



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:29 am BST

PDB ID : 6RCP  
Title : Crystal structure of the OmpK36 clinical isolate ST258 from *Klebsiella pneumoniae*  
Authors : Beis, K.; Romano, M.; Kwong, J.  
Deposited on : 2019-04-11  
Resolution : 3.23 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

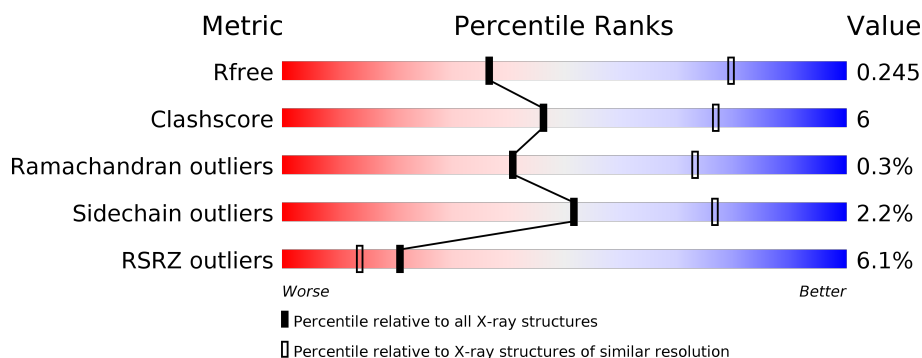
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 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	A	349	<div> <div>3%</div> <div>83% 17%</div> </div>
1	B	349	<div> <div>3%</div> <div>85% 14%</div> </div>
1	C	349	<div> <div>5%</div> <div>80% 19%</div> </div>
1	D	349	<div> <div>5%</div> <div>82% 18%</div> </div>
1	E	349	<div> <div>3%</div> <div>84% 15%</div> </div>
1	F	349	<div> <div>5%</div> <div>85% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	349	
1	H	349	
1	I	349	
1	J	349	
1	K	349	
1	L	349	
1	M	349	
1	N	349	
1	O	349	
1	P	349	
1	Q	349	
1	R	349	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 48852 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 OmpK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	B	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	E	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	G	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	H	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	I	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	K	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	L	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	N	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	O	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	P	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	Q	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	R	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	F	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	D	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	J	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			
1	C	349	Total	C	N	O	S	0	1	0
			2714	1700	450	562	2			

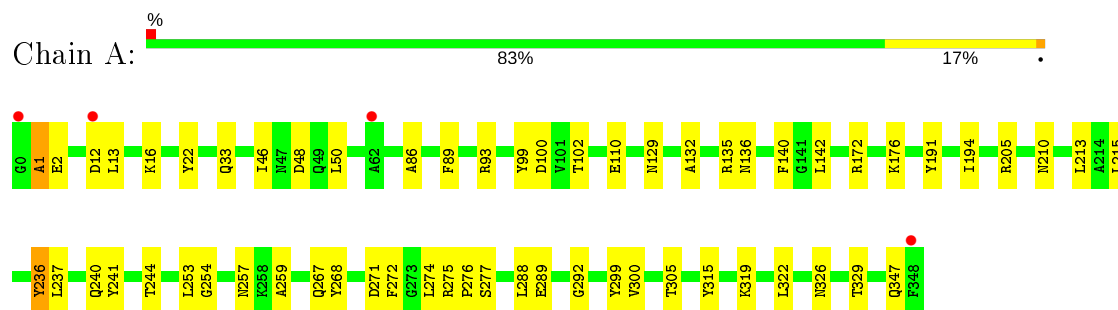
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP E5G6G2
B	0	GLY	-	expression tag	UNP E5G6G2
E	0	GLY	-	expression tag	UNP E5G6G2
G	0	GLY	-	expression tag	UNP E5G6G2
H	0	GLY	-	expression tag	UNP E5G6G2
I	0	GLY	-	expression tag	UNP E5G6G2
K	0	GLY	-	expression tag	UNP E5G6G2
L	0	GLY	-	expression tag	UNP E5G6G2
N	0	GLY	-	expression tag	UNP E5G6G2
O	0	GLY	-	expression tag	UNP E5G6G2
P	0	GLY	-	expression tag	UNP E5G6G2
Q	0	GLY	-	expression tag	UNP E5G6G2
R	0	GLY	-	expression tag	UNP E5G6G2
F	0	GLY	-	expression tag	UNP E5G6G2
D	0	GLY	-	expression tag	UNP E5G6G2
J	0	GLY	-	expression tag	UNP E5G6G2
M	0	GLY	-	expression tag	UNP E5G6G2
C	0	GLY	-	expression tag	UNP E5G6G2

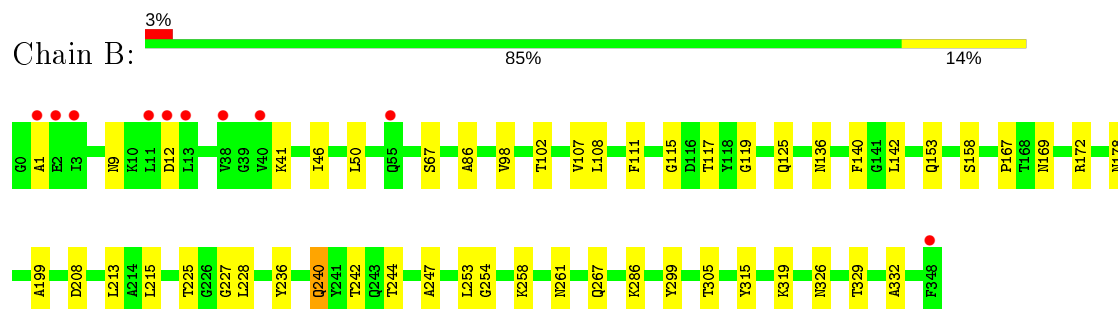
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

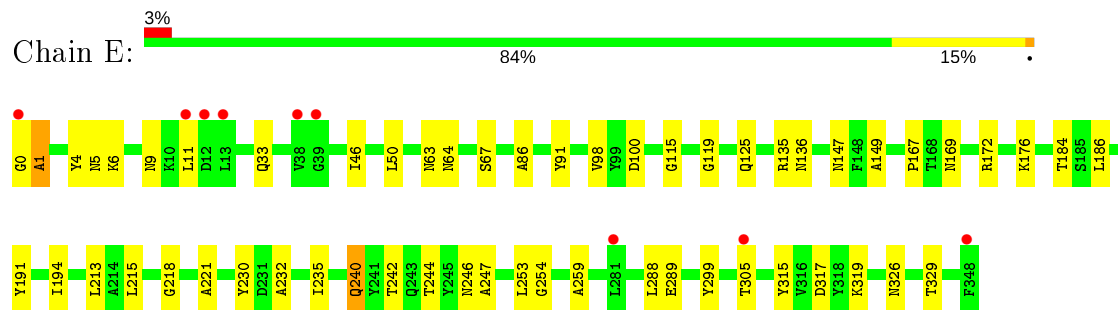
#### • Molecule 1: OmpK36



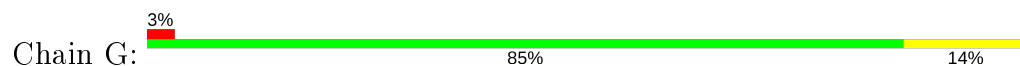
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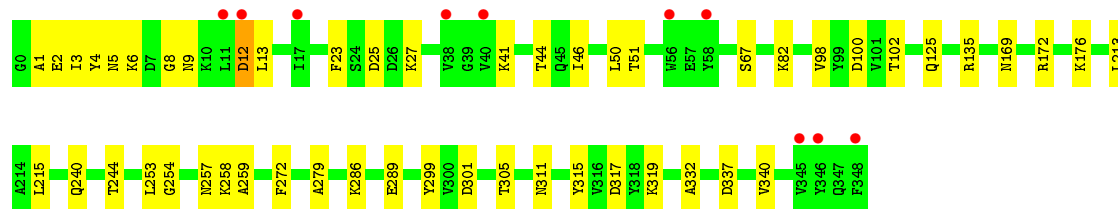


#### • Molecule 1: OmpK36

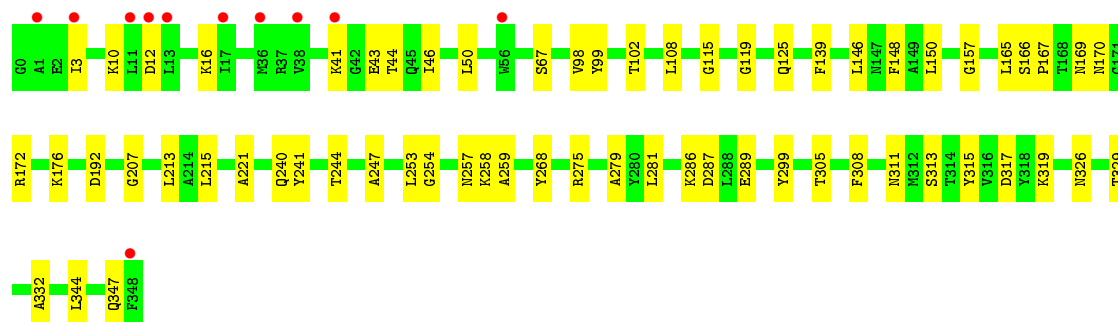
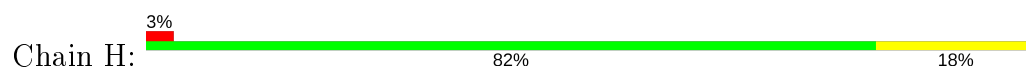


#### • Molecule 1: OmpK36

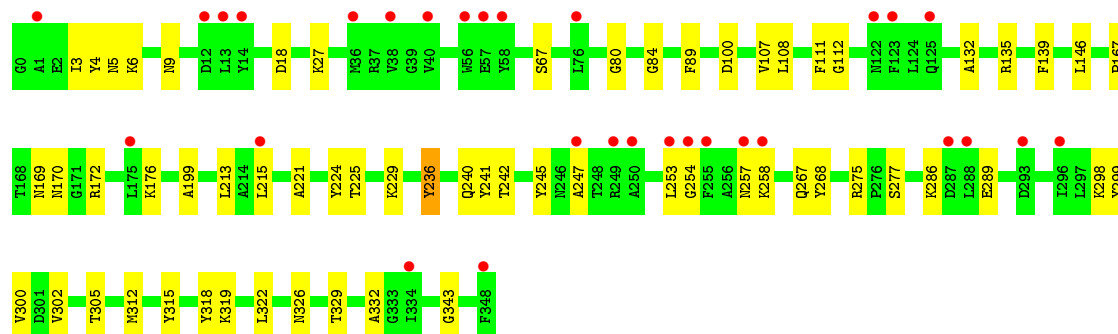
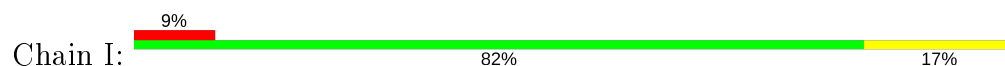




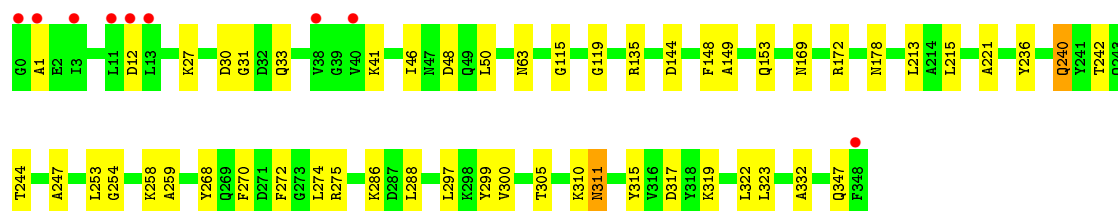
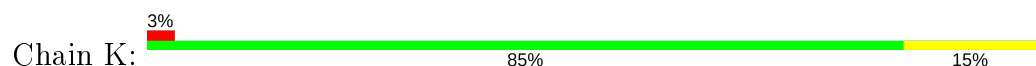
• Molecule 1: OmpK36



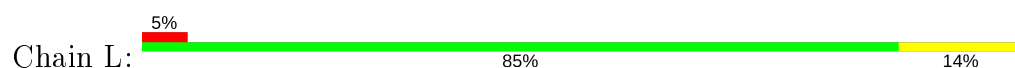
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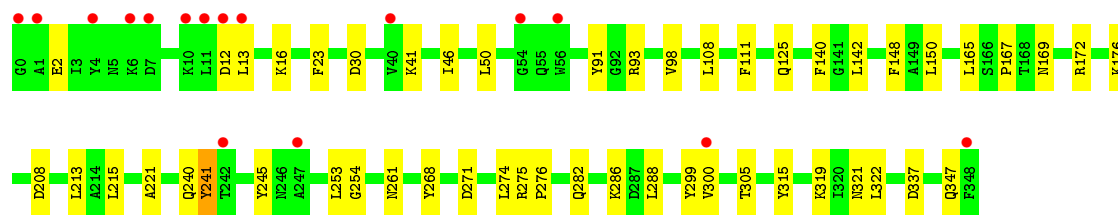


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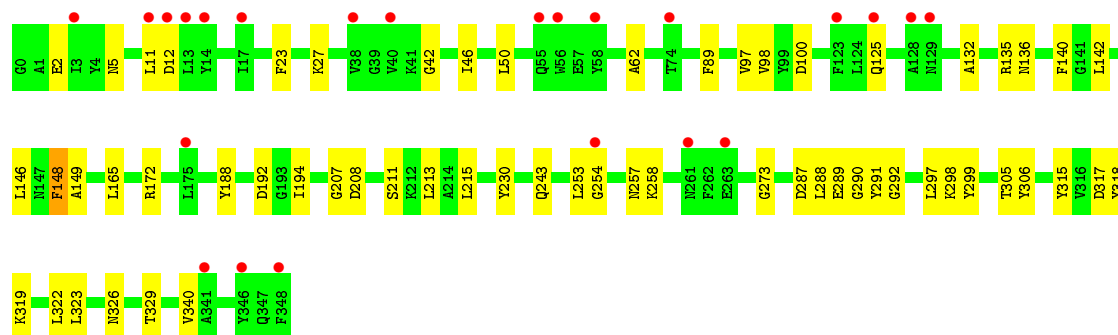
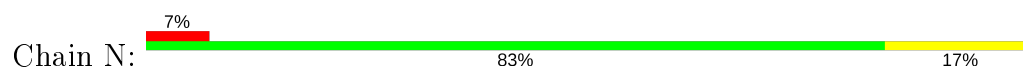


• Molecule 1: OmpK36

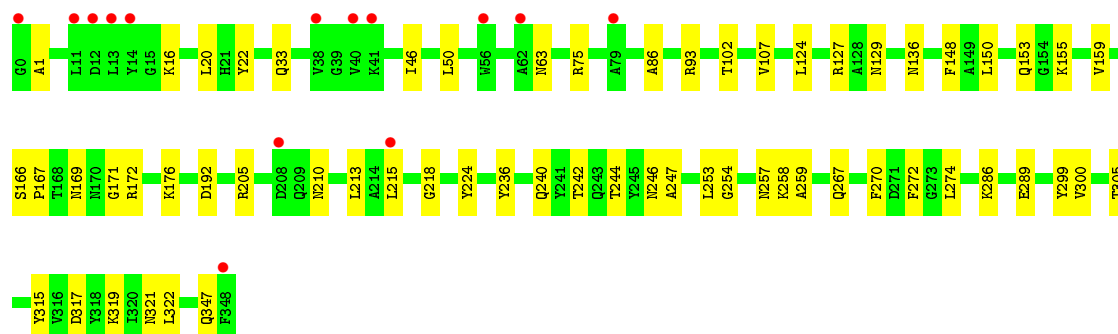
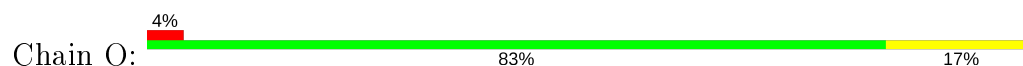




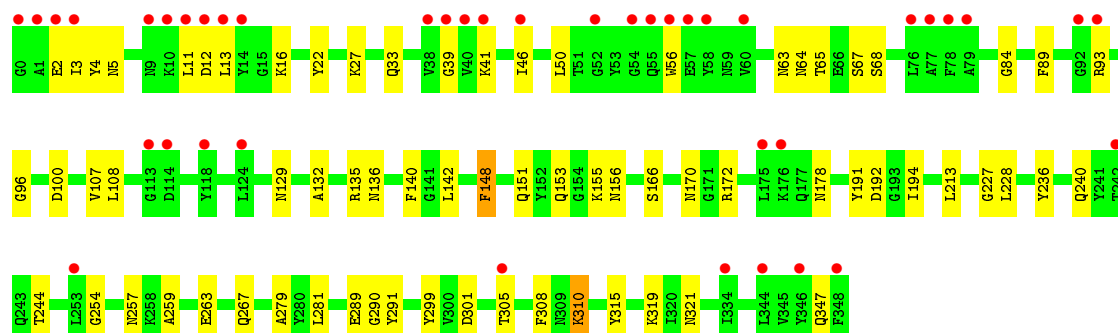
• Molecule 1: OmpK36



• Molecule 1: OmpK36

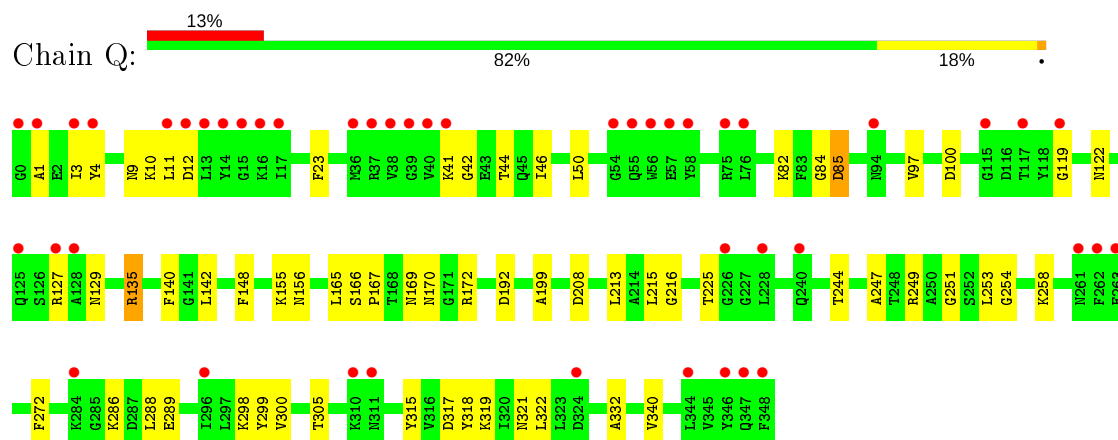


• Molecule 1: OmpK36

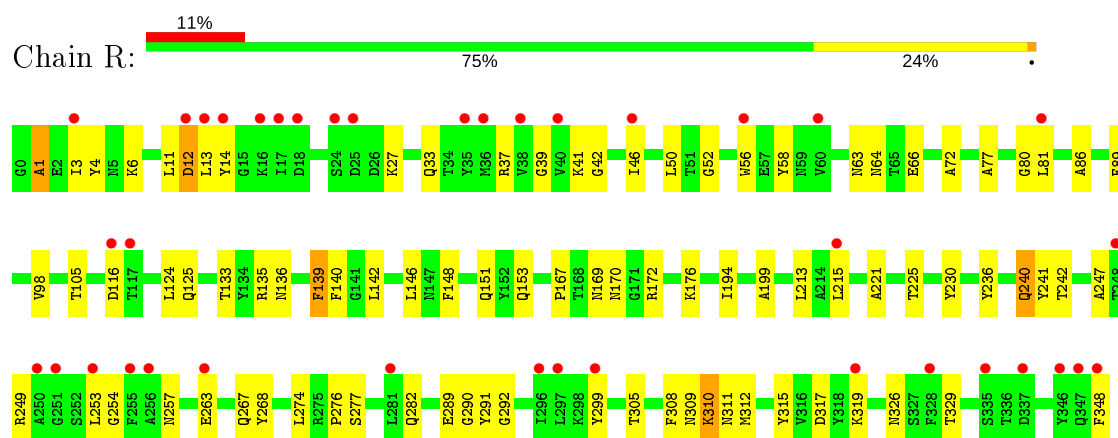




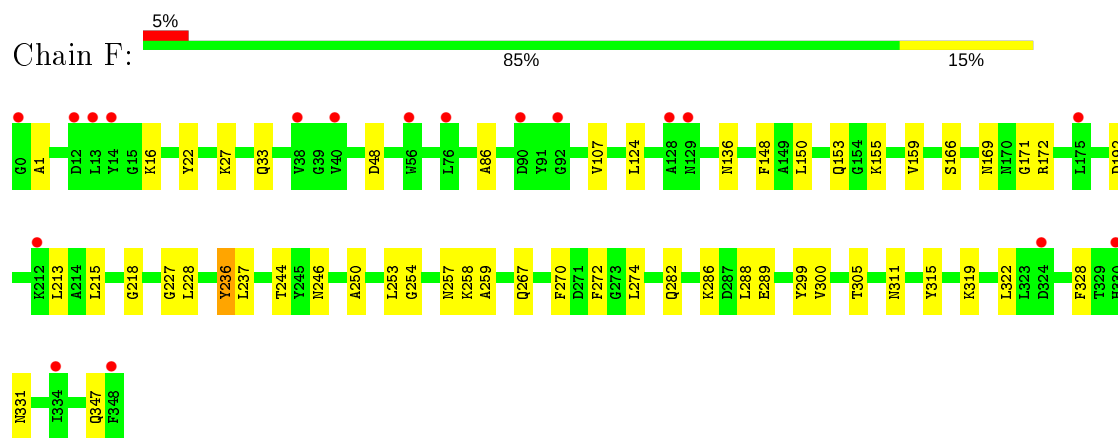
- Molecule 1: OmpK36



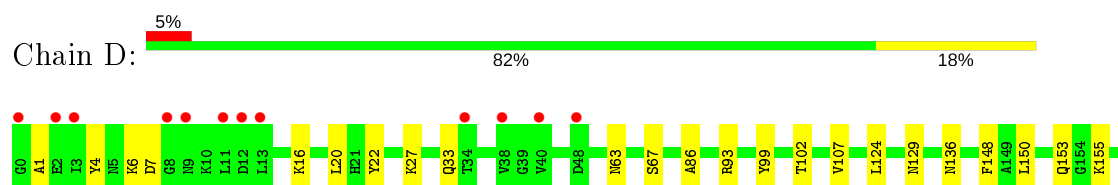
- Molecule 1: OmpK36

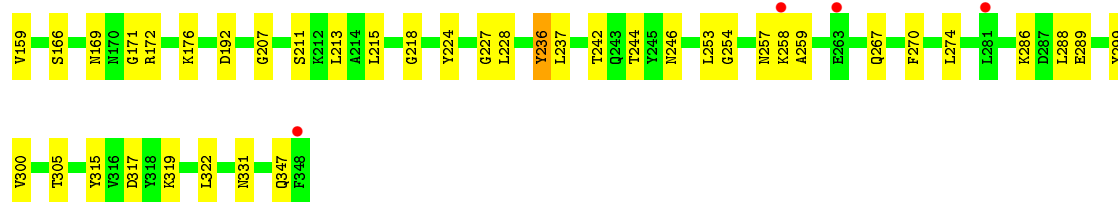


- Molecule 1: OmpK36

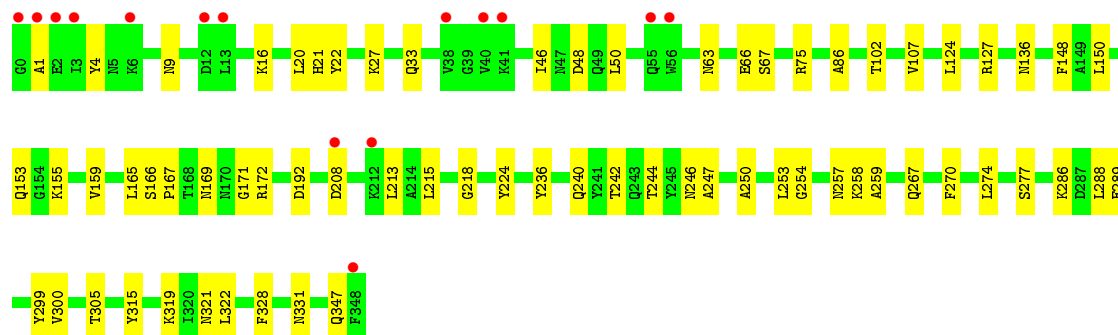
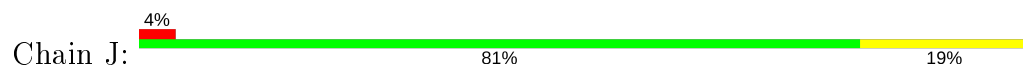


- Molecule 1: OmpK36

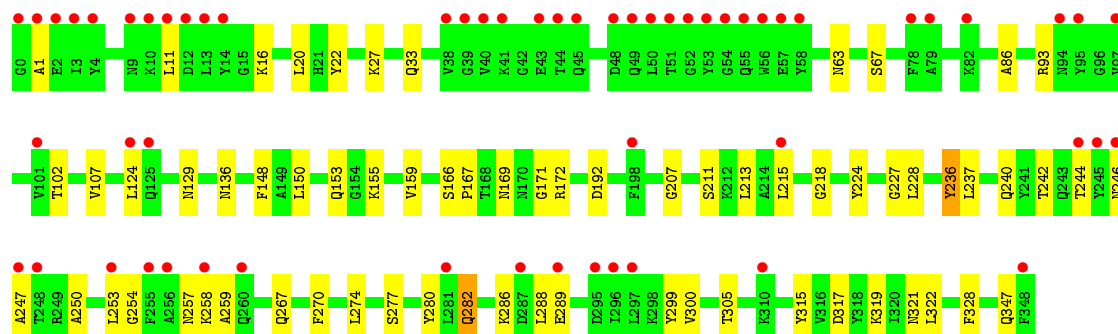
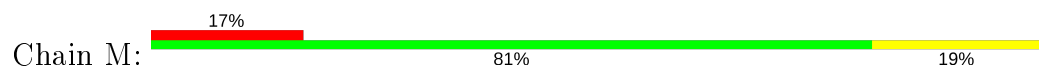




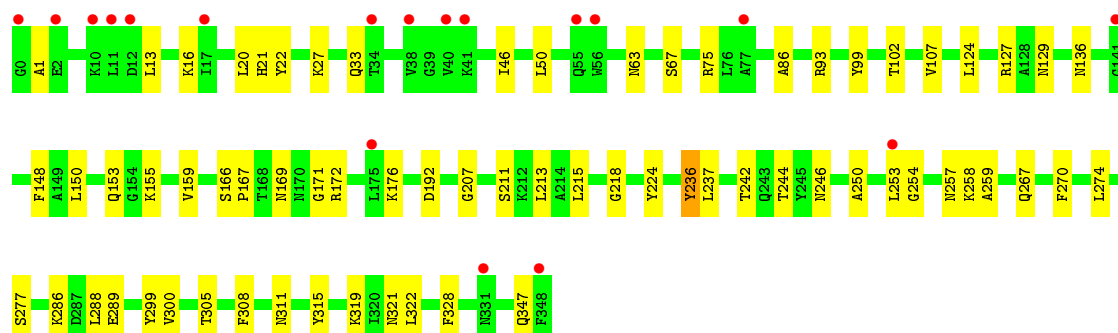
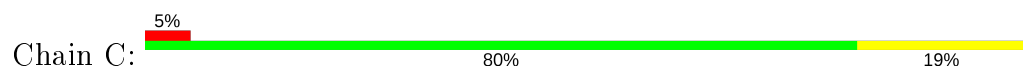
• Molecule 1: OmpK36



• Molecule 1: OmpK36



• Molecule 1: OmpK36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.04 Å   326.11 Å   164.19 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	91.51 – 3.23 286.04 – 3.23	Depositor EDS
% Data completeness (in resolution range)	51.9 (91.51-3.23) 51.9 (286.04-3.23)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.26 Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.218   ,   0.250 0.216   ,   0.245	Depositor DCC
$R_{free}$ test set	6394 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.1	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	48852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, 0.333 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	A	0.27	0/2774	0.50	0/3756
1	B	0.27	0/2774	0.51	0/3756
1	C	0.27	0/2774	0.51	0/3756
1	D	0.26	0/2774	0.50	0/3756
1	E	0.28	0/2774	0.52	0/3756
1	F	0.26	0/2774	0.49	0/3756
1	G	0.27	0/2774	0.51	0/3756
1	H	0.26	0/2774	0.50	0/3756
1	I	0.27	0/2774	0.50	0/3756
1	J	0.26	0/2774	0.50	0/3756
1	K	0.27	0/2774	0.51	0/3756
1	L	0.27	0/2774	0.50	0/3756
1	M	0.26	0/2774	0.50	0/3756
1	N	0.26	0/2774	0.50	0/3756
1	O	0.26	0/2774	0.50	0/3756
1	P	0.27	0/2774	0.51	0/3756
1	Q	0.27	0/2774	0.52	0/3756
1	R	0.27	0/2774	0.51	0/3756
All	All	0.27	0/49932	0.50	0/67608

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 ⓘ

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	2714	0	2506	35	0
1	B	2714	0	2506	28	0
1	C	2714	0	2506	39	0
1	D	2714	0	2506	33	0
1	E	2714	0	2506	34	0
1	F	2714	0	2506	26	0
1	G	2714	0	2506	29	0
1	H	2714	0	2506	38	0
1	I	2714	0	2506	42	0
1	J	2714	0	2506	37	0
1	K	2714	0	2506	27	0
1	L	2714	0	2506	29	0
1	M	2714	0	2506	36	0
1	N	2714	0	2506	33	0
1	O	2714	0	2506	30	0
1	P	2714	0	2506	44	0
1	Q	2714	0	2506	41	0
1	R	2714	0	2506	55	0
All	All	48852	0	45108	589	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 6.

All (589) 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:311:ASN:ND2	1:K:347:GLN:O	1.97	0.98
1:N:100:ASP:OD2	1:N:135:ARG:NH2	2.14	0.80
1:H:305:THR:HG23	1:H:315:TYR:HB3	1.65	0.78
1:G:100:ASP:OD2	1:G:135:ARG:NH2	2.17	0.77
1:H:258:LYS:HB3	1:H:286:LYS:HB2	1.69	0.74
1:K:311:ASN:OD1	1:J:9:ASN:ND2	2.20	0.73
1:F:213:LEU:HD22	1:F:254:GLY:HA2	1.71	0.73
1:G:305:THR:HG23	1:G:315:TYR:HB3	1.72	0.72
1:B:305:THR:HG23	1:B:315:TYR:HB3	1.71	0.70
1:D:27:LYS:HD2	1:C:167:PRO:HD2	1.74	0.70
1:G:98:VAL:HB	1:G:125:GLN:HA	1.75	0.69
1:P:305:THR:HG23	1:P:315:TYR:HB3	1.74	0.69
1:P:3:ILE:HD11	1:Q:3:ILE:HD12	1.73	0.69
1:P:4:TYR:HB3	1:P:11:LEU:HB2	1.75	0.69
1:D:213:LEU:HD22	1:D:254:GLY:HA2	1.75	0.68
1:J:213:LEU:HD22	1:J:254:GLY:HA2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:THR:HG23	1:E:315:TYR:HB3	1.74	0.68
1:P:12[B]:ASP:HB3	1:P:41:LYS:HB3	1.74	0.68
1:M:213:LEU:HD22	1:M:254:GLY:HA2	1.76	0.68
1:E:289:GLU:N	1:E:289:GLU:OE1	2.26	0.68
1:O:213:LEU:HD22	1:O:254:GLY:HA2	1.75	0.67
1:K:305:THR:HG23	1:K:315:TYR:HB3	1.76	0.67
1:B:213:LEU:HD22	1:B:254:GLY:HA2	1.77	0.67
1:C:213:LEU:HD22	1:C:254:GLY:HA2	1.77	0.67
1:F:305:THR:HG23	1:F:315:TYR:HB3	1.77	0.67
1:O:167:PRO:HD2	1:M:27:LYS:HD2	1.77	0.66
1:E:91:TYR:OH	1:C:21:HIS:ND1	2.25	0.66
1:K:213:LEU:HD22	1:K:254:GLY:HA2	1.77	0.66
1:N:305:THR:HG23	1:N:315:TYR:HB3	1.76	0.66
1:E:167:PRO:HD2	1:C:27:LYS:HD2	1.78	0.66
1:L:305:THR:HG23	1:L:315:TYR:HB3	1.77	0.66
1:E:100:ASP:OD2	1:E:135:ARG:NH2	2.23	0.65
1:R:305:THR:HG23	1:R:315:TYR:HB3	1.79	0.65
1:L:213:LEU:HD22	1:L:254:GLY:HA2	1.78	0.65
1:L:12[B]:ASP:HB3	1:L:41:LYS:HB3	1.78	0.65
1:Q:167:PRO:HD2	1:R:27:LYS:HD2	1.78	0.65
1:E:213:LEU:HD22	1:E:254:GLY:HA2	1.79	0.64
1:Q:305:THR:HG23	1:Q:315:TYR:HB3	1.79	0.64
1:R:257:ASN:ND2	1:R:289:GLU:OE2	2.30	0.64
1:G:213:LEU:HD22	1:G:254:GLY:HA2	1.79	0.64
1:L:91:TYR:OH	1:J:21:HIS:ND1	2.26	0.64
1:I:100:ASP:OD2	1:I:135:ARG:NH2	2.21	0.63
1:P:170:ASN:O	1:P:172:ARG:NH1	2.32	0.62
1:R:213:LEU:HD22	1:R:254:GLY:HA2	1.80	0.62
1:R:50:LEU:HD11	1:R:81:LEU:HD13	1.79	0.62
1:H:240:GLN:HG2	1:H:241:TYR:N	2.14	0.61
1:E:215:LEU:HD12	1:E:288:LEU:HD22	1.82	0.61
1:F:257:ASN:ND2	1:F:289:GLU:OE2	2.29	0.61
1:J:305:THR:HG23	1:J:315:TYR:HB3	1.82	0.61
1:P:257:ASN:ND2	1:P:289:GLU:OE2	2.32	0.61
1:G:258:LYS:HB3	1:G:286:LYS:HB2	1.81	0.61
1:N:290:GLY:O	1:N:292:GLY:N	2.32	0.61
1:H:12[B]:ASP:HB3	1:H:41:LYS:HB3	1.82	0.61
1:I:257:ASN:ND2	1:I:289:GLU:OE2	2.34	0.61
1:Q:213:LEU:HD22	1:Q:254:GLY:HA2	1.83	0.61
1:A:240:GLN:HG2	1:A:241:TYR:N	2.16	0.61
1:I:240:GLN:HG2	1:I:241:TYR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:310:LYS:HD3	1:P:310:LYS:H	1.64	0.61
1:O:300:VAL:HG23	1:O:322:LEU:HD11	1.84	0.60
1:Q:215:LEU:HD23	1:Q:253:LEU:HB3	1.83	0.60
1:A:213:LEU:HD22	1:A:254:GLY:HA2	1.84	0.60
1:C:215:LEU:HD23	1:C:253:LEU:HB3	1.84	0.60
1:C:300:VAL:HG23	1:C:322:LEU:HD11	1.82	0.60
1:J:257:ASN:ND2	1:J:289:GLU:OE2	2.34	0.60
1:P:12[A]:ASP:HB2	1:P:41:LYS:HB3	1.83	0.59
1:G:46:ILE:HD12	1:G:50:LEU:HG	1.84	0.59
1:R:12[B]:ASP:HB3	1:R:41:LYS:HB3	1.83	0.59
1:B:215:LEU:HD23	1:B:253:LEU:HB3	1.84	0.59
1:L:12[A]:ASP:HB2	1:L:41:LYS:HB3	1.82	0.59
1:P:16:LYS:HB3	1:P:347:GLN:HG3	1.83	0.59
1:F:215:LEU:HD23	1:F:253:LEU:HB3	1.84	0.59
1:B:9:ASN:ND2	1:F:311:ASN:OD1	2.34	0.59
1:G:2:GLU:OE2	1:G:5:ASN:ND2	2.27	0.58
1:M:300:VAL:HG23	1:M:322:LEU:HD11	1.86	0.58
1:I:300:VAL:HG23	1:I:322:LEU:HD11	1.85	0.58
1:D:257:ASN:ND2	1:D:289:GLU:OE2	2.35	0.58
1:E:46:ILE:HD12	1:E:50:LEU:HG	1.85	0.58
1:D:215:LEU:HD23	1:D:253:LEU:HB3	1.85	0.57
1:I:305:THR:HG23	1:I:315:TYR:HB3	1.86	0.57
1:N:213:LEU:HD22	1:N:254:GLY:HA2	1.85	0.57
1:E:176:LYS:HE3	1:C:67:SER:HB3	1.85	0.57
1:H:215:LEU:HD23	1:H:253:LEU:HB3	1.85	0.57
1:A:305:THR:HG23	1:A:315:TYR:HB3	1.85	0.57
1:I:215:LEU:HD23	1:I:253:LEU:HB3	1.85	0.57
1:M:257:ASN:ND2	1:M:289:GLU:OE2	2.34	0.57
1:O:215:LEU:HD23	1:O:253:LEU:HB3	1.86	0.57
1:N:297:LEU:HA	1:N:323:LEU:HD11	1.86	0.57
1:O:257:ASN:ND2	1:O:289:GLU:OE2	2.34	0.57
1:M:215:LEU:HD23	1:M:253:LEU:HB3	1.85	0.57
1:A:86:ALA:O	1:A:136:ASN:ND2	2.38	0.57
1:C:159:VAL:HA	1:C:171:GLY:HA3	1.86	0.57
1:P:170:ASN:ND2	1:P:172:ARG:HH12	2.03	0.57
1:R:12[A]:ASP:HB2	1:R:41:LYS:HB3	1.86	0.57
1:F:16:LYS:HB3	1:F:347:GLN:HG3	1.87	0.57
1:H:299:TYR:CD1	1:H:319:LYS:HG3	2.39	0.57
1:L:215:LEU:HD23	1:L:253:LEU:HB3	1.87	0.57
1:Q:156:ASN:HB3	1:Q:172:ARG:NH1	2.20	0.57
1:J:215:LEU:HD23	1:J:253:LEU:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:240:GLN:OE1	1:R:242:THR:OG1	2.18	0.56
1:B:299:TYR:CD2	1:B:319:LYS:HG3	2.40	0.56
1:P:27:LYS:HD2	1:R:167:PRO:HD2	1.87	0.56
1:B:86:ALA:O	1:B:136:ASN:ND2	2.38	0.56
1:O:270:PHE:HD2	1:O:274:LEU:HB3	1.70	0.56
1:R:86:ALA:O	1:R:136:ASN:ND2	2.38	0.56
1:H:16:LYS:HB3	1:H:347:GLN:HG3	1.87	0.56
1:B:244:THR:HB	1:B:247:ALA:HB3	1.86	0.56
1:F:270:PHE:HD2	1:F:274:LEU:HB3	1.71	0.56
1:D:305:THR:HG23	1:D:315:TYR:HB3	1.87	0.56
1:H:12[A]:ASP:HB2	1:H:41:LYS:HB3	1.86	0.56
1:O:305:THR:HG23	1:O:315:TYR:HB3	1.86	0.56
1:R:39:GLY:HA3	1:R:56:TRP:O	2.05	0.56
1:D:270:PHE:HD2	1:D:274:LEU:HB3	1.71	0.56
1:P:2:GLU:OE2	1:P:5:ASN:ND2	2.37	0.56
1:K:240:GLN:OE1	1:K:242:THR:OG1	2.23	0.56
1:M:305:THR:HG23	1:M:315:TYR:HB3	1.88	0.56
1:Q:44:THR:OG1	1:R:309:ASN:ND2	2.34	0.56
1:M:207:GLY:O	1:M:211:SER:OG	2.15	0.55
1:N:23:PHE:HB2	1:N:340:VAL:HB	1.88	0.55
1:E:191:TYR:HD2	1:E:194:ILE:HD12	1.71	0.55
1:M:86:ALA:O	1:M:136:ASN:ND2	2.39	0.55
1:N:27:LYS:HD2	1:M:167:PRO:HD2	1.88	0.55
1:L:46:ILE:HD12	1:L:50:LEU:HG	1.89	0.55
1:C:16:LYS:HB3	1:C:347:GLN:HG3	1.87	0.55
1:H:46:ILE:HD12	1:H:50:LEU:HG	1.88	0.55
1:M:16:LYS:HB3	1:M:347:GLN:HG3	1.89	0.55
1:F:86:ALA:O	1:F:136:ASN:ND2	2.39	0.55
1:O:159:VAL:HA	1:O:171:GLY:HA3	1.89	0.55
1:O:16:LYS:HB3	1:O:347:GLN:HG3	1.89	0.55
1:G:279:ALA:HB3	1:G:301:ASP:HB3	1.88	0.55
1:B:253:LEU:HG	1:B:332:ALA:HA	1.89	0.55
1:I:139:PHE:HB2	1:I:146:LEU:HD23	1.89	0.55
1:J:300:VAL:HG23	1:J:322:LEU:HD11	1.88	0.55
1:A:215:LEU:HD23	1:A:253:LEU:HB3	1.89	0.54
1:K:270:PHE:HD2	1:K:274:LEU:HB3	1.73	0.54
1:N:243:GLN:OE1	1:N:258:LYS:NZ	2.40	0.54
1:O:86:ALA:O	1:O:136:ASN:ND2	2.40	0.54
1:Q:170:ASN:O	1:Q:172:ARG:NH1	2.40	0.54
1:I:267:GLN:HG2	1:I:277:SER:HB2	1.90	0.54
1:Q:140:PHE:HB2	1:Q:142:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:ASN:ND2	1:Q:172:ARG:HH12	2.06	0.54
1:G:215:LEU:HD23	1:G:253:LEU:HB3	1.90	0.54
1:L:2:GLU:HA	1:L:12[A]:ASP:HA	1.89	0.54
1:R:33:GLN:HA	1:R:63:ASN:HD22	1.73	0.54
1:A:191:TYR:HD2	1:A:194:ILE:HD12	1.72	0.54
1:R:11:LEU:HD12	1:R:42:GLY:HA3	1.88	0.54
1:G:9:ASN:ND2	1:H:311:ASN:OD1	2.40	0.54
1:K:299:TYR:CD2	1:K:319:LYS:HG3	2.43	0.54
1:L:2:GLU:HA	1:L:12[B]:ASP:HA	1.90	0.54
1:A:176:LYS:HE3	1:B:67:SER:HB3	1.90	0.53
1:A:257:ASN:ND2	1:A:289:GLU:OE2	2.40	0.53
1:C:270:PHE:HD2	1:C:274:LEU:HB3	1.72	0.53
1:D:300:VAL:HG23	1:D:322:LEU:HD11	1.89	0.53
1:L:93:ARG:NH2	1:J:66:GLU:OE2	2.40	0.53
1:E:194:ILE:HG12	1:E:230:TYR:HD2	1.73	0.53
1:N:2:GLU:HA	1:N:12[A]:ASP:HA	1.90	0.53
1:Q:46:ILE:HD12	1:Q:50:LEU:HG	1.89	0.53
1:N:2:GLU:HA	1:N:12[B]:ASP:HA	1.90	0.53
1:D:107:VAL:O	1:D:267:GLN:NE2	2.40	0.53
1:F:299:TYR:CD1	1:F:319:LYS:HG3	2.43	0.53
1:O:22:TYR:CD1	1:O:33:GLN:HG3	2.44	0.53
1:B:140:PHE:HB2	1:B:142:LEU:HD13	1.90	0.53
1:I:89:PHE:HE1	1:I:132:ALA:HB1	1.74	0.53
1:B:167:PRO:HD2	1:F:27:LYS:HD2	1.91	0.53
1:M:270:PHE:HD2	1:M:274:LEU:HB3	1.74	0.53
1:Q:10:LYS:O	1:Q:42:GLY:HA2	2.09	0.53
1:A:110:GLU:HB2	1:A:315:TYR:HE2	1.72	0.53
1:F:258:LYS:HB3	1:F:286:LYS:HB2	1.91	0.53
1:I:213:LEU:HD22	1:I:254:GLY:HA2	1.90	0.53
1:N:98:VAL:HB	1:N:125:GLN:HA	1.91	0.53
1:R:139:PHE:HB2	1:R:146:LEU:HB3	1.91	0.53
1:R:290:GLY:O	1:R:292:GLY:N	2.39	0.53
1:C:107:VAL:O	1:C:267:GLN:NE2	2.42	0.53
1:C:22:TYR:CD1	1:C:33:GLN:HG3	2.44	0.52
1:L:176:LYS:HE3	1:J:67:SER:HB3	1.91	0.52
1:N:215:LEU:HD23	1:N:253:LEU:HB3	1.90	0.52
1:E:9:ASN:ND2	1:C:311:ASN:OD1	2.43	0.52
1:C:86:ALA:O	1:C:136:ASN:ND2	2.41	0.52
1:D:155:LYS:HE3	1:D:166:SER:HB3	1.91	0.52
1:E:240:GLN:OE1	1:E:242:THR:OG1	2.24	0.52
1:J:155:LYS:HE3	1:J:166:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:VAL:HA	1:J:171:GLY:HA3	1.92	0.52
1:L:98:VAL:HB	1:L:125:GLN:HA	1.91	0.52
1:C:305:THR:HG23	1:C:315:TYR:HB3	1.92	0.52
1:D:16:LYS:HB3	1:D:347:GLN:HG3	1.91	0.52
1:E:215:LEU:HD23	1:E:253:LEU:HB3	1.90	0.52
1:P:100:ASP:OD2	1:P:135:ARG:NH2	2.28	0.52
1:Q:119:GLY:HA3	1:Q:249:ARG:HH12	1.75	0.52
1:H:44:THR:HG21	1:I:312:MET:HB2	1.92	0.52
1:G:12[B]:ASP:HB3	1:G:41:LYS:HB3	1.92	0.52
1:M:159:VAL:HA	1:M:171:GLY:HA3	1.91	0.52
1:N:136:ASN:HB3	1:N:148:PHE:CE1	2.44	0.52
1:J:107:VAL:O	1:J:267:GLN:NE2	2.41	0.52
1:B:98:VAL:HB	1:B:125:GLN:HA	1.92	0.52
1:F:148:PHE:CZ	1:F:150:LEU:HG	2.44	0.52
1:H:257:ASN:ND2	1:H:289:GLU:OE2	2.43	0.52
1:J:270:PHE:HD2	1:J:274:LEU:HB3	1.74	0.52
1:C:155:LYS:HE3	1:C:166:SER:HB3	1.92	0.52
1:D:207:GLY:O	1:D:211:SER:OG	2.18	0.52
1:F:107:VAL:O	1:F:267:GLN:NE2	2.38	0.52
1:R:37:ARG:HA	1:R:58:TYR:O	2.10	0.51
1:C:257:ASN:ND2	1:C:289:GLU:OE2	2.37	0.51
1:O:107:VAL:O	1:O:267:GLN:NE2	2.42	0.51
1:Q:4:TYR:HB2	1:R:3:ILE:HG22	1.92	0.51
1:E:299:TYR:CD2	1:E:319:LYS:HG3	2.45	0.51
1:N:299:TYR:CD1	1:N:319:LYS:HG3	2.46	0.51
1:P:155:LYS:HE3	1:P:166:SER:HB3	1.93	0.51
1:A:140:PHE:HB2	1:A:142:LEU:HD13	1.93	0.51
1:O:155:LYS:HE3	1:O:166:SER:HB3	1.93	0.51
1:D:86:ALA:O	1:D:136:ASN:ND2	2.44	0.51
1:A:215:LEU:HD12	1:A:288:LEU:HD22	1.93	0.50
1:J:16:LYS:HB3	1:J:347:GLN:HG3	1.93	0.50
1:K:297:LEU:HA	1:K:323:LEU:HD11	1.93	0.50
1:J:86:ALA:O	1:J:136:ASN:ND2	2.44	0.50
1:J:299:TYR:CD1	1:J:319:LYS:HG3	2.46	0.50
1:R:267:GLN:HG2	1:R:277:SER:HB2	1.92	0.50
1:D:159:VAL:HA	1:D:171:GLY:HA3	1.93	0.50
1:K:258:LYS:HB3	1:K:286:LYS:HB2	1.93	0.50
1:M:155:LYS:HE3	1:M:166:SER:HB3	1.94	0.50
1:H:139:PHE:HB2	1:H:146:LEU:HB3	1.93	0.50
1:Q:300:VAL:HG23	1:Q:322:LEU:HD11	1.93	0.50
1:R:46:ILE:HD12	1:R:50:LEU:HG	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:298:LYS:HG2	1:Q:322:LEU:HB2	1.94	0.50
1:F:155:LYS:HE3	1:F:166:SER:HB3	1.93	0.50
1:D:4:TYR:CZ	1:D:6:LYS:HB3	2.47	0.49
1:E:244:THR:OG1	1:E:259:ALA:HB3	2.12	0.49
1:G:51:THR:HB	1:G:82:LYS:HB3	1.94	0.49
1:H:99:TYR:HA	1:H:102:THR:OG1	2.12	0.49
1:Q:215:LEU:HD13	1:Q:289:GLU:HG2	1.94	0.49
1:C:20:LEU:HD21	1:C:22:TYR:HE1	1.77	0.49
1:H:108:LEU:HD21	1:H:279:ALA:HB2	1.94	0.49
1:N:298:LYS:HG2	1:N:322:LEU:HB2	1.93	0.49
1:O:218:GLY:HA3	1:O:246:ASN:ND2	2.27	0.49
1:G:1:ALA:HB3	1:G:13:LEU:O	2.12	0.49
1:I:299:TYR:CD1	1:I:319:LYS:HG3	2.46	0.49
1:A:300:VAL:HG23	1:A:322:LEU:HD11	1.95	0.49
1:O:148:PHE:CZ	1:O:150:LEU:HG	2.47	0.49
1:A:2:GLU:HA	1:A:12[A]:ASP:HA	1.94	0.49
1:A:205:ARG:NH2	1:A:210:ASN:OD1	2.34	0.49
1:K:12[B]:ASP:HB3	1:K:41:LYS:HB3	1.95	0.49
1:Q:129:ASN:HB2	1:Q:172:ARG:NH2	2.28	0.49
1:I:5:ASN:HB3	1:D:7:ASP:OD1	2.13	0.49
1:J:22:TYR:CD1	1:J:33:GLN:HG3	2.48	0.49
1:G:27:LYS:NZ	1:I:167:PRO:HD2	2.28	0.49
1:L:274:LEU:HG	1:L:276:PRO:HD3	1.94	0.49
1:C:244:THR:OG1	1:C:259:ALA:HB3	2.13	0.49
1:I:315:TYR:CZ	1:I:343:GLY:HA3	2.48	0.49
1:A:288:LEU:HB2	1:A:292:GLY:H	1.77	0.48
1:E:67:SER:HB3	1:D:176:LYS:NZ	2.28	0.48
1:R:215:LEU:HD23	1:R:253:LEU:HB3	1.95	0.48
1:D:148:PHE:CZ	1:D:150:LEU:HG	2.48	0.48
1:G:299:TYR:CD1	1:G:319:LYS:HG3	2.48	0.48
1:F:159:VAL:HA	1:F:171:GLY:HA3	1.95	0.48
1:P:279:ALA:HB3	1:P:301:ASP:HB3	1.95	0.48
1:A:274:LEU:HG	1:A:276:PRO:HD3	1.95	0.48
1:B:115:GLY:H	1:B:119:GLY:HA2	1.78	0.48
1:D:33:GLN:HA	1:D:63:ASN:HD22	1.79	0.48
1:M:22:TYR:CD1	1:M:33:GLN:HG3	2.49	0.48
1:Q:122:ASN:ND2	1:Q:249:ARG:HG3	2.28	0.48
1:G:25:ASP:HB2	1:G:337:ASP:HB3	1.95	0.48
1:I:258:LYS:HB3	1:I:286:LYS:HB2	1.96	0.48
1:D:244:THR:OG1	1:D:259:ALA:HB3	2.13	0.48
1:M:124:LEU:HD21	1:M:153:GLN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:GLN:HA	1:O:63:ASN:HD22	1.78	0.48
1:A:89:PHE:HE1	1:A:132:ALA:HB1	1.79	0.48
1:L:299:TYR:CD1	1:L:319:LYS:HG3	2.49	0.48
1:N:97:VAL:O	1:N:100:ASP:HB2	2.14	0.48
1:R:4:TYR:CZ	1:R:6:LYS:HB2	2.49	0.48
1:G:311:ASN:CG	1:I:9:ASN:HD21	2.16	0.48
1:K:48:ASP:HB2	1:F:48:ASP:OD2	2.13	0.48
1:P:3:ILE:HG22	1:P:13:LEU:H	1.79	0.48
1:P:46:ILE:HD12	1:P:50:LEU:HG	1.95	0.48
1:E:86:ALA:O	1:E:136:ASN:ND2	2.47	0.47
1:A:2:GLU:HA	1:A:12[B]:ASP:HA	1.95	0.47
1:I:108:LEU:HD12	1:I:112:GLY:HA3	1.96	0.47
1:L:148:PHE:CZ	1:L:150:LEU:HG	2.48	0.47
1:R:299:TYR:CD2	1:R:319:LYS:HG3	2.49	0.47
1:A:244:THR:OG1	1:A:259:ALA:HB3	2.14	0.47
1:D:22:TYR:CD1	1:D:33:GLN:HG3	2.50	0.47
1:E:147:ASN:O	1:E:186:LEU:HA	2.14	0.47
1:I:221:ALA:HB1	1:I:247:ALA:HB2	1.95	0.47
1:L:240:GLN:O	1:L:241:TYR:HB3	2.14	0.47
1:B:107:VAL:HG21	1:B:236:TYR:CE2	2.50	0.47
1:C:33:GLN:HA	1:C:63:ASN:HD22	1.80	0.47
1:F:22:TYR:CD1	1:F:33:GLN:HG3	2.49	0.47
1:P:299:TYR:CD1	1:P:319:LYS:HG3	2.49	0.47
1:E:46:ILE:HD13	1:C:308:PHE:HB3	1.96	0.47
1:F:300:VAL:HG23	1:F:322:LEU:HD11	1.96	0.47
1:P:244:THR:OG1	1:P:259:ALA:HB3	2.15	0.47
1:G:176:LYS:HE3	1:H:67:SER:HB3	1.97	0.47
1:I:18:ASP:OD1	1:I:315:TYR:OH	2.30	0.47
1:O:244:THR:OG1	1:O:259:ALA:HB3	2.14	0.47
1:B:117:THR:HB	1:B:261:ASN:ND2	2.29	0.47
1:M:218:GLY:HA3	1:M:246:ASN:ND2	2.30	0.47
1:O:124:LEU:HD21	1:O:153:GLN:HB2	1.96	0.47
1:C:148:PHE:CZ	1:C:150:LEU:HG	2.50	0.47
1:G:257:ASN:ND2	1:G:289:GLU:OE2	2.48	0.47
1:M:148:PHE:CZ	1:M:150:LEU:HG	2.49	0.47
1:N:215:LEU:HD12	1:N:288:LEU:HD22	1.97	0.47
1:P:156:ASN:HB3	1:P:172:ARG:NH1	2.30	0.47
1:Q:97:VAL:O	1:Q:100:ASP:HB2	2.14	0.47
1:I:224:TYR:O	1:I:242:THR:HA	2.15	0.47
1:L:215:LEU:HD12	1:L:288:LEU:HD22	1.97	0.47
1:F:215:LEU:HD12	1:F:288:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:THR:OG1	1:F:259:ALA:HB3	2.14	0.46
1:R:80:GLY:HA3	1:R:89:PHE:O	2.14	0.46
1:A:48:ASP:HB2	1:J:48:ASP:OD2	2.15	0.46
1:C:124:LEU:HD21	1:C:153:GLN:HB2	1.95	0.46
1:C:258:LYS:HB3	1:C:286:LYS:HB2	1.98	0.46
1:M:258:LYS:HB3	1:M:286:LYS:HB2	1.98	0.46
1:N:89:PHE:HE1	1:N:132:ALA:HB1	1.80	0.46
1:H:213:LEU:HD22	1:H:254:GLY:HA2	1.97	0.46
1:I:298:LYS:HG2	1:I:322:LEU:HB2	1.96	0.46
1:N:62:ALA:O	1:M:129:ASN:ND2	2.48	0.46
1:M:244:THR:OG1	1:M:259:ALA:HB3	2.15	0.46
1:N:146:LEU:HD13	1:N:188:TYR:HB2	1.96	0.46
1:N:46:ILE:HD12	1:N:50:LEU:HG	1.96	0.46
1:R:221:ALA:HB1	1:R:247:ALA:HB2	1.98	0.46
1:A:299:TYR:CD1	1:A:319:LYS:HG3	2.51	0.46
1:K:253:LEU:HG	1:K:332:ALA:HA	1.97	0.46
1:H:244:THR:OG1	1:H:259:ALA:HB3	2.16	0.46
1:J:218:GLY:HA3	1:J:246:ASN:ND2	2.31	0.46
1:J:33:GLN:HA	1:J:63:ASN:HD22	1.80	0.46
1:P:308:PHE:HB3	1:R:46:ILE:HG21	1.97	0.46
1:D:218:GLY:HA3	1:D:246:ASN:ND2	2.31	0.46
1:K:215:LEU:HD12	1:K:288:LEU:HD22	1.97	0.46
1:P:153:GLN:OE1	1:P:178:ASN:ND2	2.48	0.46
1:L:167:PRO:HD2	1:J:27:LYS:HD2	1.98	0.46
1:O:93:ARG:HD2	1:O:129:ASN:ND2	2.30	0.46
1:D:93:ARG:HD2	1:D:129:ASN:ND2	2.30	0.46
1:O:299:TYR:CD1	1:O:319:LYS:HG3	2.50	0.46
1:E:221:ALA:HB1	1:E:247:ALA:HB2	1.97	0.46
1:H:139:PHE:CG	1:H:146:LEU:HD23	2.51	0.46
1:K:300:VAL:HG23	1:K:322:LEU:HD11	1.97	0.46
1:R:98:VAL:HB	1:R:125:GLN:HA	1.98	0.46
1:K:215:LEU:HD23	1:K:253:LEU:HB3	1.96	0.46
1:M:107:VAL:O	1:M:267:GLN:NE2	2.45	0.46
1:A:46:ILE:HD12	1:A:50:LEU:HG	1.99	0.45
1:C:218:GLY:HA3	1:C:246:ASN:ND2	2.31	0.45
1:D:258:LYS:HB3	1:D:286:LYS:HB2	1.97	0.45
1:L:300:VAL:HG23	1:L:322:LEU:HD11	1.97	0.45
1:P:39:GLY:HA3	1:P:56:TRP:O	2.16	0.45
1:L:108:LEU:HB2	1:L:111:PHE:O	2.16	0.45
1:O:176:LYS:NZ	1:M:67:SER:HB3	2.31	0.45
1:N:257:ASN:HB2	1:N:287:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:240:GLN:HE21	1:P:263:GLU:HG3	1.81	0.45
1:I:326:ASN:OD1	1:I:329:THR:HG23	2.17	0.45
1:M:299:TYR:CD1	1:M:319:LYS:HG3	2.51	0.45
1:Q:216:GLY:H	1:Q:289:GLU:CD	2.19	0.45
1:Q:85:ASP:N	1:Q:85:ASP:OD1	2.49	0.45
1:B:102:THR:HA	1:B:240:GLN:HG3	1.98	0.45
1:C:1:ALA:HB3	1:C:13:LEU:O	2.16	0.45
1:Q:251:GLY:HA3	1:Q:332:ALA:HB1	1.98	0.45
1:H:3:ILE:HD12	1:I:3:ILE:HD12	1.99	0.45
1:F:218:GLY:HA3	1:F:246:ASN:ND2	2.32	0.45
1:K:221:ALA:HB1	1:K:247:ALA:HB2	1.97	0.45
1:Q:258:LYS:HB3	1:Q:286:LYS:HB2	1.98	0.45
1:D:124:LEU:HD21	1:D:153:GLN:HB2	1.98	0.45
1:L:16:LYS:HB3	1:L:347:GLN:HG3	1.97	0.45
1:R:326:ASN:H	1:R:329:THR:HG22	1.82	0.45
1:R:58:TYR:CE2	1:R:72:ALA:HB1	2.52	0.45
1:C:46:ILE:HD12	1:C:50:LEU:HG	1.99	0.45
1:K:115:GLY:H	1:K:119:GLY:HA2	1.82	0.45
1:M:20:LEU:HD21	1:M:22:TYR:HE1	1.81	0.45
1:N:165:LEU:HD23	1:N:208:ASP:OD1	2.17	0.45
1:E:326:ASN:OD1	1:E:329:THR:HG23	2.16	0.45
1:Q:100:ASP:OD2	1:Q:135:ARG:NH2	2.49	0.45
1:Q:23:PHE:HB2	1:Q:340:VAL:HB	1.99	0.45
1:D:299:TYR:CD1	1:D:319:LYS:HG3	2.52	0.45
1:J:244:THR:HB	1:J:247:ALA:HB3	1.99	0.45
1:J:244:THR:OG1	1:J:259:ALA:HB3	2.16	0.45
1:L:268:TYR:O	1:L:275:ARG:HA	2.17	0.45
1:O:20:LEU:HD21	1:O:22:TYR:HE1	1.82	0.45
1:O:258:LYS:HB3	1:O:286:LYS:HB2	1.98	0.45
1:F:250:ALA:HB1	1:F:328:PHE:HZ	1.82	0.44
1:N:194:ILE:HG12	1:N:230:TYR:HD1	1.82	0.44
1:E:67:SER:HB3	1:D:176:LYS:HZ1	1.83	0.44
1:G:253:LEU:HG	1:G:332:ALA:HA	1.99	0.44
1:H:167:PRO:HD2	1:I:27:LYS:HD2	1.99	0.44
1:J:258:LYS:HB3	1:J:286:LYS:HB2	1.97	0.44
1:L:241:TYR:HA	1:L:261:ASN:O	2.17	0.44
1:J:46:ILE:HD12	1:J:50:LEU:HG	1.98	0.44
1:C:215:LEU:HD12	1:C:288:LEU:HD22	1.99	0.44
1:I:229:LYS:HG3	1:I:236:TYR:HE1	1.83	0.44
1:I:5:ASN:HA	1:I:9:ASN:O	2.17	0.44
1:J:148:PHE:CZ	1:J:150:LEU:HG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:268:TYR:O	1:K:275:ARG:HA	2.18	0.44
1:P:136:ASN:HB3	1:P:148:PHE:CE1	2.52	0.44
1:G:8:GLY:O	1:G:44:THR:HA	2.18	0.44
1:H:221:ALA:HB1	1:H:247:ALA:HB2	2.00	0.44
1:J:124:LEU:HD21	1:J:153:GLN:HB2	1.98	0.44
1:P:89:PHE:HE1	1:P:132:ALA:HB1	1.81	0.44
1:J:20:LEU:HD21	1:J:22:TYR:HE1	1.83	0.44
1:I:199:ALA:HB3	1:I:225:THR:HB	2.00	0.44
1:K:30:ASP:OD1	1:K:31:GLY:N	2.51	0.44
1:M:93:ARG:HD2	1:M:129:ASN:ND2	2.33	0.44
1:A:267:GLN:HG2	1:A:277:SER:HB2	1.99	0.44
1:B:258:LYS:HB3	1:B:286:LYS:HB2	2.00	0.44
1:D:20:LEU:HD21	1:D:22:TYR:HE1	1.83	0.44
1:H:313:SER:O	1:H:344:LEU:HD12	2.18	0.44
1:J:102:THR:HG22	1:J:240:GLN:OE1	2.18	0.44
1:M:215:LEU:HD12	1:M:288:LEU:HD22	2.00	0.44
1:M:33:GLN:HA	1:M:63:ASN:HD22	1.83	0.44
1:O:102:THR:HG22	1:O:240:GLN:OE1	2.18	0.44
1:Q:244:THR:HB	1:Q:247:ALA:HB3	2.00	0.44
1:R:176:LYS:HG2	1:R:249:ARG:NH2	2.33	0.44
1:Q:127:ARG:NE	1:R:66:GLU:OE2	2.48	0.44
1:Q:12[B]:ASP:HB3	1:Q:41:LYS:HB3	2.00	0.43
1:Q:82:LYS:NZ	1:Q:84:GLY:HA2	2.33	0.43
1:I:267:GLN:HG2	1:I:277:SER:CB	2.48	0.43
1:L:23:PHE:HA	1:L:30:ASP:OD1	2.18	0.43
1:P:65:THR:O	1:P:68:SER:OG	2.27	0.43
1:R:140:PHE:HB2	1:R:142:LEU:HD13	2.00	0.43
1:R:240:GLN:HG2	1:R:241:TYR:H	1.83	0.43
1:C:93:ARG:HD2	1:C:129:ASN:ND2	2.32	0.43
1:G:5:ASN:HA	1:G:9:ASN:O	2.17	0.43
1:K:244:THR:OG1	1:K:259:ALA:HB3	2.17	0.43
1:L:140:PHE:HB2	1:L:142:LEU:HD13	2.00	0.43
1:M:102:THR:HG22	1:M:240:GLN:OE1	2.18	0.43
1:Q:9:ASN:ND2	1:R:311:ASN:OD1	2.42	0.43
1:C:299:TYR:CD1	1:C:319:LYS:HG3	2.54	0.43
1:D:215:LEU:HD12	1:D:288:LEU:HD22	2.00	0.43
1:J:267:GLN:HG2	1:J:277:SER:HB2	2.01	0.43
1:N:257:ASN:ND2	1:N:289:GLU:OE2	2.50	0.43
1:P:107:VAL:O	1:P:267:GLN:NE2	2.46	0.43
1:A:99:TYR:HA	1:A:102:THR:OG1	2.18	0.43
1:A:236:TYR:HD2	1:A:275:ARG:HH21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:GLY:H	1:E:119:GLY:HA2	1.83	0.43
1:Q:299:TYR:CD1	1:Q:319:LYS:HG3	2.53	0.43
1:E:149:ALA:O	1:E:184:THR:HA	2.18	0.43
1:H:157:GLY:HA3	1:H:166:SER:O	2.19	0.43
1:G:3:ILE:HD12	1:I:3:ILE:HD12	1.99	0.43
1:P:93:ARG:HD2	1:P:129:ASN:ND2	2.33	0.43
1:Q:170:ASN:HD22	1:Q:172:ARG:HH22	1.67	0.43
1:B:240:GLN:OE1	1:B:242:THR:OG1	2.34	0.43
1:N:326:ASN:OD1	1:N:329:THR:HG23	2.18	0.43
1:R:3:ILE:HG12	1:R:11:LEU:O	2.18	0.43
1:B:225:THR:OG1	1:B:242:THR:HG23	2.19	0.43
1:H:268:TYR:O	1:H:275:ARG:HA	2.18	0.43
1:I:253:LEU:HG	1:I:332:ALA:HA	2.01	0.43
1:L:165:LEU:HD23	1:L:208:ASP:OD1	2.19	0.43
1:N:273:GLY:O	1:N:306:TYR:HA	2.18	0.43
1:P:22:TYR:CD1	1:P:33:GLN:HG3	2.53	0.43
1:Q:215:LEU:HD12	1:Q:288:LEU:HD22	2.01	0.43
1:K:1:ALA:HA	1:J:4:TYR:CZ	2.54	0.43
1:K:46:ILE:HD12	1:K:50:LEU:HG	2.00	0.43
1:P:33:GLN:HA	1:P:63:ASN:HD22	1.84	0.43
1:R:116:ASP:OD2	1:R:299:TYR:OH	2.36	0.43
1:K:135:ARG:HG3	1:K:149:ALA:HB2	2.01	0.42
1:P:140:PHE:HB2	1:P:142:LEU:HD13	2.01	0.42
1:Q:165:LEU:HD23	1:Q:208:ASP:OD1	2.20	0.42
1:E:33:GLN:HA	1:E:63:ASN:HD22	1.83	0.42
1:G:244:THR:OG1	1:G:259:ALA:HB3	2.19	0.42
1:Q:11:LEU:HA	1:Q:11:LEU:HD12	1.93	0.42
1:B:153:GLN:OE1	1:B:178:ASN:ND2	2.52	0.42
1:I:80:GLY:HA3	1:I:89:PHE:O	2.19	0.42
1:L:286:LYS:HB3	1:L:286:LYS:HE3	1.79	0.42
1:N:135:ARG:HD3	1:N:149:ALA:HB2	2.02	0.42
1:O:75:ARG:O	1:O:127:ARG:HD2	2.19	0.42
1:P:213:LEU:HD22	1:P:254:GLY:HA2	2.00	0.42
1:R:52:GLY:HA2	1:R:81:LEU:HD23	2.00	0.42
1:E:5:ASN:HA	1:E:9:ASN:O	2.18	0.42
1:H:98:VAL:HB	1:H:125:GLN:HA	2.01	0.42
1:C:207:GLY:O	1:C:211:SER:OG	2.29	0.42
1:C:250:ALA:HB1	1:C:328:PHE:HZ	1.85	0.42
1:G:67:SER:HB3	1:I:176:LYS:NZ	2.35	0.42
1:P:319:LYS:HE2	1:P:321:ASN:HD22	1.84	0.42
1:R:310:LYS:H	1:R:310:LYS:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:PHE:CZ	1:H:150:LEU:HG	2.54	0.42
1:I:89:PHE:CE1	1:I:132:ALA:HB1	2.53	0.42
1:I:245:TYR:HE1	1:I:258:LYS:HE2	1.85	0.42
1:I:302:VAL:HG13	1:I:318:TYR:HB3	2.01	0.42
1:B:108:LEU:HB2	1:B:111:PHE:O	2.19	0.42
1:F:227:GLY:O	1:F:228:LEU:HD12	2.19	0.42
1:H:257:ASN:HB2	1:H:287:ASP:O	2.20	0.42
1:N:207:GLY:O	1:N:211:SER:OG	2.30	0.42
1:P:108:LEU:HD21	1:P:279:ALA:HB2	2.01	0.42
1:R:274:LEU:HG	1:R:276:PRO:HD3	2.01	0.42
1:R:308:PHE:HB2	1:R:312:MET:HB3	2.01	0.42
1:D:224:TYR:O	1:D:242:THR:HA	2.19	0.42
1:G:4:TYR:CZ	1:G:6:LYS:HB3	2.55	0.42
1:J:215:LEU:HD12	1:J:288:LEU:HD22	2.01	0.42
1:J:250:ALA:HB1	1:J:328:PHE:HZ	1.84	0.42
1:Q:155:LYS:HE3	1:Q:166:SER:HB3	2.01	0.42
1:B:12[B]:ASP:HB3	1:B:41:LYS:HB3	2.01	0.42
1:B:98:VAL:HA	1:B:199:ALA:HB1	2.02	0.42
1:G:46:ILE:HD13	1:H:308:PHE:HB3	2.02	0.42
1:P:93:ARG:HD2	1:P:129:ASN:HD21	1.84	0.42
1:C:75:ARG:O	1:C:127:ARG:HD2	2.20	0.42
1:C:267:GLN:HG2	1:C:277:SER:HB2	2.01	0.42
1:D:67:SER:HB3	1:C:176:LYS:NZ	2.35	0.42
1:E:4:TYR:CZ	1:E:6:LYS:HB3	2.55	0.42
1:M:11:LEU:HD12	1:M:11:LEU:HA	1.96	0.42
1:R:56:TRP:HD1	1:R:77:ALA:HB2	1.85	0.42
1:A:16:LYS:HB3	1:A:347:GLN:HG3	2.02	0.41
1:B:46:ILE:HD12	1:B:50:LEU:HG	2.02	0.41
1:D:236:TYR:HD1	1:D:237:LEU:N	2.18	0.41
1:J:224:TYR:O	1:J:242:THR:HA	2.20	0.41
1:R:194:ILE:HG12	1:R:230:TYR:HD1	1.85	0.41
1:A:110:GLU:HB2	1:A:315:TYR:CE2	2.54	0.41
1:A:268:TYR:O	1:A:275:ARG:HA	2.20	0.41
1:C:236:TYR:HD1	1:C:237:LEU:N	2.17	0.41
1:H:10:LYS:HG2	1:H:43:GLU:HG3	2.02	0.41
1:H:165:LEU:HD11	1:H:207:GLY:HA3	2.00	0.41
1:K:27:LYS:HD2	1:J:167:PRO:HD2	2.01	0.41
1:M:224:TYR:O	1:M:242:THR:HA	2.21	0.41
1:P:3:ILE:CG2	1:P:13:LEU:H	2.33	0.41
1:P:67:SER:HB3	1:R:176:LYS:NZ	2.35	0.41
1:R:240:GLN:HG2	1:R:241:TYR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:CD1	1:A:33:GLN:HG3	2.55	0.41
1:I:111:PHE:CD2	1:I:319:LYS:HB2	2.55	0.41
1:M:280:TYR:OH	1:M:282:GLN:NE2	2.46	0.41
1:O:224:TYR:O	1:O:242:THR:HA	2.20	0.41
1:Q:4:TYR:CZ	1:R:1:ALA:HA	2.55	0.41
1:A:267:GLN:HG2	1:A:277:SER:CB	2.51	0.41
1:E:147:ASN:O	1:E:186:LEU:HD12	2.20	0.41
1:Q:12[A]:ASP:HB2	1:Q:41:LYS:HB3	2.02	0.41
1:R:133:THR:OG1	1:R:151:GLN:NE2	2.46	0.41
1:R:3:ILE:HG21	1:R:13:LEU:HB3	2.03	0.41
1:A:1:ALA:HB3	1:A:13:LEU:O	2.21	0.41
1:E:218:GLY:HA3	1:E:246:ASN:ND2	2.35	0.41
1:F:124:LEU:HD21	1:F:153:GLN:HB2	2.03	0.41
1:G:23:PHE:HB2	1:G:340:VAL:HB	2.03	0.41
1:R:268:TYR:O	1:R:276:PRO:HD2	2.21	0.41
1:C:311:ASN:ND2	1:C:347:GLN:O	2.36	0.41
1:F:236:TYR:HD1	1:F:237:LEU:N	2.19	0.41
1:H:170:ASN:OD1	1:H:170:ASN:N	2.52	0.41
1:I:4:TYR:CZ	1:I:6:LYS:HB3	2.56	0.41
1:L:221:ALA:HA	1:L:245:TYR:O	2.20	0.41
1:M:250:ALA:HB1	1:M:328:PHE:HZ	1.85	0.41
1:N:2:GLU:OE2	1:N:5:ASN:ND2	2.50	0.41
1:O:244:THR:HB	1:O:247:ALA:HB3	2.02	0.41
1:O:46:ILE:HD12	1:O:50:LEU:HG	2.02	0.41
1:R:14:TYR:HA	1:R:348:PHE:OXT	2.19	0.41
1:R:199:ALA:HB3	1:R:225:THR:HB	2.02	0.41
1:A:326:ASN:OD1	1:A:329:THR:HG23	2.21	0.41
1:H:326:ASN:OD1	1:H:329:THR:HG23	2.21	0.41
1:N:140:PHE:HB2	1:N:142:LEU:HD13	2.02	0.41
1:O:205:ARG:NH2	1:O:210:ASN:OD1	2.50	0.41
1:P:227:GLY:O	1:P:228:LEU:HD12	2.21	0.41
1:D:227:GLY:O	1:D:228:LEU:HD12	2.20	0.41
1:E:11:LEU:HD12	1:E:11:LEU:HA	1.89	0.41
1:F:150:LEU:HD23	1:F:150:LEU:HA	1.92	0.41
1:K:153:GLN:OE1	1:K:178:ASN:ND2	2.53	0.41
1:L:12[B]:ASP:OD1	1:L:13:LEU:N	2.54	0.41
1:A:236:TYR:HD1	1:A:237:LEU:N	2.19	0.41
1:B:158:SER:HB3	1:B:208:ASP:OD2	2.20	0.41
1:C:99:TYR:HA	1:C:102:THR:OG1	2.21	0.41
1:H:115:GLY:H	1:H:119:GLY:HA2	1.86	0.41
1:H:176:LYS:HE3	1:I:67:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:11:LEU:HD12	1:N:42:GLY:HA3	2.02	0.41
1:R:170:ASN:N	1:R:170:ASN:OD1	2.53	0.41
1:B:107:VAL:O	1:B:267:GLN:NE2	2.50	0.41
1:C:224:TYR:O	1:C:242:THR:HA	2.21	0.41
1:M:236:TYR:HD1	1:M:237:LEU:N	2.19	0.41
1:O:150:LEU:HA	1:O:150:LEU:HD23	1.90	0.41
1:P:96:GLY:HA2	1:P:151:GLN:HE22	1.85	0.41
1:Q:199:ALA:HB3	1:Q:225:THR:HB	2.02	0.41
1:R:267:GLN:HG2	1:R:277:SER:CB	2.51	0.41
1:B:227:GLY:O	1:B:228:LEU:HD12	2.20	0.41
1:D:99:TYR:HA	1:D:102:THR:OG1	2.21	0.41
1:H:253:LEU:HG	1:H:332:ALA:HA	2.03	0.41
1:H:299:TYR:CD2	1:H:319:LYS:HE3	2.56	0.41
1:I:170:ASN:OD1	1:I:170:ASN:N	2.51	0.41
1:K:33:GLN:HA	1:K:63:ASN:HD22	1.86	0.41
1:N:165:LEU:HD11	1:N:207:GLY:HA3	2.02	0.41
1:P:170:ASN:N	1:P:170:ASN:OD1	2.48	0.41
1:R:105:THR:OG1	1:R:263:GLU:OE1	2.29	0.41
1:A:100:ASP:OD2	1:A:135:ARG:NH2	2.39	0.40
1:A:93:ARG:HD2	1:A:129:ASN:ND2	2.36	0.40
1:B:326:ASN:OD1	1:B:329:THR:HG23	2.21	0.40
1:Q:318:TYR:HD1	1:Q:340:VAL:HG22	1.86	0.40
1:R:124:LEU:HD21	1:R:153:GLN:HB2	2.03	0.40
1:I:107:VAL:O	1:I:267:GLN:NE2	2.54	0.40
1:J:75:ARG:O	1:J:127:ARG:HD2	2.21	0.40
1:M:267:GLN:HG2	1:M:277:SER:HB2	2.03	0.40
1:P:319:LYS:HE2	1:P:321:ASN:ND2	2.36	0.40
1:E:98:VAL:HB	1:E:125:GLN:HA	2.02	0.40
1:P:281:LEU:HD13	1:P:299:TYR:CZ	2.57	0.40
1:G:102:THR:HG22	1:G:240:GLN:OE1	2.22	0.40
1:J:165:LEU:HD23	1:J:208:ASP:OD1	2.22	0.40
1:K:12[A]:ASP:HB2	1:K:41:LYS:HB3	2.02	0.40
1:M:244:THR:HB	1:M:247:ALA:HB3	2.03	0.40
1:P:191:TYR:HD2	1:P:194:ILE:HD12	1.85	0.40
1:R:3:ILE:HD13	1:R:13:LEU:CB	2.52	0.40
1:E:0:GLY:O	1:E:1:ALA:HB3	2.21	0.40
1:E:232:ALA:O	1:E:235:ILE:HB	2.22	0.40
1:H:281:LEU:HD13	1:H:299:TYR:CZ	2.57	0.40
1:I:268:TYR:O	1:I:275:ARG:HA	2.21	0.40
1:M:227:GLY:O	1:M:228:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

## 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	A	348/349 (100%)	312 (90%)	35 (10%)	1 (0%)	41	73
1	B	348/349 (100%)	314 (90%)	33 (10%)	1 (0%)	41	73
1	C	348/349 (100%)	312 (90%)	36 (10%)	0	100	100
1	D	348/349 (100%)	310 (89%)	37 (11%)	1 (0%)	41	73
1	E	348/349 (100%)	314 (90%)	33 (10%)	1 (0%)	41	73
1	F	348/349 (100%)	310 (89%)	37 (11%)	1 (0%)	41	73
1	G	348/349 (100%)	315 (90%)	33 (10%)	0	100	100
1	H	348/349 (100%)	314 (90%)	34 (10%)	0	100	100
1	I	348/349 (100%)	312 (90%)	35 (10%)	1 (0%)	41	73
1	J	348/349 (100%)	312 (90%)	35 (10%)	1 (0%)	41	73
1	K	348/349 (100%)	314 (90%)	34 (10%)	0	100	100
1	L	348/349 (100%)	310 (89%)	37 (11%)	1 (0%)	41	73
1	M	348/349 (100%)	311 (89%)	36 (10%)	1 (0%)	41	73
1	N	348/349 (100%)	313 (90%)	34 (10%)	1 (0%)	41	73
1	O	348/349 (100%)	312 (90%)	35 (10%)	1 (0%)	41	73
1	P	348/349 (100%)	312 (90%)	34 (10%)	2 (1%)	25	61
1	Q	348/349 (100%)	314 (90%)	33 (10%)	1 (0%)	41	73
1	R	348/349 (100%)	313 (90%)	32 (9%)	3 (1%)	17	52
All	All	6264/6282 (100%)	5624 (90%)	623 (10%)	17 (0%)	41	73

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	1	ALA
1	F	1	ALA
1	A	1	ALA
1	E	1	ALA

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Mol	Chain	Res	Type
1	N	291	TYR
1	O	1	ALA
1	Q	1	ALA
1	D	1	ALA
1	J	1	ALA
1	M	1	ALA
1	B	1	ALA
1	R	139	PHE
1	R	291	TYR
1	L	241	TYR
1	P	290	GLY
1	I	84	GLY
1	P	84	GLY

### 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	A	279/278 (100%)	275 (99%)	4 (1%)	67	84
1	B	279/278 (100%)	276 (99%)	3 (1%)	73	87
1	C	279/278 (100%)	274 (98%)	5 (2%)	59	80
1	D	279/278 (100%)	273 (98%)	6 (2%)	52	76
1	E	279/278 (100%)	274 (98%)	5 (2%)	59	80
1	F	279/278 (100%)	272 (98%)	7 (2%)	47	74
1	G	279/278 (100%)	273 (98%)	6 (2%)	52	76
1	H	279/278 (100%)	275 (99%)	4 (1%)	67	84
1	I	279/278 (100%)	276 (99%)	3 (1%)	73	87
1	J	279/278 (100%)	273 (98%)	6 (2%)	52	76
1	K	279/278 (100%)	269 (96%)	10 (4%)	35	66
1	L	279/278 (100%)	273 (98%)	6 (2%)	52	76
1	M	279/278 (100%)	272 (98%)	7 (2%)	47	74
1	N	279/278 (100%)	274 (98%)	5 (2%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	279/278 (100%)	272 (98%)	7 (2%)	47	74
1	P	279/278 (100%)	273 (98%)	6 (2%)	52	76
1	Q	279/278 (100%)	271 (97%)	8 (3%)	42	71
1	R	279/278 (100%)	267 (96%)	12 (4%)	29	62
All	All	5022/5004 (100%)	4912 (98%)	110 (2%)	52	76

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ARG
1	A	236	TYR
1	A	271	ASP
1	A	272	PHE
1	B	169	ASN
1	B	172	ARG
1	B	240	GLN
1	E	64	ASN
1	E	169	ASN
1	E	172	ARG
1	E	240	GLN
1	E	317	ASP
1	G	12[A]	ASP
1	G	12[B]	ASP
1	G	169	ASN
1	G	172	ARG
1	G	272	PHE
1	G	317	ASP
1	H	169	ASN
1	H	172	ARG
1	H	192	ASP
1	H	317	ASP
1	I	169	ASN
1	I	172	ARG
1	I	236	TYR
1	K	144	ASP
1	K	148	PHE
1	K	169	ASN
1	K	172	ARG
1	K	236	TYR
1	K	240	GLN
1	K	272	PHE

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Mol	Chain	Res	Type
1	K	310	LYS
1	K	311	ASN
1	K	317	ASP
1	L	169	ASN
1	L	172	ARG
1	L	271	ASP
1	L	282	GLN
1	L	321	ASN
1	L	337	ASP
1	N	148	PHE
1	N	172	ARG
1	N	192	ASP
1	N	317	ASP
1	N	318	TYR
1	O	169	ASN
1	O	172	ARG
1	O	192	ASP
1	O	236	TYR
1	O	272	PHE
1	O	317	ASP
1	O	321	ASN
1	P	64	ASN
1	P	148	PHE
1	P	192	ASP
1	P	236	TYR
1	P	291	TYR
1	P	310	LYS
1	Q	85	ASP
1	Q	135	ARG
1	Q	148	PHE
1	Q	169	ASN
1	Q	192	ASP
1	Q	272	PHE
1	Q	317	ASP
1	Q	321	ASN
1	R	12[A]	ASP
1	R	12[B]	ASP
1	R	64	ASN
1	R	135	ARG
1	R	148	PHE
1	R	169	ASN
1	R	172	ARG

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Mol	Chain	Res	Type
1	R	236	TYR
1	R	240	GLN
1	R	282	GLN
1	R	310	LYS
1	R	317	ASP
1	F	169	ASN
1	F	172	ARG
1	F	192	ASP
1	F	236	TYR
1	F	272	PHE
1	F	282	GLN
1	F	331	ASN
1	D	169	ASN
1	D	172	ARG
1	D	192	ASP
1	D	236	TYR
1	D	317	ASP
1	D	331	ASN
1	J	169	ASN
1	J	172	ARG
1	J	192	ASP
1	J	236	TYR
1	J	321	ASN
1	J	331	ASN
1	M	169	ASN
1	M	172	ARG
1	M	192	ASP
1	M	236	TYR
1	M	282	GLN
1	M	317	ASP
1	M	321	ASN
1	C	169	ASN
1	C	172	ARG
1	C	192	ASP
1	C	236	TYR
1	C	321	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	9	ASN
1	O	129	ASN

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Mol	Chain	Res	Type
1	F	282	GLN
1	M	282	GLN
1	C	282	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	349/349 (100%)	0.42	4 (1%) 80 73	28, 55, 82, 109	0
1	B	349/349 (100%)	0.39	10 (2%) 51 40	31, 56, 90, 115	0
1	C	349/349 (100%)	0.70	18 (5%) 27 17	42, 64, 100, 147	0
1	D	349/349 (100%)	0.61	16 (4%) 32 22	29, 60, 95, 140	0
1	E	349/349 (100%)	0.54	9 (2%) 56 44	31, 55, 79, 106	0
1	F	349/349 (100%)	0.61	18 (5%) 27 17	37, 59, 85, 138	0
1	G	349/349 (100%)	0.44	10 (2%) 51 40	26, 58, 88, 114	0
1	H	349/349 (100%)	0.49	11 (3%) 47 35	30, 59, 88, 116	0
1	I	349/349 (100%)	0.69	30 (8%) 10 7	33, 76, 100, 123	0
1	J	349/349 (100%)	0.54	15 (4%) 35 25	39, 72, 98, 128	0
1	K	349/349 (100%)	0.60	9 (2%) 56 44	33, 56, 82, 112	0
1	L	349/349 (100%)	0.48	16 (4%) 32 22	37, 69, 94, 121	0
1	M	349/349 (100%)	0.86	58 (16%) 1 1	59, 93, 117, 143	0
1	N	349/349 (100%)	0.61	23 (6%) 18 12	53, 86, 113, 144	0
1	O	349/349 (100%)	0.44	14 (4%) 38 28	48, 70, 101, 133	0
1	P	349/349 (100%)	0.79	41 (11%) 4 3	72, 96, 129, 162	0
1	Q	349/349 (100%)	0.81	46 (13%) 3 2	82, 111, 137, 161	0
1	R	349/349 (100%)	0.66	38 (10%) 5 4	75, 106, 140, 157	0
All	All	6282/6282 (100%)	0.59	386 (6%) 21 14	26, 70, 117, 162	0

All (386) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	348	PHE	12.1
1	P	12[A]	ASP	9.0
1	Q	0	GLY	8.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	12[A]	ASP	8.3
1	M	348	PHE	7.7
1	Q	13	LEU	7.6
1	P	55	GLN	6.9
1	P	56	TRP	6.9
1	D	0	GLY	6.8
1	Q	12[A]	ASP	6.5
1	P	13	LEU	6.3
1	J	0	GLY	6.3
1	M	0	GLY	6.0
1	B	12[A]	ASP	5.9
1	Q	40	VAL	5.7
1	P	40	VAL	5.7
1	O	348	PHE	5.5
1	E	12[A]	ASP	5.4
1	D	12[A]	ASP	5.3
1	P	11	LEU	5.3
1	Q	16	LYS	5.3
1	R	348	PHE	5.2
1	Q	55	GLN	5.2
1	H	348	PHE	5.2
1	N	12[A]	ASP	5.0
1	M	54	GLY	4.9
1	Q	15	GLY	4.8
1	Q	38	VAL	4.8
1	P	58	TYR	4.8
1	C	12[A]	ASP	4.8
1	Q	17	ILE	4.7
1	K	12[A]	ASP	4.7
1	P	54	GLY	4.6
1	P	41	LYS	4.6
1	A	12[A]	ASP	4.6
1	C	348	PHE	4.6
1	C	0	GLY	4.6
1	R	251	GLY	4.5
1	M	13	LEU	4.5
1	P	348	PHE	4.5
1	K	348	PHE	4.5
1	Q	54	GLY	4.5
1	B	348	PHE	4.4
1	D	348	PHE	4.4
1	F	348	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	256	ALA	4.3
1	M	11	LEU	4.3
1	M	41	LYS	4.3
1	Q	39	GLY	4.3
1	L	12[A]	ASP	4.3
1	M	287	ASP	4.3
1	Q	56	TRP	4.3
1	E	348	PHE	4.3
1	M	2	GLU	4.2
1	M	295	ASP	4.2
1	N	348	PHE	4.2
1	J	12[A]	ASP	4.1
1	G	348	PHE	4.1
1	E	0	GLY	4.1
1	M	296	ILE	4.1
1	J	348	PHE	4.0
1	Q	346	TYR	4.0
1	M	55	GLN	4.0
1	N	11	LEU	4.0
1	K	0	GLY	3.9
1	M	40	VAL	3.9
1	R	256	ALA	3.9
1	R	17	ILE	3.8
1	P	38	VAL	3.8
1	P	76	LEU	3.8
1	P	79	ALA	3.7
1	M	43	GLU	3.7
1	M	94	ASN	3.7
1	N	74	THR	3.7
1	P	0	GLY	3.7
1	Q	58	TYR	3.7
1	O	14	TYR	3.7
1	O	13	LEU	3.6
1	R	296	ILE	3.6
1	M	3	ILE	3.6
1	M	289	GLU	3.6
1	R	16	LYS	3.6
1	I	40	VAL	3.6
1	Q	296	ILE	3.6
1	L	0	GLY	3.5
1	M	10	LYS	3.5
1	R	40	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	O	0	GLY	3.5
1	H	38	VAL	3.5
1	Q	263	GLU	3.5
1	Q	11	LEU	3.4
1	N	38	VAL	3.4
1	I	12[A]	ASP	3.4
1	R	36	MET	3.4
1	M	247	ALA	3.4
1	R	319	LYS	3.4
1	O	12[A]	ASP	3.4
1	R	25	ASP	3.4
1	P	9	ASN	3.4
1	O	40	VAL	3.4
1	R	335	SER	3.4
1	Q	1	ALA	3.4
1	Q	3	ILE	3.4
1	R	255	PHE	3.3
1	H	36	MET	3.3
1	P	10	LYS	3.3
1	Q	41	LYS	3.3
1	L	242	THR	3.2
1	P	2	GLU	3.2
1	I	215	LEU	3.2
1	L	348	PHE	3.2
1	D	13	LEU	3.2
1	M	38	VAL	3.2
1	M	258	LYS	3.2
1	Q	347	GLN	3.2
1	P	118	TYR	3.2
1	C	11	LEU	3.2
1	K	40	VAL	3.1
1	D	9	ASN	3.1
1	L	247	ALA	3.1
1	F	12[A]	ASP	3.1
1	N	3	ILE	3.1
1	Q	37	ARG	3.1
1	C	40	VAL	3.1
1	Q	125	GLN	3.1
1	M	78	PHE	3.0
1	I	56	TRP	3.0
1	P	57	GLU	3.0
1	M	58	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	3	ILE	3.0
1	R	248	THR	3.0
1	H	13	LEU	3.0
1	O	38	VAL	3.0
1	M	53	TYR	3.0
1	E	13	LEU	3.0
1	P	52	GLY	3.0
1	I	249	ARG	3.0
1	J	212	LYS	3.0
1	C	41	LYS	2.9
1	M	56	TRP	2.9
1	I	255	PHE	2.9
1	H	12[A]	ASP	2.9
1	L	40	VAL	2.9
1	J	40	VAL	2.9
1	Q	128	ALA	2.9
1	P	92	GLY	2.9
1	R	38	VAL	2.9
1	D	38	VAL	2.9
1	N	58	TYR	2.9
1	C	56	TRP	2.8
1	M	44	THR	2.8
1	L	13	LEU	2.8
1	N	13	LEU	2.8
1	G	40	VAL	2.8
1	C	38	VAL	2.8
1	N	129	ASN	2.8
1	M	124	LEU	2.8
1	N	56	TRP	2.8
1	N	55	GLN	2.8
1	B	3	ILE	2.8
1	Q	117	THR	2.8
1	P	124	LEU	2.8
1	R	281	LEU	2.8
1	I	38	VAL	2.8
1	M	244	THR	2.8
1	L	11	LEU	2.8
1	P	1	ALA	2.8
1	P	175	LEU	2.8
1	D	11	LEU	2.8
1	I	296	ILE	2.8
1	M	255	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	12[A]	ASP	2.8
1	M	1	ALA	2.8
1	Q	14	TYR	2.7
1	P	46	ILE	2.7
1	M	79	ALA	2.7
1	R	81	LEU	2.7
1	P	39	GLY	2.7
1	J	38	VAL	2.7
1	L	10	LYS	2.7
1	I	13	LEU	2.7
1	I	175	LEU	2.7
1	Q	261	ASN	2.7
1	B	13	LEU	2.7
1	F	92	GLY	2.7
1	Q	4	TYR	2.7
1	L	4	TYR	2.7
1	M	14	TYR	2.7
1	N	14	TYR	2.7
1	K	11	LEU	2.7
1	Q	76	LEU	2.7
1	E	39	GLY	2.7
1	N	123	PHE	2.7
1	M	215	LEU	2.7
1	P	77	ALA	2.7
1	I	293	ASP	2.6
1	I	123	PHE	2.6
1	N	17	ILE	2.6
1	K	13	LEU	2.6
1	P	78	PHE	2.6
1	F	13	LEU	2.6
1	M	246	ASN	2.6
1	C	10	LYS	2.6
1	K	3	ILE	2.6
1	P	14	TYR	2.6
1	Q	94	ASN	2.6
1	P	93	ARG	2.6
1	I	287	ASP	2.6
1	N	175	LEU	2.6
1	R	56	TRP	2.6
1	B	11	LEU	2.6
1	C	55	GLN	2.6
1	N	128	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2	GLU	2.6
1	Q	57	GLU	2.6
1	R	337	ASP	2.6
1	J	208	ASP	2.6
1	M	97	VAL	2.6
1	R	215	LEU	2.6
1	O	62	ALA	2.6
1	D	8	GLY	2.6
1	I	122	ASN	2.6
1	I	254	GLY	2.5
1	H	56	TRP	2.5
1	K	38	VAL	2.5
1	I	76	LEU	2.5
1	I	250	ALA	2.5
1	P	346	TYR	2.5
1	P	60	VAL	2.5
1	R	347	GLN	2.5
1	O	215	LEU	2.5
1	F	324	ASP	2.5
1	M	51	THR	2.5
1	C	141	GLY	2.5
1	N	261	ASN	2.5
1	M	52	GLY	2.5
1	M	49	GLN	2.5
1	P	3	ILE	2.5
1	P	176	LYS	2.5
1	R	13	LEU	2.5
1	F	40	VAL	2.5
1	P	114	ASP	2.5
1	I	348	PHE	2.5
1	N	254	GLY	2.5
1	Q	240	GLN	2.5
1	F	76	LEU	2.5
1	F	56	TRP	2.4
1	Q	119	GLY	2.4
1	M	248	THR	2.4
1	O	11	LEU	2.4
1	R	328	PHE	2.4
1	F	128	ALA	2.4
1	D	258	LYS	2.4
1	B	38	VAL	2.4
1	Q	344	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	R	35	TYR	2.4
1	Q	311	ASN	2.4
1	G	17	ILE	2.4
1	Q	310	LYS	2.4
1	M	253	LEU	2.4
1	R	299	TYR	2.4
1	J	41	LYS	2.4
1	M	45	GLN	2.4
1	R	24	SER	2.4
1	R	117	THR	2.4
1	N	341	ALA	2.4
1	O	56	TRP	2.4
1	M	48	ASP	2.4
1	A	0	GLY	2.4
1	Q	226	GLY	2.4
1	C	2	GLU	2.4
1	I	334	ILE	2.4
1	L	56	TRP	2.4
1	C	17	ILE	2.4
1	H	11	LEU	2.4
1	F	175	LEU	2.4
1	J	2	GLU	2.4
1	P	242	THR	2.4
1	D	34	THR	2.4
1	R	346	TYR	2.3
1	I	253	LEU	2.3
1	R	253	LEU	2.3
1	R	12[A]	ASP	2.3
1	H	17	ILE	2.3
1	D	3	ILE	2.3
1	L	7	ASP	2.3
1	R	14	TYR	2.3
1	P	344	LEU	2.3
1	F	14	TYR	2.3
1	E	281	LEU	2.3
1	I	258	LYS	2.3
1	R	263	GLU	2.3
1	C	253	LEU	2.3
1	L	54	GLY	2.3
1	Q	75	ARG	2.3
1	Q	115	GLY	2.3
1	M	82	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	175	LEU	2.3
1	G	56	TRP	2.3
1	M	95	TYR	2.3
1	P	305	THR	2.3
1	M	310	LYS	2.3
1	I	36	MET	2.3
1	P	113	GLY	2.3
1	J	13	LEU	2.3
1	R	116	ASP	2.3
1	F	129	ASN	2.3
1	M	245	TYR	2.3
1	M	57	GLU	2.2
1	D	48	ASP	2.2
1	G	346	TYR	2.2
1	I	58	TYR	2.2
1	D	40	VAL	2.2
1	J	6	LYS	2.2
1	D	281	LEU	2.2
1	A	348	PHE	2.2
1	B	40	VAL	2.2
1	N	40	VAL	2.2
1	E	11	LEU	2.2
1	I	1	ALA	2.2
1	Q	36	MET	2.2
1	R	46	ILE	2.2
1	F	90	ASP	2.2
1	Q	127	ARG	2.2
1	E	38	VAL	2.2
1	G	38	VAL	2.2
1	M	39	GLY	2.2
1	M	4	TYR	2.2
1	Q	324	ASP	2.2
1	F	212	LYS	2.2
1	R	250	ALA	2.2
1	F	0	GLY	2.2
1	L	1	ALA	2.2
1	O	79	ALA	2.2
1	Q	228	LEU	2.2
1	O	208	ASP	2.2
1	P	253	LEU	2.1
1	M	281	LEU	2.1
1	A	62	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	198	PHE	2.1
1	Q	284	LYS	2.1
1	G	345	VAL	2.1
1	R	3	ILE	2.1
1	R	18	ASP	2.1
1	I	288	LEU	2.1
1	N	346	TYR	2.1
1	J	1	ALA	2.1
1	L	6	LYS	2.1
1	O	41	LYS	2.1
1	C	77	ALA	2.1
1	I	125	GLN	2.1
1	I	14	TYR	2.1
1	R	297	LEU	2.1
1	R	60	VAL	2.1
1	M	101	VAL	2.1
1	G	11	LEU	2.1
1	C	331	ASN	2.1
1	J	56	TRP	2.1
1	I	247	ALA	2.1
1	L	300	VAL	2.1
1	F	330	HIS	2.1
1	M	50	LEU	2.1
1	B	55	GLN	2.1
1	N	125	GLN	2.1
1	M	260	GLN	2.1
1	D	2	GLU	2.1
1	M	297	LEU	2.1
1	I	257	ASN	2.1
1	H	41	LYS	2.0
1	I	57	GLU	2.0
1	B	1	ALA	2.0
1	H	3	ILE	2.0
1	M	9	ASN	2.0
1	C	34	THR	2.0
1	H	1	ALA	2.0
1	K	1	ALA	2.0
1	F	38	VAL	2.0
1	N	263	GLU	2.0
1	G	58	TYR	2.0
1	P	334	ILE	2.0
1	F	334	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	262	PHE	2.0
1	E	305	THR	2.0
1	D	263	GLU	2.0
1	J	55	GLN	2.0
1	M	125	GLN	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.