



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:57 am BST

PDB ID : 4EP0  
Title : Structure of the bacteriophage C1 tail knob protein, gp12  
Authors : Aksyuk, A.A.; Rossmann, M.G.  
Deposited on : 2012-04-16  
Resolution : 4.00 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

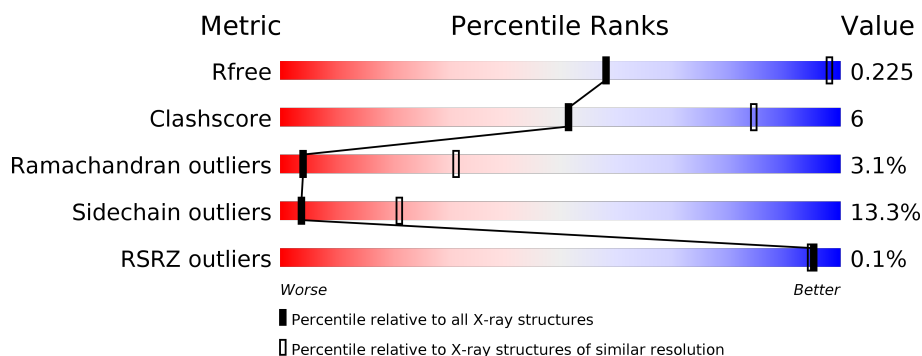
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	583	<div> <div>64%</div> <div>17%</div> <div>•</div> <div>16%</div> </div>
1	B	583	<div> <div>63%</div> <div>17%</div> <div>•</div> <div>16%</div> </div>
1	C	583	<div> <div>62%</div> <div>19%</div> <div>• •</div> <div>16%</div> </div>
1	D	583	<div> <div>62%</div> <div>18%</div> <div>•</div> <div>16%</div> </div>
1	E	583	<div> <div>62%</div> <div>18%</div> <div>•</div> <div>16%</div> </div>
1	F	583	<div> <div>63%</div> <div>17%</div> <div>•</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	583	<div><div></div><div>63%17%•16%</div></div>
1	H	583	<div><div></div><div>63%17%•16%</div></div>
1	I	583	<div><div></div><div>62%19%•16%</div></div>
1	J	583	<div><div></div><div>64%16%•16%</div></div>
1	K	583	<div><div></div><div>63%17%•16%</div></div>
1	L	583	<div><div></div><div>63%17%•16%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 47376 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 Major tail protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	B	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	C	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	D	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	E	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	F	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	G	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	H	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	I	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	J	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	K	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	L	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
A	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
A	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
A	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
A	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
A	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
A	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
A	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
B	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
B	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
B	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
B	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
B	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
B	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
B	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
B	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
B	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
C	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
C	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
C	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
C	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
C	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
C	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
C	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
C	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
C	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
D	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
D	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
D	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
D	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
D	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
D	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
D	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
D	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
D	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
E	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
E	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
E	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
E	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
E	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
E	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
E	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
E	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
E	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
F	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
F	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
F	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
F	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
F	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
F	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
F	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
F	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
G	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
G	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
G	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
G	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
G	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
G	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
G	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
G	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
G	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
H	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
H	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
H	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
H	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
H	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
H	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
H	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
H	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
H	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
I	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
I	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
I	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
I	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
I	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
I	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
I	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
I	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
I	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
J	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
J	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
J	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
J	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
J	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
J	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
J	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
J	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0

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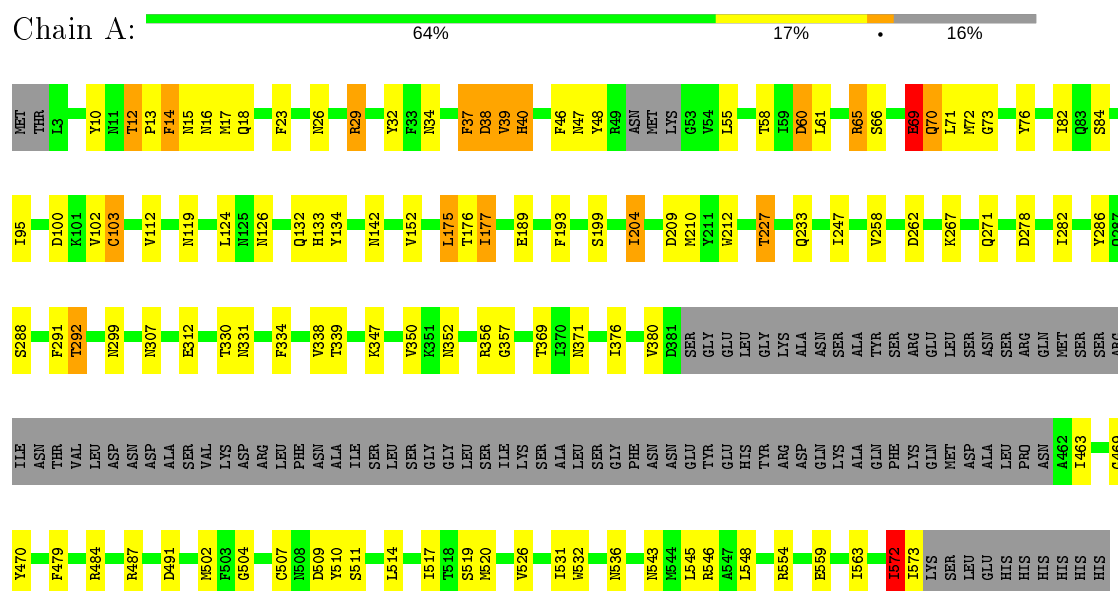
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Chain	Residue	Modelled	Actual	Comment	Reference
J	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
K	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
K	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
K	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
K	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
K	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
K	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
K	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
K	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
K	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
L	575	SER	-	EXPRESSION TAG	UNP Q7Y3F0
L	576	LEU	-	EXPRESSION TAG	UNP Q7Y3F0
L	577	GLU	-	EXPRESSION TAG	UNP Q7Y3F0
L	578	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
L	579	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
L	580	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
L	581	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
L	582	HIS	-	EXPRESSION TAG	UNP Q7Y3F0
L	583	HIS	-	EXPRESSION TAG	UNP Q7Y3F0

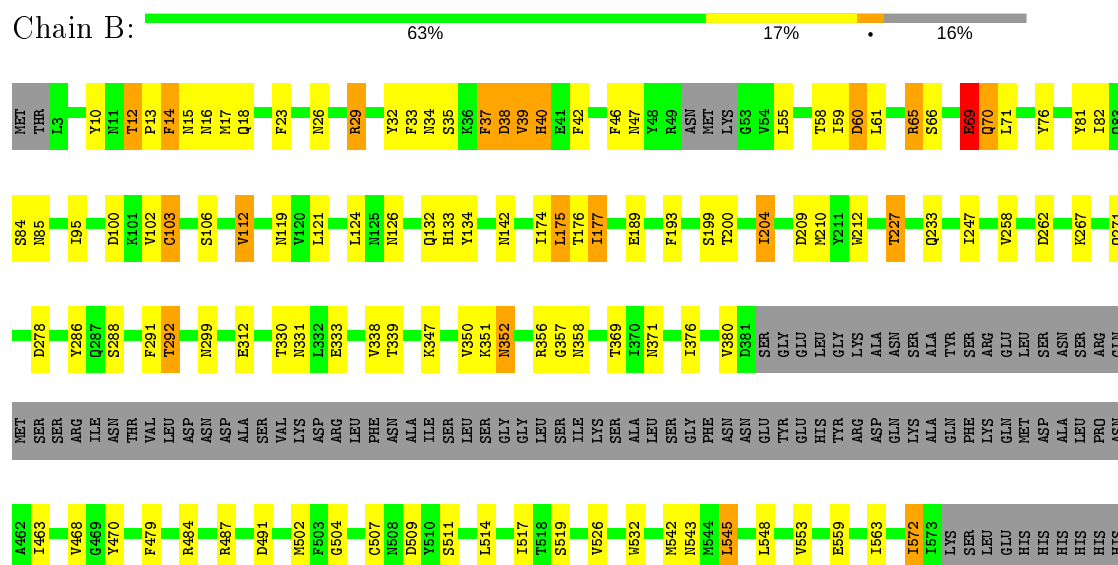
### 3 Residue-property plots

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

#### • Molecule 1: Major tail protein

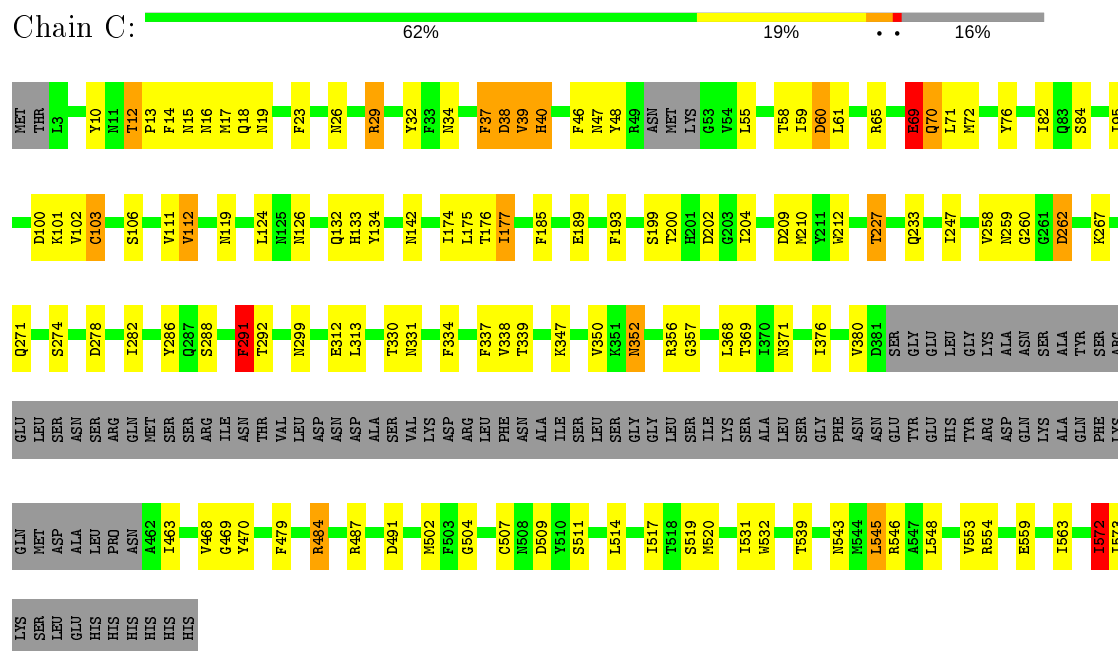


#### • Molecule 1: Major tail protein

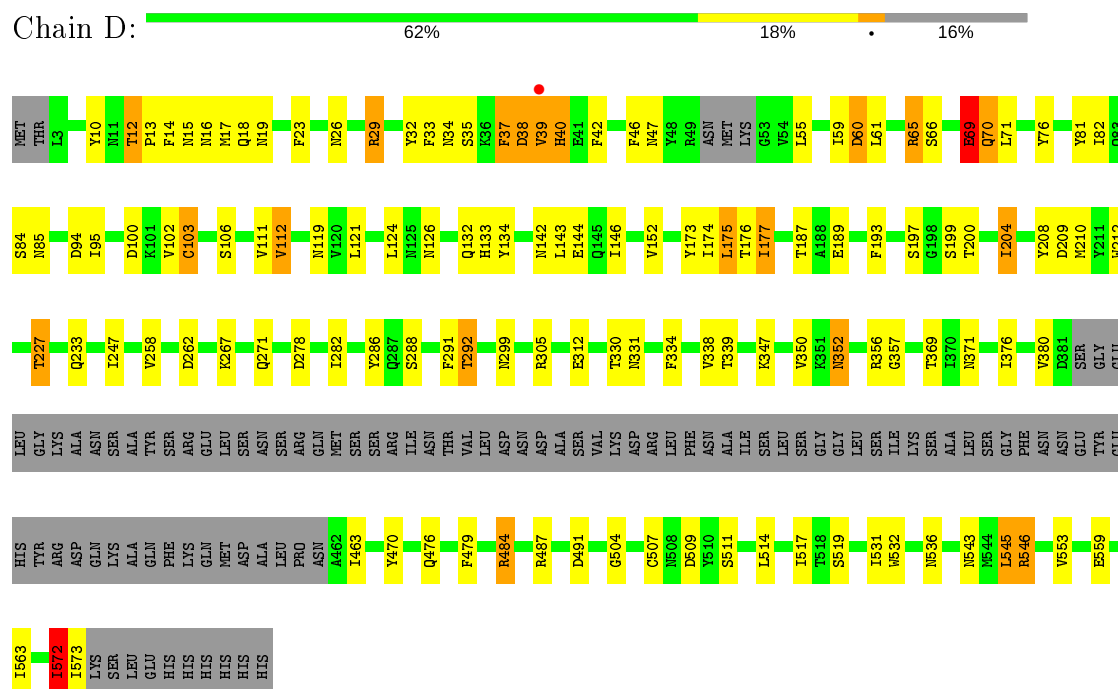




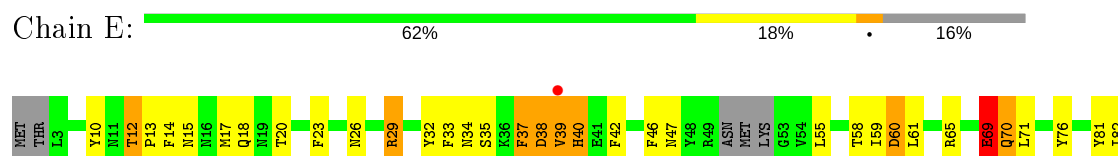
- Molecule 1: Major tail protein



- Molecule 1: Major tail protein



- Molecule 1: Major tail protein

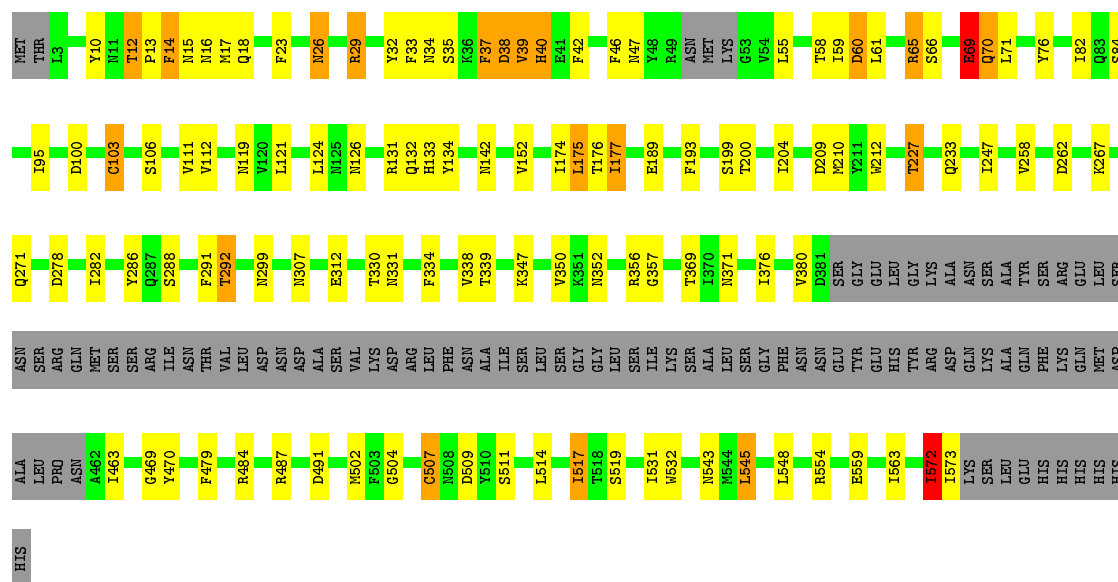






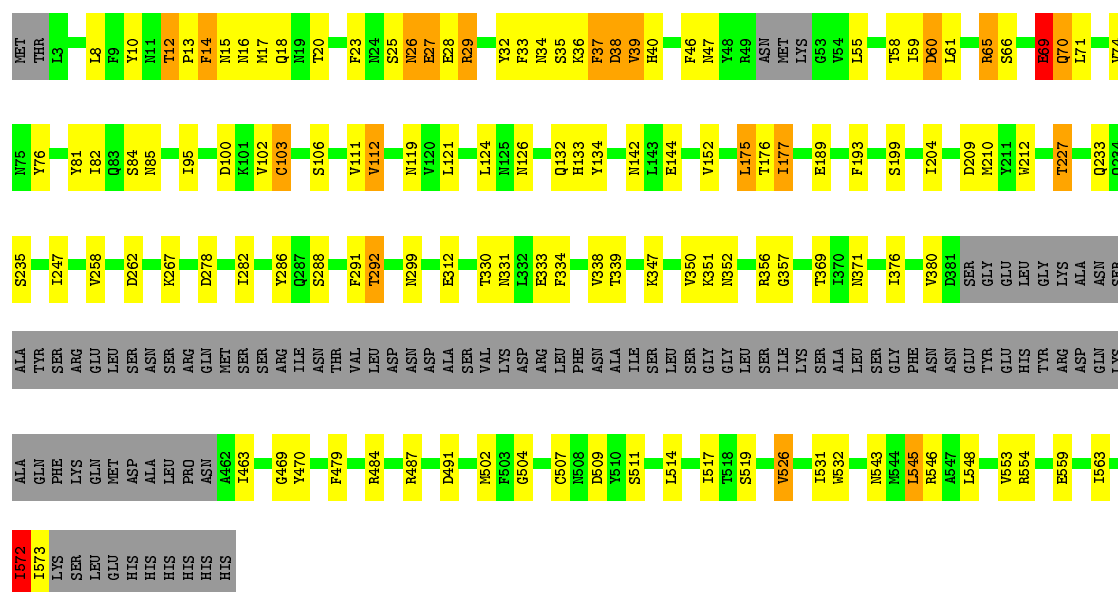
- Molecule 1: Major tail protein

Chain H: 63% 17% 16%

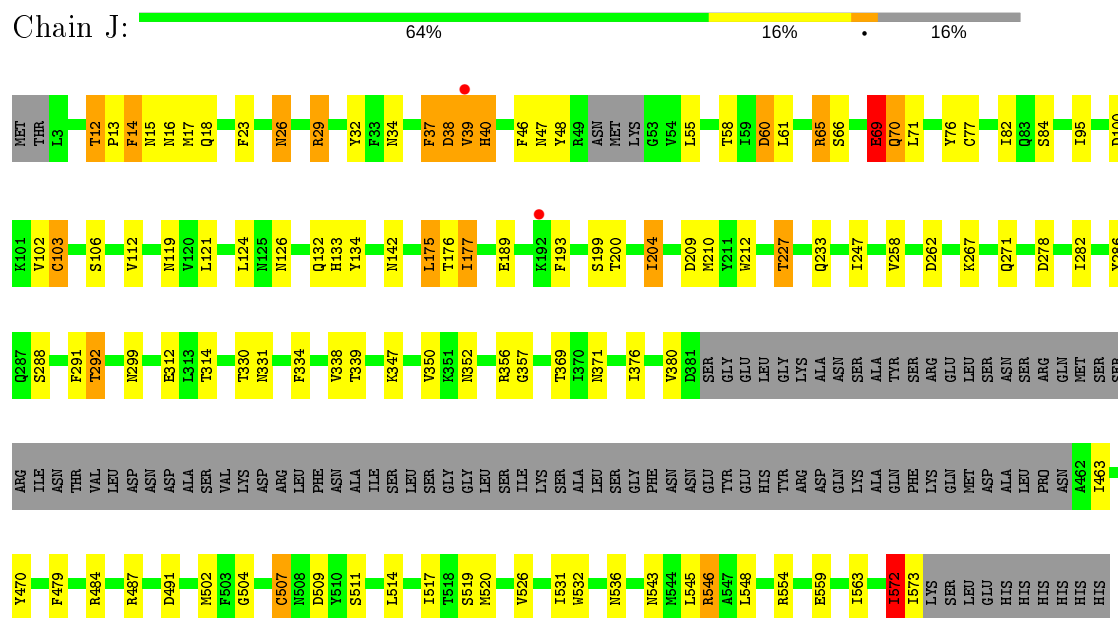


- Molecule 1: Major tail protein

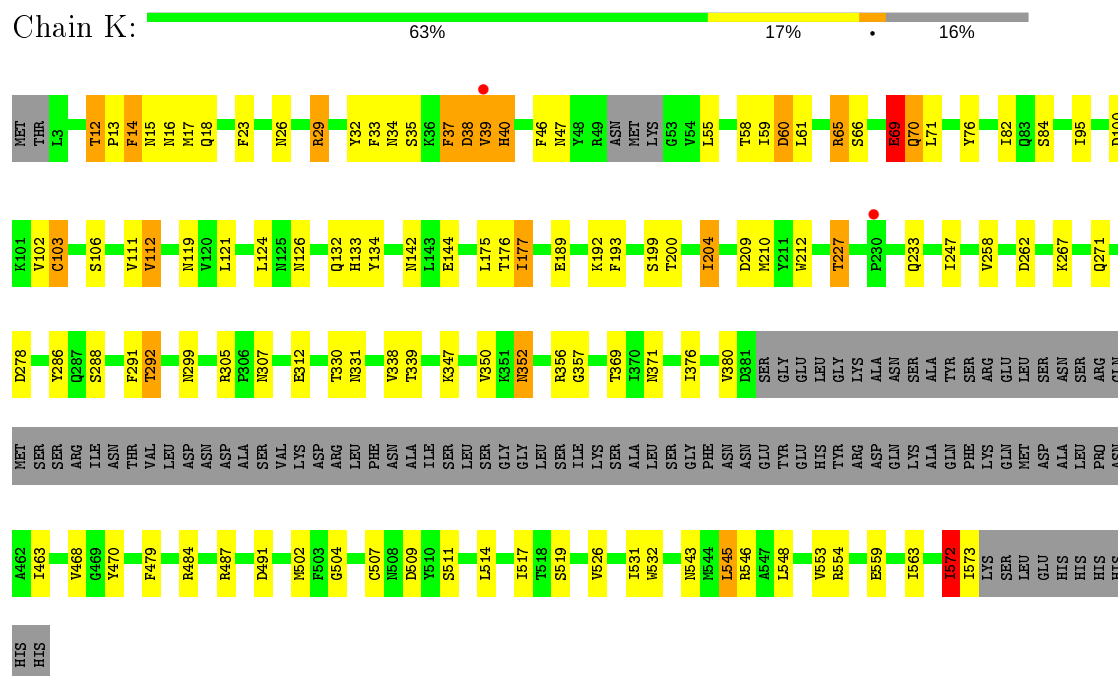
Chain I: 62% 19% 16%



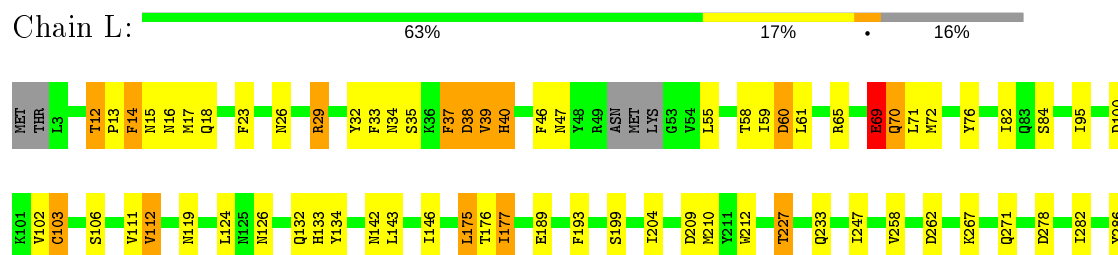
- Molecule 1: Major tail protein



- Molecule 1: Major tail protein



- Molecule 1: Major tail protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	316.87Å 211.38Å 178.60Å 90.00° 116.53° 90.00°	Depositor
Resolution (Å)	49.73 – 4.00 49.73 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.73-4.00) 99.4 (49.73-4.00)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.195 , 0.233 0.184 , 0.225	Depositor DCC
$R_{free}$ test set	4429 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 97.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	47376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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	0.50	0/4030	0.71	0/5464
1	B	0.50	0/4030	0.71	0/5464
1	C	0.55	2/4030 (0.0%)	0.73	4/5464 (0.1%)
1	D	0.52	0/4030	0.73	3/5464 (0.1%)
1	E	0.49	0/4030	0.70	0/5464
1	F	0.51	0/4030	0.72	1/5464 (0.0%)
1	G	0.47	0/4030	0.70	2/5464 (0.0%)
1	H	0.48	0/4030	0.70	1/5464 (0.0%)
1	I	0.51	0/4030	0.72	1/5464 (0.0%)
1	J	0.49	0/4030	0.71	1/5464 (0.0%)
1	K	0.48	0/4030	0.70	1/5464 (0.0%)
1	L	0.48	0/4030	0.70	1/5464 (0.0%)
All	All	0.50	2/48360 (0.0%)	0.71	15/65568 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	291	PHE	CE1-CZ	-8.24	1.21	1.37
1	C	291	PHE	CD1-CE1	-5.88	1.27	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	PHE	CB-CG-CD1	-6.34	116.36	120.80
1	G	484	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	J	546	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	291	PHE	CB-CG-CD2	5.71	124.79	120.80
1	L	546	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	484	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	H	131	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	K	305	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	305	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	484	ARG	NE-CZ-NH1	5.31	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	546	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	F	291	PHE	CB-CG-CD1	-5.14	117.20	120.80
1	I	546	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	546	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	G	291	PHE	CB-CG-CD1	-5.01	117.30	120.80

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	3948	0	3832	43	0
1	B	3948	0	3832	52	0
1	C	3948	0	3832	63	2
1	D	3948	0	3832	55	1
1	E	3948	0	3832	48	0
1	F	3948	0	3832	45	0
1	G	3948	0	3832	44	0
1	H	3948	0	3832	44	0
1	I	3948	0	3832	68	0
1	J	3948	0	3832	42	0
1	K	3948	0	3832	45	1
1	L	3948	0	3832	47	0
All	All	47376	0	45984	524	2

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 (524) 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:C:291:PHE:HZ	1:I:26:ASN:N	1.74	0.85
1:C:291:PHE:CZ	1:I:25:SER:HB2	2.22	0.74
1:L:312:GLU:OE2	1:L:484:ARG:NH1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:TYR:N	1:F:331:ASN:OD1	2.24	0.71
1:F:32:TYR:OH	1:F:559:GLU:OE2	2.09	0.70
1:D:312:GLU:OE2	1:D:484:ARG:NH1	2.24	0.70
1:E:312:GLU:OE2	1:E:484:ARG:NH1	2.25	0.70
1:A:286:TYR:N	1:A:331:ASN:OD1	2.26	0.69
1:C:286:TYR:N	1:C:331:ASN:OD1	2.26	0.68
1:B:358:ASN:HB2	1:I:36:LYS:CA	2.23	0.68
1:C:291:PHE:CZ	1:I:25:SER:C	2.67	0.68
1:E:286:TYR:N	1:E:331:ASN:OD1	2.28	0.67
1:K:286:TYR:N	1:K:331:ASN:OD1	2.27	0.67
1:B:358:ASN:HB2	1:I:36:LYS:N	2.10	0.67
1:H:312:GLU:OE2	1:H:484:ARG:NH1	2.28	0.67
1:H:286:TYR:N	1:H:331:ASN:OD1	2.28	0.66
1:C:291:PHE:CZ	1:I:26:ASN:N	2.61	0.65
1:L:286:TYR:N	1:L:331:ASN:OD1	2.29	0.65
1:C:291:PHE:CE1	1:I:25:SER:HB2	2.31	0.65
1:J:286:TYR:N	1:J:331:ASN:OD1	2.30	0.64
1:G:286:TYR:N	1:G:331:ASN:OD1	2.31	0.64
1:F:312:GLU:OE2	1:F:484:ARG:NH1	2.31	0.64
1:D:233:GLN:NE2	1:D:380:VAL:HG22	2.13	0.63
1:I:286:TYR:N	1:I:331:ASN:OD1	2.30	0.63
1:D:286:TYR:N	1:D:331:ASN:OD1	2.31	0.63
1:A:491:ASP:OD2	1:F:142:ASN:ND2	2.32	0.63
1:F:69:GLU:HA	1:F:103:CYS:SG	2.38	0.63
1:A:312:GLU:OE2	1:A:484:ARG:NH1	2.32	0.63
1:F:233:GLN:NE2	1:F:380:VAL:HG22	2.13	0.62
1:B:286:TYR:N	1:B:331:ASN:OD1	2.32	0.62
1:D:356:ARG:NH2	1:E:487:ARG:O	2.32	0.62
1:A:69:GLU:HA	1:A:103:CYS:SG	2.40	0.62
1:A:142:ASN:ND2	1:B:491:ASP:OD2	2.31	0.62
1:G:233:GLN:NE2	1:G:380:VAL:HG22	2.14	0.62
1:I:312:GLU:OE2	1:I:484:ARG:NH1	2.33	0.62
1:H:69:GLU:O	1:H:71:LEU:N	2.32	0.62
1:B:312:GLU:OE2	1:B:484:ARG:NH1	2.32	0.62
1:C:291:PHE:CZ	1:I:25:SER:CB	2.82	0.62
1:D:142:ASN:ND2	1:E:491:ASP:OD2	2.33	0.62
1:H:233:GLN:NE2	1:H:380:VAL:HG22	2.15	0.62
1:C:291:PHE:CE2	1:I:25:SER:OG	2.48	0.61
1:K:312:GLU:OE2	1:K:484:ARG:NH1	2.32	0.61
1:C:291:PHE:CD2	1:I:27:GLU:HG2	2.34	0.61
1:B:26:ASN:OD1	1:B:29:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:GLU:OE2	1:C:484:ARG:NH1	2.34	0.61
1:J:233:GLN:NE2	1:J:380:VAL:HG22	2.15	0.61
1:E:26:ASN:OD1	1:E:29:ARG:NH1	2.34	0.61
1:I:233:GLN:NE2	1:I:380:VAL:HG22	2.16	0.61
1:I:356:ARG:NH2	1:J:487:ARG:O	2.34	0.61
1:E:69:GLU:HA	1:E:103:CYS:SG	2.41	0.61
1:A:69:GLU:O	1:A:71:LEU:N	2.34	0.61
1:D:204:ILE:HD13	1:E:468:VAL:HG21	1.83	0.61
1:K:69:GLU:O	1:K:71:LEU:N	2.34	0.60
1:E:233:GLN:NE2	1:E:380:VAL:HG22	2.15	0.60
1:A:233:GLN:NE2	1:A:380:VAL:HG22	2.16	0.60
1:G:69:GLU:O	1:G:71:LEU:N	2.35	0.60
1:J:69:GLU:O	1:J:71:LEU:N	2.33	0.60
1:J:312:GLU:OE2	1:J:484:ARG:NH1	2.35	0.60
1:B:358:ASN:HB2	1:I:36:LYS:HA	1.82	0.59
1:J:26:ASN:OD1	1:J:29:ARG:NH1	2.35	0.59
1:F:26:ASN:OD1	1:F:29:ARG:NH1	2.35	0.59
1:L:32:TYR:OH	1:L:559:GLU:OE2	2.21	0.59
1:D:69:GLU:O	1:D:71:LEU:N	2.35	0.59
1:G:312:GLU:OE2	1:G:484:ARG:NH1	2.36	0.59
1:J:142:ASN:ND2	1:K:491:ASP:OD2	2.35	0.59
1:C:291:PHE:HZ	1:I:26:ASN:CA	2.15	0.59
1:E:69:GLU:O	1:E:71:LEU:N	2.35	0.59
1:A:26:ASN:OD1	1:A:29:ARG:NH1	2.36	0.59
1:L:233:GLN:NE2	1:L:380:VAL:HG22	2.17	0.59
1:L:69:GLU:O	1:L:71:LEU:N	2.35	0.59
1:C:69:GLU:HA	1:C:103:CYS:SG	2.44	0.58
1:A:16:ASN:HB2	1:F:531:ILE:HD13	1.85	0.58
1:G:142:ASN:ND2	1:H:491:ASP:OD2	2.36	0.58
1:D:133:HIS:CE1	1:D:504:GLY:HA2	2.39	0.58
1:K:233:GLN:NE2	1:K:380:VAL:HG22	2.19	0.57
1:C:291:PHE:CE2	1:I:25:SER:CB	2.88	0.57
1:H:142:ASN:ND2	1:I:491:ASP:OD2	2.38	0.57
1:A:32:TYR:OH	1:A:559:GLU:OE2	2.22	0.57
1:C:209:ASP:OD2	1:C:267:LYS:NZ	2.37	0.57
1:C:291:PHE:CD1	1:I:27:GLU:CD	2.78	0.57
1:G:491:ASP:OD2	1:L:142:ASN:ND2	2.38	0.57
1:A:288:SER:O	1:A:292:THR:OG1	2.22	0.57
1:K:32:TYR:OH	1:K:559:GLU:OE2	2.22	0.57
1:B:69:GLU:O	1:B:71:LEU:N	2.38	0.56
1:G:69:GLU:HA	1:G:103:CYS:SG	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:TYR:OH	1:C:559:GLU:OE2	2.22	0.56
1:G:26:ASN:OD1	1:G:29:ARG:NH1	2.37	0.56
1:I:32:TYR:OH	1:I:559:GLU:OE2	2.23	0.56
1:K:69:GLU:HA	1:K:103:CYS:SG	2.45	0.56
1:C:291:PHE:CZ	1:I:27:GLU:N	2.73	0.56
1:F:69:GLU:O	1:F:71:LEU:N	2.39	0.56
1:C:69:GLU:O	1:C:71:LEU:N	2.37	0.56
1:D:26:ASN:OD1	1:D:29:ARG:NH1	2.39	0.56
1:K:209:ASP:OD2	1:K:267:LYS:NZ	2.38	0.56
1:C:142:ASN:ND2	1:D:491:ASP:OD2	2.39	0.56
1:D:69:GLU:HA	1:D:103:CYS:SG	2.45	0.55
1:C:288:SER:HA	1:I:27:GLU:OE2	2.06	0.55
1:I:23:PHE:CD2	1:I:29:ARG:HB2	2.41	0.55
1:I:26:ASN:OD1	1:I:29:ARG:NH1	2.39	0.55
1:C:13:PRO:O	1:C:15:ASN:ND2	2.40	0.55
1:D:227:THR:HA	1:D:233:GLN:HE22	1.71	0.55
1:C:352:ASN:OD1	1:C:352:ASN:N	2.39	0.55
1:J:209:ASP:OD2	1:J:267:LYS:NZ	2.40	0.55
1:E:32:TYR:OH	1:E:559:GLU:OE2	2.23	0.55
1:I:133:HIS:CE1	1:I:504:GLY:HA2	2.42	0.55
1:K:26:ASN:OD1	1:K:29:ARG:NH1	2.39	0.55
1:B:288:SER:O	1:B:292:THR:OG1	2.25	0.55
1:C:119:ASN:O	1:C:119:ASN:ND2	2.40	0.55
1:B:209:ASP:OD2	1:B:267:LYS:NZ	2.39	0.54
1:B:233:GLN:NE2	1:B:380:VAL:HG22	2.21	0.54
1:I:288:SER:O	1:I:292:THR:OG1	2.24	0.54
1:L:69:GLU:HA	1:L:103:CYS:SG	2.48	0.54
1:L:209:ASP:OD2	1:L:267:LYS:NZ	2.41	0.54
1:F:502:MET:O	1:F:554:ARG:NH1	2.41	0.54
1:A:227:THR:HA	1:A:233:GLN:HE22	1.73	0.54
1:J:69:GLU:HA	1:J:103:CYS:SG	2.48	0.54
1:H:37:PHE:CZ	1:H:40:HIS:O	2.61	0.54
1:B:37:PHE:CZ	1:B:40:HIS:O	2.61	0.54
1:B:69:GLU:HA	1:B:103:CYS:SG	2.48	0.54
1:I:119:ASN:O	1:I:119:ASN:ND2	2.41	0.54
1:C:37:PHE:CZ	1:C:40:HIS:O	2.61	0.54
1:H:209:ASP:OD2	1:H:267:LYS:NZ	2.41	0.54
1:K:175:LEU:HD13	1:K:177:ILE:HG23	1.90	0.53
1:B:227:THR:HA	1:B:233:GLN:HE22	1.73	0.53
1:E:119:ASN:O	1:E:119:ASN:ND2	2.41	0.53
1:I:69:GLU:HA	1:I:103:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:PHE:CZ	1:L:40:HIS:O	2.62	0.53
1:C:233:GLN:NE2	1:C:380:VAL:HG22	2.23	0.53
1:H:69:GLU:HA	1:H:103:CYS:SG	2.48	0.53
1:K:288:SER:O	1:K:292:THR:OG1	2.27	0.53
1:K:37:PHE:CZ	1:K:40:HIS:O	2.61	0.53
1:B:119:ASN:ND2	1:B:119:ASN:O	2.42	0.53
1:H:32:TYR:OH	1:H:559:GLU:OE2	2.24	0.53
1:H:23:PHE:CD2	1:H:29:ARG:HB2	2.44	0.53
1:H:26:ASN:OD1	1:H:29:ARG:NH1	2.41	0.53
1:E:209:ASP:OD2	1:E:267:LYS:NZ	2.41	0.53
1:D:288:SER:O	1:D:292:THR:OG1	2.27	0.52
1:A:209:ASP:OD2	1:A:267:LYS:NZ	2.42	0.52
1:J:32:TYR:OH	1:J:559:GLU:OE2	2.26	0.52
1:C:26:ASN:OD1	1:C:29:ARG:NH1	2.42	0.52
1:A:13:PRO:O	1:A:15:ASN:ND2	2.42	0.52
1:L:26:ASN:OD1	1:L:29:ARG:NH1	2.42	0.52
1:J:133:HIS:CE1	1:J:504:GLY:HA2	2.44	0.52
1:G:209:ASP:OD2	1:G:267:LYS:NZ	2.42	0.52
1:I:69:GLU:O	1:I:71:LEU:N	2.42	0.52
1:I:142:ASN:ND2	1:J:491:ASP:OD2	2.42	0.52
1:J:288:SER:O	1:J:292:THR:OG1	2.27	0.52
1:L:134:TYR:CE2	1:L:142:ASN:HB2	2.45	0.52
1:G:37:PHE:CZ	1:G:40:HIS:O	2.62	0.52
1:H:119:ASN:O	1:H:119:ASN:ND2	2.43	0.52
1:G:288:SER:O	1:G:292:THR:OG1	2.28	0.51
1:H:133:HIS:CE1	1:H:504:GLY:HA2	2.45	0.51
1:D:32:TYR:OH	1:D:559:GLU:OE2	2.24	0.51
1:H:531:ILE:HD13	1:I:16:ASN:HB2	1.92	0.51
1:H:12:THR:HG21	1:H:76:TYR:HB2	1.93	0.51
1:J:531:ILE:HD13	1:K:16:ASN:HB2	1.91	0.51
1:C:133:HIS:CE1	1:C:504:GLY:HA2	2.45	0.51
1:E:288:SER:O	1:E:292:THR:OG1	2.28	0.51
1:J:356:ARG:NH2	1:K:487:ARG:O	2.43	0.51
1:L:119:ASN:ND2	1:L:119:ASN:O	2.44	0.51
1:D:134:TYR:CE2	1:D:142:ASN:HB2	2.46	0.51
1:F:119:ASN:O	1:F:119:ASN:ND2	2.44	0.51
1:F:133:HIS:CE1	1:F:504:GLY:HA2	2.45	0.51
1:H:288:SER:O	1:H:292:THR:OG1	2.28	0.51
1:B:133:HIS:CE1	1:B:504:GLY:HA2	2.46	0.51
1:F:38:ASP:OD1	1:F:38:ASP:N	2.44	0.51
1:G:227:THR:HA	1:G:233:GLN:HE22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:ASN:HB2	1:L:531:ILE:HD13	1.91	0.51
1:G:119:ASN:ND2	1:G:119:ASN:O	2.43	0.51
1:I:37:PHE:CZ	1:I:40:HIS:O	2.64	0.51
1:E:23:PHE:CD2	1:E:29:ARG:HB2	2.45	0.51
1:E:142:ASN:ND2	1:F:491:ASP:OD2	2.44	0.51
1:E:133:HIS:CE1	1:E:504:GLY:HA2	2.46	0.51
1:I:209:ASP:OD2	1:I:267:LYS:NZ	2.44	0.50
1:K:142:ASN:ND2	1:L:491:ASP:OD2	2.44	0.50
1:C:470:TYR:HB3	1:C:479:PHE:CD1	2.46	0.50
1:D:60:ASP:HB3	1:D:102:VAL:HG22	1.93	0.50
1:F:288:SER:O	1:F:292:THR:OG1	2.29	0.50
1:G:32:TYR:OH	1:G:559:GLU:OE2	2.26	0.50
1:H:227:THR:HA	1:H:233:GLN:HE22	1.76	0.50
1:K:352:ASN:OD1	1:K:352:ASN:N	2.44	0.50
1:F:23:PHE:CD2	1:F:29:ARG:HB2	2.46	0.50
1:J:227:THR:HA	1:J:233:GLN:HE22	1.77	0.50
1:D:209:ASP:OD2	1:D:267:LYS:NZ	2.45	0.50
1:D:37:PHE:CZ	1:D:40:HIS:O	2.64	0.50
1:F:209:ASP:OD2	1:F:267:LYS:NZ	2.44	0.50
1:B:32:TYR:OH	1:B:559:GLU:OE2	2.28	0.50
1:F:37:PHE:CZ	1:F:40:HIS:O	2.65	0.50
1:E:227:THR:HA	1:E:233:GLN:HE22	1.76	0.50
1:C:291:PHE:CE1	1:I:27:GLU:OE1	2.65	0.50
1:I:531:ILE:HD13	1:J:16:ASN:HB2	1.94	0.50
1:J:23:PHE:CD2	1:J:29:ARG:HB2	2.47	0.50
1:A:487:ARG:O	1:F:356:ARG:NH2	2.45	0.49
1:K:23:PHE:CD2	1:K:29:ARG:HB2	2.47	0.49
1:A:119:ASN:O	1:A:119:ASN:ND2	2.45	0.49
1:D:13:PRO:O	1:D:15:ASN:ND2	2.45	0.49
1:L:288:SER:O	1:L:292:THR:OG1	2.30	0.49
1:J:119:ASN:ND2	1:J:119:ASN:O	2.45	0.49
1:C:531:ILE:HD13	1:D:16:ASN:HB2	1.94	0.49
1:H:13:PRO:O	1:H:15:ASN:ND2	2.46	0.49
1:J:13:PRO:O	1:J:15:ASN:ND2	2.46	0.49
1:F:12:THR:HG21	1:F:76:TYR:HB2	1.93	0.49
1:G:23:PHE:CD2	1:G:29:ARG:HB2	2.46	0.49
1:K:134:TYR:CE2	1:K:142:ASN:HB2	2.47	0.49
1:D:23:PHE:CD2	1:D:29:ARG:HB2	2.47	0.49
1:L:133:HIS:CE1	1:L:504:GLY:HA2	2.47	0.49
1:L:23:PHE:CD2	1:L:29:ARG:HB2	2.47	0.49
1:K:12:THR:HG21	1:K:76:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:CZ	1:A:40:HIS:O	2.66	0.49
1:B:470:TYR:HB3	1:B:479:PHE:CD1	2.48	0.49
1:C:291:PHE:CE2	1:I:27:GLU:N	2.81	0.49
1:B:124:LEU:HD22	1:B:532:TRP:HB2	1.94	0.49
1:E:134:TYR:CE2	1:E:142:ASN:HB2	2.48	0.49
1:G:124:LEU:HD22	1:G:532:TRP:HB2	1.94	0.49
1:J:12:THR:HG21	1:J:76:TYR:HB2	1.95	0.49
1:K:119:ASN:O	1:K:119:ASN:ND2	2.46	0.49
1:K:227:THR:HA	1:K:233:GLN:HE22	1.78	0.48
1:L:38:ASP:OD1	1:L:38:ASP:N	2.46	0.48
1:I:13:PRO:O	1:I:15:ASN:ND2	2.46	0.48
1:A:133:HIS:CE1	1:A:504:GLY:HA2	2.48	0.48
1:B:352:ASN:OD1	1:B:352:ASN:N	2.43	0.48
1:A:212:TRP:CZ3	1:A:247:ILE:HG13	2.48	0.48
1:C:337:PHE:CE2	1:D:476:GLN:HG3	2.49	0.48
1:E:124:LEU:HD22	1:E:532:TRP:HB2	1.96	0.48
1:E:12:THR:HG21	1:E:76:TYR:HB2	1.96	0.48
1:F:59:ILE:HG12	1:F:60:ASP:N	2.29	0.48
1:A:502:MET:O	1:A:554:ARG:NH1	2.47	0.48
1:B:12:THR:HG21	1:B:76:TYR:HB2	1.96	0.48
1:J:314:THR:HG21	1:J:484:ARG:NH2	2.28	0.48
1:K:356:ARG:NH2	1:L:487:ARG:O	2.47	0.48
1:F:227:THR:HA	1:F:233:GLN:HE22	1.78	0.48
1:G:133:HIS:CE1	1:G:504:GLY:HA2	2.49	0.48
1:H:502:MET:O	1:H:554:ARG:NH1	2.45	0.48
1:I:33:PHE:C	1:I:35:SER:H	2.17	0.48
1:A:204:ILE:HD13	1:B:468:VAL:HG21	1.95	0.48
1:E:37:PHE:CZ	1:E:40:HIS:O	2.66	0.48
1:I:227:THR:HA	1:I:233:GLN:HE22	1.78	0.48
1:D:352:ASN:N	1:D:352:ASN:OD1	2.46	0.47
1:G:356:ARG:NH2	1:H:487:ARG:O	2.47	0.47
1:K:133:HIS:CE1	1:K:504:GLY:HA2	2.49	0.47
1:D:212:TRP:CZ3	1:D:247:ILE:HG13	2.49	0.47
1:F:212:TRP:CZ3	1:F:247:ILE:HG13	2.49	0.47
1:I:12:THR:HG21	1:I:76:TYR:HB2	1.97	0.47
1:L:12:THR:HG21	1:L:76:TYR:HB2	1.96	0.47
1:B:212:TRP:CZ3	1:B:247:ILE:HG13	2.50	0.47
1:J:38:ASP:N	1:J:38:ASP:OD1	2.48	0.47
1:E:352:ASN:N	1:E:352:ASN:OD1	2.46	0.47
1:E:38:ASP:N	1:E:38:ASP:OD1	2.48	0.47
1:L:227:THR:HA	1:L:233:GLN:HE22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:TRP:CZ3	1:C:247:ILE:HG13	2.49	0.47
1:D:119:ASN:ND2	1:D:119:ASN:O	2.47	0.47
1:E:202:ASP:OD2	1:E:274:SER:OG	2.31	0.47
1:G:13:PRO:O	1:G:15:ASN:ND2	2.48	0.47
1:K:470:TYR:HB3	1:K:479:PHE:CD1	2.49	0.47
1:B:23:PHE:CD2	1:B:29:ARG:HB2	2.49	0.47
1:B:38:ASP:OD1	1:B:38:ASP:N	2.48	0.47
1:F:175:LEU:HD13	1:F:177:ILE:HG23	1.96	0.47
1:E:356:ARG:NH2	1:F:487:ARG:O	2.47	0.47
1:G:531:ILE:HD13	1:H:16:ASN:HB2	1.97	0.47
1:E:282:ILE:HG23	1:E:334:PHE:CD2	2.50	0.47
1:F:282:ILE:HG23	1:F:334:PHE:CD2	2.50	0.47
1:F:134:TYR:CE2	1:F:142:ASN:HB2	2.50	0.47
1:A:23:PHE:CD2	1:A:29:ARG:HB2	2.49	0.47
1:I:134:TYR:CE2	1:I:142:ASN:HB2	2.49	0.47
1:I:38:ASP:N	1:I:38:ASP:OD1	2.48	0.47
1:K:13:PRO:O	1:K:15:ASN:ND2	2.47	0.47
1:C:291:PHE:CE2	1:I:25:SER:C	2.88	0.47
1:C:502:MET:O	1:C:554:ARG:NH1	2.46	0.47
1:A:352:ASN:OD1	1:A:352:ASN:N	2.46	0.46
1:A:60:ASP:HB3	1:A:102:VAL:HG22	1.97	0.46
1:H:356:ARG:NH2	1:I:487:ARG:O	2.47	0.46
1:I:23:PHE:CG	1:I:29:ARG:HB2	2.49	0.46
1:I:212:TRP:CZ3	1:I:247:ILE:HG13	2.50	0.46
1:A:531:ILE:HD11	1:B:15:ASN:OD1	2.15	0.46
1:C:12:THR:HG21	1:C:76:TYR:HB2	1.98	0.46
1:H:38:ASP:OD1	1:H:38:ASP:N	2.48	0.46
1:A:12:THR:HG21	1:A:76:TYR:HB2	1.97	0.46
1:E:112:VAL:HG11	1:E:553:VAL:HG11	1.98	0.46
1:J:60:ASP:HB3	1:J:102:VAL:HG22	1.96	0.46
1:E:502:MET:O	1:E:554:ARG:NH1	2.48	0.46
1:G:134:TYR:CE2	1:G:142:ASN:HB2	2.51	0.46
1:H:134:TYR:OH	1:H:507:CYS:SG	2.73	0.46
1:I:282:ILE:HG23	1:I:334:PHE:CD2	2.51	0.46
1:J:352:ASN:N	1:J:352:ASN:OD1	2.48	0.46
1:L:352:ASN:N	1:L:352:ASN:OD1	2.49	0.46
1:K:502:MET:O	1:K:554:ARG:NH1	2.47	0.46
1:K:71:LEU:HD21	1:K:95:ILE:HG21	1.97	0.46
1:C:175:LEU:HD13	1:C:177:ILE:HG23	1.97	0.46
1:E:174:ILE:HG13	1:E:174:ILE:O	2.15	0.46
1:L:13:PRO:O	1:L:15:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:TYR:CE2	1:C:142:ASN:HB2	2.50	0.46
1:C:71:LEU:HD21	1:C:95:ILE:HG21	1.97	0.46
1:G:212:TRP:CZ3	1:G:247:ILE:HG13	2.51	0.46
1:L:124:LEU:HD22	1:L:532:TRP:HB2	1.97	0.46
1:G:174:ILE:O	1:G:174:ILE:HG13	2.16	0.46
1:B:13:PRO:O	1:B:15:ASN:ND2	2.48	0.45
1:C:291:PHE:HE2	1:I:28:GLU:H	1.64	0.45
1:L:71:LEU:HD21	1:L:95:ILE:HG21	1.98	0.45
1:C:356:ARG:NH2	1:D:487:ARG:O	2.48	0.45
1:E:60:ASP:HB3	1:E:102:VAL:HG22	1.98	0.45
1:F:352:ASN:OD1	1:F:352:ASN:N	2.46	0.45
1:H:124:LEU:HD22	1:H:532:TRP:HB2	1.99	0.45
1:I:352:ASN:OD1	1:I:352:ASN:N	2.48	0.45
1:A:282:ILE:HG23	1:A:334:PHE:CD2	2.51	0.45
1:F:13:PRO:O	1:F:15:ASN:ND2	2.49	0.45
1:B:134:TYR:CE2	1:B:142:ASN:HB2	2.52	0.45
1:C:38:ASP:N	1:C:38:ASP:OD1	2.49	0.45
1:D:38:ASP:OD1	1:D:38:ASP:N	2.50	0.45
1:H:134:TYR:CE2	1:H:142:ASN:HB2	2.52	0.45
1:F:124:LEU:HD22	1:F:532:TRP:HB2	1.98	0.45
1:K:60:ASP:HB3	1:K:102:VAL:HG22	1.98	0.45
1:C:111:VAL:CG2	1:C:545:LEU:HD13	2.47	0.45
1:D:531:ILE:HD11	1:E:15:ASN:OD1	2.17	0.45
1:F:470:TYR:HB3	1:F:479:PHE:CD1	2.51	0.45
1:J:212:TRP:CZ3	1:J:247:ILE:HG13	2.52	0.45
1:K:124:LEU:HD22	1:K:532:TRP:HB2	1.99	0.45
1:H:352:ASN:OD1	1:H:352:ASN:N	2.48	0.45
1:K:212:TRP:CZ3	1:K:247:ILE:HG13	2.52	0.45
1:F:60:ASP:HB3	1:F:102:VAL:HG22	1.99	0.45
1:K:531:ILE:HD13	1:L:16:ASN:HB2	1.99	0.45
1:C:174:ILE:O	1:C:174:ILE:HG13	2.17	0.45
1:E:212:TRP:CZ3	1:E:247:ILE:HG13	2.51	0.45
1:G:352:ASN:N	1:G:352:ASN:OD1	2.49	0.45
1:C:23:PHE:CD2	1:C:29:ARG:HB2	2.52	0.45
1:D:572:ILE:O	1:D:573:ILE:CG1	2.65	0.45
1:G:112:VAL:HG11	1:G:553:VAL:HG11	1.99	0.45
1:F:33:PHE:C	1:F:35:SER:H	2.21	0.44
1:A:124:LEU:HD22	1:A:532:TRP:HB2	1.99	0.44
1:C:470:TYR:CG	1:C:479:PHE:CE1	3.05	0.44
1:D:12:THR:HG21	1:D:76:TYR:HB2	1.99	0.44
1:D:175:LEU:HD13	1:D:177:ILE:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:TYR:O	1:D:85:ASN:N	2.50	0.44
1:E:13:PRO:O	1:E:15:ASN:ND2	2.50	0.44
1:H:470:TYR:HB3	1:H:479:PHE:CD1	2.52	0.44
1:L:60:ASP:HB3	1:L:102:VAL:HG22	1.98	0.44
1:C:60:ASP:HB3	1:C:102:VAL:HG22	2.00	0.44
1:D:33:PHE:O	1:D:35:SER:N	2.50	0.44
1:G:12:THR:HG21	1:G:76:TYR:HB2	1.99	0.44
1:H:212:TRP:CZ3	1:H:247:ILE:HG13	2.52	0.44
1:L:175:LEU:HD13	1:L:177:ILE:HG23	1.99	0.44
1:A:356:ARG:NH2	1:B:487:ARG:O	2.48	0.44
1:B:60:ASP:HB3	1:B:102:VAL:HG22	2.00	0.44
1:I:470:TYR:HB3	1:I:479:PHE:CD1	2.52	0.44
1:I:59:ILE:HG12	1:I:60:ASP:N	2.32	0.44
1:B:71:LEU:HD21	1:B:95:ILE:HG21	1.99	0.44
1:B:358:ASN:C	1:I:35:SER:HA	2.38	0.44
1:J:134:TYR:CE2	1:J:142:ASN:HB2	2.52	0.44
1:D:124:LEU:HD22	1:D:532:TRP:HB2	1.99	0.44
1:G:38:ASP:N	1:G:38:ASP:OD1	2.50	0.44
1:I:112:VAL:HG11	1:I:553:VAL:HG11	1.99	0.44
1:J:124:LEU:HD22	1:J:532:TRP:HB2	1.99	0.44
1:C:124:LEU:HD22	1:C:532:TRP:HB2	1.99	0.44
1:C:572:ILE:O	1:C:573:ILE:CG1	2.66	0.44
1:E:42:PHE:CE1	1:E:59:ILE:HD12	2.53	0.44
1:F:23:PHE:CG	1:F:29:ARG:HB2	2.53	0.44
1:F:71:LEU:HD21	1:F:95:ILE:HG21	1.99	0.44
1:I:71:LEU:HD21	1:I:95:ILE:HG21	1.98	0.44
1:D:174:ILE:O	1:D:174:ILE:HG13	2.17	0.44
1:A:38:ASP:N	1:A:38:ASP:OD1	2.51	0.44
1:E:470:TYR:HB3	1:E:479:PHE:CD1	2.53	0.44
1:B:356:ARG:NH2	1:C:487:ARG:O	2.51	0.43
1:I:124:LEU:HD22	1:I:532:TRP:HB2	2.00	0.43
1:J:502:MET:O	1:J:554:ARG:NH1	2.51	0.43
1:K:23:PHE:CG	1:K:29:ARG:HB2	2.53	0.43
1:L:572:ILE:O	1:L:573:ILE:CG1	2.66	0.43
1:H:174:ILE:O	1:H:174:ILE:HG13	2.19	0.43
1:A:546:ARG:CZ	1:B:15:ASN:OD1	2.66	0.43
1:D:33:PHE:C	1:D:35:SER:H	2.21	0.43
1:G:42:PHE:CE1	1:G:59:ILE:HD12	2.53	0.43
1:L:212:TRP:CZ3	1:L:247:ILE:HG13	2.53	0.43
1:K:38:ASP:OD1	1:K:38:ASP:N	2.51	0.43
1:A:134:TYR:CE2	1:A:142:ASN:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:572:ILE:O	1:F:573:ILE:CG1	2.67	0.43
1:A:531:ILE:HD13	1:B:16:ASN:HB2	2.00	0.43
1:B:23:PHE:CG	1:B:29:ARG:HB2	2.54	0.43
1:F:134:TYR:OH	1:F:507:CYS:SG	2.75	0.43
1:J:23:PHE:CG	1:J:29:ARG:HB2	2.54	0.43
1:L:111:VAL:CG2	1:L:545:LEU:HD13	2.49	0.43
1:B:333:GLU:OE1	1:B:351:LYS:NZ	2.52	0.43
1:J:175:LEU:HD13	1:J:177:ILE:HG23	2.00	0.43
1:B:142:ASN:ND2	1:C:491:ASP:OD2	2.51	0.43
1:H:23:PHE:CG	1:H:29:ARG:HB2	2.53	0.43
1:I:175:LEU:HD13	1:I:177:ILE:HG23	2.01	0.43
1:J:71:LEU:HD21	1:J:95:ILE:HG21	1.99	0.43
1:L:314:THR:HG21	1:L:484:ARG:NH2	2.34	0.43
1:E:175:LEU:HD13	1:E:177:ILE:HG23	2.01	0.43
1:G:197:SER:OG	1:G:267:LYS:NZ	2.39	0.43
1:L:59:ILE:HG12	1:L:60:ASP:N	2.34	0.43
1:C:313:LEU:HB3	1:C:368:LEU:HD22	2.01	0.43
1:G:175:LEU:HD13	1:G:177:ILE:HG23	2.01	0.43
1:G:502:MET:O	1:G:554:ARG:NH1	2.50	0.43
1:J:572:ILE:O	1:J:573:ILE:CG1	2.67	0.43
1:J:572:ILE:O	1:J:573:ILE:HG13	2.18	0.43
1:B:227:THR:HA	1:B:233:GLN:NE2	2.34	0.42
1:D:282:ILE:HG23	1:D:334:PHE:CD2	2.54	0.42
1:H:59:ILE:HG12	1:H:60:ASP:N	2.34	0.42
1:I:572:ILE:O	1:I:573:ILE:CG1	2.67	0.42
1:C:227:THR:HA	1:C:233:GLN:HE22	1.84	0.42
1:E:71:LEU:HD21	1:E:95:ILE:HG21	2.01	0.42
1:G:531:ILE:HD11	1:H:15:ASN:OD1	2.19	0.42
1:H:282:ILE:HG23	1:H:334:PHE:CD2	2.55	0.42
1:H:42:PHE:CE1	1:H:59:ILE:HD12	2.54	0.42
1:J:282:ILE:HG23	1:J:334:PHE:CD2	2.53	0.42
1:J:134:TYR:OH	1:J:507:CYS:SG	2.76	0.42
1:D:42:PHE:CE1	1:D:59:ILE:HD12	2.55	0.42
1:E:59:ILE:HG12	1:E:60:ASP:N	2.34	0.42
1:I:33:PHE:O	1:I:35:SER:N	2.52	0.42
1:I:502:MET:O	1:I:554:ARG:NH1	2.51	0.42
1:L:502:MET:O	1:L:554:ARG:NH1	2.50	0.42
1:A:175:LEU:HD13	1:A:177:ILE:HG23	2.02	0.42
1:A:65:ARG:HG2	1:A:66:SER:N	2.33	0.42
1:E:23:PHE:CG	1:E:29:ARG:HB2	2.55	0.42
1:J:470:TYR:HB3	1:J:479:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:TYR:HB3	1:A:479:PHE:CD1	2.54	0.42
1:D:531:ILE:HA	1:D:531:ILE:HD12	1.93	0.42
1:F:16:ASN:OD1	1:F:19:ASN:N	2.52	0.42
1:G:60:ASP:HB3	1:G:102:VAL:HG22	2.01	0.42
1:A:71:LEU:HD21	1:A:95:ILE:HG21	2.01	0.42
1:F:111:VAL:CG2	1:F:545:LEU:HD13	2.49	0.42
1:I:60:ASP:HB3	1:I:102:VAL:HG22	2.00	0.42
1:C:291:PHE:CD1	1:I:27:GLU:OE2	2.73	0.42
1:J:204:ILE:HD13	1:K:468:VAL:HG21	2.01	0.42
1:A:510:TYR:HB3	1:B:502:MET:CE	2.50	0.42
1:C:112:VAL:HG11	1:C:553:VAL:HG11	2.01	0.42
1:D:112:VAL:HG11	1:D:553:VAL:HG11	2.01	0.42
1:F:33:PHE:O	1:F:35:SER:N	2.53	0.42
1:G:202:ASP:OD2	1:G:274:SER:OG	2.37	0.42
1:G:65:ARG:HG2	1:G:66:SER:N	2.35	0.42
1:G:71:LEU:HD21	1:G:95:ILE:HG21	2.02	0.42
1:K:204:ILE:HD13	1:L:468:VAL:HG21	2.01	0.42
1:B:175:LEU:HD13	1:B:177:ILE:HG23	2.02	0.42
1:G:572:ILE:O	1:G:573:ILE:CG1	2.68	0.42
1:J:572:ILE:C	1:J:573:ILE:HG13	2.40	0.42
1:D:173:TYR:N	1:D:173:TYR:CD2	2.87	0.42
1:E:81:TYR:O	1:E:85:ASN:N	2.53	0.42
1:G:487:ARG:O	1:L:356:ARG:NH2	2.52	0.42
1:L:572:ILE:O	1:L:573:ILE:HG13	2.20	0.42
1:A:23:PHE:CG	1:A:29:ARG:HB2	2.55	0.41
1:B:59:ILE:HG12	1:B:60:ASP:N	2.35	0.41
1:C:539:THR:HG23	1:D:94:ASP:HA	2.01	0.41
1:D:16:ASN:OD1	1:D:19:ASN:N	2.53	0.41
1:D:470:TYR:HB3	1:D:479:PHE:CD1	2.54	0.41
1:D:65:ARG:HG2	1:D:66:SER:N	2.34	0.41
1:I:111:VAL:CG2	1:I:545:LEU:HD13	2.50	0.41
1:K:33:PHE:O	1:K:35:SER:N	2.53	0.41
1:K:59:ILE:HG12	1:K:60:ASP:N	2.35	0.41
1:B:112:VAL:HG11	1:B:553:VAL:HG11	2.02	0.41
1:C:59:ILE:HG12	1:C:60:ASP:N	2.35	0.41
1:H:572:ILE:O	1:H:573:ILE:CG1	2.68	0.41
1:H:71:LEU:HD21	1:H:95:ILE:HG21	2.02	0.41
1:I:144:GLU:OE1	1:I:356:ARG:NH1	2.53	0.41
1:K:531:ILE:HD11	1:L:15:ASN:OD1	2.19	0.41
1:A:73:GLY:HA3	1:F:536:ASN:HA	2.02	0.41
1:I:333:GLU:OE1	1:I:351:LYS:NZ	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:PHE:CZ	1:J:40:HIS:O	2.73	0.41
1:L:33:PHE:O	1:L:35:SER:N	2.54	0.41
1:A:12:THR:HG23	1:A:14:PHE:N	2.35	0.41
1:D:143:LEU:HA	1:D:146:ILE:HG22	2.03	0.41
1:E:531:ILE:HD13	1:F:16:ASN:HB2	2.01	0.41
1:I:8:LEU:HD22	1:I:74:VAL:HG21	2.03	0.41
1:L:23:PHE:CG	1:L:29:ARG:HB2	2.55	0.41
1:L:33:PHE:C	1:L:35:SER:H	2.23	0.41
1:L:112:VAL:HG11	1:L:553:VAL:HG11	2.02	0.41
1:B:65:ARG:HG2	1:B:66:SER:N	2.35	0.41
1:D:71:LEU:HD21	1:D:95:ILE:HG21	2.02	0.41
1:G:572:ILE:O	1:G:573:ILE:HG13	2.21	0.41
1:I:65:ARG:HG2	1:I:66:SER:N	2.35	0.41
1:D:572:ILE:C	1:D:573:ILE:HG13	2.41	0.41
1:H:121:LEU:HD13	1:H:517:ILE:HG12	2.02	0.41
1:H:175:LEU:HD13	1:H:177:ILE:HG23	2.01	0.41
1:I:81:TYR:O	1:I:85:ASN:N	2.53	0.41
1:J:65:ARG:HG2	1:J:66:SER:N	2.34	0.41
1:K:33:PHE:C	1:K:35:SER:H	2.23	0.41
1:L:143:LEU:HA	1:L:146:ILE:HG22	2.03	0.41
1:L:282:ILE:HG23	1:L:334:PHE:CD2	2.56	0.41
1:D:111:VAL:CG2	1:D:545:LEU:HD13	2.51	0.41
1:D:204:ILE:HD13	1:E:468:VAL:CG2	2.50	0.41
1:F:209:ASP:HB3	1:F:211:TYR:CE2	2.56	0.41
1:L:470:TYR:HB3	1:L:479:PHE:CD1	2.55	0.41
1:F:65:ARG:HG2	1:F:66:SER:N	2.36	0.41
1:G:515:SER:OG	1:G:516:ASP:N	2.54	0.41
1:K:111:VAL:CG2	1:K:545:LEU:HD13	2.51	0.41
1:K:112:VAL:HG11	1:K:553:VAL:HG11	2.02	0.41
1:B:42:PHE:CE1	1:B:59:ILE:HD12	2.56	0.41
1:C:282:ILE:HG23	1:C:334:PHE:CD2	2.56	0.41
1:A:572:ILE:O	1:A:573:ILE:CG1	2.68	0.41
1:E:33:PHE:O	1:E:35:SER:N	2.54	0.41
1:K:144:GLU:OE1	1:K:356:ARG:NH1	2.52	0.41
1:B:174:ILE:O	1:B:174:ILE:HG13	2.21	0.41
1:B:204:ILE:HD13	1:C:468:VAL:HG21	2.02	0.41
1:E:572:ILE:O	1:E:573:ILE:CG1	2.69	0.41
1:H:65:ARG:HG2	1:H:66:SER:N	2.35	0.41
1:J:532:TRP:CZ2	1:J:546:ARG:HA	2.56	0.41
1:K:532:TRP:CZ2	1:K:546:ARG:HA	2.56	0.41
1:K:572:ILE:O	1:K:573:ILE:CG1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:ARG:HG2	1:K:66:SER:N	2.36	0.41
1:L:572:ILE:C	1:L:573:ILE:HG13	2.41	0.41
1:D:197:SER:OG	1:D:267:LYS:NZ	2.42	0.40
1:D:208:TYR:HE2	1:E:463:ILE:HB	1.86	0.40
1:G:470:TYR:HB3	1:G:479:PHE:CD1	2.55	0.40
1:L:542:MET:HE2	1:L:545:LEU:HD23	2.02	0.40
1:B:81:TYR:O	1:B:85:ASN:N	2.54	0.40
1:C:185:PHE:CE2	1:C:259:ASN:HB2	2.56	0.40
1:D:144:GLU:OE1	1:D:356:ARG:NH1	2.54	0.40
1:G:33:PHE:C	1:G:35:SER:H	2.25	0.40
1:H:572:ILE:O	1:H:573:ILE:HG13	2.22	0.40
1:D:59:ILE:HG12	1:D:60:ASP:N	2.36	0.40
1:E:333:GLU:OE1	1:E:351:LYS:NZ	2.51	0.40
1:F:42:PHE:CE1	1:F:59:ILE:HD12	2.57	0.40
1:A:572:ILE:C	1:A:573:ILE:HG13	2.41	0.40
1:B:470:TYR:CG	1:B:479:PHE:CE1	3.08	0.40
1:C:202:ASP:OD2	1:C:274:SER:OG	2.36	0.40
1:E:542:MET:HE2	1:E:545:LEU:HD23	2.03	0.40
1:G:59:ILE:HG12	1:G:60:ASP:N	2.36	0.40
1:H:111:VAL:CG2	1:H:545:LEU:HD13	2.51	0.40
1:B:23:PHE:N	1:B:23:PHE:CD2	2.89	0.40
1:B:33:PHE:O	1:B:35:SER:N	2.54	0.40
1:B:542:MET:HE2	1:B:545:LEU:HD23	2.04	0.40
1:C:16:ASN:OD1	1:C:19:ASN:N	2.55	0.40
1:C:23:PHE:N	1:C:23:PHE:CD2	2.89	0.40
1:D:532:TRP:CZ2	1:D:546:ARG:HA	2.57	0.40
1:E:177:ILE:HB	1:E:235:SER:O	2.22	0.40
1:H:33:PHE:C	1:H:35:SER:H	2.24	0.40
1:I:177:ILE:HB	1:I:235:SER:O	2.22	0.40

All (2) 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:C:262:ASP:O	1:K:192:LYS:NZ[4_547]	2.08	0.12
1:C:260:GLY:O	1:D:187:THR:OG1[2_556]	2.10	0.10

## 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	482/583 (83%)	408 (85%)	58 (12%)	16 (3%)	4	30
1	B	482/583 (83%)	408 (85%)	60 (12%)	14 (3%)	4	32
1	C	482/583 (83%)	407 (84%)	59 (12%)	16 (3%)	4	30
1	D	482/583 (83%)	410 (85%)	57 (12%)	15 (3%)	4	31
1	E	482/583 (83%)	412 (86%)	56 (12%)	14 (3%)	4	32
1	F	482/583 (83%)	408 (85%)	58 (12%)	16 (3%)	4	30
1	G	482/583 (83%)	409 (85%)	59 (12%)	14 (3%)	4	32
1	H	482/583 (83%)	410 (85%)	56 (12%)	16 (3%)	4	30
1	I	482/583 (83%)	406 (84%)	60 (12%)	16 (3%)	4	30
1	J	482/583 (83%)	410 (85%)	56 (12%)	16 (3%)	4	30
1	K	482/583 (83%)	411 (85%)	57 (12%)	14 (3%)	4	32
1	L	482/583 (83%)	410 (85%)	58 (12%)	14 (3%)	4	32
All	All	5784/6996 (83%)	4909 (85%)	694 (12%)	181 (3%)	4	31

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	70	GLN
1	A	84	SER
1	A	258	VAL
1	B	18	GLN
1	B	70	GLN
1	B	84	SER
1	B	258	VAL
1	C	18	GLN
1	C	70	GLN
1	C	84	SER
1	C	258	VAL

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Mol	Chain	Res	Type
1	D	18	GLN
1	D	70	GLN
1	D	84	SER
1	D	258	VAL
1	E	18	GLN
1	E	70	GLN
1	E	84	SER
1	E	258	VAL
1	F	18	GLN
1	F	26	ASN
1	F	70	GLN
1	F	84	SER
1	F	258	VAL
1	G	18	GLN
1	G	70	GLN
1	G	84	SER
1	G	258	VAL
1	H	18	GLN
1	H	70	GLN
1	H	84	SER
1	H	258	VAL
1	I	18	GLN
1	I	26	ASN
1	I	70	GLN
1	I	84	SER
1	I	258	VAL
1	J	18	GLN
1	J	70	GLN
1	J	84	SER
1	J	258	VAL
1	K	18	GLN
1	K	70	GLN
1	K	84	SER
1	K	258	VAL
1	L	18	GLN
1	L	70	GLN
1	L	84	SER
1	L	258	VAL
1	A	34	ASN
1	A	357	GLY
1	A	572	ILE
1	B	34	ASN

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Mol	Chain	Res	Type
1	B	357	GLY
1	B	572	ILE
1	C	34	ASN
1	C	357	GLY
1	C	572	ILE
1	D	34	ASN
1	D	69	GLU
1	D	100	ASP
1	D	357	GLY
1	D	572	ILE
1	E	34	ASN
1	E	100	ASP
1	E	357	GLY
1	E	572	ILE
1	F	27	GLU
1	F	34	ASN
1	F	100	ASP
1	F	357	GLY
1	F	572	ILE
1	G	34	ASN
1	G	100	ASP
1	G	357	GLY
1	G	572	ILE
1	H	34	ASN
1	H	357	GLY
1	H	572	ILE
1	I	27	GLU
1	I	34	ASN
1	I	100	ASP
1	I	357	GLY
1	I	572	ILE
1	J	34	ASN
1	J	357	GLY
1	J	572	ILE
1	K	34	ASN
1	K	357	GLY
1	K	572	ILE
1	L	34	ASN
1	L	357	GLY
1	L	572	ILE
1	A	14	PHE
1	A	69	GLU

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Mol	Chain	Res	Type
1	A	100	ASP
1	A	536	ASN
1	B	14	PHE
1	B	69	GLU
1	B	100	ASP
1	C	69	GLU
1	C	100	ASP
1	C	371	ASN
1	D	14	PHE
1	E	69	GLU
1	F	14	PHE
1	G	69	GLU
1	H	69	GLU
1	H	100	ASP
1	I	14	PHE
1	I	69	GLU
1	J	69	GLU
1	J	100	ASP
1	K	69	GLU
1	K	100	ASP
1	L	69	GLU
1	L	100	ASP
1	B	371	ASN
1	C	14	PHE
1	D	371	ASN
1	E	14	PHE
1	F	69	GLU
1	G	371	ASN
1	H	14	PHE
1	I	371	ASN
1	J	14	PHE
1	J	371	ASN
1	K	371	ASN
1	L	14	PHE
1	L	371	ASN
1	A	271	GLN
1	A	371	ASN
1	B	271	GLN
1	C	271	GLN
1	D	40	HIS
1	D	271	GLN
1	D	536	ASN

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Mol	Chain	Res	Type
1	E	271	GLN
1	E	371	ASN
1	F	40	HIS
1	F	371	ASN
1	G	14	PHE
1	G	40	HIS
1	G	271	GLN
1	H	40	HIS
1	H	271	GLN
1	H	371	ASN
1	J	40	HIS
1	J	271	GLN
1	J	536	ASN
1	K	40	HIS
1	K	271	GLN
1	L	40	HIS
1	L	271	GLN
1	A	40	HIS
1	B	40	HIS
1	C	40	HIS
1	C	101	LYS
1	E	40	HIS
1	H	26	ASN
1	J	26	ASN
1	K	14	PHE
1	A	39	VAL
1	B	39	VAL
1	C	39	VAL
1	D	39	VAL
1	E	39	VAL
1	F	39	VAL
1	G	39	VAL
1	H	39	VAL
1	I	39	VAL
1	J	39	VAL
1	K	39	VAL
1	L	39	VAL
1	F	469	GLY
1	I	469	GLY
1	I	526	VAL
1	A	469	GLY
1	C	469	GLY

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Mol	Chain	Res	Type
1	H	469	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	446/529 (84%)	386 (86%)	60 (14%)	4	21
1	B	446/529 (84%)	386 (86%)	60 (14%)	4	21
1	C	446/529 (84%)	387 (87%)	59 (13%)	4	21
1	D	446/529 (84%)	389 (87%)	57 (13%)	4	22
1	E	446/529 (84%)	385 (86%)	61 (14%)	3	20
1	F	446/529 (84%)	388 (87%)	58 (13%)	4	22
1	G	446/529 (84%)	384 (86%)	62 (14%)	3	20
1	H	446/529 (84%)	387 (87%)	59 (13%)	4	21
1	I	446/529 (84%)	386 (86%)	60 (14%)	4	21
1	J	446/529 (84%)	385 (86%)	61 (14%)	3	20
1	K	446/529 (84%)	387 (87%)	59 (13%)	4	21
1	L	446/529 (84%)	389 (87%)	57 (13%)	4	22
All	All	5352/6348 (84%)	4639 (87%)	713 (13%)	4	21

All (713) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	12	THR
1	A	17	MET
1	A	29	ARG
1	A	37	PHE
1	A	38	ASP
1	A	39	VAL
1	A	46	PHE
1	A	47	ASN

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Mol	Chain	Res	Type
1	A	48	TYR
1	A	55	LEU
1	A	58	THR
1	A	60	ASP
1	A	61	LEU
1	A	65	ARG
1	A	69	GLU
1	A	70	GLN
1	A	72	MET
1	A	82	ILE
1	A	103	CYS
1	A	112	VAL
1	A	126	ASN
1	A	132	GLN
1	A	152	VAL
1	A	175	LEU
1	A	176	THR
1	A	177	ILE
1	A	189	GLU
1	A	193	PHE
1	A	199	SER
1	A	204	ILE
1	A	210	MET
1	A	227	THR
1	A	262	ASP
1	A	278	ASP
1	A	291	PHE
1	A	292	THR
1	A	299	ASN
1	A	307	ASN
1	A	330	THR
1	A	338	VAL
1	A	339	THR
1	A	347	LYS
1	A	350	VAL
1	A	369	THR
1	A	376	ILE
1	A	463	ILE
1	A	507	CYS
1	A	509	ASP
1	A	511	SER
1	A	514	LEU

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Mol	Chain	Res	Type
1	A	517	ILE
1	A	519	SER
1	A	520	MET
1	A	526	VAL
1	A	543	ASN
1	A	545	LEU
1	A	548	LEU
1	A	563	ILE
1	A	572	ILE
1	B	10	TYR
1	B	12	THR
1	B	14	PHE
1	B	17	MET
1	B	29	ARG
1	B	37	PHE
1	B	38	ASP
1	B	39	VAL
1	B	46	PHE
1	B	47	ASN
1	B	55	LEU
1	B	58	THR
1	B	60	ASP
1	B	61	LEU
1	B	65	ARG
1	B	69	GLU
1	B	70	GLN
1	B	82	ILE
1	B	103	CYS
1	B	106	SER
1	B	112	VAL
1	B	121	LEU
1	B	126	ASN
1	B	132	GLN
1	B	175	LEU
1	B	176	THR
1	B	177	ILE
1	B	189	GLU
1	B	193	PHE
1	B	199	SER
1	B	200	THR
1	B	204	ILE
1	B	210	MET

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Mol	Chain	Res	Type
1	B	227	THR
1	B	262	ASP
1	B	278	ASP
1	B	291	PHE
1	B	292	THR
1	B	299	ASN
1	B	330	THR
1	B	338	VAL
1	B	339	THR
1	B	347	LYS
1	B	350	VAL
1	B	352	ASN
1	B	369	THR
1	B	376	ILE
1	B	463	ILE
1	B	507	CYS
1	B	509	ASP
1	B	511	SER
1	B	514	LEU
1	B	517	ILE
1	B	519	SER
1	B	526	VAL
1	B	543	ASN
1	B	545	LEU
1	B	548	LEU
1	B	563	ILE
1	B	572	ILE
1	C	10	TYR
1	C	12	THR
1	C	17	MET
1	C	29	ARG
1	C	37	PHE
1	C	38	ASP
1	C	39	VAL
1	C	46	PHE
1	C	47	ASN
1	C	48	TYR
1	C	55	LEU
1	C	58	THR
1	C	60	ASP
1	C	61	LEU
1	C	65	ARG

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Mol	Chain	Res	Type
1	C	69	GLU
1	C	70	GLN
1	C	72	MET
1	C	82	ILE
1	C	103	CYS
1	C	106	SER
1	C	112	VAL
1	C	126	ASN
1	C	132	GLN
1	C	176	THR
1	C	177	ILE
1	C	189	GLU
1	C	193	PHE
1	C	199	SER
1	C	200	THR
1	C	204	ILE
1	C	210	MET
1	C	227	THR
1	C	262	ASP
1	C	278	ASP
1	C	291	PHE
1	C	292	THR
1	C	299	ASN
1	C	330	THR
1	C	338	VAL
1	C	339	THR
1	C	347	LYS
1	C	350	VAL
1	C	352	ASN
1	C	369	THR
1	C	376	ILE
1	C	463	ILE
1	C	507	CYS
1	C	509	ASP
1	C	511	SER
1	C	514	LEU
1	C	517	ILE
1	C	519	SER
1	C	520	MET
1	C	543	ASN
1	C	545	LEU
1	C	548	LEU

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Mol	Chain	Res	Type
1	C	563	ILE
1	C	572	ILE
1	D	10	TYR
1	D	12	THR
1	D	17	MET
1	D	29	ARG
1	D	37	PHE
1	D	38	ASP
1	D	39	VAL
1	D	46	PHE
1	D	47	ASN
1	D	55	LEU
1	D	60	ASP
1	D	61	LEU
1	D	65	ARG
1	D	69	GLU
1	D	70	GLN
1	D	82	ILE
1	D	103	CYS
1	D	106	SER
1	D	112	VAL
1	D	121	LEU
1	D	126	ASN
1	D	132	GLN
1	D	152	VAL
1	D	175	LEU
1	D	176	THR
1	D	177	ILE
1	D	189	GLU
1	D	193	PHE
1	D	199	SER
1	D	200	THR
1	D	204	ILE
1	D	210	MET
1	D	227	THR
1	D	262	ASP
1	D	278	ASP
1	D	291	PHE
1	D	292	THR
1	D	299	ASN
1	D	330	THR
1	D	338	VAL

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Mol	Chain	Res	Type
1	D	339	THR
1	D	347	LYS
1	D	350	VAL
1	D	352	ASN
1	D	369	THR
1	D	376	ILE
1	D	463	ILE
1	D	507	CYS
1	D	509	ASP
1	D	511	SER
1	D	514	LEU
1	D	517	ILE
1	D	519	SER
1	D	543	ASN
1	D	545	LEU
1	D	563	ILE
1	D	572	ILE
1	E	10	TYR
1	E	12	THR
1	E	17	MET
1	E	20	THR
1	E	29	ARG
1	E	37	PHE
1	E	38	ASP
1	E	39	VAL
1	E	46	PHE
1	E	47	ASN
1	E	55	LEU
1	E	58	THR
1	E	60	ASP
1	E	61	LEU
1	E	65	ARG
1	E	69	GLU
1	E	70	GLN
1	E	82	ILE
1	E	103	CYS
1	E	106	SER
1	E	112	VAL
1	E	126	ASN
1	E	132	GLN
1	E	152	VAL
1	E	175	LEU

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Mol	Chain	Res	Type
1	E	176	THR
1	E	177	ILE
1	E	189	GLU
1	E	193	PHE
1	E	199	SER
1	E	200	THR
1	E	204	ILE
1	E	210	MET
1	E	227	THR
1	E	262	ASP
1	E	278	ASP
1	E	291	PHE
1	E	292	THR
1	E	299	ASN
1	E	330	THR
1	E	338	VAL
1	E	339	THR
1	E	347	LYS
1	E	350	VAL
1	E	352	ASN
1	E	369	THR
1	E	376	ILE
1	E	463	ILE
1	E	507	CYS
1	E	509	ASP
1	E	511	SER
1	E	514	LEU
1	E	517	ILE
1	E	519	SER
1	E	520	MET
1	E	526	VAL
1	E	543	ASN
1	E	545	LEU
1	E	548	LEU
1	E	563	ILE
1	E	572	ILE
1	F	12	THR
1	F	17	MET
1	F	29	ARG
1	F	37	PHE
1	F	38	ASP
1	F	39	VAL

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Mol	Chain	Res	Type
1	F	46	PHE
1	F	47	ASN
1	F	48	TYR
1	F	55	LEU
1	F	58	THR
1	F	60	ASP
1	F	61	LEU
1	F	65	ARG
1	F	68	PHE
1	F	69	GLU
1	F	70	GLN
1	F	82	ILE
1	F	103	CYS
1	F	106	SER
1	F	112	VAL
1	F	126	ASN
1	F	132	GLN
1	F	152	VAL
1	F	175	LEU
1	F	176	THR
1	F	177	ILE
1	F	189	GLU
1	F	193	PHE
1	F	199	SER
1	F	200	THR
1	F	204	ILE
1	F	210	MET
1	F	227	THR
1	F	262	ASP
1	F	278	ASP
1	F	291	PHE
1	F	292	THR
1	F	299	ASN
1	F	330	THR
1	F	338	VAL
1	F	339	THR
1	F	347	LYS
1	F	350	VAL
1	F	352	ASN
1	F	369	THR
1	F	376	ILE
1	F	463	ILE

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Mol	Chain	Res	Type
1	F	507	CYS
1	F	509	ASP
1	F	511	SER
1	F	514	LEU
1	F	517	ILE
1	F	519	SER
1	F	543	ASN
1	F	545	LEU
1	F	563	ILE
1	F	572	ILE
1	G	12	THR
1	G	14	PHE
1	G	17	MET
1	G	29	ARG
1	G	37	PHE
1	G	38	ASP
1	G	39	VAL
1	G	46	PHE
1	G	47	ASN
1	G	48	TYR
1	G	55	LEU
1	G	58	THR
1	G	60	ASP
1	G	61	LEU
1	G	65	ARG
1	G	69	GLU
1	G	70	GLN
1	G	82	ILE
1	G	103	CYS
1	G	106	SER
1	G	112	VAL
1	G	121	LEU
1	G	126	ASN
1	G	132	GLN
1	G	152	VAL
1	G	175	LEU
1	G	176	THR
1	G	177	ILE
1	G	189	GLU
1	G	193	PHE
1	G	199	SER
1	G	200	THR

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Mol	Chain	Res	Type
1	G	204	ILE
1	G	210	MET
1	G	227	THR
1	G	262	ASP
1	G	278	ASP
1	G	291	PHE
1	G	292	THR
1	G	299	ASN
1	G	307	ASN
1	G	330	THR
1	G	338	VAL
1	G	339	THR
1	G	347	LYS
1	G	350	VAL
1	G	369	THR
1	G	376	ILE
1	G	463	ILE
1	G	507	CYS
1	G	509	ASP
1	G	511	SER
1	G	514	LEU
1	G	517	ILE
1	G	519	SER
1	G	520	MET
1	G	526	VAL
1	G	543	ASN
1	G	545	LEU
1	G	548	LEU
1	G	563	ILE
1	G	572	ILE
1	H	10	TYR
1	H	12	THR
1	H	14	PHE
1	H	17	MET
1	H	29	ARG
1	H	37	PHE
1	H	38	ASP
1	H	39	VAL
1	H	46	PHE
1	H	47	ASN
1	H	55	LEU
1	H	58	THR

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Mol	Chain	Res	Type
1	H	60	ASP
1	H	61	LEU
1	H	65	ARG
1	H	69	GLU
1	H	70	GLN
1	H	82	ILE
1	H	103	CYS
1	H	106	SER
1	H	112	VAL
1	H	126	ASN
1	H	132	GLN
1	H	152	VAL
1	H	175	LEU
1	H	176	THR
1	H	177	ILE
1	H	189	GLU
1	H	193	PHE
1	H	199	SER
1	H	200	THR
1	H	204	ILE
1	H	210	MET
1	H	227	THR
1	H	262	ASP
1	H	278	ASP
1	H	291	PHE
1	H	292	THR
1	H	299	ASN
1	H	307	ASN
1	H	330	THR
1	H	338	VAL
1	H	339	THR
1	H	347	LYS
1	H	350	VAL
1	H	369	THR
1	H	376	ILE
1	H	463	ILE
1	H	507	CYS
1	H	509	ASP
1	H	511	SER
1	H	514	LEU
1	H	517	ILE
1	H	519	SER

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Mol	Chain	Res	Type
1	H	543	ASN
1	H	545	LEU
1	H	548	LEU
1	H	563	ILE
1	H	572	ILE
1	I	10	TYR
1	I	12	THR
1	I	14	PHE
1	I	17	MET
1	I	20	THR
1	I	29	ARG
1	I	37	PHE
1	I	38	ASP
1	I	39	VAL
1	I	46	PHE
1	I	47	ASN
1	I	55	LEU
1	I	58	THR
1	I	60	ASP
1	I	61	LEU
1	I	65	ARG
1	I	69	GLU
1	I	70	GLN
1	I	82	ILE
1	I	103	CYS
1	I	106	SER
1	I	112	VAL
1	I	121	LEU
1	I	126	ASN
1	I	132	GLN
1	I	152	VAL
1	I	175	LEU
1	I	176	THR
1	I	177	ILE
1	I	189	GLU
1	I	193	PHE
1	I	199	SER
1	I	204	ILE
1	I	210	MET
1	I	227	THR
1	I	262	ASP
1	I	278	ASP

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Mol	Chain	Res	Type
1	I	291	PHE
1	I	292	THR
1	I	299	ASN
1	I	330	THR
1	I	338	VAL
1	I	339	THR
1	I	347	LYS
1	I	350	VAL
1	I	369	THR
1	I	376	ILE
1	I	463	ILE
1	I	507	CYS
1	I	509	ASP
1	I	511	SER
1	I	514	LEU
1	I	517	ILE
1	I	519	SER
1	I	526	VAL
1	I	543	ASN
1	I	545	LEU
1	I	548	LEU
1	I	563	ILE
1	I	572	ILE
1	J	12	THR
1	J	14	PHE
1	J	17	MET
1	J	29	ARG
1	J	37	PHE
1	J	38	ASP
1	J	39	VAL
1	J	46	PHE
1	J	47	ASN
1	J	48	TYR
1	J	55	LEU
1	J	58	THR
1	J	60	ASP
1	J	61	LEU
1	J	65	ARG
1	J	69	GLU
1	J	70	GLN
1	J	77	CYS
1	J	82	ILE

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Mol	Chain	Res	Type
1	J	103	CYS
1	J	106	SER
1	J	112	VAL
1	J	121	LEU
1	J	126	ASN
1	J	132	GLN
1	J	175	LEU
1	J	176	THR
1	J	177	ILE
1	J	189	GLU
1	J	193	PHE
1	J	199	SER
1	J	200	THR
1	J	204	ILE
1	J	210	MET
1	J	227	THR
1	J	262	ASP
1	J	278	ASP
1	J	291	PHE
1	J	292	THR
1	J	299	ASN
1	J	330	THR
1	J	338	VAL
1	J	339	THR
1	J	347	LYS
1	J	350	VAL
1	J	369	THR
1	J	376	ILE
1	J	463	ILE
1	J	507	CYS
1	J	509	ASP
1	J	511	SER
1	J	514	LEU
1	J	517	ILE
1	J	519	SER
1	J	520	MET
1	J	526	VAL
1	J	543	ASN
1	J	545	LEU
1	J	548	LEU
1	J	563	ILE
1	J	572	ILE

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Mol	Chain	Res	Type
1	K	12	THR
1	K	14	PHE
1	K	17	MET
1	K	29	ARG
1	K	37	PHE
1	K	38	ASP
1	K	39	VAL
1	K	46	PHE
1	K	47	ASN
1	K	55	LEU
1	K	58	THR
1	K	60	ASP
1	K	61	LEU
1	K	65	ARG
1	K	69	GLU
1	K	70	GLN
1	K	82	ILE
1	K	103	CYS
1	K	106	SER
1	K	112	VAL
1	K	121	LEU
1	K	126	ASN
1	K	132	GLN
1	K	176	THR
1	K	177	ILE
1	K	189	GLU
1	K	193	PHE
1	K	199	SER
1	K	200	THR
1	K	204	ILE
1	K	210	MET
1	K	227	THR
1	K	262	ASP
1	K	278	ASP
1	K	291	PHE
1	K	292	THR
1	K	299	ASN
1	K	307	ASN
1	K	330	THR
1	K	338	VAL
1	K	339	THR
1	K	347	LYS

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Mol	Chain	Res	Type
1	K	350	VAL
1	K	352	ASN
1	K	369	THR
1	K	376	ILE
1	K	463	ILE
1	K	507	CYS
1	K	509	ASP
1	K	511	SER
1	K	514	LEU
1	K	517	ILE
1	K	519	SER
1	K	526	VAL
1	K	543	ASN
1	K	545	LEU
1	K	548	LEU
1	K	563	ILE
1	K	572	ILE
1	L	12	THR
1	L	14	PHE
1	L	17	MET
1	L	29	ARG
1	L	37	PHE
1	L	38	ASP
1	L	39	VAL
1	L	46	PHE
1	L	47	ASN
1	L	55	LEU
1	L	58	THR
1	L	60	ASP
1	L	61	LEU
1	L	65	ARG
1	L	69	GLU
1	L	70	GLN
1	L	72	MET
1	L	82	ILE
1	L	103	CYS
1	L	106	SER
1	L	112	VAL
1	L	126	ASN
1	L	132	GLN
1	L	175	LEU
1	L	176	THR

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Mol	Chain	Res	Type
1	L	177	ILE
1	L	189	GLU
1	L	193	PHE
1	L	199	SER
1	L	204	ILE
1	L	210	MET
1	L	227	THR
1	L	262	ASP
1	L	278	ASP
1	L	291	PHE
1	L	292	THR
1	L	299	ASN
1	L	330	THR
1	L	338	VAL
1	L	339	THR
1	L	347	LYS
1	L	350	VAL
1	L	369	THR
1	L	376	ILE
1	L	463	ILE
1	L	507	CYS
1	L	509	ASP
1	L	511	SER
1	L	514	LEU
1	L	517	ILE
1	L	519	SER
1	L	526	VAL
1	L	543	ASN
1	L	545	LEU
1	L	548	LEU
1	L	563	ILE
1	L	572	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	B	233	GLN
1	C	233	GLN
1	D	233	GLN
1	E	233	GLN
1	F	233	GLN

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Mol	Chain	Res	Type
1	G	233	GLN
1	H	233	GLN
1	I	233	GLN
1	J	233	GLN
1	K	233	GLN
1	L	233	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	488/583 (83%)	-0.51	0  	25, 83, 153, 207	0
1	B	488/583 (83%)	-0.45	0  	28, 81, 149, 232	0
1	C	488/583 (83%)	-0.54	0  	16, 72, 151, 222	0
1	D	488/583 (83%)	-0.60	1 (0%)  	18, 72, 140, 212	0
1	E	488/583 (83%)	-0.47	1 (0%)  	27, 83, 146, 215	0
1	F	488/583 (83%)	-0.52	0  	17, 79, 158, 247	0
1	G	488/583 (83%)	-0.35	1 (0%)  	41, 97, 171, 227	0
1	H	488/583 (83%)	-0.45	0  	35, 91, 170, 258	0
1	I	488/583 (83%)	-0.41	0  	20, 84, 160, 222	0
1	J	488/583 (83%)	-0.34	2 (0%)  	35, 93, 162, 211	0
1	K	488/583 (83%)	-0.39	2 (0%)  	36, 94, 159, 226	0
1	L	488/583 (83%)	-0.38	0  	37, 90, 174, 247	0
All	All	5856/6996 (83%)	-0.45	7 (0%)  	16, 85, 161, 258	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	39	VAL	3.6
1	J	39	VAL	3.0
1	E	39	VAL	3.0
1	K	230	PRO	2.9
1	D	39	VAL	2.4
1	K	39	VAL	2.1
1	J	192	LYS	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.