%)	9 (10%)	9	10
1	3-A	98/136 (72%)	88 (90%)	10 (10%)	8	9
1	3-B	94/136 (69%)	86 (92%)	8 (8%)	12	14
1	4-A	98/136 (72%)	89 (91%)	9 (9%)	10	11
1	4-B	94/136 (69%)	84 (89%)	10 (11%)	7	8
1	5-A	98/136 (72%)	88 (90%)	10 (10%)	8	9
1	5-B	94/136 (69%)	82 (87%)	12 (13%)	5	4
1	6-A	98/136 (72%)	89 (91%)	9 (9%)	10	11
1	6-B	94/136 (69%)	85 (90%)	9 (10%)	9	10
1	7-A	98/136 (72%)	89 (91%)	9 (9%)	10	11
1	7-B	94/136 (69%)	86 (92%)	8 (8%)	12	14
1	8-A	98/136 (72%)	89 (91%)	9 (9%)	10	11
1	8-B	94/136 (69%)	84 (89%)	10 (11%)	7	8
1	9-A	98/136 (72%)	87 (89%)	11 (11%)	6	7
1	9-B	94/136 (69%)	86 (92%)	8 (8%)	12	14
1	10-A	98/136 (72%)	84 (86%)	14 (14%)	3	3
1	10-B	94/136 (69%)	86 (92%)	8 (8%)	12	14
1	11-A	98/136 (72%)	88 (90%)	10 (10%)	8	9
1	11-B	94/136 (69%)	90 (96%)	4 (4%)	32	43
1	12-A	98/136 (72%)	87 (89%)	11 (11%)	6	7
1	12-B	94/136 (69%)	82 (87%)	12 (13%)	5	4
1	13-A	98/136 (72%)	80 (82%)	18 (18%)	2	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	23	PHE
1	1-A	28	GLU
1	1-A	31	LEU
1	1-A	41	PHE
1	1-A	44	GLU
1	1-A	52	GLN
1	1-A	63	GLU
1	1-A	70	LEU
1	1-A	79	PRO
1	1-A	81	PRO
1	1-A	82	GLN
1	1-A	85	PRO
1	1-A	92	LEU
1	1-A	121	LYS
1	1-A	129	TYR
1	1-B	24	ARG
1	1-B	35	ARG
1	1-B	36	ARG
1	1-B	37	LEU
1	1-B	40	GLU
1	1-B	52	GLN
1	1-B	77	THR
1	1-B	104	VAL
1	1-B	114	LEU
1	1-B	123	ASP
1	2-A	28	GLU
1	2-A	38	HIS
1	2-A	51	HIS
1	2-A	63	GLU
1	2-A	67	LEU
1	2-A	75	SER
1	2-A	77	THR
1	2-A	78	GLU
1	2-A	89	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	97	SER
1	2-A	120	SER
1	2-A	121	LYS
1	2-A	122	MSE
1	2-A	132	HIS
1	2-A	134	SER
1	2-B	37	LEU
1	2-B	44	GLU
1	2-B	46	ASP
1	2-B	52	GLN
1	2-B	79	PRO
1	2-B	89	ARG
1	2-B	95	GLU
1	2-B	120	SER
1	2-B	130	PRO
1	3-A	48	GLU
1	3-A	52	GLN
1	3-A	53	PRO
1	3-A	54	ARG
1	3-A	63	GLU
1	3-A	67	LEU
1	3-A	76	ASP
1	3-A	77	THR
1	3-A	82	GLN
1	3-A	129	TYR
1	3-B	24	ARG
1	3-B	38	HIS
1	3-B	77	THR
1	3-B	79	PRO
1	3-B	89	ARG
1	3-B	94	GLU
1	3-B	104	VAL
1	3-B	119	ILE
1	4-A	54	ARG
1	4-A	63	GLU
1	4-A	64	VAL
1	4-A	67	LEU
1	4-A	86	PRO
1	4-A	102	TYR
1	4-A	109	ARG
1	4-A	122	MSE
1	4-A	129	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	24	ARG
1	4-B	49	GLN
1	4-B	54	ARG
1	4-B	63	GLU
1	4-B	81	PRO
1	4-B	82	GLN
1	4-B	89	ARG
1	4-B	104	VAL
1	4-B	119	ILE
1	4-B	122	MSE
1	5-A	33	ASP
1	5-A	48	GLU
1	5-A	67	LEU
1	5-A	72	GLN
1	5-A	79	PRO
1	5-A	82	GLN
1	5-A	89	ARG
1	5-A	119	ILE
1	5-A	128	ARG
1	5-A	129	TYR
1	5-B	24	ARG
1	5-B	49	GLN
1	5-B	70	LEU
1	5-B	75	SER
1	5-B	77	THR
1	5-B	84	TRP
1	5-B	87	LYS
1	5-B	95	GLU
1	5-B	106	LEU
1	5-B	110	CYS
1	5-B	119	ILE
1	5-B	123	ASP
1	6-A	26	SER
1	6-A	28	GLU
1	6-A	44	GLU
1	6-A	66	GLU
1	6-A	67	LEU
1	6-A	75	SER
1	6-A	89	ARG
1	6-A	109	ARG
1	6-A	129	TYR
1	6-B	28	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-B	40	GLU
1	6-B	60	LEU
1	6-B	77	THR
1	6-B	78	GLU
1	6-B	97	SER
1	6-B	98	ASP
1	6-B	104	VAL
1	6-B	115	PRO
1	7-A	25	PHE
1	7-A	51	HIS
1	7-A	63	GLU
1	7-A	67	LEU
1	7-A	75	SER
1	7-A	82	GLN
1	7-A	87	LYS
1	7-A	129	TYR
1	7-A	133	LEU
1	7-B	24	ARG
1	7-B	77	THR
1	7-B	82	GLN
1	7-B	86	PRO
1	7-B	89	ARG
1	7-B	93	GLN
1	7-B	98	ASP
1	7-B	111	HIS
1	8-A	26	SER
1	8-A	28	GLU
1	8-A	63	GLU
1	8-A	66	GLU
1	8-A	74	LYS
1	8-A	75	SER
1	8-A	98	ASP
1	8-A	129	TYR
1	8-A	132	HIS
1	8-B	50	PHE
1	8-B	60	LEU
1	8-B	63	GLU
1	8-B	67	LEU
1	8-B	87	LYS
1	8-B	93	GLN
1	8-B	95	GLU
1	8-B	113	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	123	ASP
1	8-B	127	GLN
1	9-A	46	ASP
1	9-A	47	TRP
1	9-A	48	GLU
1	9-A	72	GLN
1	9-A	95	GLU
1	9-A	98	ASP
1	9-A	100	LEU
1	9-A	119	ILE
1	9-A	122	MSE
1	9-A	123	ASP
1	9-A	129	TYR
1	9-B	36	ARG
1	9-B	46	ASP
1	9-B	49	GLN
1	9-B	75	SER
1	9-B	78	GLU
1	9-B	89	ARG
1	9-B	93	GLN
1	9-B	129	TYR
1	10-A	28	GLU
1	10-A	46	ASP
1	10-A	48	GLU
1	10-A	64	VAL
1	10-A	72	GLN
1	10-A	75	SER
1	10-A	78	GLU
1	10-A	82	GLN
1	10-A	86	PRO
1	10-A	94	GLU
1	10-A	95	GLU
1	10-A	102	TYR
1	10-A	129	TYR
1	10-A	132	HIS
1	10-B	33	ASP
1	10-B	73	TRP
1	10-B	75	SER
1	10-B	98	ASP
1	10-B	104	VAL
1	10-B	116	GLN
1	10-B	124	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-B	126	ARG
1	11-A	26	SER
1	11-A	29	PRO
1	11-A	30	THR
1	11-A	54	ARG
1	11-A	66	GLU
1	11-A	77	THR
1	11-A	78	GLU
1	11-A	119	ILE
1	11-A	129	TYR
1	11-A	130	PRO
1	11-B	60	LEU
1	11-B	100	LEU
1	11-B	104	VAL
1	11-B	122	MSE
1	12-A	28	GLU
1	12-A	29	PRO
1	12-A	33	ASP
1	12-A	35	ARG
1	12-A	63	GLU
1	12-A	66	GLU
1	12-A	75	SER
1	12-A	81	PRO
1	12-A	86	PRO
1	12-A	92	LEU
1	12-A	129	TYR
1	12-B	24	ARG
1	12-B	35	ARG
1	12-B	52	GLN
1	12-B	54	ARG
1	12-B	60	LEU
1	12-B	70	LEU
1	12-B	71	PHE
1	12-B	77	THR
1	12-B	89	ARG
1	12-B	93	GLN
1	12-B	104	VAL
1	12-B	124	THR
1	13-A	24	ARG
1	13-A	33	ASP
1	13-A	41	PHE
1	13-A	45	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13-A	63	GLU
1	13-A	67	LEU
1	13-A	71	PHE
1	13-A	86	PRO
1	13-A	92	LEU
1	13-A	95	GLU
1	13-A	98	ASP
1	13-A	111	HIS
1	13-A	116	GLN
1	13-A	120	SER
1	13-A	121	LYS
1	13-A	125	ASN
1	13-A	129	TYR
1	13-A	132	HIS
1	13-B	28	GLU
1	13-B	32	GLU
1	13-B	37	LEU
1	13-B	40	GLU
1	13-B	52	GLN
1	13-B	75	SER
1	13-B	77	THR
1	13-B	86	PRO
1	13-B	87	LYS
1	13-B	89	ARG
1	13-B	95	GLU
1	13-B	103	LEU
1	13-B	118	VAL
1	13-B	122	MSE
1	13-B	128	ARG
1	14-A	28	GLU
1	14-A	31	LEU
1	14-A	46	ASP
1	14-A	52	GLN
1	14-A	60	LEU
1	14-A	63	GLU
1	14-A	79	PRO
1	14-A	85	PRO
1	14-A	89	ARG
1	14-A	93	GLN
1	14-A	98	ASP
1	14-A	122	MSE
1	14-A	129	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-B	24	ARG
1	14-B	32	GLU
1	14-B	33	ASP
1	14-B	37	LEU
1	14-B	40	GLU
1	14-B	44	GLU
1	14-B	48	GLU
1	14-B	49	GLN
1	14-B	63	GLU
1	14-B	71	PHE
1	14-B	72	GLN
1	14-B	77	THR
1	14-B	86	PRO
1	14-B	87	LYS
1	14-B	113	ASP
1	14-B	115	PRO
1	14-B	121	LYS
1	14-B	122	MSE
1	14-B	126	ARG
1	14-B	127	GLN
1	15-A	24	ARG
1	15-A	34	ILE
1	15-A	44	GLU
1	15-A	49	GLN
1	15-A	52	GLN
1	15-A	63	GLU
1	15-A	66	GLU
1	15-A	82	GLN
1	15-A	95	GLU
1	15-A	123	ASP
1	15-A	127	GLN
1	15-A	129	TYR
1	15-B	28	GLU
1	15-B	38	HIS
1	15-B	49	GLN
1	15-B	51	HIS
1	15-B	52	GLN
1	15-B	60	LEU
1	15-B	71	PHE
1	15-B	76	ASP
1	15-B	78	GLU
1	15-B	89	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-B	93	GLN
1	15-B	94	GLU
1	15-B	95	GLU
1	15-B	100	LEU
1	15-B	120	SER
1	15-B	122	MSE
1	15-B	125	ASN
1	15-B	127	GLN
1	15-B	128	ARG
1	16-A	28	GLU
1	16-A	35	ARG
1	16-A	46	ASP
1	16-A	48	GLU
1	16-A	50	PHE
1	16-A	53	PRO
1	16-A	56	LEU
1	16-A	60	LEU
1	16-A	66	GLU
1	16-A	67	LEU
1	16-A	77	THR
1	16-A	79	PRO
1	16-A	84	TRP
1	16-A	102	TYR
1	16-A	106	LEU
1	16-A	120	SER
1	16-A	124	THR
1	16-A	125	ASN
1	16-A	126	ARG
1	16-B	29	PRO
1	16-B	32	GLU
1	16-B	37	LEU
1	16-B	41	PHE
1	16-B	44	GLU
1	16-B	49	GLN
1	16-B	54	ARG
1	16-B	67	LEU
1	16-B	73	TRP
1	16-B	75	SER
1	16-B	77	THR
1	16-B	78	GLU
1	16-B	93	GLN
1	16-B	110	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16-B	116	GLN
1	16-B	122	MSE
1	16-B	124	THR
1	16-B	126	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	93	GLN
1	1-A	127	GLN
1	1-B	93	GLN
1	2-A	38	HIS
1	2-A	52	GLN
1	2-A	55	ASN
1	2-A	82	GLN
1	2-A	93	GLN
1	2-B	52	GLN
1	2-B	72	GLN
1	2-B	125	ASN
1	3-A	38	HIS
1	3-A	93	GLN
1	3-A	111	HIS
1	3-A	127	GLN
1	3-A	132	HIS
1	3-B	49	GLN
1	3-B	52	GLN
1	3-B	111	HIS
1	4-A	93	GLN
1	4-A	127	GLN
1	4-B	38	HIS
1	4-B	72	GLN
1	4-B	82	GLN
1	4-B	93	GLN
1	4-B	111	HIS
1	5-B	55	ASN
1	5-B	93	GLN
1	5-B	111	HIS
1	5-B	116	GLN
1	5-B	125	ASN
1	5-B	127	GLN
1	6-A	49	GLN
1	6-A	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	93	GLN
1	6-A	127	GLN
1	6-B	38	HIS
1	6-B	82	GLN
1	6-B	93	GLN
1	6-B	127	GLN
1	7-A	49	GLN
1	7-A	111	HIS
1	7-A	116	GLN
1	7-A	127	GLN
1	7-B	49	GLN
1	7-B	52	GLN
1	7-B	82	GLN
1	7-B	111	HIS
1	8-A	55	ASN
1	8-A	111	HIS
1	8-B	38	HIS
1	8-B	51	HIS
1	8-B	82	GLN
1	8-B	93	GLN
1	8-B	127	GLN
1	9-A	72	GLN
1	9-A	111	HIS
1	9-B	52	GLN
1	9-B	125	ASN
1	10-A	38	HIS
1	10-A	127	GLN
1	10-B	93	GLN
1	10-B	116	GLN
1	10-B	125	ASN
1	10-B	127	GLN
1	11-A	55	ASN
1	11-A	72	GLN
1	11-A	93	GLN
1	11-A	127	GLN
1	11-B	38	HIS
1	11-B	93	GLN
1	11-B	111	HIS
1	11-B	116	GLN
1	11-B	125	ASN
1	12-A	55	ASN
1	12-A	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-A	111	HIS
1	12-B	51	HIS
1	12-B	52	GLN
1	12-B	82	GLN
1	12-B	93	GLN
1	12-B	116	GLN
1	12-B	125	ASN
1	13-A	38	HIS
1	13-A	52	GLN
1	13-A	55	ASN
1	13-A	72	GLN
1	13-A	93	GLN
1	13-A	111	HIS
1	13-B	51	HIS
1	13-B	52	GLN
1	13-B	55	ASN
1	13-B	111	HIS
1	14-A	55	ASN
1	14-A	93	GLN
1	14-A	116	GLN
1	14-A	127	GLN
1	14-B	38	HIS
1	14-B	51	HIS
1	14-B	52	GLN
1	14-B	93	GLN
1	15-A	49	GLN
1	15-A	52	GLN
1	15-A	72	GLN
1	15-A	127	GLN
1	15-B	38	HIS
1	15-B	52	GLN
1	15-B	111	HIS
1	15-B	127	GLN
1	16-A	51	HIS
1	16-A	52	GLN
1	16-A	111	HIS
1	16-B	72	GLN
1	16-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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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