



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:16 AM UTC

PDB ID : 5LOX / pdb_00005lox
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

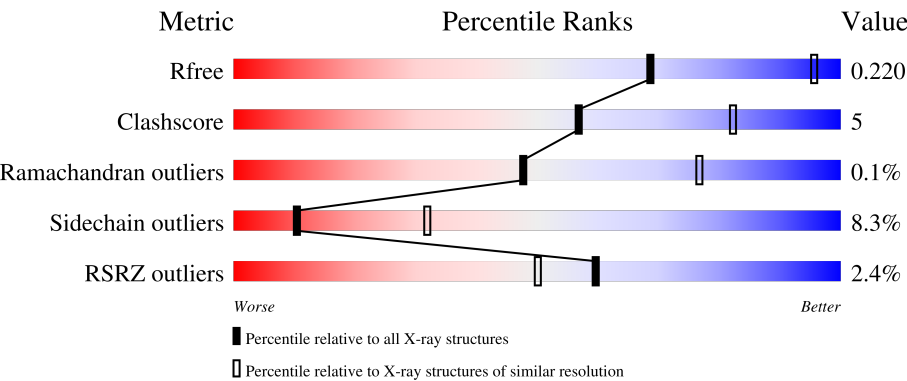
1 Overall quality at a glance i

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	242	2% 86% 12% .
1	2	242	3% 84% 14% .
1	3	242	2% 83% 14% .
1	4	242	% 86% 13% .
1	5	242	3% 87% 12% .

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Mol	Chain	Length	Quality of chain
1	6	242	
1	7	242	
1	8	242	
1	A	242	
1	B	242	
1	C	242	
1	D	242	
1	E	242	
1	F	242	
1	G	242	
1	H	242	
1	I	242	
1	J	242	
1	K	242	
1	L	242	
1	M	242	
1	N	242	
1	O	242	
1	P	242	
1	Q	242	
1	R	242	
1	S	242	
1	T	242	
1	U	242	
1	V	242	

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Mol	Chain	Length	Quality of chain
1	W	242	3% 85% 13%
1	X	242	3% 86% 12%
1	Y	242	% 85% 14%
1	Z	242	2% 86% 13%

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 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	B	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	C	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	D	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	E	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	F	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	G	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	H	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	I	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	J	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	K	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	L	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	M	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	N	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	O	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	P	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0

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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

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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

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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

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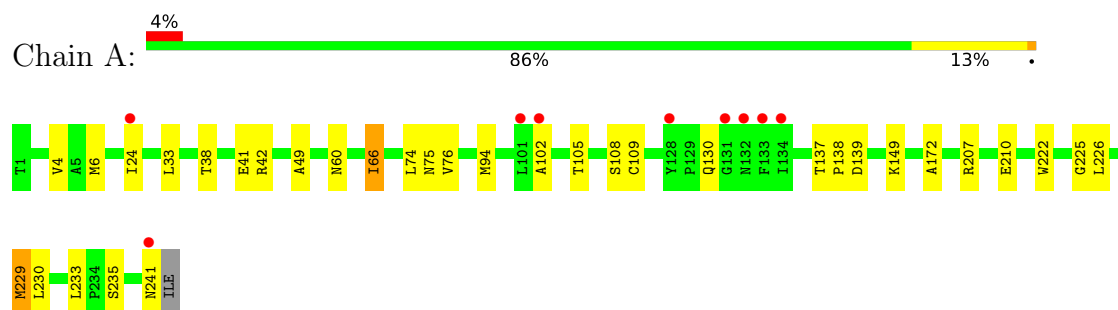
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Chain	Residue	Modelled	Actual	Comment	Reference
4	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
4	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
4	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	112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

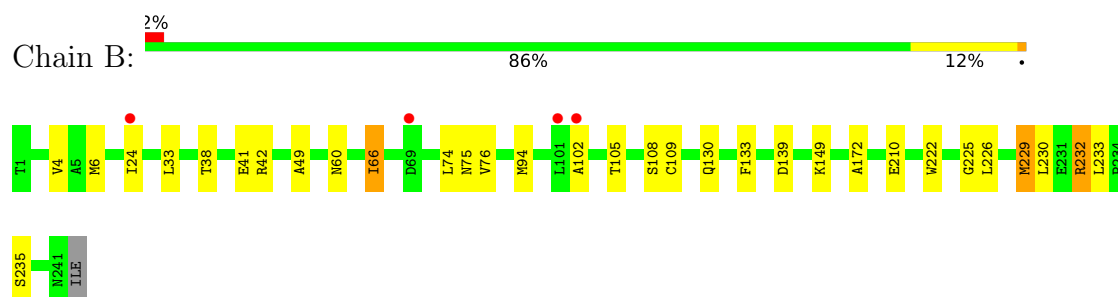
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

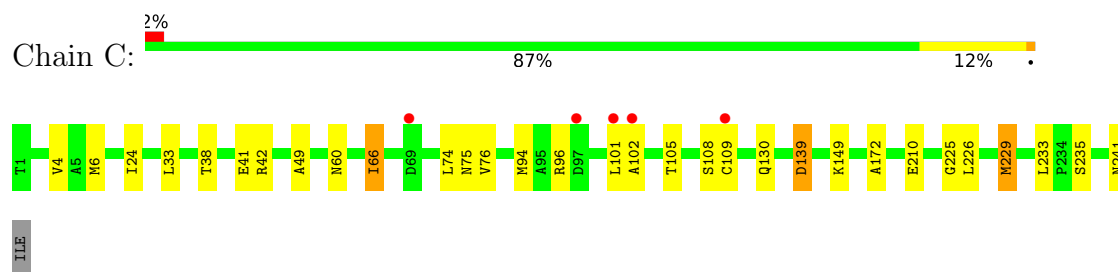
• Molecule 1: Peptidase



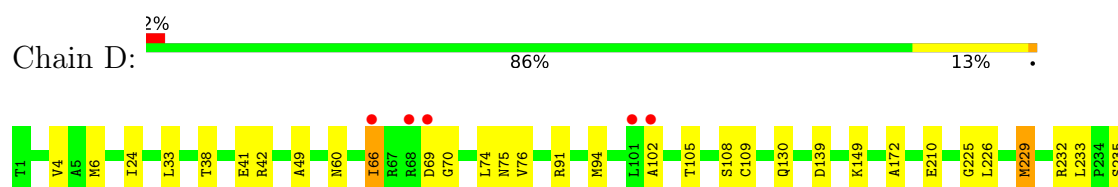
• Molecule 1: Peptidase



• Molecule 1: Peptidase

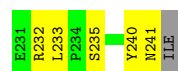
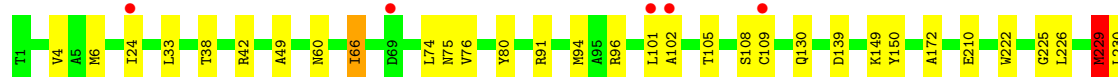
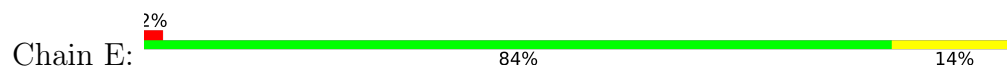


• Molecule 1: Peptidase

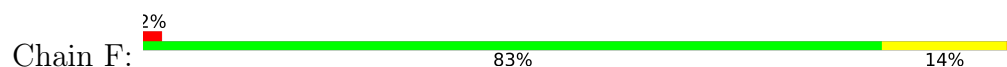




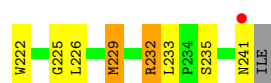
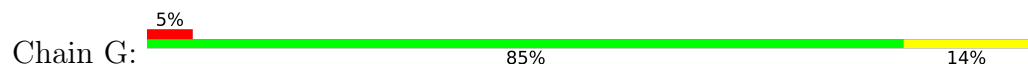
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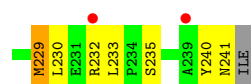
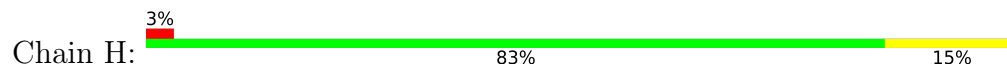
• Molecule 1: Peptidase



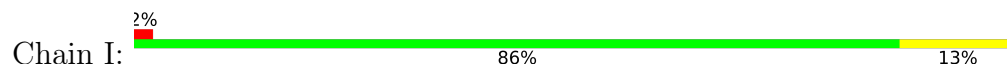
• Molecule 1: Peptidase

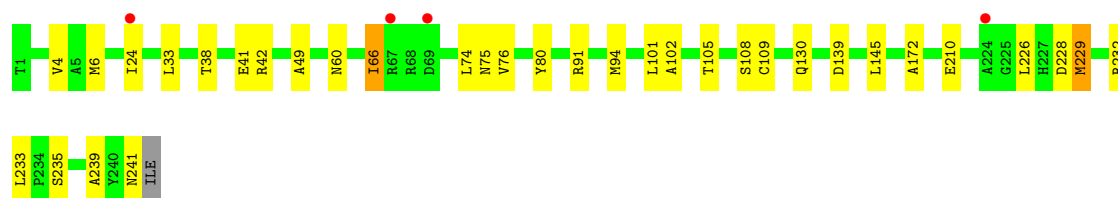


• Molecule 1: Peptidase

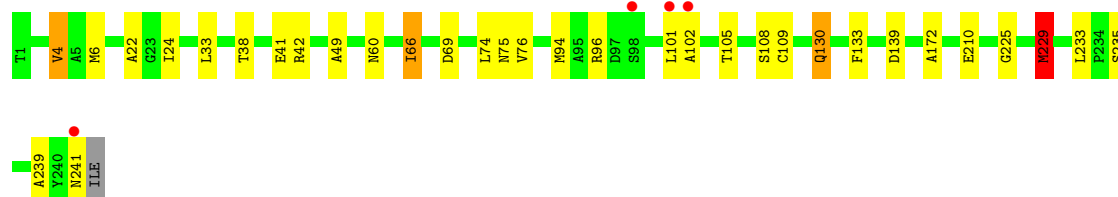
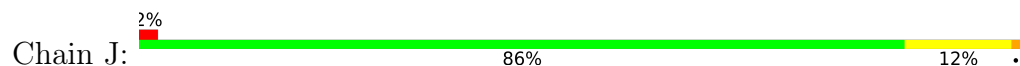


• Molecule 1: Peptidase

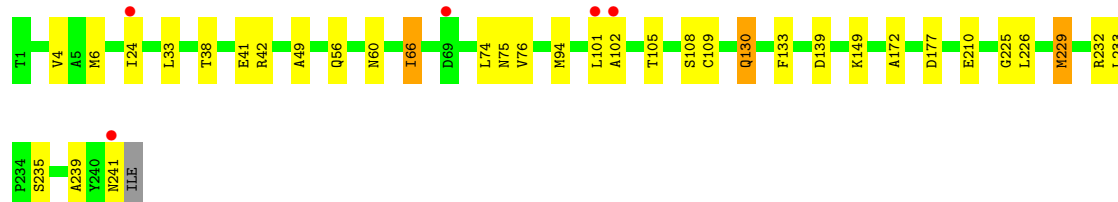
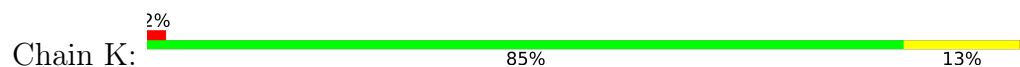




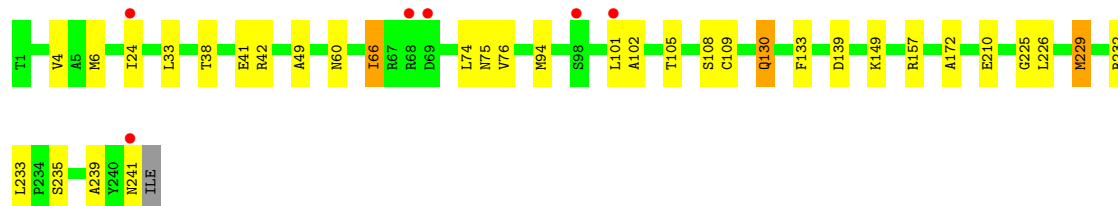
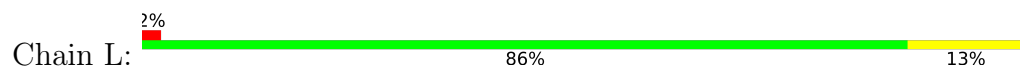
• Molecule 1: Peptidase



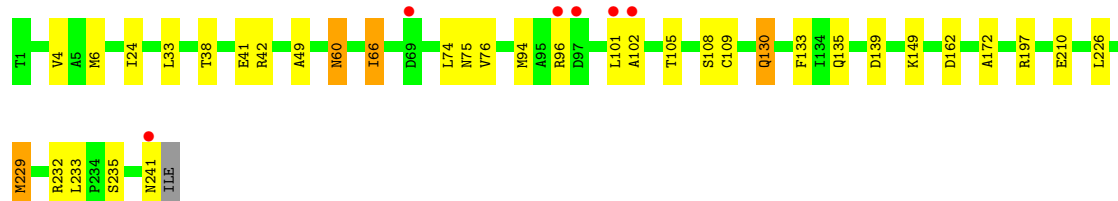
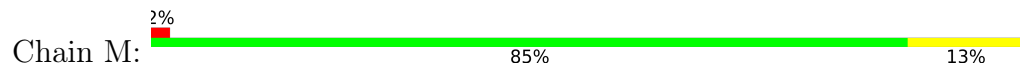
• Molecule 1: Peptidase



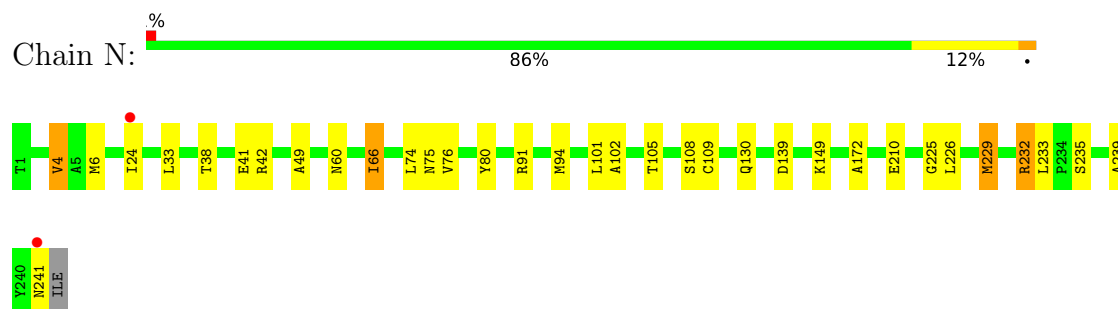
• Molecule 1: Peptidase



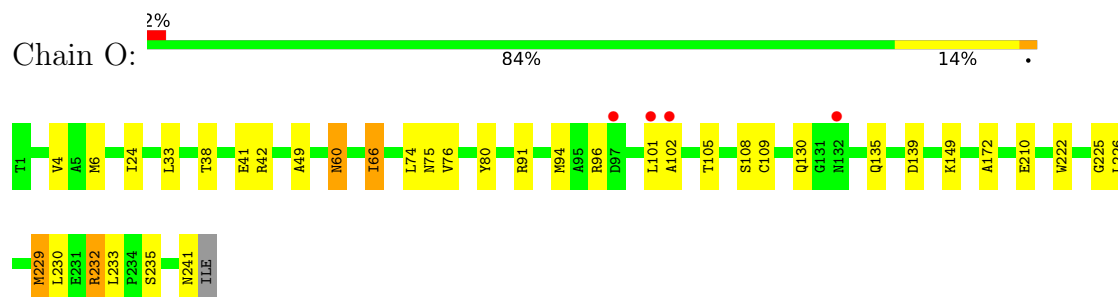
• Molecule 1: Peptidase



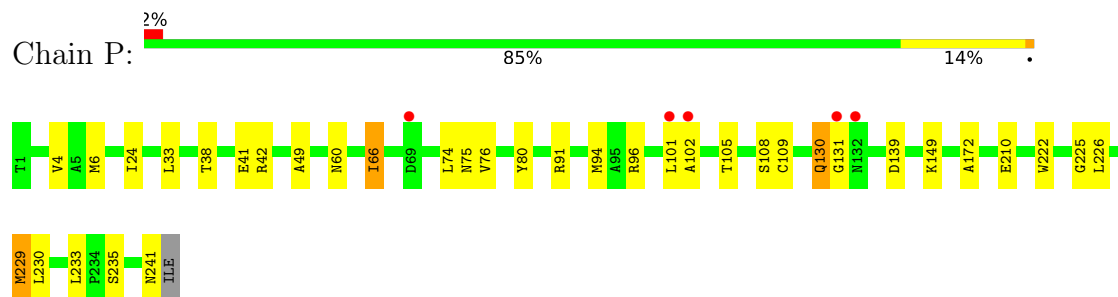
● Molecule 1: Peptidase



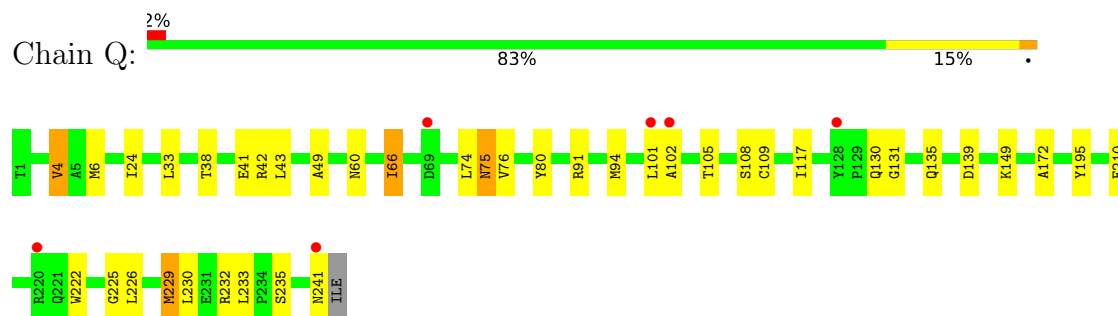
● Molecule 1: Peptidase



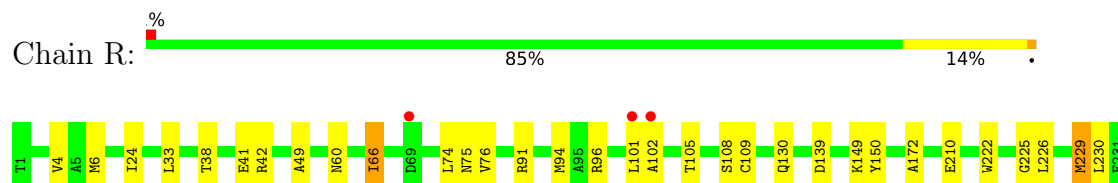
● Molecule 1: Peptidase



● Molecule 1: Peptidase

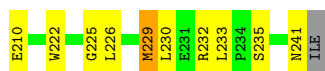
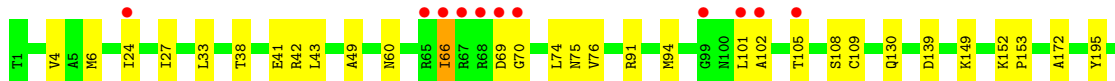
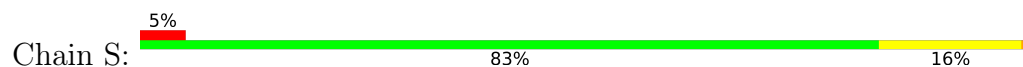


● Molecule 1: Peptidase

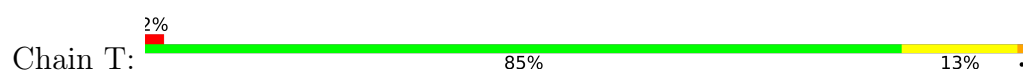




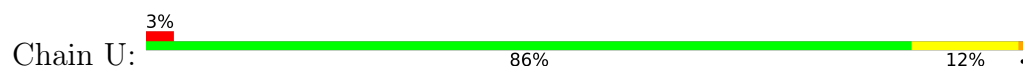
- Molecule 1: Peptidase



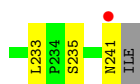
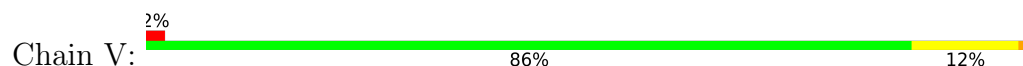
- Molecule 1: Peptidase



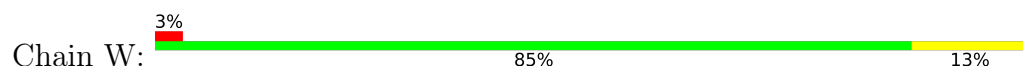
- Molecule 1: Peptidase

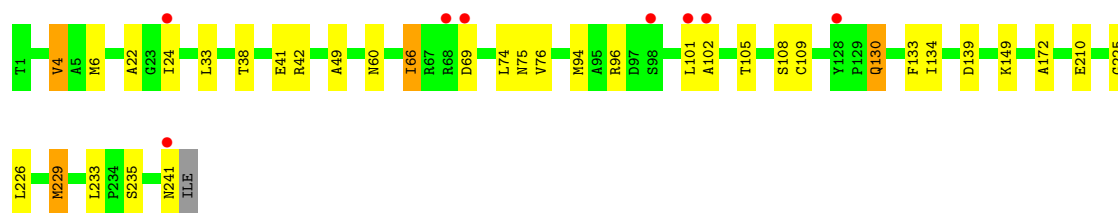


- Molecule 1: Peptidase

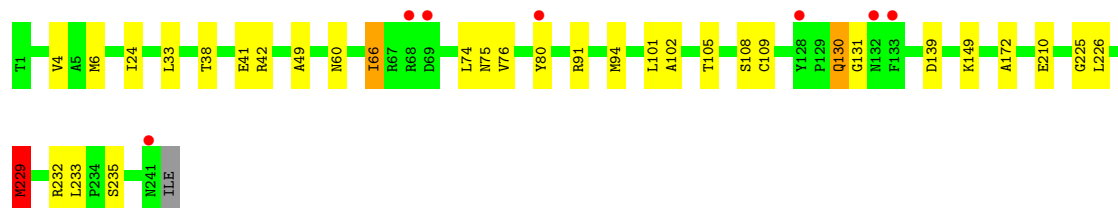
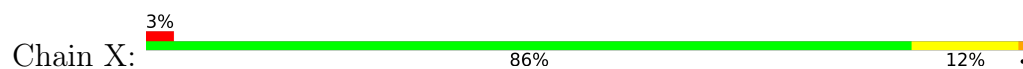


- Molecule 1: Peptidase

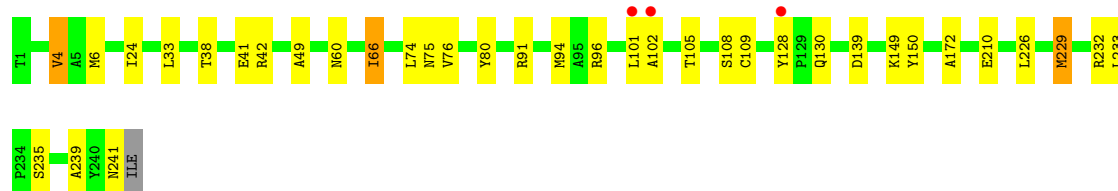
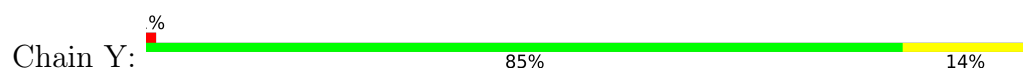




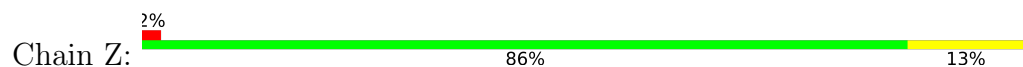
• Molecule 1: Peptidase



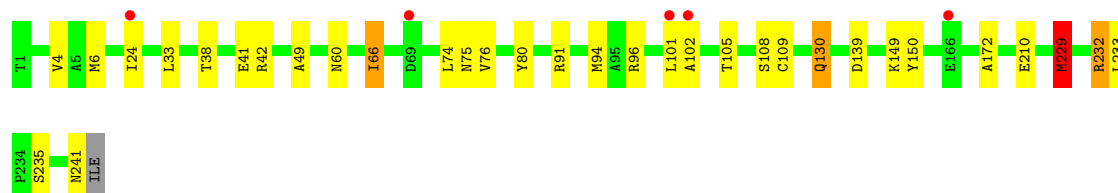
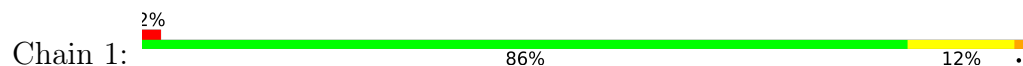
• Molecule 1: Peptidase



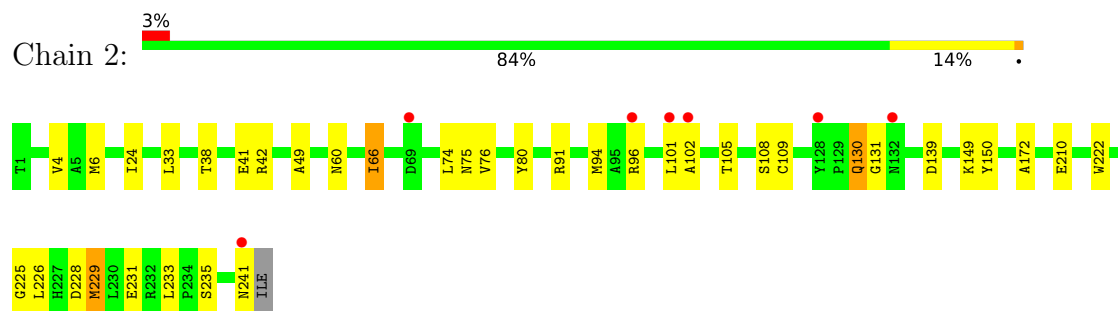
• Molecule 1: Peptidase



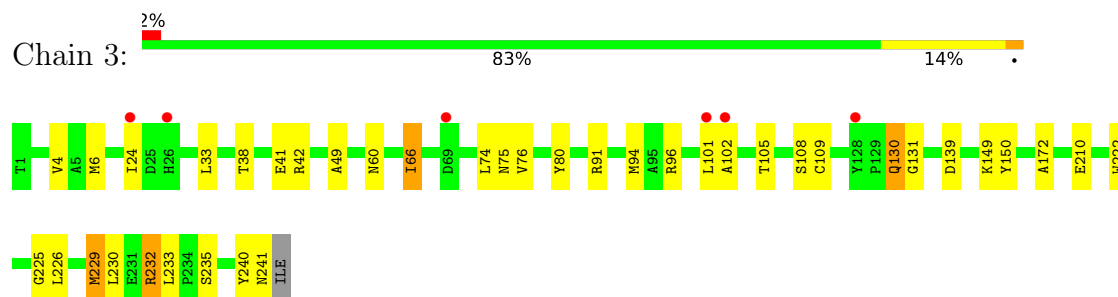
• Molecule 1: Peptidase



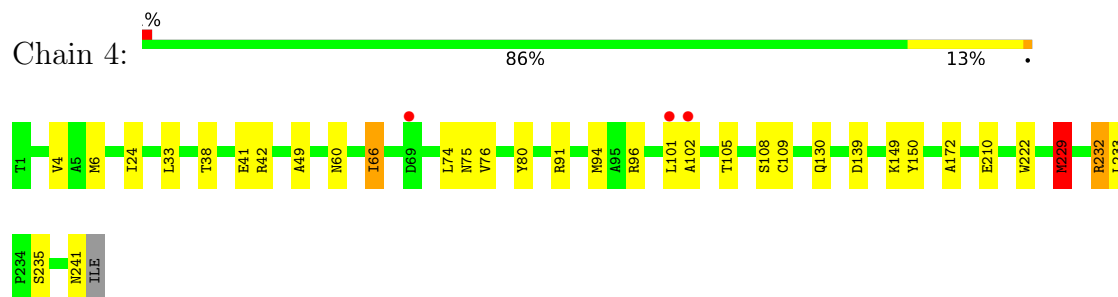
• Molecule 1: Peptidase



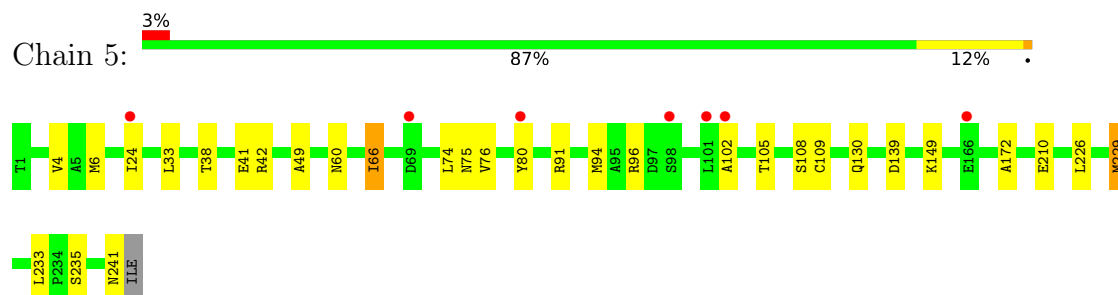
• Molecule 1: Peptidase



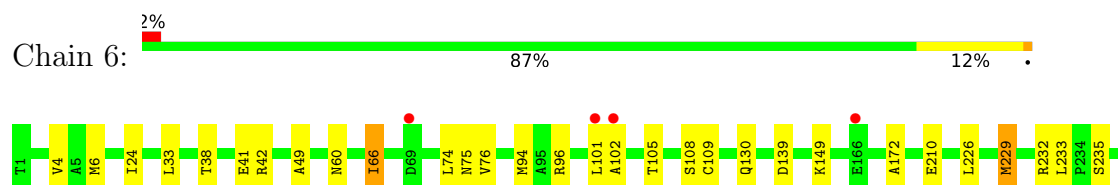
• Molecule 1: Peptidase



• Molecule 1: Peptidase

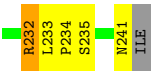
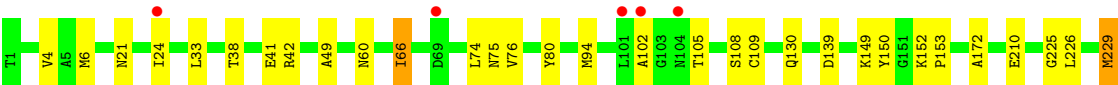
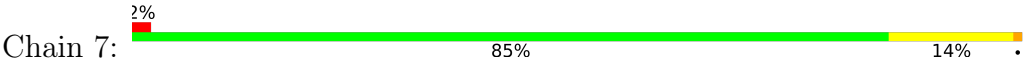


• Molecule 1: Peptidase

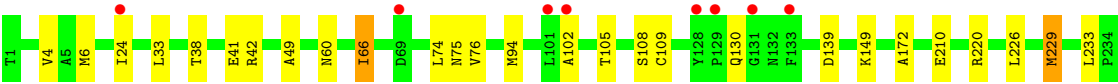
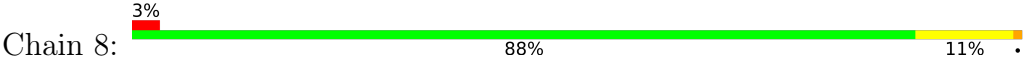




● Molecule 1: Peptidase



● Molecule 1: Peptidase



4 Data and refinement statistics

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 39.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.60-2.90) 99.9 (39.60-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.00%)	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)	0.30 , 43.0	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	0.95	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.*

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	0.81	0/1862	0.93	3/2530 (0.1%)
1	2	0.79	0/1862	0.87	0/2530
1	3	0.82	0/1862	0.89	2/2530 (0.1%)
1	4	0.81	0/1862	0.92	2/2530 (0.1%)
1	5	0.76	0/1862	0.86	0/2530
1	6	0.77	0/1862	0.87	0/2530
1	7	0.84	0/1862	0.89	2/2530 (0.1%)
1	8	0.83	0/1862	0.88	1/2530 (0.0%)
1	A	0.88	0/1862	0.89	0/2530
1	B	0.82	0/1862	0.91	3/2530 (0.1%)
1	C	0.83	0/1862	0.89	0/2530
1	D	0.84	0/1862	0.90	1/2530 (0.0%)
1	E	0.85	0/1862	0.98	7/2530 (0.3%)
1	F	0.95	2/1862 (0.1%)	0.96	5/2530 (0.2%)
1	G	0.87	0/1862	0.90	1/2530 (0.0%)
1	H	0.83	0/1862	0.90	3/2530 (0.1%)
1	I	0.86	1/1862 (0.1%)	0.88	0/2530
1	J	0.86	0/1862	0.93	4/2530 (0.2%)
1	K	0.90	0/1862	0.90	1/2530 (0.0%)
1	L	0.87	0/1862	0.91	1/2530 (0.0%)
1	M	0.90	0/1862	0.93	1/2530 (0.0%)
1	N	0.85	0/1862	0.91	3/2530 (0.1%)
1	O	0.86	0/1862	0.91	1/2530 (0.0%)
1	P	0.85	0/1862	0.88	0/2530
1	Q	0.90	0/1862	0.89	1/2530 (0.0%)
1	R	0.83	0/1862	0.88	0/2530
1	S	0.87	0/1862	0.90	0/2530
1	T	0.84	0/1862	0.89	2/2530 (0.1%)
1	U	0.84	0/1862	0.94	5/2530 (0.2%)
1	V	0.85	0/1862	0.92	3/2530 (0.1%)
1	W	0.89	0/1862	0.92	3/2530 (0.1%)
1	X	0.89	1/1862 (0.1%)	0.90	0/2530
1	Y	0.80	0/1862	0.86	1/2530 (0.0%)
1	Z	0.79	0/1862	0.88	1/2530 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.85	4/63308 (0.0%)	0.90	57/86020 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	221	GLN	CD-OE1	-7.61	1.09	1.23
1	I	145	LEU	CA-C	-5.28	1.46	1.52
1	X	229	MSE	SE-CE	5.22	2.11	1.95
1	F	221	GLN	N-CA	5.04	1.52	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	229	MSE	N-CA-CB	-13.66	89.57	110.06
1	E	229	MSE	CA-CB-CG	-11.12	91.86	114.10
1	4	229	MSE	CG-SE-CE	10.11	121.16	98.92
1	1	229	MSE	CG-SE-CE	9.57	119.97	98.92
1	U	229	MSE	CG-SE-CE	-9.33	78.40	98.92
1	U	229	MSE	N-CA-CB	-8.86	96.77	110.06
1	F	221	GLN	CG-CD-NE2	8.48	129.12	116.40
1	F	133	PHE	CB-CA-C	-8.28	91.86	110.07
1	1	232	ARG	CB-CA-C	-7.40	94.52	109.99
1	U	229	MSE	CA-CB-CG	-7.40	99.31	114.10
1	N	232	ARG	CA-CB-CG	7.39	128.89	114.10
1	J	229	MSE	CG-SE-CE	7.35	115.09	98.92
1	1	232	ARG	N-CA-C	6.30	120.71	112.89
1	T	232	ARG	CD-NE-CZ	6.20	133.08	124.40
1	8	75	ASN	CB-CG-ND2	-6.05	107.32	116.40
1	V	75	ASN	CB-CG-ND2	-6.05	107.33	116.40
1	W	75	ASN	CB-CG-ND2	-6.03	107.36	116.40
1	F	133	PHE	CA-CB-CG	6.02	119.82	113.80
1	D	75	ASN	CB-CG-ND2	-6.02	107.38	116.40
1	4	75	ASN	CB-CG-ND2	-5.99	107.42	116.40
1	E	75	ASN	CB-CG-ND2	-5.98	107.43	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASN	CB-CG-ND2	-5.96	107.46	116.40
1	F	221	GLN	CG-CD-OE1	-5.86	109.08	120.80
1	E	240	TYR	N-CA-C	5.78	120.07	113.19
1	W	133	PHE	N-CA-C	5.78	117.97	109.24
1	M	133	PHE	N-CA-C	5.74	117.91	109.24
1	O	232	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	J	229	MSE	CB-CG-SE	-5.50	96.21	112.70
1	7	232	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	Q	4	VAL	CB-CA-C	-5.44	101.98	110.69
1	W	4	VAL	CB-CA-C	-5.40	101.36	110.71
1	J	133	PHE	N-CA-C	5.40	117.39	109.24
1	N	232	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	E	229	MSE	CG-SE-CE	5.36	110.71	98.92
1	E	229	MSE	N-CA-C	5.34	117.80	111.33
1	K	133	PHE	N-CA-C	5.31	117.26	109.24
1	Z	240	TYR	N-CA-C	5.31	119.51	113.19
1	E	229	MSE	CB-CA-C	-5.29	101.68	110.68
1	H	240	TYR	N-CA-C	5.25	119.44	113.19
1	F	133	PHE	N-CA-C	5.25	117.17	109.24
1	V	133	PHE	N-CA-C	5.25	117.16	109.24
1	B	232	ARG	N-CA-CB	-5.21	102.29	110.46
1	L	133	PHE	N-CA-C	5.20	117.09	109.24
1	T	232	ARG	CB-CG-CD	-5.19	99.37	111.30
1	7	21	ASN	CB-CG-ND2	-5.13	108.70	116.40
1	3	240	TYR	N-CA-C	5.08	119.24	113.19
1	U	4	VAL	CB-CA-C	-5.08	102.56	110.69
1	H	133	PHE	N-CA-C	5.07	116.89	109.24
1	3	232	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	U	133	PHE	N-CA-C	5.06	116.88	109.24
1	J	4	VAL	CB-CA-C	-5.05	102.61	110.69
1	G	232	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	V	4	VAL	CB-CA-C	-5.04	102.64	110.69
1	N	4	VAL	CB-CA-C	-5.03	102.65	110.69
1	Y	4	VAL	CB-CA-C	-5.01	101.73	110.71
1	H	4	VAL	CB-CA-C	-5.01	102.67	110.69
1	B	133	PHE	N-CA-C	5.00	116.79	109.24

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 ⓘ

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	31	0
1	2	1829	0	1800	32	2
1	3	1829	0	1800	29	0
1	4	1829	0	1800	27	1
1	5	1829	0	1800	17	0
1	6	1829	0	1800	15	0
1	7	1829	0	1800	18	1
1	8	1829	0	1800	16	1
1	A	1829	0	1800	21	0
1	B	1829	0	1800	18	0
1	C	1829	0	1800	19	0
1	D	1829	0	1800	19	0
1	E	1829	0	1800	37	0
1	F	1829	0	1800	46	1
1	G	1829	0	1800	33	0
1	H	1829	0	1800	42	0
1	I	1829	0	1800	19	1
1	J	1829	0	1800	22	0
1	K	1829	0	1800	24	0
1	L	1829	0	1800	24	0
1	M	1829	0	1800	22	2
1	N	1829	0	1800	19	0
1	O	1829	0	1800	34	1
1	P	1829	0	1800	33	0
1	Q	1829	0	1800	37	0
1	R	1829	0	1800	34	0
1	S	1829	0	1800	29	0
1	T	1829	0	1800	19	0
1	U	1829	0	1800	18	2
1	V	1829	0	1800	18	0
1	W	1829	0	1800	29	0
1	X	1829	0	1800	27	0
1	Y	1829	0	1800	32	0
1	Z	1829	0	1800	32	0
All	All	62186	0	61200	573	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 5.

All (573) 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:W:101:LEU:HD22	1:Y:91:ARG:HG2	1.44	0.98
1:I:101:LEU:HD22	1:3:91:ARG:CG	1.93	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

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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:W:229:MSE:HE1	1:X:229:MSE:CE	2.04	0.86
1:2:91:ARG:HG3	1:4:101:LEU:HD22	1.58	0.86
1:S:229:MSE:CE	1:T:229:MSE:HE1	2.06	0.86
1:G:229:MSE:CE	1:H:229:MSE:HE1	2.05	0.85
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: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: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
1:1:101:LEU:HD22	1:3:91:ARG:HG3	1.65	0.77
1:M:229:MSE:CE	1:N:229:MSE:HE1	2.14	0.77

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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:X:80:TYR:OH	1:Z:96:ARG:NH1	2.19	0.75
1:Y:101:LEU:HD22	1:1:91:ARG:CG	2.16	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:W:229:MSE:CE	1:X:229:MSE:CE	2.66	0.69
1:2:80:TYR:OH	1:4:96:ARG:NH1	2.24	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:C:229:MSE:CE	1:D:229:MSE:CE	2.71	0.69
1:2:80:TYR:OH	1:4:96:ARG:NH2	2.25	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:L:102:ALA:O	1:L:105:THR:HG22	1.94	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: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:U:102:ALA:O	1:U: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:5:102:ALA:O	1:5:105: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:S:102:ALA:O	1:S: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: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: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
1:8:102:ALA:O	1:8:105: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:E:229:MSE:SE	1:F:229:MSE:HE2	2.47	0.64
1:5:229:MSE:CE	1:6:229:MSE:HE1	2.25	0.64
1:4:91:ARG:CG	1:6:101:LEU:HD22	2.27	0.64

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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: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
1:2:94:MSE:HE1	1:2:108:SER:HA	1.82	0.62
1:J:69:ASP:CB	1:W:69:ASP:C	2.70	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:Z:94:MSE:HE1	1:Z:108:SER:HA	1.81	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: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:R:94:MSE:HE1	1:R:108:SER:HA	1.82	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: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:F:42:ARG:HH21	1:S:69:ASP:HA	1.66	0.61
1:7:94:MSE:HE1	1:7:108:SER:HA	1.82	0.61
1:G:94:MSE:HE1	1:G:108:SER:HA	1.83	0.61
1:Q:229:MSE:SE	1:R:229:MSE:HE1	2.51	0.61
1:2:80:TYR:OH	1:4:96:ARG:CZ	2.48	0.61
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
1:4:80:TYR:OH	1:6:96:ARG:NH2	2.34	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:H:94:MSE:HE1	1:H:108:SER:HA	1.82	0.60
1:1:229:MSE:HE2	1:2:229:MSE:HE1	1.84	0.60
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
1:K:94:MSE:HE1	1:K:108:SER:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:94:MSE:HE1	1:6:108:SER:HA	1.83	0.59
1:N:94:MSE:HE1	1:N:108:SER:HA	1.84	0.59
1:X:80:TYR:OH	1:Z:96:ARG:CZ	2.50	0.59
1:X:94:MSE:HE1	1:X:108:SER:HA	1.83	0.59
1:Y:94:MSE:HE1	1:Y:108:SER:HA	1.83	0.59
1:1:94:MSE:HE1	1:1:108: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:M:96:ARG:HH22	1:O:80:TYR:HH	1.48	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:W:94:MSE:HE1	1:W:108:SER:HA	1.85	0.59
1:3:96:ARG:NH2	1:5:80:TYR:OH	2.36	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:W:226:LEU:HA	1:W:229:MSE:HE3	1.85	0.58
1:6:226:LEU:HA	1:6:229:MSE:HE3	1.86	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:X:80:TYR:OH	1:Z:96:ARG:NH2	2.37	0.57
1:5:94:MSE:HE1	1:5:108:SER:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:91:ARG:HH21	1:R:101:LEU:HD23	1.70	0.56
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: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
1:1:101:LEU:HD21	1:3:131:GLY:HA3	1.87	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:P:80:TYR:OH	1:R:96:ARG:NH2	2.40	0.55
1:Q:6:MSE:HE1	1:Q:172:ALA:HB2	1.89	0.55
1:3:226:LEU:HA	1:3:229:MSE:HE3	1.87	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: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
1:1:150:TYR:OH	1:2:149:LYS:HD3	2.07	0.54
1:P:226:LEU:HA	1:P:229:MSE:HE3	1.88	0.54
1:1:229:MSE:SE	1:2:225:GLY:HA3	2.57	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: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
1:1:6:MSE:HE1	1:1:172:ALA:HB2	1.90	0.54
1:1:149:LYS:HD3	1:2:150:TYR:OH	2.08	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
1:5:229:MSE:CE	1:6:229:MSE:CE	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:6:MSE:HE1	1:S:172:ALA:HB2	1.90	0.53
1:Y:226:LEU:HA	1:Y:229:MSE:HE3	1.90	0.53
1:A:226:LEU:HA	1:A:229:MSE:HE3	1.89	0.53
1:5:6:MSE:HE1	1:5:172: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
1:1:101: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:U:149:LYS:HB2	1:V:149:LYS:HB2	1.89	0.53
1:7:6:MSE:HE1	1:7:172: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
1:2:6:MSE:HE1	1:2:172:ALA:HB2	1.91	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:E:149:LYS:HB2	1:F:149:LYS:HB2	1.91	0.53
1:F:80:TYR:HH	1:H:96:ARG:HH12	1.48	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
1:4:6:MSE:HE1	1:4:172:ALA:HB2	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: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
1:3:6:MSE:HE1	1:3:172:ALA:HB2	1.91	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
1:7:229:MSE:SE	1:8:229:MSE:HE1	2.59	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:B:6:MSE:HE1	1:B:172:ALA:HB2	1.92	0.52
1:8:6:MSE:HE1	1:8:172:ALA:HB2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:6:MSE:HE1	1:E:172:ALA:HB2	1.92	0.50
1:3:225:GLY:HA3	1:4:229:MSE:SE	2.61	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:91:ARG:NH2	1:H:101:LEU:HD22	2.22	0.50
1:F:226:LEU:HA	1:F:229:MSE:HE3	1.94	0.50
1:P:80:TYR:HH	1:R:96:ARG:HH12	1.59	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:X:226:LEU:HA	1:X:229:MSE:HE3	1.95	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: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: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
1:3:101:LEU:HD22	1:5:91:ARG:CG	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:66:ILE:HG12	1:O:74:LEU:HG	1.95	0.48
1:P:33:LEU:C	1:P:33:LEU:HD23	2.38	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:X:33:LEU:HD23	1:X:33:LEU:C	2.39	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:S:66:ILE:HG12	1:S:74:LEU:HG	1.95	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: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:N:33:LEU:HD23	1:N:33:LEU:C	2.39	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
1:3:49:ALA:O	1:3:109:CYS:HB2	2.15	0.47
1:D:70:GLY:HA2	1:Q:75:ASN:O	2.14	0.47
1:L:66:ILE:HG12	1:L:74:LEU:HG	1.97	0.47
1:U:49:ALA:O	1:U: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: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:R:33:LEU:C	1:R:33:LEU:HD23	2.39	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
1:2:91:ARG:HH21	1:4:101:LEU:HD23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:66:ILE:HG12	1:5:74:LEU:HG	1.96	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
1:1:101: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: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
1:N:49:ALA:O	1:N:109:CYS:HB2	2.15	0.47
1:N:91:ARG:HG2	1:P:101:LEU:HD22	1.95	0.47
1:O:229:MSE:SE	1:P:225:GLY:HA3	2.64	0.47
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
1:1:66: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: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:W:96:ARG:NH1	1:Y:80:TYR:OH	2.48	0.46
1:7:49:ALA:O	1:7:109:CYS:HB2	2.15	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
1:4:49: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:X:49:ALA:O	1:X:109:CYS:HB2	2.15	0.46
1:7:66:ILE:HG12	1:7:74:LEU:HG	1.96	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:HE3	1:X:229:MSE:HB2	1.75	0.46
1:7:33:LEU:C	1:7:33:LEU:HD23	2.41	0.46
1:A:66:ILE:HG12	1:A:74:LEU:HG	1.97	0.46
1:M:33:LEU:C	1:M:33:LEU:HD23	2.41	0.46
1:A:49:ALA:O	1:A:109:CYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:3:66:ILE:HG12	1:3:74: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
1:Q:149:LYS:HD3	1:R:150:TYR:OH	2.16	0.45
1:8:66:ILE:HG12	1:8:74:LEU:HG	1.97	0.45
1:G:222:TRP:CH2	1:H:230:LEU:HD13	2.52	0.45
1:D:33:LEU:HD23	1:D:33:LEU:C	2.42	0.45
1:S:33:LEU:HD23	1:S:33:LEU:C	2.42	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
1:3:96:ARG:HH22	1:5:80:TYR:HH	1.64	0.45
1:E:101:LEU:HD22	1:G:91:ARG:HG2	1.94	0.45
1:8:33:LEU:HD23	1:8:33:LEU:C	2.42	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:HE3	1:S:229:MSE:HB2	1.79	0.45
1:2:131:GLY:HA3	1:4:101:LEU:CD2	2.46	0.45
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
1:1:150: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:D:229:MSE:HE3	1:D:229:MSE:HB2	1.76	0.44
1:I:66:ILE:HG12	1:I:74:LEU:HG	1.99	0.44
1:L:229:MSE:HE3	1:L:229:MSE:HB2	1.77	0.44
1:W:33:LEU:C	1:W:33:LEU:HD23	2.42	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:Q:43:LEU:HD22	1:Q:195:TYR:CD1	2.53	0.44
1:Y:33:LEU:C	1:Y:33:LEU:HD23	2.43	0.44
1:Z:80:TYR:OH	1:2:96:ARG:CZ	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:222:TRP:CH2	1:4:229:MSE:HE3	2.53	0.44
1:O:229:MSE:HE3	1:O:229:MSE:HB2	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:V:33:LEU:C	1:V:33:LEU:HD23	2.43	0.43
1:K:229:MSE:HE3	1:K:229:MSE:HB2	1.79	0.43
1:U:56:GLN:OE1	1:W:134:ILE:HA	2.18	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
1:3:150:TYR:OH	1:4:149:LYS:HD3	2.19	0.43
1:F:33:LEU:C	1:F:33:LEU:HD23	2.43	0.43
1:I:33:LEU:HD23	1:I:33:LEU:C	2.43	0.43
1:K:177:ASP:OD2	1:L:157:ARG:NH2	2.52	0.43
1:W:229:MSE:HE3	1:W:229:MSE:HB2	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
1:4:33:LEU:C	1:4:33:LEU:HD23	2.44	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
1:3:230:LEU:HD13	1:4:222:TRP:CH2	2.54	0.43
1:2:33:LEU:C	1:2:33:LEU:HD23	2.44	0.42
1:S:101:LEU:HG	1:U:130:GLN:HA	2.01	0.42
1:O:96:ARG:CZ	1:Q:80:TYR:OH	2.67	0.42
1:2:229:MSE:HE3	1:2:229:MSE:HB2	1.82	0.42
1:W:229:MSE:SE	1:X:225:GLY:HA3	2.69	0.42
1:7:149:LYS:HB2	1:8:149:LYS:HB2	2.01	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:K:33:LEU:C	1:K:33:LEU:HD23	2.43	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
1:1:33:LEU:HD23	1:1:33:LEU:C	2.44	0.42
1:B:33:LEU:HD23	1:B:33:LEU:C	2.44	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
1:7:152:LYS:N	1:7:153:PRO:CD	2.83	0.42
1:U:225:GLY:HA3	1:V:229:MSE:SE	2.69	0.42
1:K:56:GLN:OE1	1:M:135:GLN:N	2.40	0.42
1:K:225:GLY:HA3	1:L:229:MSE:SE	2.70	0.42
1:1:229:MSE:HE3	1:2:222:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LEU:C	1:E:33:LEU:HD23	2.44	0.42
1:Y:101:LEU:HG	1:1:130:GLN:O	2.20	0.42
1:3:33:LEU:HD23	1:3:33:LEU:C	2.45	0.42
1:P:229:MSE:HE3	1:P:229:MSE:HB2	1.76	0.41
1:S:43:LEU:HD22	1:S:195:TYR:CD1	2.55	0.41
1:7:150:TYR:OH	1:8:149:LYS:HD3	2.20	0.41
1:C:33:LEU:C	1:C:33:LEU:HD23	2.46	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
1:1:150: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:M:60:ASN:ND2	1:O:135:GLN:OE1	2.54	0.41
1:O:33:LEU:C	1:O:33:LEU:HD23	2.46	0.41
1:Y:149:LYS:HD3	1:Z:150:TYR:CZ	2.55	0.41
1:6:33:LEU:C	1:6:33:LEU:HD23	2.45	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:O:60:ASN:ND2	1:Q:135:GLN:HE22	2.18	0.41
1:H:229:MSE:HE3	1:H:229:MSE:HB2	1.78	0.41
1:K:229:MSE:SE	1:L:225:GLY:HA3	2.70	0.41
1:Y:96:ARG:NH1	1:1:80:TYR:OH	2.53	0.41
1:A:33:LEU:C	1:A:33:LEU:HD23	2.45	0.41
1:O:229:MSE:SE	1:P:229:MSE:HE1	2.71	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
1:1:149:LYS:HB2	1:2:149:LYS:HB2	2.02	0.41
1:A:229:MSE:HE3	1:A:229:MSE:HB2	1.78	0.41
1:J:33:LEU:C	1:J:33:LEU:HD23	2.46	0.41
1:Q:33:LEU:C	1:Q:33:LEU:HD23	2.46	0.41
1:S:152:LYS:N	1:S:153:PRO:CD	2.84	0.41
1:3:222:TRP:CZ2	1:4:229:MSE:HE3	2.56	0.41
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
1:3:149:LYS:HB2	1:4:149:LYS:HB2	2.02	0.40
1:C:229:MSE:HE3	1:C:229:MSE:HB2	1.78	0.40
1:T:33:LEU:C	1:T:33:LEU:HD23	2.47	0.40
1:U:33:LEU:HD23	1:U:33:LEU:C	2.46	0.40
1:A:207:ARG:NH1	1:C:139:ASP:OD2	2.29	0.40
1:L:33:LEU:C	1:L:33:LEU:HD23	2.46	0.40
1:H:51:ASN:OD1	1:H:51:ASN:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:172:ALA:O	1:T:175:SER:HB3	2.22	0.40
1:5:33:LEU:HD23	1:5:33:LEU:C	2.47	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30	59
1	J	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	30	59
1	K	239/242 (99%)	230 (96%)	8 (3%)	1 (0%)	30	59
1	L	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	30	59
1	M	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	N	239/242 (99%)	228 (95%)	10 (4%)	1 (0%)	30	59
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
1	Y	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	30	59
1	Z	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
All	All	8126/8228 (99%)	7785 (96%)	335 (4%)	6 (0%)	48	77

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

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Mol	Chain	Res	Type
1	Y	239	ALA

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	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	2	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	3	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	4	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	5	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	6	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	7	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	8	197/197 (100%)	182 (92%)	15 (8%)	12	36
1	A	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	B	197/197 (100%)	182 (92%)	15 (8%)	12	36
1	C	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	D	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	E	197/197 (100%)	182 (92%)	15 (8%)	12	36
1	F	197/197 (100%)	178 (90%)	19 (10%)	8	26
1	G	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	H	197/197 (100%)	179 (91%)	18 (9%)	9	28
1	I	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	J	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	K	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	L	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	M	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	N	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	O	197/197 (100%)	181 (92%)	16 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	Q	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	R	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	S	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	T	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	U	197/197 (100%)	183 (93%)	14 (7%)	13	40
1	V	197/197 (100%)	182 (92%)	15 (8%)	12	36
1	W	197/197 (100%)	182 (92%)	15 (8%)	12	36
1	X	197/197 (100%)	181 (92%)	16 (8%)	11	33
1	Y	197/197 (100%)	180 (91%)	17 (9%)	10	30
1	Z	197/197 (100%)	180 (91%)	17 (9%)	10	30
All	All	6698/6698 (100%)	6141 (92%)	557 (8%)	10	32

All (557) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
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	76	VAL
1	A	130	GLN
1	A	139	ASP
1	A	210	GLU
1	A	229	MSE
1	A	233	LEU
1	A	235	SER
1	A	241	ASN
1	B	4	VAL
1	B	24	ILE
1	B	38	THR
1	B	41	GLU
1	B	42	ARG
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	66	ILE
1	B	76	VAL
1	B	130	GLN
1	B	139	ASP
1	B	210	GLU
1	B	229	MSE
1	B	232	ARG
1	B	233	LEU
1	B	235	SER
1	C	4	VAL
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	76	VAL
1	C	130	GLN
1	C	139	ASP
1	C	210	GLU
1	C	229	MSE
1	C	233	LEU
1	C	235	SER
1	C	241	ASN
1	D	4	VAL
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	76	VAL
1	D	130	GLN
1	D	139	ASP
1	D	210	GLU
1	D	229	MSE
1	D	232	ARG
1	D	233	LEU
1	D	235	SER
1	D	241	ASN
1	E	4	VAL

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Mol	Chain	Res	Type
1	E	24	ILE
1	E	38	THR
1	E	42	ARG
1	E	60	ASN
1	E	66	ILE
1	E	76	VAL
1	E	130	GLN
1	E	139	ASP
1	E	210	GLU
1	E	229	MSE
1	E	232	ARG
1	E	233	LEU
1	E	235	SER
1	E	241	ASN
1	F	4	VAL
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	76	VAL
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	F	241	ASN
1	G	4	VAL
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
1	G	76	VAL

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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	G	241	ASN
1	H	4	VAL
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	76	VAL
1	H	129	PRO
1	H	130	GLN
1	H	139	ASP
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	4	VAL
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	76	VAL
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

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Mol	Chain	Res	Type
1	I	241	ASN
1	J	4	VAL
1	J	24	ILE
1	J	38	THR
1	J	41	GLU
1	J	42	ARG
1	J	60	ASN
1	J	66	ILE
1	J	75	ASN
1	J	76	VAL
1	J	130	GLN
1	J	139	ASP
1	J	210	GLU
1	J	229	MSE
1	J	233	LEU
1	J	235	SER
1	J	241	ASN
1	K	4	VAL
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	76	VAL
1	K	130	GLN
1	K	139	ASP
1	K	210	GLU
1	K	229	MSE
1	K	232	ARG
1	K	233	LEU
1	K	235	SER
1	K	241	ASN
1	L	4	VAL
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

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Mol	Chain	Res	Type
1	L	76	VAL
1	L	130	GLN
1	L	139	ASP
1	L	210	GLU
1	L	229	MSE
1	L	232	ARG
1	L	233	LEU
1	L	235	SER
1	L	241	ASN
1	M	4	VAL
1	M	24	ILE
1	M	38	THR
1	M	41	GLU
1	M	42	ARG
1	M	60	ASN
1	M	66	ILE
1	M	75	ASN
1	M	76	VAL
1	M	130	GLN
1	M	139	ASP
1	M	210	GLU
1	M	229	MSE
1	M	232	ARG
1	M	233	LEU
1	M	235	SER
1	M	241	ASN
1	N	4	VAL
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	76	VAL
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

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Mol	Chain	Res	Type
1	N	241	ASN
1	O	4	VAL
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	76	VAL
1	O	130	GLN
1	O	139	ASP
1	O	210	GLU
1	O	229	MSE
1	O	233	LEU
1	O	235	SER
1	O	241	ASN
1	P	4	VAL
1	P	24	ILE
1	P	38	THR
1	P	41	GLU
1	P	42	ARG
1	P	60	ASN
1	P	66	ILE
1	P	75	ASN
1	P	76	VAL
1	P	130	GLN
1	P	139	ASP
1	P	210	GLU
1	P	229	MSE
1	P	233	LEU
1	P	235	SER
1	P	241	ASN
1	Q	4	VAL
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	76	VAL

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Mol	Chain	Res	Type
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	Q	241	ASN
1	R	4	VAL
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	76	VAL
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	R	241	ASN
1	S	4	VAL
1	S	24	ILE
1	S	38	THR
1	S	41	GLU
1	S	42	ARG
1	S	60	ASN
1	S	66	ILE
1	S	75	ASN
1	S	76	VAL
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	S	241	ASN

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Mol	Chain	Res	Type
1	T	4	VAL
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	76	VAL
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	T	241	ASN
1	U	4	VAL
1	U	24	ILE
1	U	38	THR
1	U	42	ARG
1	U	60	ASN
1	U	66	ILE
1	U	75	ASN
1	U	76	VAL
1	U	130	GLN
1	U	139	ASP
1	U	210	GLU
1	U	229	MSE
1	U	233	LEU
1	U	235	SER
1	V	4	VAL
1	V	24	ILE
1	V	38	THR
1	V	41	GLU
1	V	42	ARG
1	V	60	ASN
1	V	66	ILE
1	V	76	VAL
1	V	130	GLN
1	V	139	ASP
1	V	210	GLU
1	V	229	MSE

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Mol	Chain	Res	Type
1	V	233	LEU
1	V	235	SER
1	V	241	ASN
1	W	4	VAL
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	76	VAL
1	W	130	GLN
1	W	139	ASP
1	W	210	GLU
1	W	229	MSE
1	W	233	LEU
1	W	235	SER
1	W	241	ASN
1	X	4	VAL
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	76	VAL
1	X	130	GLN
1	X	139	ASP
1	X	210	GLU
1	X	229	MSE
1	X	232	ARG
1	X	233	LEU
1	X	235	SER
1	Y	4	VAL
1	Y	24	ILE
1	Y	38	THR
1	Y	41	GLU
1	Y	42	ARG
1	Y	60	ASN
1	Y	66	ILE
1	Y	75	ASN

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Mol	Chain	Res	Type
1	Y	76	VAL
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	Y	241	ASN
1	Z	4	VAL
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	76	VAL
1	Z	130	GLN
1	Z	139	ASP
1	Z	210	GLU
1	Z	229	MSE
1	Z	232	ARG
1	Z	233	LEU
1	Z	235	SER
1	Z	241	ASN
1	1	4	VAL
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	76	VAL
1	1	130	GLN
1	1	139	ASP
1	1	210	GLU
1	1	229	MSE
1	1	232	ARG
1	1	233	LEU
1	1	235	SER

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Mol	Chain	Res	Type
1	1	241	ASN
1	2	4	VAL
1	2	24	ILE
1	2	38	THR
1	2	41	GLU
1	2	42	ARG
1	2	60	ASN
1	2	66	ILE
1	2	75	ASN
1	2	76	VAL
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	2	241	ASN
1	3	4	VAL
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	76	VAL
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	3	241	ASN
1	4	4	VAL
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	76	VAL

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Mol	Chain	Res	Type
1	4	130	GLN
1	4	139	ASP
1	4	210	GLU
1	4	229	MSE
1	4	232	ARG
1	4	233	LEU
1	4	235	SER
1	4	241	ASN
1	5	4	VAL
1	5	24	ILE
1	5	38	THR
1	5	41	GLU
1	5	42	ARG
1	5	60	ASN
1	5	66	ILE
1	5	75	ASN
1	5	76	VAL
1	5	130	GLN
1	5	139	ASP
1	5	210	GLU
1	5	229	MSE
1	5	233	LEU
1	5	235	SER
1	5	241	ASN
1	6	4	VAL
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	76	VAL
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	6	241	ASN
1	7	4	VAL

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Mol	Chain	Res	Type
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	76	VAL
1	7	130	GLN
1	7	139	ASP
1	7	210	GLU
1	7	229	MSE
1	7	232	ARG
1	7	233	LEU
1	7	235	SER
1	7	241	ASN
1	8	4	VAL
1	8	24	ILE
1	8	38	THR
1	8	41	GLU
1	8	42	ARG
1	8	60	ASN
1	8	66	ILE
1	8	76	VAL
1	8	130	GLN
1	8	139	ASP
1	8	210	GLU
1	8	229	MSE
1	8	233	LEU
1	8	235	SER
1	8	241	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	75	ASN
1	A	135	GLN
1	A	144	GLN
1	A	158	ASN
1	B	21	ASN
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	64	GLN
1	B	144	GLN
1	C	7	HIS
1	C	60	ASN
1	C	64	GLN
1	C	135	GLN
1	C	144	GLN
1	D	21	ASN
1	D	60	ASN
1	D	135	GLN
1	D	144	GLN
1	D	158	ASN
1	E	7	HIS
1	E	26	HIS
1	E	135	GLN
1	E	144	GLN
1	F	7	HIS
1	F	60	ASN
1	F	64	GLN
1	F	75	ASN
1	F	130	GLN
1	F	144	GLN
1	F	158	ASN
1	G	60	ASN
1	G	64	GLN
1	G	75	ASN
1	G	135	GLN
1	G	144	GLN
1	H	7	HIS
1	H	144	GLN
1	H	158	ASN
1	H	221	GLN
1	I	75	ASN
1	I	144	GLN
1	I	158	ASN
1	J	21	ASN
1	J	60	ASN
1	J	64	GLN
1	J	75	ASN
1	J	135	GLN
1	J	144	GLN
1	K	21	ASN

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Mol	Chain	Res	Type
1	K	75	ASN
1	K	144	GLN
1	K	158	ASN
1	L	75	ASN
1	L	135	GLN
1	L	144	GLN
1	L	221	GLN
1	M	60	ASN
1	M	64	GLN
1	M	135	GLN
1	M	144	GLN
1	M	158	ASN
1	N	75	ASN
1	N	144	GLN
1	O	7	HIS
1	O	60	ASN
1	O	64	GLN
1	O	135	GLN
1	O	144	GLN
1	O	158	ASN
1	O	221	GLN
1	P	21	ASN
1	P	60	ASN
1	P	64	GLN
1	P	75	ASN
1	P	144	GLN
1	P	158	ASN
1	Q	60	ASN
1	Q	64	GLN
1	Q	75	ASN
1	Q	135	GLN
1	Q	144	GLN
1	Q	158	ASN
1	R	75	ASN
1	R	135	GLN
1	R	144	GLN
1	R	158	ASN
1	S	60	ASN
1	S	64	GLN
1	S	75	ASN
1	S	135	GLN
1	S	144	GLN

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Mol	Chain	Res	Type
1	T	60	ASN
1	T	64	GLN
1	T	75	ASN
1	T	135	GLN
1	T	144	GLN
1	T	158	ASN
1	U	21	ASN
1	U	144	GLN
1	U	158	ASN
1	V	60	ASN
1	V	64	GLN
1	V	135	GLN
1	V	144	GLN
1	V	158	ASN
1	W	7	HIS
1	W	60	ASN
1	W	64	GLN
1	W	144	GLN
1	W	221	GLN
1	X	7	HIS
1	X	135	GLN
1	X	144	GLN
1	X	158	ASN
1	Y	21	ASN
1	Y	60	ASN
1	Y	64	GLN
1	Y	75	ASN
1	Y	144	GLN
1	Y	158	ASN
1	Z	7	HIS
1	Z	75	ASN
1	Z	144	GLN
1	Z	158	ASN
1	1	7	HIS
1	1	75	ASN
1	1	135	GLN
1	1	144	GLN
1	2	21	ASN
1	2	60	ASN
1	2	64	GLN
1	2	75	ASN
1	2	144	GLN

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Mol	Chain	Res	Type
1	2	158	ASN
1	3	7	HIS
1	3	21	ASN
1	3	60	ASN
1	3	64	GLN
1	3	75	ASN
1	3	144	GLN
1	3	158	ASN
1	4	7	HIS
1	4	60	ASN
1	4	64	GLN
1	4	144	GLN
1	5	26	HIS
1	5	60	ASN
1	5	64	GLN
1	5	144	GLN
1	5	158	ASN
1	6	7	HIS
1	6	60	ASN
1	6	64	GLN
1	6	144	GLN
1	6	158	ASN
1	7	60	ASN
1	7	64	GLN
1	7	144	GLN
1	8	7	HIS
1	8	60	ASN
1	8	64	GLN
1	8	144	GLN
1	8	158	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	236/242 (97%)	0.00	5 (2%) 63 54	56, 86, 131, 215	0
1	2	236/242 (97%)	0.08	7 (2%) 52 43	58, 87, 135, 203	0
1	3	236/242 (97%)	-0.01	6 (2%) 58 48	57, 80, 140, 221	0
1	4	236/242 (97%)	-0.01	3 (1%) 75 67	56, 83, 129, 220	0
1	5	236/242 (97%)	0.15	7 (2%) 52 43	60, 97, 147, 204	0
1	6	236/242 (97%)	0.06	5 (2%) 63 54	64, 94, 138, 205	0
1	7	236/242 (97%)	-0.06	5 (2%) 63 54	56, 79, 118, 227	0
1	8	236/242 (97%)	-0.03	8 (3%) 48 39	57, 79, 135, 186	0
1	A	236/242 (97%)	-0.10	9 (3%) 44 36	54, 72, 120, 163	0
1	B	236/242 (97%)	-0.10	4 (1%) 69 61	55, 76, 117, 208	0
1	C	236/242 (97%)	-0.05	5 (2%) 63 54	54, 77, 119, 208	0
1	D	236/242 (97%)	-0.14	5 (2%) 63 54	53, 70, 128, 190	0
1	E	236/242 (97%)	-0.05	5 (2%) 63 54	53, 77, 122, 216	0
1	F	236/242 (97%)	-0.10	6 (2%) 58 48	50, 66, 121, 234	0
1	G	236/242 (97%)	0.02	11 (4%) 36 28	56, 74, 127, 186	0
1	H	236/242 (97%)	-0.09	7 (2%) 52 43	52, 74, 126, 210	0
1	I	236/242 (97%)	-0.13	4 (1%) 69 61	52, 72, 107, 134	0
1	J	236/242 (97%)	-0.13	4 (1%) 69 61	50, 70, 137, 226	0
1	K	236/242 (97%)	-0.25	5 (2%) 63 54	46, 64, 106, 174	0
1	L	236/242 (97%)	-0.21	6 (2%) 58 48	48, 67, 109, 153	0
1	M	236/242 (97%)	-0.22	6 (2%) 58 48	47, 65, 113, 200	0
1	N	236/242 (97%)	-0.26	2 (0%) 82 77	43, 69, 107, 136	0
1	O	236/242 (97%)	-0.18	4 (1%) 69 61	50, 70, 117, 195	0
1	P	236/242 (97%)	-0.14	5 (2%) 63 54	50, 75, 124, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Q	236/242 (97%)	-0.16	6 (2%) 58 48	49, 66, 114, 216	0
1	R	236/242 (97%)	-0.08	3 (1%) 75 67	49, 78, 120, 199	0
1	S	236/242 (97%)	-0.06	11 (4%) 36 28	51, 69, 132, 179	0
1	T	236/242 (97%)	-0.09	5 (2%) 63 54	52, 79, 126, 202	0
1	U	236/242 (97%)	-0.06	8 (3%) 48 39	54, 79, 124, 160	0
1	V	236/242 (97%)	-0.13	5 (2%) 63 54	54, 69, 124, 206	0
1	W	236/242 (97%)	-0.07	8 (3%) 48 39	47, 70, 137, 215	0
1	X	236/242 (97%)	-0.13	7 (2%) 52 43	47, 69, 112, 148	0
1	Y	236/242 (97%)	0.04	3 (1%) 75 67	57, 89, 142, 213	0
1	Z	236/242 (97%)	0.06	5 (2%) 63 54	56, 87, 136, 199	0
All	All	8024/8228 (97%)	-0.08	195 (2%) 59 50	43, 75, 128, 234	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	69	ASP	6.7
1	S	68	ARG	6.1
1	F	101	LEU	5.4
1	F	69	ASP	5.0
1	G	102	ALA	4.9
1	Q	102	ALA	4.8
1	F	102	ALA	4.8
1	J	101	LEU	4.6
1	5	101	LEU	4.6
1	T	101	LEU	4.5
1	S	66	ILE	4.4
1	B	102	ALA	4.4
1	Q	101	LEU	4.4
1	U	69	ASP	4.3
1	3	101	LEU	4.3
1	I	69	ASP	4.3
1	S	67	ARG	4.2
1	M	101	LEU	4.2
1	C	101	LEU	4.1
1	G	131	GLY	4.1
1	5	69	ASP	4.0
1	A	128	TYR	4.0
1	2	101	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	X	69	ASP	3.9
1	G	128	TYR	3.8
1	Z	102	ALA	3.8
1	A	131	GLY	3.8
1	L	101	LEU	3.8
1	W	101	LEU	3.8
1	F	128	TYR	3.7
1	E	102	ALA	3.7
1	X	128	TYR	3.7
1	W	102	ALA	3.6
1	J	102	ALA	3.6
1	A	133	PHE	3.6
1	Y	101	LEU	3.5
1	A	102	ALA	3.5
1	M	102	ALA	3.5
1	L	69	ASP	3.5
1	C	102	ALA	3.5
1	P	102	ALA	3.5
1	1	101	LEU	3.5
1	P	69	ASP	3.5
1	D	69	ASP	3.4
1	8	101	LEU	3.4
1	2	69	ASP	3.3
1	1	102	ALA	3.3
1	B	101	LEU	3.3
1	K	101	LEU	3.3
1	T	69	ASP	3.2
1	3	69	ASP	3.2
1	S	102	ALA	3.2
1	T	102	ALA	3.2
1	R	69	ASP	3.2
1	7	69	ASP	3.2
1	H	102	ALA	3.2
1	3	128	TYR	3.2
1	G	101	LEU	3.2
1	D	68	ARG	3.1
1	K	69	ASP	3.1
1	S	70	GLY	3.1
1	S	101	LEU	3.1
1	5	98	SER	3.1
1	7	102	ALA	3.1
1	V	241	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	102	ALA	3.1
1	6	102	ALA	3.1
1	1	69	ASP	3.1
1	U	101	LEU	3.1
1	Y	102	ALA	3.1
1	3	102	ALA	3.1
1	H	69	ASP	3.1
1	5	102	ALA	3.0
1	V	69	ASP	3.0
1	Z	101	LEU	3.0
1	8	128	TYR	3.0
1	Z	69	ASP	3.0
1	8	69	ASP	3.0
1	G	134	ILE	3.0
1	C	69	ASP	3.0
1	G	69	ASP	3.0
1	N	241	ASN	3.0
1	W	241	ASN	3.0
1	X	241	ASN	3.0
1	R	102	ALA	3.0
1	8	133	PHE	3.0
1	E	101	LEU	2.9
1	Q	128	TYR	2.9
1	E	24	ILE	2.9
1	4	102	ALA	2.9
1	O	102	ALA	2.8
1	B	69	ASP	2.8
1	F	131	GLY	2.8
1	Q	69	ASP	2.8
1	I	224	ALA	2.8
1	R	101	LEU	2.8
1	V	101	LEU	2.8
1	W	98	SER	2.8
1	V	102	ALA	2.7
1	X	133	PHE	2.7
1	L	24	ILE	2.7
1	7	24	ILE	2.7
1	H	232	ARG	2.7
1	M	96	ARG	2.7
1	A	134	ILE	2.7
1	P	101	LEU	2.7
1	U	241	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	66	ILE	2.7
1	W	24	ILE	2.6
1	4	101	LEU	2.7
1	I	67	ARG	2.6
1	L	241	ASN	2.6
1	2	102	ALA	2.6
1	P	131	GLY	2.6
1	6	101	LEU	2.6
1	S	24	ILE	2.6
1	J	241	ASN	2.6
1	G	133	PHE	2.6
1	3	26	HIS	2.6
1	4	69	ASP	2.6
1	6	69	ASP	2.6
1	N	24	ILE	2.5
1	W	69	ASP	2.5
1	A	241	ASN	2.5
1	O	97	ASP	2.5
1	D	101	LEU	2.5
1	G	132	ASN	2.5
1	T	97	ASP	2.5
1	K	241	ASN	2.5
1	6	241	ASN	2.5
1	7	104	ASN	2.5
1	A	101	LEU	2.4
1	O	101	LEU	2.4
1	W	68	ARG	2.4
1	1	166	GLU	2.4
1	I	24	ILE	2.4
1	6	166	GLU	2.4
1	G	166	GLU	2.4
1	U	24	ILE	2.4
1	8	24	ILE	2.4
1	E	69	ASP	2.4
1	2	128	TYR	2.4
1	U	236	PRO	2.4
1	Z	109	CYS	2.3
1	5	166	GLU	2.3
1	K	24	ILE	2.3
1	Y	128	TYR	2.3
1	O	132	ASN	2.3
1	H	101	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	235	SER	2.3
1	V	24	ILE	2.3
1	5	80	TYR	2.3
1	A	132	ASN	2.2
1	G	241	ASN	2.2
1	M	241	ASN	2.2
1	C	97	ASP	2.2
1	A	24	ILE	2.2
1	1	24	ILE	2.2
1	5	24	ILE	2.2
1	X	68	ARG	2.2
1	W	128	TYR	2.2
1	8	102	ALA	2.2
1	7	101	LEU	2.2
1	P	132	ASN	2.2
1	Q	220	ARG	2.2
1	2	96	ARG	2.2
1	S	99	GLY	2.2
1	8	129	PRO	2.2
1	2	241	ASN	2.1
1	Z	22	ALA	2.1
1	L	68	ARG	2.1
1	M	69	ASP	2.1
1	8	131	GLY	2.1
1	Q	241	ASN	2.1
1	S	65	ARG	2.1
1	K	102	ALA	2.1
1	E	109	CYS	2.1
1	H	109	CYS	2.1
1	J	98	SER	2.1
1	L	98	SER	2.1
1	X	132	ASN	2.1
1	G	24	ILE	2.1
1	X	80	TYR	2.1
1	2	132	ASN	2.0
1	U	68	ARG	2.0
1	B	24	ILE	2.0
1	S	105	THR	2.0
1	3	24	ILE	2.0
1	F	41	GLU	2.0
1	T	166	GLU	2.0
1	C	109	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	132	ASN	2.0
1	H	239	ALA	2.0
1	U	102	ALA	2.0
1	M	97	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.