



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:13 AM UTC

PDB ID : 8WK4 / pdb_00008wk4
EMDB ID : EMD-37595
Title : Cryo-EM structure of the MS ring with FlgB and FliE within the flagellar motor-hook complex in the CW state.
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-27
Resolution : 3.70 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

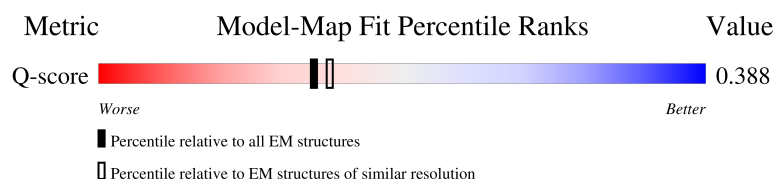
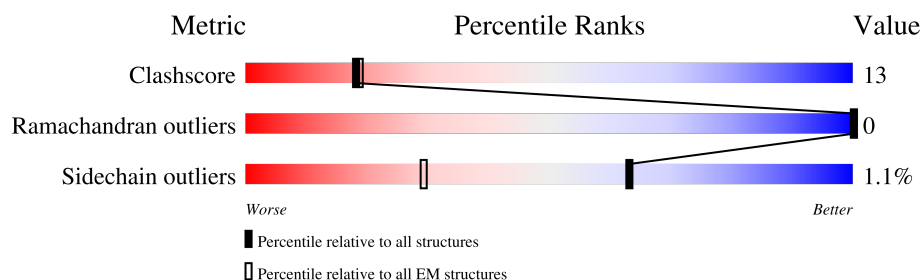
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



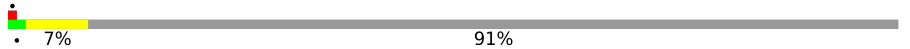
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	i	104	
1	j	104	
1	k	104	
1	l	104	

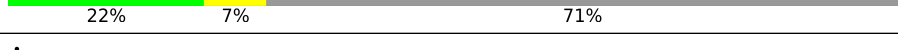
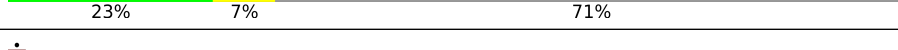
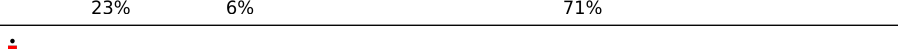
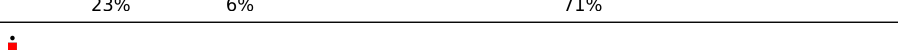
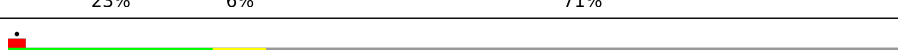
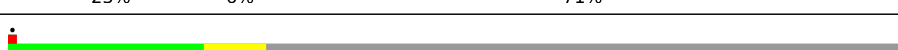
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Mol	Chain	Length	Quality of chain
1	m	104	 9% 9% 82%
1	n	104	 8% 10% 82%
2	o	138	 8% 88%
2	p	138	 7% 91%
2	q	138	 5% 6% 88%
2	r	138	 6% 6% 88%
2	s	138	 7% 88%
3	A	560	 22% 7% 71%
3	B	560	 23% 7% 71%
3	C	560	 23% 6% 71%
3	D	560	 23% 6% 71%
3	E	560	 23% 7% 71%
3	F	560	 23% 7% 71%
3	G	560	 22% 8% 71%
3	H	560	 22% 8% 71%
3	I	560	 23% 6% 71%
3	J	560	 23% 6% 71%
3	K	560	 23% 7% 71%
3	L	560	 23% 7% 71%
3	M	560	 22% 7% 71%
3	N	560	 22% 7% 71%
3	O	560	 23% 6% 71%
3	P	560	 23% 6% 71%
3	Q	560	 23% 6% 71%
3	R	560	 23% 6% 71%

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Mol	Chain	Length	Quality of chain
3	S	560	 22% 7% 71%
3	T	560	 23% 7% 71%
3	U	560	 22% 7% 71%
3	V	560	 23% 6% 71%
3	W	560	 23% 6% 71%
3	X	560	 23% 6% 71%
3	Y	560	 22% 7% 71%
3	Z	560	 23% 7% 71%
3	a	560	 23% 6% 71%
3	b	560	 23% 6% 71%
3	c	560	 23% 6% 71%
3	d	560	 23% 6% 71%
3	e	560	 22% 7% 71%
3	f	560	 22% 7% 71%
3	g	560	 22% 7% 71%
3	h	560	 22% 7% 71%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 44690 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 hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	19	Total	C	N	O	S	0	0
			129	80	22	26	1		
1	j	19	Total	C	N	O	S	0	0
			129	80	22	26	1		
1	k	19	Total	C	N	O	S	0	0
			129	80	22	26	1		
1	l	19	Total	C	N	O	S	0	0
			129	80	22	26	1		
1	m	19	Total	C	N	O	S	0	0
			129	80	22	26	1		
1	n	19	Total	C	N	O	S	0	0
			129	80	22	26	1		

- Molecule 2 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	o	17	Total	C	N	O	0	0
			116	72	22	22		
2	p	13	Total	C	N	O	0	0
			94	60	17	17		
2	q	17	Total	C	N	O	0	0
			119	75	22	22		
2	r	17	Total	C	N	O	0	0
			119	75	22	22		
2	s	17	Total	C	N	O	0	0
			118	74	22	22		

- Molecule 3 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
3	B	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	D	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	E	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	F	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	G	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	H	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	I	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	J	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	K	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	L	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	M	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	N	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	O	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	P	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	Q	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	R	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	S	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	T	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	U	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	V	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	W	164	Total 1275	C 776	N 237	O 259	S 3	0	0

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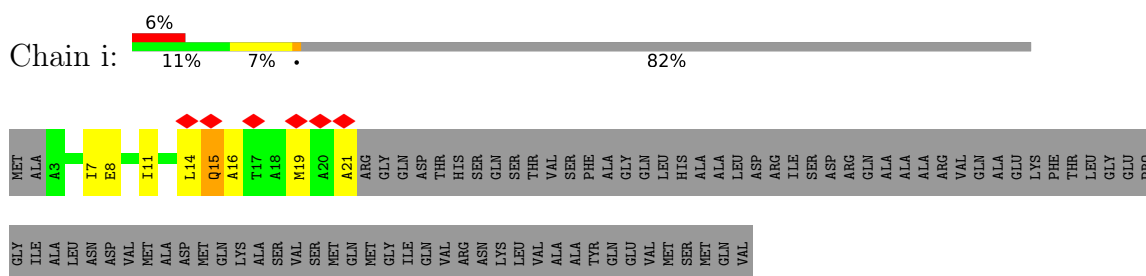
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	Y	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	Z	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	a	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	b	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	c	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	d	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	e	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	f	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	g	164	Total 1275	C 776	N 237	O 259	S 3	0	0
3	h	164	Total 1275	C 776	N 237	O 259	S 3	0	0

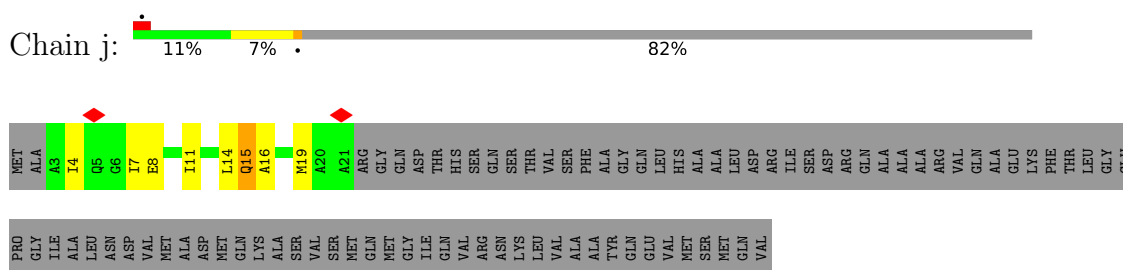
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

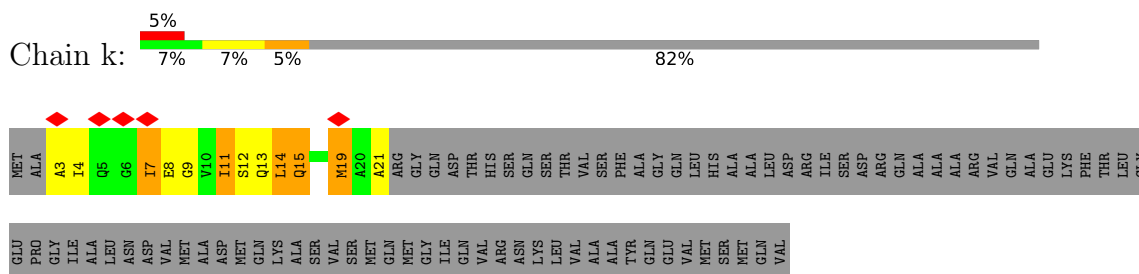
- Molecule 1: Flagellar hook-basal body complex protein FliE



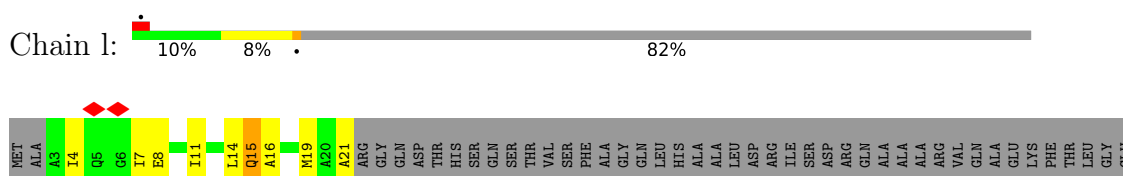
- Molecule 1: Flagellar hook-basal body complex protein FliE

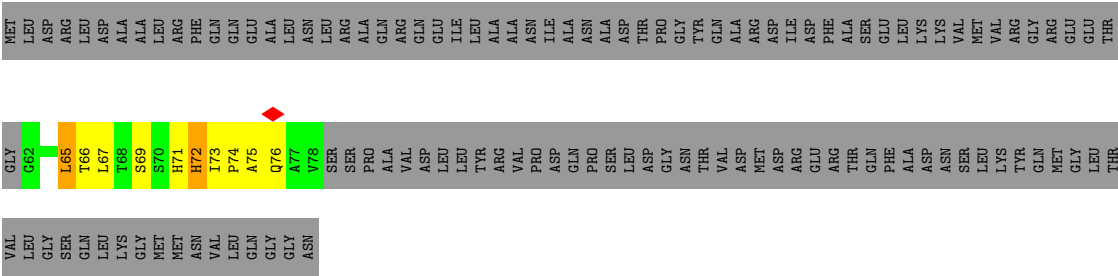


- Molecule 1: Flagellar hook-basal body complex protein FliE

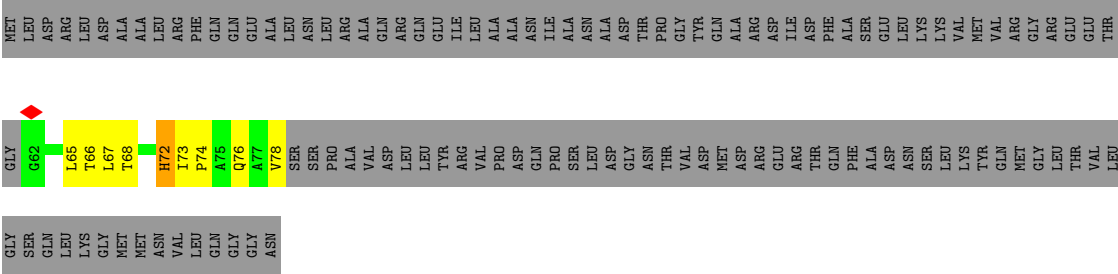


- Molecule 1: Flagellar hook-basal body complex protein FliE

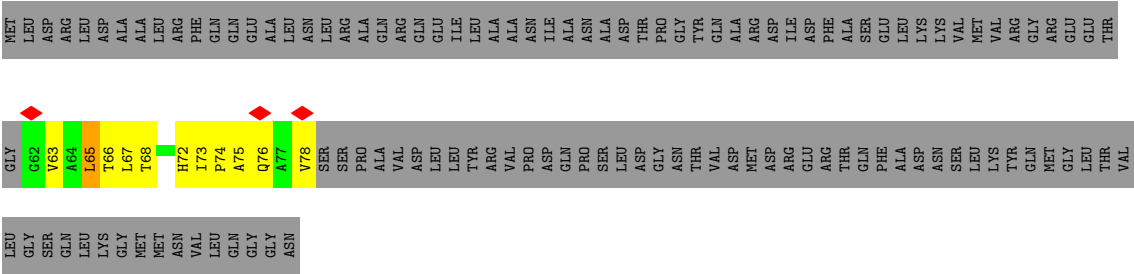




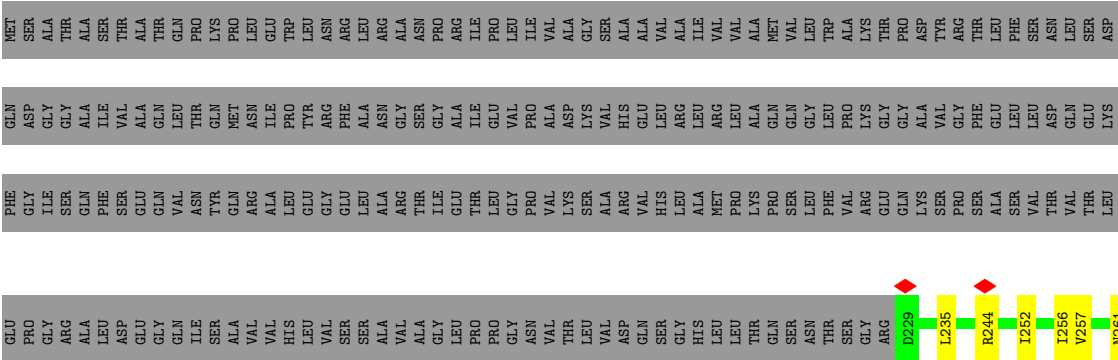
● Molecule 2: Flagellar basal body rod protein FlgB



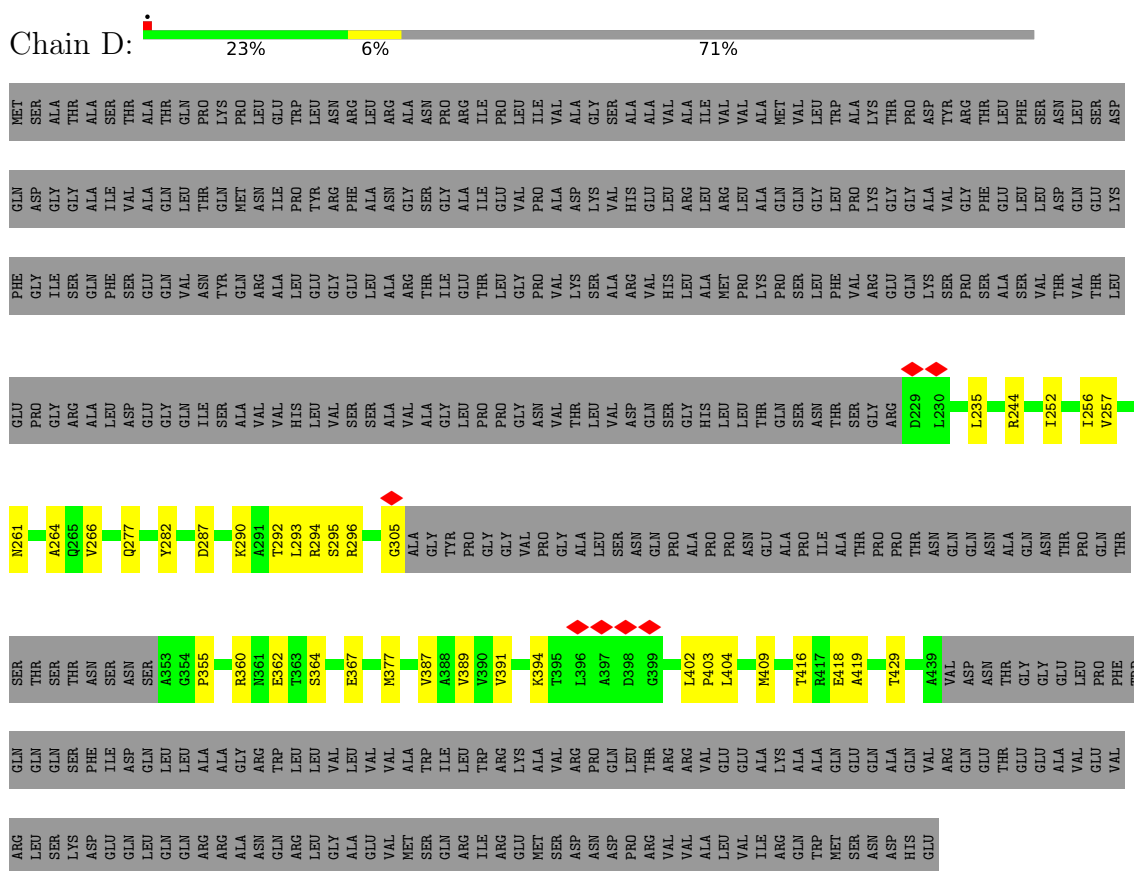
● Molecule 2: Flagellar basal body rod protein FlgB



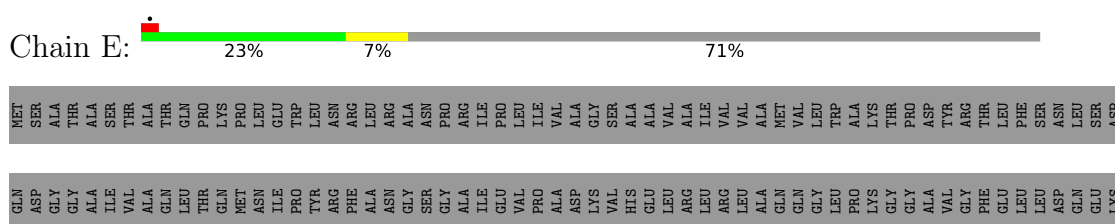
● Molecule 3: Flagellar M-ring protein

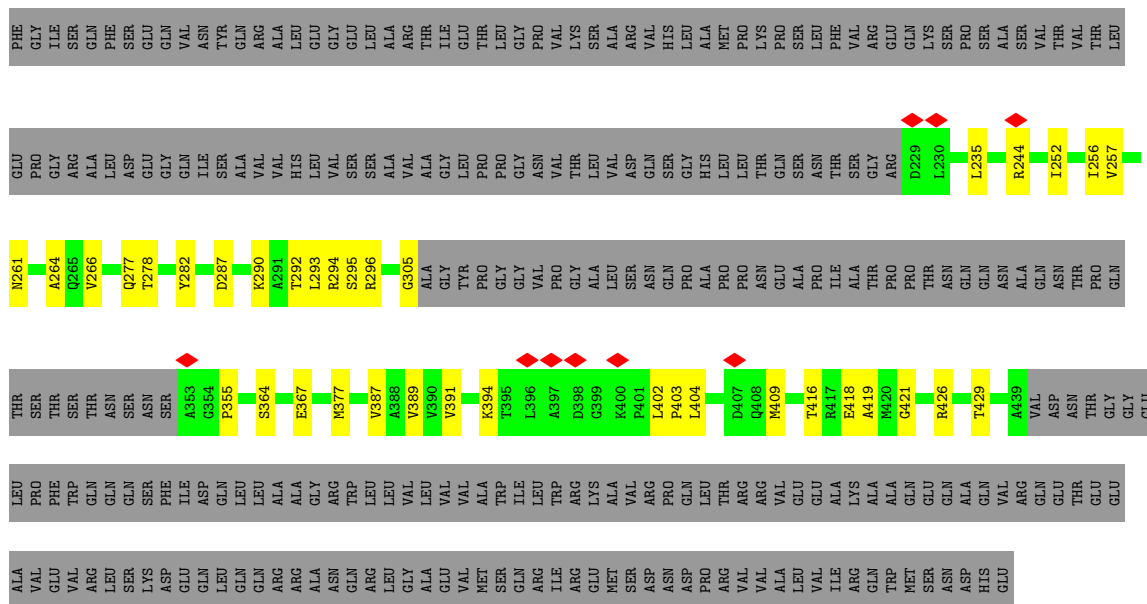


- Molecule 3: Flagellar M-ring protein

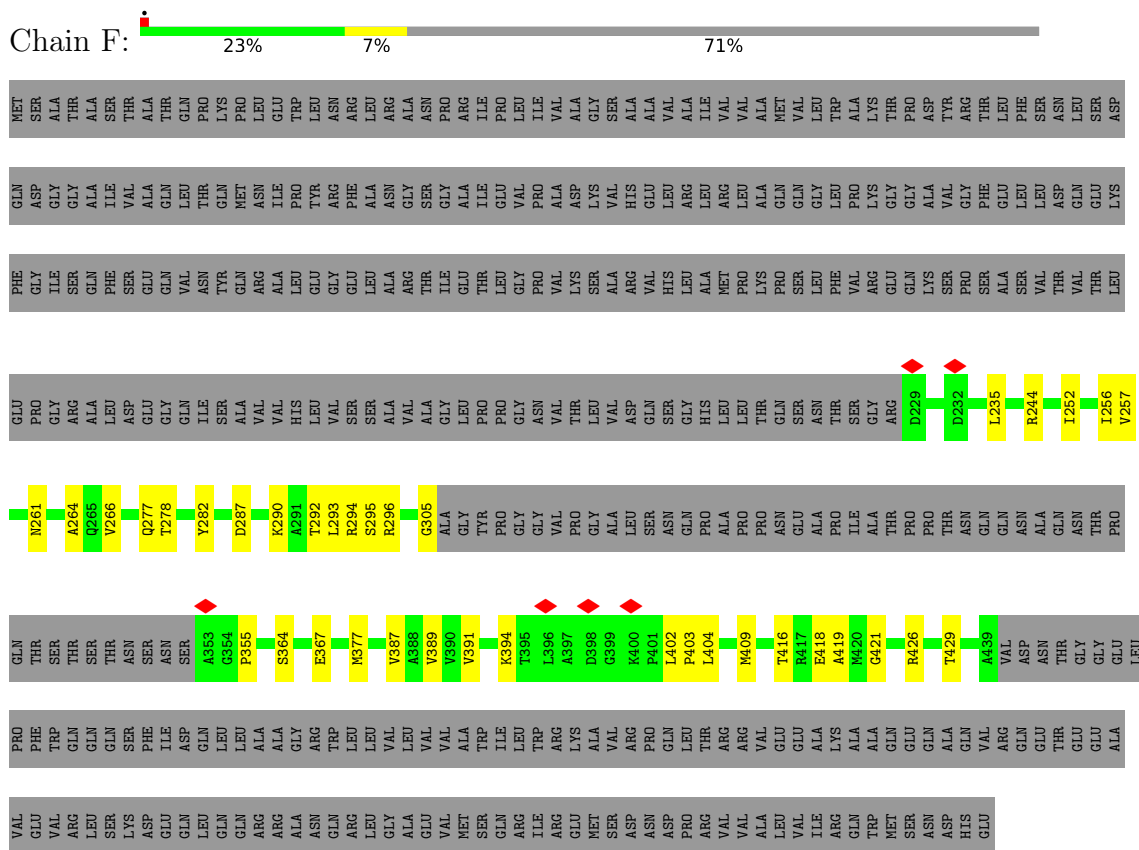


- Molecule 3: Flagellar M-ring protein

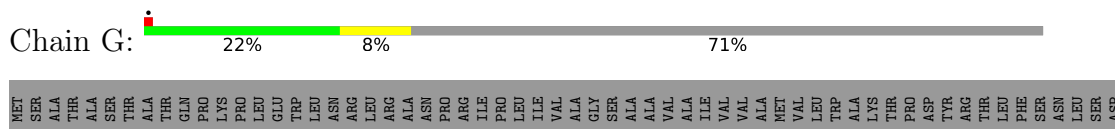




- Molecule 3: Flagellar M-ring protein



- Molecule 3: Flagellar M-ring protein





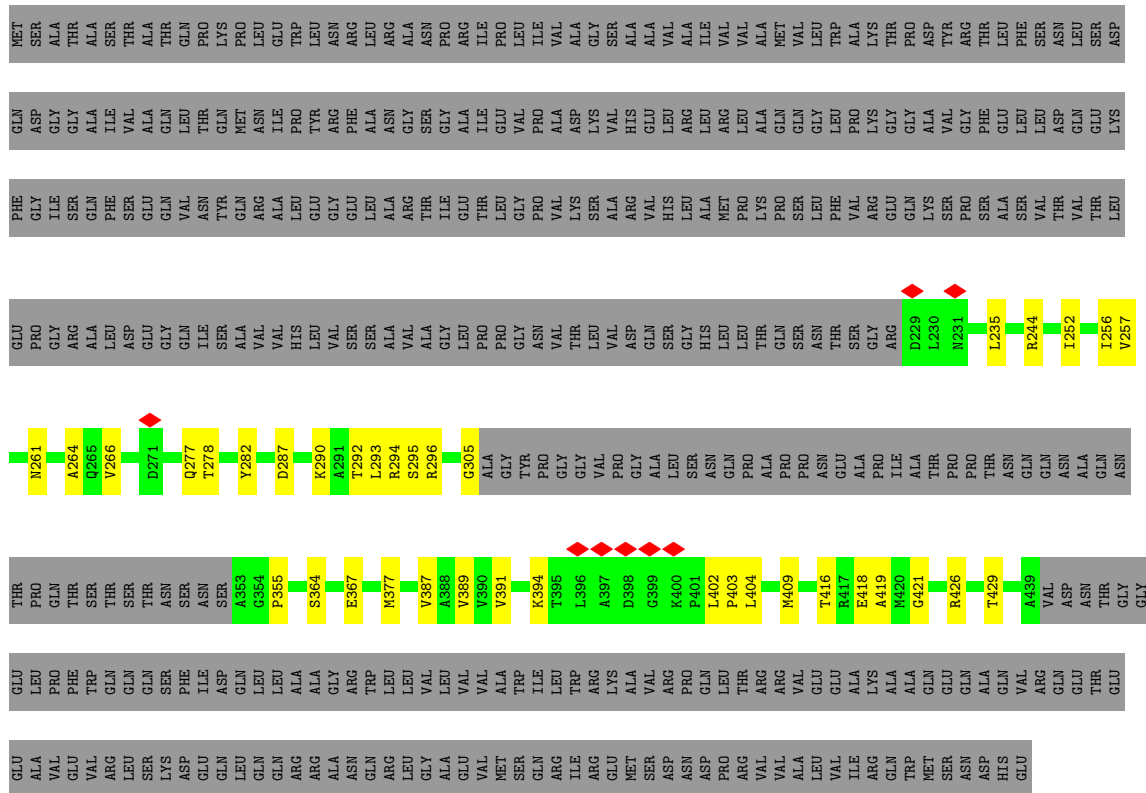
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SER	LYS	SER	SER	GLY	GLY	GLY	ILE	SER	ILE	GLY	THR
ASP	GLU	PHE	ASN	ALA	ALA	GLN	PHE	GLN	ALA	ALA	THR
GLN	GLN	ASP	ASN	LEU	LEU	LEU	ASP	SER	VAL	VAL	THR
LEU	GLN	LEU	SER	GLY	GLY	GLN	Y282	GLY	ALA	ALA	THR
GLN	ARG	ALA	A353	ALA	LEU	GLN	D287	VAL	GLN	LEU	THR
ARG	ALA	ALA	G354	GLY	ILE	ILE	Y282	GLN	THR	LEU	GLN
ALA	ALA	GLY	P355	GLY	SER	TYR	K290	ASN	ASN	THR	PRO
ASN	ASN	TRP	S364	ARG	VAL	GLN	T292	GLN	ARG	GLN	LEU
GLN	GLN	ARG	E367	LEU	HIS	VAL	L293	ALA	ASN	ASN	PRO
ARG	LEU	LEU	M377	VAL	VAL	VAL	R294	ALA	ILE	ILE	GLY
GLY	GLY	VAL	V387	VAL	VAL	VAL	S295	GLY	GLY	GLY	PRO
ALA	GLU	VAL	V387	VAL	VAL	SER	Q297	GLY	GLY	GLY	LEU
VAL	MET	ALA	A386	ALA	ASN	ALA	G305	ALA	ALA	ASN	ARG
MET	SER	TRP	V389	ILE	GLY	VAL	ALA	VAL	ARG	GLY	ALA
GLN	ARG	LEU	V391	LEU	TYR	GLY	TYR	GLY	THR	GLY	THR
ARG	ILE	TRP	K394	TRP	PRO	LEU	PRO	LEU	GLY	LEU	ARG
ILE	ARG	ARG	T395	ARG	GLY	PRO	GLY	PRO	THR	THR	ILE
GLY	GLY	LYS	L396	LYS	GLY	PRO	GLY	PRO	ILE	ILE	GLY
MET	MET	ALA	A397	ALA	VAL	GLY	VAL	GLY	GLY	GLY	LEU
ASP	ASP	VAL	D398	VAL	PRO	ASN	THR	THR	VAL	VAL	LEU
ASN	ASN	GLN	L402	GLN	ARG	LEU	ALA	ALA	GLY	ASP	ILE
ASP	PRO	LEU	P403	LEU	THR	SER	SER	VAL	VAL	LYS	VAL
ARG	ARG	THR	L404	THR	ARG	ASN	ASN	ASP	ASP	ARG	ALA
VAL	VAL	ARG	M409	ARG	ARG	GLN	GLN	GLN	GLN	HIS	ALA
VAL	ALA	VAL	T416	VAL	VAL	ALA	ALA	GLY	GLY	LEU	ALA
LEU	LEU	GLY	T416	GLY	GLY	PRO	PRO	HIS	ALA	LEU	VAL
VAL	VAL	GLY	R417	GLY	ARG	ASN	ASN	LEU	MET	ARG	VAL
ILE	ILE	ALA	E418	GLY	ALA	PRO	PRO	LEU	PRO	LEU	VAL
ARG	ARG	LYS	A419	LYS	ALA	GLY	GLY	LEU	LYS	ALA	ALA
GLN	TRP	ALA	M420	GLN	ALA	GLN	PRO	SER	PRO	GLN	MET
MET	MET	GLN	G421	GLN	ALA	ILE	ILE	ASN	LEU	GLY	LEU
SER	SER	GLY	R426	GLY	VAL	ALA	THR	THR	PHE	LEU	TRP
ASN	ASN	GLN	T429	GLN	ALA	GLN	PRO	SER	VAL	PRO	ALA
ASP	HIS	GLY	A439	GLN	VAL	THR	PRO	ARG	GLY	GLY	LYS
GLY		VAL	VAL	VAL	ARG	ASN	THR	ASN	GLN	VAL	ASP
		GLN	ASP	GLN	GLN	ASN	GLN	SER	VAL	ALA	TVR
		GLY	ASN	GLY	GLY	THR	GLN	PRO	GLY	GLY	ARG
		THR	THR	GLY	GLY	GLY	ALA	SER	PHE	PHE	THR
		GLY	GLY	GLY	GLY	GLY	T252	ALA	GLU	GLU	THR
		ALA	GLY	GLY	GLY	ASN	T252	SER	LEU	LEU	PHE
		VAL	LEU	VAL	ALA	THR	T256	VAL	LEU	LEU	SER
		VAL	LEU	VAL	VAL	THR	V257	THR	ASP	ASP	ASN
		GLY	PRO	GLY	GLY	PRO	V257	VAL	GLN	GLN	LEU
		ARG	TRP	VAL	ARG	THR	N261	THR	LEU	GLY	SER
		VAL		VAL	VAL				LYS	ASP	ASP

● Molecule 3: Flagellar M-ring protein

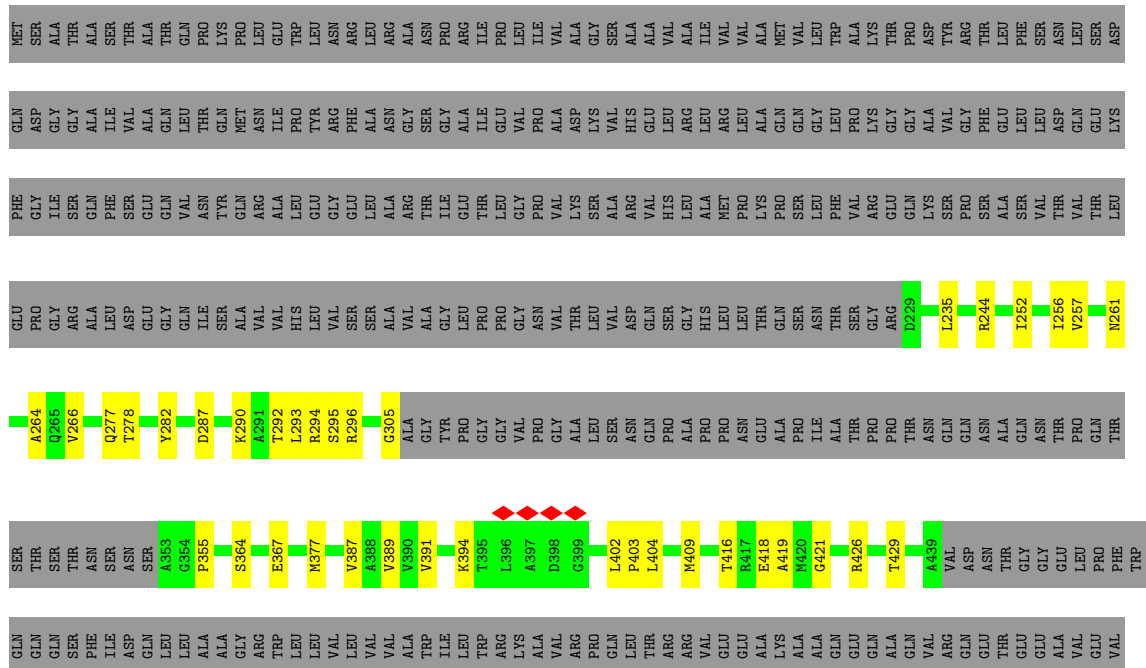


MET	SER	ALA	THR	THR	SER	THR	ALA	THR	THR	GLN	PRO	LYS	PRO	LEU	ASN	ARG	LEU	ARG	ALA	GLY	SER	ALA	ALA	VAL	VAL	ILE	PRO	LEU	PRO	ILE	VAL	ALA	GLY	ALA	GLN	ASP	GLN	ASP	
GLN	ASP	GLY	THR	GLY	ILE	SER	GLN	ARG	ALA	VAL	GLN	GLN	TYR	GLN	ASN	PHE	ALA	ALA	GLY	GLY	THR	GLY	GLN	VAL	VAL	GLY	VAL	ASN	PRO	GLY	VAL	GLN	GLY	VAL	GLY	VAL	LYS		
PHE	GLY	ILE	SER	SER	GLN	PHE	SER	GLY	GLN	VAL	GLN	ASN	TYR	GLN	ARG	GLY	LEU	ALA	GLY	GLY	THR	GLY	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU		
GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLY	GLY	GLN	VAL	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	GLY	VAL	SER	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU		
A264	Q265	Q266	Q277	Y282	D287	K290	K291	T292	L293	R294	S295	R296	G305	ALA	GLY	TYR	PRO	GLY	GLY	GLY	VAL	PRO	PRO	GLY	GLY	ASN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL		
THR	SER	THR	ASN	SER	SER	SER	A353	G354	P355	S364	E367	M377	D381	V387	A388	V389	V390	V391	K394	T395	L396	A397	D398	G399	L402	P403	L404	M409	T416	R417	E418	A419	M420	G421	R425	R426	T429	A439	VAL
PHE	THR	THR	GLN	GLN	PHE	ILE	ASP	GLN	GLN	VAL	GLN	ASN	TYR	GLN	ARG	GLY	LEU	ALA	GLY	GLY	THR	GLY	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
GLU	VAL	ARG	LEU	SER	LYS	ASP	GLY	GLN	GLN	GLN	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	

Chain K:



Chain L:



Chain M: 22% 7% 71%



[illegible]

- Molecule 3: Flagellar M-ring protein

[illegible][illegible]

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

[illegible]

Y261	Y262	Y263	Y264	Y265	Y266	Y267	Y268	Y269	Y270	Y271	Y272	Y273	Y274	Y275	Y276	Y277	Y278	Y279	Y280	Y281	Y282	Y283	Y284	Y285	Y286	Y287	Y288	Y289	Y290	Y291	Y292	Y293	Y294	Y295	Y296	Y297	Y298	Y299	Y300	Y301	Y302	Y303	Y304	Y305	Y306	Y307	Y308	Y309	Y310	Y311	Y312	Y313	Y314	Y315	Y316	Y317	Y318	Y319	Y320	Y321	Y322	Y323	Y324	Y325	Y326	Y327	Y328	Y329	Y330	Y331	Y332	Y333	Y334	Y335	Y336	Y337	Y338	Y339	Y340	Y341	Y342	Y343	Y344	Y345	Y346	Y347	Y348	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403	Y404	Y405	Y406	Y407	Y408	Y409	Y410	Y411	Y412	Y413	Y414	Y415	Y416	Y417	Y418	Y419	Y420	Y421	Y422	Y423	Y424	Y425	Y426	Y427	Y428	Y429	Y430	Y431	Y432	Y433	Y434	Y435	Y436	Y437	Y438	Y439	Y440	Y441	Y442	Y443	Y444	Y445	Y446	Y447	Y448	Y449	Y450	Y451	Y452	Y453	Y454	Y455	Y456	Y457	Y458	Y459	Y460	Y461	Y462	Y463	Y464	Y465	Y466	Y467	Y468	Y469	Y470	Y471	Y472	Y473	Y474	Y475	Y476	Y477	Y478	Y479	Y480	Y481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789	Y790	Y791	Y792	Y793	Y794	Y795	Y796	Y797	Y798	Y799	Y800	Y801	Y802	Y803	Y804	Y805	Y806	Y807	Y808	Y809	Y810	Y811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000
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	TBR	SER	THR	SER	THR	SER	THR	ASV	SER	ASN	A363	G364	P365	S366	E367	M377	V387	X388	V389	V390	Z391	K394	T395	L402	P403	L404	M409	T416	R417	E418	A419	M420	G421	K425	R426	T429	A439	VAL	ASP	ASN	THR	GLY	GLU	LEU	PRO	HIS
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TRP	GLN	GLN	GLN	SER	PHE	ILE	ASP	ILE	GLN	GLN	LEU	LEU	ALA	ALA	GLY	ARG	TRP	LEU	LEU	VAL	VAL	VAL	ALA	ALA	TRP	TRP	ILE	LEU	TRP	LEU	ARG	LYS	VAL	VAL	ARG	PRO	GLN	GLN	LEU	THR	ARG	ARG	VAL	GLU	GLU	ALA	ALA	LYS	ALA	ALA	ALA	GLN	GLN	GLN	VAL	ARG	GLN	GLU	THR	GLU	GLU	ALA	ALA	VAL	THR
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VAL	ARG	SER	LYS	ASP	GLU	GLN	LEU	GLN	GLN	ARG	ARG	ALA	ASN	GLN	GLN	LEU	GLY	GLU	VAL	VAL	SER	SER	GLN	ARG	ARG	ILE	ARG	GLU	GLU	VAL	VAL	ASP	ASP	PRO	ARG	VAL	VAL	ALA	LEU	VAL	ILE	ARG	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU
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- Molecule 3: Flagellar M-ring protein



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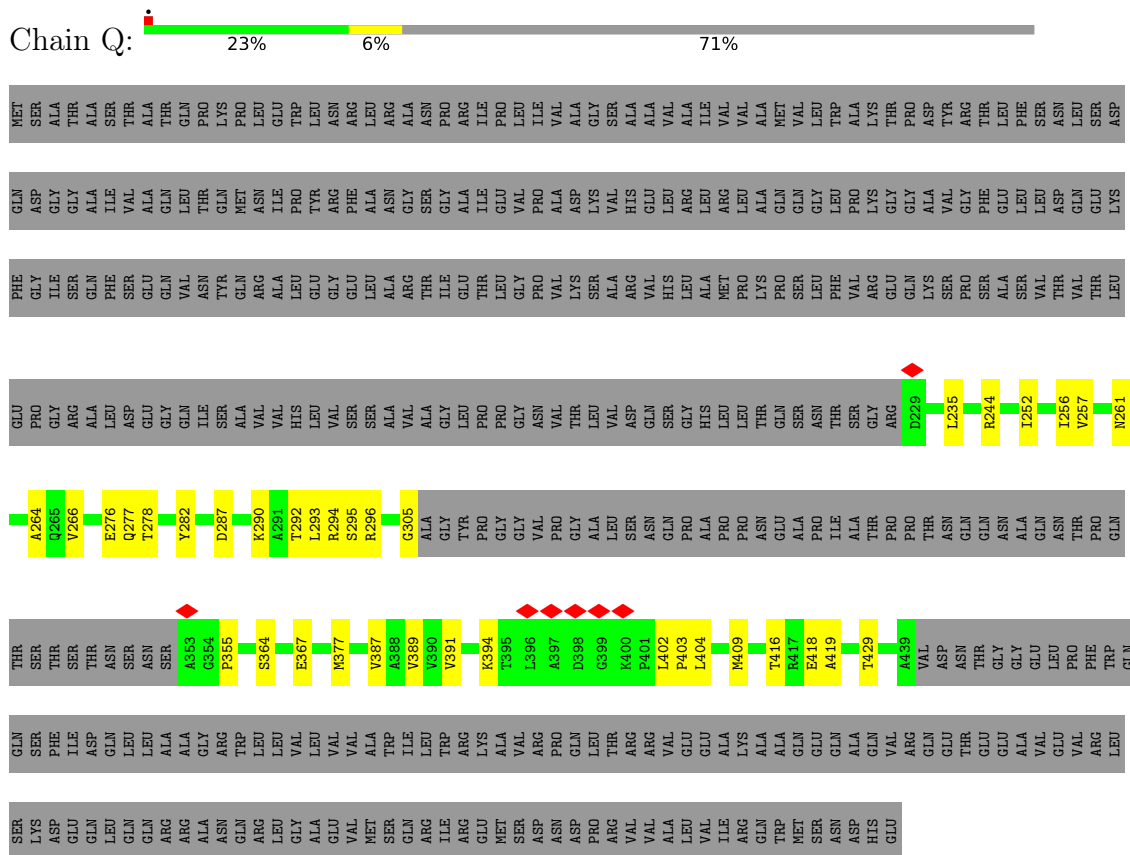
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PHE GLY ILE SER GLN PHE SER GLU GLN VAL VAL TYR GLN ARG ALA LEU GLU GLY GLU LEU LEU THR THR ILE GLU THR LEU GLY GLY VAL LYS SER SER ALA ARG ARG VAL HIS LEU LEU MET MET PRO PRO LYS PRO PRO SER SER PHE VAL VAL ARG ARG GLU GLN LYS SER SER PRO PRO ALA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

GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	LEU	VAL	ASP	GLN	SER	GLY	HIS	LEU	LEU	THR	GLN	SER	ASN	THR	THR	GLY	ARG	D229	L235	E242	R244	T252	T256
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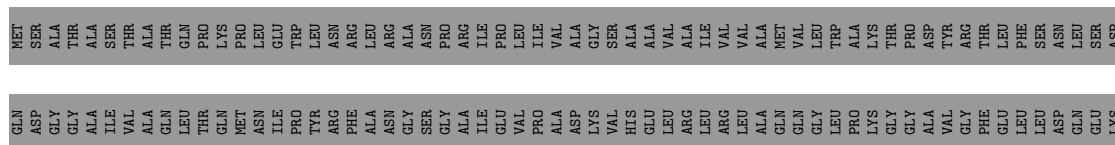
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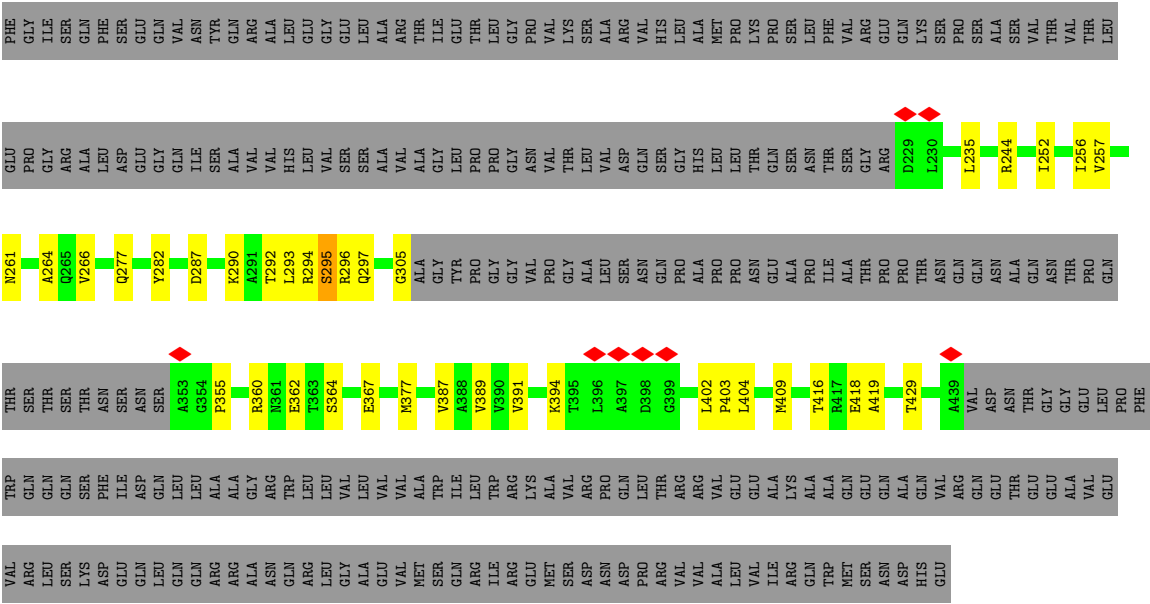
- Molecule 3: Flagellar M-ring protein



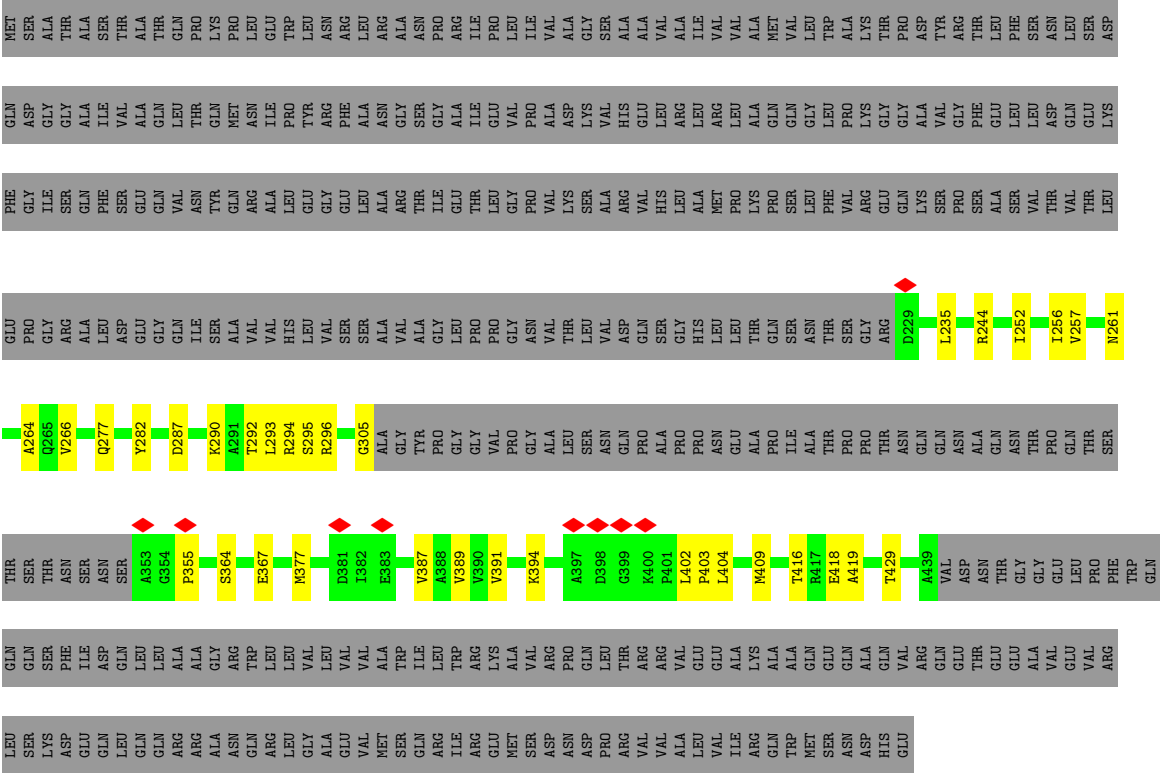
- Molecule 3: Flagellar M-ring protein



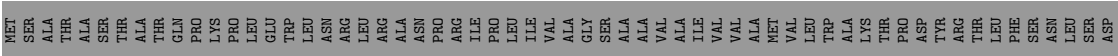




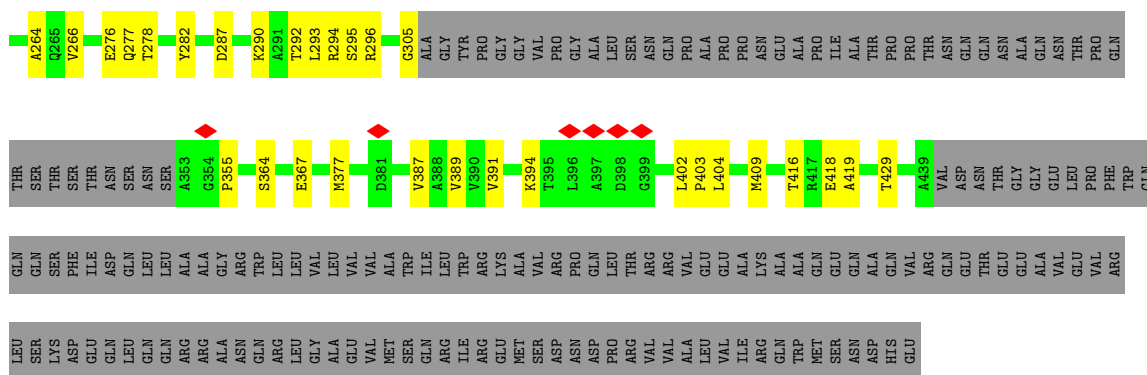
• Molecule 3: Flagellar M-ring protein



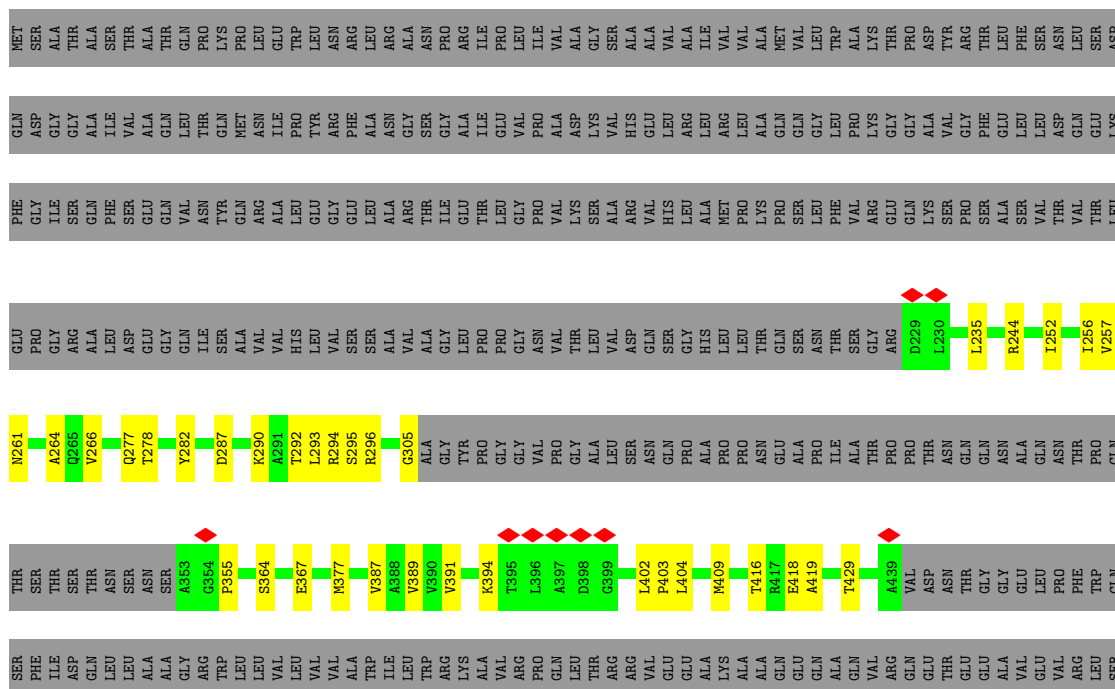
• Molecule 3: Flagellar M-ring protein



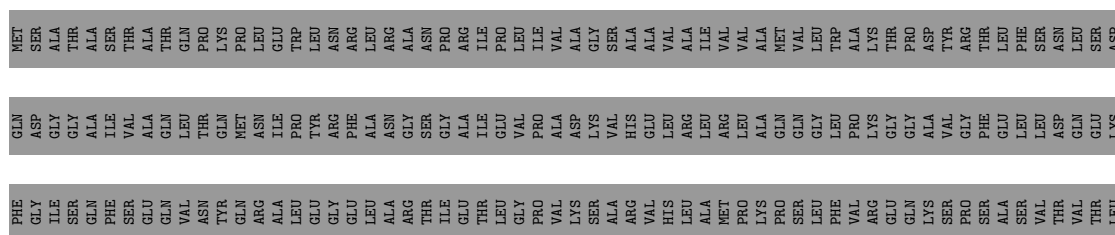


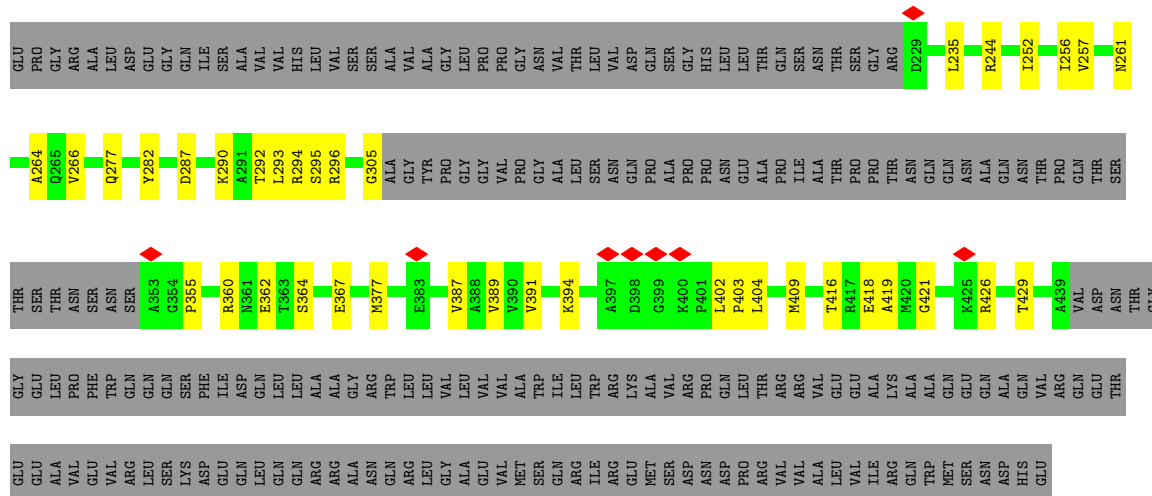


- Molecule 3: Flagellar M-ring protein

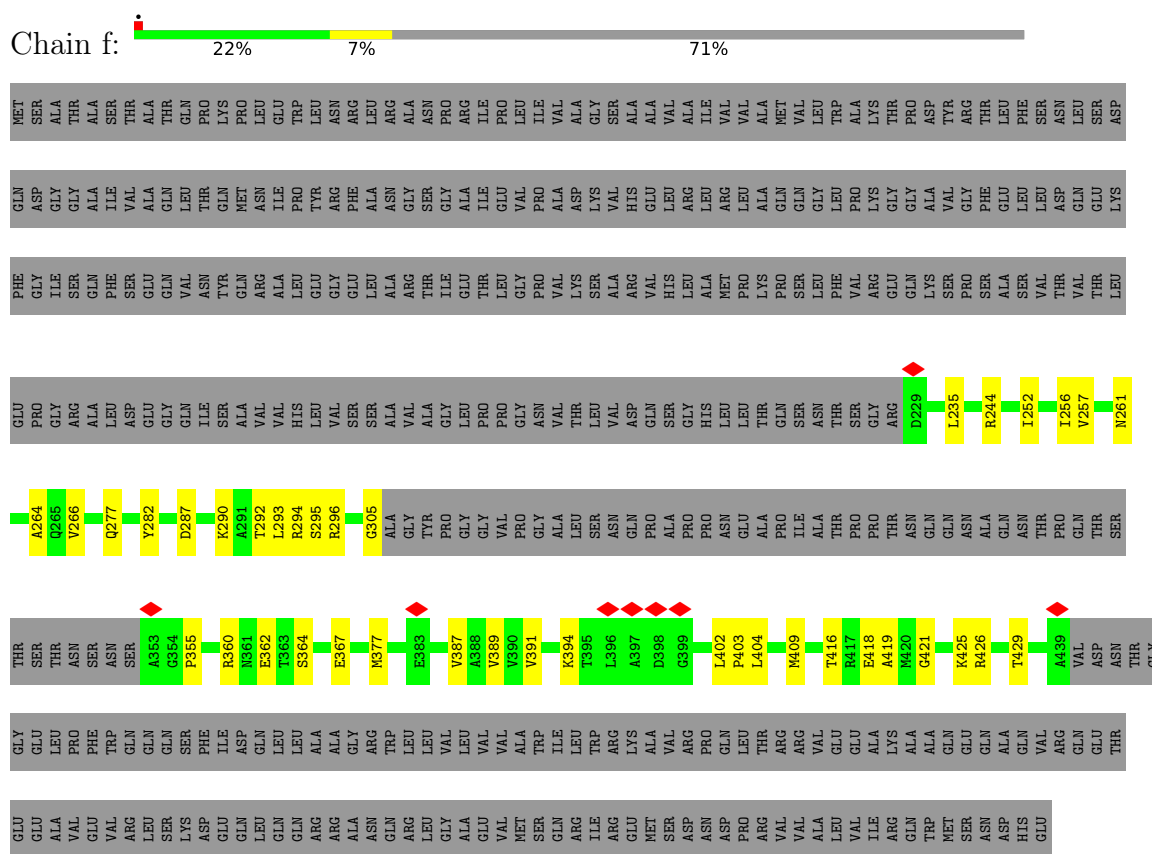


- Molecule 3: Flagellar M-ring protein

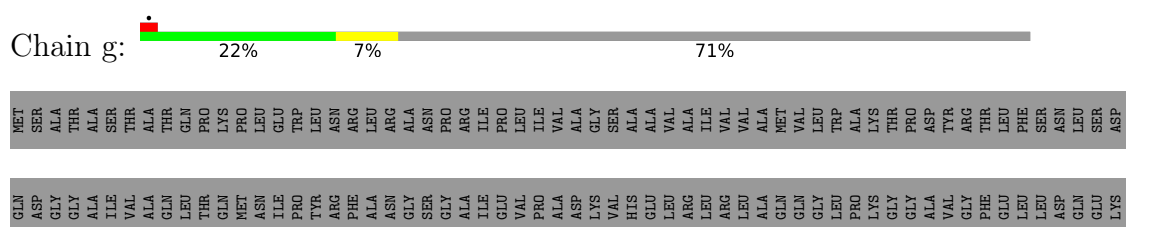




• Molecule 3: Flagellar M-ring protein



• Molecule 3: Flagellar M-ring protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.175	Depositor
Minimum map value	-0.712	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.19	Depositor
Map size ($\text{\AA}$)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	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	i	0.92	0/128	1.38	0/172
1	j	0.92	0/128	1.37	0/172
1	k	0.92	0/128	1.51	0/172
1	l	0.92	0/128	1.38	0/172
1	m	0.93	0/128	1.39	0/172
1	n	0.93	0/128	1.39	0/172
2	o	1.02	0/118	1.06	0/161
2	p	1.02	0/96	1.04	0/132
2	q	1.04	0/121	1.28	0/166
2	r	1.02	0/121	1.58	3/166 (1.8%)
2	s	1.01	0/120	1.16	0/164
3	A	0.22	0/1289	0.44	1/1741 (0.1%)
3	B	0.22	0/1289	0.44	1/1741 (0.1%)
3	C	0.22	0/1289	0.44	1/1741 (0.1%)
3	D	0.22	0/1289	0.44	1/1741 (0.1%)
3	E	0.22	0/1289	0.44	1/1741 (0.1%)
3	F	0.22	0/1289	0.44	1/1741 (0.1%)
3	G	0.22	0/1289	0.44	1/1741 (0.1%)
3	H	0.22	0/1289	0.44	1/1741 (0.1%)
3	I	0.22	0/1289	0.44	1/1741 (0.1%)
3	J	0.22	0/1289	0.44	1/1741 (0.1%)
3	K	0.22	0/1289	0.44	1/1741 (0.1%)
3	L	0.22	0/1289	0.44	1/1741 (0.1%)
3	M	0.22	0/1289	0.44	1/1741 (0.1%)
3	N	0.22	0/1289	0.44	1/1741 (0.1%)
3	O	0.22	0/1289	0.44	1/1741 (0.1%)
3	P	0.22	0/1289	0.44	1/1741 (0.1%)
3	Q	0.22	0/1289	0.44	1/1741 (0.1%)
3	R	0.22	0/1289	0.44	1/1741 (0.1%)
3	S	0.22	0/1289	0.44	1/1741 (0.1%)
3	T	0.22	0/1289	0.44	1/1741 (0.1%)
3	U	0.22	0/1289	0.44	1/1741 (0.1%)
3	V	0.22	0/1289	0.44	1/1741 (0.1%)
3	W	0.22	0/1289	0.44	1/1741 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	X	0.22	0/1289	0.44	1/1741 (0.1%)
3	Y	0.22	0/1289	0.44	1/1741 (0.1%)
3	Z	0.22	0/1289	0.44	1/1741 (0.1%)
3	a	0.22	0/1289	0.44	1/1741 (0.1%)
3	b	0.22	0/1289	0.44	1/1741 (0.1%)
3	c	0.22	0/1289	0.44	1/1741 (0.1%)
3	d	0.22	0/1289	0.44	1/1741 (0.1%)
3	e	0.22	0/1289	0.44	1/1741 (0.1%)
3	f	0.22	0/1289	0.44	1/1741 (0.1%)
3	g	0.22	0/1289	0.44	1/1741 (0.1%)
3	h	0.22	0/1289	0.44	1/1741 (0.1%)
All	All	0.27	0/45170	0.49	37/61015 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	72	HIS	CA-C-N	-7.35	116.28	123.04
2	r	72	HIS	C-N-CA	-7.35	116.28	123.04
2	r	72	HIS	CA-CB-CG	-7.30	106.50	113.80
3	h	261	ASN	N-CA-C	-5.41	106.53	113.02
3	K	261	ASN	N-CA-C	-5.40	106.54	113.02
3	E	261	ASN	N-CA-C	-5.40	106.54	113.02
3	G	261	ASN	N-CA-C	-5.40	106.54	113.02
3	Q	261	ASN	N-CA-C	-5.40	106.54	113.02
3	g	261	ASN	N-CA-C	-5.39	106.55	113.02
3	d	261	ASN	N-CA-C	-5.37	106.58	113.02
3	R	261	ASN	N-CA-C	-5.37	106.58	113.02
3	O	261	ASN	N-CA-C	-5.36	106.58	113.02
3	J	261	ASN	N-CA-C	-5.36	106.59	113.02
3	Y	261	ASN	N-CA-C	-5.36	106.59	113.02
3	e	261	ASN	N-CA-C	-5.36	106.59	113.02
3	f	261	ASN	N-CA-C	-5.36	106.59	113.02
3	D	261	ASN	N-CA-C	-5.36	106.59	113.02
3	N	261	ASN	N-CA-C	-5.35	106.60	113.02
3	X	261	ASN	N-CA-C	-5.35	106.59	113.02
3	B	261	ASN	N-CA-C	-5.35	106.60	113.02
3	U	261	ASN	N-CA-C	-5.35	106.60	113.02
3	b	261	ASN	N-CA-C	-5.35	106.60	113.02
3	S	261	ASN	N-CA-C	-5.35	106.60	113.02
3	c	261	ASN	N-CA-C	-5.35	106.60	113.02
3	V	261	ASN	N-CA-C	-5.35	106.60	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	261	ASN	N-CA-C	-5.35	106.60	113.02
3	Z	261	ASN	N-CA-C	-5.35	106.60	113.02
3	A	261	ASN	N-CA-C	-5.35	106.61	113.02
3	T	261	ASN	N-CA-C	-5.34	106.61	113.02
3	I	261	ASN	N-CA-C	-5.34	106.61	113.02
3	L	261	ASN	N-CA-C	-5.34	106.61	113.02
3	M	261	ASN	N-CA-C	-5.34	106.61	113.02
3	F	261	ASN	N-CA-C	-5.34	106.61	113.02
3	H	261	ASN	N-CA-C	-5.34	106.62	113.02
3	W	261	ASN	N-CA-C	-5.33	106.62	113.02
3	C	261	ASN	N-CA-C	-5.33	106.63	113.02
3	a	261	ASN	N-CA-C	-5.31	106.65	113.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	i	129	0	134	25	0
1	j	129	0	134	43	0
1	k	129	0	134	44	0
1	l	129	0	134	34	0
1	m	129	0	134	35	0
1	n	129	0	134	32	0
2	o	116	0	115	7	0
2	p	94	0	96	22	0
2	q	119	0	121	38	0
2	r	119	0	121	23	0
2	s	118	0	117	38	0
3	A	1275	0	1254	45	0
3	B	1275	0	1254	32	0
3	C	1275	0	1254	28	0
3	D	1275	0	1254	30	0
3	E	1275	0	1254	33	0
3	F	1275	0	1254	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1275	0	1254	51	0
3	H	1275	0	1254	58	0
3	I	1275	0	1254	37	0
3	J	1275	0	1254	31	0
3	K	1275	0	1254	37	0
3	L	1275	0	1254	32	0
3	M	1275	0	1254	50	0
3	N	1275	0	1254	54	0
3	O	1275	0	1254	30	0
3	P	1275	0	1254	32	0
3	Q	1275	0	1254	34	0
3	R	1275	0	1254	30	0
3	S	1275	0	1254	43	0
3	T	1275	0	1254	47	0
3	U	1275	0	1254	47	0
3	V	1275	0	1254	46	0
3	W	1275	0	1254	29	0
3	X	1275	0	1254	30	0
3	Y	1275	0	1254	53	0
3	Z	1275	0	1254	48	0
3	a	1275	0	1254	42	0
3	b	1275	0	1254	41	0
3	c	1275	0	1254	39	0
3	d	1275	0	1254	35	0
3	e	1275	0	1254	30	0
3	f	1275	0	1254	32	0
3	g	1275	0	1254	40	0
3	h	1275	0	1254	34	0
All	All	44690	0	44010	1171	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 13.

All (1171) 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:j:11:ILE:HG22	3:Y:372:ILE:CD1	1.58	1.32
2:s:72:HIS:CD2	3:H:365:ASN:HB3	1.64	1.32
1:m:7:ILE:HG21	3:G:278:THR:CG2	1.56	1.31
2:q:73:ILE:CD1	3:V:297:GLN:HB2	1.61	1.31
1:m:7:ILE:CG2	3:G:278:THR:HG21	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:72:HIS:ND1	3:a:365:ASN:HB3	1.47	1.25
1:j:7:ILE:HD11	3:Z:370:ARG:NH2	1.54	1.23
1:i:7:ILE:HG21	3:d:278:THR:CG2	1.69	1.22
1:j:11:ILE:CG2	3:Y:372:ILE:HG21	1.68	1.21
1:n:7:ILE:CG2	3:A:278:THR:HG21	1.70	1.20
2:r:72:HIS:CD2	3:N:365:ASN:HB3	1.79	1.17
2:s:78:VAL:CG1	3:H:299:ASN:HD22	1.58	1.17
1:j:11:ILE:HG21	3:Y:372:ILE:CG2	1.74	1.15
2:s:78:VAL:HG11	3:H:299:ASN:ND2	1.61	1.15
1:m:21:ALA:CB	3:E:278:THR:HG21	1.78	1.14
2:r:68:THR:HG21	3:N:367:GLU:OE1	1.49	1.13
2:s:68:THR:HG21	3:H:367:GLU:OE1	1.49	1.13
1:k:11:ILE:HD12	1:k:12:SER:N	1.64	1.12
1:n:7:ILE:HG21	3:A:278:THR:HG21	1.21	1.12
1:i:14:LEU:HD23	3:c:278:THR:CG2	1.78	1.12
2:s:78:VAL:CG1	3:H:299:ASN:ND2	2.14	1.11
1:i:7:ILE:HG21	3:d:278:THR:HG21	1.20	1.10
1:n:19:MET:HA	3:g:276:GLU:OE2	1.51	1.10
1:j:14:LEU:HD21	3:Y:370:ARG:HH21	1.07	1.10
1:n:21:ALA:CB	3:g:278:THR:HG21	1.80	1.10
1:k:7:ILE:HB	3:S:278:THR:HG21	1.16	1.09
1:j:4:ILE:HG12	3:Z:372:ILE:CG2	1.81	1.08
1:n:21:ALA:HB1	3:g:278:THR:HG21	1.29	1.08
1:j:11:ILE:HG22	3:Y:372:ILE:HD13	1.36	1.07
2:q:72:HIS:ND1	3:U:365:ASN:HB3	1.67	1.07
1:i:7:ILE:CG2	3:d:278:THR:HG21	1.85	1.07
1:i:21:ALA:CB	3:b:278:THR:HG21	1.83	1.07
1:l:21:ALA:CB	3:K:278:THR:HG21	1.84	1.07
1:j:7:ILE:CD1	3:Z:370:ARG:HH21	1.67	1.06
2:q:65:LEU:HB2	3:U:295:SER:HB2	1.35	1.06
2:r:68:THR:OG1	2:r:72:HIS:CE1	2.07	1.05
1:i:14:LEU:HD23	3:c:278:THR:HG21	1.37	1.05
1:m:7:ILE:CG2	3:G:278:THR:CG2	2.25	1.05
2:q:72:HIS:CB	3:V:295:SER:HB3	1.87	1.04
1:k:11:ILE:HG22	3:S:372:ILE:CG2	1.87	1.04
1:j:11:ILE:HG22	3:Y:372:ILE:HD12	1.38	1.03
1:m:7:ILE:HG21	3:G:278:THR:HG22	1.36	1.03
1:j:7:ILE:HD11	3:Z:370:ARG:HH21	1.00	1.03
1:n:7:ILE:HG21	3:A:278:THR:CG2	1.87	1.03
2:p:73:ILE:HG13	3:b:295:SER:HB2	1.38	1.02
1:k:11:ILE:HD12	1:k:11:ILE:C	1.84	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:65:LEU:CD2	3:H:297:GLN:HB2	1.90	1.01
1:l:21:ALA:HB3	3:K:278:THR:HG21	1.43	1.00
1:m:21:ALA:HB1	3:E:278:THR:HG21	1.43	1.00
2:s:78:VAL:HG11	3:H:299:ASN:HD22	0.86	1.00
1:k:11:ILE:CG2	3:S:372:ILE:HG21	1.92	0.99
1:k:11:ILE:CG2	3:S:372:ILE:CG2	2.42	0.98
2:r:78:VAL:C	3:N:299:ASN:HD21	1.70	0.97
1:m:14:LEU:HD11	3:G:370:ARG:HH21	1.29	0.97
1:k:14:LEU:HB3	3:R:278:THR:HG21	1.45	0.97
1:j:11:ILE:HG21	3:Y:372:ILE:HG21	1.34	0.97
2:r:78:VAL:O	3:N:299:ASN:ND2	1.99	0.96
2:s:72:HIS:HD2	3:H:365:ASN:HB3	0.98	0.96
1:k:11:ILE:HG22	3:S:372:ILE:HG21	1.44	0.96
1:j:4:ILE:CG1	3:Z:372:ILE:CG2	2.44	0.95
2:p:72:HIS:CE1	3:a:365:ASN:HB3	2.02	0.95
1:j:11:ILE:CG2	3:Y:372:ILE:CG2	2.38	0.95
1:m:7:ILE:HG21	3:G:278:THR:HG21	1.31	0.94
2:o:65:LEU:HD22	3:h:295:SER:HB2	1.49	0.93
2:q:72:HIS:HB2	3:V:295:SER:HB3	1.48	0.93
1:j:4:ILE:HD11	3:Z:372:ILE:HG22	1.49	0.93
1:j:4:ILE:HG12	3:Z:372:ILE:CB	1.99	0.92
2:r:72:HIS:HD2	3:N:365:ASN:HB3	1.15	0.92
1:i:14:LEU:CD2	3:c:278:THR:HG21	2.01	0.90
1:j:14:LEU:CD2	3:Y:370:ARG:HH21	1.83	0.90
1:m:14:LEU:HB3	3:F:278:THR:HG21	1.52	0.90
2:q:73:ILE:HD13	3:V:297:GLN:HB2	1.53	0.90
1:i:14:LEU:HD23	3:c:278:THR:HG22	1.54	0.89
1:m:7:ILE:CB	3:G:278:THR:HG21	2.02	0.89
1:m:21:ALA:HB3	3:E:278:THR:HG21	1.53	0.89
2:q:65:LEU:HB2	3:U:295:SER:CB	2.03	0.88
2:r:72:HIS:HD2	3:N:365:ASN:CB	1.87	0.88
1:j:4:ILE:HG12	3:Z:372:ILE:HB	1.55	0.87
2:q:73:ILE:HD12	3:V:297:GLN:HB2	1.57	0.86
1:j:4:ILE:HG12	3:Z:372:ILE:HG21	1.57	0.86
1:j:4:ILE:CG1	3:Z:372:ILE:HG21	2.04	0.86
1:i:21:ALA:HB1	3:b:278:THR:HG21	1.56	0.85
2:s:65:LEU:HD22	3:H:297:GLN:HB2	1.57	0.85
2:r:68:THR:HG1	2:r:72:HIS:CE1	1.95	0.84
2:r:78:VAL:HG12	3:M:361:ASN:HD22	1.40	0.84
1:j:4:ILE:CD1	3:Z:372:ILE:HG22	2.08	0.84
2:q:76:GLN:O	3:U:297:GLN:OE1	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:7:ILE:HB	3:S:278:THR:CG2	2.07	0.83
1:n:7:ILE:CG2	3:A:278:THR:CG2	2.52	0.83
1:j:14:LEU:HD21	3:Y:370:ARG:NH2	1.91	0.83
1:j:7:ILE:HD11	3:Z:370:ARG:CZ	2.08	0.82
1:l:11:ILE:HG22	3:M:372:ILE:HD12	1.62	0.82
1:m:14:LEU:HD23	3:F:278:THR:CG2	2.09	0.82
1:k:21:ALA:HB1	3:Q:278:THR:HG21	1.62	0.82
2:s:78:VAL:HG12	3:H:299:ASN:ND2	1.93	0.81
1:n:21:ALA:HB1	3:g:278:THR:CG2	2.10	0.81
2:s:72:HIS:HD2	3:H:365:ASN:CB	1.88	0.80
1:k:11:ILE:HG22	3:S:372:ILE:CB	2.11	0.80
1:n:14:LEU:HB3	3:h:278:THR:HG21	1.64	0.80
1:k:7:ILE:HD11	3:T:370:ARG:HE	1.46	0.80
1:l:11:ILE:HG22	3:M:372:ILE:CD1	2.14	0.78
2:p:67:LEU:HD11	2:p:74:PRO:HA	1.64	0.78
2:q:72:HIS:HA	3:V:295:SER:OG	1.83	0.78
2:q:72:HIS:ND1	3:U:365:ASN:CB	2.47	0.77
1:m:14:LEU:HD23	3:F:278:THR:HG22	1.66	0.77
1:n:19:MET:CA	3:g:276:GLU:OE2	2.32	0.77
2:q:73:ILE:HD11	3:V:297:GLN:HB2	1.63	0.77
1:l:21:ALA:HB1	3:K:278:THR:HG21	1.65	0.77
1:k:11:ILE:C	1:k:11:ILE:CD1	2.57	0.76
1:k:21:ALA:CB	3:Q:278:THR:HG21	2.16	0.76
2:p:73:ILE:HG13	3:b:295:SER:CB	2.14	0.76
2:s:73:ILE:HG13	3:I:295:SER:HB2	1.67	0.76
1:n:4:ILE:CD1	3:B:374:HIS:HB2	2.16	0.75
1:l:7:ILE:CG2	3:M:278:THR:HG21	2.17	0.75
2:s:68:THR:CG2	3:H:294:ARG:CD	2.65	0.75
1:k:4:ILE:HD12	3:T:374:HIS:HB2	1.68	0.74
1:l:7:ILE:HG21	3:M:278:THR:CG2	2.16	0.74
1:i:21:ALA:HB1	3:b:278:THR:CG2	2.17	0.74
1:k:4:ILE:HG12	3:T:372:ILE:HB	1.68	0.74
1:m:14:LEU:HD11	3:G:370:ARG:NH2	2.02	0.73
2:s:65:LEU:HB2	3:H:295:SER:HB2	1.69	0.73
1:m:7:ILE:HB	3:G:278:THR:HG21	1.70	0.73
1:i:21:ALA:CB	3:b:278:THR:CG2	2.64	0.73
1:j:11:ILE:CG2	3:Y:372:ILE:HD13	2.16	0.72
1:j:11:ILE:CG2	3:Y:372:ILE:CB	2.67	0.72
1:k:4:ILE:HG13	3:T:372:ILE:CG2	2.20	0.72
1:j:11:ILE:HG21	3:Y:372:ILE:CB	2.18	0.72
1:i:7:ILE:CG2	3:d:278:THR:CG2	2.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:72:HIS:CE1	3:I:294:ARG:HG3	2.25	0.71
1:i:21:ALA:HB3	3:b:278:THR:HG21	1.71	0.71
1:k:4:ILE:CD1	3:T:374:HIS:HB2	2.20	0.71
1:n:11:ILE:CG2	3:A:372:ILE:HG21	2.21	0.71
2:p:72:HIS:ND1	3:a:365:ASN:CB	2.40	0.71
2:r:78:VAL:HG12	3:M:361:ASN:ND2	2.06	0.71
2:s:68:THR:HG22	3:H:294:ARG:HD3	1.73	0.71
2:s:68:THR:HG21	3:H:294:ARG:HD2	1.71	0.70
2:p:71:HIS:HB2	3:b:294:ARG:HG2	1.74	0.70
1:i:14:LEU:HB3	3:c:278:THR:HG21	1.72	0.70
2:q:72:HIS:HB3	3:V:295:SER:HB3	1.72	0.69
1:k:11:ILE:HG22	3:S:372:ILE:HB	1.74	0.69
2:s:76:GLN:N	3:H:297:GLN:HE22	1.91	0.69
1:k:4:ILE:CG1	3:T:372:ILE:CG2	2.70	0.68
1:n:7:ILE:HG22	3:A:278:THR:HG21	1.73	0.68
2:p:68:THR:CG2	3:a:294:ARG:HD3	2.23	0.68
1:j:4:ILE:CG1	3:Z:372:ILE:HG22	2.25	0.67
1:m:7:ILE:HD11	3:H:370:ARG:HE	1.58	0.67
1:n:21:ALA:HB3	3:g:278:THR:HG21	1.73	0.67
2:s:65:LEU:HD21	3:H:297:GLN:HB2	1.73	0.67
3:F:391:VAL:HG21	3:F:409:MET:HE1	1.78	0.66
1:l:14:LEU:HB3	3:L:278:THR:HG21	1.77	0.66
3:E:391:VAL:HG21	3:E:409:MET:HE1	1.78	0.66
3:G:391:VAL:HG21	3:G:409:MET:HE1	1.78	0.66
3:W:391:VAL:HG21	3:W:409:MET:HE1	1.78	0.66
3:D:391:VAL:HG21	3:D:409:MET:HE1	1.78	0.66
3:V:391:VAL:HG21	3:V:409:MET:HE1	1.78	0.66
3:X:391:VAL:HG21	3:X:409:MET:HE1	1.78	0.66
3:Y:391:VAL:HG21	3:Y:409:MET:HE1	1.78	0.66
1:n:15:GLN:HB2	3:h:374:HIS:CD2	2.30	0.66
2:q:73:ILE:CD1	3:V:297:GLN:CB	2.56	0.66
3:C:391:VAL:HG21	3:C:409:MET:HE1	1.78	0.66
3:H:391:VAL:HG21	3:H:409:MET:HE1	1.78	0.66
3:U:391:VAL:HG21	3:U:409:MET:HE1	1.78	0.66
1:i:7:ILE:CB	3:d:278:THR:HG21	2.24	0.66
3:T:391:VAL:HG21	3:T:409:MET:HE1	1.78	0.66
3:Z:391:VAL:HG21	3:Z:409:MET:HE1	1.78	0.66
3:B:391:VAL:HG21	3:B:409:MET:HE1	1.78	0.66
3:I:391:VAL:HG21	3:I:409:MET:HE1	1.78	0.66
3:J:391:VAL:HG21	3:J:409:MET:HE1	1.78	0.66
3:a:391:VAL:HG21	3:a:409:MET:HE1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:391:VAL:HG21	3:S:409:MET:HE1	1.78	0.66
3:b:391:VAL:HG21	3:b:409:MET:HE1	1.78	0.66
1:m:21:ALA:HB1	3:E:278:THR:CG2	2.22	0.65
2:r:78:VAL:C	3:N:299:ASN:ND2	2.48	0.65
3:R:391:VAL:HG21	3:R:409:MET:HE1	1.78	0.65
1:l:7:ILE:HG21	3:M:278:THR:HG21	1.76	0.65
3:A:391:VAL:HG21	3:A:409:MET:HE1	1.78	0.65
1:m:11:ILE:HG22	3:G:372:ILE:HB	1.77	0.65
3:K:391:VAL:HG21	3:K:409:MET:HE1	1.78	0.65
3:Q:391:VAL:HG21	3:Q:409:MET:HE1	1.78	0.65
3:h:391:VAL:HG21	3:h:409:MET:HE1	1.78	0.65
3:K:389:VAL:HG21	3:K:416:THR:HG21	1.79	0.65
3:P:391:VAL:HG21	3:P:409:MET:HE1	1.78	0.65
3:c:391:VAL:HG21	3:c:409:MET:HE1	1.78	0.65
3:d:391:VAL:HG21	3:d:409:MET:HE1	1.78	0.65
3:H:389:VAL:HG21	3:H:416:THR:HG21	1.79	0.65
3:L:391:VAL:HG21	3:L:409:MET:HE1	1.78	0.65
3:b:389:VAL:HG21	3:b:416:THR:HG21	1.79	0.65
3:d:389:VAL:HG21	3:d:416:THR:HG21	1.79	0.65
3:J:389:VAL:HG21	3:J:416:THR:HG21	1.79	0.65
3:Z:389:VAL:HG21	3:Z:416:THR:HG21	1.79	0.65
3:f:391:VAL:HG21	3:f:409:MET:HE1	1.78	0.65
3:g:391:VAL:HG21	3:g:409:MET:HE1	1.78	0.65
1:l:7:ILE:HD11	3:N:370:ARG:HH21	1.62	0.65
2:s:72:HIS:CD2	3:H:365:ASN:CB	2.60	0.65
3:I:389:VAL:HG21	3:I:416:THR:HG21	1.79	0.65
3:O:391:VAL:HG21	3:O:409:MET:HE1	1.78	0.65
3:e:391:VAL:HG21	3:e:409:MET:HE1	1.78	0.65
2:q:72:HIS:HA	3:V:295:SER:CB	2.27	0.65
2:s:76:GLN:H	3:H:297:GLN:NE2	1.95	0.65
3:F:389:VAL:HG21	3:F:416:THR:HG21	1.79	0.65
3:M:389:VAL:HG21	3:M:416:THR:HG21	1.79	0.65
3:a:389:VAL:HG21	3:a:416:THR:HG21	1.79	0.65
3:c:389:VAL:HG21	3:c:416:THR:HG21	1.79	0.65
3:e:389:VAL:HG21	3:e:416:THR:HG21	1.79	0.65
3:G:389:VAL:HG21	3:G:416:THR:HG21	1.79	0.65
3:X:389:VAL:HG21	3:X:416:THR:HG21	1.79	0.65
3:L:389:VAL:HG21	3:L:416:THR:HG21	1.79	0.64
3:M:391:VAL:HG21	3:M:409:MET:HE1	1.78	0.64
3:N:391:VAL:HG21	3:N:409:MET:HE1	1.78	0.64
3:g:389:VAL:HG21	3:g:416:THR:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:68:THR:CG2	3:H:294:ARG:HD2	2.25	0.64
3:A:389:VAL:HG21	3:A:416:THR:HG21	1.79	0.64
3:D:389:VAL:HG21	3:D:416:THR:HG21	1.79	0.64
3:N:389:VAL:HG21	3:N:416:THR:HG21	1.79	0.64
3:f:389:VAL:HG21	3:f:416:THR:HG21	1.79	0.64
1:k:4:ILE:HG13	3:T:372:ILE:HG21	1.79	0.64
3:V:389:VAL:HG21	3:V:416:THR:HG21	1.79	0.64
3:Y:389:VAL:HG21	3:Y:416:THR:HG21	1.79	0.64
3:C:389:VAL:HG21	3:C:416:THR:HG21	1.79	0.64
3:O:389:VAL:HG21	3:O:416:THR:HG21	1.79	0.64
2:p:74:PRO:O	2:p:75:ALA:C	2.40	0.64
3:B:389:VAL:HG21	3:B:416:THR:HG21	1.79	0.64
3:E:389:VAL:HG21	3:E:416:THR:HG21	1.79	0.64
3:c:235:LEU:HD22	3:d:244:ARG:HH12	1.63	0.64
3:D:235:LEU:HD22	3:E:244:ARG:HH12	1.63	0.64
3:F:235:LEU:HD22	3:G:244:ARG:HH12	1.63	0.64
3:L:394:LYS:HE3	3:L:394:LYS:HA	1.80	0.64
3:O:394:LYS:HA	3:O:394:LYS:HE3	1.80	0.64
3:Q:235:LEU:HD22	3:R:244:ARG:HH12	1.63	0.64
3:V:394:LYS:HA	3:V:394:LYS:HE3	1.80	0.64
3:a:235:LEU:HD22	3:b:244:ARG:HH12	1.63	0.64
3:e:235:LEU:HD22	3:f:244:ARG:HH12	1.63	0.64
3:h:389:VAL:HG21	3:h:416:THR:HG21	1.79	0.64
3:B:235:LEU:HD22	3:C:244:ARG:HH12	1.63	0.64
3:N:394:LYS:HE3	3:N:394:LYS:HA	1.80	0.64
3:P:389:VAL:HG21	3:P:416:THR:HG21	1.79	0.64
3:T:394:LYS:HE3	3:T:394:LYS:HA	1.80	0.64
3:W:389:VAL:HG21	3:W:416:THR:HG21	1.79	0.64
3:X:394:LYS:HE3	3:X:394:LYS:HA	1.80	0.64
1:k:3:ALA:C	3:T:372:ILE:CD1	2.70	0.64
1:l:7:ILE:HD11	3:N:370:ARG:HE	1.62	0.64
1:n:21:ALA:CB	3:g:278:THR:CG2	2.67	0.64
2:r:72:HIS:CD2	3:N:365:ASN:CB	2.66	0.64
3:H:235:LEU:HD22	3:I:244:ARG:HH12	1.63	0.64
3:J:394:LYS:HA	3:J:394:LYS:HE3	1.80	0.64
3:M:394:LYS:HE3	3:M:394:LYS:HA	1.80	0.64
3:O:235:LEU:HD22	3:P:244:ARG:HH12	1.63	0.64
3:Q:394:LYS:HA	3:Q:394:LYS:HE3	1.80	0.64
3:S:235:LEU:HD22	3:T:244:ARG:HH12	1.63	0.64
3:S:394:LYS:HE3	3:S:394:LYS:HA	1.80	0.64
3:d:287:ASP:HB3	3:d:290:LYS:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:11:ILE:CG2	3:G:372:ILE:HG21	2.28	0.64
3:K:287:ASP:HB3	3:K:290:LYS:HE2	1.80	0.64
3:R:389:VAL:HG21	3:R:416:THR:HG21	1.79	0.64
3:R:394:LYS:HE3	3:R:394:LYS:HA	1.80	0.64
3:S:389:VAL:HG21	3:S:416:THR:HG21	1.79	0.64
3:T:389:VAL:HG21	3:T:416:THR:HG21	1.79	0.64
3:V:235:LEU:HD22	3:W:244:ARG:HH12	1.63	0.64
1:n:7:ILE:HD12	3:B:372:ILE:HD12	1.80	0.63
3:A:244:ARG:HH12	3:h:235:LEU:HD22	1.63	0.63
3:L:287:ASP:HB3	3:L:290:LYS:HE2	1.80	0.63
3:Q:389:VAL:HG21	3:Q:416:THR:HG21	1.79	0.63
3:g:235:LEU:HD22	3:h:244:ARG:HH12	1.63	0.63
1:i:14:LEU:CD2	3:c:278:THR:CG2	2.62	0.63
1:l:11:ILE:CG2	3:M:372:ILE:HG21	2.28	0.63
3:J:235:LEU:HD22	3:K:244:ARG:HH12	1.63	0.63
3:M:235:LEU:HD22	3:N:244:ARG:HH12	1.63	0.63
3:P:394:LYS:HE3	3:P:394:LYS:HA	1.80	0.63
3:U:389:VAL:HG21	3:U:416:THR:HG21	1.79	0.63
3:U:394:LYS:HE3	3:U:394:LYS:HA	1.80	0.63
3:X:235:LEU:HD22	3:Y:244:ARG:HH12	1.63	0.63
3:Y:235:LEU:HD22	3:Z:244:ARG:HH12	1.63	0.63
3:Y:394:LYS:HE3	3:Y:394:LYS:HA	1.80	0.63
3:c:287:ASP:HB3	3:c:290:LYS:HE2	1.80	0.63
3:e:287:ASP:HB3	3:e:290:LYS:HE2	1.80	0.63
2:o:63:VAL:HG21	3:g:297:GLN:HB2	1.80	0.63
2:r:66:THR:OG1	3:N:294:ARG:HG2	1.98	0.63
2:s:72:HIS:HE1	3:I:294:ARG:HE	1.43	0.63
3:H:394:LYS:HE3	3:H:394:LYS:HA	1.80	0.63
3:J:287:ASP:HB3	3:J:290:LYS:HE2	1.80	0.63
3:K:394:LYS:HE3	3:K:394:LYS:HA	1.80	0.63
3:W:394:LYS:HE3	3:W:394:LYS:HA	1.80	0.63
3:L:235:LEU:HD22	3:M:244:ARG:HH12	1.63	0.63
3:P:287:ASP:HB3	3:P:290:LYS:HE2	1.80	0.63
3:Q:287:ASP:HB3	3:Q:290:LYS:HE2	1.80	0.63
3:T:235:LEU:HD22	3:U:244:ARG:HH12	1.63	0.63
3:U:235:LEU:HD22	3:V:244:ARG:HH12	1.63	0.63
3:I:394:LYS:HE3	3:I:394:LYS:HA	1.80	0.63
3:N:235:LEU:HD22	3:O:244:ARG:HH12	1.63	0.63
3:Z:394:LYS:HE3	3:Z:394:LYS:HA	1.80	0.63
3:f:235:LEU:HD22	3:g:244:ARG:HH12	1.63	0.63
3:M:287:ASP:HB3	3:M:290:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:287:ASP:HB3	3:C:290:LYS:HE2	1.80	0.63
3:D:287:ASP:HB3	3:D:290:LYS:HE2	1.80	0.63
3:P:235:LEU:HD22	3:Q:244:ARG:HH12	1.63	0.63
3:b:287:ASP:HB3	3:b:290:LYS:HE2	1.80	0.63
2:p:65:LEU:HD21	3:Z:363:THR:HG23	1.80	0.63
3:A:235:LEU:HD22	3:B:244:ARG:HH12	1.63	0.63
3:B:287:ASP:HB3	3:B:290:LYS:HE2	1.80	0.63
3:W:235:LEU:HD22	3:X:244:ARG:HH12	1.63	0.63
3:Y:287:ASP:HB3	3:Y:290:LYS:HE2	1.80	0.63
3:a:394:LYS:HE3	3:a:394:LYS:HA	1.80	0.63
3:f:287:ASP:HB3	3:f:290:LYS:HE2	1.80	0.63
3:A:394:LYS:HE3	3:A:394:LYS:HA	1.80	0.63
3:G:394:LYS:HE3	3:G:394:LYS:HA	1.80	0.63
3:I:287:ASP:HB3	3:I:290:LYS:HE2	1.80	0.63
3:K:235:LEU:HD22	3:L:244:ARG:HH12	1.63	0.63
3:O:287:ASP:HB3	3:O:290:LYS:HE2	1.80	0.63
3:R:235:LEU:HD22	3:S:244:ARG:HH12	1.63	0.63
3:R:287:ASP:HB3	3:R:290:LYS:HE2	1.80	0.63
3:Z:235:LEU:HD22	3:a:244:ARG:HH12	1.63	0.63
3:Z:287:ASP:HB3	3:Z:290:LYS:HE2	1.80	0.63
3:d:235:LEU:HD22	3:e:244:ARG:HH12	1.63	0.63
2:q:76:GLN:H	3:U:297:GLN:HE22	1.46	0.62
3:f:394:LYS:HE3	3:f:394:LYS:HA	1.80	0.62
2:p:73:ILE:CG1	3:b:295:SER:HB2	2.22	0.62
3:E:287:ASP:HB3	3:E:290:LYS:HE2	1.80	0.62
3:X:287:ASP:HB3	3:X:290:LYS:HE2	1.80	0.62
1:j:11:ILE:HG23	3:Y:372:ILE:HG21	1.76	0.62
3:A:287:ASP:HB3	3:A:290:LYS:HE2	1.80	0.62
3:C:235:LEU:HD22	3:D:244:ARG:HH12	1.63	0.62
3:U:287:ASP:HB3	3:U:290:LYS:HE2	1.80	0.62
3:b:235:LEU:HD22	3:c:244:ARG:HH12	1.63	0.62
1:k:4:ILE:CG1	3:T:372:ILE:HG22	2.29	0.62
2:q:72:HIS:CB	3:V:295:SER:CB	2.73	0.62
3:B:394:LYS:HE3	3:B:394:LYS:HA	1.80	0.62
3:F:394:LYS:HE3	3:F:394:LYS:HA	1.80	0.62
3:I:235:LEU:HD22	3:J:244:ARG:HH12	1.63	0.62
3:b:394:LYS:HA	3:b:394:LYS:HE3	1.80	0.62
3:E:235:LEU:HD22	3:F:244:ARG:HH12	1.63	0.62
3:D:394:LYS:HE3	3:D:394:LYS:HA	1.80	0.62
3:T:287:ASP:HB3	3:T:290:LYS:HE2	1.80	0.62
3:V:287:ASP:HB3	3:V:290:LYS:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:394:LYS:HA	3:g:394:LYS:HE3	1.80	0.62
3:N:287:ASP:HB3	3:N:290:LYS:HE2	1.80	0.62
2:q:72:HIS:CE1	3:U:365:ASN:HB3	2.33	0.62
2:s:78:VAL:HG12	3:H:299:ASN:HD21	1.62	0.62
3:E:394:LYS:HA	3:E:394:LYS:HE3	1.80	0.62
3:G:235:LEU:HD22	3:H:244:ARG:HH12	1.63	0.62
3:a:287:ASP:HB3	3:a:290:LYS:HE2	1.80	0.62
1:j:4:ILE:HG13	3:Z:372:ILE:HG21	1.82	0.62
2:q:65:LEU:HD12	2:q:65:LEU:C	2.25	0.62
3:c:394:LYS:HE3	3:c:394:LYS:HA	1.80	0.62
3:F:287:ASP:HB3	3:F:290:LYS:HE2	1.80	0.62
3:g:287:ASP:HB3	3:g:290:LYS:HE2	1.80	0.62
3:H:287:ASP:HB3	3:H:290:LYS:HE2	1.80	0.61
3:S:287:ASP:HB3	3:S:290:LYS:HE2	1.80	0.61
3:h:287:ASP:HB3	3:h:290:LYS:HE2	1.80	0.61
3:h:394:LYS:HE3	3:h:394:LYS:HA	1.80	0.61
3:e:394:LYS:HE3	3:e:394:LYS:HA	1.80	0.61
3:W:287:ASP:HB3	3:W:290:LYS:HE2	1.81	0.61
3:U:277:GLN:HB3	3:U:377:MET:HE1	1.83	0.61
3:V:277:GLN:HB3	3:V:377:MET:HE1	1.83	0.61
3:Y:277:GLN:HB3	3:Y:377:MET:HE1	1.83	0.61
3:a:277:GLN:HB3	3:a:377:MET:HE1	1.83	0.61
3:d:394:LYS:HE3	3:d:394:LYS:HA	1.80	0.61
3:W:277:GLN:HB3	3:W:377:MET:HE1	1.83	0.61
1:k:11:ILE:CD1	1:k:12:SER:N	2.55	0.61
1:n:11:ILE:CG2	3:A:372:ILE:CG2	2.78	0.61
3:R:277:GLN:HB3	3:R:377:MET:HE1	1.83	0.61
3:T:277:GLN:HB3	3:T:377:MET:HE1	1.83	0.61
3:C:394:LYS:HE3	3:C:394:LYS:HA	1.80	0.61
3:S:277:GLN:HB3	3:S:377:MET:HE1	1.83	0.61
3:X:277:GLN:HB3	3:X:377:MET:HE1	1.83	0.61
1:m:14:LEU:CD1	3:G:370:ARG:HH21	2.10	0.61
3:Z:277:GLN:HB3	3:Z:377:MET:HE1	1.83	0.61
3:c:277:GLN:HB3	3:c:377:MET:HE1	1.83	0.61
1:k:3:ALA:C	3:T:372:ILE:HD13	2.26	0.61
1:k:11:ILE:HD12	1:k:12:SER:CA	2.31	0.61
3:G:287:ASP:HB3	3:G:290:LYS:HE2	1.80	0.61
1:m:14:LEU:HD23	3:F:278:THR:HG21	1.83	0.61
3:Q:277:GLN:HB3	3:Q:377:MET:HE1	1.83	0.61
3:b:277:GLN:HB3	3:b:377:MET:HE1	1.83	0.61
3:D:277:GLN:HB3	3:D:377:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:277:GLN:HB3	3:P:377:MET:HE1	1.83	0.60
3:H:277:GLN:HB3	3:H:377:MET:HE1	1.83	0.60
3:e:277:GLN:HB3	3:e:377:MET:HE1	1.83	0.60
3:C:277:GLN:HB3	3:C:377:MET:HE1	1.83	0.60
3:I:277:GLN:HB3	3:I:377:MET:HE1	1.83	0.60
3:d:277:GLN:HB3	3:d:377:MET:HE1	1.83	0.60
3:E:277:GLN:HB3	3:E:377:MET:HE1	1.83	0.60
3:O:277:GLN:HB3	3:O:377:MET:HE1	1.83	0.60
3:d:402:LEU:HD12	3:d:403:PRO:HD2	1.84	0.60
3:K:402:LEU:HD12	3:K:403:PRO:HD2	1.84	0.60
3:G:277:GLN:HB3	3:G:377:MET:HE1	1.83	0.60
3:L:402:LEU:HD12	3:L:403:PRO:HD2	1.84	0.60
3:N:277:GLN:HB3	3:N:377:MET:HE1	1.83	0.60
3:H:402:LEU:HD12	3:H:403:PRO:HD2	1.84	0.60
3:I:402:LEU:HD12	3:I:403:PRO:HD2	1.84	0.60
3:N:402:LEU:HD12	3:N:403:PRO:HD2	1.84	0.60
3:O:402:LEU:HD12	3:O:403:PRO:HD2	1.84	0.60
3:X:402:LEU:HD12	3:X:403:PRO:HD2	1.84	0.60
3:Y:402:LEU:HD12	3:Y:403:PRO:HD2	1.84	0.60
3:c:402:LEU:HD12	3:c:403:PRO:HD2	1.84	0.60
3:f:277:GLN:HB3	3:f:377:MET:HE1	1.83	0.60
1:k:11:ILE:CG2	3:S:372:ILE:HG22	2.31	0.59
3:J:402:LEU:HD12	3:J:403:PRO:HD2	1.84	0.59
3:M:277:GLN:HB3	3:M:377:MET:HE1	1.83	0.59
3:M:402:LEU:HD12	3:M:403:PRO:HD2	1.84	0.59
3:e:402:LEU:HD12	3:e:403:PRO:HD2	1.84	0.59
3:g:277:GLN:HB3	3:g:377:MET:HE1	1.83	0.59
3:J:277:GLN:HB3	3:J:377:MET:HE1	1.83	0.59
2:s:68:THR:CG2	3:H:294:ARG:HD3	2.31	0.59
3:B:277:GLN:HB3	3:B:377:MET:HE1	1.83	0.59
2:r:65:LEU:HB2	3:N:295:SER:CB	2.32	0.59
3:G:402:LEU:HD12	3:G:403:PRO:HD2	1.84	0.59
3:W:402:LEU:HD12	3:W:403:PRO:HD2	1.84	0.59
3:f:402:LEU:HD12	3:f:403:PRO:HD2	1.84	0.59
3:F:402:LEU:HD12	3:F:403:PRO:HD2	1.84	0.59
3:L:277:GLN:HB3	3:L:377:MET:HE1	1.83	0.59
3:P:402:LEU:HD12	3:P:403:PRO:HD2	1.84	0.59
3:Q:402:LEU:HD12	3:Q:403:PRO:HD2	1.84	0.59
3:Z:402:LEU:HD12	3:Z:403:PRO:HD2	1.84	0.59
3:h:277:GLN:HB3	3:h:377:MET:HE1	1.83	0.59
2:p:68:THR:CG2	3:a:294:ARG:CD	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:402:LEU:HD12	3:E:403:PRO:HD2	1.84	0.59
3:b:402:LEU:HD12	3:b:403:PRO:HD2	1.84	0.59
3:R:402:LEU:HD12	3:R:403:PRO:HD2	1.84	0.59
3:A:402:LEU:HD12	3:A:403:PRO:HD2	1.84	0.59
3:F:277:GLN:HB3	3:F:377:MET:HE1	1.83	0.59
3:a:252:ILE:HD11	3:a:419:ALA:HB2	1.85	0.59
1:j:7:ILE:CG2	3:Y:278:THR:HG21	2.33	0.59
3:B:377:MET:SD	3:B:377:MET:N	2.76	0.59
3:B:402:LEU:HD12	3:B:403:PRO:HD2	1.84	0.59
3:N:377:MET:SD	3:N:377:MET:N	2.76	0.59
3:P:377:MET:SD	3:P:377:MET:N	2.76	0.59
3:Y:252:ILE:HD11	3:Y:419:ALA:HB2	1.85	0.59
3:Z:252:ILE:HD11	3:Z:419:ALA:HB2	1.85	0.59
1:j:7:ILE:HD11	3:Z:370:ARG:NE	2.17	0.58
1:n:11:ILE:HG22	3:A:372:ILE:HG21	1.85	0.58
3:D:402:LEU:HD12	3:D:403:PRO:HD2	1.84	0.58
3:L:377:MET:SD	3:L:377:MET:N	2.76	0.58
3:U:377:MET:SD	3:U:377:MET:N	2.76	0.58
3:W:377:MET:SD	3:W:377:MET:N	2.76	0.58
3:h:377:MET:SD	3:h:377:MET:N	2.76	0.58
1:j:11:ILE:CG2	3:Y:372:ILE:HB	2.33	0.58
3:D:377:MET:SD	3:D:377:MET:N	2.76	0.58
3:K:277:GLN:HB3	3:K:377:MET:HE1	1.83	0.58
3:e:377:MET:SD	3:e:377:MET:N	2.76	0.58
3:G:252:ILE:HD11	3:G:419:ALA:HB2	1.85	0.58
3:H:252:ILE:HD11	3:H:419:ALA:HB2	1.85	0.58
3:K:252:ILE:HD11	3:K:419:ALA:HB2	1.85	0.58
3:R:377:MET:SD	3:R:377:MET:N	2.76	0.58
3:T:252:ILE:HD11	3:T:419:ALA:HB2	1.85	0.58
3:U:252:ILE:HD11	3:U:419:ALA:HB2	1.85	0.58
3:U:305:GLY:HA3	3:U:355:PRO:HG2	1.86	0.58
3:V:402:LEU:HD12	3:V:403:PRO:HD2	1.84	0.58
3:h:402:LEU:HD12	3:h:403:PRO:HD2	1.84	0.58
2:q:67:LEU:HA	2:q:72:HIS:NE2	2.18	0.58
2:r:65:LEU:HB2	3:N:295:SER:HB2	1.84	0.58
3:A:277:GLN:HB3	3:A:377:MET:HE1	1.83	0.58
3:J:252:ILE:HD11	3:J:419:ALA:HB2	1.85	0.58
3:K:305:GLY:HA3	3:K:355:PRO:HG2	1.86	0.58
3:Q:305:GLY:HA3	3:Q:355:PRO:HG2	1.86	0.58
3:S:377:MET:SD	3:S:377:MET:N	2.76	0.58
3:T:377:MET:N	3:T:377:MET:SD	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:377:MET:N	3:Y:377:MET:SD	2.76	0.58
3:b:252:ILE:HD11	3:b:419:ALA:HB2	1.85	0.58
3:f:252:ILE:HD11	3:f:419:ALA:HB2	1.85	0.58
3:F:252:ILE:HD11	3:F:419:ALA:HB2	1.85	0.58
3:L:305:GLY:HA3	3:L:355:PRO:HG2	1.86	0.58
3:P:305:GLY:HA3	3:P:355:PRO:HG2	1.86	0.58
3:S:402:LEU:HD12	3:S:403:PRO:HD2	1.84	0.58
3:V:305:GLY:HA3	3:V:355:PRO:HG2	1.86	0.58
3:e:252:ILE:HD11	3:e:419:ALA:HB2	1.85	0.58
3:g:377:MET:SD	3:g:377:MET:N	2.76	0.58
3:E:252:ILE:HD11	3:E:419:ALA:HB2	1.85	0.58
3:J:377:MET:SD	3:J:377:MET:N	2.76	0.58
3:S:252:ILE:HD11	3:S:419:ALA:HB2	1.85	0.58
3:V:252:ILE:HD11	3:V:419:ALA:HB2	1.85	0.58
3:a:402:LEU:HD12	3:a:403:PRO:HD2	1.84	0.58
3:f:377:MET:SD	3:f:377:MET:N	2.76	0.58
3:g:402:LEU:HD12	3:g:403:PRO:HD2	1.84	0.58
2:p:66:THR:OG1	3:a:294:ARG:HG2	2.03	0.58
3:M:252:ILE:HD11	3:M:419:ALA:HB2	1.85	0.58
3:V:377:MET:SD	3:V:377:MET:N	2.76	0.58
3:c:377:MET:SD	3:c:377:MET:N	2.76	0.58
1:j:11:ILE:HG22	3:Y:372:ILE:CB	2.32	0.58
3:C:402:LEU:HD12	3:C:403:PRO:HD2	1.84	0.58
3:D:252:ILE:HD11	3:D:419:ALA:HB2	1.85	0.58
3:E:377:MET:SD	3:E:377:MET:N	2.76	0.58
3:I:252:ILE:HD11	3:I:419:ALA:HB2	1.85	0.58
3:K:377:MET:SD	3:K:377:MET:N	2.76	0.58
3:Q:377:MET:SD	3:Q:377:MET:N	2.76	0.58
3:X:252:ILE:HD11	3:X:419:ALA:HB2	1.85	0.58
3:g:252:ILE:HD11	3:g:419:ALA:HB2	1.85	0.58
1:i:11:ILE:CD1	3:c:276:GLU:OE2	2.52	0.58
1:k:7:ILE:CB	3:S:278:THR:HG21	2.11	0.58
3:A:377:MET:SD	3:A:377:MET:N	2.76	0.58
3:L:252:ILE:HD11	3:L:419:ALA:HB2	1.85	0.58
3:M:377:MET:SD	3:M:377:MET:N	2.76	0.58
3:Z:305:GLY:HA3	3:Z:355:PRO:HG2	1.86	0.58
3:a:305:GLY:HA3	3:a:355:PRO:HG2	1.86	0.58
3:M:305:GLY:HA3	3:M:355:PRO:HG2	1.86	0.58
3:N:252:ILE:HD11	3:N:419:ALA:HB2	1.85	0.58
3:O:305:GLY:HA3	3:O:355:PRO:HG2	1.86	0.58
3:R:305:GLY:HA3	3:R:355:PRO:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:402:LEU:HD12	3:T:403:PRO:HD2	1.84	0.58
3:W:305:GLY:HA3	3:W:355:PRO:HG2	1.86	0.58
3:a:377:MET:SD	3:a:377:MET:N	2.76	0.58
3:G:377:MET:SD	3:G:377:MET:N	2.76	0.57
3:J:305:GLY:HA3	3:J:355:PRO:HG2	1.86	0.57
3:T:305:GLY:HA3	3:T:355:PRO:HG2	1.86	0.57
3:d:252:ILE:HD11	3:d:419:ALA:HB2	1.85	0.57
1:k:19:MET:HA	3:Q:276:GLU:OE2	2.04	0.57
3:H:377:MET:SD	3:H:377:MET:N	2.76	0.57
3:I:377:MET:SD	3:I:377:MET:N	2.76	0.57
3:X:377:MET:SD	3:X:377:MET:N	2.76	0.57
2:o:67:LEU:HD11	2:o:74:PRO:HA	1.85	0.57
3:A:305:GLY:HA3	3:A:355:PRO:HG2	1.85	0.57
3:C:252:ILE:HD11	3:C:419:ALA:HB2	1.85	0.57
3:F:377:MET:SD	3:F:377:MET:N	2.76	0.57
3:U:402:LEU:HD12	3:U:403:PRO:HD2	1.84	0.57
3:Y:305:GLY:HA3	3:Y:355:PRO:HG2	1.86	0.57
3:b:305:GLY:HA3	3:b:355:PRO:HG2	1.86	0.57
1:m:11:ILE:HG22	3:G:372:ILE:CB	2.34	0.57
2:s:72:HIS:HE1	3:I:294:ARG:NE	2.01	0.57
3:O:377:MET:SD	3:O:377:MET:N	2.76	0.57
3:c:252:ILE:HD11	3:c:419:ALA:HB2	1.85	0.57
1:k:4:ILE:HG12	3:T:372:ILE:CB	2.34	0.57
3:R:252:ILE:HD11	3:R:419:ALA:HB2	1.85	0.57
3:b:377:MET:SD	3:b:377:MET:N	2.76	0.57
3:h:305:GLY:HA3	3:h:355:PRO:HG2	1.86	0.57
1:m:11:ILE:CG2	3:G:372:ILE:CG2	2.83	0.57
3:B:252:ILE:HD11	3:B:419:ALA:HB2	1.85	0.57
3:G:305:GLY:HA3	3:G:355:PRO:HG2	1.86	0.57
3:O:252:ILE:HD11	3:O:419:ALA:HB2	1.85	0.57
3:W:252:ILE:HD11	3:W:419:ALA:HB2	1.85	0.57
3:Z:377:MET:SD	3:Z:377:MET:N	2.76	0.57
3:g:305:GLY:HA3	3:g:355:PRO:HG2	1.86	0.57
1:j:11:ILE:HG21	3:Y:372:ILE:HB	1.87	0.57
2:q:65:LEU:CD1	3:U:365:ASN:ND2	2.67	0.57
3:A:252:ILE:HD11	3:A:419:ALA:HB2	1.85	0.57
3:C:377:MET:N	3:C:377:MET:SD	2.76	0.57
3:D:305:GLY:HA3	3:D:355:PRO:HG2	1.86	0.57
3:h:252:ILE:HD11	3:h:419:ALA:HB2	1.85	0.57
3:B:305:GLY:HA3	3:B:355:PRO:HG2	1.86	0.57
3:C:305:GLY:HA3	3:C:355:PRO:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:305:GLY:HA3	3:X:355:PRO:HG2	1.86	0.57
1:m:8:GLU:O	1:m:11:ILE:HG13	2.05	0.57
2:p:65:LEU:HD22	3:a:295:SER:HB2	1.86	0.57
3:F:305:GLY:HA3	3:F:355:PRO:HG2	1.86	0.57
3:P:252:ILE:HD11	3:P:419:ALA:HB2	1.85	0.57
3:d:377:MET:SD	3:d:377:MET:N	2.76	0.57
3:N:305:GLY:HA3	3:N:355:PRO:HG2	1.86	0.56
3:e:305:GLY:HA3	3:e:355:PRO:HG2	1.86	0.56
3:f:305:GLY:HA3	3:f:355:PRO:HG2	1.86	0.56
3:I:305:GLY:HA3	3:I:355:PRO:HG2	1.86	0.56
3:S:305:GLY:HA3	3:S:355:PRO:HG2	1.86	0.56
1:j:8:GLU:O	1:j:11:ILE:HG13	2.06	0.56
1:n:8:GLU:O	1:n:11:ILE:HG13	2.06	0.56
3:H:305:GLY:HA3	3:H:355:PRO:HG2	1.86	0.56
3:Q:252:ILE:HD11	3:Q:419:ALA:HB2	1.85	0.56
3:c:305:GLY:HA3	3:c:355:PRO:HG2	1.86	0.56
1:i:8:GLU:O	1:i:11:ILE:HG13	2.05	0.56
3:E:305:GLY:HA3	3:E:355:PRO:HG2	1.86	0.56
1:j:11:ILE:HG22	3:Y:372:ILE:CG1	2.32	0.56
3:d:305:GLY:HA3	3:d:355:PRO:HG2	1.86	0.56
1:i:14:LEU:CB	3:c:278:THR:HG21	2.35	0.56
1:l:14:LEU:HD11	3:M:370:ARG:HH21	1.71	0.56
1:m:7:ILE:HG22	3:G:278:THR:HG21	1.78	0.56
2:o:73:ILE:HG13	3:A:295:SER:HB2	1.88	0.55
1:k:12:SER:O	1:k:15:GLN:HG3	2.06	0.55
3:O:264:ALA:HB2	3:O:389:VAL:HG13	1.89	0.55
1:l:21:ALA:HB1	3:K:278:THR:CG2	2.35	0.55
3:L:264:ALA:HB2	3:L:389:VAL:HG13	1.89	0.55
3:C:264:ALA:HB2	3:C:389:VAL:HG13	1.89	0.55
3:h:264:ALA:HB2	3:h:389:VAL:HG13	1.89	0.55
1:j:11:ILE:HG21	3:Y:372:ILE:HG22	1.83	0.55
3:C:409:MET:HA	3:C:409:MET:HE2	1.89	0.55
3:D:409:MET:HE2	3:D:409:MET:HA	1.89	0.55
3:F:264:ALA:HB2	3:F:389:VAL:HG13	1.89	0.55
3:I:264:ALA:HB2	3:I:389:VAL:HG13	1.89	0.55
3:B:264:ALA:HB2	3:B:389:VAL:HG13	1.89	0.55
3:E:409:MET:HE2	3:E:409:MET:HA	1.89	0.55
3:R:264:ALA:HB2	3:R:389:VAL:HG13	1.89	0.55
3:d:409:MET:HE2	3:d:409:MET:HA	1.89	0.55
3:e:409:MET:HA	3:e:409:MET:HE2	1.89	0.55
1:l:8:GLU:O	1:l:11:ILE:HG13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:409:MET:HA	3:A:409:MET:HE2	1.89	0.55
3:B:409:MET:HE2	3:B:409:MET:HA	1.89	0.55
3:E:264:ALA:HB2	3:E:389:VAL:HG13	1.89	0.55
3:F:409:MET:HA	3:F:409:MET:HE2	1.89	0.55
3:M:264:ALA:HB2	3:M:389:VAL:HG13	1.89	0.55
3:c:409:MET:HA	3:c:409:MET:HE2	1.89	0.55
3:f:409:MET:HE2	3:f:409:MET:HA	1.89	0.55
3:P:264:ALA:HB2	3:P:389:VAL:HG13	1.89	0.55
3:e:264:ALA:HB2	3:e:389:VAL:HG13	1.89	0.55
3:g:264:ALA:HB2	3:g:389:VAL:HG13	1.89	0.55
3:g:409:MET:HE2	3:g:409:MET:HA	1.89	0.55
3:G:409:MET:HE2	3:G:409:MET:HA	1.89	0.54
3:b:409:MET:HE2	3:b:409:MET:HA	1.89	0.54
3:h:409:MET:HA	3:h:409:MET:HE2	1.89	0.54
3:H:264:ALA:HB2	3:H:389:VAL:HG13	1.89	0.54
3:a:409:MET:HE2	3:a:409:MET:HA	1.89	0.54
1:l:21:ALA:CB	3:K:278:THR:CG2	2.74	0.54
3:H:409:MET:HA	3:H:409:MET:HE2	1.89	0.54
3:J:264:ALA:HB2	3:J:389:VAL:HG13	1.89	0.54
3:K:264:ALA:HB2	3:K:389:VAL:HG13	1.89	0.54
3:N:264:ALA:HB2	3:N:389:VAL:HG13	1.89	0.54
3:Q:264:ALA:HB2	3:Q:389:VAL:HG13	1.89	0.54
3:S:409:MET:HE2	3:S:409:MET:HA	1.89	0.54
3:N:409:MET:HE2	3:N:409:MET:HA	1.89	0.54
3:P:409:MET:HE2	3:P:409:MET:HA	1.89	0.54
3:Z:409:MET:HE2	3:Z:409:MET:HA	1.89	0.54
1:l:11:ILE:HG22	3:M:372:ILE:HB	1.88	0.54
3:G:264:ALA:HB2	3:G:389:VAL:HG13	1.89	0.54
3:I:409:MET:HE2	3:I:409:MET:HA	1.89	0.54
3:Q:409:MET:HE2	3:Q:409:MET:HA	1.89	0.54
3:T:264:ALA:HB2	3:T:389:VAL:HG13	1.89	0.54
3:U:264:ALA:HB2	3:U:389:VAL:HG13	1.89	0.54
3:U:409:MET:HE2	3:U:409:MET:HA	1.89	0.54
3:A:264:ALA:HB2	3:A:389:VAL:HG13	1.89	0.54
3:D:264:ALA:HB2	3:D:389:VAL:HG13	1.89	0.54
3:Y:409:MET:HA	3:Y:409:MET:HE2	1.89	0.54
3:b:264:ALA:HB2	3:b:389:VAL:HG13	1.89	0.54
3:V:282:TYR:HB3	3:W:292:THR:HG21	1.90	0.54
3:W:264:ALA:HB2	3:W:389:VAL:HG13	1.89	0.54
1:n:4:ILE:HD11	3:B:374:HIS:HB2	1.90	0.54
3:T:282:TYR:HB3	3:U:292:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:282:TYR:HB3	3:V:292:THR:HG21	1.90	0.54
3:Z:264:ALA:HB2	3:Z:389:VAL:HG13	1.89	0.54
3:f:264:ALA:HB2	3:f:389:VAL:HG13	1.89	0.54
3:E:282:TYR:HB3	3:F:292:THR:HG21	1.90	0.53
3:J:409:MET:HA	3:J:409:MET:HE2	1.89	0.53
3:S:264:ALA:HB2	3:S:389:VAL:HG13	1.89	0.53
3:S:282:TYR:HB3	3:T:292:THR:HG21	1.90	0.53
3:W:282:TYR:HB3	3:X:292:THR:HG21	1.90	0.53
3:X:282:TYR:HB3	3:Y:292:THR:HG21	1.90	0.53
1:l:7:ILE:CG2	3:M:278:THR:CG2	2.80	0.53
2:q:65:LEU:HD13	3:U:365:ASN:ND2	2.24	0.53
3:X:409:MET:HE2	3:X:409:MET:HA	1.89	0.53
3:c:264:ALA:HB2	3:c:389:VAL:HG13	1.89	0.53
3:H:282:TYR:HB3	3:I:292:THR:HG21	1.90	0.53
3:R:409:MET:HA	3:R:409:MET:HE2	1.89	0.53
3:V:409:MET:HE2	3:V:409:MET:HA	1.89	0.53
3:Y:264:ALA:HB2	3:Y:389:VAL:HG13	1.89	0.53
2:p:65:LEU:HB3	3:a:295:SER:HB2	1.90	0.53
3:B:282:TYR:HB3	3:C:292:THR:HG21	1.90	0.53
3:C:282:TYR:HB3	3:D:292:THR:HG21	1.90	0.53
3:G:282:TYR:HB3	3:H:292:THR:HG21	1.90	0.53
3:J:282:TYR:HB3	3:K:292:THR:HG21	1.90	0.53
3:R:282:TYR:HB3	3:S:292:THR:HG21	1.90	0.53
3:X:264:ALA:HB2	3:X:389:VAL:HG13	1.89	0.53
3:Y:282:TYR:HB3	3:Z:292:THR:HG21	1.90	0.53
3:d:264:ALA:HB2	3:d:389:VAL:HG13	1.89	0.53
1:k:4:ILE:HG12	3:T:372:ILE:CG2	2.37	0.53
3:K:409:MET:HE2	3:K:409:MET:HA	1.89	0.53
3:Z:282:TYR:HB3	3:a:292:THR:HG21	1.90	0.53
1:k:11:ILE:HG21	3:S:372:ILE:HG22	1.90	0.53
1:m:10:VAL:HG12	3:G:372:ILE:CD1	2.39	0.53
3:A:292:THR:HG21	3:h:282:TYR:HB3	1.90	0.53
3:L:409:MET:HE2	3:L:409:MET:HA	1.89	0.53
3:W:409:MET:HA	3:W:409:MET:HE2	1.89	0.53
3:Q:282:TYR:HB3	3:R:292:THR:HG21	1.90	0.53
3:a:264:ALA:HB2	3:a:389:VAL:HG13	1.89	0.53
3:a:282:TYR:HB3	3:b:292:THR:HG21	1.90	0.53
3:b:282:TYR:HB3	3:c:292:THR:HG21	1.90	0.53
1:l:11:ILE:CG2	3:M:372:ILE:CG2	2.87	0.53
3:H:293:LEU:HD21	3:H:364:SER:HB3	1.91	0.53
3:J:293:LEU:HD21	3:J:364:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:293:LEU:HD21	3:Q:364:SER:HB3	1.91	0.53
3:V:264:ALA:HB2	3:V:389:VAL:HG13	1.89	0.53
3:M:409:MET:HA	3:M:409:MET:HE2	1.89	0.53
3:O:293:LEU:HD21	3:O:364:SER:HB3	1.91	0.53
3:O:409:MET:HA	3:O:409:MET:HE2	1.89	0.53
3:T:293:LEU:HD21	3:T:364:SER:HB3	1.91	0.53
3:T:409:MET:HA	3:T:409:MET:HE2	1.89	0.53
3:G:293:LEU:HD21	3:G:364:SER:HB3	1.91	0.53
3:P:282:TYR:HB3	3:Q:292:THR:HG21	1.90	0.53
3:R:293:LEU:HD21	3:R:364:SER:HB3	1.91	0.53
1:m:7:ILE:HG22	3:G:278:THR:CG2	2.32	0.52
3:F:282:TYR:HB3	3:G:292:THR:HG21	1.90	0.52
3:L:293:LEU:HD21	3:L:364:SER:HB3	1.91	0.52
3:S:293:LEU:HD21	3:S:364:SER:HB3	1.91	0.52
3:V:293:LEU:HD21	3:V:364:SER:HB3	1.91	0.52
2:r:72:HIS:HD2	3:N:365:ASN:CG	2.16	0.52
3:D:282:TYR:HB3	3:E:292:THR:HG21	1.90	0.52
3:F:293:LEU:HD21	3:F:364:SER:HB3	1.91	0.52
3:M:293:LEU:HD21	3:M:364:SER:HB3	1.91	0.52
3:c:282:TYR:HB3	3:d:292:THR:HG21	1.90	0.52
3:K:282:TYR:HB3	3:L:292:THR:HG21	1.90	0.52
3:L:282:TYR:HB3	3:M:292:THR:HG21	1.90	0.52
3:M:282:TYR:HB3	3:N:292:THR:HG21	1.90	0.52
3:U:293:LEU:HD21	3:U:364:SER:HB3	1.91	0.52
3:I:282:TYR:HB3	3:J:292:THR:HG21	1.90	0.52
3:I:293:LEU:HD21	3:I:364:SER:HB3	1.91	0.52
3:K:293:LEU:HD21	3:K:364:SER:HB3	1.91	0.52
3:N:293:LEU:HD21	3:N:364:SER:HB3	1.91	0.52
3:O:282:TYR:HB3	3:P:292:THR:HG21	1.90	0.52
3:X:293:LEU:HD21	3:X:364:SER:HB3	1.91	0.52
3:d:282:TYR:HB3	3:e:292:THR:HG21	1.90	0.52
3:A:282:TYR:HB3	3:B:292:THR:HG21	1.90	0.52
3:E:293:LEU:HD21	3:E:364:SER:HB3	1.91	0.52
1:l:7:ILE:HG21	3:M:278:THR:HG22	1.91	0.52
3:P:293:LEU:HD21	3:P:364:SER:HB3	1.91	0.52
3:f:282:TYR:HB3	3:g:292:THR:HG21	1.90	0.52
3:B:235:LEU:HB3	3:C:244:ARG:HH22	1.75	0.52
3:H:235:LEU:HB3	3:I:244:ARG:HH22	1.75	0.52
3:W:293:LEU:HD21	3:W:364:SER:HB3	1.91	0.52
3:Y:235:LEU:HB3	3:Z:244:ARG:HH22	1.75	0.52
3:D:293:LEU:HD21	3:D:364:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:235:LEU:HB3	3:L:244:ARG:HH22	1.75	0.52
3:d:235:LEU:HB3	3:e:244:ARG:HH22	1.75	0.52
3:g:282:TYR:HB3	3:h:292:THR:HG21	1.90	0.52
3:C:293:LEU:HD21	3:C:364:SER:HB3	1.91	0.52
3:E:235:LEU:HB3	3:F:244:ARG:HH22	1.75	0.52
3:F:235:LEU:HB3	3:G:244:ARG:HH22	1.75	0.52
3:V:235:LEU:HB3	3:W:244:ARG:HH22	1.75	0.52
3:a:235:LEU:HB3	3:b:244:ARG:HH22	1.75	0.52
3:e:282:TYR:HB3	3:f:292:THR:HG21	1.90	0.52
3:C:235:LEU:HB3	3:D:244:ARG:HH22	1.75	0.52
3:N:282:TYR:HB3	3:O:292:THR:HG21	1.90	0.52
3:Z:293:LEU:HD21	3:Z:364:SER:HB3	1.91	0.52
3:c:235:LEU:HB3	3:d:244:ARG:HH22	1.75	0.52
3:f:235:LEU:HB3	3:g:244:ARG:HH22	1.75	0.52
3:g:235:LEU:HB3	3:h:244:ARG:HH22	1.75	0.52
3:Q:235:LEU:HB3	3:R:244:ARG:HH22	1.75	0.51
3:T:235:LEU:HB3	3:U:244:ARG:HH22	1.75	0.51
3:Y:293:LEU:HD21	3:Y:364:SER:HB3	1.91	0.51
2:p:67:LEU:HG	2:p:72:HIS:HB3	1.92	0.51
3:A:235:LEU:HB3	3:B:244:ARG:HH22	1.75	0.51
3:I:235:LEU:HB3	3:J:244:ARG:HH22	1.75	0.51
3:b:235:LEU:HB3	3:c:244:ARG:HH22	1.75	0.51
3:f:293:LEU:HD21	3:f:364:SER:HB3	1.91	0.51
2:q:67:LEU:HA	2:q:72:HIS:HE2	1.74	0.51
3:J:235:LEU:HB3	3:K:244:ARG:HH22	1.75	0.51
3:M:235:LEU:HB3	3:N:244:ARG:HH22	1.75	0.51
3:N:235:LEU:HB3	3:O:244:ARG:HH22	1.75	0.51
3:a:256:ILE:HG13	3:a:257:VAL:N	2.26	0.51
1:j:7:ILE:CD1	3:Z:370:ARG:HE	2.24	0.51
3:B:293:LEU:HD21	3:B:364:SER:HB3	1.91	0.51
3:L:256:ILE:HG13	3:L:257:VAL:N	2.26	0.51
3:X:235:LEU:HB3	3:Y:244:ARG:HH22	1.75	0.51
1:k:8:GLU:O	1:k:11:ILE:HG13	2.09	0.51
2:p:68:THR:HG21	3:a:294:ARG:HD2	1.92	0.51
2:s:65:LEU:CB	3:H:295:SER:HB2	2.39	0.51
3:A:293:LEU:HD21	3:A:364:SER:HB3	1.91	0.51
3:N:256:ILE:HG13	3:N:257:VAL:N	2.26	0.51
3:P:256:ILE:HG13	3:P:257:VAL:N	2.26	0.51
3:S:235:LEU:HB3	3:T:244:ARG:HH22	1.75	0.51
3:Y:256:ILE:HG13	3:Y:257:VAL:N	2.26	0.51
3:c:256:ILE:HG13	3:c:257:VAL:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:293:LEU:HD21	3:c:364:SER:HB3	1.91	0.51
3:O:256:ILE:HG13	3:O:257:VAL:N	2.26	0.51
3:P:235:LEU:HB3	3:Q:244:ARG:HH22	1.75	0.51
3:d:256:ILE:HG13	3:d:257:VAL:N	2.26	0.51
3:e:293:LEU:HD21	3:e:364:SER:HB3	1.91	0.51
1:m:14:LEU:CB	3:F:278:THR:HG21	2.31	0.51
3:W:235:LEU:HB3	3:X:244:ARG:HH22	1.75	0.51
3:a:293:LEU:HD21	3:a:364:SER:HB3	1.91	0.51
3:b:293:LEU:HD21	3:b:364:SER:HB3	1.91	0.51
3:f:256:ILE:HG13	3:f:257:VAL:N	2.26	0.51
3:D:235:LEU:HB3	3:E:244:ARG:HH22	1.75	0.51
3:I:256:ILE:HG13	3:I:257:VAL:N	2.26	0.51
3:h:293:LEU:HD21	3:h:364:SER:HB3	1.91	0.51
3:J:256:ILE:HG13	3:J:257:VAL:N	2.26	0.51
3:K:256:ILE:HG13	3:K:257:VAL:N	2.26	0.51
3:A:244:ARG:HH22	3:h:235:LEU:HB3	1.75	0.50
3:W:256:ILE:HG13	3:W:257:VAL:N	2.26	0.50
3:d:293:LEU:HD21	3:d:364:SER:HB3	1.91	0.50
1:l:11:ILE:HG22	3:M:372:ILE:CB	2.40	0.50
3:A:256:ILE:HG13	3:A:257:VAL:N	2.26	0.50
3:g:256:ILE:HG13	3:g:257:VAL:N	2.26	0.50
3:L:235:LEU:HB3	3:M:244:ARG:HH22	1.75	0.50
3:R:235:LEU:HB3	3:S:244:ARG:HH22	1.75	0.50
3:U:256:ILE:HG13	3:U:257:VAL:N	2.26	0.50
3:Z:256:ILE:HG13	3:Z:257:VAL:N	2.26	0.50
3:g:293:LEU:HD21	3:g:364:SER:HB3	1.92	0.50
3:U:235:LEU:HB3	3:V:244:ARG:HH22	1.75	0.50
3:Z:235:LEU:HB3	3:a:244:ARG:HH22	1.75	0.50
3:F:256:ILE:HG13	3:F:257:VAL:N	2.26	0.50
3:M:256:ILE:HG13	3:M:257:VAL:N	2.26	0.50
3:e:235:LEU:HB3	3:f:244:ARG:HH22	1.75	0.50
3:D:256:ILE:HG13	3:D:257:VAL:N	2.26	0.50
3:G:235:LEU:HB3	3:H:244:ARG:HH22	1.75	0.50
3:S:256:ILE:HG13	3:S:257:VAL:N	2.26	0.50
1:n:11:ILE:HG22	3:A:372:ILE:CG2	2.41	0.50
3:R:256:ILE:HG13	3:R:257:VAL:N	2.26	0.50
3:G:256:ILE:HG13	3:G:257:VAL:N	2.26	0.50
3:C:256:ILE:HG13	3:C:257:VAL:N	2.26	0.50
3:I:294:ARG:HD2	3:I:367:GLU:OE1	2.12	0.50
3:Q:256:ILE:HG13	3:Q:257:VAL:N	2.26	0.50
2:s:66:THR:HG23	3:G:365:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:294:ARG:HD2	3:A:367:GLU:OE1	2.12	0.49
3:B:294:ARG:HD2	3:B:367:GLU:OE1	2.12	0.49
3:C:294:ARG:HD2	3:C:367:GLU:OE1	2.12	0.49
3:E:294:ARG:HD2	3:E:367:GLU:OE1	2.12	0.49
3:H:294:ARG:HD2	3:H:367:GLU:OE1	2.12	0.49
3:O:235:LEU:HB3	3:P:244:ARG:HH22	1.75	0.49
3:d:294:ARG:HD2	3:d:367:GLU:OE1	2.12	0.49
3:f:294:ARG:HD2	3:f:367:GLU:OE1	2.13	0.49
3:g:294:ARG:HD2	3:g:367:GLU:OE1	2.12	0.49
3:D:294:ARG:HD2	3:D:367:GLU:OE1	2.12	0.49
3:F:294:ARG:HD2	3:F:367:GLU:OE1	2.12	0.49
3:G:294:ARG:HD2	3:G:367:GLU:OE1	2.13	0.49
3:H:256:ILE:HG13	3:H:257:VAL:N	2.26	0.49
3:V:256:ILE:HG13	3:V:257:VAL:N	2.26	0.49
3:e:256:ILE:HG13	3:e:257:VAL:N	2.26	0.49
3:e:294:ARG:HD2	3:e:367:GLU:OE1	2.12	0.49
3:h:294:ARG:HD2	3:h:367:GLU:OE1	2.13	0.49
2:q:66:THR:OG1	3:U:294:ARG:HG2	2.11	0.49
3:B:256:ILE:HG13	3:B:257:VAL:N	2.26	0.49
3:b:256:ILE:HG13	3:b:257:VAL:N	2.26	0.49
3:h:256:ILE:HG13	3:h:257:VAL:N	2.26	0.49
3:E:256:ILE:HG13	3:E:257:VAL:N	2.26	0.49
3:J:294:ARG:HD2	3:J:367:GLU:OE1	2.13	0.49
3:c:294:ARG:HD2	3:c:367:GLU:OE1	2.12	0.49
2:q:76:GLN:N	3:U:297:GLN:HE22	2.08	0.49
3:K:294:ARG:HD2	3:K:367:GLU:OE1	2.12	0.49
3:T:256:ILE:HG13	3:T:257:VAL:N	2.26	0.49
3:X:256:ILE:HG13	3:X:257:VAL:N	2.26	0.49
2:r:68:THR:CG2	3:N:294:ARG:CD	2.91	0.49
3:D:266:VAL:HG22	3:D:387:VAL:HG22	1.95	0.49
3:S:266:VAL:HG22	3:S:387:VAL:HG22	1.95	0.49
3:b:294:ARG:HD2	3:b:367:GLU:OE1	2.12	0.49
3:C:266:VAL:HG22	3:C:387:VAL:HG22	1.95	0.49
3:T:266:VAL:HG22	3:T:387:VAL:HG22	1.95	0.49
2:p:68:THR:HG21	3:a:294:ARG:CD	2.42	0.49
3:E:266:VAL:HG22	3:E:387:VAL:HG22	1.95	0.49
1:i:7:ILE:HG21	3:d:278:THR:HG22	1.81	0.48
1:j:11:ILE:CG2	3:Y:372:ILE:HD12	2.28	0.48
2:q:72:HIS:ND1	3:U:365:ASN:CG	2.70	0.48
3:R:266:VAL:HG22	3:R:387:VAL:HG22	1.95	0.48
3:S:294:ARG:HD2	3:S:367:GLU:OE1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:4:ILE:HG12	3:N:372:ILE:CG2	2.43	0.48
2:p:68:THR:HG21	3:a:294:ARG:HH11	1.78	0.48
2:q:65:LEU:HD11	3:U:365:ASN:HD21	1.78	0.48
3:K:266:VAL:HG22	3:K:387:VAL:HG22	1.95	0.48
3:L:294:ARG:HD2	3:L:367:GLU:OE1	2.13	0.48
3:R:294:ARG:HD2	3:R:367:GLU:OE1	2.12	0.48
3:T:294:ARG:HD2	3:T:367:GLU:OE1	2.12	0.48
3:a:294:ARG:HD2	3:a:367:GLU:OE1	2.12	0.48
1:n:11:ILE:HD11	3:h:276:GLU:CD	2.37	0.48
2:r:67:LEU:HD21	2:r:74:PRO:HB3	1.94	0.48
3:L:266:VAL:HG22	3:L:387:VAL:HG22	1.95	0.48
3:N:294:ARG:HD2	3:N:367:GLU:OE1	2.12	0.48
3:O:294:ARG:HD2	3:O:367:GLU:OE1	2.12	0.48
3:U:294:ARG:HD2	3:U:367:GLU:OE1	2.12	0.48
3:X:266:VAL:HG22	3:X:387:VAL:HG22	1.95	0.48
3:Y:266:VAL:HG22	3:Y:387:VAL:HG22	1.95	0.48
3:P:294:ARG:HD2	3:P:367:GLU:OE1	2.12	0.48
3:Q:294:ARG:HD2	3:Q:367:GLU:OE1	2.13	0.48
3:F:266:VAL:HG22	3:F:387:VAL:HG22	1.95	0.48
3:J:266:VAL:HG22	3:J:387:VAL:HG22	1.95	0.48
3:Q:266:VAL:HG22	3:Q:387:VAL:HG22	1.95	0.48
3:U:266:VAL:HG22	3:U:387:VAL:HG22	1.95	0.48
3:V:294:ARG:HD2	3:V:367:GLU:OE1	2.12	0.48
3:M:294:ARG:HD2	3:M:367:GLU:OE1	2.13	0.48
3:W:294:ARG:HD2	3:W:367:GLU:OE1	2.12	0.48
3:X:294:ARG:HD2	3:X:367:GLU:OE1	2.12	0.48
3:Z:294:ARG:HD2	3:Z:367:GLU:OE1	2.12	0.48
3:g:266:VAL:HG22	3:g:387:VAL:HG22	1.95	0.48
1:m:4:ILE:HG12	3:H:372:ILE:CG2	2.43	0.48
3:B:266:VAL:HG22	3:B:387:VAL:HG22	1.95	0.48
3:I:266:VAL:HG22	3:I:387:VAL:HG22	1.95	0.48
3:M:266:VAL:HG22	3:M:387:VAL:HG22	1.95	0.48
3:W:266:VAL:HG22	3:W:387:VAL:HG22	1.95	0.48
3:Y:294:ARG:HD2	3:Y:367:GLU:OE1	2.13	0.48
3:Z:266:VAL:HG22	3:Z:387:VAL:HG22	1.95	0.48
3:h:266:VAL:HG22	3:h:387:VAL:HG22	1.95	0.48
3:b:296:ARG:HG2	3:b:296:ARG:HH11	1.79	0.48
1:i:7:ILE:CD1	3:d:278:THR:HG21	2.44	0.48
1:k:11:ILE:HG23	3:S:372:ILE:HG21	1.89	0.48
3:f:266:VAL:HG22	3:f:387:VAL:HG22	1.95	0.48
3:U:296:ARG:HG2	3:U:296:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:266:VAL:HG22	3:V:387:VAL:HG22	1.95	0.47
3:X:296:ARG:HG2	3:X:296:ARG:HH11	1.79	0.47
1:i:11:ILE:CD1	3:c:276:GLU:CD	2.88	0.47
1:n:7:ILE:CB	3:A:278:THR:HG21	2.41	0.47
3:P:296:ARG:HH11	3:P:296:ARG:HG2	1.80	0.47
3:c:266:VAL:HG22	3:c:387:VAL:HG22	1.95	0.47
3:e:296:ARG:HG2	3:e:296:ARG:HH11	1.79	0.47
2:o:63:VAL:CG2	3:g:297:GLN:NE2	2.77	0.47
3:B:296:ARG:HG2	3:B:296:ARG:HH11	1.80	0.47
3:h:296:ARG:HH11	3:h:296:ARG:HG2	1.80	0.47
3:G:266:VAL:HG22	3:G:387:VAL:HG22	1.95	0.47
3:K:296:ARG:HH11	3:K:296:ARG:HG2	1.79	0.47
3:N:266:VAL:HG22	3:N:387:VAL:HG22	1.95	0.47
3:N:296:ARG:HG2	3:N:296:ARG:HH11	1.80	0.47
3:P:266:VAL:HG22	3:P:387:VAL:HG22	1.95	0.47
3:R:296:ARG:HH11	3:R:296:ARG:HG2	1.79	0.47
3:S:296:ARG:HG2	3:S:296:ARG:HH11	1.79	0.47
3:Y:296:ARG:HG2	3:Y:296:ARG:HH11	1.79	0.47
3:a:296:ARG:HH11	3:a:296:ARG:HG2	1.79	0.47
3:b:266:VAL:HG22	3:b:387:VAL:HG22	1.95	0.47
3:g:296:ARG:HG2	3:g:296:ARG:HH11	1.79	0.47
3:A:266:VAL:HG22	3:A:387:VAL:HG22	1.95	0.47
3:H:266:VAL:HG22	3:H:387:VAL:HG22	1.95	0.47
3:E:296:ARG:HG2	3:E:296:ARG:HH11	1.80	0.47
3:H:296:ARG:HG2	3:H:296:ARG:HH11	1.79	0.47
3:M:296:ARG:HH11	3:M:296:ARG:HG2	1.80	0.47
3:a:266:VAL:HG22	3:a:387:VAL:HG22	1.95	0.47
3:d:266:VAL:HG22	3:d:387:VAL:HG22	1.95	0.47
1:k:4:ILE:HG13	3:T:372:ILE:HG22	1.93	0.47
2:s:72:HIS:CE1	3:I:294:ARG:CG	2.96	0.47
3:C:296:ARG:HG2	3:C:296:ARG:HH11	1.79	0.47
3:G:296:ARG:HG2	3:G:296:ARG:HH11	1.79	0.47
3:Q:296:ARG:HG2	3:Q:296:ARG:HH11	1.79	0.47
3:T:296:ARG:HG2	3:T:296:ARG:HH11	1.79	0.47
1:l:4:ILE:HG12	3:N:372:ILE:HB	1.96	0.47
2:q:72:HIS:CA	3:V:295:SER:CB	2.93	0.47
2:r:73:ILE:HD12	2:r:74:PRO:HD2	1.95	0.47
3:V:296:ARG:HG2	3:V:296:ARG:HH11	1.79	0.47
3:Z:296:ARG:HG2	3:Z:296:ARG:HH11	1.79	0.47
3:e:266:VAL:HG22	3:e:387:VAL:HG22	1.95	0.47
3:c:296:ARG:HH11	3:c:296:ARG:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:73:ILE:HG22	2:q:75:ALA:H	1.80	0.47
2:s:67:LEU:HD11	2:s:74:PRO:HA	1.97	0.47
3:O:266:VAL:HG22	3:O:387:VAL:HG22	1.95	0.47
3:f:296:ARG:HH11	3:f:296:ARG:HG2	1.79	0.47
1:k:7:ILE:O	1:k:11:ILE:HG23	2.16	0.46
1:l:4:ILE:CG1	3:N:372:ILE:HG21	2.45	0.46
3:D:296:ARG:HG2	3:D:296:ARG:HH11	1.79	0.46
3:d:296:ARG:HG2	3:d:296:ARG:HH11	1.80	0.46
1:i:21:ALA:HB3	3:b:278:THR:CG2	2.39	0.46
2:q:65:LEU:HD13	3:U:295:SER:OG	2.14	0.46
3:F:296:ARG:HH11	3:F:296:ARG:HG2	1.79	0.46
3:J:296:ARG:HG2	3:J:296:ARG:HH11	1.80	0.46
1:j:15:GLN:HG3	1:j:16:ALA:N	2.30	0.46
3:I:296:ARG:HG2	3:I:296:ARG:HH11	1.79	0.46
3:W:296:ARG:HH11	3:W:296:ARG:HG2	1.79	0.46
2:q:76:GLN:H	3:U:297:GLN:NE2	2.12	0.46
1:n:7:ILE:HG21	3:A:278:THR:HG22	1.89	0.46
3:A:296:ARG:HH11	3:A:296:ARG:HG2	1.79	0.46
3:L:296:ARG:HG2	3:L:296:ARG:HH11	1.80	0.46
3:O:296:ARG:HG2	3:O:296:ARG:HH11	1.80	0.46
3:b:235:LEU:HD13	3:c:244:ARG:HH22	1.81	0.46
1:l:11:ILE:CG2	3:M:372:ILE:HB	2.45	0.46
2:s:65:LEU:HG	2:s:75:ALA:CA	2.46	0.46
3:A:244:ARG:HH22	3:h:235:LEU:HD13	1.81	0.46
3:L:235:LEU:HD13	3:M:244:ARG:HH22	1.81	0.46
3:O:235:LEU:HD13	3:P:244:ARG:HH22	1.81	0.46
3:Q:235:LEU:HD13	3:R:244:ARG:HH22	1.81	0.46
3:e:235:LEU:HD13	3:f:244:ARG:HH22	1.81	0.46
2:s:76:GLN:OE1	3:I:297:GLN:OE1	2.33	0.46
3:E:235:LEU:HD13	3:F:244:ARG:HH22	1.81	0.46
3:J:235:LEU:HD13	3:K:244:ARG:HH22	1.81	0.46
3:Y:235:LEU:HD13	3:Z:244:ARG:HH22	1.81	0.46
3:H:235:LEU:HD13	3:I:244:ARG:HH22	1.81	0.46
1:m:14:LEU:CD2	3:F:278:THR:HG21	2.46	0.46
2:p:66:THR:OG1	3:a:294:ARG:CG	2.64	0.46
3:G:235:LEU:HD13	3:H:244:ARG:HH22	1.81	0.46
3:T:235:LEU:HD13	3:U:244:ARG:HH22	1.81	0.46
3:A:235:LEU:HD13	3:B:244:ARG:HH22	1.81	0.45
3:f:235:LEU:HD13	3:g:244:ARG:HH22	1.81	0.45
3:C:235:LEU:HD13	3:D:244:ARG:HH22	1.81	0.45
3:M:235:LEU:HD13	3:N:244:ARG:HH22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:235:LEU:HD13	3:T:244:ARG:HH22	1.81	0.45
3:V:235:LEU:HD13	3:W:244:ARG:HH22	1.81	0.45
1:l:7:ILE:HD11	3:N:370:ARG:NH2	2.30	0.45
1:n:15:GLN:HG3	1:n:16:ALA:N	2.30	0.45
3:N:235:LEU:HD13	3:O:244:ARG:HH22	1.81	0.45
3:R:235:LEU:HD13	3:S:244:ARG:HH22	1.81	0.45
3:X:235:LEU:HD13	3:Y:244:ARG:HH22	1.81	0.45
3:Z:235:LEU:HD13	3:a:244:ARG:HH22	1.81	0.45
3:c:235:LEU:HD13	3:d:244:ARG:HH22	1.81	0.45
1:l:15:GLN:HG3	1:l:16:ALA:N	2.30	0.45
3:I:235:LEU:HD13	3:J:244:ARG:HH22	1.81	0.45
3:a:235:LEU:HD13	3:b:244:ARG:HH22	1.81	0.45
1:m:15:GLN:HG3	1:m:16:ALA:N	2.30	0.45
2:r:78:VAL:CG1	3:M:361:ASN:ND2	2.78	0.45
3:D:235:LEU:HD13	3:E:244:ARG:HH22	1.81	0.45
3:B:235:LEU:HD13	3:C:244:ARG:HH22	1.81	0.45
3:P:235:LEU:HD13	3:Q:244:ARG:HH22	1.81	0.45
3:d:235:LEU:HD13	3:e:244:ARG:HH22	1.81	0.45
1:n:7:ILE:HD11	3:B:370:ARG:HH21	1.82	0.45
2:q:65:LEU:HD11	3:U:365:ASN:ND2	2.32	0.45
3:W:235:LEU:HD13	3:X:244:ARG:HH22	1.81	0.45
2:q:73:ILE:HD13	3:V:297:GLN:CB	2.35	0.44
3:F:235:LEU:HD13	3:G:244:ARG:HH22	1.81	0.44
3:K:235:LEU:HD13	3:L:244:ARG:HH22	1.81	0.44
1:j:7:ILE:CG1	3:Z:370:ARG:HH21	2.26	0.44
1:k:3:ALA:C	3:T:372:ILE:HD12	2.42	0.44
2:q:73:ILE:HD12	3:U:363:THR:HG23	1.98	0.44
3:g:235:LEU:HD13	3:h:244:ARG:HH22	1.81	0.44
1:i:15:GLN:HG3	1:i:16:ALA:N	2.30	0.44
1:k:21:ALA:HB3	3:Q:278:THR:HG21	1.97	0.44
2:q:72:HIS:CA	3:V:295:SER:HB3	2.45	0.44
3:U:235:LEU:HD13	3:V:244:ARG:HH22	1.81	0.44
1:n:14:LEU:HD21	3:A:370:ARG:HH21	1.83	0.44
2:o:77:ALA:HB3	3:g:297:GLN:HE22	1.83	0.44
1:m:11:ILE:HG22	3:G:372:ILE:CG2	2.47	0.44
3:B:429:THR:OG1	3:C:418:GLU:OE2	2.36	0.44
3:G:429:THR:OG1	3:H:418:GLU:OE2	2.36	0.44
3:D:429:THR:OG1	3:E:418:GLU:OE2	2.36	0.44
3:g:429:THR:OG1	3:h:418:GLU:OE2	2.36	0.44
1:l:21:ALA:HB3	3:K:278:THR:CG2	2.31	0.44
2:q:67:LEU:HD21	2:q:74:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:429:THR:OG1	3:U:418:GLU:OE2	2.36	0.44
3:J:429:THR:OG1	3:K:418:GLU:OE2	2.36	0.43
2:s:73:ILE:HG13	3:I:295:SER:CB	2.43	0.43
3:A:429:THR:OG1	3:B:418:GLU:OE2	2.36	0.43
3:E:429:THR:OG1	3:F:418:GLU:OE2	2.36	0.43
3:I:429:THR:OG1	3:J:418:GLU:OE2	2.36	0.43
3:R:429:THR:OG1	3:S:418:GLU:OE2	2.36	0.43
3:V:429:THR:OG1	3:W:418:GLU:OE2	2.36	0.43
3:W:429:THR:OG1	3:X:418:GLU:OE2	2.36	0.43
1:l:7:ILE:HD11	3:N:370:ARG:NE	2.32	0.43
2:p:68:THR:CG2	3:a:294:ARG:HD2	2.49	0.43
3:Y:429:THR:OG1	3:Z:418:GLU:OE2	2.36	0.43
3:d:429:THR:OG1	3:e:418:GLU:OE2	2.36	0.43
2:s:63:VAL:H	3:G:297:GLN:NE2	2.16	0.43
3:F:429:THR:OG1	3:G:418:GLU:OE2	2.36	0.43
3:e:429:THR:OG1	3:f:418:GLU:OE2	2.36	0.43
3:A:418:GLU:OE2	3:h:429:THR:OG1	2.36	0.43
3:H:429:THR:OG1	3:I:418:GLU:OE2	2.36	0.43
3:L:429:THR:OG1	3:M:418:GLU:OE2	2.36	0.43
1:l:14:LEU:HD23	3:L:278:THR:CG2	2.49	0.43
2:r:68:THR:CG2	3:N:294:ARG:HD2	2.48	0.43
3:K:290:LYS:HE3	3:K:290:LYS:HB2	1.93	0.43
3:U:429:THR:OG1	3:V:418:GLU:OE2	2.36	0.43
3:f:429:THR:OG1	3:g:418:GLU:OE2	2.36	0.43
1:l:14:LEU:HD11	3:M:370:ARG:NH2	2.32	0.43
2:q:65:LEU:HD23	2:q:75:ALA:CB	2.48	0.43
3:M:429:THR:OG1	3:N:418:GLU:OE2	2.36	0.43
3:Q:429:THR:OG1	3:R:418:GLU:OE2	2.36	0.43
3:a:429:THR:OG1	3:b:418:GLU:OE2	2.36	0.43
1:m:4:ILE:HG12	3:H:372:ILE:HB	2.00	0.43
1:n:15:GLN:HB2	3:h:374:HIS:CG	2.53	0.43
2:r:68:THR:HG21	3:N:294:ARG:HD2	2.01	0.43
3:P:429:THR:OG1	3:Q:418:GLU:OE2	2.36	0.43
3:X:429:THR:OG1	3:Y:418:GLU:OE2	2.36	0.43
2:p:69:SER:OG	3:b:294:ARG:HD3	2.19	0.42
3:J:421:GLY:O	3:J:426:ARG:NH2	2.51	0.42
3:K:421:GLY:O	3:K:426:ARG:NH2	2.51	0.42
3:L:421:GLY:O	3:L:426:ARG:NH2	2.51	0.42
3:O:429:THR:OG1	3:P:418:GLU:OE2	2.36	0.42
3:S:429:THR:OG1	3:T:418:GLU:OE2	2.36	0.42
1:j:7:ILE:HG22	3:Y:278:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:421:GLY:O	3:I:426:ARG:NH2	2.51	0.42
3:K:429:THR:OG1	3:L:418:GLU:OE2	2.36	0.42
3:a:290:LYS:HE3	3:a:290:LYS:HB2	1.93	0.42
3:g:296:ARG:HG2	3:g:296:ARG:NH1	2.35	0.42
1:k:7:ILE:HD11	3:T:370:ARG:NE	2.23	0.42
1:l:7:ILE:CB	3:M:278:THR:HG21	2.50	0.42
1:m:4:ILE:CD1	3:H:374:HIS:HB2	2.50	0.42
1:n:11:ILE:HG22	3:A:372:ILE:CB	2.49	0.42
3:C:429:THR:OG1	3:D:418:GLU:OE2	2.36	0.42
3:L:296:ARG:HG2	3:L:296:ARG:NH1	2.35	0.42
3:M:421:GLY:O	3:M:426:ARG:NH2	2.51	0.42
3:R:296:ARG:HG2	3:R:296:ARG:NH1	2.35	0.42
3:h:296:ARG:HG2	3:h:296:ARG:NH1	2.35	0.42
1:k:4:ILE:CD1	3:T:374:HIS:CB	2.93	0.42
3:K:296:ARG:HG2	3:K:296:ARG:NH1	2.35	0.42
3:Q:296:ARG:HG2	3:Q:296:ARG:NH1	2.35	0.42
3:S:296:ARG:HG2	3:S:296:ARG:NH1	2.35	0.42
3:Z:404:LEU:HD22	3:Z:409:MET:HE3	2.02	0.42
3:b:429:THR:OG1	3:c:418:GLU:OE2	2.36	0.42
1:k:9:GLY:O	1:k:13:GLN:HG3	2.18	0.42
2:r:68:THR:HG22	3:N:294:ARG:HD3	2.01	0.42
3:F:296:ARG:HG2	3:F:296:ARG:NH1	2.35	0.42
3:H:421:GLY:O	3:H:426:ARG:NH2	2.51	0.42
3:M:296:ARG:HG2	3:M:296:ARG:NH1	2.35	0.42
3:Y:404:LEU:HD22	3:Y:409:MET:HE3	2.02	0.42
3:a:404:LEU:HD22	3:a:409:MET:HE3	2.02	0.42
3:c:429:THR:OG1	3:d:418:GLU:OE2	2.36	0.42
3:A:296:ARG:HG2	3:A:296:ARG:NH1	2.35	0.42
3:G:296:ARG:HG2	3:G:296:ARG:NH1	2.35	0.42
3:I:296:ARG:HG2	3:I:296:ARG:NH1	2.35	0.42
3:N:421:GLY:O	3:N:426:ARG:NH2	2.51	0.42
3:T:296:ARG:HG2	3:T:296:ARG:NH1	2.35	0.42
3:X:404:LEU:HD22	3:X:409:MET:HE3	2.02	0.42
3:b:404:LEU:HD22	3:b:409:MET:HE3	2.02	0.42
3:c:404:LEU:HD22	3:c:409:MET:HE3	2.02	0.42
3:f:296:ARG:HG2	3:f:296:ARG:NH1	2.35	0.42
3:E:296:ARG:HG2	3:E:296:ARG:NH1	2.35	0.42
3:G:421:GLY:O	3:G:426:ARG:NH2	2.51	0.42
3:H:296:ARG:HG2	3:H:296:ARG:NH1	2.35	0.42
3:b:296:ARG:HG2	3:b:296:ARG:NH1	2.35	0.42
3:f:290:LYS:HE3	3:f:290:LYS:HB2	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:404:LEU:HD22	3:g:409:MET:HE3	2.02	0.42
3:h:404:LEU:HD22	3:h:409:MET:HE3	2.02	0.42
3:P:296:ARG:HG2	3:P:296:ARG:NH1	2.35	0.42
3:U:296:ARG:HG2	3:U:296:ARG:NH1	2.35	0.42
3:W:404:LEU:HD22	3:W:409:MET:HE3	2.02	0.42
3:f:404:LEU:HD22	3:f:409:MET:HE3	2.02	0.42
3:A:404:LEU:HD22	3:A:409:MET:HE3	2.02	0.42
3:D:296:ARG:HG2	3:D:296:ARG:NH1	2.35	0.42
3:d:404:LEU:HD22	3:d:409:MET:HE3	2.02	0.42
3:e:404:LEU:HD22	3:e:409:MET:HE3	2.02	0.42
1:n:7:ILE:HG22	3:A:278:THR:CG2	2.42	0.41
3:D:290:LYS:HE3	3:D:290:LYS:HB2	1.93	0.41
3:J:404:LEU:HD22	3:J:409:MET:HE3	2.02	0.41
3:N:296:ARG:HG2	3:N:296:ARG:NH1	2.35	0.41
3:N:429:THR:OG1	3:O:418:GLU:OE2	2.36	0.41
3:O:404:LEU:HD22	3:O:409:MET:HE3	2.02	0.41
3:O:421:GLY:O	3:O:426:ARG:NH2	2.51	0.41
3:Q:290:LYS:HE3	3:Q:290:LYS:HB2	1.93	0.41
3:V:296:ARG:HG2	3:V:296:ARG:NH1	2.35	0.41
3:W:296:ARG:HG2	3:W:296:ARG:NH1	2.35	0.41
3:Z:429:THR:OG1	3:a:418:GLU:OE2	2.36	0.41
3:c:296:ARG:HG2	3:c:296:ARG:NH1	2.35	0.41
1:n:11:ILE:HG22	3:A:372:ILE:HB	2.03	0.41
3:B:404:LEU:HD22	3:B:409:MET:HE3	2.02	0.41
3:C:296:ARG:HG2	3:C:296:ARG:NH1	2.35	0.41
3:C:404:LEU:HD22	3:C:409:MET:HE3	2.02	0.41
3:J:296:ARG:HG2	3:J:296:ARG:NH1	2.35	0.41
3:L:404:LEU:HD22	3:L:409:MET:HE3	2.02	0.41
3:V:404:LEU:HD22	3:V:409:MET:HE3	2.02	0.41
3:X:296:ARG:HG2	3:X:296:ARG:NH1	2.35	0.41
3:M:404:LEU:HD22	3:M:409:MET:HE3	2.02	0.41
3:a:296:ARG:HG2	3:a:296:ARG:NH1	2.35	0.41
1:k:3:ALA:HA	3:T:372:ILE:HD13	2.02	0.41
1:k:7:ILE:CD1	3:T:370:ARG:HE	2.24	0.41
2:s:66:THR:HG23	3:G:365:ASN:CG	2.44	0.41
3:B:296:ARG:HG2	3:B:296:ARG:NH1	2.35	0.41
3:F:421:GLY:O	3:F:426:ARG:NH2	2.51	0.41
3:U:404:LEU:HD22	3:U:409:MET:HE3	2.02	0.41
3:V:290:LYS:HE3	3:V:290:LYS:HB2	1.93	0.41
3:d:296:ARG:HG2	3:d:296:ARG:NH1	2.35	0.41
3:e:296:ARG:HG2	3:e:296:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:421:GLY:O	3:g:426:ARG:NH2	2.51	0.41
1:l:4:ILE:HG12	3:N:372:ILE:HG21	2.02	0.41
3:D:404:LEU:HD22	3:D:409:MET:HE3	2.02	0.41
3:Q:404:LEU:HD22	3:Q:409:MET:HE3	2.02	0.41
3:O:296:ARG:HG2	3:O:296:ARG:NH1	2.35	0.41
3:V:235:LEU:HB3	3:W:244:ARG:NH2	2.36	0.41
3:Y:296:ARG:HG2	3:Y:296:ARG:NH1	2.35	0.41
3:G:404:LEU:HD22	3:G:409:MET:HE3	2.02	0.41
3:H:404:LEU:HD22	3:H:409:MET:HE3	2.02	0.41
3:N:404:LEU:HD22	3:N:409:MET:HE3	2.02	0.41
3:P:290:LYS:HE3	3:P:290:LYS:HB2	1.93	0.41
3:Y:235:LEU:HB3	3:Z:244:ARG:NH2	2.36	0.41
3:Z:296:ARG:HG2	3:Z:296:ARG:NH1	2.35	0.41
3:f:421:GLY:O	3:f:426:ARG:NH2	2.51	0.41
2:s:68:THR:HG22	3:H:294:ARG:CD	2.36	0.41
2:s:72:HIS:CE1	3:H:366:TYR:O	2.74	0.41
3:E:404:LEU:HD22	3:E:409:MET:HE3	2.02	0.41
3:M:235:LEU:HB3	3:N:244:ARG:NH2	2.36	0.41
3:P:235:LEU:HB3	3:Q:244:ARG:NH2	2.36	0.41
3:P:421:GLY:O	3:P:426:ARG:NH2	2.51	0.41
3:S:235:LEU:HB3	3:T:244:ARG:NH2	2.36	0.41
3:T:404:LEU:HD22	3:T:409:MET:HE3	2.02	0.41
1:i:11:ILE:HD13	3:c:276:GLU:CD	2.46	0.41
3:I:404:LEU:HD22	3:I:409:MET:HE3	2.02	0.41
3:K:404:LEU:HD22	3:K:409:MET:HE3	2.02	0.41
3:O:235:LEU:HB3	3:P:244:ARG:NH2	2.36	0.41
3:R:404:LEU:HD22	3:R:409:MET:HE3	2.02	0.41
3:b:235:LEU:HB3	3:c:244:ARG:NH2	2.36	0.41
3:f:425:LYS:HE3	3:f:425:LYS:HB3	1.96	0.41
3:J:290:LYS:HE3	3:J:290:LYS:HB2	1.93	0.40
3:L:235:LEU:HB3	3:M:244:ARG:NH2	2.36	0.40
3:R:235:LEU:HB3	3:S:244:ARG:NH2	2.36	0.40
1:m:7:ILE:O	1:m:11:ILE:HG23	2.21	0.40
3:A:360:ARG:NH1	3:A:362:GLU:OE1	2.55	0.40
3:D:360:ARG:NH1	3:D:362:GLU:OE1	2.55	0.40
3:E:421:GLY:O	3:E:426:ARG:NH2	2.51	0.40
3:J:235:LEU:HB3	3:K:244:ARG:NH2	2.36	0.40
1:j:7:ILE:O	1:j:11:ILE:HG23	2.21	0.40
3:F:404:LEU:HD22	3:F:409:MET:HE3	2.02	0.40
3:S:404:LEU:HD22	3:S:409:MET:HE3	2.02	0.40
3:U:360:ARG:NH1	3:U:362:GLU:OE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:360:ARG:NH1	3:V:362:GLU:OE1	2.55	0.40
3:X:360:ARG:NH1	3:X:362:GLU:OE1	2.55	0.40
3:Y:360:ARG:NH1	3:Y:362:GLU:OE1	2.55	0.40
3:b:360:ARG:NH1	3:b:362:GLU:OE1	2.55	0.40
3:e:421:GLY:O	3:e:426:ARG:NH2	2.51	0.40
3:f:360:ARG:NH1	3:f:362:GLU:OE1	2.55	0.40
3:G:360:ARG:NH1	3:G:362:GLU:OE1	2.55	0.40
3:S:360:ARG:NH1	3:S:362:GLU:OE1	2.55	0.40
3:e:360:ARG:NH1	3:e:362:GLU:OE1	2.55	0.40
1:j:4:ILE:HA	3:Z:372:ILE:HD12	2.03	0.40
1:l:7:ILE:HB	3:M:278:THR:HG21	2.02	0.40
2:o:63:VAL:HG23	3:g:297:GLN:NE2	2.37	0.40
2:q:67:LEU:CA	2:q:72:HIS:HE2	2.34	0.40
2:s:72:HIS:HA	3:I:295:SER:HB3	2.02	0.40
3:P:404:LEU:HD22	3:P:409:MET:HE3	2.02	0.40
3:U:235:LEU:HB3	3:V:244:ARG:NH2	2.36	0.40
3:X:235:LEU:HB3	3:Y:244:ARG:NH2	2.36	0.40
3:h:360:ARG:NH1	3:h:362:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	i	17/104 (16%)	17 (100%)	0	0	100	100
1	j	17/104 (16%)	17 (100%)	0	0	100	100
1	k	17/104 (16%)	17 (100%)	0	0	100	100
1	l	17/104 (16%)	17 (100%)	0	0	100	100
1	m	17/104 (16%)	17 (100%)	0	0	100	100
1	n	17/104 (16%)	17 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	o	15/138 (11%)	14 (93%)	1 (7%)	0	100	100
2	p	11/138 (8%)	11 (100%)	0	0	100	100
2	q	15/138 (11%)	13 (87%)	2 (13%)	0	100	100
2	r	15/138 (11%)	14 (93%)	1 (7%)	0	100	100
2	s	15/138 (11%)	14 (93%)	1 (7%)	0	100	100
3	A	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	B	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	C	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	D	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	E	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	F	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	G	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	H	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	I	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	J	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	K	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	L	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	M	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	N	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	O	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	P	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	Q	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	R	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	S	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	T	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	U	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	V	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	W	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	X	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	Y	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	Z	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	b	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	c	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	d	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	e	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	f	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	g	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
3	h	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
All	All	5613/20354 (28%)	5540 (99%)	73 (1%)	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	i	12/79 (15%)	10 (83%)	2 (17%)	2	14
1	j	12/79 (15%)	10 (83%)	2 (17%)	2	14
1	k	12/79 (15%)	7 (58%)	5 (42%)	0	0
1	l	12/79 (15%)	10 (83%)	2 (17%)	2	14
1	m	12/79 (15%)	10 (83%)	2 (17%)	2	14
1	n	12/79 (15%)	10 (83%)	2 (17%)	2	14
2	o	12/113 (11%)	11 (92%)	1 (8%)	10	35
2	p	11/113 (10%)	11 (100%)	0	100	100
2	q	13/113 (12%)	9 (69%)	4 (31%)	0	2
2	r	13/113 (12%)	12 (92%)	1 (8%)	12	38
2	s	13/113 (12%)	12 (92%)	1 (8%)	12	38
3	A	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	B	141/467 (30%)	140 (99%)	1 (1%)	76	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	D	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	E	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	F	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	G	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	H	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	I	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	J	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	K	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	L	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	M	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	N	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	O	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	P	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	Q	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	R	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	S	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	T	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	U	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	V	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	W	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	X	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	Y	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	Z	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	a	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	b	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	c	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	d	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	e	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	f	141/467 (30%)	140 (99%)	1 (1%)	76	77
3	g	141/467 (30%)	140 (99%)	1 (1%)	76	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	h	141/467 (30%)	140 (99%)	1 (1%)	76	77
All	All	4928/16917 (29%)	4872 (99%)	56 (1%)	63	73

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	i	15	GLN
1	i	19	MET
1	j	15	GLN
1	j	19	MET
1	k	7	ILE
1	k	11	ILE
1	k	14	LEU
1	k	15	GLN
1	k	19	MET
1	l	15	GLN
1	l	19	MET
1	m	15	GLN
1	m	19	MET
1	n	15	GLN
1	n	19	MET
2	o	63	VAL
2	q	65	LEU
2	q	69	SER
2	q	71	HIS
2	q	72	HIS
2	r	76	GLN
2	s	65	LEU
3	A	295	SER
3	B	295	SER
3	C	295	SER
3	D	295	SER
3	E	295	SER
3	F	295	SER
3	G	295	SER
3	H	295	SER
3	I	295	SER
3	J	295	SER
3	K	295	SER
3	L	295	SER
3	M	295	SER
3	N	295	SER

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Mol	Chain	Res	Type
3	O	295	SER
3	P	295	SER
3	Q	295	SER
3	R	295	SER
3	S	295	SER
3	T	295	SER
3	U	295	SER
3	V	295	SER
3	W	295	SER
3	X	295	SER
3	Y	295	SER
3	Z	295	SER
3	a	295	SER
3	b	295	SER
3	c	295	SER
3	d	295	SER
3	e	295	SER
3	f	295	SER
3	g	295	SER
3	h	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	13	GLN
1	k	15	GLN
2	o	71	HIS
2	q	76	GLN
2	r	72	HIS
2	r	76	GLN
2	s	72	HIS
2	s	76	GLN
3	A	234	GLN
3	A	263	HIS
3	A	303	GLN
3	A	378	ASN
3	A	434	ASN
3	B	234	GLN
3	B	281	HIS
3	B	303	GLN
3	B	374	HIS
3	B	378	ASN

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Mol	Chain	Res	Type
3	B	434	ASN
3	C	234	GLN
3	C	303	GLN
3	C	374	HIS
3	C	378	ASN
3	C	434	ASN
3	D	234	GLN
3	D	303	GLN
3	D	374	HIS
3	D	378	ASN
3	D	434	ASN
3	E	234	GLN
3	E	303	GLN
3	E	374	HIS
3	E	378	ASN
3	E	434	ASN
3	F	234	GLN
3	F	303	GLN
3	F	374	HIS
3	F	378	ASN
3	F	434	ASN
3	G	231	ASN
3	G	234	GLN
3	G	303	GLN
3	G	374	HIS
3	G	378	ASN
3	G	434	ASN
3	H	231	ASN
3	H	234	GLN
3	H	297	GLN
3	H	299	ASN
3	H	303	GLN
3	H	374	HIS
3	H	378	ASN
3	H	434	ASN
3	I	231	ASN
3	I	234	GLN
3	I	303	GLN
3	I	374	HIS
3	I	378	ASN
3	I	434	ASN
3	J	231	ASN

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Mol	Chain	Res	Type
3	J	234	GLN
3	J	281	HIS
3	J	303	GLN
3	J	374	HIS
3	J	378	ASN
3	J	434	ASN
3	K	231	ASN
3	K	234	GLN
3	K	303	GLN
3	K	374	HIS
3	K	378	ASN
3	K	434	ASN
3	L	231	ASN
3	L	234	GLN
3	L	263	HIS
3	L	281	HIS
3	L	303	GLN
3	L	374	HIS
3	L	378	ASN
3	L	434	ASN
3	M	231	ASN
3	M	234	GLN
3	M	281	HIS
3	M	297	GLN
3	M	303	GLN
3	M	374	HIS
3	M	378	ASN
3	M	434	ASN
3	N	231	ASN
3	N	234	GLN
3	N	281	HIS
3	N	299	ASN
3	N	303	GLN
3	N	374	HIS
3	N	378	ASN
3	N	434	ASN
3	O	231	ASN
3	O	234	GLN
3	O	303	GLN
3	O	374	HIS
3	O	378	ASN
3	O	434	ASN

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Mol	Chain	Res	Type
3	P	231	ASN
3	P	234	GLN
3	P	303	GLN
3	P	374	HIS
3	P	378	ASN
3	P	434	ASN
3	Q	231	ASN
3	Q	234	GLN
3	Q	281	HIS
3	Q	303	GLN
3	Q	374	HIS
3	Q	378	ASN
3	Q	434	ASN
3	R	231	ASN
3	R	234	GLN
3	R	303	GLN
3	R	374	HIS
3	R	378	ASN
3	R	434	ASN
3	S	231	ASN
3	S	234	GLN
3	S	303	GLN
3	S	374	HIS
3	S	378	ASN
3	S	434	ASN
3	T	231	ASN
3	T	234	GLN
3	T	281	HIS
3	T	303	GLN
3	T	374	HIS
3	T	378	ASN
3	T	434	ASN
3	U	231	ASN
3	U	234	GLN
3	U	297	GLN
3	U	303	GLN
3	U	365	ASN
3	U	374	HIS
3	U	378	ASN
3	U	434	ASN
3	V	231	ASN
3	V	234	GLN

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Mol	Chain	Res	Type
3	V	297	GLN
3	V	303	GLN
3	V	374	HIS
3	V	378	ASN
3	V	434	ASN
3	W	231	ASN
3	W	234	GLN
3	W	246	GLN
3	W	281	HIS
3	W	303	GLN
3	W	374	HIS
3	W	378	ASN
3	W	434	ASN
3	X	231	ASN
3	X	234	GLN
3	X	303	GLN
3	X	378	ASN
3	X	434	ASN
3	Y	231	ASN
3	Y	234	GLN
3	Y	281	HIS
3	Y	303	GLN
3	Y	374	HIS
3	Y	378	ASN
3	Y	434	ASN
3	Z	231	ASN
3	Z	234	GLN
3	Z	303	GLN
3	Z	374	HIS
3	Z	378	ASN
3	Z	434	ASN
3	a	231	ASN
3	a	234	GLN
3	a	281	HIS
3	a	303	GLN
3	a	374	HIS
3	a	378	ASN
3	a	434	ASN
3	b	231	ASN
3	b	234	GLN
3	b	281	HIS
3	b	303	GLN

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Mol	Chain	Res	Type
3	b	374	HIS
3	b	378	ASN
3	b	434	ASN
3	c	234	GLN
3	c	281	HIS
3	c	303	GLN
3	c	374	HIS
3	c	378	ASN
3	c	434	ASN
3	d	234	GLN
3	d	303	GLN
3	d	374	HIS
3	d	378	ASN
3	d	434	ASN
3	e	234	GLN
3	e	303	GLN
3	e	374	HIS
3	e	378	ASN
3	e	434	ASN
3	f	234	GLN
3	f	303	GLN
3	f	374	HIS
3	f	378	ASN
3	f	434	ASN
3	g	234	GLN
3	g	297	GLN
3	g	303	GLN
3	g	374	HIS
3	g	378	ASN
3	g	434	ASN
3	h	234	GLN
3	h	303	GLN
3	h	374	HIS
3	h	378	ASN
3	h	434	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

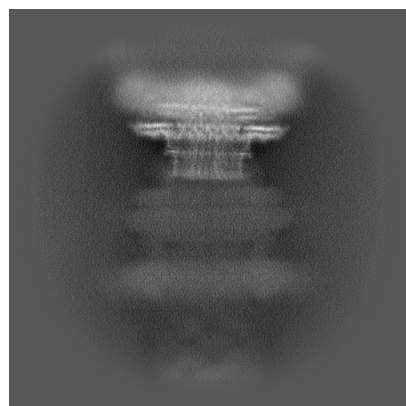
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37595. These allow visual inspection of the internal detail of the map and identification of artifacts.

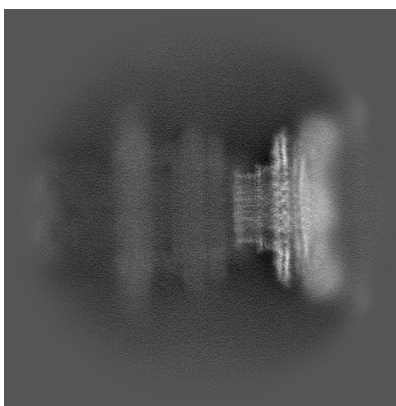
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

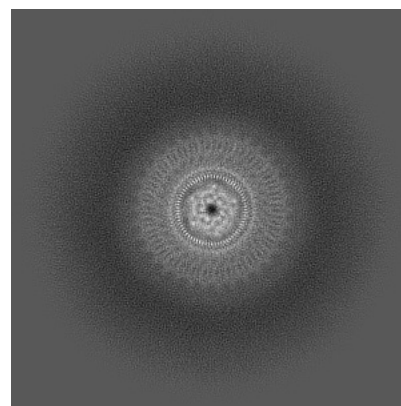
6.1.1 Primary map



X

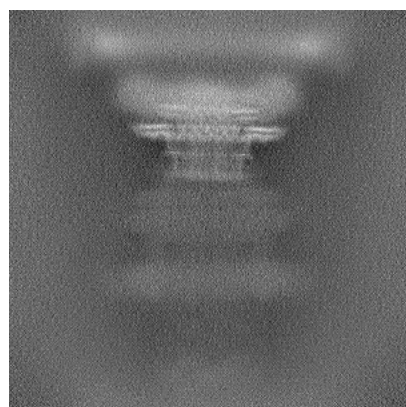


Y

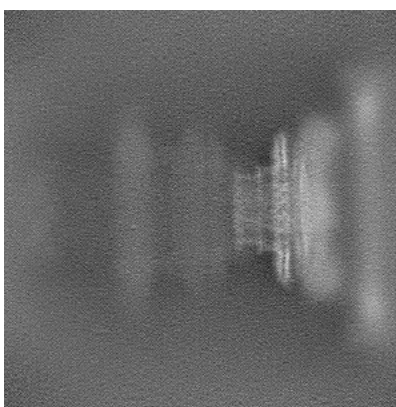


Z

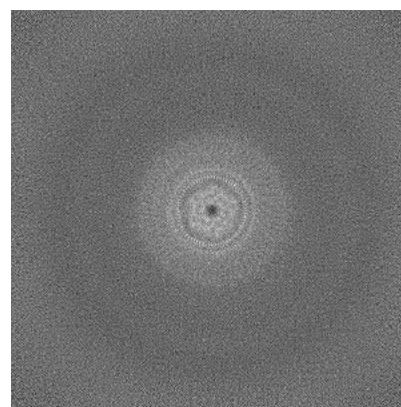
6.1.2 Raw map



X



Y



Z

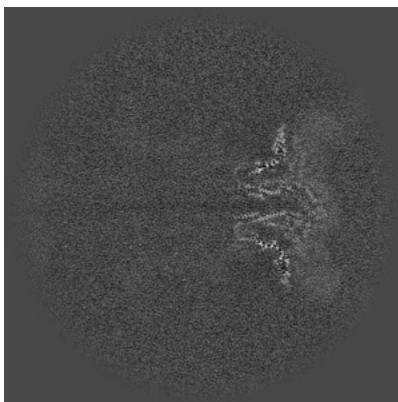
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

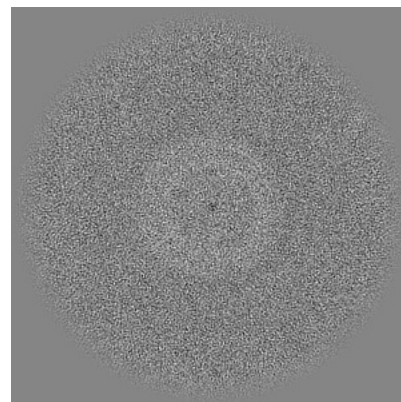
6.2.1 Primary map



X Index: 256



Y Index: 256

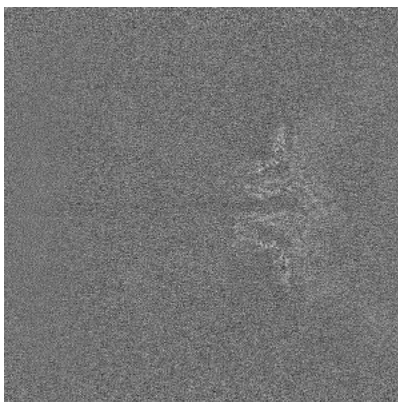


Z Index: 256

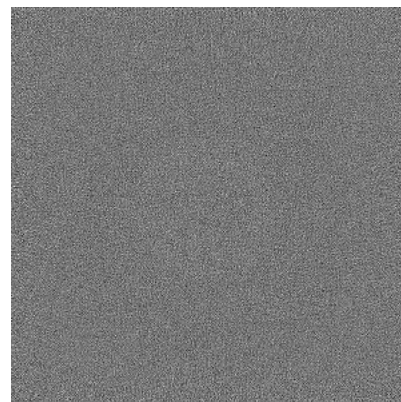
6.2.2 Raw map



X Index: 256



Y Index: 256

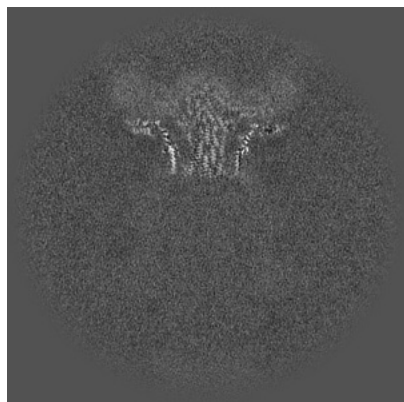


Z Index: 256

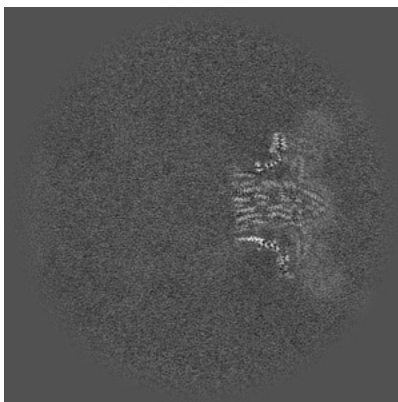
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

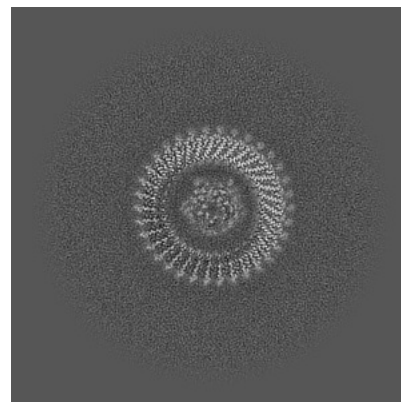
6.3.1 Primary map



X Index: 245

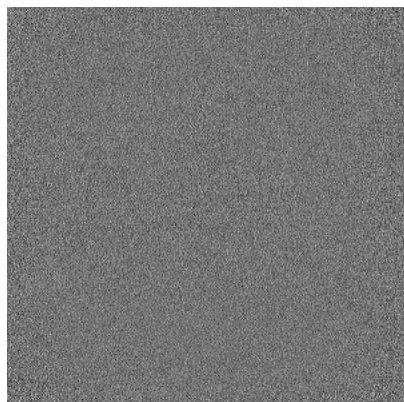


Y Index: 265

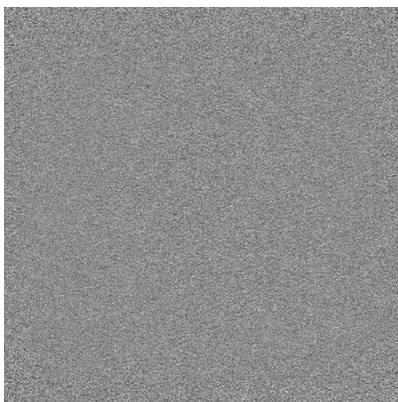


Z Index: 358

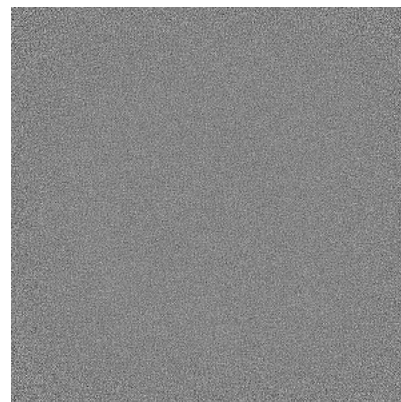
6.3.2 Raw map



X Index: 0



Y Index: 0

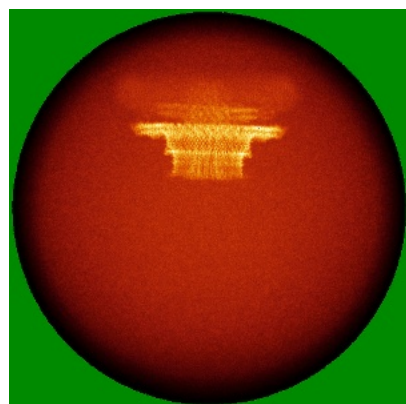


Z Index: 0

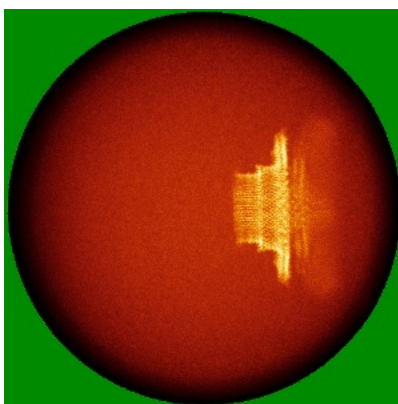
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

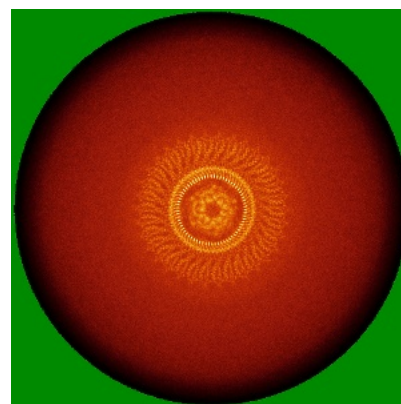
6.4.1 Primary map



X

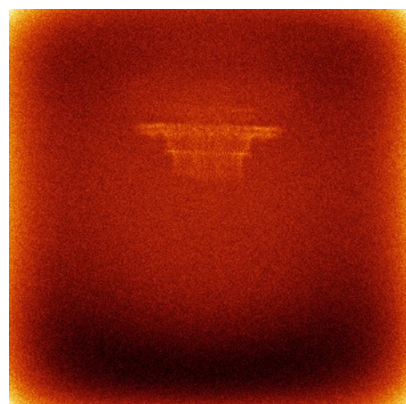


Y

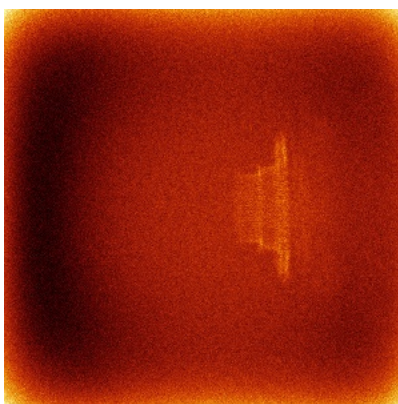


Z

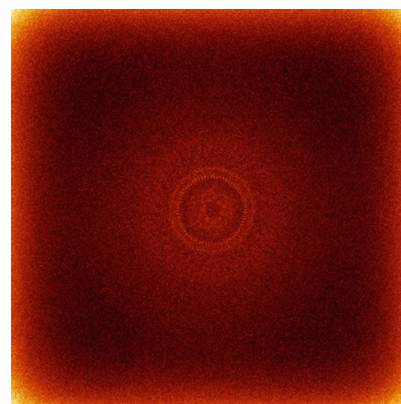
6.4.2 Raw map



X



Y

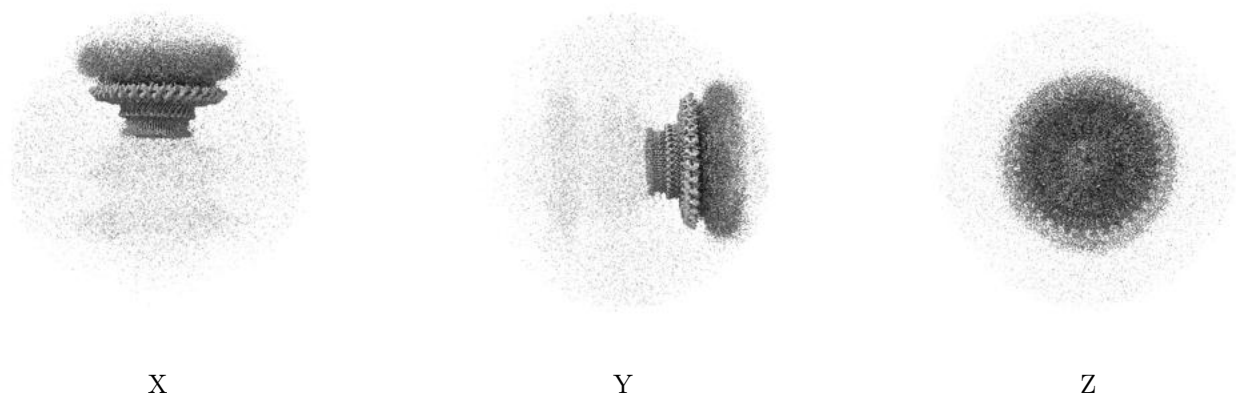


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

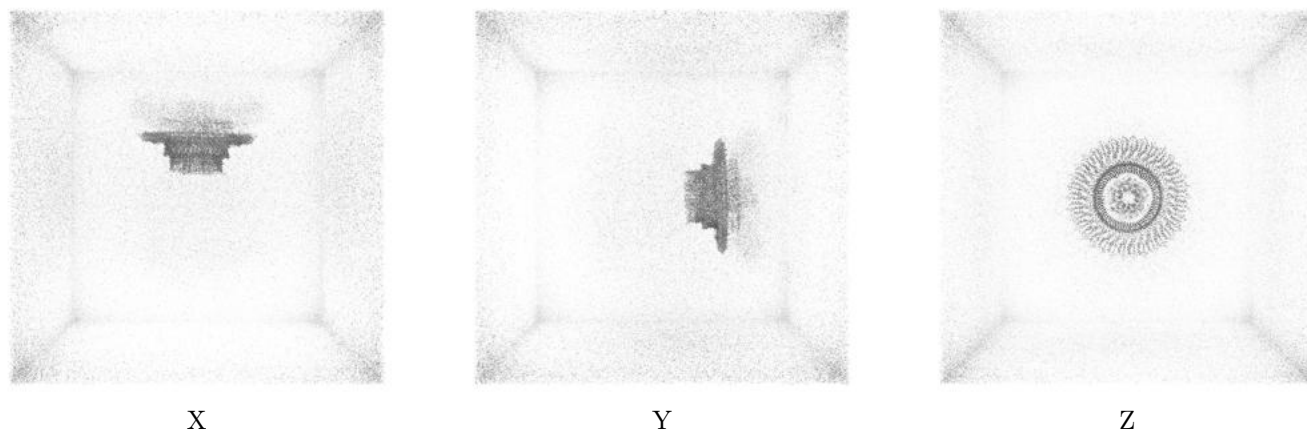
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

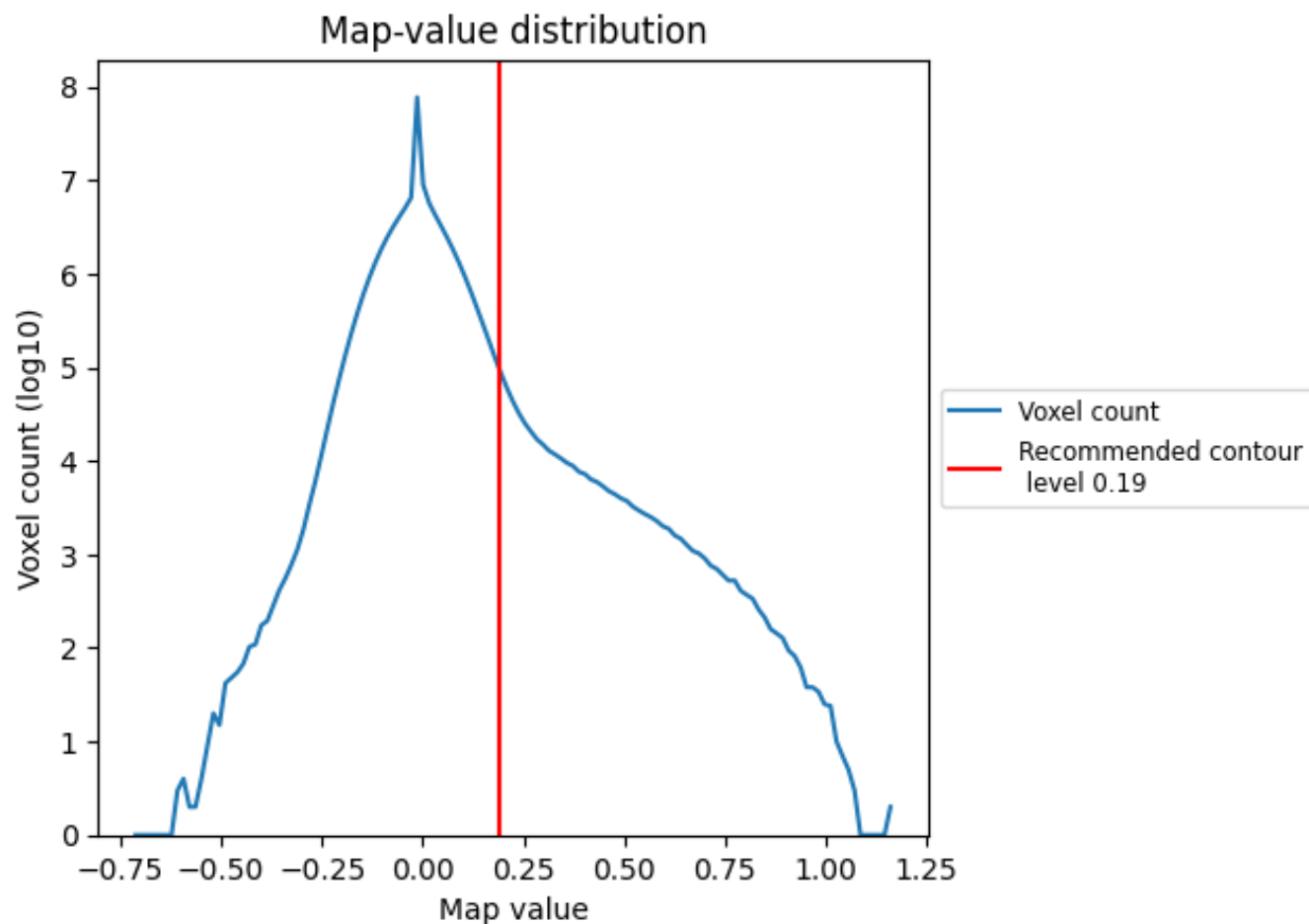
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

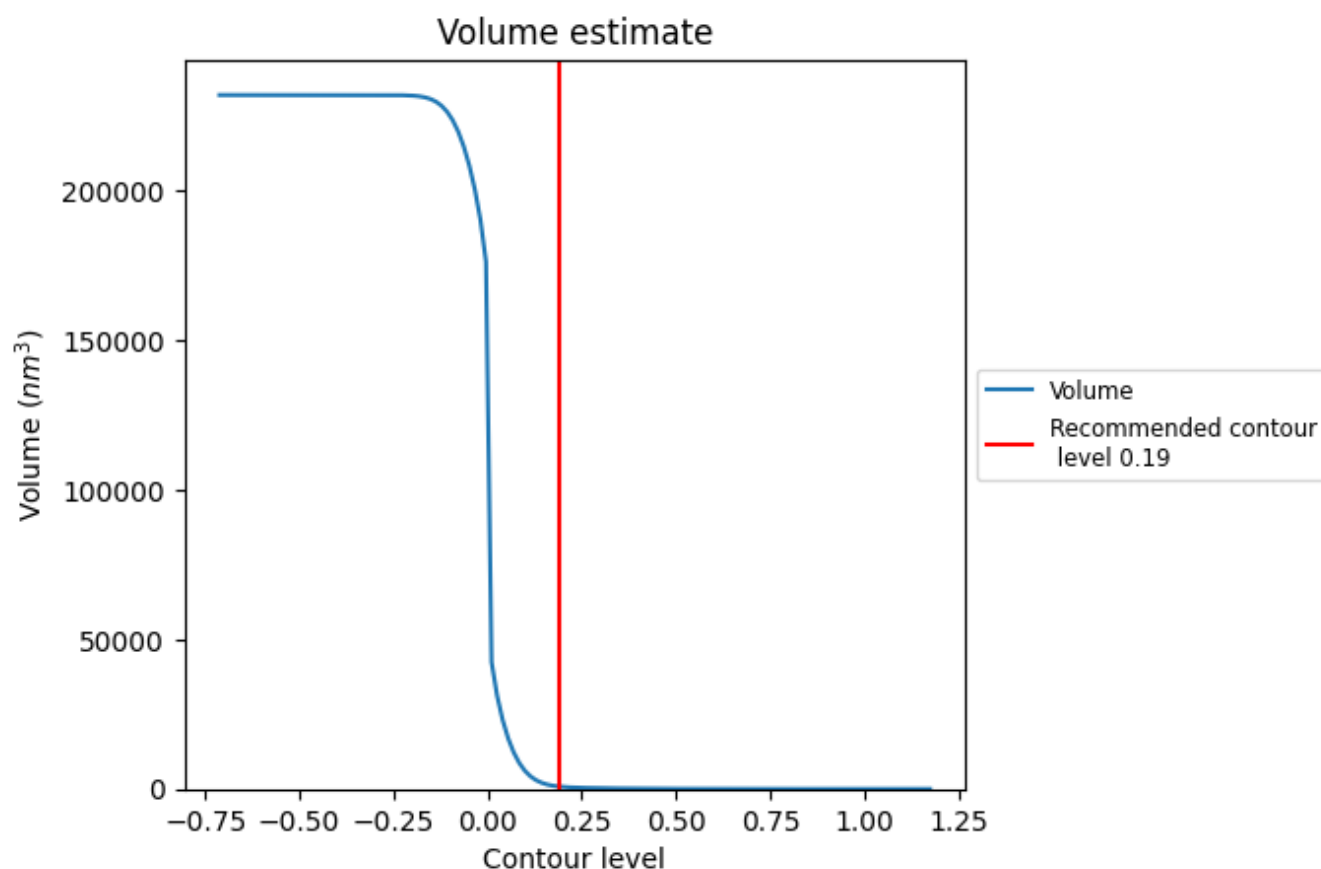
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

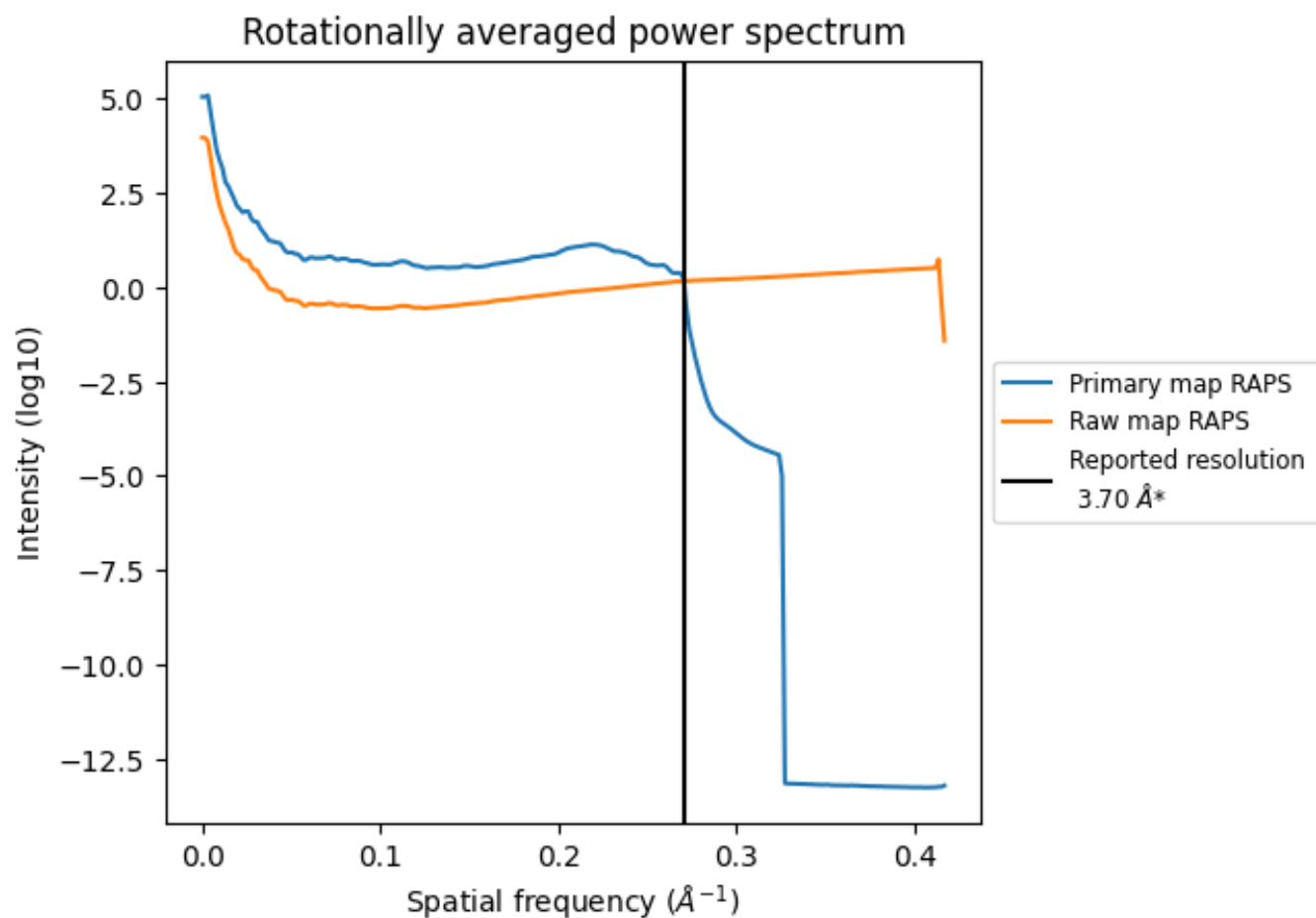
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 804 nm³; this corresponds to an approximate mass of 727 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

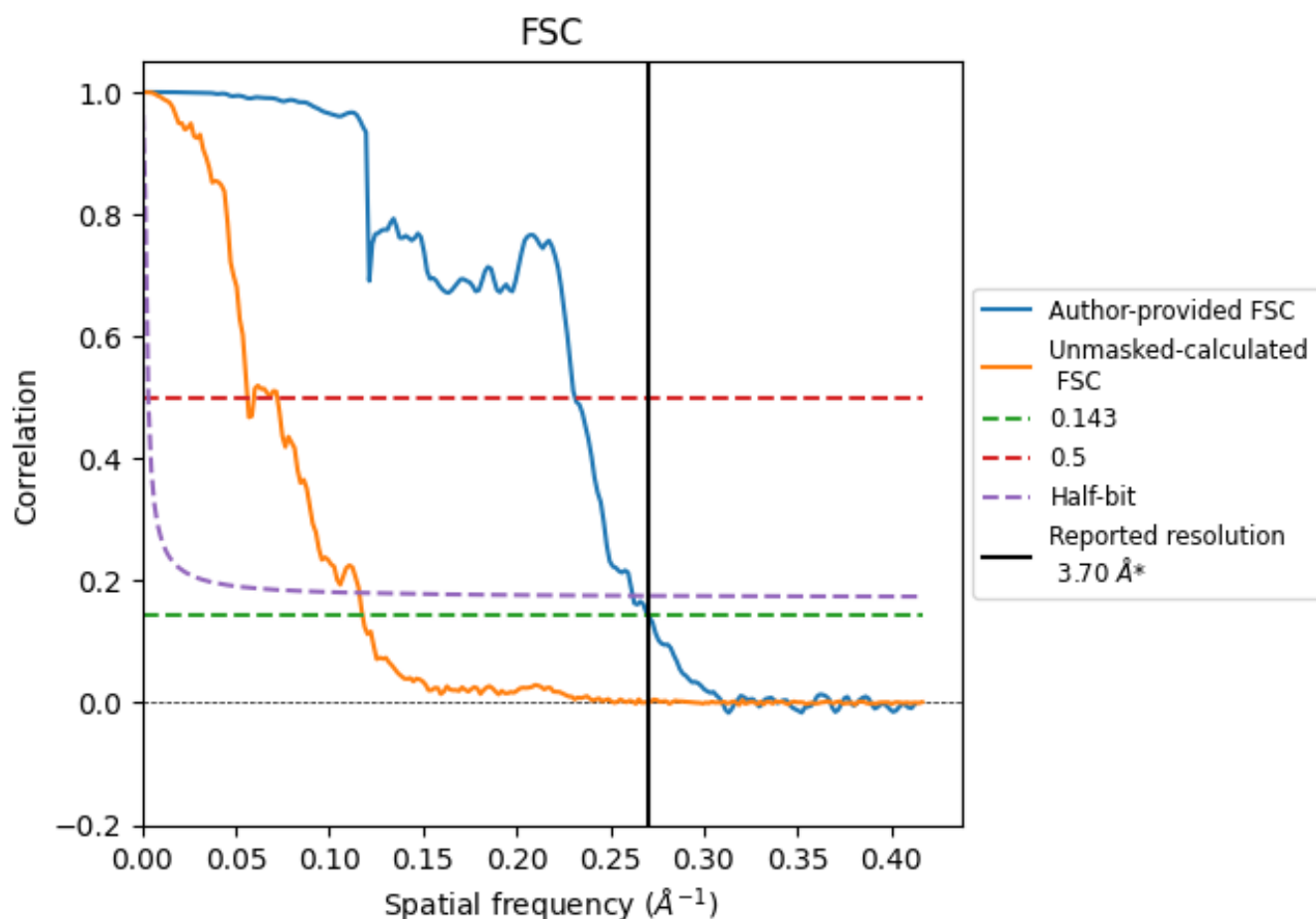


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

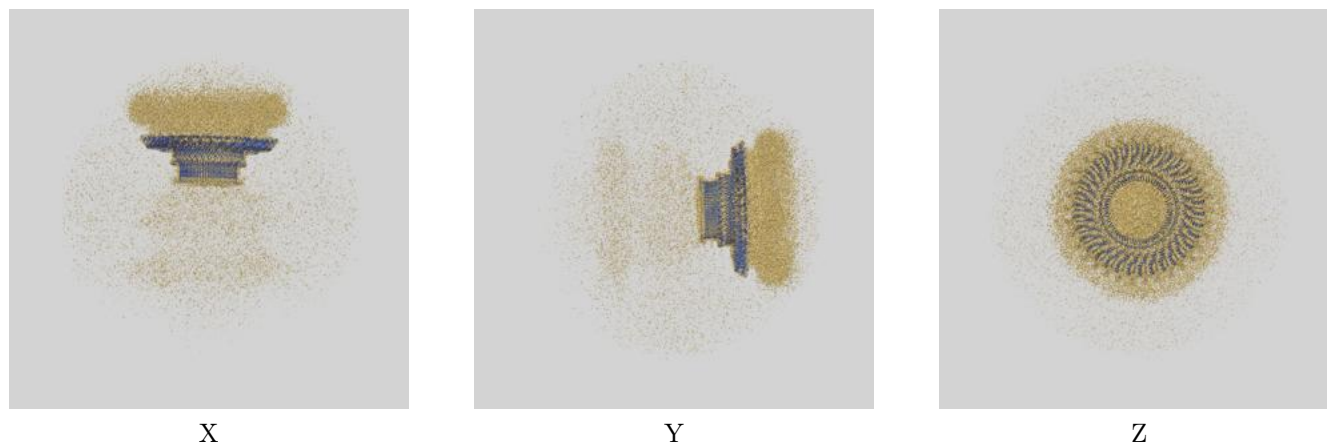
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.32	3.82
Unmasked-calculated*	8.50	17.79	8.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.50 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

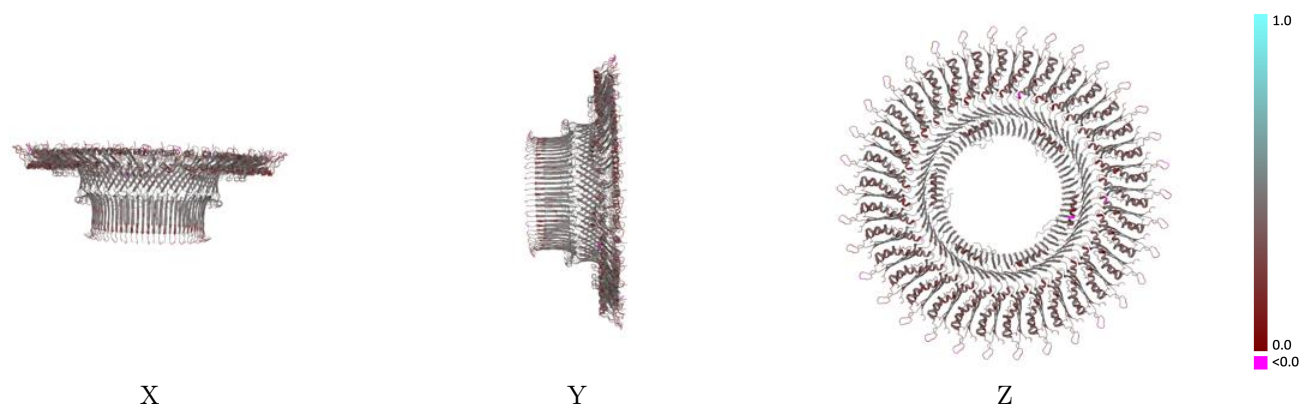
This section contains information regarding the fit between EMDB map EMD-37595 and PDB model 8WK4. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



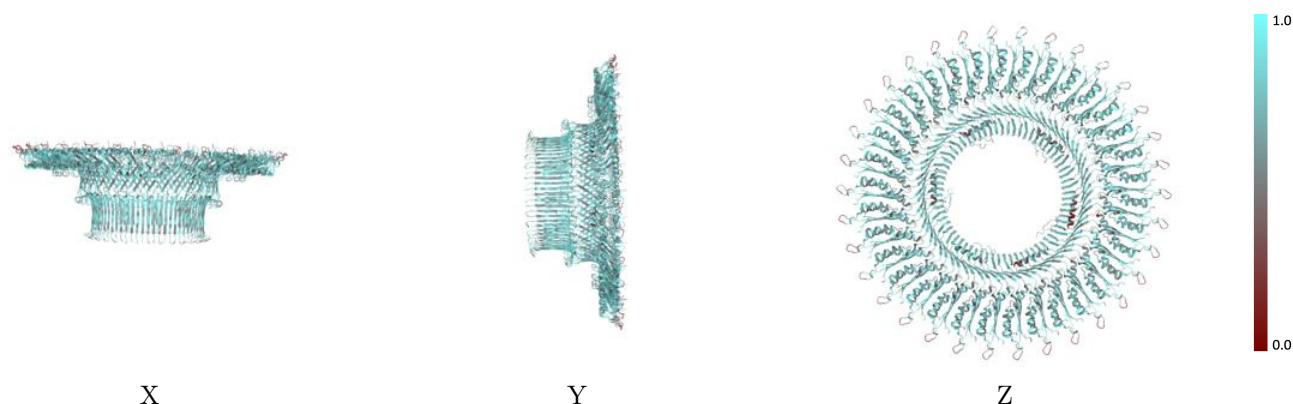
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



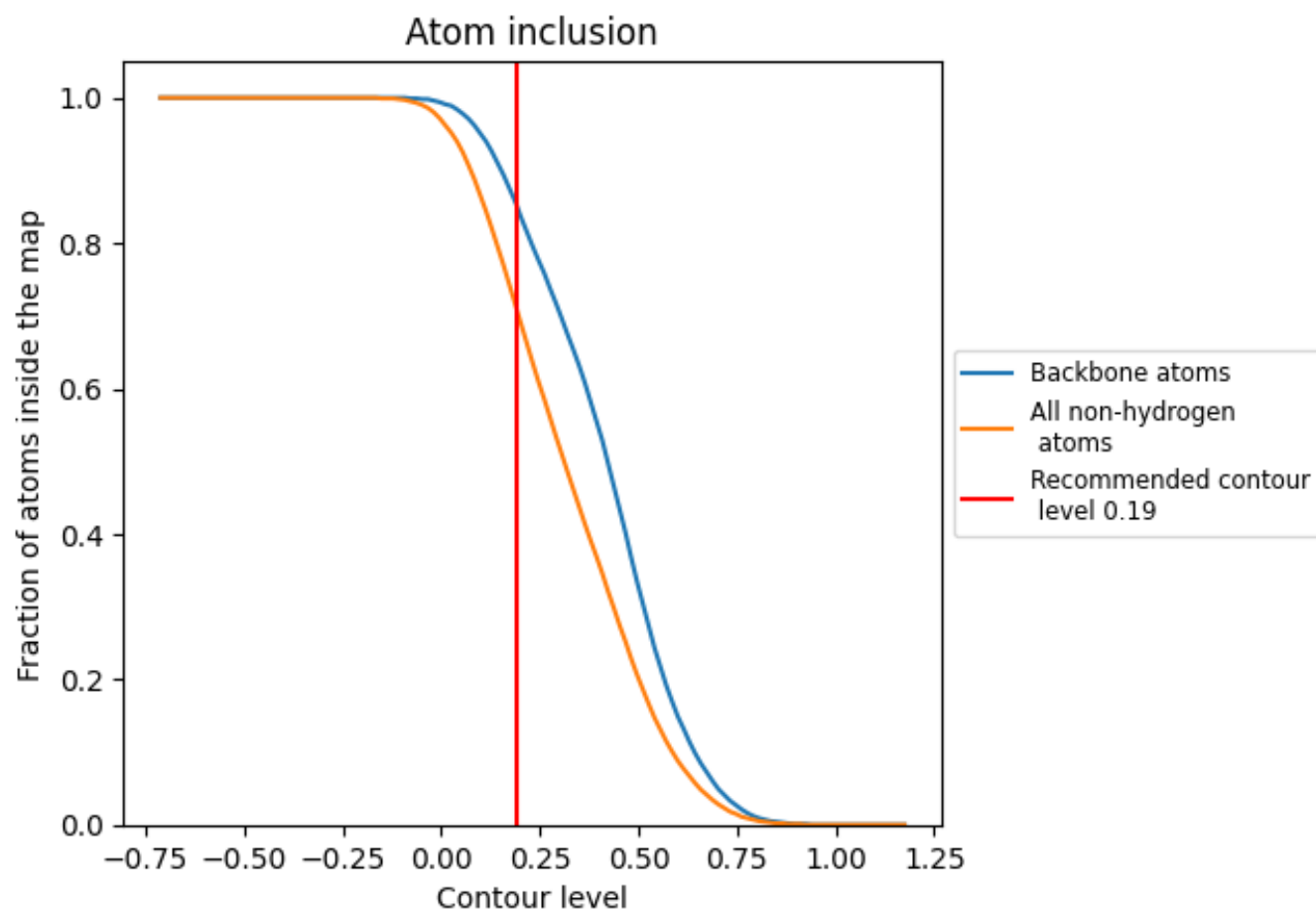
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.3880
A	 0.7230	 0.3960
B	 0.7160	 0.3810
C	 0.7120	 0.3920
D	 0.7290	 0.3950
E	 0.7200	 0.3910
F	 0.7100	 0.3970
G	 0.7160	 0.3920
H	 0.7140	 0.3810
I	 0.7380	 0.3930
J	 0.7140	 0.3900
K	 0.7240	 0.3890
L	 0.7200	 0.3980
M	 0.7240	 0.3950
N	 0.7110	 0.3910
O	 0.7200	 0.4030
P	 0.7420	 0.4030
Q	 0.7200	 0.3980
R	 0.7180	 0.3900
S	 0.7190	 0.3900
T	 0.7110	 0.3880
U	 0.7250	 0.3840
V	 0.7080	 0.3800
W	 0.7180	 0.3750
X	 0.6880	 0.3710
Y	 0.7000	 0.3730
Z	 0.7040	 0.3830
a	 0.7030	 0.3860
b	 0.7020	 0.3860
c	 0.7000	 0.3810
d	 0.7000	 0.3840
e	 0.7130	 0.3920
f	 0.7080	 0.3930
g	 0.7040	 0.3890
h	 0.7140	 0.3910



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Chain	Atom inclusion	Q-score
i	 0.5350	 0.3330
j	 0.6120	 0.3150
k	 0.5270	 0.3360
l	 0.5890	 0.3350
m	 0.5580	 0.3250
n	 0.4570	 0.2610
o	 0.6900	 0.4740
p	 0.7450	 0.4520
q	 0.6980	 0.4230
r	 0.6720	 0.4750
s	 0.6190	 0.4460