



Full wwPDB EM Model Validation Report ⓘ

Mar 9, 2020 – 02:50 PM EDT

PDB ID : 6SD1
EMDB ID : EMD-10145
Title : Structure of the RBM3/collar region of the Salmonella flagella MS-ring protein
FliF with 33-fold symmetry applied
Authors : Johnson, S.; Fong, Y.H.; Deme, J.C.; Furlong, E.J.; Kuhlen, L.; Lea, S.M.
Deposited on : 2019-07-26
Resolution : 2.60 Å(reported)

This is a Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

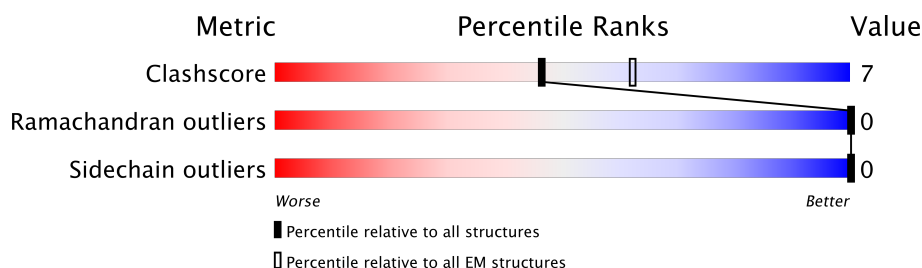
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	560	20% 7% 73%
1	B	560	19% 8% 73%
1	C	560	20% 7% 73%
1	D	560	20% 7% 73%
1	E	560	21% 6% 73%
1	F	560	21% 6% 73%
1	G	560	20% 7% 73%
1	H	560	20% 7% 73%
1	I	560	21% 6% 73%

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Mol	Chain	Length	Quality of chain
1	J	560	 21% 6% 73%
1	K	560	 22% 5% 73%
1	L	560	 21% 6% 73%
1	M	560	 20% 7% 73%
1	N	560	 21% 6% 73%
1	O	560	 20% 7% 73%
1	P	560	 20% 7% 73%
1	Q	560	 21% 6% 73%
1	R	560	 21% 6% 73%
1	S	560	 21% 6% 73%
1	T	560	 21% 6% 73%
1	U	560	 21% 6% 73%
1	V	560	 21% 6% 73%
1	W	560	 21% 6% 73%
1	X	560	 20% 7% 73%
1	Y	560	 20% 7% 73%
1	Z	560	 21% 6% 73%
1	a	560	 27% 73%
1	b	560	 27% 73%
1	c	560	 27% 73%
1	d	560	 27% 73%
1	e	560	 27% 73%
1	f	560	 27% 73%
1	g	560	 27% 73%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39369 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Flagellar M-ring protein.

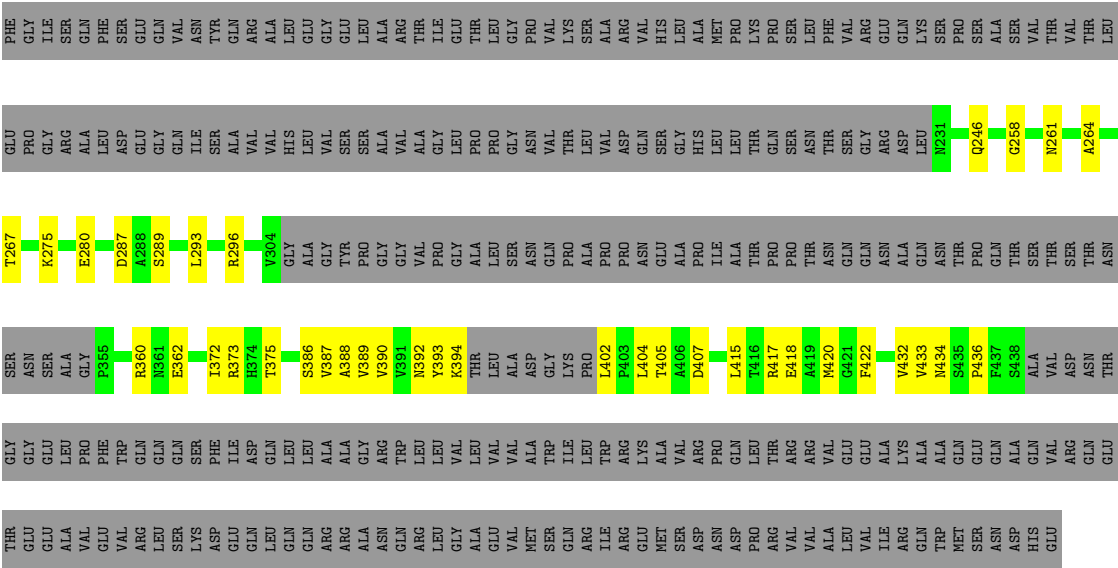
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	B	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	C	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	D	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	E	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	F	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	G	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	H	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	I	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	J	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	K	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	L	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	M	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	N	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	O	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	P	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	Q	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		

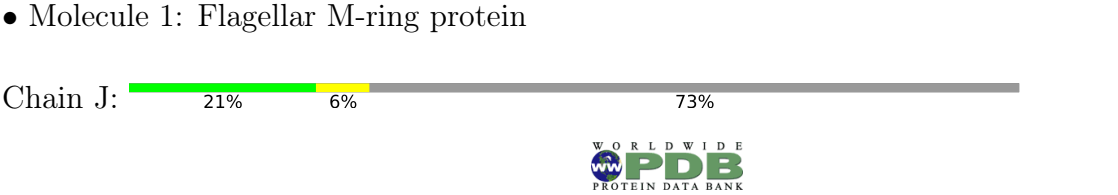
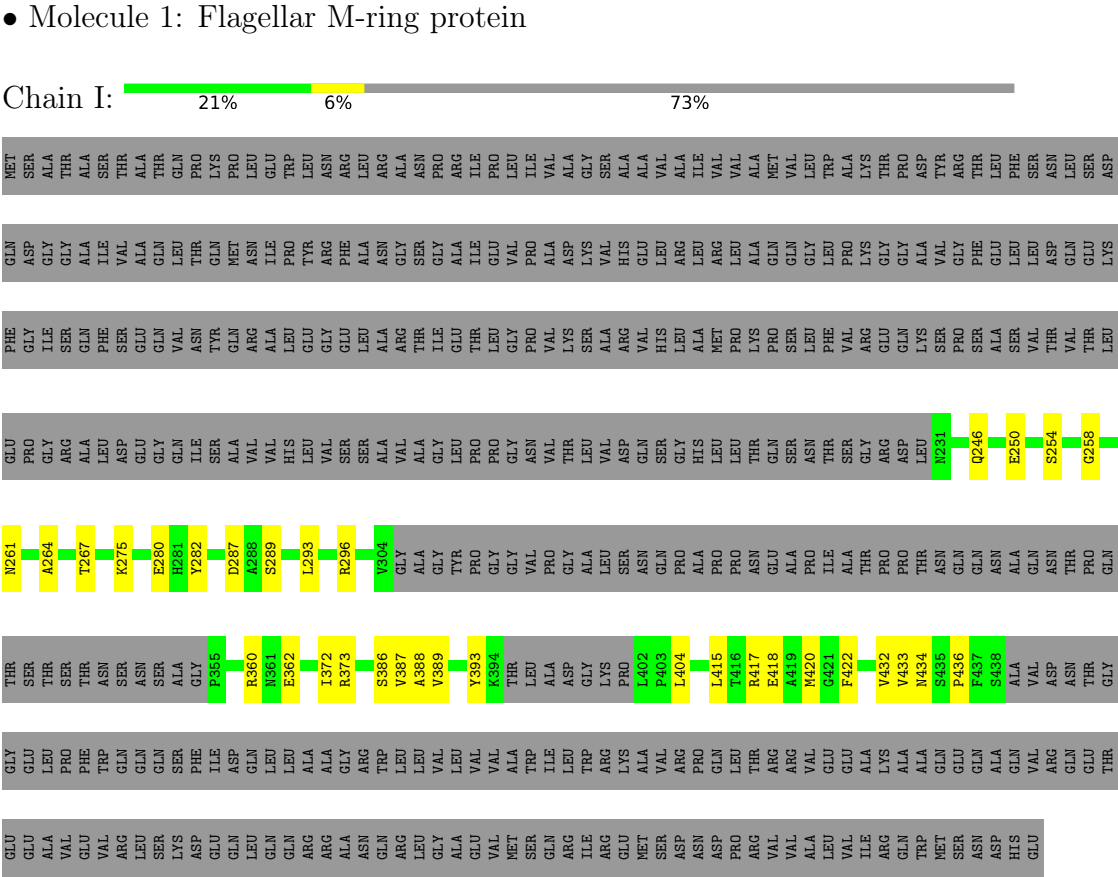
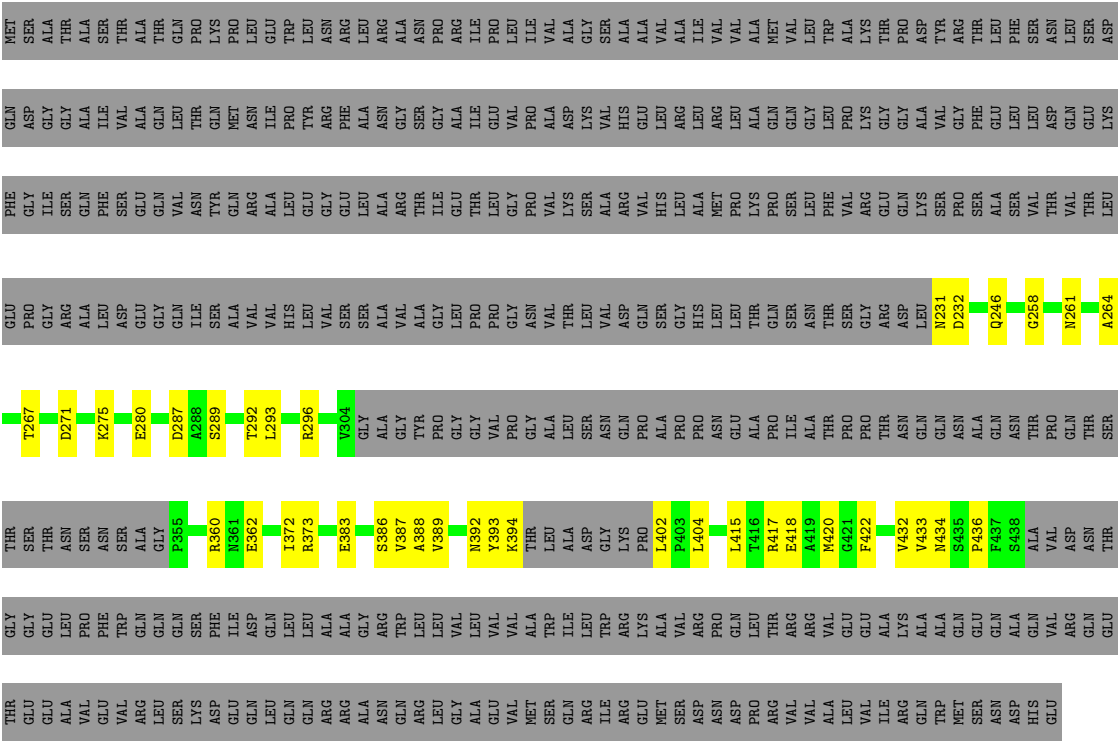
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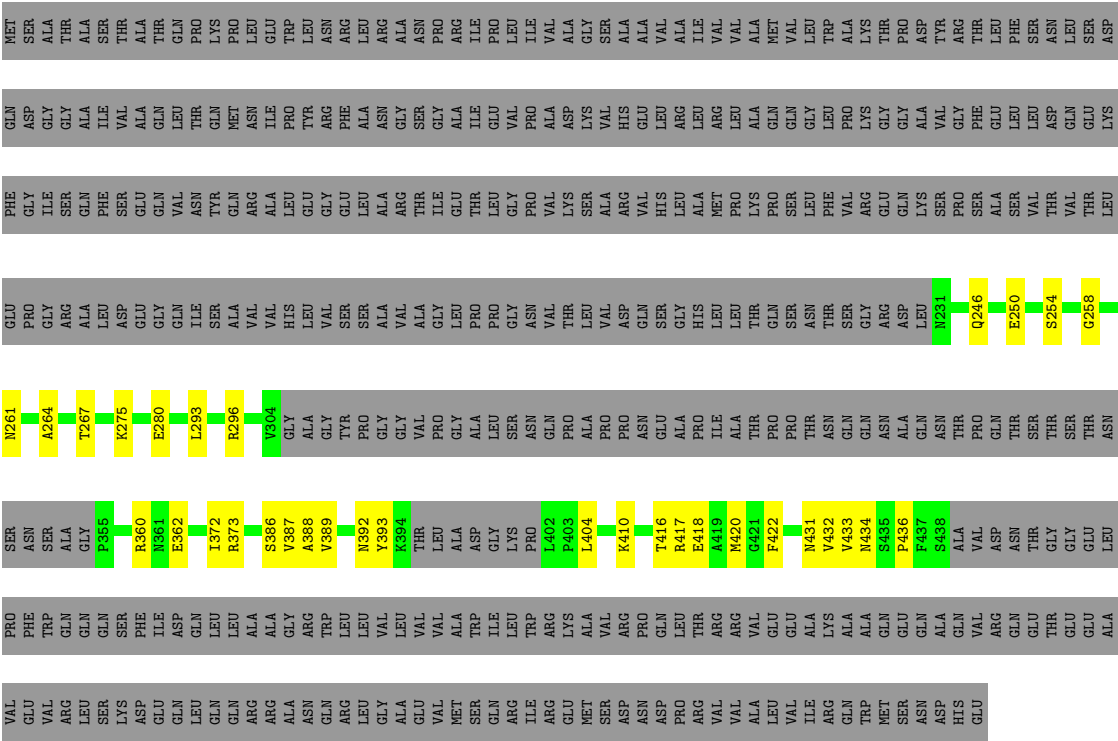
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	S	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	T	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	U	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	V	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	W	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	X	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	Y	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	Z	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	a	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	b	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	c	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	d	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	e	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	f	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	g	151	Total 1193	C 726	N 223	O 241	S 3	0	0



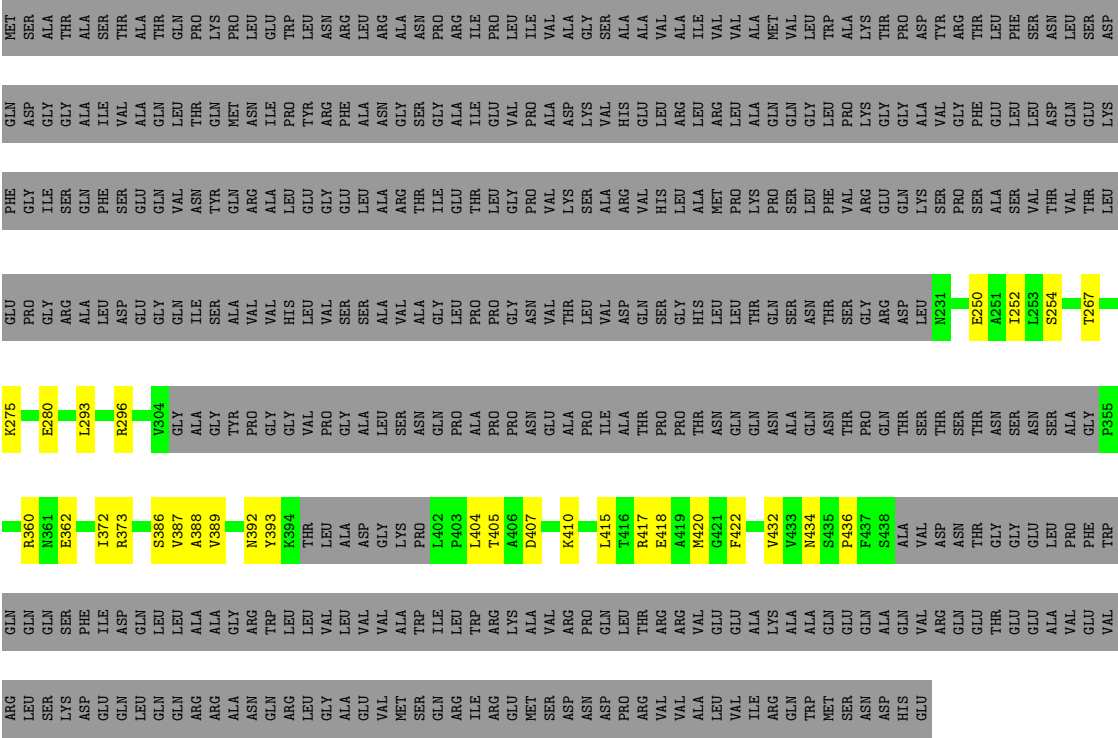






• Molecule 1: Flagellar M-ring protein

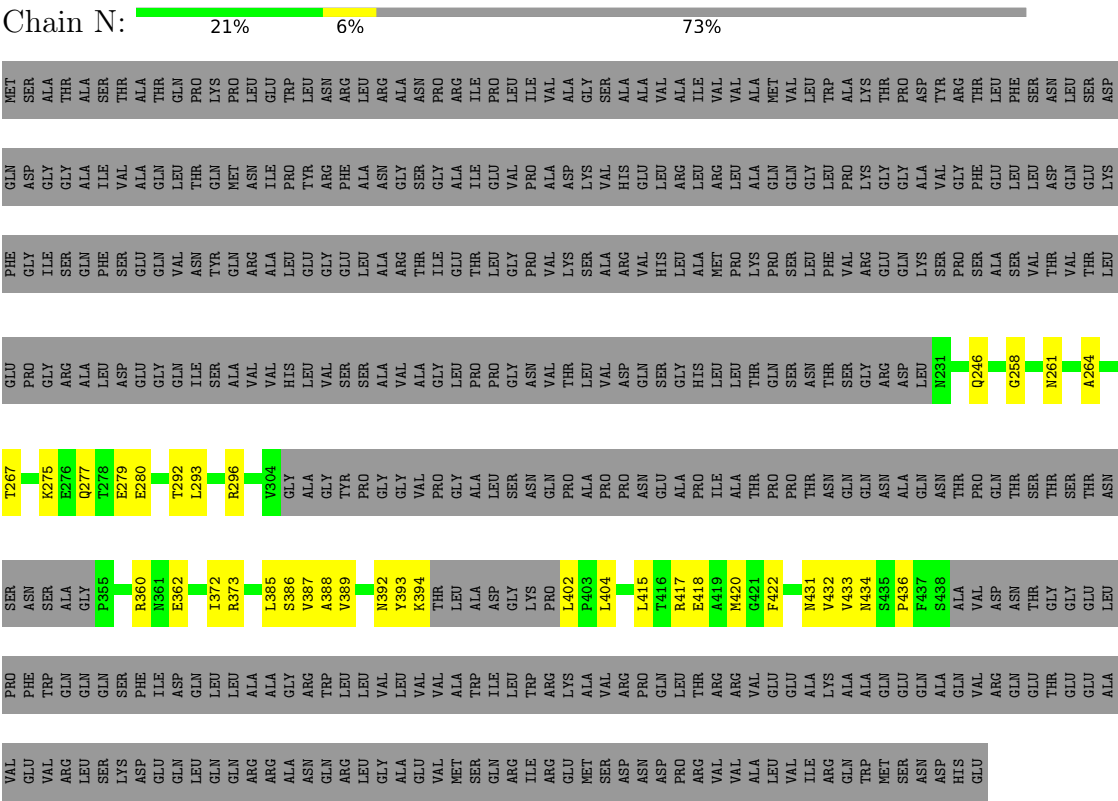
Chain K: 22% 5% 73%



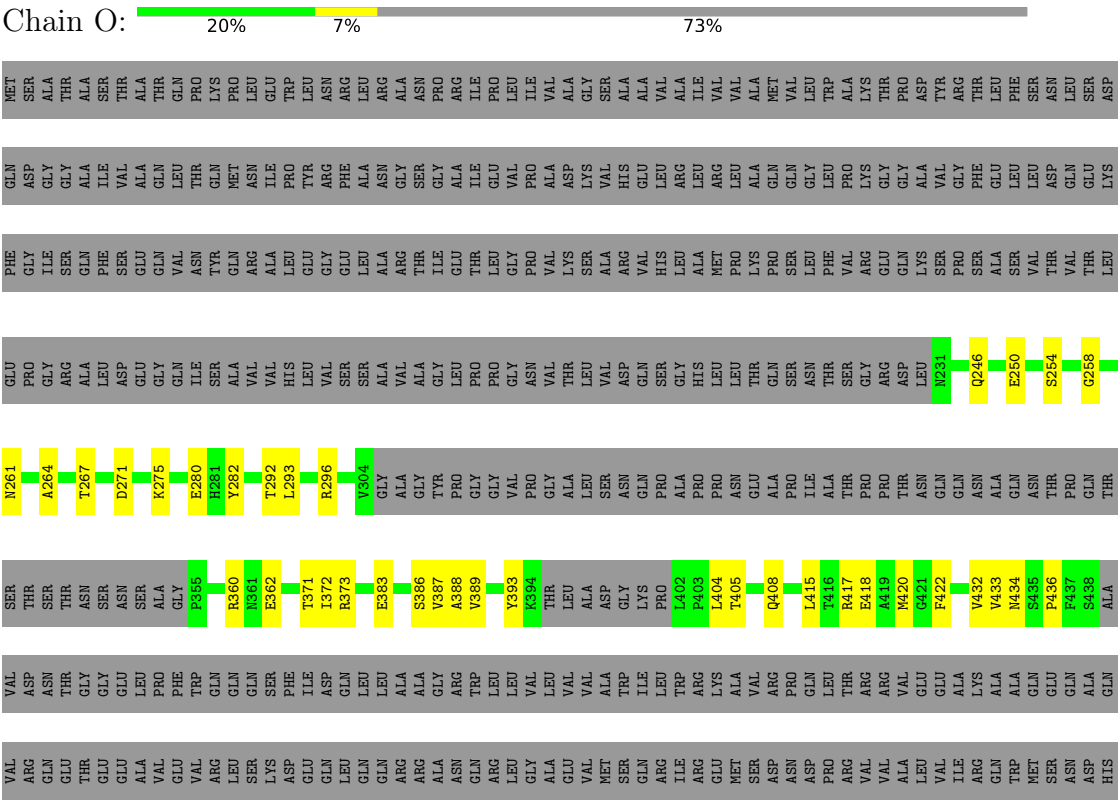
• Molecule 1: Flagellar M-ring protein

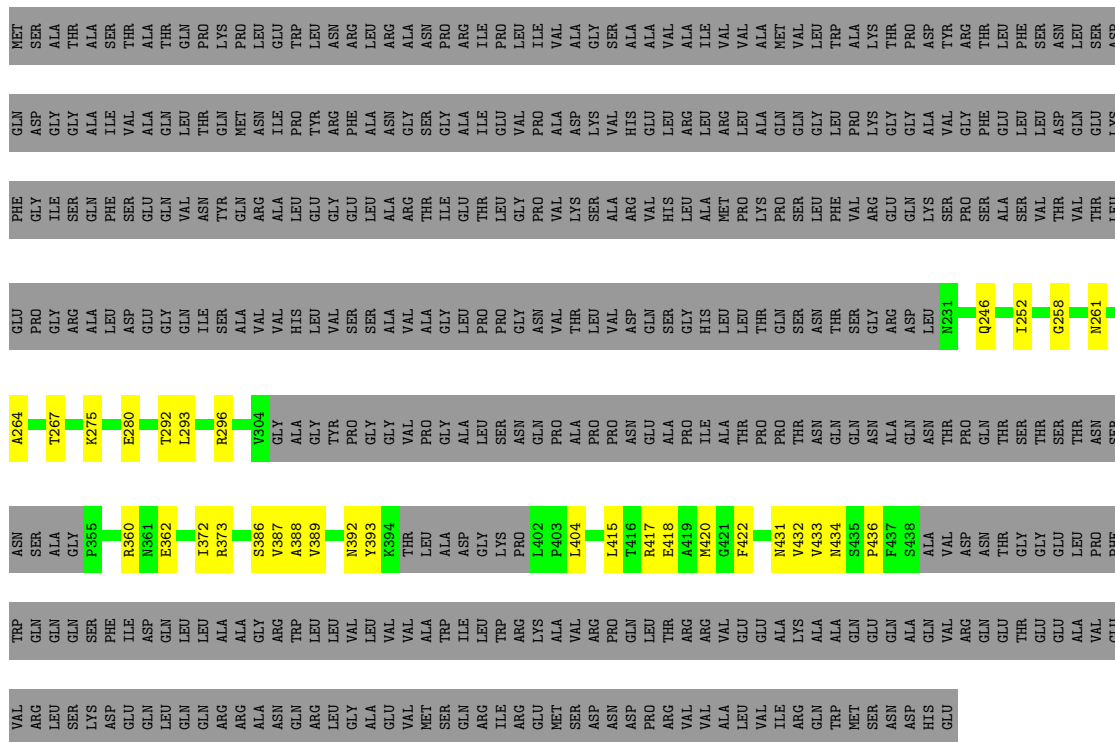
Chain L: 21% 6% 73%





● Molecule 1: Flagellar M-ring protein





ASN	SER	ASN	SER	ALA	GLY	P365	R360	N361	E362	R373	S386	V387	A388	V389	N392	Y393	K394	THR	LEU	ALA	ASP	GLY	PRO	L402	P403	L404	L415	T416	R417	E418	A419	M420	F422	N431	V432	V433	N434	S435	P436	F437	S438	ALA	VAL	ASP	ASN	THR	GLY	GLY	LEU	PRO
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PHE	TRP	GLN	GLN	ALA	SER	PHE	ILE	ASP	LEU	LEU	ALA	GLY	TRP	LEU	VAL	LEU	VAL	VAL	TRP	ILE	TRP	ARG	ARG	LYS	ALA	VAL	ARG	PRO	ASN	GLN	THR	ARG	ARG	VAL	ALA	GLY	LEU	VAL	GLU	ALA	LYS	ALA	ALA	ALA	GLN	VAL	ARG	ASN	GLN	THR	GLY	GLY	ALA	VAL
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GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	ARG	ALA	ASN	ARG	GLY	ALA	VAL	MET	SER	GLN	ARG	ILE	TRP	ILE	GLY	MET	SER	ASP	ASN	GLN	PRO	ARG	VAL	ILE	ARG	VAL	LEU	VAL	ILE	ALA	ARG	GLN	TRP	MET	SER	ASN	GLY	ASP	HIS	GLU
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● Molecule 1: Flagellar M-ring protein



MET	SER	ALA	THR	GLY	ALA	SER	THR	ALA	THR	THR	PRO	LYS	PRO	LEU	ARG	ASN	TRP	LEU	GLY	ASN	ARG	ILE	PRO	ILE	ILE	VAL	ALA	GLY	SER	GLN	ALA	VAL	THR	TRP	ALA	LYS	THR	THR	GLY	ASP	PRO	ASP	THR	THR	LEU	ASP	ASP
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GLN	ASP	GLY	GLY	ALA	ILE	VAL	ALA	GLN	LEU	THR	GLN	MET	ASN	ILE	PRO	TYR	GLY	ARG	PHE	ALA	ASN	ILE	GLY	ALA	THR	ILE	GLY	LYS	ASP	VAL	GLN	GLY	LEU	THR	PRO	GLN	GLY	VAL	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS
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PHE	GLY	ILE	SER	GLN	PHE	SER	GLU	ALA	GLU	VAL	ASN	TYR	GLN	ARG	ALA	GLY	GLY	LEU	LEU	GLU	THR	ILE	GLY	VAL	VAL	LYS	SER	ALA	THR	LEU	ALA	PRO	PHE	VAL	ARG	LYS	GLY	GLY	THR	GLY	VAL	THR	VAL	THR	LEU	LEU
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GLU	PRO	ARG	GLY	LEU	ASP	GLU	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	GLY	PRO	PRO	GLY	ASN	VAL	THR	LEU	THR	LEU	VAL	VAL	GLN	ASN	THR	THR	GLN	ASP	LEU	R231	Q246	E250	S254	G258
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N261	A264	T267	K275	E280	D287	A288	S289	L293	R296	V304	GLY	ALA	GLY	TYR	PRO	GLY	GLY	VAL	PRO	GLY	ASN	VAL	THR	LEU	SER	ASN	GLN	PRO	ALA	PRO	ASN	THR	ASN	GLN	ALA	ASN	ALA	GLN	ASN	THR	PRO	GLN	THR	SER
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THR	SER	ASN	SER	GLY	P365	E362	I372	S386	V387	A388	V389	V390	V391	N392	Y393	K394	THR	LEU	ALA	ASP	GLY	LYS	PRO	L402	P403	L404	L415	T416	R417	E418	A419	M420	G421	F422	V432	V433	N434	S435	P436	F437	S438	ALA	VAL	ASP	THR	THR	GLY	GLY	GLU	LEU
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PRO	PHE	TRP	GLN	SER	PHE	ILE	ASP	GLN	LEU	LEU	ALA	ALA	GLY	GLY	ALA	VAL	THR	ILE	TRP	ILE	TRP	ILE	ARG	LYS	ALA	VAL	VAL	GLN	ARG	THR	ARG	VAL	ALA	GLU	ALA	LYS	ALA	GLN	ALA	GLN	VAL	VAL	GLY	THR	THR	GLU	GLU	ALA
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VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLN	GLN	GLN	ARG	ARG	ALA	ASN	TYR	ARG	PHE	ALA	GLY	GLY	ALA	GLY	ILE	GLY	MET	GLU	VAL	VAL	ASN	PRO	ARG	VAL	VAL	ALA	LEU	VAL	ILE	ARG	GLN	TRP	ALA	THR	SER	ASP	ASN	HIS	GLU
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● Molecule 1: Flagellar M-ring protein



MET	SER	THR	THR	ALA	SER	THR	ALA	THR	THR	PRO	LYS	PRO	LEU	ARG	LEU	VAL	ASN	TRP	LEU	ASN	ARG	ILE	PRO	ILE	PRO	GLY	SER	ALA	VAL	THR	VAL	ALA	THR	ALA	LYS	THR	ALA	VAL	THR	THR	ARG	TYR	THR	THR	LEU	ASP
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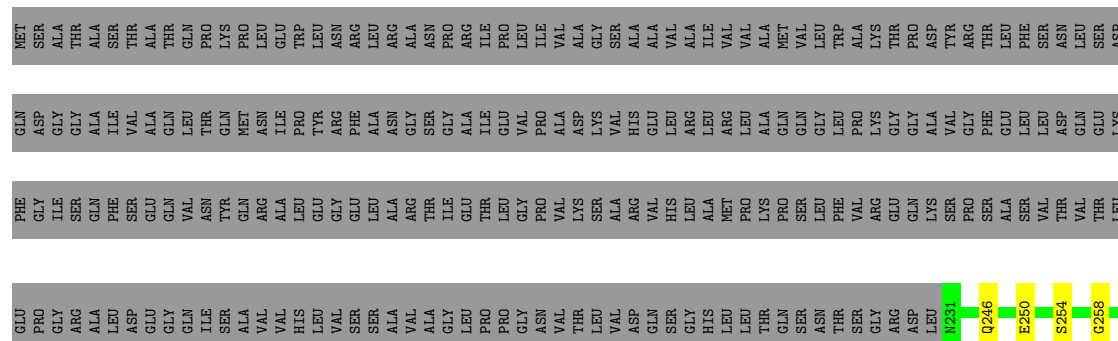
GLN	ASP	GLY	GLY	ALA	ILE	VAL	VAL	GLN	LEU	THR	GLN	MET	ASN	ILE	PRO	TYR	GLY	ARG	PHE	ALA	ASN	ALA	GLY	VAL	VAL	GLN	HIS	ARG	LEU	LEU	ARG	VAL	ALA	GLY	LYS	PRO	GLY	GLY	ALA	VAL	VAL	PHE	LEU	SER	ASN	GLN	THR	LEU	LYS
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PHE	GLY	ILE	GLN	PHE	SER	GLU	GLN	VAL	ASN	THR	TYR	GLN	ARG	ALA	GLY	GLY	GLY	LEU	LEU	ALA	THR	ILE	GLY	PRO	PRO	GLY	VAL	LYS	ALA	VAL	PRO	GLN	SER	GLY	LEU	ASN	SER	THR	THR	GLY	VAL	THR	THR	GLY	GLY	GLY	LEU
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GLU	PRO	GLY	ALA	LEU	ASP	GLU	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	GLY	VAL	SER	ALA	GLY	PRO	PRO	GLY	VAL	VAL	THR	VAL	GLN	ASN	THR	THR	ALA	THR	SER	THR	GLY	THR	ARG	ASP	LEU	R231	Q246	E250	A261	T267	L292	L293	S254
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G258	M261	A264	T267	E280	D287	A288	S289	T292	L293	R296	V304	GLY	ALA	GLY	TYR	PRO	GLY	GLY	VAL	ASN	VAL	ALA	LEU	SER	VAL	VAL	GLN	ASN	GLY	ALA	PRO	PRO	ASN	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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● Molecule 1: Flagellar M-ring protein

Chain b:

27%

73%

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- Molecule 1: Flagellar M-ring protein

Chain d: 27% 73%

NET	SER	ALA	THR	ALA	SER	THR	ALA	THR	GLN	PRO	PRO	LYS	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ARG	LEU	ARG	ALA	ALA	ASN	PRO	ARG	ILE	ILE	VAL	ALA	GLY	SER	ALA	ALA	ALA	VAL	VAL	ALA	ILE	VAL	VAL	VAL	VAL	VAL	MET	VAL	VAL	LEU	TRP	ALA	ALA	LYS	THR	PRO	PRO	ASP	TYR	THR	ARG	THR	LEU	PHE	SER	ASN	LEU	LEU	SER	ASP
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GLU	PRO	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	ALA	VAL	VAL	GLY	LEU	PRO	PRO	GLY	ASN	THR	VAL	THR	THR	CLN	SER	ASN	THR	SER	SER	GLY	HIS	LEU	LEU	THR	THR	CLN	SER	ASP	ARG	GLY	ASP	LEU	M231	G046	GLY	ALA	GLY	Tyr	PRO	PRO	GLY	GLY
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THR	GLY	GLU	LEU	PRO	PHE	TRP	GLN	GLN	SER	PHE	ILE	ASP	GLN	LEU	LEU	ALA	ALA	GLY	ARG	TRP	LEU	VAL	VAL	VAL	ALA	TRP	ILE	LEU	TRP	ARG	LYS	ALA	VAL	ARG	PRO	GLN	LEU	THR	ARG	VAL	GLU	ALA	LYS	ALA	ALA	ALA	GLN	VAL	VAL	ARG	GLN
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GLU	THR	GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	GLN	ARG	ARG	ALA	ASN	GLN	GLN	GLN	LEU	GLY	ALA	GLU	VAL	VAL	SER	SER	GLN	ARG	ILE	ILE	ARG	GLU	MET	ASP	ASN	ASP	ASN	PRO	ARG	VAL	ALA	VAL	ALA	LEU	VAL	ILE	ILE	ARG	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU
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- Molecule 1: Flagellar M-ring protein

Chain e: 27% 73%

MET	SER	ALA	THR	ALA	SER	THR	ALA	THR	GLN	PRO	PRO	LYS	PRO	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ARG	LEU	ARG	ALA	ALA	ASN	PRO	PRO	ARG	ILE	ILE	ILE	VAL	ALA	GLY	SER	ALA	ALA	VAL	VAL	ALA	ALA	ILE	VAL	VAL	VAL	VAL	MET	VAL	VAL	LEU	LEU	TRP	ALA	ALA	ALA	LYS	THR	THR	PRO	ASP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	LEU	SER	SER	ASN	SER
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GLN ASP GLY GLY ALA ALA ILE VAL ALA ALA LEU LEU THR MET ASN ILE PRO ARG PHE ASN GLY GLY SER GLY ALA ILE GLU VAL PRO ASP LYS VAL HIS GLU LEU LEU LEU GLN GLN GLY GLY VAL VAL PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLN LYS

PHE GLY ILE SER GLN PHE SER GLU VAL TYR GLN ARG ALA LEU GLU GLY GLU LEU THR GLY THR LEU PRO GLY VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO PRO LYS PRO SER PHE VAL ARG GLN GLN LYS SER PRO PRO SER ALA SER VAL THR VAL THR THR

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THR	GLY	GLU	LEU	PRO	PHE	TRP	GLN	GLN	SER	PHE	ILE	ASP	GLN	LEU	LEU	LEU	ALA	ALA	GLY	ARG	TRP	LEU	LEU	VAL	VAL	VAL	ALA	ALA	ILE	LEU	TRP	ARG	ARG	PRO	GLN	LEU	THR	ARG	VAL	GLU	GLU	ALA	ALA	LYS	ALA	ALA	ALA	ALA	GLN	GLN	GLU	GLN	VAL	VAL	GLN	ARG	GLN
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GLU	THR	GLU	GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	GLN	ARG	ARG	ALA	ASN	GLN	GLN	ARG	GLU	LEU	GLY	ALA	GLU	VAL	VAL	SER	SER	GLN	ARG	ILE	ILE	ARG	ARG	GLU	GLU	MET	SER	ASP	ASP	ASN	ASP	PRO	ARG	ARG	VAL	VAL	ALA	ALA	VAL	LEU	VAL	ILE	ILE	ARG	GLN	TRP	ASN	ASP	HIS	GLU
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Chain f: 27% 73%

Chain g: 27% 73%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C33	Depositor
Number of particles used	77849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

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	0.26	0/1205	0.42	0/1624
1	B	0.26	0/1205	0.42	0/1624
1	C	0.26	0/1205	0.42	0/1624
1	D	0.26	0/1205	0.42	0/1624
1	E	0.26	0/1205	0.43	0/1624
1	F	0.26	0/1205	0.43	0/1624
1	G	0.26	0/1205	0.42	0/1624
1	H	0.26	0/1205	0.42	0/1624
1	I	0.26	0/1205	0.42	0/1624
1	J	0.26	0/1205	0.42	0/1624
1	K	0.26	0/1205	0.42	0/1624
1	L	0.26	0/1205	0.43	0/1624
1	M	0.26	0/1205	0.42	0/1624
1	N	0.26	0/1205	0.42	0/1624
1	O	0.26	0/1205	0.42	0/1624
1	P	0.26	0/1205	0.42	0/1624
1	Q	0.26	0/1205	0.42	0/1624
1	R	0.26	0/1205	0.43	0/1624
1	S	0.26	0/1205	0.42	0/1624
1	T	0.26	0/1205	0.43	0/1624
1	U	0.26	0/1205	0.42	0/1624
1	V	0.26	0/1205	0.42	0/1624
1	W	0.26	0/1205	0.42	0/1624
1	X	0.26	0/1205	0.42	0/1624
1	Y	0.26	0/1205	0.42	0/1624
1	Z	0.26	0/1205	0.43	0/1624
1	a	0.26	0/1205	0.42	0/1624
1	b	0.26	0/1205	0.42	0/1624
1	c	0.26	0/1205	0.42	0/1624
1	d	0.26	0/1205	0.43	0/1624
1	e	0.26	0/1205	0.42	0/1624
1	f	0.26	0/1205	0.42	0/1624
1	g	0.26	0/1205	0.42	0/1624
All	All	0.26	0/39765	0.42	0/53592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1193	0	1173	29	0
1	B	1193	0	1173	29	0
1	C	1193	0	1173	26	0
1	D	1193	0	1173	25	0
1	E	1193	0	1173	26	0
1	F	1193	0	1173	26	0
1	G	1193	0	1173	32	0
1	H	1193	0	1173	26	0
1	I	1193	0	1173	23	0
1	J	1193	0	1173	24	0
1	K	1193	0	1173	22	0
1	L	1193	0	1173	24	0
1	M	1193	0	1173	26	0
1	N	1193	0	1173	25	0
1	O	1193	0	1173	26	0
1	P	1193	0	1173	27	0
1	Q	1193	0	1173	26	0
1	R	1193	0	1173	24	0
1	S	1193	0	1173	25	0
1	T	1193	0	1173	22	0
1	U	1193	0	1173	24	0
1	V	1193	0	1173	23	0
1	W	1193	0	1173	24	0
1	X	1193	0	1173	27	0
1	Y	1193	0	1173	27	0
1	Z	1193	0	1173	23	0
1	a	1193	0	1173	0	0
1	b	1193	0	1173	0	0
1	c	1193	0	1173	0	0
1	d	1193	0	1173	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	1193	0	1173	0	0
1	f	1193	0	1173	0	0
1	g	1193	0	1173	0	0
All	All	39369	0	38709	553	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (553) 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:Q:280:GLU:HG3	1:Q:372:ILE:HG12	1.80	0.64
1:B:250:GLU:O	1:B:254:SER:OG	2.15	0.63
1:H:360:ARG:NH1	1:H:362:GLU:OE1	2.31	0.63
1:P:405:THR:HG22	1:P:407:ASP:H	1.64	0.62
1:G:405:THR:HG22	1:G:407:ASP:H	1.64	0.61
1:D:405:THR:HG22	1:D:407:ASP:H	5.29	0.61
1:Y:387:VAL:HG21	1:Y:420:MET:HG2	1.82	0.61
1:U:404:LEU:H	1:U:434:ASN:HD21	1.47	0.61
1:B:405:THR:HG22	1:B:407:ASP:H	5.14	0.61
1:P:360:ARG:NH1	1:P:362:GLU:OE1	2.34	0.61
1:K:405:THR:HG22	1:K:407:ASP:H	1.66	0.61
1:N:277:GLN:NE2	1:N:279:GLU:OE2	2.33	0.61
1:P:404:LEU:H	1:P:434:ASN:HD21	1.49	0.60
1:F:387:VAL:HG21	1:F:420:MET:HG2	1.84	0.60
1:L:387:VAL:HG21	1:L:420:MET:HG2	1.84	0.60
1:D:404:LEU:H	1:D:434:ASN:HD21	1.49	0.60
1:M:405:THR:HG23	1:M:408:GLN:H	1.67	0.60
1:M:404:LEU:H	1:M:434:ASN:HD21	1.47	0.60
1:J:404:LEU:H	1:J:434:ASN:HD21	1.47	0.60
1:S:258:GLY:HA3	1:S:261:ASN:HD22	1.67	0.60
1:A:404:LEU:H	1:A:434:ASN:HD21	1.50	0.60
1:R:258:GLY:HA3	1:R:261:ASN:HD22	1.66	0.60
1:W:404:LEU:H	1:W:434:ASN:HD21	1.50	0.60
1:X:404:LEU:H	1:X:434:ASN:HD21	1.50	0.59
1:G:387:VAL:HG21	1:G:420:MET:HG2	1.85	0.59
1:B:387:VAL:HG21	1:B:420:MET:HG2	1.86	0.59
1:O:293:LEU:HD11	1:O:296:ARG:HH11	1.67	0.59
1:X:293:LEU:HD11	1:X:296:ARG:HH11	1.68	0.59
1:C:387:VAL:HG21	1:C:420:MET:HG2	1.87	0.59
1:E:404:LEU:H	1:E:434:ASN:HD21	1.52	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:293:LEU:HD11	1:U:296:ARG:HH11	1.67	0.59
1:D:293:LEU:HD11	1:D:296:ARG:HH11	1.70	0.59
1:W:405:THR:HG23	1:W:408:GLN:H	1.67	0.59
1:H:258:GLY:HA3	1:H:261:ASN:HD22	1.66	0.59
1:S:404:LEU:H	1:S:434:ASN:HD21	1.50	0.59
1:I:293:LEU:HD11	1:I:296:ARG:HH11	1.67	0.59
1:O:387:VAL:HG21	1:O:420:MET:HG2	1.84	0.59
1:O:404:LEU:H	1:O:434:ASN:HD21	1.51	0.59
1:N:404:LEU:H	1:N:434:ASN:HD21	1.51	0.58
1:P:387:VAL:HG21	1:P:420:MET:HG2	1.86	0.58
1:G:404:LEU:H	1:G:434:ASN:ND2	2.00	0.58
1:J:258:GLY:HA3	1:J:261:ASN:HD22	1.69	0.58
1:C:404:LEU:H	1:C:434:ASN:HD21	1.54	0.58
1:F:404:LEU:H	1:F:434:ASN:HD21	1.52	0.58
1:L:258:GLY:HA3	1:L:261:ASN:HD22	1.68	0.58
1:C:293:LEU:HD11	1:C:296:ARG:HH11	1.71	0.58
1:C:405:THR:HG23	1:C:408:GLN:H	4.47	0.58
1:P:293:LEU:HD11	1:P:296:ARG:HH11	1.68	0.58
1:V:404:LEU:H	1:V:434:ASN:HD21	1.50	0.58
1:F:415:LEU:HD11	1:G:433:VAL:HG21	1.86	0.58
1:J:293:LEU:HD11	1:J:296:ARG:HH11	1.69	0.58
1:D:258:GLY:HA3	1:D:261:ASN:HD22	1.68	0.57
1:I:258:GLY:HA3	1:I:261:ASN:HD22	1.70	0.57
1:Q:405:THR:HG23	1:Q:408:GLN:H	1.68	0.57
1:W:293:LEU:HD11	1:W:296:ARG:HH11	1.69	0.57
1:I:404:LEU:H	1:I:434:ASN:HD21	1.52	0.57
1:N:258:GLY:HA3	1:N:261:ASN:HD22	1.69	0.57
1:X:387:VAL:HG21	1:X:420:MET:HG2	1.86	0.57
1:H:404:LEU:H	1:H:434:ASN:HD21	1.52	0.57
1:J:404:LEU:H	1:J:434:ASN:ND2	2.02	0.57
1:H:293:LEU:HD11	1:H:296:ARG:HH11	1.68	0.57
1:D:387:VAL:HG21	1:D:420:MET:HG2	1.90	0.57
1:L:404:LEU:H	1:L:434:ASN:HD21	1.51	0.57
1:Q:387:VAL:HG21	1:Q:420:MET:HG2	1.87	0.57
1:V:387:VAL:HG21	1:V:420:MET:HG2	1.86	0.57
1:X:258:GLY:HA3	1:X:261:ASN:HD22	1.69	0.57
1:E:293:LEU:HD11	1:E:296:ARG:HH11	1.70	0.57
1:P:404:LEU:H	1:P:434:ASN:ND2	2.01	0.57
1:W:258:GLY:HA3	1:W:261:ASN:HD22	1.69	0.57
1:M:293:LEU:HD11	1:M:296:ARG:HH11	1.69	0.56
1:V:293:LEU:HD11	1:V:296:ARG:HH11	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:293:LEU:HD11	1:K:296:ARG:HH11	1.71	0.56
1:F:293:LEU:HD11	1:F:296:ARG:HH11	1.71	0.56
1:T:293:LEU:HD11	1:T:296:ARG:HH11	1.68	0.56
1:X:405:THR:HG23	1:X:408:GLN:H	1.70	0.56
1:B:293:LEU:HD11	1:B:296:ARG:HH11	1.70	0.56
1:I:387:VAL:HG21	1:I:420:MET:HG2	1.87	0.56
1:T:404:LEU:H	1:T:434:ASN:HD21	1.51	0.56
1:O:405:THR:HG23	1:O:408:GLN:H	1.69	0.56
1:U:405:THR:HG23	1:U:408:GLN:H	1.70	0.56
1:Y:293:LEU:HD11	1:Y:296:ARG:HH11	1.70	0.56
1:Z:293:LEU:HD11	1:Z:296:ARG:HH11	1.69	0.56
1:A:258:GLY:HA3	1:A:261:ASN:HD22	1.78	0.56
1:B:404:LEU:H	1:B:434:ASN:HD21	1.52	0.56
1:N:387:VAL:HG21	1:N:420:MET:HG2	1.87	0.56
1:Q:404:LEU:H	1:Q:434:ASN:HD21	1.52	0.56
1:R:404:LEU:H	1:R:434:ASN:HD21	1.52	0.56
1:A:293:LEU:HD11	1:A:296:ARG:HH11	1.71	0.56
1:D:404:LEU:H	1:D:434:ASN:ND2	2.07	0.56
1:K:387:VAL:HG21	1:K:420:MET:HG2	1.88	0.56
1:V:404:LEU:H	1:V:434:ASN:ND2	2.03	0.56
1:H:387:VAL:HG21	1:H:420:MET:HG2	1.86	0.56
1:T:387:VAL:HG21	1:T:420:MET:HG2	1.85	0.56
1:R:387:VAL:HG21	1:R:420:MET:HG2	1.88	0.56
1:S:387:VAL:HG21	1:S:420:MET:HG2	1.87	0.56
1:K:404:LEU:H	1:K:434:ASN:ND2	2.04	0.56
1:Y:258:GLY:HA3	1:Y:261:ASN:HD22	1.70	0.56
1:B:404:LEU:H	1:B:434:ASN:ND2	2.05	0.55
1:N:293:LEU:HD11	1:N:296:ARG:HH11	1.69	0.55
1:G:404:LEU:H	1:G:434:ASN:HD21	1.57	0.55
1:K:404:LEU:H	1:K:434:ASN:HD21	1.54	0.55
1:A:404:LEU:H	1:A:434:ASN:ND2	2.04	0.55
1:O:258:GLY:HA3	1:O:261:ASN:HD22	1.71	0.55
1:J:280:GLU:HG3	1:J:372:ILE:HG12	1.88	0.55
1:P:258:GLY:HA3	1:P:261:ASN:HD22	1.72	0.55
1:F:287:ASP:OD2	1:F:289:SER:OG	2.24	0.55
1:B:258:GLY:HA3	1:B:261:ASN:HD22	1.73	0.55
1:E:258:GLY:HA3	1:E:261:ASN:HD22	1.96	0.55
1:E:387:VAL:HG21	1:E:420:MET:HG2	1.88	0.55
1:X:277:GLN:NE2	1:X:279:GLU:OE2	2.40	0.55
1:V:287:ASP:OD2	1:V:289:SER:OG	2.24	0.55
1:Z:387:VAL:HG21	1:Z:420:MET:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:VAL:HG21	1:A:420:MET:HG2	1.95	0.55
1:H:404:LEU:H	1:H:434:ASN:ND2	2.05	0.55
1:F:258:GLY:HA3	1:F:261:ASN:HD22	1.75	0.54
1:N:404:LEU:H	1:N:434:ASN:ND2	2.05	0.54
1:U:250:GLU:O	1:U:254:SER:OG	2.18	0.54
1:U:417:ARG:HG3	1:U:422:PHE:HB3	1.89	0.54
1:C:258:GLY:HA3	1:C:261:ASN:HD22	1.71	0.54
1:E:404:LEU:H	1:E:434:ASN:ND2	2.06	0.54
1:G:287:ASP:OD2	1:G:289:SER:OG	2.26	0.54
1:W:387:VAL:HG21	1:W:420:MET:HG2	1.88	0.54
1:Z:404:LEU:H	1:Z:434:ASN:HD21	1.53	0.54
1:G:293:LEU:HD11	1:G:296:ARG:HH11	1.76	0.54
1:X:287:ASP:OD2	1:X:289:SER:OG	2.24	0.54
1:Y:360:ARG:NH1	1:Y:362:GLU:OE1	2.39	0.54
1:B:287:ASP:OD2	1:B:289:SER:OG	2.26	0.54
1:B:360:ARG:NH1	1:B:362:GLU:OE1	2.41	0.54
1:D:287:ASP:OD2	1:D:289:SER:OG	2.23	0.54
1:P:280:GLU:HG3	1:P:372:ILE:HG12	1.90	0.54
1:W:287:ASP:OD2	1:W:289:SER:OG	2.24	0.54
1:X:404:LEU:H	1:X:434:ASN:ND2	2.05	0.54
1:C:287:ASP:OD2	1:C:289:SER:OG	2.26	0.54
1:S:293:LEU:HD11	1:S:296:ARG:HH11	1.72	0.54
1:W:404:LEU:H	1:W:434:ASN:ND2	2.04	0.54
1:C:280:GLU:HG3	1:C:372:ILE:HG12	1.90	0.54
1:Y:404:LEU:H	1:Y:434:ASN:HD21	1.55	0.54
1:H:417:ARG:HG3	1:H:422:PHE:HB3	1.90	0.53
1:Z:280:GLU:HG3	1:Z:372:ILE:HG12	1.90	0.53
1:A:287:ASP:OD2	1:A:289:SER:OG	2.27	0.53
1:E:287:ASP:OD2	1:E:289:SER:OG	2.28	0.53
1:J:389:VAL:HB	1:J:432:VAL:HG22	1.90	0.53
1:R:293:LEU:HD11	1:R:296:ARG:HH11	1.73	0.53
1:O:404:LEU:H	1:O:434:ASN:ND2	2.05	0.53
1:F:246:GLN:NE2	1:F:264:ALA:O	2.42	0.53
1:M:404:LEU:H	1:M:434:ASN:ND2	2.07	0.53
1:P:287:ASP:OD2	1:P:289:SER:OG	2.25	0.53
1:Q:293:LEU:HD11	1:Q:296:ARG:HH11	1.73	0.53
1:U:287:ASP:OD2	1:U:289:SER:OG	2.27	0.53
1:A:360:ARG:NH1	1:A:362:GLU:OE1	2.38	0.53
1:L:360:ARG:NH1	1:L:362:GLU:OE1	2.36	0.53
1:Y:418:GLU:HB2	1:Z:388:ALA:HB2	1.91	0.53
1:J:387:VAL:HG21	1:J:420:MET:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:360:ARG:NH1	1:O:362:GLU:OE1	2.40	0.53
1:Q:287:ASP:OD2	1:Q:289:SER:OG	2.26	0.53
1:Q:360:ARG:NH1	1:Q:362:GLU:OE1	2.41	0.53
1:U:258:GLY:HA3	1:U:261:ASN:HD22	1.74	0.53
1:X:360:ARG:NH1	1:X:362:GLU:OE1	2.40	0.52
1:Y:287:ASP:OD2	1:Y:289:SER:OG	2.27	0.52
1:N:417:ARG:HG3	1:N:422:PHE:HB3	1.91	0.52
1:A:280:GLU:HG3	1:A:372:ILE:HG12	1.91	0.52
1:G:258:GLY:HA3	1:G:261:ASN:HD22	1.75	0.52
1:L:389:VAL:HB	1:L:432:VAL:HG22	1.91	0.52
1:R:360:ARG:NH1	1:R:362:GLU:OE1	2.39	0.52
1:C:404:LEU:H	1:C:434:ASN:ND2	2.08	0.52
1:N:280:GLU:HG3	1:N:372:ILE:HG12	1.91	0.52
1:Z:360:ARG:NH1	1:Z:362:GLU:OE1	2.42	0.52
1:D:417:ARG:HG3	1:D:422:PHE:HB3	1.92	0.52
1:O:417:ARG:HG3	1:O:422:PHE:HB3	1.91	0.52
1:Q:267:THR:HB	1:Q:386:SER:HB2	1.92	0.52
1:Y:280:GLU:HG3	1:Y:372:ILE:HG12	1.92	0.52
1:L:293:LEU:HD11	1:L:296:ARG:HH11	1.75	0.52
1:G:389:VAL:HB	1:G:432:VAL:HG22	1.92	0.51
1:E:380:GLY:HA3	1:F:231:ASN:HD21	2.56	0.51
1:F:404:LEU:H	1:F:434:ASN:ND2	2.11	0.51
1:A:246:GLN:NE2	1:A:264:ALA:O	2.44	0.51
1:F:360:ARG:NH1	1:F:362:GLU:OE1	2.43	0.51
1:S:287:ASP:OD2	1:S:289:SER:OG	2.28	0.51
1:U:404:LEU:H	1:U:434:ASN:ND2	2.09	0.51
1:Q:417:ARG:HG3	1:Q:422:PHE:HB3	1.92	0.51
1:O:250:GLU:O	1:O:254:SER:OG	2.21	0.51
1:N:360:ARG:NH1	1:N:362:GLU:OE1	2.42	0.51
1:Z:267:THR:HB	1:Z:386:SER:HB2	1.93	0.51
1:B:393:TYR:CE2	1:B:436:PRO:HD3	2.53	0.51
1:C:373:ARG:NH2	1:D:275:LYS:HD3	2.26	0.51
1:I:250:GLU:O	1:I:254:SER:OG	2.18	0.51
1:T:258:GLY:HA3	1:T:261:ASN:HD22	1.75	0.51
1:Y:417:ARG:HG3	1:Y:422:PHE:HB3	1.93	0.51
1:A:373:ARG:NH2	1:B:275:LYS:HD3	2.27	0.51
1:S:373:ARG:NH2	1:T:275:LYS:HD3	2.26	0.51
1:F:418:GLU:HB2	1:G:388:ALA:HB2	1.97	0.50
1:Z:287:ASP:OD2	1:Z:289:SER:OG	2.29	0.50
1:R:389:VAL:HB	1:R:432:VAL:HG22	1.93	0.50
1:Q:373:ARG:NH2	1:R:275:LYS:HD3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ARG:HG3	1:A:422:PHE:HB3	1.93	0.50
1:B:280:GLU:HG3	1:B:372:ILE:HG12	1.93	0.50
1:I:287:ASP:OD2	1:I:289:SER:OG	2.29	0.50
1:D:360:ARG:NH1	1:D:362:GLU:OE1	2.43	0.50
1:L:404:LEU:H	1:L:434:ASN:ND2	2.10	0.50
1:A:275:LYS:HD3	1:G:373:ARG:NH2	82.97	0.50
1:D:393:TYR:CE2	1:D:436:PRO:HD3	2.47	0.50
1:M:417:ARG:HG3	1:M:422:PHE:HB3	1.94	0.50
1:U:246:GLN:NE2	1:U:264:ALA:O	2.44	0.50
1:Z:250:GLU:O	1:Z:254:SER:OG	2.19	0.50
1:E:393:TYR:CE2	1:E:436:PRO:HD3	2.47	0.50
1:J:373:ARG:NH2	1:K:275:LYS:HD3	2.27	0.50
1:M:258:GLY:HA3	1:M:261:ASN:HD22	1.76	0.49
1:R:373:ARG:NH2	1:S:275:LYS:HD3	2.27	0.49
1:G:417:ARG:HG3	1:G:422:PHE:HB3	1.94	0.49
1:A:388:ALA:HB2	1:Z:418:GLU:HB2	115.15	0.49
1:C:360:ARG:NH1	1:C:362:GLU:OE1	2.42	0.49
1:C:393:TYR:CE2	1:C:436:PRO:HD3	2.49	0.49
1:M:267:THR:HB	1:M:386:SER:HB2	1.94	0.49
1:M:387:VAL:HG21	1:M:420:MET:HG2	1.93	0.49
1:M:373:ARG:NH2	1:N:275:LYS:HD3	2.27	0.49
1:P:246:GLN:NE2	1:P:264:ALA:O	2.45	0.49
1:R:417:ARG:HG3	1:R:422:PHE:HB3	1.93	0.49
1:S:404:LEU:H	1:S:434:ASN:ND2	2.08	0.49
1:T:267:THR:HB	1:T:386:SER:HB2	1.94	0.49
1:U:387:VAL:HG21	1:U:420:MET:HG2	1.93	0.49
1:E:417:ARG:HG3	1:E:422:PHE:HB3	1.95	0.49
1:F:417:ARG:HG3	1:F:422:PHE:HB3	1.97	0.49
1:H:373:ARG:NH2	1:I:275:LYS:HD3	2.27	0.49
1:Q:283:SER:HB2	1:Q:369:ASP:HB2	1.95	0.49
1:V:373:ARG:NH2	1:W:275:LYS:HD3	2.27	0.49
1:G:393:TYR:CE2	1:G:436:PRO:HD3	2.47	0.49
1:I:373:ARG:NH2	1:J:275:LYS:HD3	2.28	0.49
1:P:373:ARG:NH2	1:Q:275:LYS:HD3	2.27	0.49
1:I:360:ARG:NH1	1:I:362:GLU:OE1	2.44	0.49
1:K:373:ARG:NH2	1:L:275:LYS:HD3	2.27	0.49
1:D:267:THR:HB	1:D:386:SER:HB2	2.02	0.49
1:G:360:ARG:NH1	1:G:362:GLU:OE1	2.43	0.49
1:I:267:THR:HB	1:I:386:SER:HB2	1.94	0.49
1:U:360:ARG:NH1	1:U:362:GLU:OE1	2.39	0.49
1:W:418:GLU:HB2	1:X:388:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:LEU:HD11	1:E:433:VAL:HG21	1.95	0.49
1:G:373:ARG:NH2	1:H:275:LYS:HD3	2.28	0.49
1:W:373:ARG:NH2	1:X:275:LYS:HD3	2.27	0.49
1:I:393:TYR:CE2	1:I:436:PRO:HD3	2.48	0.48
1:S:267:THR:HB	1:S:386:SER:HB2	1.95	0.48
1:S:393:TYR:CE2	1:S:436:PRO:HD3	2.48	0.48
1:V:393:TYR:CE2	1:V:436:PRO:HD3	2.48	0.48
1:X:415:LEU:HD11	1:Y:433:VAL:HG21	1.94	0.48
1:U:393:TYR:CE2	1:U:436:PRO:HD3	2.48	0.48
1:X:280:GLU:HG3	1:X:372:ILE:HG12	1.94	0.48
1:B:389:VAL:HB	1:B:432:VAL:HG22	1.95	0.48
1:G:267:THR:HB	1:G:386:SER:HB2	2.06	0.48
1:T:404:LEU:H	1:T:434:ASN:ND2	2.11	0.48
1:Y:410:LYS:HB3	1:Y:410:LYS:HE2	1.67	0.48
1:A:275:LYS:HD3	1:Z:373:ARG:NH2	83.50	0.48
1:A:393:TYR:CE2	1:A:436:PRO:HD3	2.48	0.48
1:H:287:ASP:OD2	1:H:289:SER:OG	2.31	0.48
1:X:418:GLU:HB2	1:Y:388:ALA:HB2	1.96	0.48
1:O:393:TYR:CE2	1:O:436:PRO:HD3	2.49	0.48
1:H:267:THR:HB	1:H:386:SER:HB2	1.95	0.48
1:K:280:GLU:HG3	1:K:372:ILE:HG12	1.95	0.48
1:Q:393:TYR:CE2	1:Q:436:PRO:HD3	2.49	0.48
1:H:393:TYR:CE2	1:H:436:PRO:HD3	2.49	0.48
1:K:250:GLU:O	1:K:254:SER:OG	2.21	0.48
1:M:393:TYR:CE2	1:M:436:PRO:HD3	2.48	0.48
1:O:418:GLU:HB2	1:P:388:ALA:HB2	1.96	0.48
1:Q:404:LEU:H	1:Q:434:ASN:ND2	2.12	0.48
1:T:393:TYR:CE2	1:T:436:PRO:HD3	2.48	0.48
1:V:258:GLY:HA3	1:V:261:ASN:HD22	1.77	0.48
1:Y:404:LEU:H	1:Y:434:ASN:ND2	2.11	0.48
1:B:417:ARG:HG3	1:B:422:PHE:HB3	1.96	0.48
1:I:246:GLN:NE2	1:I:264:ALA:O	2.46	0.48
1:I:280:GLU:HG3	1:I:372:ILE:HG12	1.96	0.48
1:N:415:LEU:HD11	1:O:433:VAL:HG21	1.95	0.48
1:T:287:ASP:OD2	1:T:289:SER:OG	2.29	0.48
1:A:250:GLU:O	1:A:254:SER:OG	2.22	0.48
1:D:418:GLU:HB2	1:E:388:ALA:HB2	2.00	0.48
1:F:393:TYR:CE2	1:F:436:PRO:HD3	2.54	0.48
1:X:373:ARG:NH2	1:Y:275:LYS:HD3	2.28	0.48
1:Z:246:GLN:NE2	1:Z:264:ALA:O	2.46	0.48
1:A:418:GLU:HB2	1:B:388:ALA:HB2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:GLU:HB2	1:F:388:ALA:HB2	1.96	0.48
1:J:250:GLU:O	1:J:254:SER:OG	2.20	0.48
1:L:393:TYR:CE2	1:L:436:PRO:HD3	2.49	0.48
1:C:267:THR:HB	1:C:386:SER:HB2	1.95	0.47
1:G:250:GLU:O	1:G:254:SER:OG	2.21	0.47
1:V:267:THR:HB	1:V:386:SER:HB2	1.95	0.47
1:A:267:THR:HB	1:A:386:SER:HB2	1.97	0.47
1:D:280:GLU:HG3	1:D:372:ILE:HG12	1.96	0.47
1:H:389:VAL:HB	1:H:432:VAL:HG22	1.96	0.47
1:J:393:TYR:CE2	1:J:436:PRO:HD3	2.50	0.47
1:P:418:GLU:HB2	1:Q:388:ALA:HB2	1.96	0.47
1:C:250:GLU:O	1:C:254:SER:OG	2.18	0.47
1:I:404:LEU:H	1:I:434:ASN:ND2	2.12	0.47
1:W:360:ARG:NH1	1:W:362:GLU:OE1	2.42	0.47
1:X:246:GLN:NE2	1:X:264:ALA:O	2.47	0.47
1:Y:393:TYR:CE2	1:Y:436:PRO:HD3	2.49	0.47
1:J:267:THR:HB	1:J:386:SER:HB2	1.96	0.47
1:E:392:ASN:OD1	1:E:393:TYR:N	2.48	0.47
1:G:246:GLN:NE2	1:G:264:ALA:O	2.48	0.47
1:G:415:LEU:HD11	1:H:433:VAL:HG21	1.97	0.47
1:O:292:THR:HG21	1:P:282:TYR:HB3	1.97	0.47
1:F:389:VAL:HB	1:F:432:VAL:HG22	1.99	0.47
1:I:389:VAL:HB	1:I:432:VAL:HG22	1.96	0.47
1:K:418:GLU:HB2	1:L:388:ALA:HB2	1.97	0.47
1:S:418:GLU:HB2	1:T:388:ALA:HB2	1.96	0.47
1:V:246:GLN:NE2	1:V:264:ALA:O	2.47	0.47
1:Z:404:LEU:H	1:Z:434:ASN:ND2	2.13	0.47
1:C:389:VAL:HB	1:C:432:VAL:HG22	1.97	0.47
1:N:267:THR:HB	1:N:386:SER:HB2	1.95	0.47
1:R:404:LEU:H	1:R:434:ASN:ND2	2.12	0.47
1:V:250:GLU:O	1:V:254:SER:OG	2.19	0.47
1:P:389:VAL:HB	1:P:432:VAL:HG22	1.96	0.47
1:X:250:GLU:O	1:X:254:SER:OG	2.21	0.47
1:M:246:GLN:NE2	1:M:264:ALA:O	2.47	0.47
1:N:389:VAL:HB	1:N:432:VAL:HG22	1.96	0.47
1:B:414:ASP:HB3	1:C:431:ASN:ND2	2.70	0.47
1:E:389:VAL:HB	1:E:432:VAL:HG22	1.97	0.47
1:F:392:ASN:OD1	1:F:393:TYR:N	2.48	0.47
1:J:410:LYS:HB3	1:J:410:LYS:HE2	1.68	0.47
1:K:360:ARG:NH1	1:K:362:GLU:OE1	2.47	0.47
1:N:373:ARG:NH2	1:O:275:LYS:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:373:ARG:NH2	1:Z:275:LYS:HD3	2.30	0.47
1:D:373:ARG:NH2	1:E:275:LYS:HD3	2.50	0.46
1:E:267:THR:HB	1:E:386:SER:HB2	2.00	0.46
1:H:246:GLN:NE2	1:H:264:ALA:O	2.48	0.46
1:H:418:GLU:HB2	1:I:388:ALA:HB2	1.98	0.46
1:T:280:GLU:HG3	1:T:372:ILE:HG12	1.97	0.46
1:T:417:ARG:HG3	1:T:422:PHE:HB3	1.96	0.46
1:C:418:GLU:HB2	1:D:388:ALA:HB2	1.98	0.46
1:D:389:VAL:HB	1:D:432:VAL:HG22	1.97	0.46
1:J:417:ARG:HG3	1:J:422:PHE:HB3	1.97	0.46
1:Q:389:VAL:HB	1:Q:432:VAL:HG22	1.96	0.46
1:V:360:ARG:NH1	1:V:362:GLU:OE1	2.44	0.46
1:P:415:LEU:HD11	1:Q:433:VAL:HG21	1.97	0.46
1:Z:393:TYR:CE2	1:Z:436:PRO:HD3	2.50	0.46
1:N:418:GLU:HB2	1:O:388:ALA:HB2	1.98	0.46
1:O:280:GLU:HG3	1:O:372:ILE:HG12	1.98	0.46
1:O:373:ARG:NH2	1:P:275:LYS:HD3	2.30	0.46
1:R:393:TYR:CE2	1:R:436:PRO:HD3	2.50	0.46
1:U:389:VAL:HB	1:U:432:VAL:HG22	1.97	0.46
1:V:410:LYS:HB3	1:V:410:LYS:HE2	1.68	0.46
1:W:389:VAL:HB	1:W:432:VAL:HG22	1.98	0.46
1:L:246:GLN:NE2	1:L:264:ALA:O	2.49	0.46
1:B:410:LYS:HB3	1:B:410:LYS:HE2	1.70	0.46
1:B:418:GLU:HB2	1:C:388:ALA:HB2	1.98	0.46
1:T:250:GLU:O	1:T:254:SER:OG	2.16	0.46
1:U:280:GLU:HG3	1:U:372:ILE:HG12	1.97	0.46
1:W:267:THR:HB	1:W:386:SER:HB2	1.98	0.46
1:X:394:LYS:O	1:X:402:LEU:N	2.48	0.46
1:B:373:ARG:NH2	1:C:275:LYS:HD3	2.52	0.46
1:B:415:LEU:HD11	1:C:433:VAL:HG21	1.98	0.46
1:E:415:LEU:HD11	1:F:433:VAL:HG21	1.97	0.46
1:I:418:GLU:HB2	1:J:388:ALA:HB2	1.98	0.46
1:K:417:ARG:HG3	1:K:422:PHE:HB3	1.98	0.46
1:W:250:GLU:O	1:W:254:SER:OG	2.20	0.46
1:R:280:GLU:HG3	1:R:372:ILE:HG12	1.98	0.46
1:S:360:ARG:NH1	1:S:362:GLU:OE1	2.43	0.46
1:P:301:SER:HB3	1:P:359:GLN:HB3	1.97	0.46
1:Q:418:GLU:HB2	1:R:388:ALA:HB2	1.98	0.46
1:V:418:GLU:HB2	1:W:388:ALA:HB2	1.98	0.46
1:A:388:ALA:HB2	1:G:418:GLU:HB2	113.74	0.45
1:L:267:THR:HB	1:L:386:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:393:TYR:CE2	1:N:436:PRO:HD3	2.52	0.45
1:Q:415:LEU:HD11	1:R:433:VAL:HG21	1.97	0.45
1:V:389:VAL:HB	1:V:432:VAL:HG22	1.97	0.45
1:X:252:ILE:HD13	1:Y:265:GLN:HG2	1.98	0.45
1:A:392:ASN:OD1	1:A:393:TYR:N	2.58	0.45
1:C:415:LEU:HD11	1:D:433:VAL:HG21	1.98	0.45
1:M:389:VAL:HB	1:M:432:VAL:HG22	1.98	0.45
1:P:417:ARG:HG3	1:P:422:PHE:HB3	1.98	0.45
1:X:389:VAL:HB	1:X:432:VAL:HG22	1.97	0.45
1:Z:410:LYS:HB3	1:Z:410:LYS:HE2	1.68	0.45
1:J:360:ARG:NH1	1:J:362:GLU:OE1	2.48	0.45
1:T:389:VAL:HB	1:T:432:VAL:HG22	1.97	0.45
1:T:415:LEU:HD11	1:U:433:VAL:HG21	1.98	0.45
1:B:292:THR:HG21	1:C:282:TYR:HB3	1.99	0.45
1:P:267:THR:HB	1:P:386:SER:HB2	1.98	0.45
1:Y:246:GLN:NE2	1:Y:264:ALA:O	2.50	0.45
1:D:246:GLN:NE2	1:D:264:ALA:O	2.50	0.45
1:M:418:GLU:HG3	1:N:431:ASN:HB2	1.97	0.45
1:U:292:THR:HG21	1:V:282:TYR:HB3	1.99	0.45
1:B:394:LYS:O	1:B:402:LEU:N	2.50	0.45
1:I:417:ARG:HG3	1:I:422:PHE:HB3	1.99	0.45
1:L:415:LEU:HD11	1:M:433:VAL:HG21	1.97	0.45
1:Y:267:THR:HB	1:Y:386:SER:HB2	1.98	0.45
1:X:371:THR:HG23	1:Y:279:GLU:HG3	1.99	0.45
1:A:389:VAL:HB	1:A:432:VAL:HG22	1.99	0.45
1:B:267:THR:HB	1:B:386:SER:HB2	1.98	0.45
1:K:392:ASN:OD1	1:K:393:TYR:N	2.50	0.45
1:R:415:LEU:HD11	1:S:433:VAL:HG21	1.98	0.45
1:W:246:GLN:NE2	1:W:264:ALA:O	2.50	0.45
1:A:394:LYS:O	1:A:402:LEU:N	2.62	0.45
1:F:267:THR:HB	1:F:386:SER:HB2	2.00	0.45
1:U:392:ASN:OD1	1:U:393:TYR:N	2.50	0.45
1:D:296:ARG:NH2	1:D:362:GLU:OE2	2.50	0.45
1:E:292:THR:HG21	1:F:282:TYR:HB3	2.00	0.45
1:I:415:LEU:HD11	1:J:433:VAL:HG21	1.98	0.45
1:L:418:GLU:HB2	1:M:388:ALA:HB2	1.99	0.45
1:P:393:TYR:CE2	1:P:436:PRO:HD3	2.52	0.45
1:P:392:ASN:OD1	1:P:393:TYR:N	2.50	0.45
1:Z:389:VAL:HB	1:Z:432:VAL:HG22	1.99	0.45
1:D:394:LYS:O	1:D:402:LEU:N	2.50	0.44
1:X:392:ASN:OD1	1:X:393:TYR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ARG:NH2	1:F:275:LYS:HD3	2.35	0.44
1:U:252:ILE:HD13	1:V:265:GLN:HG2	2.00	0.44
1:G:296:ARG:NH2	1:G:362:GLU:OE2	2.55	0.44
1:J:418:GLU:HB2	1:K:388:ALA:HB2	2.00	0.44
1:L:392:ASN:OD1	1:L:393:TYR:N	2.51	0.44
1:Q:389:VAL:HG21	1:Q:416:THR:HG21	1.98	0.44
1:R:292:THR:HG21	1:S:282:TYR:HB3	2.00	0.44
1:T:246:GLN:NE2	1:T:264:ALA:O	2.51	0.44
1:V:417:ARG:HG3	1:V:422:PHE:HB3	1.98	0.44
1:R:246:GLN:NE2	1:R:264:ALA:O	2.51	0.44
1:W:415:LEU:HD11	1:X:433:VAL:HG21	1.99	0.44
1:C:417:ARG:HG3	1:C:422:PHE:HB3	2.05	0.44
1:O:267:THR:HB	1:O:386:SER:HB2	2.00	0.44
1:F:410:LYS:HB3	1:F:410:LYS:HE2	3.12	0.44
1:O:389:VAL:HB	1:O:432:VAL:HG22	1.98	0.44
1:S:415:LEU:HD11	1:T:433:VAL:HG21	2.00	0.44
1:X:393:TYR:CE2	1:X:436:PRO:HD3	2.52	0.44
1:B:276:GLU:HG2	1:B:376:LYS:HG3	1.99	0.44
1:Q:390:VAL:HG12	1:Q:433:VAL:HG22	1.99	0.44
1:E:246:GLN:NE2	1:E:264:ALA:O	2.50	0.44
1:L:417:ARG:HG3	1:L:422:PHE:HB3	1.99	0.44
1:U:418:GLU:HB2	1:V:388:ALA:HB2	1.99	0.44
1:D:390:VAL:HG12	1:D:433:VAL:HG22	2.00	0.44
1:F:280:GLU:HG3	1:F:372:ILE:HG12	2.01	0.44
1:A:296:ARG:NH2	1:A:362:GLU:OE2	2.51	0.43
1:W:394:LYS:O	1:W:402:LEU:N	2.51	0.43
1:A:433:VAL:HG21	1:G:415:LEU:HD11	122.81	0.43
1:B:392:ASN:OD1	1:B:393:TYR:N	2.57	0.43
1:K:393:TYR:CE2	1:K:436:PRO:HD3	2.53	0.43
1:R:275:LYS:HB2	1:R:275:LYS:HE3	1.71	0.43
1:R:418:GLU:HB2	1:S:388:ALA:HB2	2.00	0.43
1:V:296:ARG:NH2	1:V:362:GLU:OE2	2.50	0.43
1:Y:389:VAL:HB	1:Y:432:VAL:HG22	1.99	0.43
1:K:296:ARG:NH2	1:K:362:GLU:OE2	2.51	0.43
1:M:392:ASN:OD1	1:M:393:TYR:N	2.51	0.43
1:O:271:ASP:HB2	1:O:383:GLU:HG3	2.00	0.43
1:B:296:ARG:NH2	1:B:362:GLU:OE2	2.52	0.43
1:G:418:GLU:HB2	1:H:388:ALA:HB2	2.01	0.43
1:S:394:LYS:O	1:S:402:LEU:N	2.52	0.43
1:W:393:TYR:CE2	1:W:436:PRO:HD3	2.53	0.43
1:G:280:GLU:HG3	1:G:372:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:418:GLU:HG3	1:L:431:ASN:HB2	2.00	0.43
1:K:415:LEU:HD11	1:L:433:VAL:HG21	1.99	0.43
1:N:392:ASN:OD1	1:N:393:TYR:N	2.52	0.43
1:V:415:LEU:HD11	1:W:433:VAL:HG21	2.00	0.43
1:A:415:LEU:HD11	1:B:433:VAL:HG21	2.01	0.43
1:X:301:SER:HB2	1:X:359:GLN:HB3	2.00	0.43
1:E:360:ARG:NH1	1:E:362:GLU:OE1	2.44	0.43
1:E:418:GLU:HG3	1:F:431:ASN:HB2	2.01	0.43
1:H:271:ASP:HB2	1:H:383:GLU:HG2	2.01	0.43
1:F:418:GLU:HG3	1:G:431:ASN:HB2	2.00	0.43
1:H:275:LYS:HB2	1:H:275:LYS:HE3	1.74	0.43
1:H:292:THR:HG21	1:I:282:TYR:HB3	2.01	0.43
1:M:418:GLU:HB2	1:N:388:ALA:HB2	2.01	0.43
1:N:394:LYS:O	1:N:402:LEU:N	2.52	0.43
1:R:418:GLU:HG3	1:S:431:ASN:HB2	2.01	0.43
1:T:418:GLU:HB2	1:U:388:ALA:HB2	2.01	0.43
1:T:390:VAL:HG12	1:T:433:VAL:HG22	2.01	0.43
1:Y:296:ARG:NH2	1:Y:362:GLU:OE2	2.52	0.43
1:F:296:ARG:NH2	1:F:362:GLU:OE2	2.52	0.43
1:Q:410:LYS:HE2	1:Q:410:LYS:HB3	1.70	0.43
1:W:410:LYS:HB3	1:W:410:LYS:HE2	1.67	0.43
1:B:246:GLN:NE2	1:B:264:ALA:O	2.55	0.43
1:E:280:GLU:HG3	1:E:372:ILE:HG12	2.03	0.43
1:S:275:LYS:HE3	1:S:275:LYS:HB2	1.73	0.43
1:T:275:LYS:HE3	1:T:275:LYS:HB2	1.74	0.43
1:T:296:ARG:NH2	1:T:362:GLU:OE2	2.52	0.43
1:D:392:ASN:OD1	1:D:393:TYR:N	2.52	0.42
1:E:394:LYS:O	1:E:402:LEU:N	2.55	0.42
1:O:371:THR:HG23	1:P:279:GLU:HG3	2.01	0.42
1:S:389:VAL:HB	1:S:432:VAL:HG22	1.99	0.42
1:K:267:THR:HB	1:K:386:SER:HB2	2.01	0.42
1:M:296:ARG:NH2	1:M:362:GLU:OE2	2.52	0.42
1:M:280:GLU:HG3	1:M:372:ILE:HG12	2.02	0.42
1:K:389:VAL:HB	1:K:432:VAL:HG22	2.01	0.42
1:L:371:THR:HG23	1:M:279:GLU:HG3	2.02	0.42
1:N:246:GLN:NE2	1:N:264:ALA:O	2.52	0.42
1:M:415:LEU:HD11	1:N:433:VAL:HG21	2.01	0.42
1:R:267:THR:HB	1:R:386:SER:HB2	2.00	0.42
1:E:296:ARG:NH2	1:E:362:GLU:OE2	2.52	0.42
1:G:410:LYS:HB3	1:G:410:LYS:HE2	4.33	0.42
1:V:392:ASN:OD1	1:V:393:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ARG:NH2	1:C:362:GLU:OE2	2.58	0.42
1:C:392:ASN:OD1	1:C:393:TYR:N	2.57	0.42
1:H:231:ASN:CG	1:H:232:ASP:H	2.22	0.42
1:H:392:ASN:OD1	1:H:393:TYR:N	2.52	0.42
1:H:394:LYS:O	1:H:402:LEU:N	2.52	0.42
1:I:296:ARG:NH2	1:I:362:GLU:OE2	2.52	0.42
1:L:280:GLU:HG3	1:L:372:ILE:HG12	2.02	0.42
1:S:246:GLN:NE2	1:S:264:ALA:O	2.52	0.42
1:S:392:ASN:OD1	1:S:393:TYR:N	2.53	0.42
1:J:296:ARG:NH2	1:J:362:GLU:OE2	2.53	0.42
1:P:275:LYS:HB2	1:P:275:LYS:HE3	1.75	0.42
1:Q:418:GLU:HG3	1:R:431:ASN:HB2	2.02	0.42
1:L:271:ASP:HB2	1:L:383:GLU:HG2	2.01	0.42
1:S:417:ARG:HG3	1:S:422:PHE:HB3	2.00	0.42
1:T:392:ASN:OD1	1:T:393:TYR:N	2.52	0.42
1:Z:296:ARG:NH2	1:Z:362:GLU:OE2	2.53	0.42
1:K:410:LYS:HB3	1:K:410:LYS:HE2	1.66	0.42
1:M:360:ARG:NH1	1:M:362:GLU:OE1	2.48	0.42
1:X:418:GLU:HG3	1:Y:431:ASN:HB2	2.02	0.42
1:S:296:ARG:NH2	1:S:362:GLU:OE2	2.52	0.42
1:Y:283:SER:HB2	1:Y:369:ASP:HB2	2.01	0.42
1:G:392:ASN:OD1	1:G:393:TYR:N	2.54	0.42
1:H:280:GLU:HG3	1:H:372:ILE:HG12	2.02	0.41
1:W:392:ASN:OD1	1:W:393:TYR:N	2.53	0.41
1:K:252:ILE:HD13	1:L:265:GLN:HG2	2.02	0.41
1:M:250:GLU:O	1:M:254:SER:OG	2.20	0.41
1:U:415:LEU:HD11	1:V:433:VAL:HG21	2.02	0.41
1:Z:390:VAL:HG12	1:Z:433:VAL:HG22	2.02	0.41
1:H:415:LEU:HD11	1:I:433:VAL:HG21	2.02	0.41
1:J:246:GLN:NE2	1:J:264:ALA:O	2.53	0.41
1:Q:296:ARG:NH2	1:Q:362:GLU:OE2	2.53	0.41
1:U:267:THR:HB	1:U:386:SER:HB2	2.03	0.41
1:J:389:VAL:HG21	1:J:416:THR:HG21	2.03	0.41
1:P:252:ILE:HD13	1:Q:265:GLN:HG2	2.03	0.41
1:O:418:GLU:HG3	1:P:431:ASN:HB2	2.02	0.41
1:G:390:VAL:HG12	1:G:433:VAL:HG22	2.30	0.41
1:J:392:ASN:OD1	1:J:393:TYR:N	2.53	0.41
1:N:292:THR:HG21	1:O:282:TYR:HB3	2.03	0.41
1:A:275:LYS:HB2	1:A:275:LYS:HE3	1.66	0.41
1:D:375:THR:HG23	1:E:275:LYS:HE2	2.97	0.41
1:G:231:ASN:N	1:G:231:ASN:OD1	4.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:296:ARG:NH2	1:W:362:GLU:OE2	2.53	0.41
1:B:252:ILE:HD13	1:C:265:GLN:HG2	2.06	0.41
1:C:277:GLN:NE2	1:C:279:GLU:OE2	2.54	0.41
1:G:293:LEU:HD13	1:G:296:ARG:HD2	2.03	0.41
1:M:295:SER:HB2	1:M:365:ASN:HD22	1.86	0.41
1:R:252:ILE:HD13	1:S:265:GLN:HG2	2.03	0.41
1:I:418:GLU:HG3	1:J:431:ASN:HB2	2.02	0.41
1:U:413:GLU:HG2	1:U:417:ARG:HH12	1.86	0.41
1:H:296:ARG:NH2	1:H:362:GLU:OE2	2.54	0.41
1:Y:292:THR:HG21	1:Z:282:TYR:HB3	2.03	0.41
1:M:301:SER:HB3	1:M:359:GLN:HB3	2.03	0.41
1:A:282:TYR:HB3	1:G:292:THR:HG21	72.75	0.41
1:F:292:THR:HG21	1:G:282:TYR:HB3	2.04	0.41
1:O:415:LEU:HD11	1:P:433:VAL:HG21	2.03	0.41
1:O:296:ARG:NH2	1:O:362:GLU:OE2	2.53	0.40
1:Q:246:GLN:NE2	1:Q:264:ALA:O	2.54	0.40
1:W:275:LYS:HE3	1:W:275:LYS:HB2	1.89	0.40
1:Y:392:ASN:OD1	1:Y:393:TYR:N	2.54	0.40
1:J:275:LYS:HE3	1:J:275:LYS:HB2	1.70	0.40
1:O:246:GLN:NE2	1:O:264:ALA:O	2.54	0.40
1:U:296:ARG:NH2	1:U:362:GLU:OE2	2.54	0.40
1:X:275:LYS:HE3	1:X:275:LYS:HB2	1.72	0.40
1:Z:412:ILE:O	1:Z:416:THR:HG22	2.21	0.40
1:A:433:VAL:HG21	1:Z:415:LEU:HD11	124.42	0.40
1:L:292:THR:HG21	1:M:282:TYR:HB3	2.04	0.40
1:N:296:ARG:NH2	1:N:362:GLU:OE2	2.54	0.40
1:R:392:ASN:OD1	1:R:393:TYR:N	2.54	0.40
1:A:265:GLN:HG2	1:Z:252:ILE:HD13	114.56	0.40
1:L:296:ARG:NH2	1:L:362:GLU:OE2	2.54	0.40
1:N:385:LEU:HA	1:N:385:LEU:HD23	1.96	0.40
1:Y:250:GLU:O	1:Y:254:SER:OG	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	B	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	C	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	D	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	E	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	F	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	G	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	H	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	I	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	J	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	K	145/560 (26%)	136 (94%)	9 (6%)	0	100	100
1	L	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	M	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	N	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	O	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	P	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	Q	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	R	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	S	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	T	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	U	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	V	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	W	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	X	145/560 (26%)	137 (94%)	8 (6%)	0	100	100
1	Y	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	Z	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	a	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	b	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	c	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	d	145/560 (26%)	139 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	f	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	g	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
All	All	4785/18480 (26%)	4579 (96%)	206 (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 PDB entries followed by that with respect to all EM entries.

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	134/467 (29%)	134 (100%)	0	100	100
1	B	134/467 (29%)	134 (100%)	0	100	100
1	C	134/467 (29%)	134 (100%)	0	100	100
1	D	134/467 (29%)	134 (100%)	0	100	100
1	E	134/467 (29%)	134 (100%)	0	100	100
1	F	134/467 (29%)	134 (100%)	0	100	100
1	G	134/467 (29%)	134 (100%)	0	100	100
1	H	134/467 (29%)	134 (100%)	0	100	100
1	I	134/467 (29%)	134 (100%)	0	100	100
1	J	134/467 (29%)	134 (100%)	0	100	100
1	K	134/467 (29%)	134 (100%)	0	100	100
1	L	134/467 (29%)	134 (100%)	0	100	100
1	M	134/467 (29%)	134 (100%)	0	100	100
1	N	134/467 (29%)	134 (100%)	0	100	100
1	O	134/467 (29%)	134 (100%)	0	100	100
1	P	134/467 (29%)	134 (100%)	0	100	100
1	Q	134/467 (29%)	134 (100%)	0	100	100
1	R	134/467 (29%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	134/467 (29%)	134 (100%)	0	100	100
1	T	134/467 (29%)	134 (100%)	0	100	100
1	U	134/467 (29%)	134 (100%)	0	100	100
1	V	134/467 (29%)	134 (100%)	0	100	100
1	W	134/467 (29%)	134 (100%)	0	100	100
1	X	134/467 (29%)	134 (100%)	0	100	100
1	Y	134/467 (29%)	134 (100%)	0	100	100
1	Z	134/467 (29%)	134 (100%)	0	100	100
1	a	134/467 (29%)	134 (100%)	0	100	100
1	b	134/467 (29%)	134 (100%)	0	100	100
1	c	134/467 (29%)	134 (100%)	0	100	100
1	d	134/467 (29%)	134 (100%)	0	100	100
1	e	134/467 (29%)	134 (100%)	0	100	100
1	f	134/467 (29%)	134 (100%)	0	100	100
1	g	134/467 (29%)	134 (100%)	0	100	100
All	All	4422/15411 (29%)	4422 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	263	HIS
1	A	365	ASN
1	A	434	ASN
1	B	261	ASN
1	B	263	HIS
1	B	434	ASN
1	C	261	ASN
1	C	277	GLN
1	C	365	ASN
1	C	434	ASN
1	D	261	ASN
1	D	263	HIS
1	D	365	ASN

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Mol	Chain	Res	Type
1	D	434	ASN
1	E	263	HIS
1	E	365	ASN
1	E	434	ASN
1	F	261	ASN
1	F	263	HIS
1	F	365	ASN
1	F	434	ASN
1	G	261	ASN
1	G	263	HIS
1	G	365	ASN
1	G	434	ASN
1	H	261	ASN
1	H	434	ASN
1	I	231	ASN
1	I	261	ASN
1	I	263	HIS
1	I	431	ASN
1	I	434	ASN
1	J	261	ASN
1	J	434	ASN
1	K	263	HIS
1	K	277	GLN
1	K	365	ASN
1	K	434	ASN
1	L	261	ASN
1	L	263	HIS
1	L	365	ASN
1	L	434	ASN
1	M	261	ASN
1	M	263	HIS
1	M	365	ASN
1	M	434	ASN
1	N	261	ASN
1	N	263	HIS
1	N	365	ASN
1	N	434	ASN
1	O	261	ASN
1	O	263	HIS
1	O	365	ASN
1	O	434	ASN
1	P	261	ASN

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Mol	Chain	Res	Type
1	P	263	HIS
1	P	365	ASN
1	P	434	ASN
1	Q	261	ASN
1	Q	263	HIS
1	Q	365	ASN
1	Q	434	ASN
1	R	261	ASN
1	R	263	HIS
1	R	365	ASN
1	R	431	ASN
1	R	434	ASN
1	S	261	ASN
1	S	263	HIS
1	S	274	ASN
1	S	365	ASN
1	S	434	ASN
1	T	261	ASN
1	T	263	HIS
1	T	277	GLN
1	T	365	ASN
1	T	434	ASN
1	U	261	ASN
1	U	263	HIS
1	U	434	ASN
1	V	261	ASN
1	V	263	HIS
1	V	365	ASN
1	V	434	ASN
1	W	261	ASN
1	W	263	HIS
1	W	277	GLN
1	W	365	ASN
1	W	434	ASN
1	X	261	ASN
1	X	263	HIS
1	X	277	GLN
1	X	365	ASN
1	X	434	ASN
1	Y	261	ASN
1	Y	263	HIS
1	Y	434	ASN

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Mol	Chain	Res	Type
1	Z	365	ASN
1	Z	434	ASN
1	a	261	ASN
1	a	263	HIS
1	a	365	ASN
1	a	434	ASN
1	b	261	ASN
1	b	263	HIS
1	b	365	ASN
1	b	434	ASN
1	c	261	ASN
1	c	365	ASN
1	c	434	ASN
1	d	261	ASN
1	d	263	HIS
1	d	434	ASN
1	e	261	ASN
1	e	263	HIS
1	e	434	ASN
1	f	231	ASN
1	f	261	ASN
1	f	263	HIS
1	f	434	ASN
1	g	231	ASN
1	g	261	ASN
1	g	263	HIS
1	g	365	ASN
1	g	434	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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.