



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:07 PM GMT

PDB ID : 3STJ  
Title : Crystal structure of the protease + PDZ1 domain of DegQ from Escherichia coli  
Authors : Sawa, J.; Malet, H.; Krojer, T.; Canellas, F.; Ehrmann, M.; Clausen, T.  
Deposited on : 2011-07-11  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

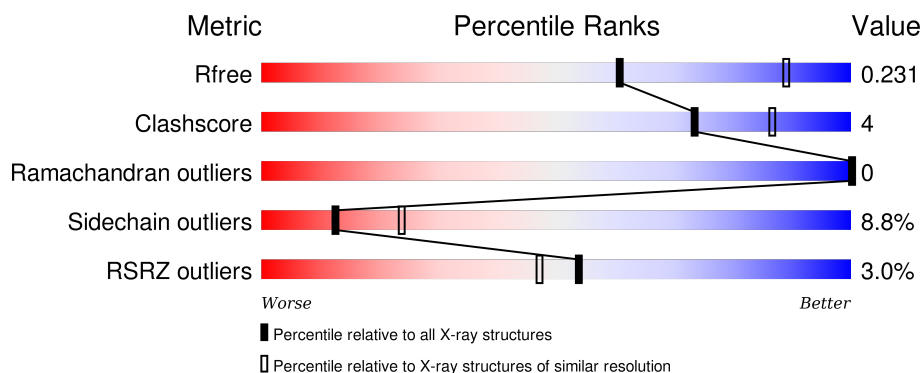
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	345	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	345	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	345	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	345	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	345	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	345	 3% 75% 11% • 13%
1	G	345	 3% 74% 12% • 13%
1	H	345	 % 74% 12% • 13%
1	I	345	 3% 74% 12% • 13%
1	J	345	 2% 72% 14% • 13%
1	K	345	 2% 73% 13% • 13%
1	L	345	 4% 74% 12% • 13%
2	M	7	 71% 29%
2	N	7	 71% 29%
2	O	7	 71% 29%
2	P	7	 71% 29%
2	Q	7	 71% 29%
2	R	7	 71% 29%
2	S	7	 71% 29%
2	T	7	 71% 29%
2	U	7	 71% 29%
2	V	7	 71% 29%
2	W	7	 71% 29%
2	X	7	 71% 29%
2	Z	7	 86% 14%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26483 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 Protease degQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	B	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	C	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	D	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	E	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	F	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	G	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	H	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	I	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	J	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	K	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			
1	L	300	Total	C	N	O	S	0	0	0
			2179	1366	382	428	3			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	338	LEU	-	EXPRESSION TAG	UNP P39099
A	339	GLU	-	EXPRESSION TAG	UNP P39099
A	340	HIS	-	EXPRESSION TAG	UNP P39099
A	341	HIS	-	EXPRESSION TAG	UNP P39099
A	342	HIS	-	EXPRESSION TAG	UNP P39099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	343	HIS	-	EXPRESSION TAG	UNP P39099
A	344	HIS	-	EXPRESSION TAG	UNP P39099
A	345	HIS	-	EXPRESSION TAG	UNP P39099
B	338	LEU	-	EXPRESSION TAG	UNP P39099
B	339	GLU	-	EXPRESSION TAG	UNP P39099
B	340	HIS	-	EXPRESSION TAG	UNP P39099
B	341	HIS	-	EXPRESSION TAG	UNP P39099
B	342	HIS	-	EXPRESSION TAG	UNP P39099
B	343	HIS	-	EXPRESSION TAG	UNP P39099
B	344	HIS	-	EXPRESSION TAG	UNP P39099
B	345	HIS	-	EXPRESSION TAG	UNP P39099
C	338	LEU	-	EXPRESSION TAG	UNP P39099
C	339	GLU	-	EXPRESSION TAG	UNP P39099
C	340	HIS	-	EXPRESSION TAG	UNP P39099
C	341	HIS	-	EXPRESSION TAG	UNP P39099
C	342	HIS	-	EXPRESSION TAG	UNP P39099
C	343	HIS	-	EXPRESSION TAG	UNP P39099
C	344	HIS	-	EXPRESSION TAG	UNP P39099
C	345	HIS	-	EXPRESSION TAG	UNP P39099
D	338	LEU	-	EXPRESSION TAG	UNP P39099
D	339	GLU	-	EXPRESSION TAG	UNP P39099
D	340	HIS	-	EXPRESSION TAG	UNP P39099
D	341	HIS	-	EXPRESSION TAG	UNP P39099
D	342	HIS	-	EXPRESSION TAG	UNP P39099
D	343	HIS	-	EXPRESSION TAG	UNP P39099
D	344	HIS	-	EXPRESSION TAG	UNP P39099
D	345	HIS	-	EXPRESSION TAG	UNP P39099
E	338	LEU	-	EXPRESSION TAG	UNP P39099
E	339	GLU	-	EXPRESSION TAG	UNP P39099
E	340	HIS	-	EXPRESSION TAG	UNP P39099
E	341	HIS	-	EXPRESSION TAG	UNP P39099
E	342	HIS	-	EXPRESSION TAG	UNP P39099
E	343	HIS	-	EXPRESSION TAG	UNP P39099
E	344	HIS	-	EXPRESSION TAG	UNP P39099
E	345	HIS	-	EXPRESSION TAG	UNP P39099
F	338	LEU	-	EXPRESSION TAG	UNP P39099
F	339	GLU	-	EXPRESSION TAG	UNP P39099
F	340	HIS	-	EXPRESSION TAG	UNP P39099
F	341	HIS	-	EXPRESSION TAG	UNP P39099
F	342	HIS	-	EXPRESSION TAG	UNP P39099
F	343	HIS	-	EXPRESSION TAG	UNP P39099
F	344	HIS	-	EXPRESSION TAG	UNP P39099

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Chain	Residue	Modelled	Actual	Comment	Reference
F	345	HIS	-	EXPRESSION TAG	UNP P39099
G	338	LEU	-	EXPRESSION TAG	UNP P39099
G	339	GLU	-	EXPRESSION TAG	UNP P39099
G	340	HIS	-	EXPRESSION TAG	UNP P39099
G	341	HIS	-	EXPRESSION TAG	UNP P39099
G	342	HIS	-	EXPRESSION TAG	UNP P39099
G	343	HIS	-	EXPRESSION TAG	UNP P39099
G	344	HIS	-	EXPRESSION TAG	UNP P39099
G	345	HIS	-	EXPRESSION TAG	UNP P39099
H	338	LEU	-	EXPRESSION TAG	UNP P39099
H	339	GLU	-	EXPRESSION TAG	UNP P39099
H	340	HIS	-	EXPRESSION TAG	UNP P39099
H	341	HIS	-	EXPRESSION TAG	UNP P39099
H	342	HIS	-	EXPRESSION TAG	UNP P39099
H	343	HIS	-	EXPRESSION TAG	UNP P39099
H	344	HIS	-	EXPRESSION TAG	UNP P39099
H	345	HIS	-	EXPRESSION TAG	UNP P39099
I	338	LEU	-	EXPRESSION TAG	UNP P39099
I	339	GLU	-	EXPRESSION TAG	UNP P39099
I	340	HIS	-	EXPRESSION TAG	UNP P39099
I	341	HIS	-	EXPRESSION TAG	UNP P39099
I	342	HIS	-	EXPRESSION TAG	UNP P39099
I	343	HIS	-	EXPRESSION TAG	UNP P39099
I	344	HIS	-	EXPRESSION TAG	UNP P39099
I	345	HIS	-	EXPRESSION TAG	UNP P39099
J	338	LEU	-	EXPRESSION TAG	UNP P39099
J	339	GLU	-	EXPRESSION TAG	UNP P39099
J	340	HIS	-	EXPRESSION TAG	UNP P39099
J	341	HIS	-	EXPRESSION TAG	UNP P39099
J	342	HIS	-	EXPRESSION TAG	UNP P39099
J	343	HIS	-	EXPRESSION TAG	UNP P39099
J	344	HIS	-	EXPRESSION TAG	UNP P39099
J	345	HIS	-	EXPRESSION TAG	UNP P39099
K	338	LEU	-	EXPRESSION TAG	UNP P39099
K	339	GLU	-	EXPRESSION TAG	UNP P39099
K	340	HIS	-	EXPRESSION TAG	UNP P39099
K	341	HIS	-	EXPRESSION TAG	UNP P39099
K	342	HIS	-	EXPRESSION TAG	UNP P39099
K	343	HIS	-	EXPRESSION TAG	UNP P39099
K	344	HIS	-	EXPRESSION TAG	UNP P39099
K	345	HIS	-	EXPRESSION TAG	UNP P39099
L	338	LEU	-	EXPRESSION TAG	UNP P39099

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Chain	Residue	Modelled	Actual	Comment	Reference
L	339	GLU	-	EXPRESSION TAG	UNP P39099
L	340	HIS	-	EXPRESSION TAG	UNP P39099
L	341	HIS	-	EXPRESSION TAG	UNP P39099
L	342	HIS	-	EXPRESSION TAG	UNP P39099
L	343	HIS	-	EXPRESSION TAG	UNP P39099
L	344	HIS	-	EXPRESSION TAG	UNP P39099
L	345	HIS	-	EXPRESSION TAG	UNP P39099

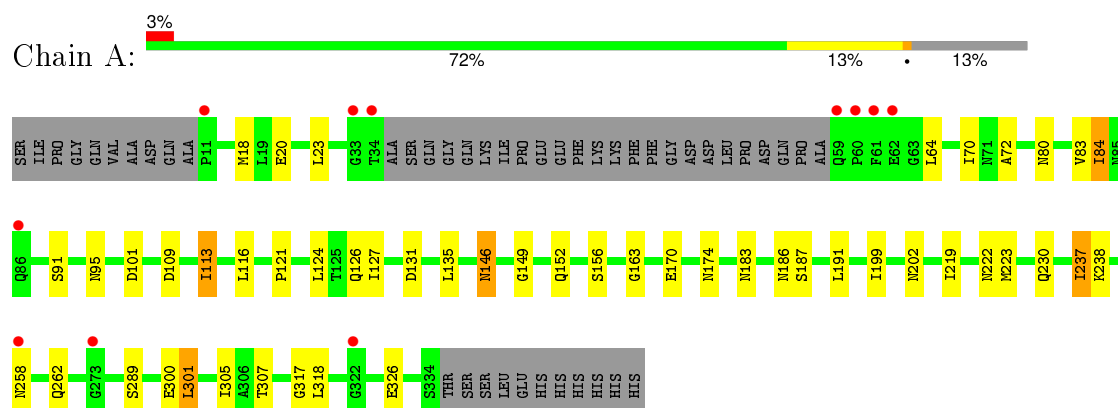
- Molecule 2 is a protein called peptide (UNK).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	N	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	O	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	P	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	Q	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	R	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	S	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	T	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	U	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	V	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	W	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	X	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	Z	7	Total	C	N	O	0	0	0
			35	21	7	7			

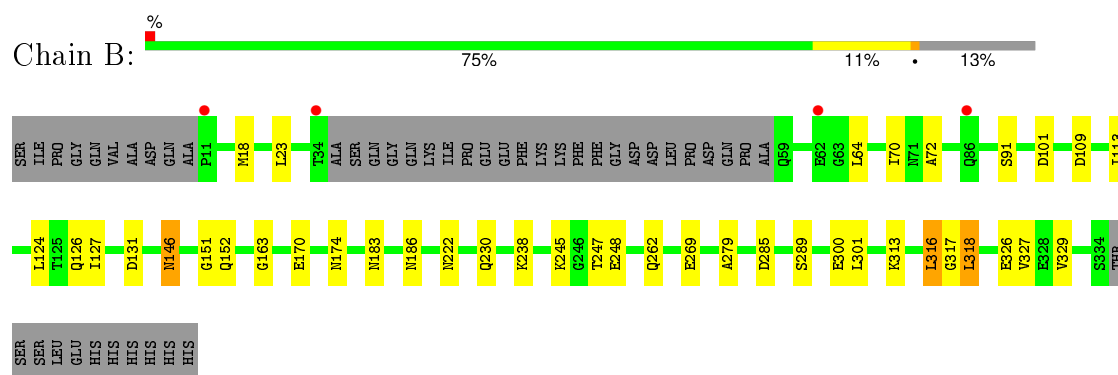
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

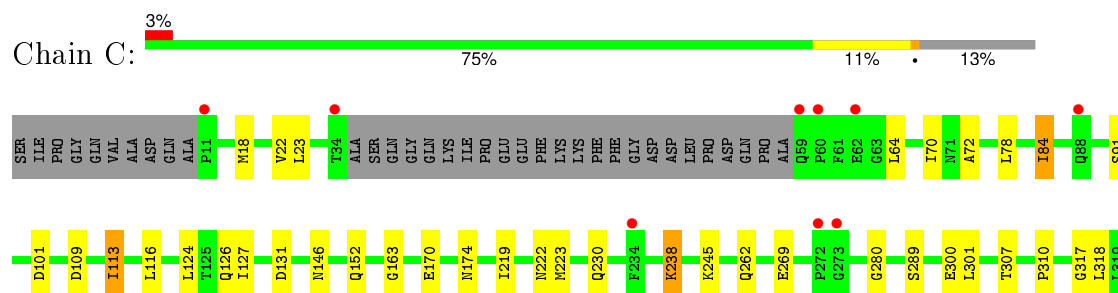
#### • Molecule 1: Protease degQ



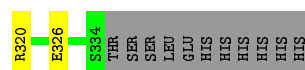
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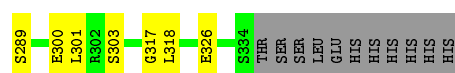
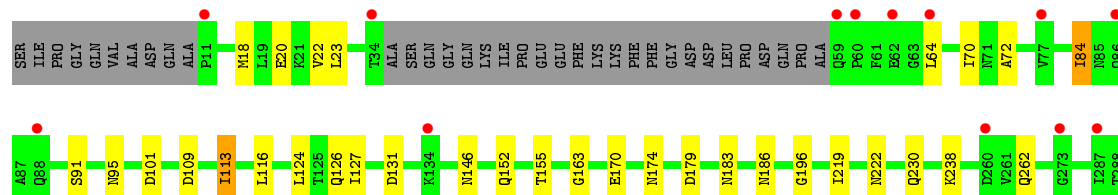
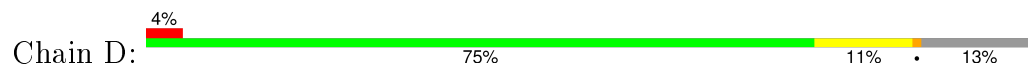
#### • Molecule 1: Protease degQ



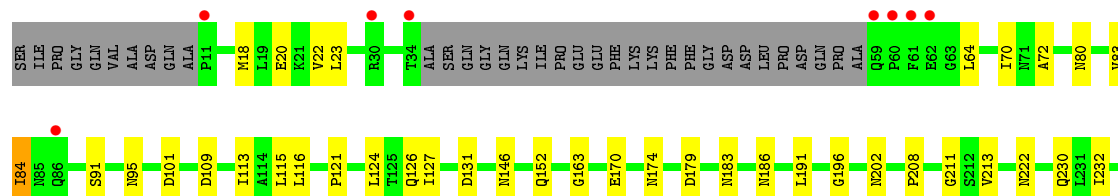




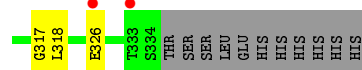
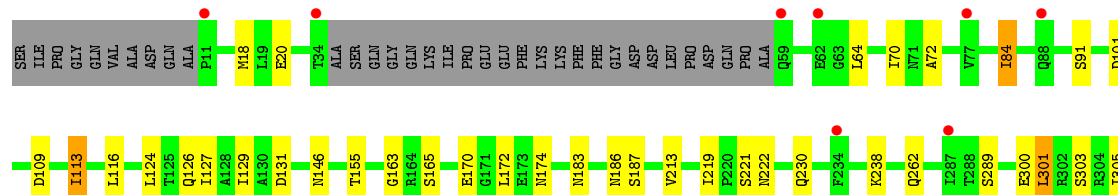
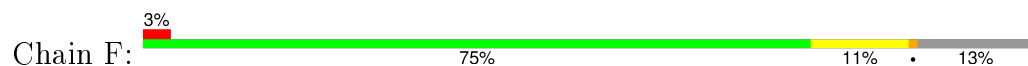
• Molecule 1: Protease degQ



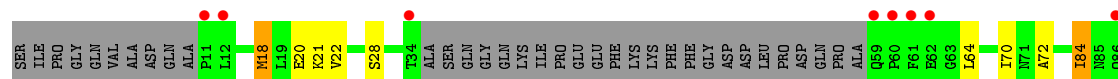
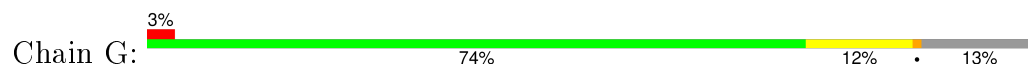
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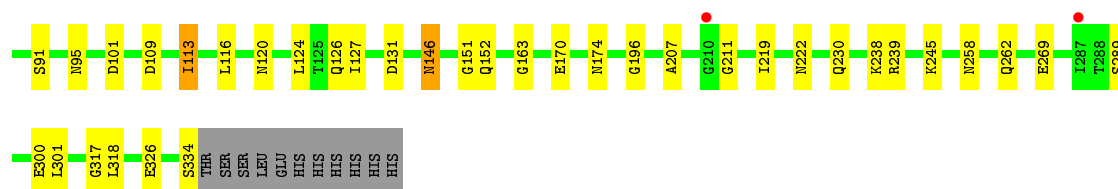


• Molecule 1: Protease degQ

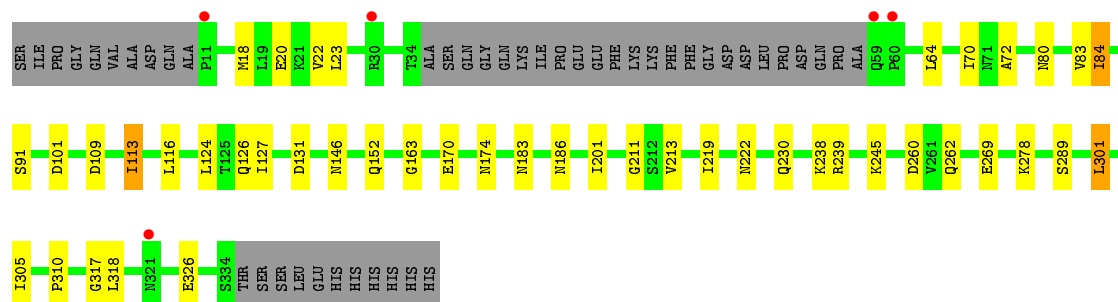
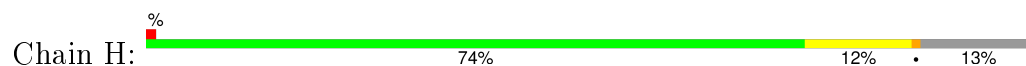


• Molecule 1: Protease degQ

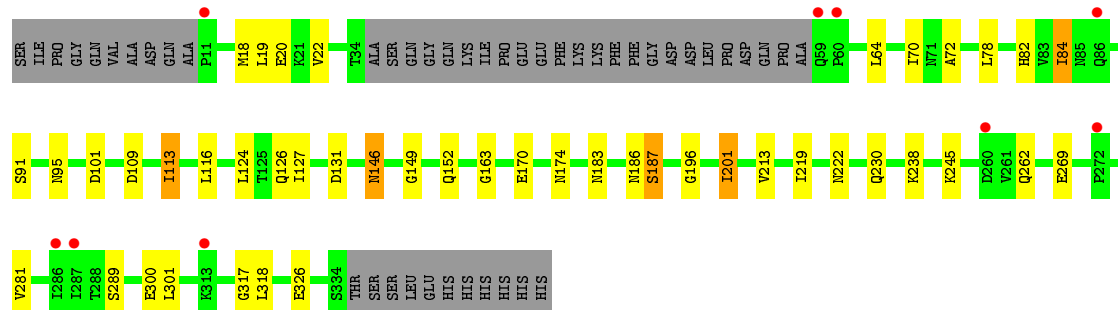
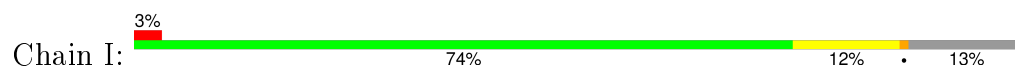




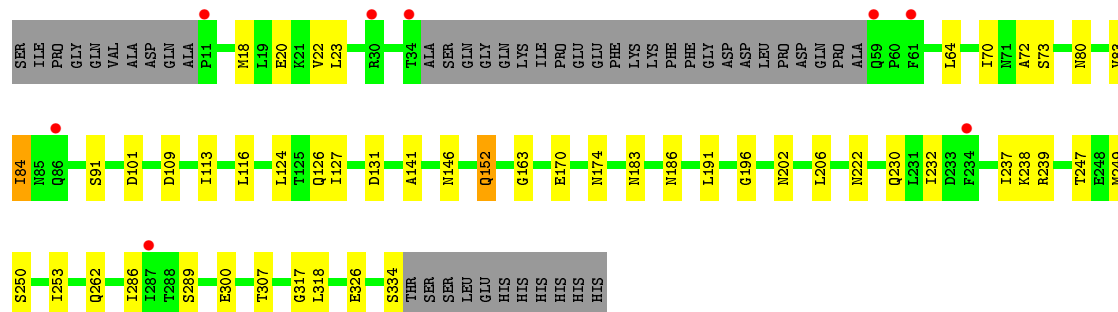
• Molecule 1: Protease degQ



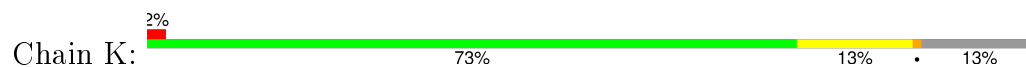
• Molecule 1: Protease degQ

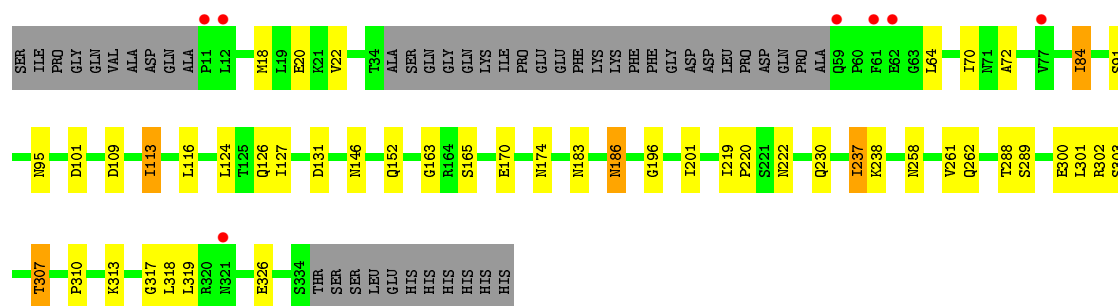


• Molecule 1: Protease degQ

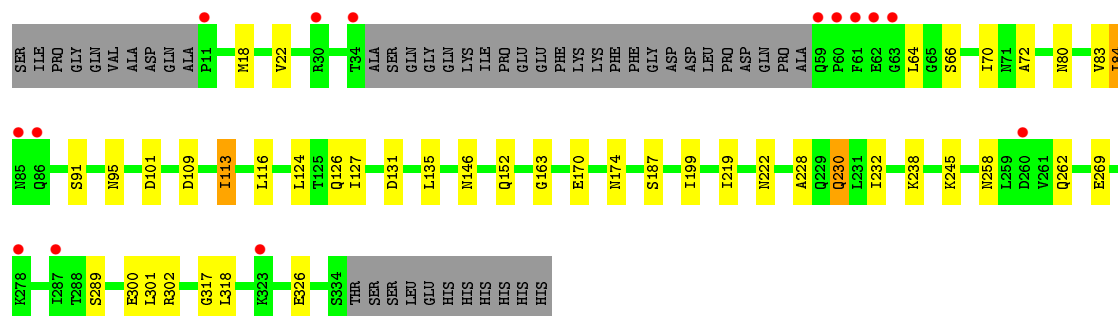
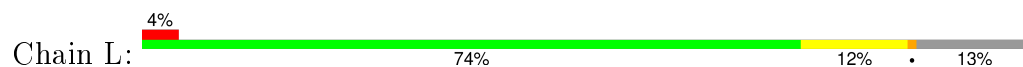


• Molecule 1: Protease degQ

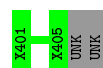




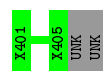
- Molecule 1: Protease degQ



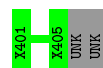
- Molecule 2: peptide (UNK)



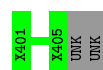
- Molecule 2: peptide (UNK)



- Molecule 2: peptide (UNK)

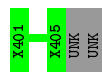


- Molecule 2: peptide (UNK)



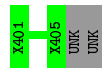
- Molecule 2: peptide (UNK)

Chain Q:  71% 29%



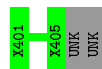
- Molecule 2: peptide (UNK)

Chain R:  71% 29%



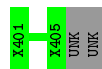
- Molecule 2: peptide (UNK)

Chain S:  71% 29%



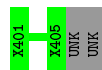
- Molecule 2: peptide (UNK)

Chain T:  71% 29%



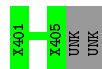
- Molecule 2: peptide (UNK)

Chain U:  71% 29%



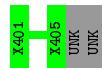
- Molecule 2: peptide (UNK)

Chain V:  71% 29%



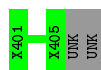
- Molecule 2: peptide (UNK)

Chain W:  71% 29%




- Molecule 2: peptide (UNK)

Chain X:  71% 29%



- Molecule 2: peptide (UNK)

Chain Z:  86% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.32Å 115.32Å 287.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.94-2.60) 95.2 (19.93-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.184 , 0.212 0.203 , 0.231	Depositor DCC
$R_{free}$ test set	6289 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.1	EDS
Estimated twinning fraction	0.019 for -h,-k,l 0.048 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 124692 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	A	0.51	0/2202	0.74	0/2977
1	B	0.53	0/2202	0.74	0/2977
1	C	0.50	0/2202	0.73	0/2977
1	D	0.46	0/2202	0.73	0/2977
1	E	0.49	0/2202	0.75	0/2977
1	F	0.48	0/2202	0.72	0/2977
1	G	0.49	0/2202	0.74	0/2977
1	H	0.49	0/2202	0.74	0/2977
1	I	0.48	0/2202	0.74	0/2977
1	J	0.48	0/2202	0.75	0/2977
1	K	0.50	0/2202	0.73	0/2977
1	L	0.48	0/2202	0.73	0/2977
All	All	0.49	0/26424	0.74	0/35724

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2179	0	2249	24	0
1	B	2179	0	2249	17	0
1	C	2179	0	2249	14	0
1	D	2179	0	2249	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2179	0	2249	27	0
1	F	2179	0	2249	17	0
1	G	2179	0	2249	19	0
1	H	2179	0	2249	17	0
1	I	2179	0	2249	19	0
1	J	2179	0	2249	20	0
1	K	2179	0	2249	21	0
1	L	2179	0	2249	13	0
2	M	25	0	7	0	0
2	N	25	0	7	0	0
2	O	25	0	7	0	0
2	P	25	0	7	0	0
2	Q	25	0	7	0	0
2	R	25	0	7	0	0
2	S	25	0	7	0	0
2	T	25	0	7	0	0
2	U	25	0	7	0	0
2	V	25	0	7	0	0
2	W	25	0	7	0	0
2	X	25	0	7	0	0
2	Z	35	0	9	1	0
All	All	26483	0	27081	218	0

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 (218) 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:K:237:ILE:CG1	1:K:237:ILE:CD1	1.76	1.57
1:A:223:MET:HG3	1:A:307:THR:HG21	1.65	0.79
1:A:183:ASN:H	1:A:186:ASN:HD22	1.31	0.79
1:H:183:ASN:H	1:H:186:ASN:HD22	1.33	0.76
1:L:230:GLN:HE21	1:L:238:LYS:H	1.34	0.76
1:I:230:GLN:HE21	1:I:238:LYS:H	1.35	0.72
1:D:183:ASN:H	1:D:186:ASN:HD22	1.37	0.72
1:G:72:ALA:H	1:G:126:GLN:HE21	1.39	0.70
1:H:72:ALA:H	1:H:126:GLN:HE21	1.39	0.70
1:E:72:ALA:H	1:E:126:GLN:HE21	1.40	0.70
1:K:303:SER:O	1:K:307:THR:HB	1.93	0.69
1:H:183:ASN:H	1:H:186:ASN:ND2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:ALA:H	1:J:126:GLN:HE21	1.40	0.68
1:G:230:GLN:HE21	1:G:238:LYS:H	1.43	0.67
1:K:72:ALA:H	1:K:126:GLN:HE21	1.43	0.67
1:A:72:ALA:H	1:A:126:GLN:HE21	1.42	0.67
1:L:72:ALA:H	1:L:126:GLN:HE21	1.41	0.66
1:C:72:ALA:H	1:C:126:GLN:HE21	1.41	0.66
1:K:261:VAL:HG21	1:K:288:THR:HG23	1.78	0.66
1:F:72:ALA:H	1:F:126:GLN:HE21	1.43	0.66
1:D:72:ALA:H	1:D:126:GLN:HE21	1.42	0.66
1:I:72:ALA:H	1:I:126:GLN:HE21	1.44	0.65
1:F:183:ASN:H	1:F:186:ASN:HD22	1.44	0.65
1:B:72:ALA:H	1:B:126:GLN:HE21	1.43	0.65
1:D:230:GLN:HE21	1:D:238:LYS:H	1.44	0.64
1:E:230:GLN:HE21	1:E:238:LYS:H	1.44	0.64
1:F:230:GLN:NE2	1:F:238:LYS:H	1.96	0.63
1:E:183:ASN:H	1:E:186:ASN:HD22	1.47	0.63
1:A:183:ASN:H	1:A:186:ASN:ND2	1.96	0.63
1:C:230:GLN:NE2	1:C:238:LYS:H	1.97	0.62
1:J:183:ASN:H	1:J:186:ASN:ND2	1.97	0.62
1:A:230:GLN:HE21	1:A:238:LYS:H	1.47	0.62
1:F:230:GLN:HE21	1:F:238:LYS:H	1.46	0.62
1:E:230:GLN:NE2	1:E:238:LYS:H	1.98	0.61
1:G:230:GLN:NE2	1:G:238:LYS:H	1.99	0.61
1:D:22:VAL:HG21	1:D:196:GLY:HA3	1.83	0.60
1:D:230:GLN:NE2	1:D:238:LYS:H	1.98	0.60
1:A:237:ILE:HD13	1:A:237:ILE:H	1.66	0.60
1:E:237:ILE:H	1:E:237:ILE:HD13	1.67	0.59
1:I:183:ASN:H	1:I:186:ASN:HD22	1.50	0.59
1:K:131:ASP:HA	1:K:222:ASN:HD21	1.68	0.58
1:B:183:ASN:O	1:B:186:ASN:HB2	2.03	0.58
1:K:237:ILE:H	1:K:237:ILE:HD13	1.68	0.58
1:J:183:ASN:H	1:J:186:ASN:HD22	1.50	0.58
1:D:183:ASN:H	1:D:186:ASN:ND2	2.01	0.58
1:J:230:GLN:HE21	1:J:238:LYS:H	1.52	0.58
1:J:22:VAL:HG21	1:J:196:GLY:HA3	1.85	0.57
1:C:23:LEU:HB3	1:C:152:GLN:HE22	1.69	0.57
1:C:230:GLN:HE21	1:C:238:LYS:H	1.50	0.57
1:G:131:ASP:HA	1:G:222:ASN:HD21	1.70	0.57
1:B:230:GLN:HE21	1:B:238:LYS:H	1.52	0.57
1:E:163:GLY:HA2	1:E:174:ASN:ND2	2.20	0.56
1:A:230:GLN:NE2	1:A:238:LYS:H	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:GLN:NE2	1:K:238:LYS:H	2.04	0.56
1:L:131:ASP:HA	1:L:222:ASN:HD21	1.71	0.56
1:I:84:ILE:HG12	1:I:116:LEU:HD21	1.88	0.56
1:J:163:GLY:HA2	1:J:174:ASN:ND2	2.21	0.56
1:C:163:GLY:HA2	1:C:174:ASN:ND2	2.22	0.55
1:B:131:ASP:HA	1:B:222:ASN:HD21	1.71	0.55
1:A:163:GLY:HA2	1:A:174:ASN:ND2	2.22	0.55
1:C:131:ASP:HA	1:C:222:ASN:HD21	1.71	0.55
1:D:131:ASP:HA	1:D:222:ASN:HD21	1.71	0.55
1:E:131:ASP:HA	1:E:222:ASN:HD21	1.72	0.55
1:D:163:GLY:HA2	1:D:174:ASN:ND2	2.22	0.55
1:A:131:ASP:HA	1:A:222:ASN:HD21	1.71	0.55
1:J:230:GLN:NE2	1:J:238:LYS:H	2.03	0.54
1:I:131:ASP:HA	1:I:222:ASN:HD21	1.72	0.54
1:H:131:ASP:HA	1:H:222:ASN:HD21	1.71	0.54
1:G:95:ASN:HD22	1:G:152:GLN:HE22	1.55	0.54
1:J:131:ASP:HA	1:J:222:ASN:HD21	1.72	0.54
1:F:163:GLY:HA2	1:F:174:ASN:ND2	2.23	0.54
1:L:84:ILE:HG12	1:L:116:LEU:HD21	1.88	0.54
1:F:131:ASP:HA	1:F:222:ASN:HD21	1.73	0.54
1:E:95:ASN:HD22	1:E:152:GLN:HE22	1.55	0.54
1:E:84:ILE:HG12	1:E:116:LEU:HD21	1.90	0.54
1:F:84:ILE:HG12	1:F:116:LEU:HD21	1.90	0.53
1:C:84:ILE:HG12	1:C:116:LEU:HD21	1.90	0.53
1:K:113:ILE:HD11	1:K:219:ILE:HG21	1.90	0.53
1:L:80:ASN:HB2	1:L:83:VAL:HG23	1.90	0.53
1:H:84:ILE:HG12	1:H:116:LEU:HD21	1.91	0.53
1:B:163:GLY:HA2	1:B:174:ASN:ND2	2.23	0.53
1:G:163:GLY:HA2	1:G:174:ASN:ND2	2.24	0.53
1:B:23:LEU:HB3	1:B:152:GLN:HE22	1.73	0.53
1:G:84:ILE:HG12	1:G:116:LEU:HD21	1.91	0.52
1:D:84:ILE:HG12	1:D:116:LEU:HD21	1.91	0.52
1:J:84:ILE:HG12	1:J:116:LEU:HD21	1.92	0.52
1:I:230:GLN:NE2	1:I:238:LYS:H	2.06	0.52
1:I:183:ASN:O	1:I:186:ASN:HB2	2.09	0.52
1:E:80:ASN:HB2	1:E:83:VAL:HG23	1.92	0.52
1:L:163:GLY:HA2	1:L:174:ASN:ND2	2.25	0.52
1:J:289:SER:HB2	1:J:317:GLY:HA3	1.91	0.51
1:A:95:ASN:HD22	1:A:152:GLN:HE22	1.57	0.51
1:E:208:PRO:HD2	1:E:213:VAL:HG11	1.92	0.51
1:G:289:SER:HB2	1:G:317:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:ILE:HG12	1:K:116:LEU:HD21	1.92	0.51
1:H:163:GLY:HA2	1:H:174:ASN:ND2	2.25	0.51
1:E:289:SER:HB2	1:E:317:GLY:HA3	1.93	0.51
1:E:115:LEU:HD21	1:E:232:ILE:HG22	1.92	0.51
1:E:303:SER:O	1:E:307:THR:HB	2.11	0.51
1:I:163:GLY:HA2	1:I:174:ASN:ND2	2.26	0.51
1:I:95:ASN:HD22	1:I:152:GLN:HE22	1.57	0.51
1:K:183:ASN:O	1:K:186:ASN:HB2	2.12	0.50
1:F:289:SER:HB2	1:F:317:GLY:HA3	1.93	0.50
1:J:250:SER:OG	1:J:253:ILE:HG12	2.10	0.50
1:E:301:LEU:O	1:E:305:ILE:HD13	2.10	0.50
1:A:289:SER:HB2	1:A:317:GLY:HA3	1.93	0.50
1:L:289:SER:HB2	1:L:317:GLY:HA3	1.93	0.50
1:E:115:LEU:CD2	1:E:232:ILE:HG22	2.41	0.50
1:A:301:LEU:HD22	1:A:305:ILE:HG12	1.94	0.50
1:C:289:SER:HB2	1:C:317:GLY:HA3	1.94	0.50
1:H:23:LEU:HB3	1:H:152:GLN:HE22	1.76	0.50
1:I:113:ILE:HD11	1:I:219:ILE:HG21	1.93	0.50
1:D:289:SER:HB2	1:D:317:GLY:HA3	1.93	0.50
1:A:191:LEU:HB2	1:A:202:ASN:HD21	1.77	0.49
1:K:95:ASN:HD22	1:K:152:GLN:HE22	1.61	0.49
1:K:163:GLY:HA2	1:K:174:ASN:ND2	2.27	0.49
1:I:183:ASN:H	1:I:186:ASN:ND2	2.10	0.49
1:E:183:ASN:O	1:E:186:ASN:HB2	2.13	0.49
1:B:230:GLN:NE2	1:B:238:LYS:H	2.10	0.48
1:K:289:SER:HB2	1:K:317:GLY:HA3	1.95	0.48
1:I:289:SER:HB2	1:I:317:GLY:HA3	1.95	0.48
1:D:95:ASN:HD22	1:D:152:GLN:HE22	1.61	0.48
1:H:230:GLN:NE2	1:H:238:LYS:H	2.12	0.47
1:A:23:LEU:HB3	1:A:152:GLN:HE22	1.79	0.47
1:H:289:SER:HB2	1:H:317:GLY:HA3	1.97	0.47
1:G:18:MET:HA	1:G:21:LYS:HE3	1.97	0.47
1:L:95:ASN:HD22	1:L:152:GLN:HE22	1.63	0.47
1:L:113:ILE:HD11	1:L:219:ILE:HG21	1.97	0.46
1:E:247:THR:HG22	1:E:248:GLU:N	2.30	0.46
1:F:183:ASN:O	1:F:186:ASN:HB2	2.15	0.46
1:J:80:ASN:HB2	1:J:83:VAL:HG23	1.96	0.46
1:E:22:VAL:HG21	1:E:196:GLY:HA3	1.97	0.46
1:B:289:SER:HB2	1:B:317:GLY:HA3	1.98	0.46
1:C:280:GLY:O	1:C:320:ARG:NH2	2.48	0.45
1:D:179:ASP:HB3	1:F:155:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:LEU:HD11	1:L:199:ILE:HB	1.99	0.45
1:F:174:ASN:ND2	1:F:300:GLU:HG3	2.32	0.45
1:I:174:ASN:ND2	1:I:300:GLU:HG3	2.31	0.45
1:A:146:ASN:HD22	1:A:149:GLY:HA2	1.82	0.45
1:J:249:MET:HE1	1:J:286:ILE:HG12	1.99	0.44
1:H:113:ILE:HD11	1:H:219:ILE:HG21	2.00	0.44
1:C:223:MET:HG3	1:C:307:THR:HG21	2.00	0.44
1:G:211:GLY:HA3	1:H:213:VAL:HG11	1.99	0.44
1:D:113:ILE:HD11	1:D:219:ILE:HG21	2.00	0.44
1:B:313:LYS:NZ	1:E:121:PRO:O	2.51	0.44
1:I:22:VAL:HG21	1:I:196:GLY:HA3	2.00	0.44
1:L:228:ALA:O	1:L:232:ILE:HG23	2.18	0.44
1:I:146:ASN:HD22	1:I:149:GLY:HA2	1.83	0.43
1:G:238:LYS:HD3	1:G:238:LYS:HA	1.85	0.43
1:E:211:GLY:HA3	1:F:213:VAL:HG11	1.99	0.43
1:B:316:LEU:HD22	1:B:329:VAL:HG21	1.98	0.43
1:F:72:ALA:H	1:F:126:GLN:NE2	2.14	0.43
1:C:238:LYS:HB3	1:C:310:PRO:HD2	2.00	0.43
1:G:174:ASN:ND2	1:G:300:GLU:HG3	2.34	0.43
1:K:174:ASN:ND2	1:K:300:GLU:HG3	2.33	0.43
1:C:174:ASN:ND2	1:C:300:GLU:HG3	2.33	0.43
1:K:261:VAL:HG21	1:K:288:THR:CG2	2.48	0.43
1:G:207:ALA:HB1	1:G:211:GLY:O	2.18	0.43
1:A:80:ASN:HB2	1:A:83:VAL:HG23	2.00	0.43
1:K:22:VAL:HG21	1:K:196:GLY:HA3	2.00	0.43
1:G:239:ARG:HB3	1:G:334:SER:HB3	2.01	0.43
1:E:183:ASN:H	1:E:186:ASN:ND2	2.13	0.43
1:H:211:GLY:HA3	1:I:213:VAL:HG11	2.00	0.43
1:A:121:PRO:O	1:K:313:LYS:NZ	2.51	0.43
1:A:135:LEU:HD11	1:A:199:ILE:HB	1.99	0.42
1:H:80:ASN:HB2	1:H:83:VAL:HG23	2.01	0.42
1:G:146:ASN:ND2	1:G:151:GLY:H	2.17	0.42
1:B:146:ASN:HD21	1:B:151:GLY:H	1.67	0.42
1:H:72:ALA:H	1:H:126:GLN:NE2	2.13	0.42
1:J:72:ALA:H	1:J:126:GLN:NE2	2.13	0.42
1:G:245:LYS:HB2	1:G:269:GLU:HB3	2.01	0.42
1:I:78:LEU:HD13	1:I:201:ILE:HD13	2.01	0.42
1:D:72:ALA:H	1:D:126:GLN:NE2	2.14	0.42
1:B:174:ASN:ND2	1:B:300:GLU:HG3	2.34	0.42
1:B:279:ALA:HB1	1:B:327:VAL:HG13	2.01	0.42
1:D:155:THR:HG22	1:E:179:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ILE:HD11	1:C:219:ILE:HG21	2.02	0.42
1:B:285:ASP:OD2	1:B:318:LEU:HD21	2.19	0.42
1:E:191:LEU:HB2	1:E:202:ASN:HD21	1.84	0.42
1:A:187:SER:OG	2:Z:6:UNK:C	2.67	0.42
1:I:82:HIS:CE1	1:I:187:SER:HG	2.37	0.42
1:F:172:LEU:HD22	1:F:303:SER:HA	2.02	0.42
1:I:245:LYS:HB2	1:I:269:GLU:HB3	2.01	0.42
1:A:113:ILE:HD11	1:A:219:ILE:HG21	2.00	0.41
1:A:84:ILE:HG12	1:A:116:LEU:HD21	2.01	0.41
1:K:113:ILE:CD1	1:K:219:ILE:HG21	2.50	0.41
1:B:245:LYS:HB2	1:B:269:GLU:HB3	2.03	0.41
1:B:146:ASN:ND2	1:B:151:GLY:H	2.18	0.41
1:G:113:ILE:HD11	1:G:219:ILE:HG21	2.03	0.41
1:J:174:ASN:ND2	1:J:300:GLU:HG3	2.35	0.41
1:D:23:LEU:HB3	1:D:152:GLN:HE22	1.85	0.41
1:J:23:LEU:HD22	1:J:152:GLN:NE2	2.36	0.41
1:H:301:LEU:HD22	1:H:305:ILE:HG12	2.01	0.41
1:J:141:ALA:HB1	1:J:191:LEU:HD11	2.03	0.41
1:C:245:LYS:HB2	1:C:269:GLU:HB3	2.01	0.41
1:F:301:LEU:HD22	1:F:305:ILE:HG12	2.03	0.41
1:E:23:LEU:HB3	1:E:152:GLN:NE2	2.36	0.41
1:J:191:LEU:HB2	1:J:202:ASN:HD21	1.86	0.41
1:E:72:ALA:H	1:E:126:GLN:NE2	2.13	0.41
1:K:72:ALA:H	1:K:126:GLN:NE2	2.14	0.41
1:D:174:ASN:ND2	1:D:300:GLU:HG3	2.35	0.41
1:E:23:LEU:HB3	1:E:152:GLN:HE22	1.86	0.41
1:J:239:ARG:HB3	1:J:334:SER:HB3	2.03	0.41
1:F:129:ILE:HG23	1:F:221:SER:HB2	2.03	0.41
1:A:183:ASN:O	1:A:186:ASN:HB2	2.21	0.41
1:A:174:ASN:ND2	1:A:300:GLU:HG3	2.36	0.41
1:B:247:THR:HG22	1:B:248:GLU:N	2.35	0.41
1:L:174:ASN:ND2	1:L:300:GLU:HG3	2.36	0.40
1:A:23:LEU:HB3	1:A:152:GLN:NE2	2.36	0.40
1:L:245:LYS:HB2	1:L:269:GLU:HB3	2.03	0.40
1:K:238:LYS:HB3	1:K:310:PRO:HD2	2.03	0.40
1:H:238:LYS:HB3	1:H:310:PRO:HD2	2.04	0.40
1:H:245:LYS:HB2	1:H:269:GLU:HB3	2.04	0.40
1:G:22:VAL:HG21	1:G:196:GLY:HA3	2.02	0.40
1:G:72:ALA:H	1:G:126:GLN:NE2	2.13	0.40
1:K:174:ASN:O	1:K:220:PRO:HG3	2.22	0.40
1:J:249:MET:CE	1:J:286:ILE:HG12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ILE:HD11	1:F:219:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/345 (86%)	291 (98%)	5 (2%)	0	100	100
1	B	296/345 (86%)	292 (99%)	4 (1%)	0	100	100
1	C	296/345 (86%)	291 (98%)	5 (2%)	0	100	100
1	D	296/345 (86%)	291 (98%)	5 (2%)	0	100	100
1	E	296/345 (86%)	292 (99%)	4 (1%)	0	100	100
1	F	296/345 (86%)	290 (98%)	6 (2%)	0	100	100
1	G	296/345 (86%)	289 (98%)	7 (2%)	0	100	100
1	H	296/345 (86%)	290 (98%)	6 (2%)	0	100	100
1	I	296/345 (86%)	291 (98%)	5 (2%)	0	100	100
1	J	296/345 (86%)	292 (99%)	4 (1%)	0	100	100
1	K	296/345 (86%)	291 (98%)	5 (2%)	0	100	100
1	L	296/345 (86%)	291 (98%)	5 (2%)	0	100	100
All	All	3552/4140 (86%)	3491 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	234/272 (86%)	214 (92%)	20 (8%)	13	25
1	B	234/272 (86%)	218 (93%)	16 (7%)	20	39
1	C	234/272 (86%)	215 (92%)	19 (8%)	15	28
1	D	234/272 (86%)	216 (92%)	18 (8%)	16	31
1	E	234/272 (86%)	212 (91%)	22 (9%)	11	20
1	F	234/272 (86%)	215 (92%)	19 (8%)	15	28
1	G	234/272 (86%)	214 (92%)	20 (8%)	13	25
1	H	234/272 (86%)	212 (91%)	22 (9%)	11	20
1	I	234/272 (86%)	213 (91%)	21 (9%)	12	23
1	J	234/272 (86%)	211 (90%)	23 (10%)	10	19
1	K	234/272 (86%)	209 (89%)	25 (11%)	8	15
1	L	234/272 (86%)	212 (91%)	22 (9%)	11	20
All	All	2808/3264 (86%)	2561 (91%)	247 (9%)	12	24

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	20	GLU
1	A	64	LEU
1	A	70	ILE
1	A	84	ILE
1	A	91	SER
1	A	101	ASP
1	A	109	ASP
1	A	113	ILE
1	A	124	LEU
1	A	127	ILE
1	A	146	ASN
1	A	156	SER
1	A	170	GLU
1	A	237	ILE
1	A	258	ASN
1	A	262	GLN
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	318	LEU
1	A	326	GLU
1	B	18	MET
1	B	64	LEU
1	B	70	ILE
1	B	91	SER
1	B	101	ASP
1	B	109	ASP
1	B	113	ILE
1	B	124	LEU
1	B	127	ILE
1	B	146	ASN
1	B	170	GLU
1	B	262	GLN
1	B	301	LEU
1	B	316	LEU
1	B	318	LEU
1	B	326	GLU
1	C	18	MET
1	C	22	VAL
1	C	64	LEU
1	C	70	ILE
1	C	78	LEU
1	C	84	ILE
1	C	91	SER
1	C	101	ASP
1	C	109	ASP
1	C	113	ILE
1	C	124	LEU
1	C	127	ILE
1	C	146	ASN
1	C	170	GLU
1	C	238	LYS
1	C	262	GLN
1	C	301	LEU
1	C	318	LEU
1	C	326	GLU
1	D	18	MET
1	D	20	GLU
1	D	64	LEU
1	D	70	ILE
1	D	84	ILE

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Mol	Chain	Res	Type
1	D	91	SER
1	D	101	ASP
1	D	109	ASP
1	D	113	ILE
1	D	124	LEU
1	D	127	ILE
1	D	146	ASN
1	D	170	GLU
1	D	262	GLN
1	D	301	LEU
1	D	303	SER
1	D	318	LEU
1	D	326	GLU
1	E	18	MET
1	E	20	GLU
1	E	64	LEU
1	E	70	ILE
1	E	84	ILE
1	E	91	SER
1	E	101	ASP
1	E	109	ASP
1	E	113	ILE
1	E	124	LEU
1	E	127	ILE
1	E	146	ASN
1	E	170	GLU
1	E	237	ILE
1	E	258	ASN
1	E	262	GLN
1	E	281	VAL
1	E	301	LEU
1	E	305	ILE
1	E	307	THR
1	E	318	LEU
1	E	326	GLU
1	F	18	MET
1	F	20	GLU
1	F	64	LEU
1	F	70	ILE
1	F	84	ILE
1	F	91	SER
1	F	101	ASP

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Mol	Chain	Res	Type
1	F	109	ASP
1	F	113	ILE
1	F	124	LEU
1	F	127	ILE
1	F	146	ASN
1	F	165	SER
1	F	170	GLU
1	F	187	SER
1	F	262	GLN
1	F	301	LEU
1	F	318	LEU
1	F	326	GLU
1	G	18	MET
1	G	20	GLU
1	G	28	SER
1	G	64	LEU
1	G	70	ILE
1	G	84	ILE
1	G	91	SER
1	G	101	ASP
1	G	109	ASP
1	G	113	ILE
1	G	120	ASN
1	G	124	LEU
1	G	127	ILE
1	G	146	ASN
1	G	170	GLU
1	G	258	ASN
1	G	262	GLN
1	G	301	LEU
1	G	318	LEU
1	G	326	GLU
1	H	18	MET
1	H	20	GLU
1	H	22	VAL
1	H	64	LEU
1	H	70	ILE
1	H	84	ILE
1	H	91	SER
1	H	101	ASP
1	H	109	ASP
1	H	113	ILE

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Mol	Chain	Res	Type
1	H	124	LEU
1	H	127	ILE
1	H	146	ASN
1	H	170	GLU
1	H	201	ILE
1	H	239	ARG
1	H	260	ASP
1	H	262	GLN
1	H	278	LYS
1	H	301	LEU
1	H	318	LEU
1	H	326	GLU
1	I	18	MET
1	I	19	LEU
1	I	20	GLU
1	I	64	LEU
1	I	70	ILE
1	I	84	ILE
1	I	91	SER
1	I	101	ASP
1	I	109	ASP
1	I	113	ILE
1	I	124	LEU
1	I	127	ILE
1	I	146	ASN
1	I	170	GLU
1	I	187	SER
1	I	201	ILE
1	I	262	GLN
1	I	281	VAL
1	I	301	LEU
1	I	318	LEU
1	I	326	GLU
1	J	18	MET
1	J	20	GLU
1	J	64	LEU
1	J	70	ILE
1	J	73	SER
1	J	84	ILE
1	J	91	SER
1	J	101	ASP
1	J	109	ASP

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Mol	Chain	Res	Type
1	J	113	ILE
1	J	124	LEU
1	J	127	ILE
1	J	146	ASN
1	J	152	GLN
1	J	170	GLU
1	J	206	LEU
1	J	232	ILE
1	J	237	ILE
1	J	247	THR
1	J	262	GLN
1	J	307	THR
1	J	318	LEU
1	J	326	GLU
1	K	18	MET
1	K	20	GLU
1	K	64	LEU
1	K	70	ILE
1	K	84	ILE
1	K	91	SER
1	K	101	ASP
1	K	109	ASP
1	K	113	ILE
1	K	124	LEU
1	K	127	ILE
1	K	146	ASN
1	K	165	SER
1	K	170	GLU
1	K	186	ASN
1	K	201	ILE
1	K	237	ILE
1	K	258	ASN
1	K	262	GLN
1	K	301	LEU
1	K	302	ARG
1	K	307	THR
1	K	318	LEU
1	K	319	LEU
1	K	326	GLU
1	L	18	MET
1	L	22	VAL
1	L	64	LEU

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Mol	Chain	Res	Type
1	L	66	SER
1	L	70	ILE
1	L	84	ILE
1	L	91	SER
1	L	101	ASP
1	L	109	ASP
1	L	113	ILE
1	L	124	LEU
1	L	127	ILE
1	L	146	ASN
1	L	170	GLU
1	L	187	SER
1	L	230	GLN
1	L	258	ASN
1	L	262	GLN
1	L	301	LEU
1	L	302	ARG
1	L	318	LEU
1	L	326	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	146	ASN
1	A	152	GLN
1	A	174	ASN
1	A	186	ASN
1	A	202	ASN
1	A	222	ASN
1	A	230	GLN
1	B	126	GLN
1	B	146	ASN
1	B	152	GLN
1	B	174	ASN
1	B	186	ASN
1	B	202	ASN
1	B	222	ASN
1	B	230	GLN
1	C	126	GLN
1	C	146	ASN
1	C	152	GLN

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Mol	Chain	Res	Type
1	C	174	ASN
1	C	186	ASN
1	C	202	ASN
1	C	222	ASN
1	C	230	GLN
1	D	126	GLN
1	D	152	GLN
1	D	174	ASN
1	D	186	ASN
1	D	202	ASN
1	D	222	ASN
1	D	230	GLN
1	E	126	GLN
1	E	146	ASN
1	E	152	GLN
1	E	174	ASN
1	E	186	ASN
1	E	202	ASN
1	E	222	ASN
1	E	230	GLN
1	F	126	GLN
1	F	152	GLN
1	F	174	ASN
1	F	186	ASN
1	F	202	ASN
1	F	222	ASN
1	F	230	GLN
1	G	126	GLN
1	G	146	ASN
1	G	152	GLN
1	G	174	ASN
1	G	186	ASN
1	G	202	ASN
1	G	222	ASN
1	G	230	GLN
1	H	126	GLN
1	H	152	GLN
1	H	174	ASN
1	H	186	ASN
1	H	202	ASN
1	H	222	ASN
1	H	230	GLN

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Mol	Chain	Res	Type
1	I	126	GLN
1	I	152	GLN
1	I	174	ASN
1	I	186	ASN
1	I	202	ASN
1	I	222	ASN
1	I	230	GLN
1	J	126	GLN
1	J	152	GLN
1	J	174	ASN
1	J	186	ASN
1	J	202	ASN
1	J	222	ASN
1	J	230	GLN
1	K	110	GLN
1	K	126	GLN
1	K	152	GLN
1	K	174	ASN
1	K	202	ASN
1	K	222	ASN
1	K	230	GLN
1	L	126	GLN
1	L	146	ASN
1	L	152	GLN
1	L	174	ASN
1	L	186	ASN
1	L	202	ASN
1	L	222	ASN
1	L	230	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	300/345 (86%)	-0.12	11 (3%) 45 37	30, 55, 82, 121	0
1	B	300/345 (86%)	-0.28	4 (1%) 79 75	29, 47, 73, 126	0
1	C	300/345 (86%)	-0.13	9 (3%) 54 47	32, 53, 78, 126	0
1	D	300/345 (86%)	0.12	13 (4%) 39 31	40, 67, 91, 116	0
1	E	300/345 (86%)	-0.06	9 (3%) 54 47	35, 57, 84, 127	0
1	F	300/345 (86%)	-0.01	10 (3%) 50 43	35, 62, 85, 122	0
1	G	300/345 (86%)	-0.07	10 (3%) 50 43	33, 53, 78, 124	0
1	H	300/345 (86%)	-0.16	5 (1%) 73 68	34, 54, 77, 124	0
1	I	300/345 (86%)	-0.05	9 (3%) 54 47	31, 57, 87, 122	0
1	J	300/345 (86%)	0.00	8 (2%) 58 51	35, 62, 89, 121	0
1	K	300/345 (86%)	-0.14	7 (2%) 64 57	36, 54, 79, 117	0
1	L	300/345 (86%)	0.05	14 (4%) 35 28	39, 62, 89, 131	0
2	M	0/7	-	-	-	-
2	N	0/7	-	-	-	-
2	O	0/7	-	-	-	-
2	P	0/7	-	-	-	-
2	Q	0/7	-	-	-	-
2	R	0/7	-	-	-	-
2	S	0/7	-	-	-	-
2	T	0/7	-	-	-	-
2	U	0/7	-	-	-	-
2	V	0/7	-	-	-	-
2	W	0/7	-	-	-	-
2	X	0/7	-	-	-	-
2	Z	0/7	-	-	-	-
All	All	3600/4231 (85%)	-0.07	109 (3%) 54 47	29, 57, 84, 131	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	59	GLN	6.7
1	D	11	PRO	6.0
1	K	11	PRO	5.8
1	E	59	GLN	5.7
1	E	11	PRO	5.3
1	F	11	PRO	5.2
1	L	60	PRO	5.2
1	C	11	PRO	5.0
1	G	11	PRO	4.9
1	C	59	GLN	4.9
1	C	34	THR	4.7
1	L	34	THR	4.7
1	F	34	THR	4.6
1	E	34	THR	4.6
1	H	59	GLN	4.6
1	E	60	PRO	4.3
1	B	11	PRO	4.3
1	L	63	GLY	4.2
1	D	59	GLN	4.1
1	J	59	GLN	4.1
1	J	11	PRO	4.1
1	I	59	GLN	4.0
1	D	88	GLN	4.0
1	K	59	GLN	4.0
1	I	11	PRO	3.9
1	G	34	THR	3.9
1	A	59	GLN	3.9
1	K	62	GLU	3.8
1	H	11	PRO	3.8
1	L	11	PRO	3.7
1	F	59	GLN	3.7
1	L	59	GLN	3.6
1	L	61	PHE	3.6
1	L	287	ILE	3.4
1	A	86	GLN	3.3
1	I	313	LYS	3.2
1	A	11	PRO	3.2
1	C	88	GLN	3.1
1	B	62	GLU	3.1
1	G	62	GLU	3.1
1	L	62	GLU	3.1
1	B	34	THR	3.0
1	H	60	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	322	GLY	3.0
1	A	33	GLY	2.9
1	D	86	GLN	2.9
1	G	86	GLN	2.9
1	D	273	GLY	2.9
1	J	287	ILE	2.9
1	J	234	PHE	2.9
1	J	30	ARG	2.8
1	H	30	ARG	2.8
1	A	273	GLY	2.8
1	A	60	PRO	2.8
1	D	60	PRO	2.8
1	G	287	ILE	2.7
1	I	60	PRO	2.7
1	L	86	GLN	2.7
1	I	260	ASP	2.7
1	G	210	GLY	2.7
1	L	85	ASN	2.7
1	D	287	ILE	2.7
1	F	77	VAL	2.7
1	A	62	GLU	2.7
1	E	86	GLN	2.6
1	D	260	ASP	2.6
1	I	86	GLN	2.5
1	B	86	GLN	2.5
1	F	88	GLN	2.5
1	L	278	LYS	2.5
1	G	60	PRO	2.5
1	L	323	LYS	2.4
1	F	287	ILE	2.4
1	K	61	PHE	2.4
1	C	62	GLU	2.4
1	K	77	VAL	2.4
1	A	34	THR	2.4
1	F	333	THR	2.4
1	I	272	PRO	2.4
1	G	61	PHE	2.4
1	D	34	THR	2.3
1	D	77	VAL	2.3
1	J	34	THR	2.3
1	D	64	LEU	2.3
1	K	12	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	260	ASP	2.3
1	D	134	LYS	2.3
1	I	286	ILE	2.3
1	C	60	PRO	2.3
1	A	258	ASN	2.3
1	E	286	ILE	2.3
1	J	86	GLN	2.3
1	E	61	PHE	2.2
1	I	287	ILE	2.2
1	C	234	PHE	2.2
1	C	272	PRO	2.2
1	A	61	PHE	2.2
1	L	30	ARG	2.2
1	F	234	PHE	2.2
1	D	62	GLU	2.1
1	E	62	GLU	2.1
1	G	12	LEU	2.1
1	C	273	GLY	2.1
1	H	321	ASN	2.1
1	F	62	GLU	2.1
1	K	321	ASN	2.1
1	J	61	PHE	2.0
1	E	30	ARG	2.0
1	F	326	GLU	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.