Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:24 am BST

PDB ID	:	5LOX
Title	:	Helical Assembly of the Anbu Complex from Pseudomonas aeruginosa
Authors	:	Fuchs, A.C.D.; Albrecht, R.; Martin, J.; Hartmann, M.D.
Deposited on	:	2016-08-10
Resolution	:	2.90 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:

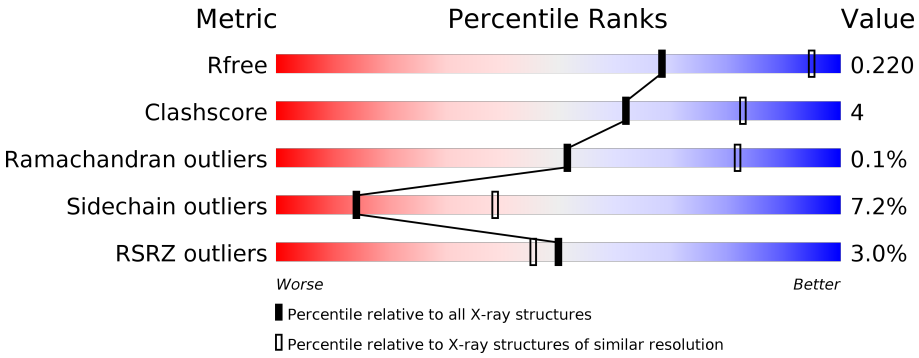
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	242	5% 87% 11% •
1	2	242	5% 86% 13% •
1	3	242	4% 86% 12% •
1	4	242	3% 87% 11% •
1	5	242	5% 88% 10% •
1	6	242	5% 88% 10% •

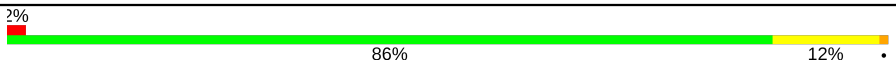
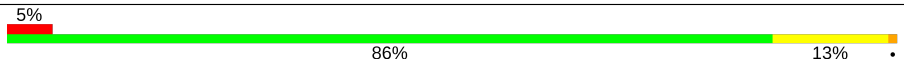
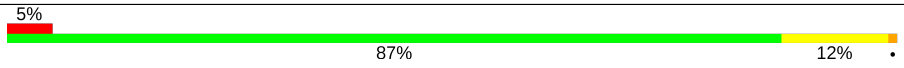
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	7	242	4% 86% 12%
1	8	242	2% 89% 10%
1	A	242	3% 86% 12%
1	B	242	2% 88% 10%
1	C	242	3% 88% 10%
1	D	242	3% 87% 12%
1	E	242	3% 86% 13%
1	F	242	3% 85% 12%
1	G	242	2% 86% 13%
1	H	242	2% 86% 13%
1	I	242	88% 11%
1	J	242	3% 88% 10%
1	K	242	2% 87% 11%
1	L	242	2% 87% 12%
1	M	242	4% 87% 12%
1	N	242	87% 12%
1	O	242	3% 86% 12%
1	P	242	2% 85% 13%
1	Q	242	3% 85% 14%
1	R	242	2% 86% 13%
1	S	242	2% 83% 15%
1	T	242	3% 87% 12%
1	U	242	2% 87% 10%
1	V	242	2% 87% 11%
1	W	242	3% 87% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	X	242	
1	Y	242	
1	Z	242	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 62186 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 Peptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	B	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	C	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	D	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	E	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	F	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	G	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	H	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	I	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	J	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	K	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	L	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	M	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	N	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	O	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	P	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	R	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	S	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	T	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	U	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	V	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	W	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	X	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	Y	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	Z	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	1	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	2	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	3	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	4	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	5	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	6	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	7	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			
1	8	241	Total	C	N	O	S	Se	0	0	0
			1829	1155	315	351	3	5			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
A	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
A	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
B	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
B	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
C	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
C	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
C	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
D	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
D	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
D	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
E	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
E	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
E	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
F	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
F	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
F	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
G	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
G	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
G	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
H	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
H	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
H	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
I	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
I	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
I	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
J	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
J	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
J	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
K	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
K	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
K	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
L	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
L	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
L	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
M	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
M	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
M	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
N	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
N	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
N	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
O	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
O	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
O	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
P	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
P	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Q	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Q	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Q	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
R	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
R	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
R	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
S	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
S	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
S	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
T	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
T	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
T	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
U	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
U	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
U	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
V	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
V	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
V	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
W	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
W	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
W	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
X	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
X	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
X	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Y	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Y	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Y	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Z	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Z	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Z	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
1	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
1	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
1	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
2	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
2	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
2	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
3	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
3	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
3	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

Continued on next page...

Continued from previous page...

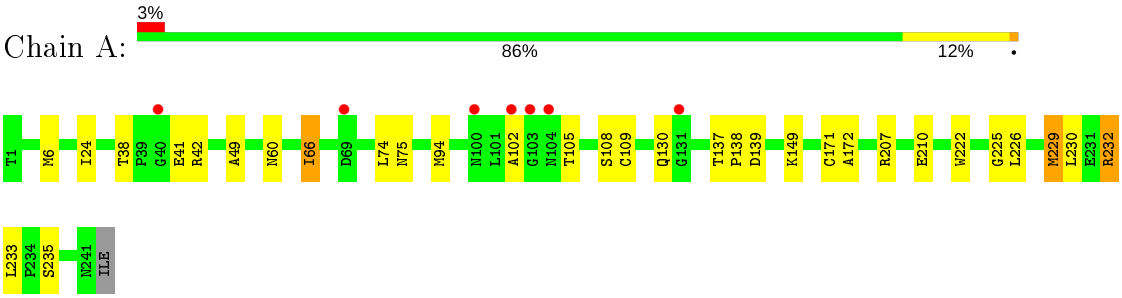
Chain	Residue	Modelled	Actual	Comment	Reference
4	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
4	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
4	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
6	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
6	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
6	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
7	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
7	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
7	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
8	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
8	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
8	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

3 Residue-property plots

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 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.

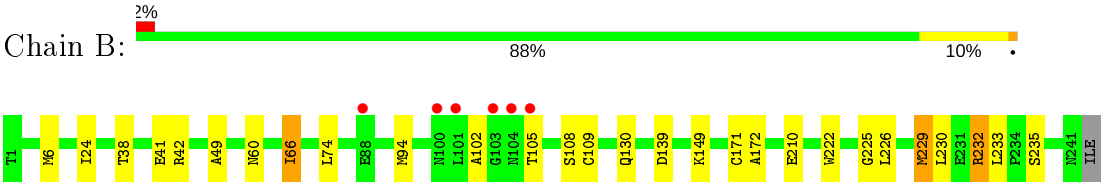
- Molecule 1: Peptidase

Chain A:



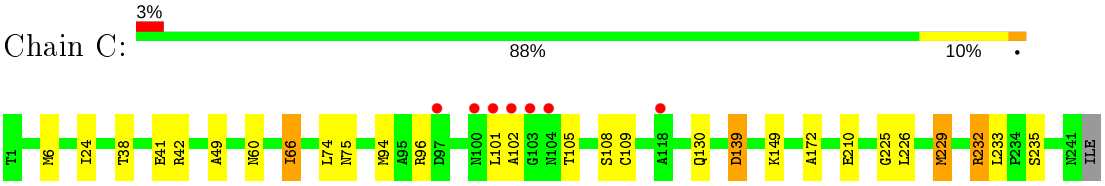
- Molecule 1: Peptidase

Chain B:



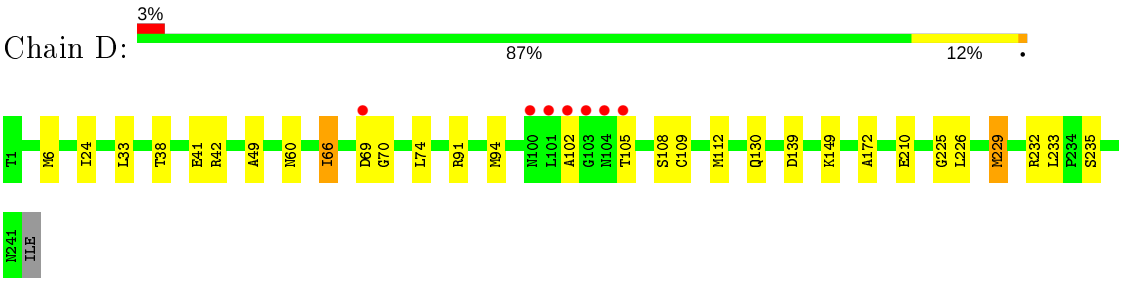
- Molecule 1: Peptidase

Chain C:



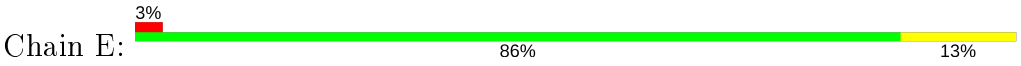
- Molecule 1: Peptidase

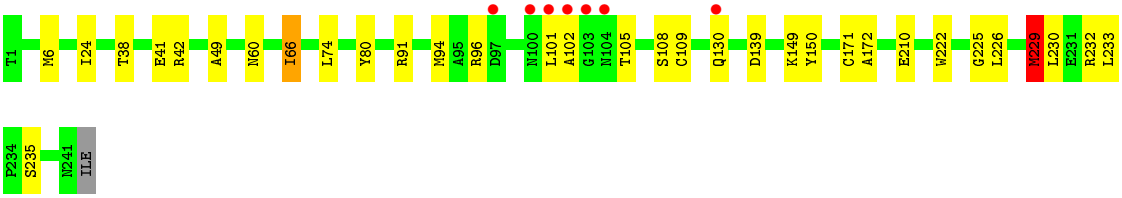
Chain D:



- Molecule 1: Peptidase

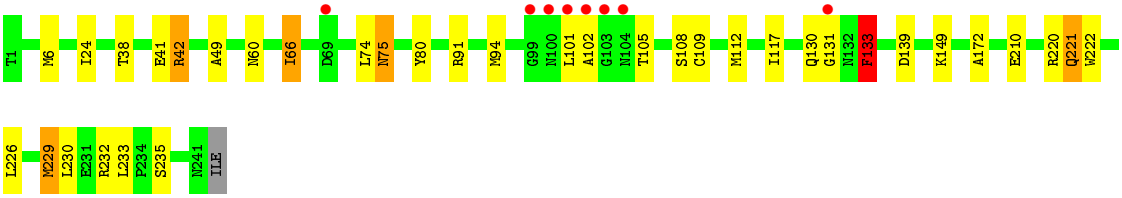
Chain E:





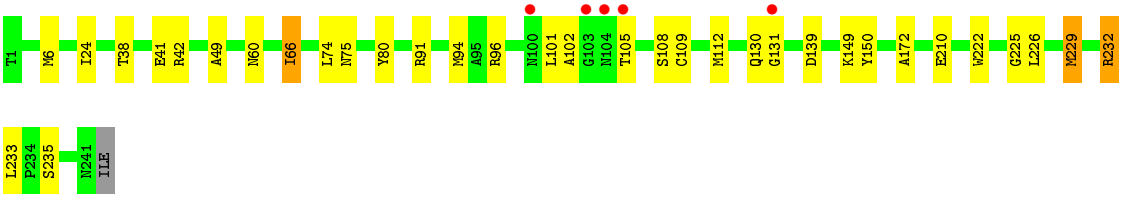
- Molecule 1: Peptidase

Chain F:



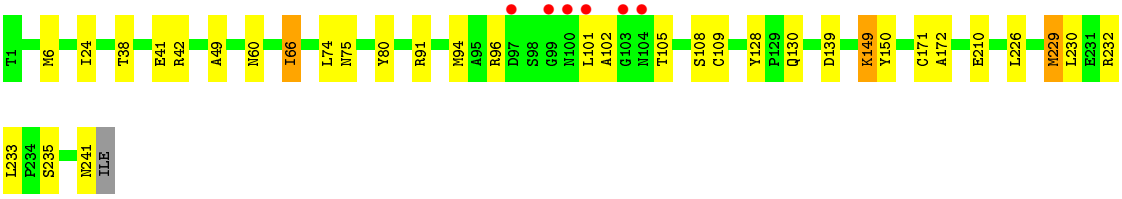
- Molecule 1: Peptidase

Chain G:



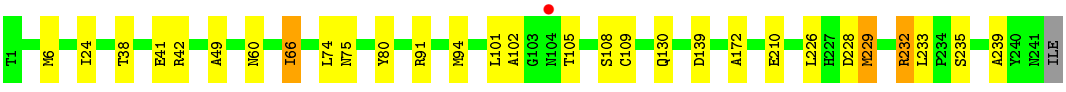
- Molecule 1: Peptidase

Chain H:



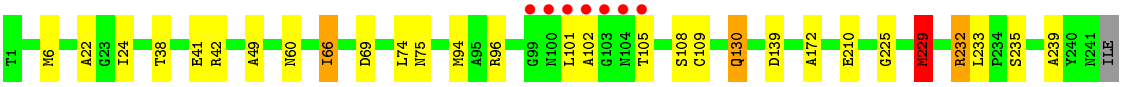
- Molecule 1: Peptidase

Chain I:



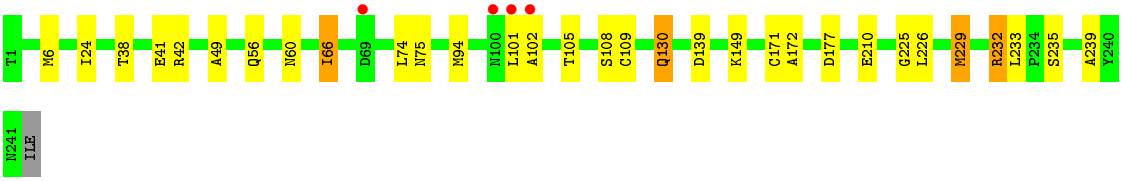
- Molecule 1: Peptidase

Chain J:



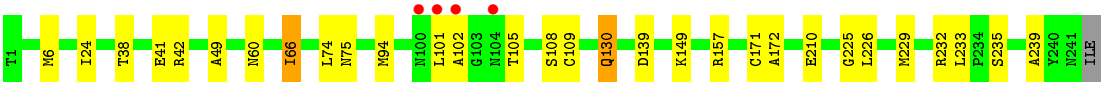
• Molecule 1: Peptidase

Chain K:



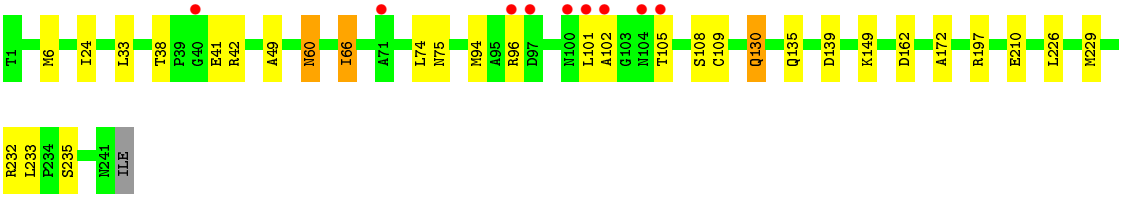
• Molecule 1: Peptidase

Chain L:



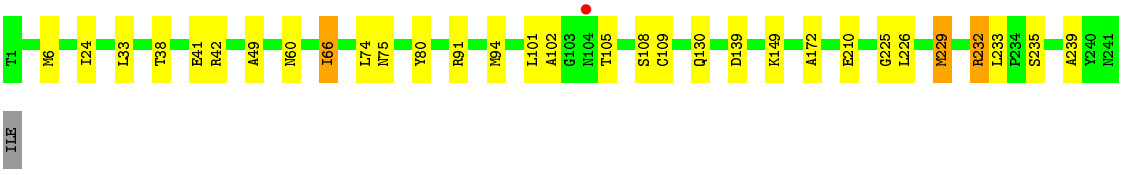
• Molecule 1: Peptidase

Chain M:



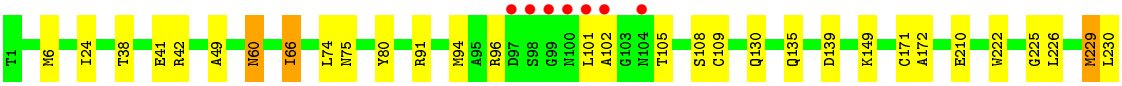
• Molecule 1: Peptidase

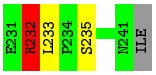
Chain N:



• Molecule 1: Peptidase

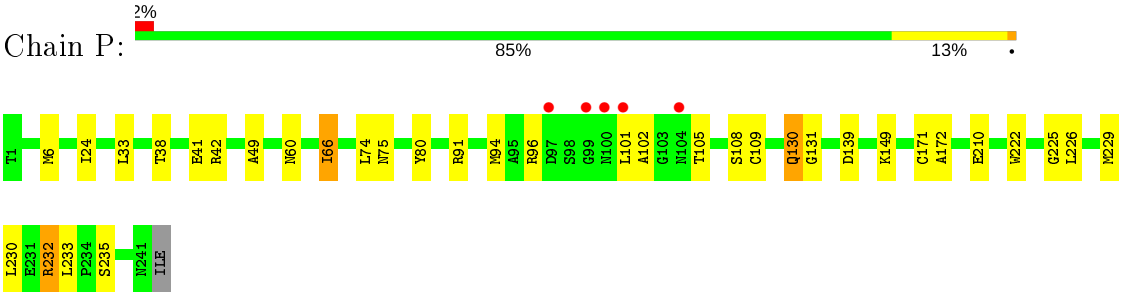
Chain O:





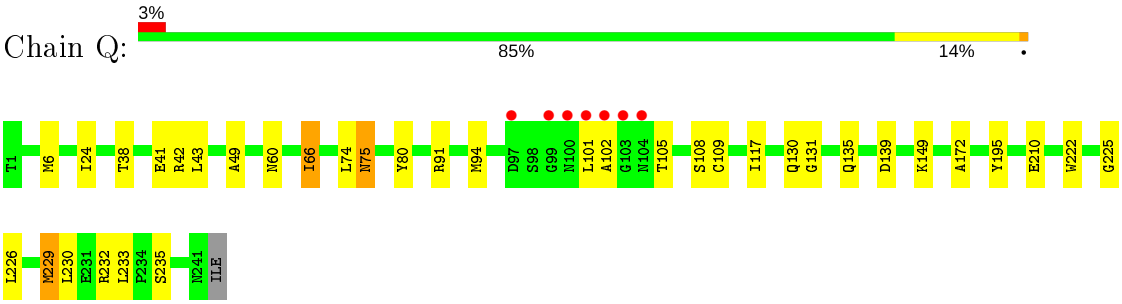
- Molecule 1: Peptidase

Chain P:



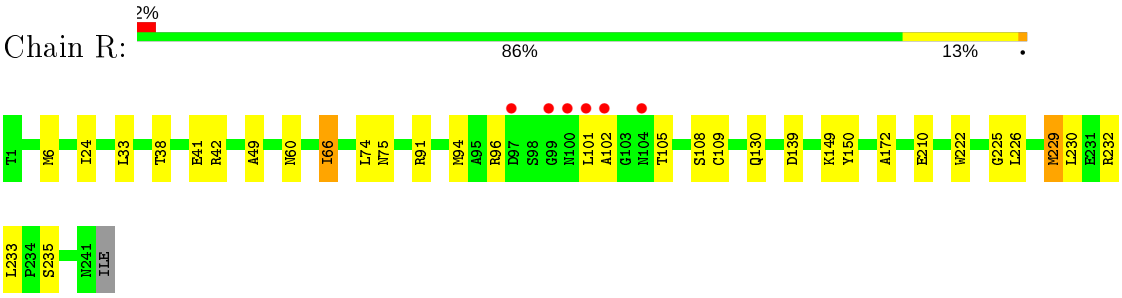
- Molecule 1: Peptidase

Chain Q:



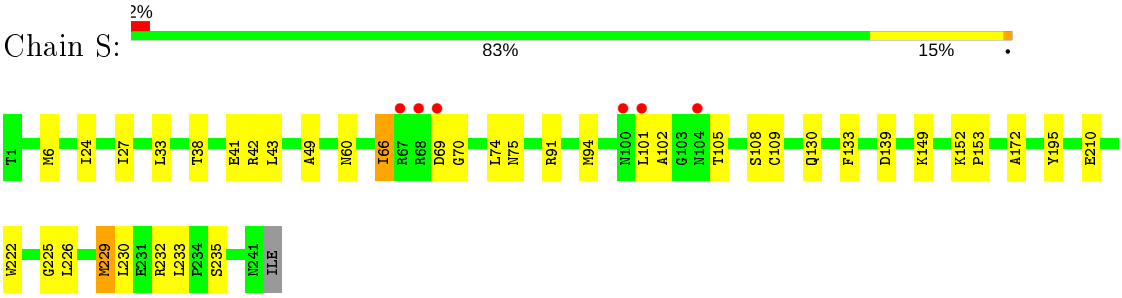
- Molecule 1: Peptidase

Chain R:



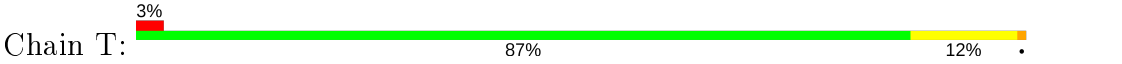
- Molecule 1: Peptidase

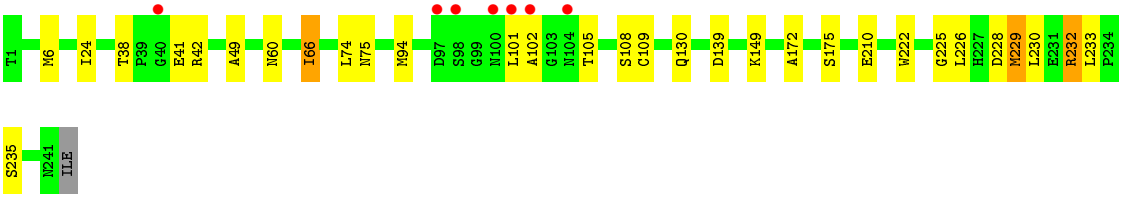
Chain S:



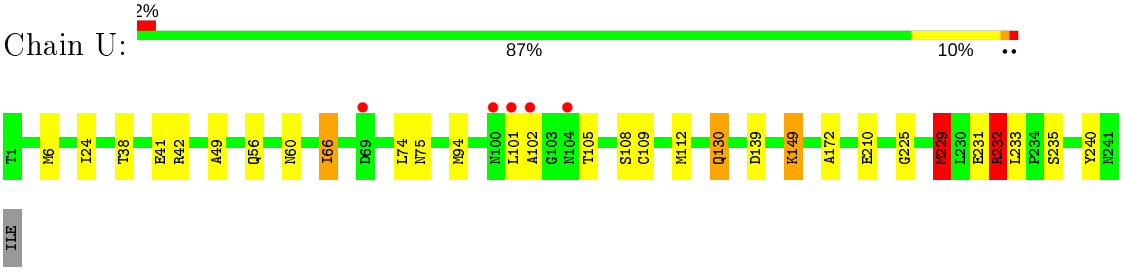
- Molecule 1: Peptidase

Chain T:

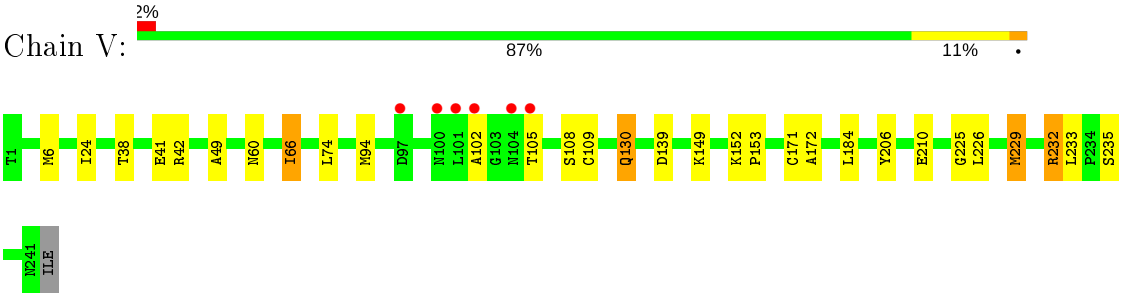




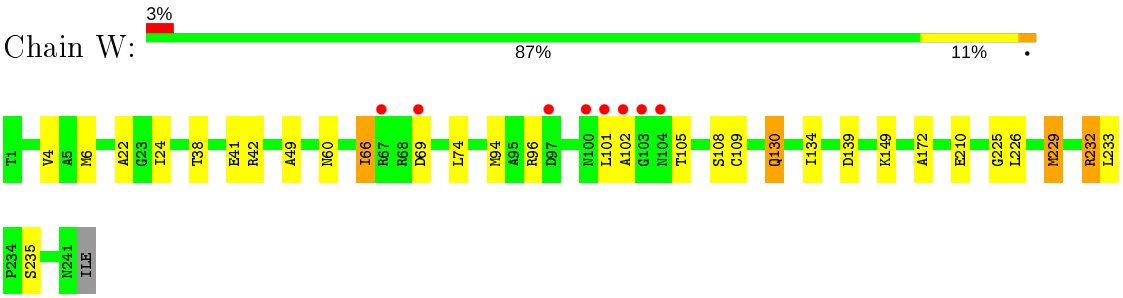
• Molecule 1: Peptidase



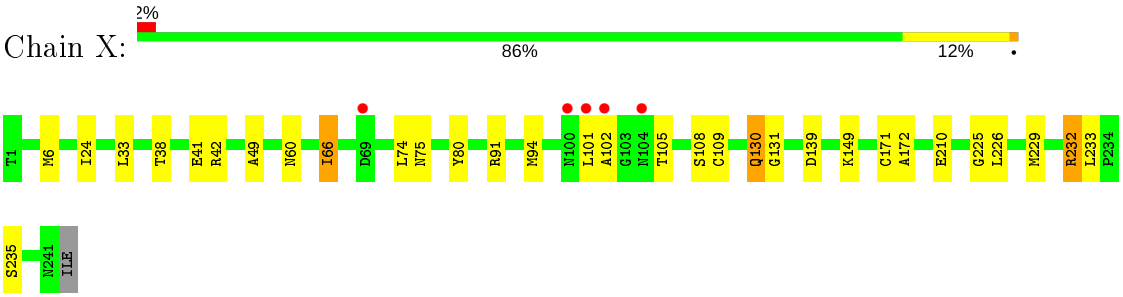
• Molecule 1: Peptidase



• Molecule 1: Peptidase

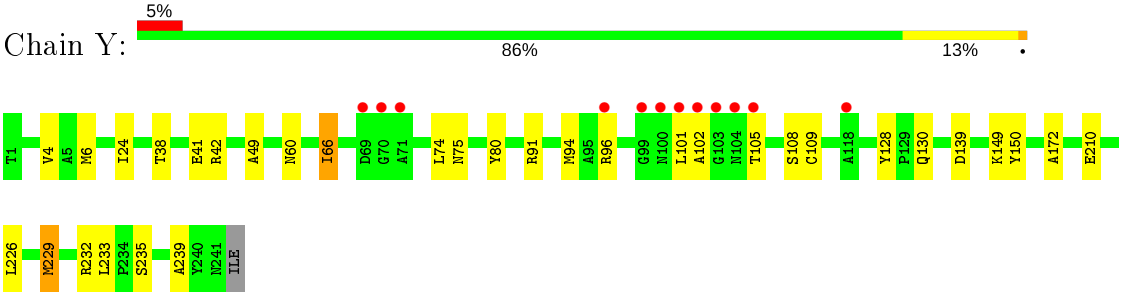


• Molecule 1: Peptidase



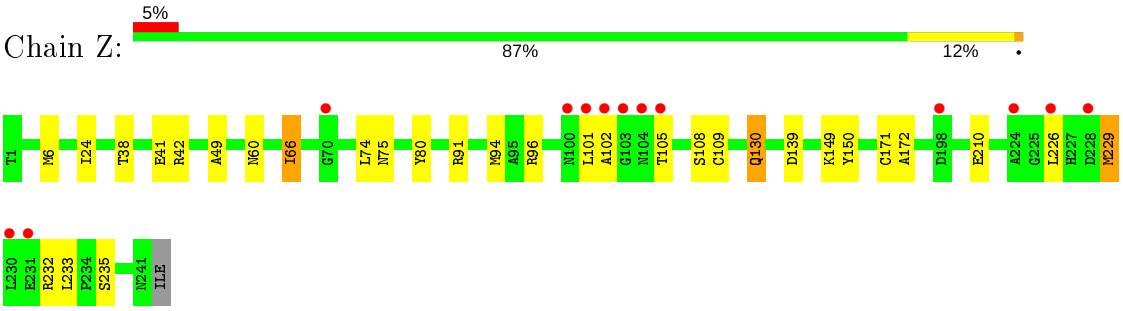
• Molecule 1: Peptidase

Chain Y:



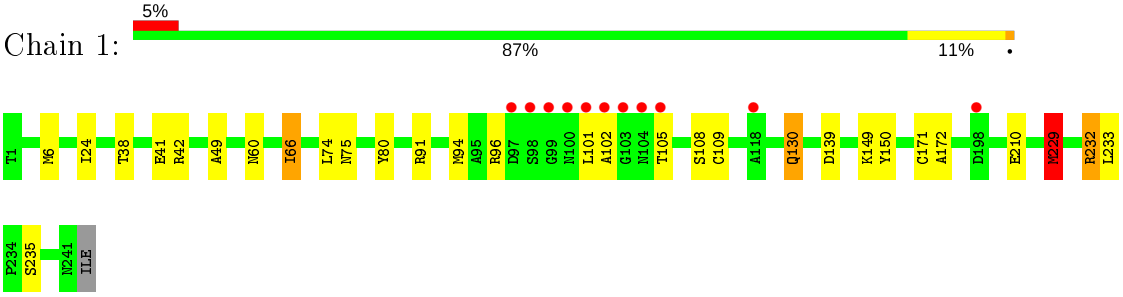
• Molecule 1: Peptidase

Chain Z:



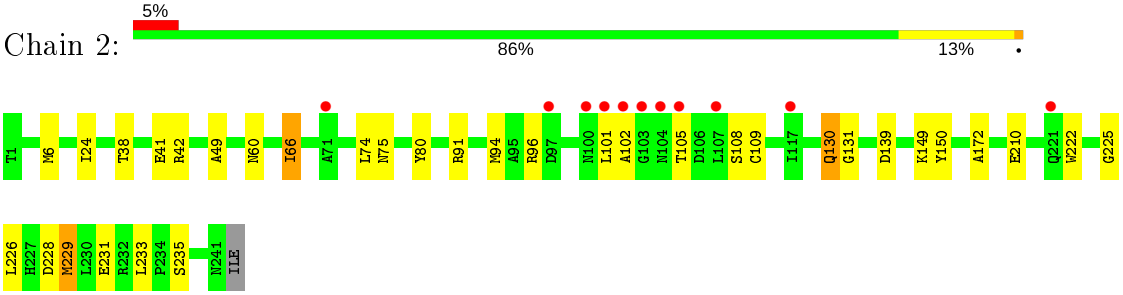
• Molecule 1: Peptidase

Chain 1:



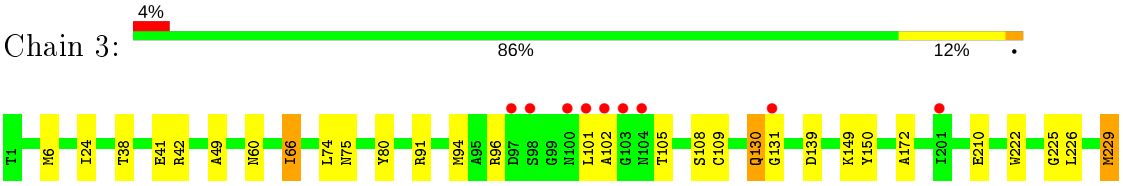
• Molecule 1: Peptidase

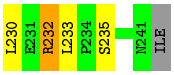
Chain 2:



• Molecule 1: Peptidase

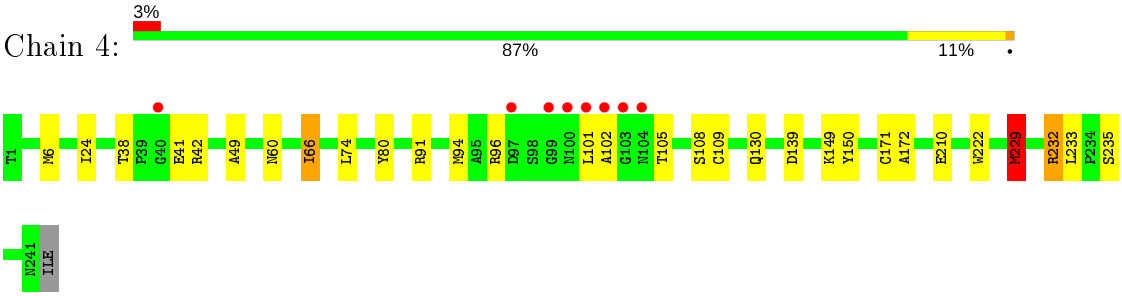
Chain 3:





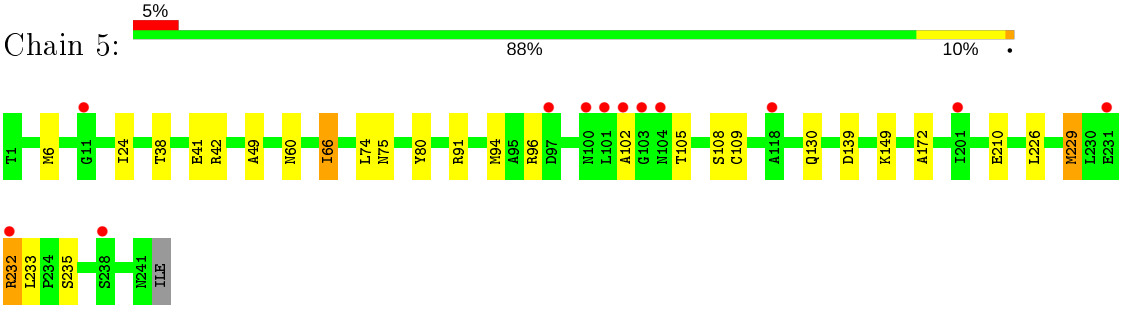
- Molecule 1: Peptidase

Chain 4:



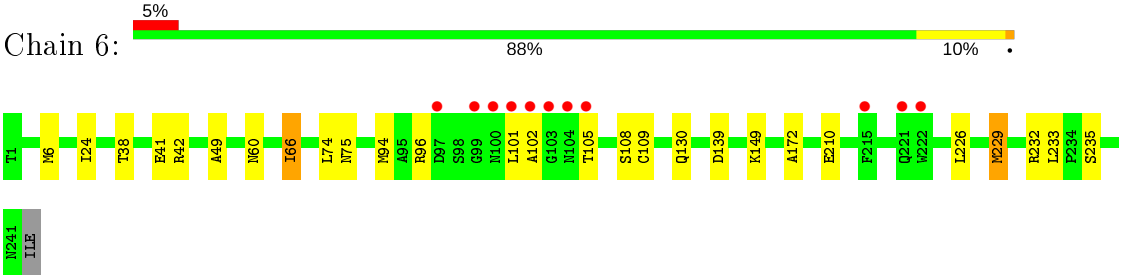
- Molecule 1: Peptidase

Chain 5:



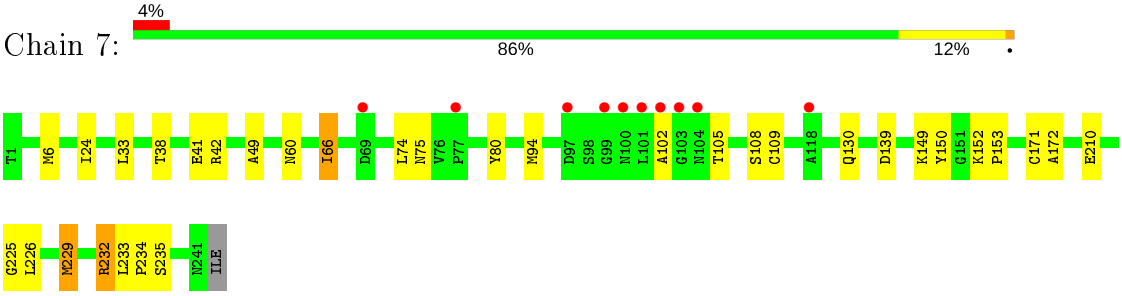
- Molecule 1: Peptidase

Chain 6:



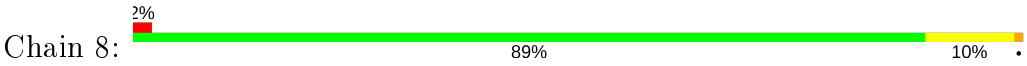
- Molecule 1: Peptidase

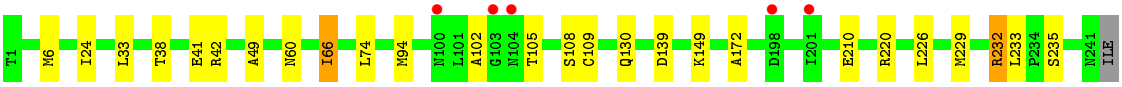
Chain 7:



- Molecule 1: Peptidase

Chain 8:




T1
M6
L24
L33
T38
E41
R42
A49
N60
I66
L74
M94
N100
L101
A102
G103
N104
T105
S108
C109
Q130
D139
K149
A172
D198
I201
E210
R220
L226
M229
R232
L233
P234
S235
N241
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	150.07Å 230.08Å 171.72Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	39.60 – 2.90 39.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.60-2.90) 99.7 (39.57-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.198 , 0.218 0.203 , 0.220	Depositor DCC
R_{free} test set	12254 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	62186	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.57	0/1862	0.80	3/2530 (0.1%)
1	2	0.56	0/1862	0.74	0/2530
1	3	0.58	0/1862	0.78	2/2530 (0.1%)
1	4	0.57	0/1862	0.77	1/2530 (0.0%)
1	5	0.53	0/1862	0.75	1/2530 (0.0%)
1	6	0.54	0/1862	0.72	0/2530
1	7	0.61	0/1862	0.78	2/2530 (0.1%)
1	8	0.59	0/1862	0.76	1/2530 (0.0%)
1	A	0.61	0/1862	0.77	1/2530 (0.0%)
1	B	0.59	0/1862	0.78	1/2530 (0.0%)
1	C	0.58	0/1862	0.76	2/2530 (0.1%)
1	D	0.60	0/1862	0.74	1/2530 (0.0%)
1	E	0.60	0/1862	0.83	3/2530 (0.1%)
1	F	0.68	1/1862 (0.1%)	0.80	4/2530 (0.2%)
1	G	0.62	0/1862	0.79	2/2530 (0.1%)
1	H	0.59	0/1862	0.74	0/2530
1	I	0.59	0/1862	0.77	2/2530 (0.1%)
1	J	0.62	0/1862	0.79	4/2530 (0.2%)
1	K	0.63	0/1862	0.78	2/2530 (0.1%)
1	L	0.62	0/1862	0.75	0/2530
1	M	0.66	0/1862	0.75	0/2530
1	N	0.63	0/1862	0.78	3/2530 (0.1%)
1	O	0.62	0/1862	0.81	2/2530 (0.1%)
1	P	0.59	0/1862	0.77	2/2530 (0.1%)
1	Q	0.64	0/1862	0.75	0/2530
1	R	0.59	0/1862	0.73	0/2530
1	S	0.63	0/1862	0.79	2/2530 (0.1%)
1	T	0.60	0/1862	0.78	3/2530 (0.1%)
1	U	0.60	0/1862	0.83	6/2530 (0.2%)
1	V	0.61	0/1862	0.79	1/2530 (0.0%)
1	W	0.63	0/1862	0.79	2/2530 (0.1%)
1	X	0.62	0/1862	0.79	2/2530 (0.1%)
1	Y	0.56	0/1862	0.72	1/2530 (0.0%)
1	Z	0.56	0/1862	0.73	0/2530

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.60	1/63308 (0.0%)	0.77	56/86020 (0.1%)

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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	221	GLN	CD-OE1	-6.75	1.09	1.24

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	229	MSE	CA-CB-CG	-12.61	91.86	113.30
1	O	232	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	7	232	ARG	NE-CZ-NH2	-12.03	114.29	120.30
1	E	229	MSE	N-CA-CB	-11.69	89.57	110.60
1	3	232	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	G	232	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	X	232	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	4	229	MSE	CG-SE-CE	10.12	121.16	98.90
1	K	232	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	U	232	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	S	133	PHE	CB-CG-CD2	-9.81	113.93	120.80
1	V	232	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	I	232	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	P	232	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	1	229	MSE	CG-SE-CE	9.58	119.97	98.90
1	5	232	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	A	232	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	C	232	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	U	229	MSE	CG-SE-CE	-9.32	78.40	98.90
1	F	133	PHE	CB-CA-C	-9.27	91.86	110.40
1	8	232	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	O	232	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	B	232	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	T	232	ARG	NE-CZ-NH1	8.90	124.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	232	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	T	232	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	U	229	MSE	CA-CB-CG	-8.23	99.31	113.30
1	1	232	ARG	CB-CA-C	-7.94	94.52	110.40
1	S	133	PHE	CB-CG-CD1	7.78	126.24	120.80
1	U	229	MSE	N-CA-CB	-7.68	96.77	110.60
1	X	232	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	N	232	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	J	229	MSE	CG-SE-CE	7.36	115.09	98.90
1	N	232	ARG	CA-CB-CG	7.04	128.89	113.40
1	I	232	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	K	232	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	T	232	ARG	CD-NE-CZ	6.77	133.08	123.60
1	J	232	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	3	232	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	J	232	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	F	221	GLN	CG-CD-OE1	-6.26	109.08	121.60
1	1	232	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	J	229	MSE	CB-CG-SE	-5.50	96.21	112.70
1	F	112	MSE	CA-CB-CG	-5.40	104.12	113.30
1	U	232	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	229	MSE	CG-SE-CE	5.37	110.71	98.90
1	W	4	VAL	CB-CA-C	-5.28	101.36	111.40
1	7	232	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	F	221	GLN	CG-CD-NE2	5.18	129.12	116.70
1	P	232	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	G	112	MSE	CA-CB-CG	-5.11	104.61	113.30
1	U	112	MSE	CA-CB-CG	-5.11	104.62	113.30
1	N	232	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	Y	4	VAL	CB-CA-C	-5.09	101.73	111.40
1	D	112	MSE	CA-CB-CG	-5.03	104.75	113.30
1	C	232	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	133	PHE	Mainchain

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	1829	0	1800	30	0
1	2	1829	0	1800	31	2
1	3	1829	0	1800	27	0
1	4	1829	0	1800	26	1
1	5	1829	0	1800	15	0
1	6	1829	0	1800	14	0
1	7	1829	0	1800	18	1
1	8	1829	0	1800	16	1
1	A	1829	0	1800	20	0
1	B	1829	0	1800	17	0
1	C	1829	0	1800	18	0
1	D	1829	0	1800	19	0
1	E	1829	0	1800	36	0
1	F	1829	0	1800	45	1
1	G	1829	0	1800	33	0
1	H	1829	0	1800	41	0
1	I	1829	0	1800	18	1
1	J	1829	0	1800	21	0
1	K	1829	0	1800	23	0
1	L	1829	0	1800	23	0
1	M	1829	0	1800	21	2
1	N	1829	0	1800	19	0
1	O	1829	0	1800	32	1
1	P	1829	0	1800	32	0
1	Q	1829	0	1800	36	0
1	R	1829	0	1800	33	0
1	S	1829	0	1800	29	0
1	T	1829	0	1800	18	0
1	U	1829	0	1800	17	2
1	V	1829	0	1800	17	0
1	W	1829	0	1800	28	0
1	X	1829	0	1800	27	0
1	Y	1829	0	1800	31	0
1	Z	1829	0	1800	32	0
All	All	62186	0	61200	547	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (547) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:ILE:HG21	1:S:69:ASP:CB	1.26	1.64
1:F:117:ILE:CG2	1:S:69:ASP:CB	1.97	1.40
1:J:69:ASP:CB	1:W:69:ASP:O	1.73	1.34
1:A:229:MSE:HE1	1:B:229:MSE:HE1	1.19	1.18
1:D:69:ASP:CB	1:Q:117:ILE:HG21	1.74	1.16
1:F:80:TYR:OH	1:H:96:ARG:NH1	1.79	1.15
1:F:91:ARG:HH21	1:H:101:LEU:CD2	1.61	1.14
1:S:229:MSE:HE1	1:T:229:MSE:HE1	1.28	1.14
1:Q:229:MSE:HE1	1:R:229:MSE:HE1	1.19	1.12
1:7:229:MSE:HE1	1:8:229:MSE:HE1	1.31	1.10
1:W:229:MSE:HE1	1:X:229:MSE:HE1	1.29	1.10
1:O:229:MSE:HE1	1:P:229:MSE:HE1	1.26	1.09
1:O:101:LEU:HD22	1:Q:91:ARG:CG	1.83	1.06
1:C:229:MSE:HE1	1:D:229:MSE:HE1	1.35	1.06
1:G:229:MSE:HE1	1:H:229:MSE:HE1	1.34	1.06
1:W:101:LEU:HD22	1:Y:91:ARG:CG	1.85	1.05
1:Y:229:MSE:HE1	1:Z:229:MSE:HE1	1.41	1.03
1:2:91:ARG:CG	1:4:101:LEU:HD22	1.88	1.03
1:F:91:ARG:HH21	1:H:101:LEU:HD23	1.23	1.02
1:J:94:MSE:HE3	1:L:101:LEU:HD11	1.40	1.02
1:M:229:MSE:HE1	1:N:229:MSE:HE1	1.40	1.02
1:D:69:ASP:CB	1:Q:117:ILE:CG2	2.38	1.01
1:Q:229:MSE:CE	1:R:229:MSE:HE1	1.91	0.99
1:K:229:MSE:HE1	1:L:229:MSE:HE1	1.41	0.99
1:Q:229:MSE:HE1	1:R:229:MSE:CE	1.91	0.99
1:1:101:LEU:HD22	1:3:91:ARG:CG	1.93	0.98
1:W:101:LEU:HD22	1:Y:91:ARG:HG2	1.44	0.98
1:U:229:MSE:HE1	1:V:225:GLY:HA3	1.45	0.97
1:I:101:LEU:HD11	1:K:94:MSE:HE3	1.45	0.97
1:A:229:MSE:HE1	1:B:229:MSE:CE	1.93	0.97
1:U:229:MSE:CE	1:V:225:GLY:HA3	1.93	0.97
1:A:229:MSE:CE	1:B:229:MSE:HE1	1.94	0.96
1:F:91:ARG:CG	1:H:101:LEU:HD22	1.96	0.95
1:K:101:LEU:HD11	1:M:94:MSE:HE3	1.50	0.94
1:L:94:MSE:HE3	1:N:101:LEU:HD11	1.49	0.94
1:J:94:MSE:HE3	1:L:101:LEU:CD1	1.98	0.94
1:O:229:MSE:CE	1:P:229:MSE:HE1	1.99	0.92
1:E:96:ARG:NH1	1:G:80:TYR:OH	2.04	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ARG:CD	1:H:101:LEU:HD22	2.02	0.90
1:O:229:MSE:HE1	1:P:229:MSE:CE	2.02	0.90
1:S:229:MSE:HE1	1:T:229:MSE:CE	2.02	0.89
1:P:91:ARG:CG	1:R:101:LEU:HD22	2.02	0.88
1:X:91:ARG:CG	1:Z:101:LEU:HD22	2.04	0.88
1:K:101:LEU:CD1	1:M:94:MSE:HE3	2.03	0.87
1:G:229:MSE:HE1	1:H:229:MSE:CE	2.04	0.87
1:W:229:MSE:CE	1:X:229:MSE:HE1	2.05	0.87
1:7:229:MSE:HE1	1:8:229:MSE:CE	2.04	0.86
1:K:102:ALA:HA	1:M:130:GLN:HB3	1.56	0.86
1:Y:96:ARG:NH2	1:1:80:TYR:OH	2.08	0.86
1:2:91:ARG:HG3	1:4:101:LEU:HD22	1.58	0.86
1:W:229:MSE:HE1	1:X:229:MSE:CE	2.04	0.86
1:S:229:MSE:CE	1:T:229:MSE:HE1	2.06	0.86
1:5:229:MSE:HE1	1:6:229:MSE:HE1	1.55	0.85
1:7:229:MSE:CE	1:8:229:MSE:HE1	2.05	0.85
1:G:229:MSE:CE	1:H:229:MSE:HE1	2.05	0.85
1:E:229:MSE:CE	1:F:229:MSE:HE1	2.05	0.85
1:2:91:ARG:HG2	1:4:101:LEU:HD22	1.58	0.85
1:E:101:LEU:HD22	1:G:91:ARG:CG	2.07	0.84
1:W:101:LEU:HD22	1:Y:91:ARG:HG3	1.57	0.84
1:L:94:MSE:HE3	1:N:101:LEU:CD1	2.08	0.84
1:Q:229:MSE:CE	1:R:229:MSE:CE	2.53	0.83
1:O:101:LEU:HD22	1:Q:91:ARG:HG2	1.59	0.82
1:C:229:MSE:HE1	1:D:229:MSE:CE	2.08	0.82
1:E:101:LEU:CD2	1:G:91:ARG:HH21	1.93	0.82
1:F:91:ARG:HD3	1:H:101:LEU:HD22	1.61	0.82
1:C:229:MSE:CE	1:D:229:MSE:HE1	2.11	0.80
1:M:229:MSE:HE1	1:N:229:MSE:CE	2.12	0.80
1:P:80:TYR:OH	1:R:96:ARG:NH1	2.14	0.80
1:1:101:LEU:HD22	1:3:91:ARG:HG2	1.63	0.79
1:I:101:LEU:CD1	1:K:94:MSE:HE3	2.13	0.79
1:J:130:GLN:HB3	1:L:102:ALA:HA	1.64	0.79
1:A:229:MSE:CE	1:B:229:MSE:CE	2.56	0.79
1:F:91:ARG:NH2	1:H:101:LEU:HD23	1.97	0.79
1:U:101:LEU:HD11	1:W:94:MSE:HE3	1.65	0.79
1:Z:91:ARG:CG	1:2:101:LEU:HD22	2.12	0.78
1:1:101:LEU:HD22	1:3:91:ARG:HG3	1.65	0.77
1:F:91:ARG:HH21	1:H:101:LEU:HD22	1.45	0.77
1:M:96:ARG:NH2	1:O:80:TYR:OH	2.16	0.77
1:M:229:MSE:CE	1:N:229:MSE:HE1	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:MSE:SE	1:F:229:MSE:CE	2.84	0.76
1:Z:80:TYR:OH	1:2:96:ARG:NH2	2.19	0.76
1:Z:91:ARG:HG2	1:2:101:LEU:HD22	1.68	0.76
1:E:229:MSE:SE	1:F:229:MSE:HE1	2.37	0.75
1:Y:101:LEU:HD22	1:1:91:ARG:CG	2.16	0.75
1:X:80:TYR:OH	1:Z:96:ARG:NH1	2.19	0.75
1:Y:229:MSE:CE	1:Z:229:MSE:HE1	2.14	0.75
1:O:101:LEU:HD22	1:Q:91:ARG:HG3	1.68	0.74
1:Y:229:MSE:HE1	1:Z:229:MSE:CE	2.15	0.74
1:K:229:MSE:CE	1:L:229:MSE:HE1	2.16	0.74
1:T:228:ASP:O	1:T:232:ARG:HG3	1.88	0.74
1:K:229:MSE:HE1	1:L:229:MSE:CE	2.15	0.73
1:E:101:LEU:HD23	1:G:91:ARG:HH21	1.53	0.73
1:X:91:ARG:HG2	1:Z:101:LEU:HD22	1.71	0.73
1:Y:101:LEU:HD22	1:1:91:ARG:HG2	1.69	0.72
1:C:101:LEU:HD22	1:E:91:ARG:HG2	1.71	0.72
1:O:229:MSE:CE	1:P:229:MSE:CE	2.63	0.72
1:G:229:MSE:CE	1:H:229:MSE:CE	2.65	0.72
1:O:96:ARG:NH1	1:Q:80:TYR:OH	2.24	0.71
1:4:91:ARG:HG2	1:6:101:LEU:HD22	1.71	0.70
1:L:130:GLN:HB3	1:N:102:ALA:HA	1.73	0.70
1:2:80:TYR:OH	1:4:96:ARG:NH1	2.24	0.69
1:W:229:MSE:CE	1:X:229:MSE:CE	2.66	0.69
1:F:117:ILE:HG22	1:S:69:ASP:CB	2.19	0.69
1:F:91:ARG:HG3	1:H:101:LEU:HD22	1.74	0.69
1:S:229:MSE:CE	1:T:229:MSE:CE	2.67	0.69
1:2:80:TYR:OH	1:4:96:ARG:NH2	2.25	0.69
1:C:229:MSE:CE	1:D:229:MSE:CE	2.71	0.69
1:F:91:ARG:NH2	1:H:101:LEU:CD2	2.46	0.69
1:P:91:ARG:HG2	1:R:101:LEU:HD22	1.75	0.68
1:E:101:LEU:HD22	1:G:91:ARG:CD	2.23	0.68
1:1:102:ALA:O	1:1:105:THR:HG22	1.94	0.68
1:2:102:ALA:O	1:2:105:THR:HG22	1.94	0.68
1:4:102:ALA:O	1:4:105:THR:HG22	1.94	0.68
1:L:102:ALA:O	1:L:105:THR:HG22	1.94	0.68
1:D:102:ALA:O	1:D:105:THR:HG22	1.94	0.68
1:K:102:ALA:O	1:K:105:THR:HG22	1.94	0.68
1:P:102:ALA:O	1:P:105:THR:HG22	1.94	0.68
1:3:102:ALA:O	1:3:105:THR:HG22	1.94	0.68
1:6:102:ALA:O	1:6:105:THR:HG22	1.94	0.68
1:U:102:ALA:O	1:U:105:THR:HG22	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:102:ALA:O	1:5:105:THR:HG22	1.94	0.68
1:A:102:ALA:O	1:A:105:THR:HG22	1.94	0.68
1:X:102:ALA:O	1:X:105:THR:HG22	1.94	0.68
1:C:102:ALA:O	1:C:105:THR:HG22	1.94	0.68
1:F:102:ALA:O	1:F:105:THR:HG22	1.93	0.68
1:M:102:ALA:O	1:M:105:THR:HG22	1.94	0.68
1:J:102:ALA:O	1:J:105:THR:HG22	1.94	0.68
1:1:96:ARG:NH1	1:3:80:TYR:OH	2.26	0.68
1:7:229:MSE:CE	1:8:229:MSE:CE	2.68	0.68
1:S:102:ALA:O	1:S:105:THR:HG22	1.94	0.68
1:Z:102:ALA:O	1:Z:105:THR:HG22	1.94	0.67
1:E:102:ALA:O	1:E:105:THR:HG22	1.94	0.67
1:G:102:ALA:O	1:G:105:THR:HG22	1.94	0.67
1:O:101:LEU:HD23	1:Q:91:ARG:HH21	1.58	0.67
1:W:102:ALA:O	1:W:105:THR:HG22	1.94	0.67
1:B:102:ALA:O	1:B:105:THR:HG22	1.94	0.67
1:H:102:ALA:O	1:H:105:THR:HG22	1.94	0.67
1:I:102:ALA:O	1:I:105:THR:HG22	1.94	0.67
1:N:102:ALA:O	1:N:105:THR:HG22	1.94	0.67
1:U:101:LEU:CD1	1:W:94:MSE:HE3	2.25	0.67
1:E:96:ARG:NH1	1:G:80:TYR:HH	1.92	0.67
1:H:80:TYR:OH	1:J:96:ARG:NH2	2.26	0.67
1:8:102:ALA:O	1:8:105:THR:HG22	1.94	0.67
1:F:91:ARG:HG2	1:H:101:LEU:HD13	1.77	0.67
1:I:229:MSE:HE1	1:J:229:MSE:HE1	1.77	0.67
1:O:102:ALA:O	1:O:105:THR:HG22	1.94	0.67
1:7:102:ALA:O	1:7:105:THR:HG22	1.94	0.66
1:Q:102:ALA:O	1:Q:105:THR:HG22	1.93	0.66
1:R:102:ALA:O	1:R:105:THR:HG22	1.94	0.66
1:V:102:ALA:O	1:V:105:THR:HG22	1.94	0.66
1:U:102:ALA:HA	1:W:130:GLN:HB3	1.77	0.66
1:Y:102:ALA:O	1:Y:105:THR:HG22	1.94	0.66
1:T:102:ALA:O	1:T:105:THR:HG22	1.94	0.65
1:F:91:ARG:HD3	1:H:101:LEU:CD2	2.27	0.65
1:O:101:LEU:HD22	1:Q:91:ARG:CD	2.25	0.65
1:E:101:LEU:HD22	1:G:91:ARG:HD3	1.77	0.65
1:I:102:ALA:HA	1:K:130:GLN:HB3	1.78	0.65
1:H:91:ARG:HG2	1:J:101:LEU:HD22	1.79	0.64
1:5:229:MSE:CE	1:6:229:MSE:HE1	2.25	0.64
1:E:229:MSE:SE	1:F:229:MSE:HE2	2.47	0.64
1:4:91:ARG:CG	1:6:101:LEU:HD22	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:229:MSE:HE1	1:4:229:MSE:HE2	1.81	0.63
1:E:226:LEU:HD23	1:E:229:MSE:HE2	1.80	0.63
1:I:229:MSE:HE1	1:J:229:MSE:SE	2.49	0.62
1:2:94:MSE:HE1	1:2:108:SER:HA	1.82	0.62
1:W:96:ARG:NH2	1:Y:80:TYR:OH	2.33	0.62
1:Z:91:ARG:HG3	1:2:101:LEU:HD22	1.79	0.62
1:3:101:LEU:HD22	1:5:91:ARG:HG2	1.80	0.62
1:M:229:MSE:CE	1:N:229:MSE:CE	2.74	0.62
1:3:94:MSE:HE1	1:3:108:SER:HA	1.82	0.62
1:5:229:MSE:HE1	1:6:229:MSE:CE	2.26	0.62
1:Z:94:MSE:HE1	1:Z:108:SER:HA	1.81	0.62
1:P:80:TYR:OH	1:R:96:ARG:CZ	2.48	0.61
1:F:91:ARG:HD3	1:H:101:LEU:CB	2.30	0.61
1:1:96:ARG:NH2	1:3:80:TYR:OH	2.32	0.61
1:4:94:MSE:HE1	1:4:108:SER:HA	1.82	0.61
1:R:94:MSE:HE1	1:R:108:SER:HA	1.82	0.61
1:P:94:MSE:HE1	1:P:108:SER:HA	1.82	0.61
1:F:91:ARG:HD3	1:H:101:LEU:HB2	1.80	0.61
1:7:94:MSE:HE1	1:7:108:SER:HA	1.82	0.61
1:F:42:ARG:HH21	1:S:69:ASP:HA	1.66	0.61
1:F:80:TYR:HH	1:H:96:ARG:NH1	1.95	0.61
1:G:94:MSE:HE1	1:G:108:SER:HA	1.83	0.61
1:2:80:TYR:OH	1:4:96:ARG:CZ	2.48	0.61
1:Q:229:MSE:SE	1:R:229:MSE:HE1	2.51	0.61
1:4:80:TYR:OH	1:6:96:ARG:NH2	2.34	0.60
1:B:94:MSE:HE1	1:B:108:SER:HA	1.82	0.60
1:V:94:MSE:HE1	1:V:108:SER:HA	1.82	0.60
1:E:94:MSE:HE1	1:E:108:SER:HA	1.83	0.60
1:F:80:TYR:OH	1:H:96:ARG:CZ	2.48	0.60
1:U:94:MSE:HE1	1:U:108:SER:HA	1.83	0.60
1:O:94:MSE:HE1	1:O:108:SER:HA	1.83	0.60
1:Q:94:MSE:HE1	1:Q:108:SER:HA	1.83	0.60
1:E:225:GLY:HA3	1:F:229:MSE:SE	2.51	0.60
1:I:94:MSE:HE1	1:I:108:SER:HA	1.81	0.60
1:P:131:GLY:HA3	1:R:101:LEU:HD21	1.84	0.60
1:8:94:MSE:HE1	1:8:108:SER:HA	1.83	0.60
1:1:229:MSE:HE2	1:2:229:MSE:HE1	1.84	0.60
1:H:94:MSE:HE1	1:H:108:SER:HA	1.82	0.60
1:6:94:MSE:HE1	1:6:108:SER:HA	1.83	0.59
1:A:94:MSE:HE1	1:A:108:SER:HA	1.84	0.59
1:F:94:MSE:HE1	1:F:108:SER:HA	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:MSE:HE1	1:K:108:SER:HA	1.82	0.59
1:N:94:MSE:HE1	1:N:108:SER:HA	1.84	0.59
1:1:94:MSE:HE1	1:1:108:SER:HA	1.83	0.59
1:X:94:MSE:HE1	1:X:108:SER:HA	1.83	0.59
1:X:80:TYR:OH	1:Z:96:ARG:CZ	2.50	0.59
1:Y:94:MSE:HE1	1:Y:108:SER:HA	1.83	0.59
1:E:101:LEU:HD21	1:G:131:GLY:HA3	1.83	0.59
1:L:94:MSE:HE1	1:L:108:SER:HA	1.83	0.59
1:S:94:MSE:HE1	1:S:108:SER:HA	1.85	0.59
1:T:94:MSE:HE1	1:T:108:SER:HA	1.84	0.59
1:C:94:MSE:HE1	1:C:108:SER:HA	1.84	0.59
1:E:229:MSE:HE1	1:F:229:MSE:HE1	1.81	0.59
1:G:101:LEU:HD22	1:I:91:ARG:HG2	1.85	0.59
1:J:94:MSE:HE1	1:J:108:SER:HA	1.83	0.59
1:Y:229:MSE:CE	1:Z:229:MSE:CE	2.79	0.59
1:K:229:MSE:CE	1:L:229:MSE:CE	2.77	0.59
1:R:91:ARG:HG2	1:T:101:LEU:HD22	1.84	0.59
1:W:22:ALA:O	1:Y:128:TYR:OH	2.17	0.59
1:3:96:ARG:NH2	1:5:80:TYR:OH	2.36	0.59
1:W:94:MSE:HE1	1:W:108:SER:HA	1.85	0.59
1:E:96:ARG:CZ	1:G:80:TYR:OH	2.51	0.58
1:S:149:LYS:HB2	1:T:149:LYS:HB2	1.85	0.58
1:D:94:MSE:HE1	1:D:108:SER:HA	1.84	0.58
1:5:96:ARG:NH2	1:7:80:TYR:OH	2.36	0.58
1:Y:101:LEU:HD22	1:1:91:ARG:HG3	1.84	0.58
1:M:94:MSE:HE1	1:M:108:SER:HA	1.84	0.58
1:V:130:GLN:HB3	1:X:102:ALA:HA	1.84	0.58
1:Q:226:LEU:HA	1:Q:229:MSE:HE3	1.85	0.58
1:P:91:ARG:HG3	1:R:101:LEU:HD22	1.85	0.58
1:6:226:LEU:HA	1:6:229:MSE:HE3	1.86	0.58
1:W:226:LEU:HA	1:W:229:MSE:HE3	1.85	0.58
1:X:91:ARG:HG3	1:Z:101:LEU:HD22	1.81	0.57
1:E:101:LEU:HD22	1:G:91:ARG:HH21	1.69	0.57
1:H:91:ARG:CG	1:J:101:LEU:HD22	2.35	0.57
1:K:101:LEU:HD13	1:M:94:MSE:HE3	1.86	0.57
1:O:101:LEU:CD2	1:Q:91:ARG:HH21	2.16	0.57
1:5:94:MSE:HE1	1:5:108:SER:HA	1.85	0.57
1:X:80:TYR:OH	1:Z:96:ARG:NH2	2.37	0.57
1:I:229:MSE:CE	1:J:229:MSE:SE	3.03	0.57
1:7:226:LEU:HA	1:7:229:MSE:HE3	1.87	0.57
1:P:91:ARG:HH21	1:R:101:LEU:HD23	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:101:LEU:HD22	1:S:91:ARG:HG2	1.86	0.56
1:C:101:LEU:HD22	1:E:91:ARG:CG	2.35	0.56
1:2:226:LEU:HA	1:2:229:MSE:HE3	1.86	0.56
1:C:226:LEU:HA	1:C:229:MSE:HE3	1.88	0.56
1:1:96:ARG:CZ	1:3:80:TYR:OH	2.53	0.56
1:5:226:LEU:HA	1:5:229:MSE:HE3	1.88	0.56
1:F:75:ASN:O	1:S:70:GLY:HA2	2.05	0.56
1:J:94:MSE:HE3	1:L:101:LEU:HD13	1.86	0.56
1:L:226:LEU:HA	1:L:229:MSE:HE3	1.88	0.56
1:T:226:LEU:HA	1:T:229:MSE:HE3	1.88	0.56
1:1:101:LEU:HD21	1:3:131:GLY:HA3	1.87	0.56
1:E:101:LEU:HD22	1:G:91:ARG:HG3	1.88	0.56
1:K:149:LYS:HB2	1:L:149:LYS:HB2	1.89	0.56
1:Y:149:LYS:HD3	1:Z:150:TYR:OH	2.06	0.55
1:D:226:LEU:HA	1:D:229:MSE:HE3	1.88	0.55
1:H:226:LEU:HA	1:H:229:MSE:HE3	1.88	0.55
1:S:226:LEU:HA	1:S:229:MSE:HE3	1.89	0.55
1:N:226:LEU:HA	1:N:229:MSE:HE3	1.87	0.55
1:X:131:GLY:HA3	1:Z:101:LEU:HD21	1.89	0.55
1:Q:230:LEU:HD13	1:R:222:TRP:CH2	2.42	0.55
1:3:226:LEU:HA	1:3:229:MSE:HE3	1.87	0.55
1:Q:6:MSE:HE1	1:Q:172:ALA:HB2	1.89	0.55
1:P:80:TYR:OH	1:R:96:ARG:NH2	2.40	0.55
1:K:226:LEU:HA	1:K:229:MSE:HE3	1.89	0.54
1:M:149:LYS:HB2	1:N:149:LYS:HB2	1.89	0.54
1:1:150:TYR:OH	1:2:149:LYS:HD3	2.07	0.54
1:A:225:GLY:HA3	1:B:229:MSE:SE	2.58	0.54
1:G:226:LEU:HA	1:G:229:MSE:HE3	1.89	0.54
1:1:229:MSE:SE	1:2:225:GLY:HA3	2.57	0.54
1:P:226:LEU:HA	1:P:229:MSE:HE3	1.88	0.54
1:P:6:MSE:HE1	1:P:172:ALA:HB2	1.90	0.54
1:S:229:MSE:SE	1:T:225:GLY:HA3	2.57	0.54
1:1:6:MSE:HE1	1:1:172:ALA:HB2	1.90	0.54
1:O:6:MSE:HE1	1:O:172:ALA:HB2	1.90	0.54
1:V:226:LEU:HA	1:V:229:MSE:HE3	1.89	0.54
1:1:149:LYS:HD3	1:2:150:TYR:OH	2.08	0.54
1:5:229:MSE:CE	1:6:229:MSE:CE	2.86	0.54
1:K:6:MSE:HE1	1:K:172:ALA:HB2	1.90	0.54
1:M:6:MSE:HE1	1:M:172:ALA:HB2	1.89	0.54
1:M:226:LEU:HA	1:M:229:MSE:HE3	1.90	0.54
1:S:6:MSE:HE1	1:S:172:ALA:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:226:LEU:HA	1:Y:229:MSE:HE3	1.90	0.53
1:5:6:MSE:HE1	1:5:172:ALA:HB2	1.90	0.53
1:A:226:LEU:HA	1:A:229:MSE:HE3	1.89	0.53
1:1:101:LEU:HG	1:3:130:GLN:O	2.08	0.53
1:6:6:MSE:HE1	1:6:172:ALA:HB2	1.90	0.53
1:D:6:MSE:HE1	1:D:172:ALA:HB2	1.90	0.53
1:Y:6:MSE:HE1	1:Y:172:ALA:HB2	1.90	0.53
1:7:6:MSE:HE1	1:7:172:ALA:HB2	1.91	0.53
1:U:149:LYS:HB2	1:V:149:LYS:HB2	1.89	0.53
1:2:6:MSE:HE1	1:2:172:ALA:HB2	1.91	0.53
1:A:222:TRP:CH2	1:B:230:LEU:HD13	2.43	0.53
1:G:96:ARG:NH2	1:I:80:TYR:OH	2.40	0.53
1:B:226:LEU:HA	1:B:229:MSE:HE3	1.91	0.53
1:J:6:MSE:HE1	1:J:172:ALA:HB2	1.91	0.53
1:O:226:LEU:HA	1:O:229:MSE:HE3	1.91	0.53
1:4:6:MSE:HE1	1:4:172:ALA:HB2	1.90	0.53
1:E:149:LYS:HB2	1:F:149:LYS:HB2	1.91	0.53
1:P:91:ARG:HH21	1:R:101:LEU:CD2	2.22	0.53
1:Z:226:LEU:HA	1:Z:229:MSE:HE3	1.90	0.53
1:R:6:MSE:HE1	1:R:172:ALA:HB2	1.91	0.53
1:X:130:GLN:O	1:Z:101:LEU:HG	2.08	0.53
1:3:6:MSE:HE1	1:3:172:ALA:HB2	1.91	0.52
1:N:6:MSE:HE1	1:N:172:ALA:HB2	1.91	0.52
1:O:230:LEU:HD13	1:P:222:TRP:CH2	2.44	0.52
1:X:6:MSE:HE1	1:X:172:ALA:HB2	1.90	0.52
1:7:229:MSE:SE	1:8:229:MSE:HE1	2.59	0.52
1:V:6:MSE:HE1	1:V:172:ALA:HB2	1.91	0.52
1:W:6:MSE:HE1	1:W:172:ALA:HB2	1.91	0.52
1:C:6:MSE:HE1	1:C:172:ALA:HB2	1.92	0.52
1:G:6:MSE:HE1	1:G:172:ALA:HB2	1.92	0.52
1:I:6:MSE:HE1	1:I:172:ALA:HB2	1.90	0.52
1:R:226:LEU:HA	1:R:229:MSE:HE3	1.91	0.52
1:8:6:MSE:HE1	1:8:172:ALA:HB2	1.90	0.52
1:B:6:MSE:HE1	1:B:172:ALA:HB2	1.92	0.52
1:F:131:GLY:HA3	1:H:101:LEU:HD21	1.92	0.52
1:T:6:MSE:HE1	1:T:172:ALA:HB2	1.92	0.52
1:A:6:MSE:HE1	1:A:172:ALA:HB2	1.91	0.51
1:W:225:GLY:HA3	1:X:229:MSE:SE	2.60	0.51
1:F:117:ILE:HG23	1:S:69:ASP:CB	2.24	0.51
1:U:6:MSE:HE1	1:U:172:ALA:HB2	1.92	0.51
1:E:150:TYR:OH	1:F:149:LYS:HD3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:149:LYS:HB2	1:X:149:LYS:HB2	1.93	0.51
1:F:6:MSE:HE1	1:F:172:ALA:HB2	1.91	0.51
1:O:101:LEU:HD22	1:Q:91:ARG:HD3	1.91	0.51
1:I:229:MSE:HE1	1:J:229:MSE:CE	2.40	0.51
1:P:91:ARG:CD	1:R:101:LEU:HD22	2.40	0.51
1:I:226:LEU:HA	1:I:229:MSE:HE3	1.93	0.51
1:H:6:MSE:HE1	1:H:172:ALA:HB2	1.91	0.51
1:W:101:LEU:CD2	1:Y:91:ARG:CG	2.75	0.51
1:W:101:LEU:CD2	1:Y:91:ARG:HG2	2.27	0.51
1:Z:6:MSE:HE1	1:Z:172:ALA:HB2	1.92	0.51
1:Q:149:LYS:HB2	1:R:149:LYS:HB2	1.92	0.51
1:3:225:GLY:HA3	1:4:229:MSE:SE	2.61	0.50
1:E:6:MSE:HE1	1:E:172:ALA:HB2	1.92	0.50
1:2:131:GLY:HA3	1:4:101:LEU:HD21	1.93	0.50
1:8:226:LEU:HA	1:8:229:MSE:HE3	1.93	0.50
1:I:229:MSE:SE	1:J:225:GLY:HA3	2.62	0.50
1:L:6:MSE:HE1	1:L:172:ALA:HB2	1.92	0.50
1:Q:229:MSE:SE	1:R:229:MSE:CE	3.08	0.50
1:F:226:LEU:HA	1:F:229:MSE:HE3	1.94	0.50
1:F:91:ARG:NH2	1:H:101:LEU:HD22	2.22	0.50
1:S:225:GLY:HA3	1:T:229:MSE:SE	2.62	0.50
1:1:101:LEU:HD23	1:3:91:ARG:HH21	1.76	0.50
1:C:149:LYS:HB2	1:D:149:LYS:HB2	1.94	0.49
1:V:94:MSE:HE3	1:X:101:LEU:HD11	1.94	0.49
1:A:229:MSE:SE	1:B:229:MSE:HE1	2.62	0.49
1:G:66:ILE:HG12	1:G:74:LEU:HG	1.95	0.49
1:P:130:GLN:O	1:R:101:LEU:HG	2.12	0.49
1:Y:96:ARG:CZ	1:1:80:TYR:OH	2.61	0.49
1:2:130:GLN:O	1:4:101:LEU:HG	2.11	0.49
1:7:225:GLY:HA3	1:8:229:MSE:SE	2.62	0.49
1:X:226:LEU:HA	1:X:229:MSE:HE3	1.95	0.49
1:D:66:ILE:HG12	1:D:74:LEU:HG	1.95	0.49
1:W:49:ALA:O	1:W:109:CYS:HB2	2.13	0.49
1:3:101:LEU:HD22	1:5:91:ARG:CG	2.43	0.49
1:E:230:LEU:HD13	1:F:222:TRP:CH2	2.47	0.49
1:S:222:TRP:CH2	1:T:230:LEU:HD13	2.48	0.49
1:2:66:ILE:HG12	1:2:74:LEU:HG	1.96	0.48
1:F:117:ILE:CG2	1:S:69:ASP:CA	2.88	0.48
1:G:150:TYR:OH	1:H:149:LYS:HD3	2.14	0.48
1:J:49:ALA:O	1:J:109:CYS:HB2	2.13	0.48
1:R:66:ILE:HG12	1:R:74:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:ILE:HG12	1:O:74:LEU:HG	1.95	0.48
1:Q:49:ALA:O	1:Q:109:CYS:HB2	2.13	0.48
1:T:66:ILE:HG12	1:T:74:LEU:HG	1.96	0.48
1:G:229:MSE:HE1	1:H:229:MSE:SE	2.63	0.48
1:G:49:ALA:O	1:G:109:CYS:HB2	2.14	0.48
1:V:49:ALA:O	1:V:109:CYS:HB2	2.14	0.48
1:Y:150:TYR:OH	1:Z:149:LYS:HD3	2.13	0.48
1:6:49:ALA:O	1:6:109:CYS:HB2	2.14	0.48
1:8:49:ALA:O	1:8:109:CYS:HB2	2.14	0.48
1:S:66:ILE:HG12	1:S:74:LEU:HG	1.95	0.48
1:C:96:ARG:NH2	1:E:80:TYR:OH	2.46	0.48
1:F:49:ALA:O	1:F:109:CYS:HB2	2.14	0.48
1:O:49:ALA:O	1:O:109:CYS:HB2	2.14	0.48
1:Q:66:ILE:HG12	1:Q:74:LEU:HG	1.95	0.48
1:Y:49:ALA:O	1:Y:109:CYS:HB2	2.14	0.48
1:3:49:ALA:O	1:3:109:CYS:HB2	2.15	0.47
1:S:49:ALA:O	1:S:109:CYS:HB2	2.14	0.47
1:T:49:ALA:O	1:T:109:CYS:HB2	2.14	0.47
1:1:49:ALA:O	1:1:109:CYS:HB2	2.14	0.47
1:5:49:ALA:O	1:5:109:CYS:HB2	2.14	0.47
1:L:66:ILE:HG12	1:L:74:LEU:HG	1.97	0.47
1:D:70:GLY:HA2	1:Q:75:ASN:O	2.14	0.47
1:U:49:ALA:O	1:U:109:CYS:HB2	2.14	0.47
1:B:49:ALA:O	1:B:109:CYS:HB2	2.15	0.47
1:C:66:ILE:HG12	1:C:74:LEU:HG	1.96	0.47
1:K:49:ALA:O	1:K:109:CYS:HB2	2.14	0.47
1:R:49:ALA:O	1:R:109:CYS:HB2	2.14	0.47
1:H:49:ALA:O	1:H:109:CYS:HB2	2.14	0.47
1:O:149:LYS:HB2	1:P:149:LYS:HB2	1.95	0.47
1:2:91:ARG:HH21	1:4:101:LEU:HD23	1.80	0.47
1:5:66:ILE:HG12	1:5:74:LEU:HG	1.96	0.47
1:C:49:ALA:O	1:C:109:CYS:HB2	2.14	0.47
1:I:49:ALA:O	1:I:109:CYS:HB2	2.15	0.47
1:Q:225:GLY:HA3	1:R:229:MSE:SE	2.64	0.47
1:U:66:ILE:HG12	1:U:74:LEU:HG	1.96	0.47
1:1:101:LEU:CD2	1:3:131:GLY:HA3	2.45	0.47
1:2:49:ALA:O	1:2:109:CYS:HB2	2.15	0.47
1:V:66:ILE:HG12	1:V:74:LEU:HG	1.96	0.47
1:Y:66:ILE:HG12	1:Y:74:LEU:HG	1.96	0.47
1:A:229:MSE:SE	1:B:225:GLY:HA3	2.65	0.47
1:M:49:ALA:O	1:M:109:CYS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:66:ILE:HG12	1:W:74:LEU:HG	1.97	0.47
1:6:66:ILE:HG12	1:6:74:LEU:HG	1.97	0.47
1:N:49:ALA:O	1:N:109:CYS:HB2	2.15	0.47
1:O:229:MSE:SE	1:P:225:GLY:HA3	2.64	0.47
1:N:91:ARG:HG2	1:P:101:LEU:HD22	1.95	0.47
1:1:66:ILE:HG12	1:1:74:LEU:HG	1.97	0.47
1:C:229:MSE:SE	1:D:225:GLY:HA3	2.65	0.47
1:Q:229:MSE:HE1	1:R:229:MSE:SE	2.65	0.47
1:A:149:LYS:HB2	1:B:149:LYS:HB2	1.95	0.47
1:7:49:ALA:O	1:7:109:CYS:HB2	2.15	0.46
1:F:66:ILE:HG12	1:F:74:LEU:HG	1.96	0.46
1:G:149:LYS:HD3	1:H:150:TYR:OH	2.15	0.46
1:J:69:ASP:CB	1:W:69:ASP:C	2.70	0.46
1:W:96:ARG:NH1	1:Y:80:TYR:OH	2.48	0.46
1:4:49:ALA:O	1:4:109:CYS:HB2	2.14	0.46
1:4:66:ILE:HG12	1:4:74:LEU:HG	1.97	0.46
1:E:49:ALA:O	1:E:109:CYS:HB2	2.15	0.46
1:P:49:ALA:O	1:P:109:CYS:HB2	2.14	0.46
1:Z:66:ILE:HG12	1:Z:74:LEU:HG	1.98	0.46
1:7:66:ILE:HG12	1:7:74:LEU:HG	1.96	0.46
1:X:49:ALA:O	1:X:109:CYS:HB2	2.15	0.46
1:E:226:LEU:O	1:E:229:MSE:HB2	2.16	0.46
1:I:226:LEU:HD23	1:J:229:MSE:HE1	1.98	0.46
1:Z:49:ALA:O	1:Z:109:CYS:HB2	2.15	0.46
1:L:49:ALA:O	1:L:109:CYS:HB2	2.14	0.46
1:A:230:LEU:HD13	1:B:222:TRP:CH2	2.50	0.46
1:D:49:ALA:O	1:D:109:CYS:HB2	2.16	0.46
1:X:91:ARG:HH21	1:Z:101:LEU:HD23	1.81	0.46
1:Q:222:TRP:CH2	1:R:230:LEU:HD13	2.50	0.46
1:S:230:LEU:HD13	1:T:222:TRP:CH2	2.50	0.46
1:X:229:MSE:HB2	1:X:229:MSE:HE3	1.75	0.46
1:A:66:ILE:HG12	1:A:74:LEU:HG	1.97	0.46
1:A:49:ALA:O	1:A:109:CYS:HB2	2.15	0.46
1:3:66:ILE:HG12	1:3:74:LEU:HG	1.97	0.45
1:B:66:ILE:HG12	1:B:74:LEU:HG	1.97	0.45
1:G:229:MSE:SE	1:H:229:MSE:HE1	2.67	0.45
1:P:66:ILE:HG12	1:P:74:LEU:HG	1.98	0.45
1:S:27:ILE:HG21	1:V:184:LEU:HD12	1.98	0.45
1:8:66:ILE:HG12	1:8:74:LEU:HG	1.97	0.45
1:D:91:ARG:HG2	1:F:101:LEU:HD22	1.98	0.45
1:G:149:LYS:HB2	1:H:149:LYS:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:149:LYS:HD3	1:R:150:TYR:OH	2.16	0.45
1:G:222:TRP:CH2	1:H:230:LEU:HD13	2.52	0.45
1:H:66:ILE:HG12	1:H:74:LEU:HG	1.98	0.45
1:M:66:ILE:HG12	1:M:74:LEU:HG	1.98	0.45
1:V:152:LYS:N	1:V:153:PRO:CD	2.80	0.45
1:X:66:ILE:HG12	1:X:74:LEU:HG	1.97	0.45
1:Y:149:LYS:HB2	1:Z:149:LYS:HB2	1.98	0.45
1:E:101:LEU:HD22	1:G:91:ARG:HG2	1.94	0.45
1:2:131:GLY:HA3	1:4:101:LEU:CD2	2.46	0.45
1:A:229:MSE:HE1	1:B:229:MSE:SE	2.67	0.45
1:I:229:MSE:HE3	1:I:229:MSE:HB2	1.82	0.45
1:J:66:ILE:HG12	1:J:74:LEU:HG	1.99	0.45
1:N:66:ILE:HG12	1:N:74:LEU:HG	1.99	0.45
1:S:229:MSE:HB2	1:S:229:MSE:HE3	1.79	0.45
1:1:150:TYR:CZ	1:2:149:LYS:CD	3.01	0.44
1:5:149:LYS:HB2	1:6:149:LYS:HB2	1.98	0.44
1:7:229:MSE:SE	1:8:229:MSE:CE	3.15	0.44
1:E:66:ILE:HG12	1:E:74:LEU:HG	1.98	0.44
1:K:66:ILE:HG12	1:K:74:LEU:HG	1.98	0.44
1:D:229:MSE:HB2	1:D:229:MSE:HE3	1.76	0.44
1:I:66:ILE:HG12	1:I:74:LEU:HG	1.99	0.44
1:L:229:MSE:HB2	1:L:229:MSE:HE3	1.77	0.44
1:M:101:LEU:HD22	1:O:91:ARG:HG2	1.98	0.44
1:O:225:GLY:HA3	1:P:229:MSE:SE	2.68	0.44
1:Y:149:LYS:CD	1:Z:150:TYR:CZ	3.00	0.44
1:Z:80:TYR:OH	1:2:96:ARG:CZ	2.66	0.44
1:Q:43:LEU:HD22	1:Q:195:TYR:CD1	2.53	0.44
1:3:222:TRP:CH2	1:4:229:MSE:HE3	2.53	0.44
1:O:229:MSE:HB2	1:O:229:MSE:HE3	1.81	0.44
1:E:222:TRP:CH2	1:F:230:LEU:HD13	2.52	0.43
1:P:91:ARG:HD3	1:R:101:LEU:HD22	2.00	0.43
1:Q:229:MSE:SE	1:R:225:GLY:HA3	2.69	0.43
1:X:33:LEU:HD23	1:X:33:LEU:C	2.39	0.43
1:K:229:MSE:HE3	1:K:229:MSE:HB2	1.79	0.43
1:P:33:LEU:HD23	1:P:33:LEU:C	2.38	0.43
1:U:56:GLN:OE1	1:W:134:ILE:HA	2.18	0.43
1:3:150:TYR:OH	1:4:149:LYS:HD3	2.19	0.43
1:E:150:TYR:CZ	1:F:149:LYS:CD	3.01	0.43
1:O:101:LEU:HD21	1:Q:131:GLY:HA3	1.99	0.43
1:K:177:ASP:OD2	1:L:157:ARG:NH2	2.52	0.43
1:N:33:LEU:C	1:N:33:LEU:HD23	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:229:MSE:HB2	1:W:229:MSE:HE3	1.84	0.43
1:Y:149:LYS:HD2	1:Z:150:TYR:CZ	2.54	0.43
1:Z:130:GLN:O	1:2:101:LEU:HG	2.18	0.43
1:3:230:LEU:HD13	1:4:222:TRP:CH2	2.54	0.43
1:C:225:GLY:HA3	1:D:229:MSE:SE	2.68	0.43
1:M:229:MSE:SE	1:N:225:GLY:HA3	2.69	0.43
1:S:101:LEU:HG	1:U:130:GLN:HA	2.01	0.42
1:2:229:MSE:HE3	1:2:229:MSE:HB2	1.82	0.42
1:O:96:ARG:CZ	1:Q:80:TYR:OH	2.67	0.42
1:7:149:LYS:HB2	1:8:149:LYS:HB2	2.01	0.42
1:W:229:MSE:SE	1:X:225:GLY:HA3	2.69	0.42
1:G:225:GLY:HA3	1:H:229:MSE:SE	2.69	0.42
1:U:240:TYR:CE1	1:V:206:TYR:CE2	3.07	0.42
1:O:101:LEU:CD2	1:Q:91:ARG:HD3	2.50	0.42
1:U:229:MSE:HE1	1:V:225:GLY:CA	2.33	0.42
1:7:152:LYS:N	1:7:153:PRO:CD	2.83	0.42
1:H:128:TYR:OH	1:J:22:ALA:O	2.25	0.42
1:O:222:TRP:CH2	1:P:230:LEU:HD13	2.55	0.42
1:U:225:GLY:HA3	1:V:229:MSE:SE	2.69	0.42
1:1:229:MSE:HE3	1:2:222:TRP:CH2	2.55	0.42
1:K:225:GLY:HA3	1:L:229:MSE:SE	2.70	0.42
1:K:56:GLN:OE1	1:M:135:GLN:N	2.40	0.42
1:R:33:LEU:C	1:R:33:LEU:HD23	2.39	0.42
1:Y:101:LEU:HG	1:1:130:GLN:O	2.20	0.42
1:7:150:TYR:OH	1:8:149:LYS:HD3	2.20	0.41
1:P:229:MSE:HB2	1:P:229:MSE:HE3	1.76	0.41
1:S:43:LEU:HD22	1:S:195:TYR:CD1	2.55	0.41
1:1:150:TYR:CZ	1:2:149:LYS:HD2	2.54	0.41
1:3:149:LYS:HD3	1:4:150:TYR:OH	2.19	0.41
1:E:150:TYR:CZ	1:F:149:LYS:HD3	2.55	0.41
1:X:131:GLY:HA3	1:Z:101:LEU:CD2	2.50	0.41
1:M:60:ASN:ND2	1:O:135:GLN:OE1	2.54	0.41
1:Y:149:LYS:HD3	1:Z:150:TYR:CZ	2.55	0.41
1:E:101:LEU:HD23	1:G:91:ARG:NH2	2.29	0.41
1:L:94:MSE:HE3	1:N:101:LEU:HD13	1.95	0.41
1:M:33:LEU:HD23	1:M:33:LEU:C	2.41	0.41
1:O:60:ASN:ND2	1:Q:135:GLN:HE22	2.18	0.41
1:Y:96:ARG:NH1	1:1:80:TYR:OH	2.53	0.41
1:H:229:MSE:HB2	1:H:229:MSE:HE3	1.78	0.41
1:K:229:MSE:SE	1:L:225:GLY:HA3	2.70	0.41
1:7:33:LEU:HD23	1:7:33:LEU:C	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:MSE:SE	1:P:229:MSE:HE1	2.71	0.41
1:1:149:LYS:HB2	1:2:149:LYS:HB2	2.02	0.41
1:A:137:THR:HB	1:A:138:PRO:HD2	2.03	0.41
1:N:80:TYR:OH	1:P:96:ARG:NH2	2.51	0.41
1:U:229:MSE:SE	1:V:229:MSE:HE1	2.71	0.41
1:3:222:TRP:CZ2	1:4:229:MSE:HE3	2.56	0.41
1:A:229:MSE:HE3	1:A:229:MSE:HB2	1.78	0.41
1:S:152:LYS:N	1:S:153:PRO:CD	2.84	0.41
1:3:149:LYS:HB2	1:4:149:LYS:HB2	2.02	0.40
1:E:150:TYR:CE2	1:F:149:LYS:HD2	2.57	0.40
1:G:150:TYR:CZ	1:H:149:LYS:CD	3.04	0.40
1:S:33:LEU:C	1:S:33:LEU:HD23	2.42	0.40
1:C:229:MSE:HE3	1:C:229:MSE:HB2	1.78	0.40
1:D:33:LEU:C	1:D:33:LEU:HD23	2.42	0.40
1:A:207:ARG:NH1	1:C:139:ASP:OD2	2.29	0.40
1:8:33:LEU:C	1:8:33:LEU:HD23	2.42	0.40
1:T:172:ALA:O	1:T:175:SER:HB3	2.22	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:ARG:NH2	1:U:232:ARG:O[1_655]	1.65	0.55
1:M:162:ASP:OD1	1:U:231:GLU:OE1[1_655]	1.71	0.49
1:2:228:ASP:OD2	1:8:220:ARG:NH1[2_744]	1.91	0.29
1:2:231:GLU:OE1	1:7:234:PRO:CB[2_744]	2.03	0.17
1:F:220:ARG:NH1	1:4:232:ARG:O[1_556]	2.08	0.12
1:I:228:ASP:OD2	1:O:232:ARG:NH2[2_845]	2.18	0.02

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	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	2	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	3	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	4	239/242 (99%)	228 (95%)	11 (5%)	0	100	100
1	5	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	6	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	7	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	8	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	A	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	B	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	C	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	D	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	E	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	F	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	G	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	H	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	I	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	34	66
1	J	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	34	66
1	K	239/242 (99%)	230 (96%)	8 (3%)	1 (0%)	34	66
1	L	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	34	66
1	M	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	N	239/242 (99%)	228 (95%)	10 (4%)	1 (0%)	34	66
1	O	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	P	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	Q	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	R	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	S	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	T	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	U	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	V	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	W	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	X	239/242 (99%)	229 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Y	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	34 66
1	Z	239/242 (99%)	229 (96%)	10 (4%)	0	100 100
All	All	8126/8228 (99%)	7785 (96%)	335 (4%)	6 (0%)	51 82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	239	ALA
1	N	239	ALA
1	I	239	ALA
1	K	239	ALA
1	L	239	ALA
1	Y	239	ALA

5.3.2 Protein sidechains (i)

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	197/197 (100%)	182 (92%)	15 (8%)	13 36
1	2	197/197 (100%)	184 (93%)	13 (7%)	16 44
1	3	197/197 (100%)	183 (93%)	14 (7%)	14 40
1	4	197/197 (100%)	183 (93%)	14 (7%)	14 40
1	5	197/197 (100%)	183 (93%)	14 (7%)	14 40
1	6	197/197 (100%)	183 (93%)	14 (7%)	14 40
1	7	197/197 (100%)	182 (92%)	15 (8%)	13 36
1	8	197/197 (100%)	185 (94%)	12 (6%)	18 48
1	A	197/197 (100%)	182 (92%)	15 (8%)	13 36
1	B	197/197 (100%)	183 (93%)	14 (7%)	14 40
1	C	197/197 (100%)	183 (93%)	14 (7%)	14 40
1	D	197/197 (100%)	184 (93%)	13 (7%)	16 44
1	E	197/197 (100%)	183 (93%)	14 (7%)	14 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	G	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	H	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	I	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	J	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	K	197/197 (100%)	182 (92%)	15 (8%)	13	36
1	L	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	M	197/197 (100%)	184 (93%)	13 (7%)	16	44
1	N	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	O	197/197 (100%)	182 (92%)	15 (8%)	13	36
1	P	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	Q	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	R	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	S	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	T	197/197 (100%)	184 (93%)	13 (7%)	16	44
1	U	197/197 (100%)	182 (92%)	15 (8%)	13	36
1	V	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	W	197/197 (100%)	184 (93%)	13 (7%)	16	44
1	X	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	Y	197/197 (100%)	183 (93%)	14 (7%)	14	40
1	Z	197/197 (100%)	182 (92%)	15 (8%)	13	36
All	All	6698/6698 (100%)	6217 (93%)	481 (7%)	14	39

All (481) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	38	THR
1	A	41	GLU
1	A	42	ARG
1	A	60	ASN
1	A	66	ILE
1	A	75	ASN
1	A	130	GLN
1	A	139	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	171	CYS
1	A	210	GLU
1	A	229	MSE
1	A	232	ARG
1	A	233	LEU
1	A	235	SER
1	B	24	ILE
1	B	38	THR
1	B	41	GLU
1	B	42	ARG
1	B	60	ASN
1	B	66	ILE
1	B	130	GLN
1	B	139	ASP
1	B	171	CYS
1	B	210	GLU
1	B	229	MSE
1	B	232	ARG
1	B	233	LEU
1	B	235	SER
1	C	24	ILE
1	C	38	THR
1	C	41	GLU
1	C	42	ARG
1	C	60	ASN
1	C	66	ILE
1	C	75	ASN
1	C	130	GLN
1	C	139	ASP
1	C	210	GLU
1	C	229	MSE
1	C	232	ARG
1	C	233	LEU
1	C	235	SER
1	D	24	ILE
1	D	38	THR
1	D	41	GLU
1	D	42	ARG
1	D	60	ASN
1	D	66	ILE
1	D	130	GLN
1	D	139	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	210	GLU
1	D	229	MSE
1	D	232	ARG
1	D	233	LEU
1	D	235	SER
1	E	24	ILE
1	E	38	THR
1	E	41	GLU
1	E	42	ARG
1	E	60	ASN
1	E	66	ILE
1	E	130	GLN
1	E	139	ASP
1	E	171	CYS
1	E	210	GLU
1	E	229	MSE
1	E	232	ARG
1	E	233	LEU
1	E	235	SER
1	F	24	ILE
1	F	38	THR
1	F	41	GLU
1	F	42	ARG
1	F	60	ASN
1	F	66	ILE
1	F	75	ASN
1	F	130	GLN
1	F	133	PHE
1	F	139	ASP
1	F	210	GLU
1	F	221	GLN
1	F	229	MSE
1	F	232	ARG
1	F	233	LEU
1	F	235	SER
1	G	24	ILE
1	G	38	THR
1	G	41	GLU
1	G	42	ARG
1	G	60	ASN
1	G	66	ILE
1	G	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	130	GLN
1	G	139	ASP
1	G	210	GLU
1	G	229	MSE
1	G	232	ARG
1	G	233	LEU
1	G	235	SER
1	H	24	ILE
1	H	38	THR
1	H	41	GLU
1	H	42	ARG
1	H	60	ASN
1	H	66	ILE
1	H	75	ASN
1	H	130	GLN
1	H	139	ASP
1	H	149	LYS
1	H	171	CYS
1	H	210	GLU
1	H	229	MSE
1	H	232	ARG
1	H	233	LEU
1	H	235	SER
1	H	241	ASN
1	I	24	ILE
1	I	38	THR
1	I	41	GLU
1	I	42	ARG
1	I	60	ASN
1	I	66	ILE
1	I	75	ASN
1	I	130	GLN
1	I	139	ASP
1	I	210	GLU
1	I	229	MSE
1	I	232	ARG
1	I	233	LEU
1	I	235	SER
1	J	24	ILE
1	J	38	THR
1	J	41	GLU
1	J	42	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	60	ASN
1	J	66	ILE
1	J	75	ASN
1	J	130	GLN
1	J	139	ASP
1	J	210	GLU
1	J	229	MSE
1	J	232	ARG
1	J	233	LEU
1	J	235	SER
1	K	24	ILE
1	K	38	THR
1	K	41	GLU
1	K	42	ARG
1	K	60	ASN
1	K	66	ILE
1	K	75	ASN
1	K	130	GLN
1	K	139	ASP
1	K	171	CYS
1	K	210	GLU
1	K	229	MSE
1	K	232	ARG
1	K	233	LEU
1	K	235	SER
1	L	24	ILE
1	L	38	THR
1	L	41	GLU
1	L	42	ARG
1	L	60	ASN
1	L	66	ILE
1	L	75	ASN
1	L	130	GLN
1	L	139	ASP
1	L	171	CYS
1	L	210	GLU
1	L	232	ARG
1	L	233	LEU
1	L	235	SER
1	M	24	ILE
1	M	38	THR
1	M	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	42	ARG
1	M	60	ASN
1	M	66	ILE
1	M	75	ASN
1	M	130	GLN
1	M	139	ASP
1	M	210	GLU
1	M	232	ARG
1	M	233	LEU
1	M	235	SER
1	N	24	ILE
1	N	38	THR
1	N	41	GLU
1	N	42	ARG
1	N	60	ASN
1	N	66	ILE
1	N	75	ASN
1	N	130	GLN
1	N	139	ASP
1	N	210	GLU
1	N	229	MSE
1	N	232	ARG
1	N	233	LEU
1	N	235	SER
1	O	24	ILE
1	O	38	THR
1	O	41	GLU
1	O	42	ARG
1	O	60	ASN
1	O	66	ILE
1	O	75	ASN
1	O	130	GLN
1	O	139	ASP
1	O	171	CYS
1	O	210	GLU
1	O	229	MSE
1	O	232	ARG
1	O	233	LEU
1	O	235	SER
1	P	24	ILE
1	P	38	THR
1	P	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	42	ARG
1	P	60	ASN
1	P	66	ILE
1	P	75	ASN
1	P	130	GLN
1	P	139	ASP
1	P	171	CYS
1	P	210	GLU
1	P	232	ARG
1	P	233	LEU
1	P	235	SER
1	Q	24	ILE
1	Q	38	THR
1	Q	41	GLU
1	Q	42	ARG
1	Q	60	ASN
1	Q	66	ILE
1	Q	75	ASN
1	Q	130	GLN
1	Q	139	ASP
1	Q	210	GLU
1	Q	229	MSE
1	Q	232	ARG
1	Q	233	LEU
1	Q	235	SER
1	R	24	ILE
1	R	38	THR
1	R	41	GLU
1	R	42	ARG
1	R	60	ASN
1	R	66	ILE
1	R	75	ASN
1	R	130	GLN
1	R	139	ASP
1	R	210	GLU
1	R	229	MSE
1	R	232	ARG
1	R	233	LEU
1	R	235	SER
1	S	24	ILE
1	S	38	THR
1	S	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	42	ARG
1	S	60	ASN
1	S	66	ILE
1	S	75	ASN
1	S	130	GLN
1	S	139	ASP
1	S	210	GLU
1	S	229	MSE
1	S	232	ARG
1	S	233	LEU
1	S	235	SER
1	T	24	ILE
1	T	38	THR
1	T	41	GLU
1	T	42	ARG
1	T	60	ASN
1	T	66	ILE
1	T	75	ASN
1	T	130	GLN
1	T	139	ASP
1	T	210	GLU
1	T	229	MSE
1	T	233	LEU
1	T	235	SER
1	U	24	ILE
1	U	38	THR
1	U	41	GLU
1	U	42	ARG
1	U	60	ASN
1	U	66	ILE
1	U	75	ASN
1	U	130	GLN
1	U	139	ASP
1	U	149	LYS
1	U	210	GLU
1	U	229	MSE
1	U	232	ARG
1	U	233	LEU
1	U	235	SER
1	V	24	ILE
1	V	38	THR
1	V	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	42	ARG
1	V	60	ASN
1	V	66	ILE
1	V	130	GLN
1	V	139	ASP
1	V	171	CYS
1	V	210	GLU
1	V	229	MSE
1	V	232	ARG
1	V	233	LEU
1	V	235	SER
1	W	24	ILE
1	W	38	THR
1	W	41	GLU
1	W	42	ARG
1	W	60	ASN
1	W	66	ILE
1	W	130	GLN
1	W	139	ASP
1	W	210	GLU
1	W	229	MSE
1	W	232	ARG
1	W	233	LEU
1	W	235	SER
1	X	24	ILE
1	X	38	THR
1	X	41	GLU
1	X	42	ARG
1	X	60	ASN
1	X	66	ILE
1	X	75	ASN
1	X	130	GLN
1	X	139	ASP
1	X	171	CYS
1	X	210	GLU
1	X	232	ARG
1	X	233	LEU
1	X	235	SER
1	Y	24	ILE
1	Y	38	THR
1	Y	41	GLU
1	Y	42	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	60	ASN
1	Y	66	ILE
1	Y	75	ASN
1	Y	130	GLN
1	Y	139	ASP
1	Y	210	GLU
1	Y	229	MSE
1	Y	232	ARG
1	Y	233	LEU
1	Y	235	SER
1	Z	24	ILE
1	Z	38	THR
1	Z	41	GLU
1	Z	42	ARG
1	Z	60	ASN
1	Z	66	ILE
1	Z	75	ASN
1	Z	130	GLN
1	Z	139	ASP
1	Z	171	CYS
1	Z	210	GLU
1	Z	229	MSE
1	Z	232	ARG
1	Z	233	LEU
1	Z	235	SER
1	1	24	ILE
1	1	38	THR
1	1	41	GLU
1	1	42	ARG
1	1	60	ASN
1	1	66	ILE
1	1	75	ASN
1	1	130	GLN
1	1	139	ASP
1	1	171	CYS
1	1	210	GLU
1	1	229	MSE
1	1	232	ARG
1	1	233	LEU
1	1	235	SER
1	2	24	ILE
1	2	38	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	41	GLU
1	2	42	ARG
1	2	60	ASN
1	2	66	ILE
1	2	75	ASN
1	2	130	GLN
1	2	139	ASP
1	2	210	GLU
1	2	229	MSE
1	2	233	LEU
1	2	235	SER
1	3	24	ILE
1	3	38	THR
1	3	41	GLU
1	3	42	ARG
1	3	60	ASN
1	3	66	ILE
1	3	75	ASN
1	3	130	GLN
1	3	139	ASP
1	3	210	GLU
1	3	229	MSE
1	3	232	ARG
1	3	233	LEU
1	3	235	SER
1	4	24	ILE
1	4	38	THR
1	4	41	GLU
1	4	42	ARG
1	4	60	ASN
1	4	66	ILE
1	4	130	GLN
1	4	139	ASP
1	4	171	CYS
1	4	210	GLU
1	4	229	MSE
1	4	232	ARG
1	4	233	LEU
1	4	235	SER
1	5	24	ILE
1	5	38	THR
1	5	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	42	ARG
1	5	60	ASN
1	5	66	ILE
1	5	75	ASN
1	5	130	GLN
1	5	139	ASP
1	5	210	GLU
1	5	229	MSE
1	5	232	ARG
1	5	233	LEU
1	5	235	SER
1	6	24	ILE
1	6	38	THR
1	6	41	GLU
1	6	42	ARG
1	6	60	ASN
1	6	66	ILE
1	6	75	ASN
1	6	130	GLN
1	6	139	ASP
1	6	210	GLU
1	6	229	MSE
1	6	232	ARG
1	6	233	LEU
1	6	235	SER
1	7	24	ILE
1	7	38	THR
1	7	41	GLU
1	7	42	ARG
1	7	60	ASN
1	7	66	ILE
1	7	75	ASN
1	7	130	GLN
1	7	139	ASP
1	7	171	CYS
1	7	210	GLU
1	7	229	MSE
1	7	232	ARG
1	7	233	LEU
1	7	235	SER
1	8	24	ILE
1	8	38	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8	41	GLU
1	8	42	ARG
1	8	60	ASN
1	8	66	ILE
1	8	130	GLN
1	8	139	ASP
1	8	210	GLU
1	8	232	ARG
1	8	233	LEU
1	8	235	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	75	ASN
1	A	130	GLN
1	B	130	GLN
1	C	75	ASN
1	C	130	GLN
1	C	135	GLN
1	D	60	ASN
1	D	130	GLN
1	E	130	GLN
1	F	75	ASN
1	F	130	GLN
1	F	135	GLN
1	G	60	ASN
1	G	64	GLN
1	G	75	ASN
1	G	130	GLN
1	H	75	ASN
1	H	130	GLN
1	H	135	GLN
1	I	75	ASN
1	I	130	GLN
1	I	135	GLN
1	J	60	ASN
1	J	64	GLN
1	J	75	ASN
1	J	130	GLN
1	J	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	60	ASN
1	K	75	ASN
1	K	130	GLN
1	L	60	ASN
1	L	75	ASN
1	L	130	GLN
1	M	60	ASN
1	M	64	GLN
1	M	75	ASN
1	M	135	GLN
1	N	75	ASN
1	N	130	GLN
1	O	60	ASN
1	O	64	GLN
1	O	75	ASN
1	O	130	GLN
1	O	135	GLN
1	P	75	ASN
1	P	130	GLN
1	Q	75	ASN
1	Q	130	GLN
1	R	75	ASN
1	R	130	GLN
1	S	75	ASN
1	S	130	GLN
1	T	75	ASN
1	T	130	GLN
1	U	75	ASN
1	U	130	GLN
1	V	130	GLN
1	V	135	GLN
1	W	60	ASN
1	W	64	GLN
1	W	130	GLN
1	X	60	ASN
1	X	75	ASN
1	X	130	GLN
1	Y	60	ASN
1	Y	64	GLN
1	Y	75	ASN
1	Y	130	GLN
1	Y	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	75	ASN
1	Z	130	GLN
1	Z	135	GLN
1	1	75	ASN
1	1	130	GLN
1	1	135	GLN
1	2	60	ASN
1	2	64	GLN
1	2	75	ASN
1	2	130	GLN
1	2	135	GLN
1	3	60	ASN
1	3	64	GLN
1	3	75	ASN
1	3	130	GLN
1	4	60	ASN
1	4	64	GLN
1	4	130	GLN
1	4	135	GLN
1	5	60	ASN
1	5	64	GLN
1	5	75	ASN
1	5	130	GLN
1	5	135	GLN
1	6	60	ASN
1	6	64	GLN
1	6	75	ASN
1	6	130	GLN
1	7	75	ASN
1	7	130	GLN
1	7	135	GLN
1	8	130	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

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, 95^{th} 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	236/242 (97%)	0.05	11 (4%)	31	28	56, 86, 131, 215	0
1	2	236/242 (97%)	-0.04	11 (4%)	31	28	59, 87, 135, 203	0
1	3	236/242 (97%)	-0.09	9 (3%)	40	36	57, 80, 140, 221	0
1	4	236/242 (97%)	-0.05	8 (3%)	45	40	56, 83, 129, 220	0
1	5	236/242 (97%)	0.16	12 (5%)	28	24	60, 97, 147, 204	0
1	6	236/242 (97%)	0.13	11 (4%)	31	28	64, 94, 138, 205	0
1	7	236/242 (97%)	0.02	10 (4%)	36	32	56, 79, 118, 227	0
1	8	236/242 (97%)	-0.13	5 (2%)	63	61	57, 79, 135, 186	0
1	A	236/242 (97%)	-0.12	7 (2%)	50	45	54, 72, 120, 163	0
1	B	236/242 (97%)	-0.20	6 (2%)	57	55	55, 76, 117, 208	0
1	C	236/242 (97%)	-0.07	7 (2%)	50	45	54, 77, 119, 208	0
1	D	236/242 (97%)	-0.16	7 (2%)	50	45	53, 70, 128, 190	0
1	E	236/242 (97%)	-0.13	7 (2%)	50	45	53, 77, 122, 216	0
1	F	236/242 (97%)	-0.13	8 (3%)	45	40	50, 66, 121, 234	0
1	G	236/242 (97%)	-0.14	5 (2%)	63	61	56, 74, 127, 186	0
1	H	236/242 (97%)	-0.12	6 (2%)	57	55	52, 74, 126, 210	0
1	I	236/242 (97%)	-0.34	1 (0%)	92	93	52, 72, 107, 134	0
1	J	236/242 (97%)	-0.17	7 (2%)	50	45	50, 70, 137, 226	0
1	K	236/242 (97%)	-0.23	4 (1%)	70	69	46, 64, 106, 174	0
1	L	236/242 (97%)	-0.20	4 (1%)	70	69	48, 67, 109, 153	0
1	M	236/242 (97%)	-0.16	9 (3%)	40	36	47, 65, 113, 200	0
1	N	236/242 (97%)	-0.25	1 (0%)	92	93	43, 69, 107, 136	0
1	O	236/242 (97%)	-0.15	7 (2%)	50	45	50, 70, 117, 195	0
1	P	236/242 (97%)	-0.13	5 (2%)	63	61	50, 75, 124, 192	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Q	236/242 (97%)	-0.12	7 (2%) 50 45	49, 66, 114, 216	0
1	R	236/242 (97%)	-0.19	6 (2%) 57 55	49, 78, 120, 199	0
1	S	236/242 (97%)	-0.04	6 (2%) 57 55	51, 69, 132, 179	0
1	T	236/242 (97%)	-0.14	7 (2%) 50 45	52, 79, 126, 202	0
1	U	236/242 (97%)	-0.06	5 (2%) 63 61	54, 79, 124, 160	0
1	V	236/242 (97%)	-0.21	6 (2%) 57 55	54, 69, 124, 206	0
1	W	236/242 (97%)	-0.15	8 (3%) 45 40	47, 70, 137, 215	0
1	X	236/242 (97%)	-0.20	5 (2%) 63 61	47, 69, 112, 148	0
1	Y	236/242 (97%)	-0.00	12 (5%) 28 24	57, 89, 142, 213	0
1	Z	236/242 (97%)	0.05	13 (5%) 25 21	56, 87, 136, 199	0
All	All	8024/8228 (97%)	-0.11	243 (3%) 50 45	43, 75, 128, 234	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	69	ASP	15.2
1	H	100	ASN	11.1
1	O	100	ASN	11.0
1	Q	100	ASN	10.7
1	H	101	LEU	10.2
1	J	101	LEU	10.0
1	4	100	ASN	10.0
1	7	104	ASN	9.3
1	J	100	ASN	9.3
1	E	100	ASN	9.1
1	R	100	ASN	8.6
1	P	100	ASN	8.5
1	F	101	LEU	7.9
1	E	104	ASN	7.9
1	4	101	LEU	7.8
1	Y	101	LEU	7.7
1	W	100	ASN	7.6
1	D	100	ASN	7.6
1	F	100	ASN	7.6
1	D	69	ASP	7.3
1	1	100	ASN	7.2
1	B	104	ASN	7.2
1	C	104	ASN	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	6	102	ALA	6.8
1	7	102	ALA	6.7
1	R	101	LEU	6.7
1	V	101	LEU	6.6
1	K	100	ASN	6.6
1	M	100	ASN	6.5
1	V	100	ASN	6.5
1	Y	100	ASN	6.5
1	O	104	ASN	6.4
1	S	100	ASN	6.4
1	6	104	ASN	6.3
1	V	104	ASN	6.3
1	C	101	LEU	6.2
1	Q	101	LEU	6.2
1	8	100	ASN	6.1
1	7	100	ASN	6.1
1	7	101	LEU	6.0
1	Z	104	ASN	6.0
1	4	104	ASN	5.9
1	8	104	ASN	5.9
1	F	99	GLY	5.8
1	K	101	LEU	5.8
1	W	104	ASN	5.6
1	F	104	ASN	5.5
1	6	101	LEU	5.4
1	E	101	LEU	5.3
1	A	104	ASN	5.3
1	H	104	ASN	5.2
1	6	103	GLY	5.2
1	3	104	ASN	5.2
1	T	104	ASN	5.2
1	X	100	ASN	5.1
1	6	100	ASN	5.1
1	Z	103	GLY	5.1
1	U	102	ALA	5.1
1	Z	101	LEU	5.1
1	Y	104	ASN	5.0
1	5	100	ASN	5.0
1	S	68	ARG	5.0
1	O	101	LEU	5.0
1	S	67	ARG	4.9
1	Q	99	GLY	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	100	ASN	4.9
1	H	99	GLY	4.9
1	Q	104	ASN	4.9
1	D	101	LEU	4.9
1	7	103	GLY	4.8
1	B	100	ASN	4.7
1	M	101	LEU	4.7
1	2	104	ASN	4.6
1	C	100	ASN	4.6
1	T	101	LEU	4.6
1	A	69	ASP	4.6
1	3	101	LEU	4.6
1	6	97	ASP	4.5
1	Y	102	ALA	4.5
1	Z	100	ASN	4.5
1	M	102	ALA	4.4
1	D	104	ASN	4.4
1	2	100	ASN	4.2
1	W	101	LEU	4.2
1	6	105	THR	4.2
1	2	101	LEU	4.2
1	1	102	ALA	4.2
1	R	97	ASP	4.2
1	Y	70	GLY	4.2
1	X	104	ASN	4.1
1	1	101	LEU	4.1
1	G	104	ASN	4.1
1	Q	103	GLY	4.1
1	M	105	THR	4.0
1	O	99	GLY	4.0
1	U	100	ASN	4.0
1	5	104	ASN	3.9
1	O	97	ASP	3.9
1	M	104	ASN	3.9
1	2	102	ALA	3.8
1	3	100	ASN	3.8
1	L	101	LEU	3.8
1	B	103	GLY	3.8
1	3	103	GLY	3.8
1	P	101	LEU	3.7
1	V	102	ALA	3.7
1	5	101	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1	98	SER	3.7
1	Z	228	ASP	3.7
1	5	97	ASP	3.7
1	J	104	ASN	3.7
1	L	102	ALA	3.7
1	1	99	GLY	3.6
1	R	102	ALA	3.6
1	C	103	GLY	3.6
1	W	67	ARG	3.6
1	G	100	ASN	3.6
1	4	102	ALA	3.5
1	C	102	ALA	3.5
1	1	104	ASN	3.5
1	S	101	LEU	3.5
1	5	201	ILE	3.5
1	2	103	GLY	3.5
1	F	102	ALA	3.5
1	J	102	ALA	3.5
1	Z	230	LEU	3.5
1	E	103	GLY	3.4
1	5	103	GLY	3.4
1	V	105	THR	3.4
1	O	98	SER	3.3
1	W	69	ASP	3.3
1	R	104	ASN	3.3
1	I	104	ASN	3.3
1	5	118	ALA	3.3
1	Y	105	THR	3.3
1	C	97	ASP	3.2
1	5	102	ALA	3.2
1	Z	102	ALA	3.1
1	3	102	ALA	3.1
1	H	97	ASP	3.1
1	7	99	GLY	3.1
1	N	104	ASN	3.1
1	4	99	GLY	3.1
1	G	131	GLY	3.0
1	P	97	ASP	3.0
1	W	103	GLY	3.0
1	Y	69	ASP	3.0
1	R	99	GLY	3.0
1	P	104	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	103	GLY	2.9
1	T	97	ASP	2.9
1	6	222	TRP	2.9
1	D	102	ALA	2.9
1	4	103	GLY	2.9
1	U	101	LEU	2.9
1	O	102	ALA	2.9
1	W	97	ASP	2.8
1	X	101	LEU	2.8
1	A	100	ASN	2.8
1	S	104	ASN	2.8
1	A	131	GLY	2.8
1	5	231	GLU	2.7
1	Y	99	GLY	2.7
1	7	77	PRO	2.6
1	D	103	GLY	2.6
1	J	103	GLY	2.6
1	L	104	ASN	2.6
1	Q	102	ALA	2.6
1	Z	226	LEU	2.6
1	L	100	ASN	2.6
1	5	238	SER	2.6
1	E	130	GLN	2.5
1	Z	231	GLU	2.5
1	E	97	ASP	2.5
1	M	71	ALA	2.5
1	Y	103	GLY	2.5
1	3	97	ASP	2.4
1	1	97	ASP	2.4
1	J	99	GLY	2.4
1	7	97	ASP	2.4
1	2	105	THR	2.4
1	3	131	GLY	2.4
1	U	104	ASN	2.4
1	V	97	ASP	2.3
1	D	105	THR	2.3
1	B	101	LEU	2.3
1	P	99	GLY	2.3
1	M	96	ARG	2.3
1	U	69	ASP	2.3
1	1	103	GLY	2.3
1	K	69	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	W	102	ALA	2.3
1	G	103	GLY	2.3
1	K	102	ALA	2.3
1	X	102	ALA	2.3
1	Z	224	ALA	2.3
1	T	40	GLY	2.3
1	4	40	GLY	2.3
1	2	97	ASP	2.3
1	4	97	ASP	2.3
1	7	69	ASP	2.3
1	B	105	THR	2.3
1	A	102	ALA	2.3
1	8	201	ILE	2.3
1	8	103	GLY	2.2
1	J	105	THR	2.2
1	2	117	ILE	2.2
1	A	40	GLY	2.2
1	F	69	ASP	2.2
1	C	118	ALA	2.2
1	A	103	GLY	2.2
1	Q	97	ASP	2.2
1	6	99	GLY	2.2
1	3	201	ILE	2.2
1	H	103	GLY	2.2
1	1	198	ASP	2.2
1	T	98	SER	2.2
1	5	232	ARG	2.2
1	1	118	ALA	2.1
1	Y	118	ALA	2.1
1	M	97	ASP	2.1
1	2	71	ALA	2.1
1	5	11	GLY	2.1
1	G	105	THR	2.1
1	B	88	GLU	2.1
1	Y	96	ARG	2.1
1	7	118	ALA	2.1
1	Z	70	GLY	2.1
1	F	131	GLY	2.1
1	6	221	GLN	2.1
1	8	198	ASP	2.1
1	6	215	PHE	2.1
1	Z	198	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2	221	GLN	2.0
1	X	69	ASP	2.0
1	3	98	SER	2.0
1	Z	105	THR	2.0
1	2	107	LEU	2.0
1	E	102	ALA	2.0
1	M	40	GLY	2.0
1	1	105	THR	2.0
1	T	102	ALA	2.0
1	Y	71	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.