



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:39 PM EDT

PDB ID : 4BWY  
Title : P4 PROTEIN FROM BACTERIOPHAGE PHI8 (R32)  
Authors : El Omari, K.; Meier, C.; Kainov, D.; Sutton, G.; Grimes, J.M.; Poranen, M.M.; Bamford, D.H.; Tuma, R.; Stuart, D.I.; Mancini, E.J.  
Deposited on : 2013-07-05  
Resolution : 3.10 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.

The types of validation reports are described at

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

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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)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

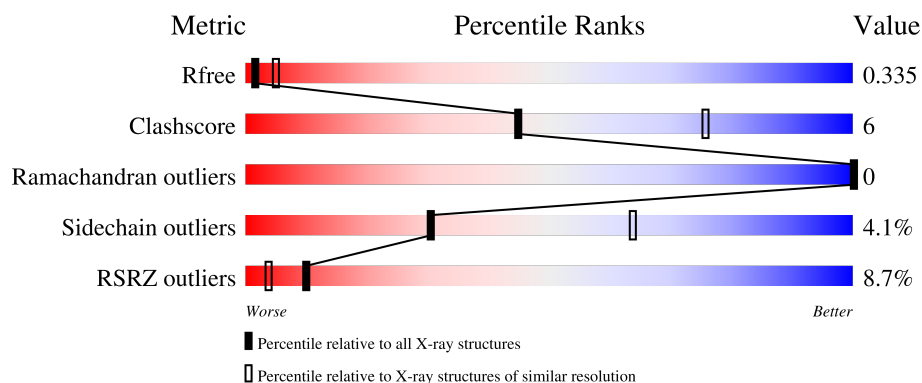
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	321	<div> <div>4%</div> <div>78%</div> <div>10%</div> <div>•</div> <div>10%</div> </div>
1	B	321	<div> <div>7%</div> <div>78%</div> <div>11%</div> <div>•</div> <div>10%</div> </div>
1	C	321	<div> <div>7%</div> <div>77%</div> <div>12%</div> <div>•</div> <div>10%</div> </div>
1	D	321	<div> <div>11%</div> <div>78%</div> <div>11%</div> <div>•</div> <div>10%</div> </div>
1	E	321	<div> <div>9%</div> <div>70%</div> <div>11%</div> <div>•</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	321	<p>9% 77% 11% • 10%</p>
1	G	321	<p>4% 78% 11% • 10%</p>
1	H	321	<p>6% 75% 13% • 10%</p>
1	I	321	<p>6% 78% 11% • 10%</p>
1	J	321	<p>9% 79% 10% • 10%</p>
1	K	321	<p>11% 78% 11% • 10%</p>
1	L	321	<p>10% 78% 11% • 10%</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25719 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.

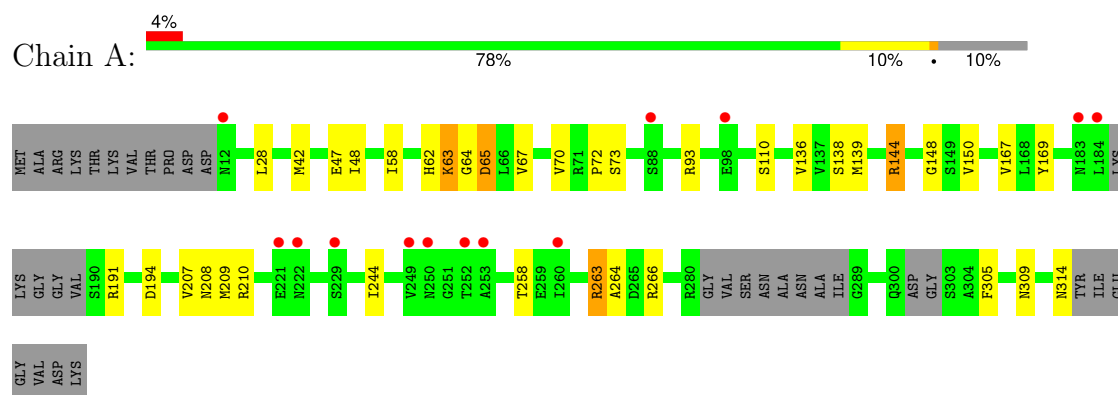
- Molecule 1 is a protein called P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	B	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	C	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	D	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	E	264	Total	C	N	O	S	0	0	0
			1981	1233	357	381	10			
1	F	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	G	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	H	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	I	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	J	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	K	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	L	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			

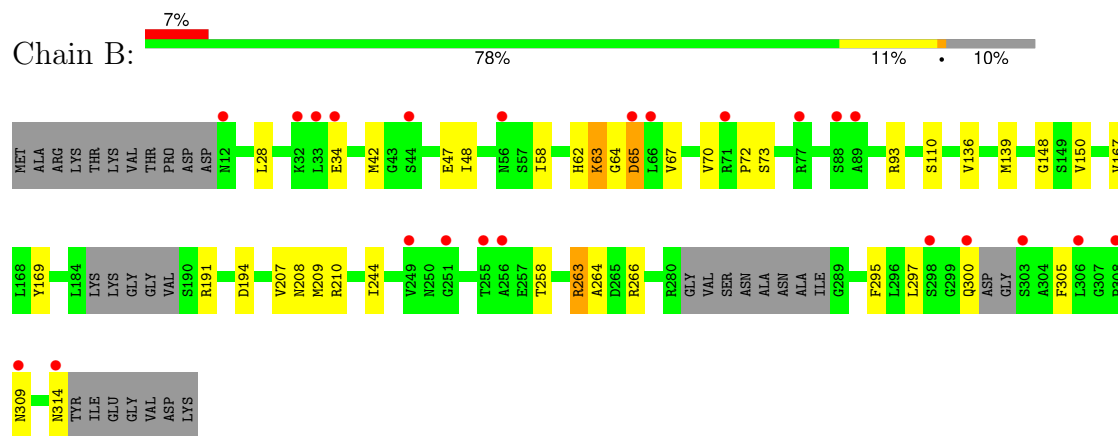
### 3 Residue-property plots [i](#)

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

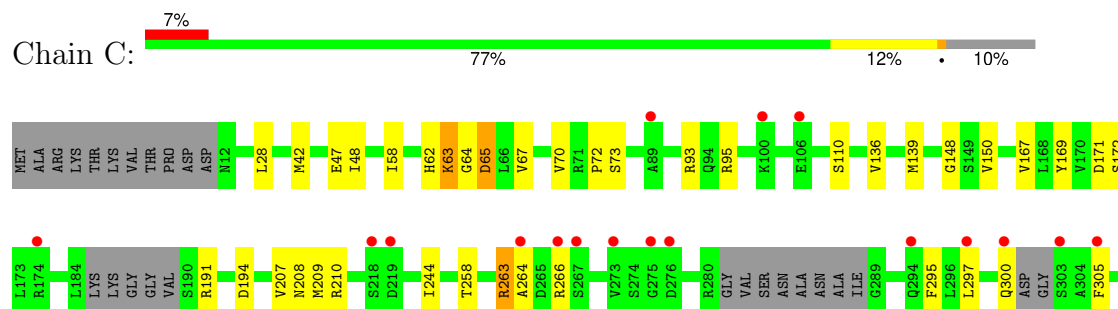
#### • Molecule 1: P4

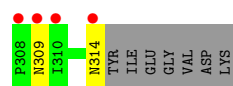


#### • Molecule 1: P4

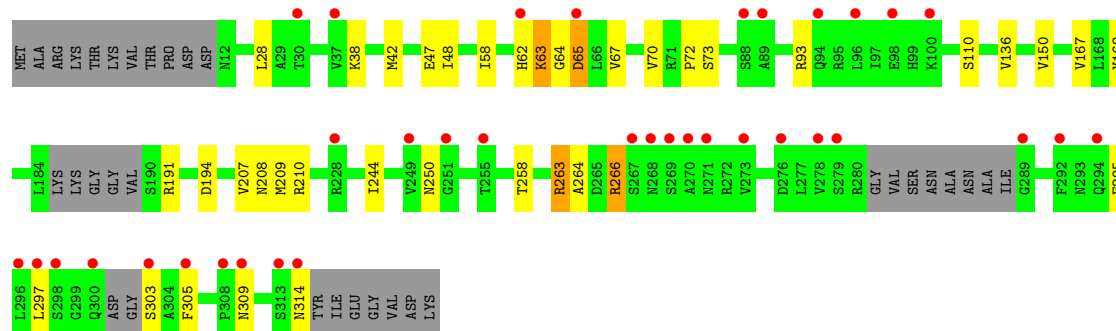
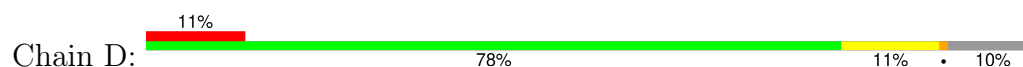


#### • Molecule 1: P4

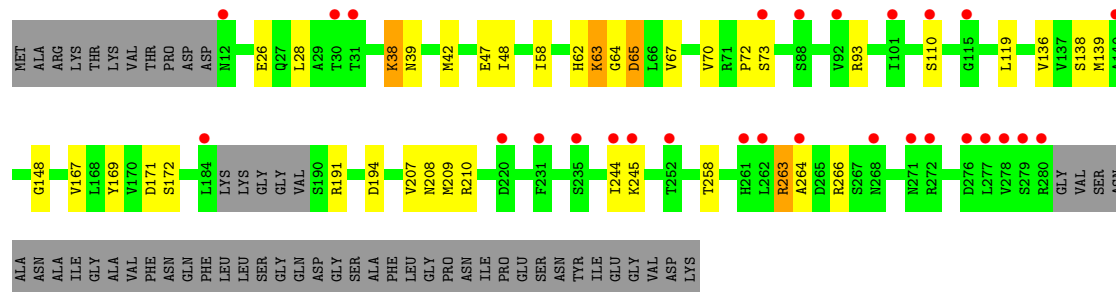




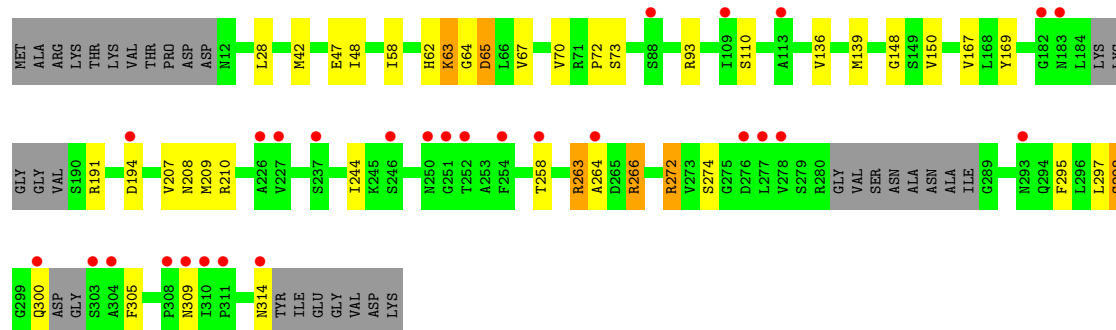
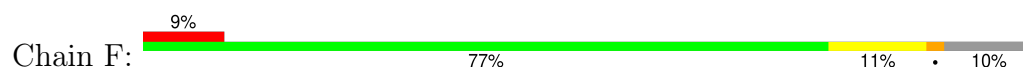
• Molecule 1: P4



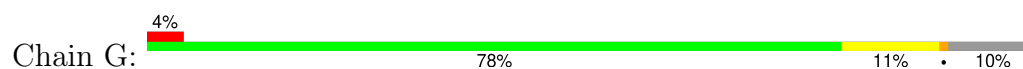
• Molecule 1: P4

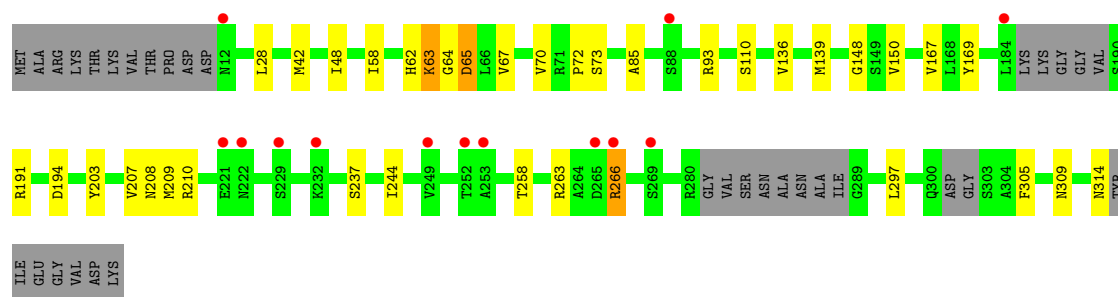


• Molecule 1: P4

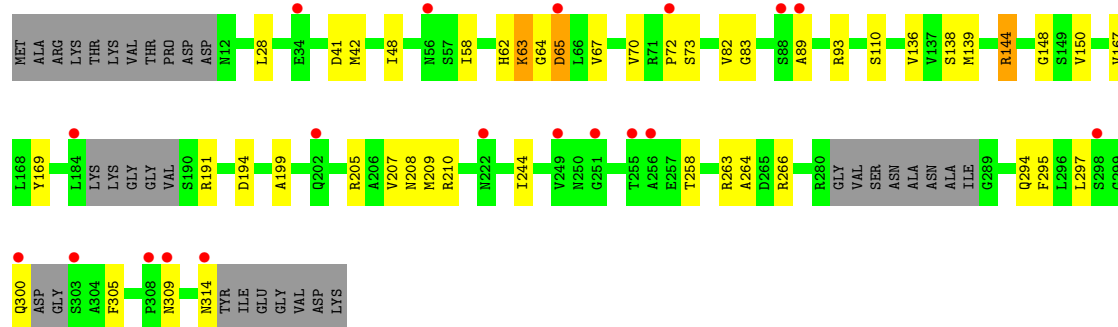
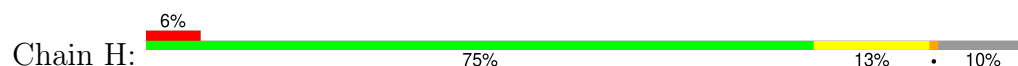


• Molecule 1: P4

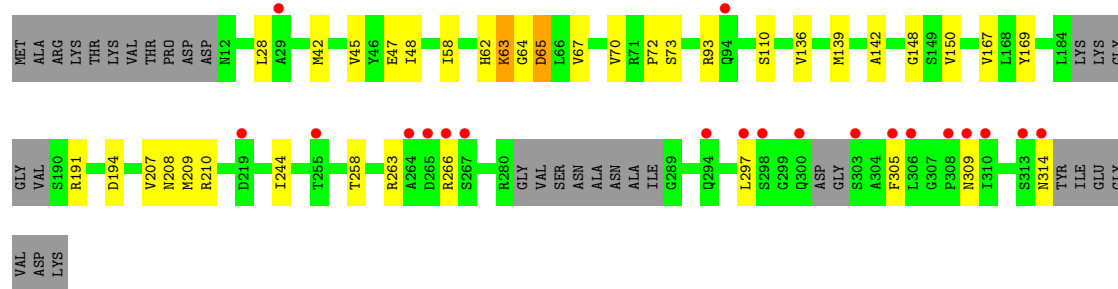
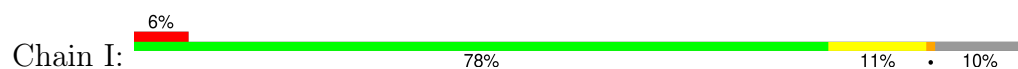




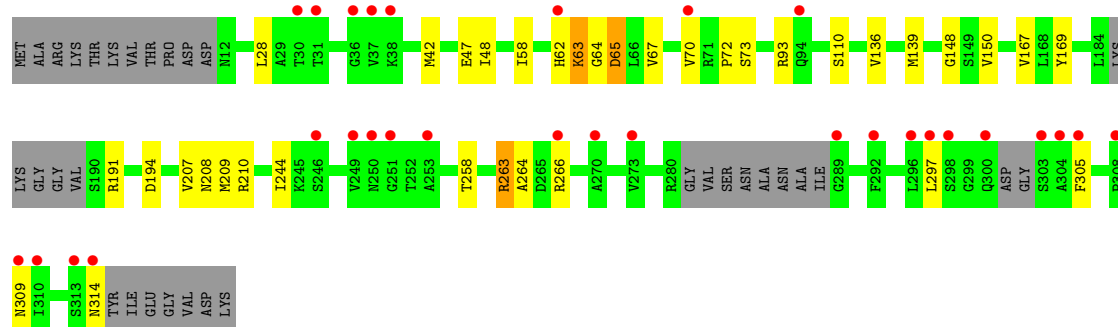
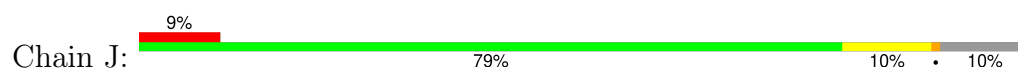
• Molecule 1: P4




• Molecule 1: P4

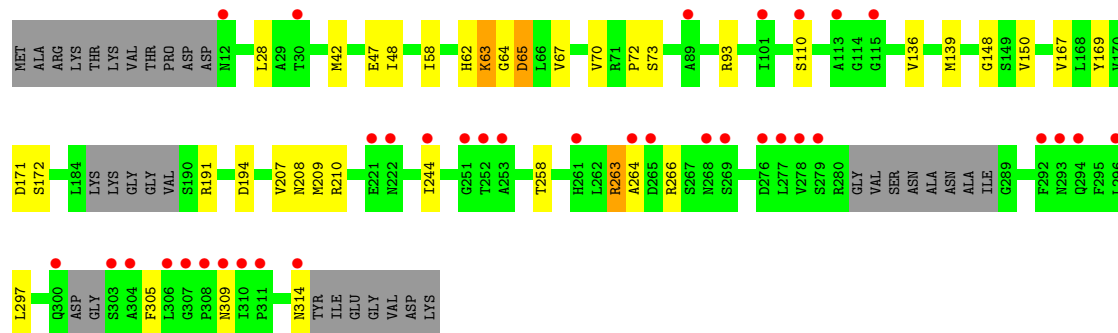


• Molecule 1: P4




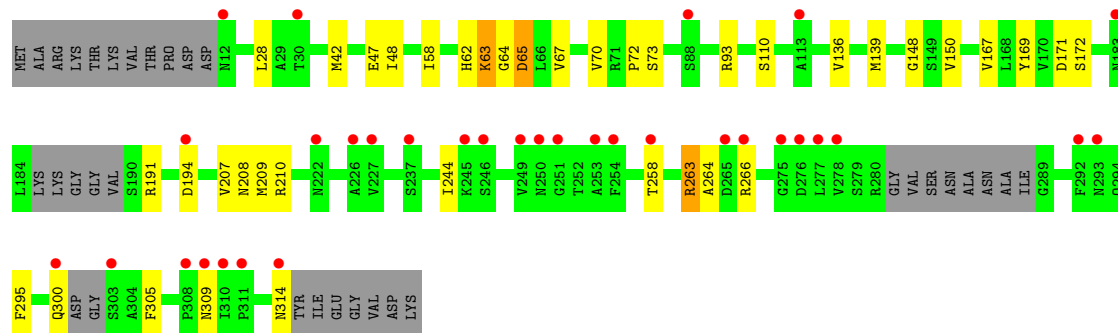
## ● Molecule 1: P4

Chain K: 



## ● Molecule 1: P4

Chain L: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.72Å 197.72Å 562.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.39 – 3.10 49.43 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.39-3.10) 99.9 (49.43-3.10)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.295 , 0.309 0.319 , 0.335	Depositor DCC
$R_{free}$ test set	3868 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	25719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3095e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.40	0/2183	0.64	0/2951
1	B	0.41	0/2183	0.64	0/2951
1	C	0.41	0/2183	0.64	0/2951
1	D	0.42	0/2183	0.64	0/2951
1	E	0.43	0/2003	0.65	0/2709
1	F	0.41	0/2183	0.64	0/2951
1	G	0.40	0/2183	0.64	0/2951
1	H	0.41	0/2183	0.64	0/2951
1	I	0.41	0/2183	0.64	0/2951
1	J	0.41	0/2183	0.64	0/2951
1	K	0.42	0/2183	0.65	0/2951
1	L	0.41	0/2183	0.64	0/2951
All	All	0.41	0/26016	0.64	0/35170

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ASP	Peptide
1	B	65	ASP	Peptide
1	C	65	ASP	Peptide
1	D	65	ASP	Peptide
1	E	65	ASP	Peptide
1	F	65	ASP	Peptide
1	G	65	ASP	Peptide
1	H	65	ASP	Peptide
1	I	65	ASP	Peptide
1	J	65	ASP	Peptide
1	K	65	ASP	Peptide
1	L	65	ASP	Peptide

## 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	2158	0	2181	25	0
1	B	2158	0	2181	28	0
1	C	2158	0	2181	28	1
1	D	2158	0	2181	30	5
1	E	1981	0	2015	28	2
1	F	2158	0	2181	31	3
1	G	2158	0	2181	30	0
1	H	2158	0	2181	49	1
1	I	2158	0	2181	30	0
1	J	2158	0	2181	25	0
1	K	2158	0	2181	26	0
1	L	2158	0	2181	26	0
All	All	25719	0	26006	335	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (335) 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:H:205:ARG:NH1	1:H:263:ARG:NH2	1.80	1.27
1:H:82:VAL:HG21	1:H:199:ALA:HB2	1.36	1.04
1:H:205:ARG:HH12	1:H:263:ARG:HH22	1.00	0.99
1:H:82:VAL:HG21	1:H:199:ALA:CB	1.94	0.97
1:A:138:SER:HB3	1:A:144:ARG:HG2	1.48	0.96
1:D:62:HIS:HB3	1:D:65:ASP:OD1	1.67	0.95
1:H:205:ARG:HH12	1:H:263:ARG:NH2	1.44	0.95
1:H:62:HIS:HB3	1:H:65:ASP:OD1	1.67	0.95
1:G:62:HIS:HB3	1:G:65:ASP:OD1	1.67	0.94
1:I:62:HIS:HB3	1:I:65:ASP:OD1	1.67	0.94
1:B:62:HIS:HB3	1:B:65:ASP:OD1	1.67	0.94
1:A:62:HIS:HB3	1:A:65:ASP:OD1	1.67	0.94
1:F:62:HIS:HB3	1:F:65:ASP:OD1	1.67	0.94
1:E:62:HIS:HB3	1:E:65:ASP:OD1	1.67	0.93
1:K:62:HIS:HB3	1:K:65:ASP:OD1	1.67	0.93
1:L:62:HIS:HB3	1:L:65:ASP:OD1	1.67	0.93
1:J:62:HIS:HB3	1:J:65:ASP:OD1	1.67	0.93
1:H:205:ARG:NH1	1:H:263:ARG:HH21	1.58	0.92
1:C:62:HIS:HB3	1:C:65:ASP:OD1	1.67	0.92
1:F:298:SER:HB2	1:H:41:ASP:HB2	1.50	0.92
1:A:63:LYS:H	1:A:63:LYS:HD2	1.35	0.92
1:G:63:LYS:H	1:G:63:LYS:HD2	1.35	0.92
1:H:205:ARG:NH1	1:H:263:ARG:HH22	1.55	0.92
1:B:63:LYS:H	1:B:63:LYS:HD2	1.35	0.91
1:H:138:SER:HB3	1:H:144:ARG:HG2	1.50	0.91
1:I:63:LYS:H	1:I:63:LYS:HD2	1.35	0.91
1:H:144:ARG:HG3	1:H:144:ARG:HH11	1.35	0.91
1:C:63:LYS:HD2	1:C:63:LYS:H	1.35	0.91
1:J:63:LYS:H	1:J:63:LYS:HD2	1.35	0.90
1:H:63:LYS:H	1:H:63:LYS:HD2	1.35	0.90
1:F:63:LYS:H	1:F:63:LYS:HD2	1.35	0.90
1:D:63:LYS:H	1:D:63:LYS:HD2	1.35	0.89
1:E:63:LYS:H	1:E:63:LYS:HD2	1.35	0.89
1:L:63:LYS:H	1:L:63:LYS:HD2	1.35	0.89
1:K:63:LYS:H	1:K:63:LYS:HD2	1.35	0.87
1:H:205:ARG:CZ	1:H:263:ARG:NH2	2.41	0.83
1:H:82:VAL:CG2	1:H:199:ALA:HB2	2.11	0.80
1:G:266:ARG:HA	1:G:266:ARG:NE	1.97	0.79
1:H:82:VAL:HG23	1:H:83:GLY:H	1.48	0.78
1:F:298:SER:HB2	1:H:41:ASP:CB	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ILE:O	1:D:63:LYS:HB3	1.86	0.75
1:G:48:ILE:O	1:G:63:LYS:HB3	1.87	0.75
1:J:48:ILE:O	1:J:63:LYS:HB3	1.86	0.74
1:B:48:ILE:O	1:B:63:LYS:HB3	1.88	0.74
1:E:48:ILE:O	1:E:63:LYS:HB3	1.88	0.74
1:L:48:ILE:O	1:L:63:LYS:HB3	1.88	0.74
1:A:48:ILE:O	1:A:63:LYS:HB3	1.87	0.73
1:I:48:ILE:O	1:I:63:LYS:HB3	1.88	0.73
1:H:82:VAL:CG2	1:H:199:ALA:CB	2.67	0.73
1:K:48:ILE:O	1:K:63:LYS:HB3	1.88	0.73
1:F:48:ILE:O	1:F:63:LYS:HB3	1.88	0.73
1:C:48:ILE:O	1:C:63:LYS:HB3	1.89	0.72
1:H:48:ILE:O	1:H:63:LYS:HB3	1.89	0.72
1:H:144:ARG:HG3	1:H:144:ARG:NH1	2.07	0.70
1:H:82:VAL:HG23	1:H:83:GLY:N	2.07	0.70
1:E:62:HIS:CB	1:E:65:ASP:OD1	2.40	0.70
1:J:62:HIS:CB	1:J:65:ASP:OD1	2.40	0.70
1:K:62:HIS:CB	1:K:65:ASP:OD1	2.40	0.69
1:I:62:HIS:CB	1:I:65:ASP:OD1	2.40	0.69
1:F:62:HIS:CB	1:F:65:ASP:OD1	2.40	0.69
1:G:62:HIS:CB	1:G:65:ASP:OD1	2.40	0.69
1:H:62:HIS:CB	1:H:65:ASP:OD1	2.40	0.69
1:D:62:HIS:CB	1:D:65:ASP:OD1	2.40	0.69
1:A:62:HIS:CB	1:A:65:ASP:OD1	2.40	0.68
1:L:62:HIS:CB	1:L:65:ASP:OD1	2.40	0.68
1:C:62:HIS:CB	1:C:65:ASP:OD1	2.40	0.67
1:B:62:HIS:CB	1:B:65:ASP:OD1	2.40	0.66
1:E:136:VAL:HG22	1:E:169:TYR:HB2	1.78	0.65
1:K:136:VAL:HG22	1:K:169:TYR:HB2	1.79	0.65
1:A:136:VAL:HG22	1:A:169:TYR:HB2	1.79	0.65
1:B:136:VAL:HG22	1:B:169:TYR:HB2	1.79	0.65
1:E:38:LYS:HD2	1:H:294:GLN:HE22	1.61	0.65
1:H:136:VAL:HG22	1:H:169:TYR:HB2	1.79	0.64
1:D:38:LYS:HG2	1:I:45:VAL:HG13	1.79	0.64
1:L:136:VAL:HG22	1:L:169:TYR:HB2	1.79	0.64
1:F:136:VAL:HG22	1:F:169:TYR:HB2	1.79	0.64
1:G:136:VAL:HG22	1:G:169:TYR:HB2	1.79	0.64
1:J:136:VAL:HG22	1:J:169:TYR:HB2	1.79	0.64
1:H:205:ARG:CZ	1:H:263:ARG:HH22	2.06	0.64
1:C:136:VAL:HG22	1:C:169:TYR:HB2	1.79	0.64
1:D:63:LYS:O	1:D:63:LYS:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:LYS:O	1:F:63:LYS:HG2	1.99	0.63
1:K:63:LYS:O	1:K:63:LYS:HG2	1.99	0.63
1:C:63:LYS:HG2	1:C:63:LYS:O	1.99	0.62
1:E:63:LYS:O	1:E:63:LYS:HG2	1.99	0.62
1:I:63:LYS:O	1:I:63:LYS:HG2	1.99	0.62
1:H:63:LYS:HG2	1:H:63:LYS:O	1.99	0.62
1:D:136:VAL:HG22	1:D:169:TYR:HB2	1.79	0.62
1:A:63:LYS:O	1:A:63:LYS:HG2	1.99	0.62
1:L:63:LYS:O	1:L:63:LYS:HG2	1.99	0.62
1:B:63:LYS:O	1:B:63:LYS:HG2	1.99	0.62
1:G:63:LYS:O	1:G:63:LYS:HG2	1.99	0.62
1:J:63:LYS:O	1:J:63:LYS:HG2	1.99	0.61
1:G:266:ARG:O	1:G:266:ARG:NH1	2.34	0.60
1:I:136:VAL:HG22	1:I:169:TYR:HB2	1.84	0.59
1:F:266:ARG:H	1:F:266:ARG:CD	2.16	0.58
1:K:63:LYS:H	1:K:63:LYS:CD	2.15	0.57
1:I:63:LYS:H	1:I:63:LYS:CD	2.15	0.57
1:A:63:LYS:H	1:A:63:LYS:CD	2.15	0.57
1:D:38:LYS:HD3	1:I:45:VAL:CG1	2.34	0.57
1:G:63:LYS:H	1:G:63:LYS:CD	2.15	0.56
1:F:272:ARG:NH1	1:F:274:SER:OG	2.38	0.56
1:B:63:LYS:H	1:B:63:LYS:CD	2.15	0.56
1:C:63:LYS:H	1:C:63:LYS:CD	2.15	0.55
1:G:63:LYS:HD2	1:G:63:LYS:N	2.15	0.55
1:D:38:LYS:CG	1:I:45:VAL:HG13	2.37	0.55
1:D:63:LYS:H	1:D:63:LYS:CD	2.15	0.55
1:J:63:LYS:HD2	1:J:63:LYS:N	2.15	0.54
1:C:63:LYS:HD2	1:C:63:LYS:N	2.15	0.54
1:A:63:LYS:HD2	1:A:63:LYS:N	2.15	0.53
1:F:63:LYS:H	1:F:63:LYS:CD	2.15	0.53
1:H:82:VAL:CG2	1:H:83:GLY:H	2.18	0.53
1:E:62:HIS:CE1	1:F:297:LEU:HD21	2.44	0.53
1:J:63:LYS:H	1:J:63:LYS:CD	2.15	0.52
1:L:63:LYS:H	1:L:63:LYS:CD	2.15	0.51
1:D:38:LYS:HD3	1:I:45:VAL:HG13	1.93	0.51
1:E:28:LEU:HD11	1:E:67:VAL:HG11	1.93	0.51
1:K:63:LYS:HD2	1:K:63:LYS:N	2.15	0.51
1:C:28:LEU:HD11	1:C:67:VAL:HG11	1.93	0.51
1:E:63:LYS:H	1:E:63:LYS:CD	2.15	0.51
1:E:63:LYS:HD2	1:E:63:LYS:N	2.15	0.51
1:I:28:LEU:HD11	1:I:67:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:HIS:O	1:J:64:GLY:N	2.45	0.50
1:L:42:MET:HB2	1:L:64:GLY:HA2	1.94	0.50
1:I:62:HIS:O	1:I:64:GLY:N	2.45	0.50
1:I:63:LYS:HD2	1:I:63:LYS:N	2.15	0.50
1:F:42:MET:HB2	1:F:64:GLY:HA2	1.93	0.49
1:K:28:LEU:HD11	1:K:67:VAL:HG11	1.94	0.49
1:B:62:HIS:O	1:B:64:GLY:N	2.45	0.49
1:F:62:HIS:O	1:F:64:GLY:N	2.45	0.49
1:B:63:LYS:HD2	1:B:63:LYS:N	2.15	0.49
1:H:28:LEU:HD11	1:H:67:VAL:HG11	1.93	0.49
1:J:28:LEU:HD11	1:J:67:VAL:HG11	1.94	0.49
1:K:42:MET:HB2	1:K:64:GLY:HA2	1.95	0.49
1:L:28:LEU:HD11	1:L:67:VAL:HG11	1.94	0.49
1:D:28:LEU:HD11	1:D:67:VAL:HG11	1.94	0.49
1:B:28:LEU:HD11	1:B:67:VAL:HG11	1.94	0.49
1:F:28:LEU:HD11	1:F:67:VAL:HG11	1.94	0.49
1:B:42:MET:HB2	1:B:64:GLY:HA2	1.94	0.49
1:D:62:HIS:O	1:D:64:GLY:N	2.45	0.49
1:G:62:HIS:O	1:G:64:GLY:N	2.45	0.49
1:C:167:VAL:HG13	1:C:210:ARG:HG3	1.95	0.48
1:E:42:MET:HB2	1:E:64:GLY:HA2	1.95	0.48
1:A:62:HIS:O	1:A:64:GLY:N	2.45	0.48
1:B:58:ILE:HB	1:B:70:VAL:HG22	1.95	0.48
1:J:65:ASP:OD1	1:J:65:ASP:N	2.47	0.48
1:G:28:LEU:HD11	1:G:67:VAL:HG11	1.94	0.48
1:K:62:HIS:O	1:K:64:GLY:N	2.45	0.48
1:A:28:LEU:HD11	1:A:67:VAL:HG11	1.94	0.48
1:D:42:MET:HB2	1:D:64:GLY:HA2	1.96	0.48
1:E:167:VAL:HG13	1:E:210:ARG:HG3	1.95	0.48
1:G:65:ASP:OD1	1:G:65:ASP:N	2.46	0.48
1:H:63:LYS:H	1:H:63:LYS:CD	2.15	0.48
1:L:65:ASP:OD1	1:L:65:ASP:N	2.47	0.48
1:H:42:MET:HB2	1:H:64:GLY:HA2	1.96	0.48
1:I:207:VAL:HG12	1:I:209:MET:HB2	1.96	0.48
1:K:167:VAL:HG13	1:K:210:ARG:HG3	1.96	0.48
1:L:167:VAL:HG13	1:L:210:ARG:HG3	1.95	0.48
1:A:167:VAL:HG13	1:A:210:ARG:HG3	1.95	0.48
1:A:62:HIS:CE1	1:C:297:LEU:HD21	2.49	0.48
1:B:65:ASP:OD1	1:B:65:ASP:N	2.47	0.48
1:D:65:ASP:OD1	1:D:65:ASP:N	2.47	0.48
1:F:110:SER:HB2	1:F:244:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HG13	1:B:210:ARG:HG3	1.96	0.48
1:B:207:VAL:HG12	1:B:209:MET:HB2	1.96	0.48
1:J:42:MET:HB2	1:J:64:GLY:HA2	1.95	0.48
1:C:62:HIS:O	1:C:64:GLY:N	2.45	0.48
1:E:58:ILE:HB	1:E:70:VAL:HG22	1.96	0.48
1:F:207:VAL:HG12	1:F:209:MET:HB2	1.96	0.48
1:H:62:HIS:O	1:H:64:GLY:N	2.45	0.47
1:L:62:HIS:O	1:L:64:GLY:N	2.45	0.47
1:C:58:ILE:HB	1:C:70:VAL:HG22	1.96	0.47
1:I:42:MET:HB2	1:I:64:GLY:HA2	1.96	0.47
1:I:58:ILE:HB	1:I:70:VAL:HG22	1.97	0.47
1:I:65:ASP:OD1	1:I:65:ASP:N	2.47	0.47
1:A:65:ASP:OD1	1:A:65:ASP:N	2.47	0.47
1:E:65:ASP:OD1	1:E:65:ASP:N	2.47	0.47
1:G:62:HIS:CE1	1:I:297:LEU:HD21	2.49	0.47
1:I:167:VAL:HG13	1:I:210:ARG:HG3	1.96	0.47
1:C:65:ASP:OD1	1:C:65:ASP:N	2.47	0.47
1:H:65:ASP:OD1	1:H:65:ASP:N	2.46	0.47
1:A:58:ILE:HB	1:A:70:VAL:HG22	1.97	0.47
1:E:62:HIS:O	1:E:64:GLY:N	2.45	0.47
1:G:58:ILE:HB	1:G:70:VAL:HG22	1.97	0.47
1:G:110:SER:HB2	1:G:244:ILE:HD12	1.97	0.47
1:J:110:SER:HB2	1:J:244:ILE:HD12	1.97	0.47
1:L:207:VAL:HG12	1:L:209:MET:HB2	1.96	0.47
1:C:110:SER:HB2	1:C:244:ILE:HD12	1.97	0.47
1:C:207:VAL:HG12	1:C:209:MET:HB2	1.96	0.47
1:D:110:SER:HB2	1:D:244:ILE:HD12	1.97	0.47
1:D:207:VAL:HG12	1:D:209:MET:HB2	1.96	0.47
1:H:167:VAL:HG13	1:H:210:ARG:HG3	1.96	0.47
1:J:167:VAL:HG13	1:J:210:ARG:HG3	1.97	0.47
1:J:207:VAL:HG12	1:J:209:MET:HB2	1.96	0.47
1:A:207:VAL:HG12	1:A:209:MET:HB2	1.96	0.47
1:G:42:MET:HB2	1:G:64:GLY:HA2	1.97	0.47
1:G:167:VAL:HG13	1:G:210:ARG:HG3	1.96	0.47
1:H:207:VAL:HG12	1:H:209:MET:HB2	1.95	0.47
1:K:62:HIS:HB3	1:K:65:ASP:CG	2.35	0.47
1:J:150:VAL:HG11	1:J:314:ASN:HD22	1.80	0.47
1:K:110:SER:HB2	1:K:244:ILE:HD12	1.96	0.47
1:K:150:VAL:HG11	1:K:314:ASN:HD22	1.80	0.47
1:A:42:MET:HB2	1:A:64:GLY:HA2	1.96	0.46
1:G:150:VAL:HG11	1:G:314:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:ILE:HB	1:H:70:VAL:HG22	1.97	0.46
1:K:58:ILE:HB	1:K:70:VAL:HG22	1.97	0.46
1:A:150:VAL:HG11	1:A:314:ASN:HD22	1.80	0.46
1:C:150:VAL:HG11	1:C:314:ASN:HD22	1.80	0.46
1:E:207:VAL:HG12	1:E:209:MET:HB2	1.96	0.46
1:F:58:ILE:HB	1:F:70:VAL:HG22	1.97	0.46
1:G:207:VAL:HG12	1:G:209:MET:HB2	1.95	0.46
1:K:207:VAL:HG12	1:K:209:MET:HB2	1.96	0.46
1:C:42:MET:HB2	1:C:64:GLY:HA2	1.97	0.46
1:E:110:SER:HB2	1:E:244:ILE:HD12	1.96	0.46
1:F:167:VAL:HG13	1:F:210:ARG:HG3	1.96	0.46
1:H:110:SER:HB2	1:H:244:ILE:HD12	1.97	0.46
1:L:63:LYS:HD2	1:L:63:LYS:N	2.15	0.46
1:A:110:SER:HB2	1:A:244:ILE:HD12	1.97	0.46
1:L:58:ILE:HB	1:L:70:VAL:HG22	1.96	0.46
1:L:110:SER:HB2	1:L:244:ILE:HD12	1.97	0.46
1:E:39:ASN:HB2	1:H:294:GLN:HG2	1.97	0.46
1:B:150:VAL:HG11	1:B:314:ASN:HD22	1.80	0.46
1:F:150:VAL:HG11	1:F:314:ASN:HD22	1.81	0.46
1:G:266:ARG:HA	1:G:266:ARG:CZ	2.46	0.46
1:H:139:MET:HB2	1:H:148:GLY:HA2	1.97	0.46
1:H:205:ARG:NH2	1:H:263:ARG:HH22	2.13	0.46
1:E:62:HIS:HB3	1:E:65:ASP:CG	2.35	0.46
1:D:150:VAL:HG11	1:D:314:ASN:HD22	1.80	0.46
1:J:58:ILE:HB	1:J:70:VAL:HG22	1.97	0.46
1:D:167:VAL:HG13	1:D:210:ARG:HG3	1.96	0.46
1:I:150:VAL:HG11	1:I:314:ASN:HD22	1.81	0.46
1:L:150:VAL:HG11	1:L:314:ASN:HD22	1.80	0.46
1:D:38:LYS:CD	1:I:45:VAL:HG13	2.46	0.45
1:H:150:VAL:HG11	1:H:314:ASN:HD22	1.80	0.45
1:I:93:ARG:HG3	1:I:208:ASN:O	2.16	0.45
1:L:62:HIS:HB3	1:L:65:ASP:CG	2.35	0.45
1:D:47:GLU:HA	1:D:63:LYS:HG3	1.99	0.45
1:F:65:ASP:OD1	1:F:65:ASP:N	2.47	0.45
1:J:93:ARG:HG3	1:J:208:ASN:O	2.17	0.45
1:H:297:LEU:HD21	1:I:62:HIS:CE1	2.51	0.45
1:K:93:ARG:HG3	1:K:208:ASN:O	2.17	0.45
1:K:139:MET:HB2	1:K:148:GLY:HA2	1.99	0.45
1:B:62:HIS:HB3	1:B:65:ASP:CG	2.35	0.45
1:I:139:MET:HB2	1:I:148:GLY:HA2	1.99	0.45
1:A:93:ARG:HG3	1:A:208:ASN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:MET:HB2	1:E:148:GLY:HA2	1.99	0.45
1:C:93:ARG:HG3	1:C:208:ASN:O	2.17	0.45
1:A:263:ARG:HA	1:A:264:ALA:HA	1.75	0.45
1:B:110:SER:HB2	1:B:244:ILE:HD12	1.97	0.45
1:B:139:MET:HB2	1:B:148:GLY:HA2	1.99	0.45
1:E:93:ARG:HG3	1:E:208:ASN:O	2.17	0.45
1:F:62:HIS:HB3	1:F:65:ASP:CG	2.35	0.45
1:C:139:MET:HB2	1:C:148:GLY:HA2	1.99	0.44
1:G:62:HIS:HB3	1:G:65:ASP:CG	2.35	0.44
1:H:63:LYS:HD2	1:H:63:LYS:N	2.15	0.44
1:L:93:ARG:HG3	1:L:208:ASN:O	2.17	0.44
1:G:93:ARG:HG3	1:G:208:ASN:O	2.17	0.44
1:H:62:HIS:CE1	1:J:297:LEU:HD21	2.52	0.44
1:K:65:ASP:OD1	1:K:65:ASP:N	2.47	0.44
1:A:70:VAL:HG23	1:A:72:PRO:HD3	2.00	0.44
1:D:93:ARG:HG3	1:D:208:ASN:O	2.17	0.44
1:E:171:ASP:HA	1:E:172:SER:HA	1.83	0.44
1:B:70:VAL:HG23	1:B:72:PRO:HD3	1.98	0.44
1:F:93:ARG:HG3	1:F:208:ASN:O	2.17	0.44
1:G:70:VAL:HG23	1:G:72:PRO:HD3	2.00	0.44
1:A:139:MET:HB2	1:A:148:GLY:HA2	2.00	0.44
1:L:70:VAL:HG23	1:L:72:PRO:HD3	2.00	0.44
1:G:297:LEU:HD21	1:L:62:HIS:CE1	2.53	0.44
1:H:70:VAL:HG23	1:H:72:PRO:HD3	1.99	0.44
1:L:263:ARG:HA	1:L:264:ALA:HA	1.74	0.44
1:G:139:MET:HB2	1:G:148:GLY:HA2	2.00	0.44
1:I:110:SER:HB2	1:I:244:ILE:HD12	1.99	0.44
1:H:144:ARG:NH1	1:H:144:ARG:CG	2.73	0.43
1:I:70:VAL:HG23	1:I:72:PRO:HD3	2.00	0.43
1:L:139:MET:HB2	1:L:148:GLY:HA2	1.99	0.43
1:F:70:VAL:HG23	1:F:72:PRO:HD3	2.00	0.43
1:F:139:MET:HB2	1:F:148:GLY:HA2	1.99	0.43
1:H:93:ARG:HG3	1:H:208:ASN:O	2.17	0.43
1:F:266:ARG:H	1:F:266:ARG:NE	2.16	0.43
1:D:62:HIS:HB3	1:D:65:ASP:CG	2.35	0.43
1:J:62:HIS:HB3	1:J:65:ASP:CG	2.35	0.43
1:E:70:VAL:HG23	1:E:72:PRO:HD3	1.99	0.43
1:F:263:ARG:HA	1:F:264:ALA:HA	1.74	0.43
1:H:62:HIS:HB3	1:H:65:ASP:CG	2.35	0.43
1:D:58:ILE:HB	1:D:70:VAL:HG22	2.01	0.43
1:J:47:GLU:HA	1:J:63:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:70:VAL:HG23	1:J:72:PRO:HD3	2.00	0.43
1:K:70:VAL:HG23	1:K:72:PRO:HD3	2.01	0.43
1:F:63:LYS:HD2	1:F:63:LYS:N	2.15	0.43
1:C:70:VAL:HG23	1:C:72:PRO:HD3	2.00	0.43
1:K:171:ASP:HA	1:K:172:SER:HA	1.85	0.43
1:B:93:ARG:HG3	1:B:208:ASN:O	2.19	0.42
1:B:297:LEU:HD21	1:C:62:HIS:CE1	2.54	0.42
1:J:139:MET:HB2	1:J:148:GLY:HA2	2.00	0.42
1:B:34:GLU:HB3	1:D:303:SER:N	2.35	0.42
1:B:62:HIS:CE1	1:D:297:LEU:HD21	2.55	0.42
1:D:263:ARG:HA	1:D:264:ALA:HA	1.74	0.42
1:H:263:ARG:HA	1:H:264:ALA:HA	1.72	0.42
1:I:62:HIS:HB3	1:I:65:ASP:CG	2.35	0.42
1:K:47:GLU:HA	1:K:63:LYS:HG3	2.02	0.42
1:K:62:HIS:CG	1:K:65:ASP:OD1	2.73	0.42
1:J:263:ARG:HA	1:J:264:ALA:HA	1.74	0.42
1:D:70:VAL:HG23	1:D:72:PRO:HD3	2.02	0.42
1:E:47:GLU:HA	1:E:63:LYS:HG3	2.01	0.42
1:L:47:GLU:HA	1:L:63:LYS:HG3	2.02	0.42
1:E:62:HIS:CG	1:E:65:ASP:OD1	2.73	0.42
1:C:171:ASP:HA	1:C:172:SER:HA	1.85	0.42
1:G:62:HIS:CG	1:G:65:ASP:OD1	2.73	0.41
1:I:47:GLU:HA	1:I:63:LYS:HG3	2.02	0.41
1:G:266:ARG:NE	1:G:266:ARG:CA	2.78	0.41
1:A:62:HIS:CG	1:A:65:ASP:OD1	2.73	0.41
1:E:263:ARG:HA	1:E:264:ALA:HA	1.74	0.41
1:J:62:HIS:CE1	1:K:297:LEU:HD21	2.56	0.41
1:C:263:ARG:HA	1:C:264:ALA:HA	1.74	0.41
1:F:47:GLU:HA	1:F:63:LYS:HG3	2.02	0.41
1:G:85:ALA:HB2	1:G:203:TYR:CE2	2.55	0.41
1:H:205:ARG:NH2	1:H:263:ARG:NH2	2.68	0.41
1:B:70:VAL:HG12	1:D:295:PHE:CE1	2.56	0.41
1:B:263:ARG:HA	1:B:264:ALA:HA	1.74	0.41
1:B:295:PHE:CE2	1:B:300:GLN:HG2	2.56	0.41
1:D:62:HIS:CG	1:D:65:ASP:OD1	2.73	0.41
1:H:295:PHE:CE2	1:H:300:GLN:HG2	2.56	0.41
1:K:263:ARG:HA	1:K:264:ALA:HA	1.74	0.41
1:L:171:ASP:HA	1:L:172:SER:HA	1.84	0.41
1:A:47:GLU:HA	1:A:63:LYS:HG3	2.03	0.41
1:C:47:GLU:HA	1:C:63:LYS:HG3	2.02	0.40
1:F:272:ARG:HD3	1:F:272:ARG:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:HIS:CG	1:C:65:ASP:OD1	2.73	0.40
1:F:295:PHE:CE2	1:F:300:GLN:HG2	2.56	0.40
1:G:237:SER:HA	1:I:142:ALA:HB1	2.04	0.40
1:L:295:PHE:CE2	1:L:300:GLN:HG2	2.56	0.40
1:C:295:PHE:CE2	1:C:300:GLN:HG2	2.56	0.40
1:B:47:GLU:HA	1:B:63:LYS:HG3	2.03	0.40
1:C:62:HIS:HB3	1:C:65:ASP:CG	2.35	0.40
1:E:119:LEU:HD23	1:E:119:LEU:HA	1.96	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ASN:ND2	1:F:272:ARG:NH2[4_555]	0.76	1.44
1:D:266:ARG:NH1	1:E:245:LYS:NZ[4_555]	1.49	0.71
1:D:250:ASN:CG	1:F:272:ARG:NH2[4_555]	1.65	0.55
1:D:250:ASN:ND2	1:F:272:ARG:CZ[4_555]	1.89	0.31
1:D:266:ARG:CZ	1:E:245:LYS:NZ[4_555]	1.99	0.21
1:C:95:ARG:NH2	1:H:89:ALA:CB[2_665]	2.08	0.12

## 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	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	B	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	C	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	D	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	E	260/321 (81%)	250 (96%)	10 (4%)	0	100	100
1	F	280/321 (87%)	269 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	H	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	I	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	J	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	K	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	L	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
All	All	3340/3852 (87%)	3209 (96%)	131 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	232/257 (90%)	222 (96%)	10 (4%)	29	62
1	B	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	C	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	D	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	E	213/257 (83%)	203 (95%)	10 (5%)	26	59
1	F	232/257 (90%)	221 (95%)	11 (5%)	26	59
1	G	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	H	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	I	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	J	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	K	232/257 (90%)	223 (96%)	9 (4%)	32	65
1	L	232/257 (90%)	223 (96%)	9 (4%)	32	65
All	All	2765/3084 (90%)	2653 (96%)	112 (4%)	30	64

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	73	SER
1	A	144	ARG
1	A	191	ARG
1	A	194	ASP
1	A	258	THR
1	A	263	ARG
1	A	266	ARG
1	A	305	PHE
1	A	309	ASN
1	B	63	LYS
1	B	73	SER
1	B	191	ARG
1	B	194	ASP
1	B	258	THR
1	B	263	ARG
1	B	266	ARG
1	B	305	PHE
1	B	309	ASN
1	C	63	LYS
1	C	73	SER
1	C	191	ARG
1	C	194	ASP
1	C	258	THR
1	C	263	ARG
1	C	266	ARG
1	C	305	PHE
1	C	309	ASN
1	D	63	LYS
1	D	73	SER
1	D	191	ARG
1	D	194	ASP
1	D	258	THR
1	D	263	ARG
1	D	266	ARG
1	D	305	PHE
1	D	309	ASN
1	E	26	GLU
1	E	38	LYS
1	E	63	LYS
1	E	73	SER
1	E	138	SER
1	E	191	ARG

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Mol	Chain	Res	Type
1	E	194	ASP
1	E	258	THR
1	E	263	ARG
1	E	266	ARG
1	F	63	LYS
1	F	73	SER
1	F	191	ARG
1	F	194	ASP
1	F	258	THR
1	F	263	ARG
1	F	266	ARG
1	F	272	ARG
1	F	298	SER
1	F	305	PHE
1	F	309	ASN
1	G	63	LYS
1	G	73	SER
1	G	191	ARG
1	G	194	ASP
1	G	258	THR
1	G	263	ARG
1	G	266	ARG
1	G	305	PHE
1	G	309	ASN
1	H	63	LYS
1	H	73	SER
1	H	144	ARG
1	H	191	ARG
1	H	194	ASP
1	H	258	THR
1	H	266	ARG
1	H	305	PHE
1	H	309	ASN
1	I	63	LYS
1	I	73	SER
1	I	191	ARG
1	I	194	ASP
1	I	258	THR
1	I	263	ARG
1	I	266	ARG
1	I	305	PHE
1	I	309	ASN

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Mol	Chain	Res	Type
1	J	63	LYS
1	J	73	SER
1	J	191	ARG
1	J	194	ASP
1	J	258	THR
1	J	263	ARG
1	J	266	ARG
1	J	305	PHE
1	J	309	ASN
1	K	63	LYS
1	K	73	SER
1	K	191	ARG
1	K	194	ASP
1	K	258	THR
1	K	263	ARG
1	K	266	ARG
1	K	305	PHE
1	K	309	ASN
1	L	63	LYS
1	L	73	SER
1	L	191	ARG
1	L	194	ASP
1	L	258	THR
1	L	263	ARG
1	L	266	ARG
1	L	305	PHE
1	L	309	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	B	314	ASN
1	C	314	ASN
1	D	39	ASN
1	D	314	ASN
1	E	39	ASN
1	F	314	ASN
1	G	314	ASN
1	H	294	GLN
1	H	314	ASN
1	I	314	ASN

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Mol	Chain	Res	Type
1	J	314	ASN
1	K	314	ASN
1	L	314	ASN

### 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 monosaccharides 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	288/321 (89%)	0.21	13 (4%) 33 16	34, 53, 78, 109	0
1	B	288/321 (89%)	0.51	23 (7%) 12 5	39, 61, 99, 124	0
1	C	288/321 (89%)	0.43	21 (7%) 15 6	29, 54, 102, 137	0
1	D	288/321 (89%)	0.71	36 (12%) 3 1	40, 69, 120, 155	0
1	E	264/321 (82%)	0.81	28 (10%) 6 2	44, 70, 109, 135	0
1	F	288/321 (89%)	0.53	28 (9%) 7 2	41, 59, 100, 137	0
1	G	288/321 (89%)	0.24	13 (4%) 33 16	32, 53, 85, 127	0
1	H	288/321 (89%)	0.46	19 (6%) 18 7	36, 58, 102, 149	0
1	I	288/321 (89%)	0.45	20 (6%) 16 7	35, 55, 112, 156	0
1	J	288/321 (89%)	0.67	30 (10%) 6 2	36, 68, 119, 152	0
1	K	288/321 (89%)	0.93	36 (12%) 3 1	44, 75, 123, 162	0
1	L	288/321 (89%)	0.58	33 (11%) 4 2	40, 61, 119, 147	0
All	All	3432/3852 (89%)	0.54	300 (8%) 10 4	29, 61, 110, 162	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	264	ALA	8.3
1	I	300	GLN	8.3
1	K	308	PRO	7.1
1	E	264	ALA	6.7
1	K	276	ASP	6.2
1	E	279	SER	6.1
1	K	307	GLY	5.9
1	J	298	SER	5.8
1	L	308	PRO	5.7
1	J	251	GLY	5.7
1	J	309	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
1	H	300	GLN	5.5
1	C	309	ASN	5.4
1	E	30	THR	5.4
1	E	252	THR	5.3
1	D	300	GLN	5.2
1	C	303	SER	5.1
1	K	314	ASN	5.1
1	K	303	SER	5.0
1	L	293	ASN	5.0
1	C	310	ILE	4.9
1	I	310	ILE	4.8
1	L	309	ASN	4.8
1	B	309	ASN	4.7
1	L	310	ILE	4.7
1	J	270	ALA	4.7
1	J	314	ASN	4.6
1	K	306	LEU	4.5
1	L	300	GLN	4.5
1	B	255	THR	4.4
1	L	250	ASN	4.4
1	J	308	PRO	4.3
1	I	309	ASN	4.3
1	E	115	GLY	4.3
1	K	279	SER	4.2
1	D	303	SER	4.1
1	F	250	ASN	4.1
1	D	251	GLY	4.1
1	I	314	ASN	4.0
1	E	268	ASN	4.0
1	K	252	THR	4.0
1	F	310	ILE	4.0
1	J	300	GLN	3.9
1	C	308	PRO	3.9
1	D	271	ASN	3.9
1	K	221	GLU	3.9
1	H	309	ASN	3.9
1	F	300	GLN	3.9
1	C	314	ASN	3.9
1	J	30	THR	3.9
1	J	296	LEU	3.9
1	B	306	LEU	3.8
1	E	12	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	37	VAL	3.8
1	D	297	LEU	3.8
1	E	245	LYS	3.8
1	I	305	PHE	3.8
1	I	294	GLN	3.7
1	B	33	LEU	3.7
1	K	110	SER	3.6
1	K	311	PRO	3.6
1	C	275	GLY	3.6
1	G	12	ASN	3.6
1	A	184	LEU	3.6
1	F	277	LEU	3.6
1	D	296	LEU	3.5
1	L	277	LEU	3.5
1	H	255	THR	3.5
1	B	300	GLN	3.5
1	E	277	LEU	3.4
1	D	270	ALA	3.4
1	K	12	ASN	3.4
1	D	313	SER	3.4
1	C	300	GLN	3.4
1	B	88	SER	3.4
1	J	62	HIS	3.4
1	K	309	ASN	3.4
1	D	88	SER	3.4
1	J	94	GLN	3.4
1	D	249	VAL	3.4
1	D	94	GLN	3.4
1	J	289	GLY	3.4
1	D	30	THR	3.3
1	F	246	SER	3.3
1	L	276	ASP	3.3
1	L	292	PHE	3.3
1	C	267	SER	3.3
1	E	110	SER	3.3
1	F	311	PRO	3.3
1	J	249	VAL	3.3
1	A	12	ASN	3.3
1	G	222	ASN	3.2
1	B	303	SER	3.2
1	A	253	ALA	3.2
1	F	88	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	88	SER	3.2
1	K	278	VAL	3.2
1	E	278	VAL	3.2
1	I	264	ALA	3.2
1	L	113	ALA	3.2
1	E	276	ASP	3.2
1	L	303	SER	3.1
1	H	89	ALA	3.1
1	B	256	ALA	3.1
1	H	298	SER	3.1
1	I	297	LEU	3.1
1	F	276	ASP	3.1
1	L	246	SER	3.1
1	E	31	THR	3.1
1	F	303	SER	3.0
1	K	269	SER	3.0
1	J	38	LYS	3.0
1	E	261	HIS	3.0
1	D	309	ASN	3.0
1	J	303	SER	3.0
1	C	219	ASP	3.0
1	F	113	ALA	3.0
1	H	256	ALA	3.0
1	L	311	PRO	3.0
1	B	56	ASN	3.0
1	G	252	THR	3.0
1	A	88	SER	2.9
1	K	268	ASN	2.9
1	J	266	ARG	2.9
1	K	277	LEU	2.9
1	D	298	SER	2.9
1	K	244	ILE	2.9
1	E	244	ILE	2.9
1	L	254	PHE	2.9
1	E	220	ASP	2.9
1	J	292	PHE	2.9
1	I	303	SER	2.9
1	K	261	HIS	2.9
1	L	237	SER	2.9
1	J	310	ILE	2.9
1	I	94	GLN	2.9
1	B	12	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	218	SER	2.8
1	D	289	GLY	2.8
1	E	140	ALA	2.8
1	F	293	ASN	2.8
1	J	297	LEU	2.8
1	K	115	GLY	2.8
1	D	37	VAL	2.8
1	D	62	HIS	2.8
1	B	89	ALA	2.8
1	K	294	GLN	2.8
1	C	264	ALA	2.8
1	D	314	ASN	2.8
1	D	305	PHE	2.8
1	D	100	LYS	2.8
1	I	267	SER	2.8
1	K	265	ASP	2.8
1	G	229	SER	2.8
1	H	56	ASN	2.8
1	I	266	ARG	2.7
1	A	252	THR	2.7
1	F	237	SER	2.7
1	F	258	THR	2.7
1	B	298	SER	2.7
1	F	309	ASN	2.7
1	I	265	ASP	2.7
1	D	267	SER	2.7
1	F	308	PRO	2.7
1	G	184	LEU	2.7
1	L	251	GLY	2.7
1	L	227	VAL	2.7
1	A	260	ILE	2.7
1	K	30	THR	2.7
1	L	258	THR	2.7
1	D	292	PHE	2.7
1	D	89	ALA	2.7
1	B	314	ASN	2.6
1	F	194	ASP	2.6
1	K	292	PHE	2.6
1	I	308	PRO	2.6
1	B	65	ASP	2.6
1	D	279	SER	2.6
1	E	272	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	89	ALA	2.6
1	A	222	ASN	2.6
1	G	88	SER	2.6
1	J	250	ASN	2.6
1	C	297	LEU	2.6
1	C	100	LYS	2.5
1	B	308	PRO	2.5
1	L	278	VAL	2.5
1	J	246	SER	2.5
1	B	77	ARG	2.5
1	I	219	ASP	2.5
1	B	34	GLU	2.5
1	L	183	ASN	2.5
1	H	251	GLY	2.5
1	B	251	GLY	2.5
1	D	273	VAL	2.5
1	F	278	VAL	2.5
1	C	273	VAL	2.5
1	B	32	LYS	2.5
1	G	221	GLU	2.5
1	L	222	ASN	2.5
1	A	221	GLU	2.5
1	B	71	ARG	2.4
1	H	308	PRO	2.4
1	D	278	VAL	2.4
1	K	296	LEU	2.4
1	H	34	GLU	2.4
1	D	269	SER	2.4
1	E	73	SER	2.4
1	F	304	ALA	2.4
1	C	276	ASP	2.4
1	F	109	ILE	2.4
1	L	249	VAL	2.4
1	K	101	ILE	2.4
1	F	254	PHE	2.4
1	J	305	PHE	2.4
1	F	182	GLY	2.4
1	I	313	SER	2.4
1	J	273	VAL	2.3
1	I	255	THR	2.3
1	K	251	GLY	2.3
1	L	266	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	222	ASN	2.3
1	L	253	ALA	2.3
1	E	231	PHE	2.3
1	J	253	ALA	2.3
1	K	304	ALA	2.3
1	F	314	ASN	2.3
1	G	253	ALA	2.3
1	H	314	ASN	2.3
1	H	72	PRO	2.3
1	L	265	ASP	2.3
1	E	262	LEU	2.3
1	D	65	ASP	2.3
1	A	98	GLU	2.2
1	I	29	ALA	2.2
1	E	184	LEU	2.2
1	G	265	ASP	2.2
1	L	314	ASN	2.2
1	F	227	VAL	2.2
1	L	12	ASN	2.2
1	J	304	ALA	2.2
1	L	275	GLY	2.2
1	E	235	SER	2.2
1	F	251	GLY	2.2
1	H	65	ASP	2.2
1	F	264	ALA	2.2
1	L	30	THR	2.2
1	D	96	LEU	2.2
1	L	226	ALA	2.2
1	B	66	LEU	2.2
1	D	268	ASN	2.2
1	J	31	THR	2.2
1	D	294	GLN	2.2
1	G	266	ARG	2.2
1	D	98	GLU	2.2
1	I	298	SER	2.2
1	D	308	PRO	2.2
1	K	310	ILE	2.2
1	E	271	ASN	2.2
1	K	89	ALA	2.1
1	F	183	ASN	2.1
1	C	174	ARG	2.1
1	C	266	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	255	THR	2.1
1	H	222	ASN	2.1
1	K	253	ALA	2.1
1	J	70	VAL	2.1
1	E	280	ARG	2.1
1	E	92	VAL	2.1
1	L	194	ASP	2.1
1	C	305	PHE	2.1
1	E	88	SER	2.1
1	G	232	LYS	2.1
1	A	250	ASN	2.1
1	E	101	ILE	2.1
1	B	44	SER	2.1
1	C	106	GLU	2.0
1	A	183	ASN	2.0
1	G	249	VAL	2.0
1	D	276	ASP	2.0
1	H	202	GLN	2.0
1	J	313	SER	2.0
1	L	88	SER	2.0
1	J	36	GLY	2.0
1	H	303	SER	2.0
1	B	249	VAL	2.0
1	H	249	VAL	2.0
1	H	184	LEU	2.0
1	L	245	LYS	2.0
1	D	228	ARG	2.0
1	K	300	GLN	2.0
1	A	229	SER	2.0
1	F	252	THR	2.0
1	K	293	ASN	2.0
1	A	249	VAL	2.0
1	G	269	SER	2.0
1	F	226	ALA	2.0
1	K	113	ALA	2.0
1	C	294	GLN	2.0
1	I	306	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.