



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:58 PM UTC

PDB ID : 7E81 / pdb_00007e81
EMDB ID : EMD-31007
Title : Cryo-EM structure of the flagellar MS ring with FlgB-Dc loop and FliE-helix 1 from Salmonella
Authors : Tan, J.X.; Chang, S.H.; Wang, X.F.; Xu, C.H.; Zhou, Y.; Zhang, X.; Zhu, Y.Q.
Deposited on : 2021-02-28
Resolution : 4.50 Å(reported)

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

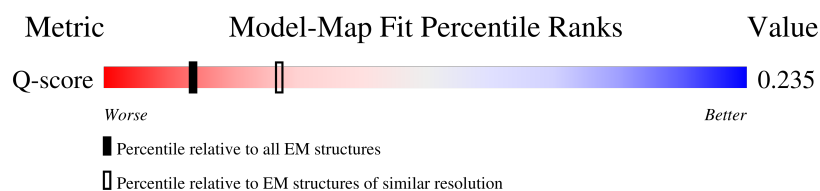
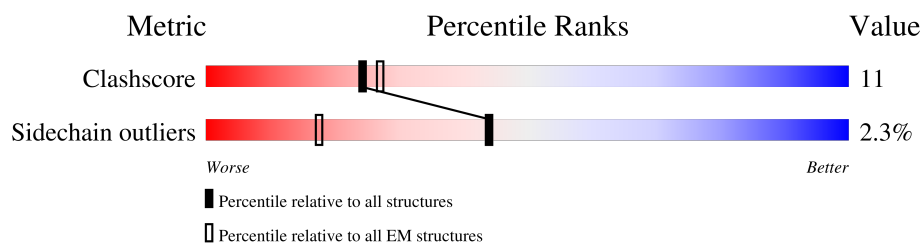
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



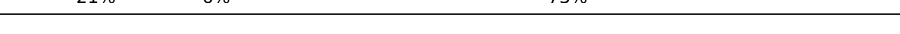
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	Ca	560	21% 6% 73%
1	Cb	560	20% 6% 73%
1	Cc	560	20% 7% 73%
1	Cd	560	20% 6% 73%
1	Ce	560	22% 5% 73%

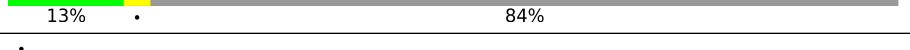
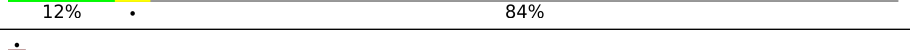
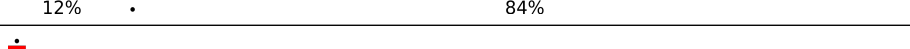
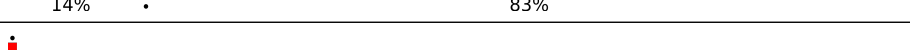
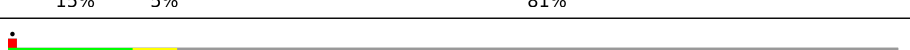
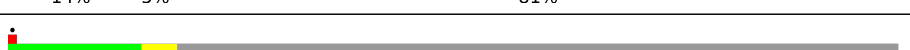
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Mol	Chain	Length	Quality of chain
1	Cf	560	 21% 6% 73%
1	Ch	560	 21% 6% 73%
1	Ci	560	 21% 6% 73%
1	Cj	560	 21% 6% 73%
1	Ck	560	 20% 6% 73%
1	Cl	560	 21% 6% 73%
1	Cm	560	 20% 7% 73%
1	Cn	560	 20% 6% 73%
1	Co	560	 21% 6% 73%
1	Cp	560	 20% 6% 73%
1	Cq	560	 22% 5% 73%
1	Cr	560	 21% 6% 73%
1	Cs	560	 21% 6% 73%
1	Ct	560	 20% 7% 73%
1	Cu	560	 21% 6% 73%
1	Cv	560	 21% 6% 73%
1	Cw	560	 20% 6% 73%
1	Cx	560	 21% 6% 73%
1	Cy	560	 21% 6% 73%
1	Cz	560	 21% 5% 73%
1	Da	560	 15% 5% 81%
1	Db	560	 15% 5% 81%
1	Dc	560	 14% 5% 81%
1	Dd	560	 17% 5% 81%
1	De	560	 14% 5% 82%

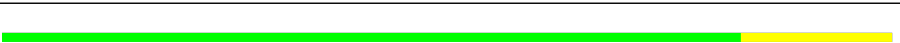
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Mol	Chain	Length	Quality of chain
1	Df	560	 14% 83%
1	Dg	560	 13% 84%
1	Dh	560	 12% 84%
1	Di	560	 12% 84%
1	Dj	560	 12% 84%
1	Dk	560	 12% 84%
1	Di	560	 13% 84%
1	Dm	560	 12% 84%
1	Dn	560	 12% 84%
1	Do	560	 14% 83%
1	Dp	560	 15% 5% 81%
1	Dq	560	 14% 5% 81%
1	Dr	560	 15% 81%
1	Ds	560	 16% 81%
1	Dt	560	 14% 5% 81%
1	Du	560	 15% 81%
1	Dv	560	 14% 5% 81%
1	Dw	560	 15% 81%
1	Ea	560	 20% 6% 73%
1	Eb	560	 21% 5% 73%
1	Ec	560	 21% 6% 73%
1	Ed	560	 20% 6% 73%
1	Ee	560	 21% 6% 73%
1	Ef	560	 21% 6% 73%
1	Eg	560	 21% 6% 73%

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Mol	Chain	Length	Quality of chain
1	Fh	560	
1	cg	560	
2	GA	12	
2	GB	12	
2	GC	12	
2	GD	12	
2	GE	12	
3	GF	18	
3	GG	18	
3	GH	18	
3	GI	18	
3	GJ	18	
3	GK	18	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 57178 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Da	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Db	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Dc	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Dd	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	De	99	Total	C	N	O	S	0	0
			696	432	125	138	1		
1	Df	97	Total	C	N	O	S	0	0
			687	427	123	136	1		
1	Dg	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Dh	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Di	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Dj	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Dk	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Dl	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Dm	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Dn	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
1	Do	97	Total	C	N	O	S	0	0
			687	427	123	136	1		
1	Dp	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Dq	109	Total	C	N	O	S	0	0
			746	462	135	148	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Dr	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Ds	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Dt	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Du	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Dv	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Dw	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
1	Ca	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cb	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cc	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cd	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Ce	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cf	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	cg	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Ch	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Ci	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cj	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Ck	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cl	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cm	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Cn	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
1	Co	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Cp	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cq	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cr	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cs	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Ct	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cu	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cv	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cw	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cx	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cy	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Cz	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Ea	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Eb	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Ec	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Ed	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Ee	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Ef	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Eg	150	Total 1185	C 722	N 221	O 239	S 3	0	0
1	Fh	150	Total 1185	C 722	N 221	O 239	S 3	0	0

- Molecule 2 is a protein called FlgB-Dc loop.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	GA	11	Total	C	N	O	0	0
			55	33	11	11		
2	GC	11	Total	C	N	O	0	0
			55	33	11	11		
2	GE	12	Total	C	N	O	0	0
			60	36	12	12		
2	GD	10	Total	C	N	O	0	0
			50	30	10	10		
2	GB	5	Total	C	N	O	0	0
			25	15	5	5		

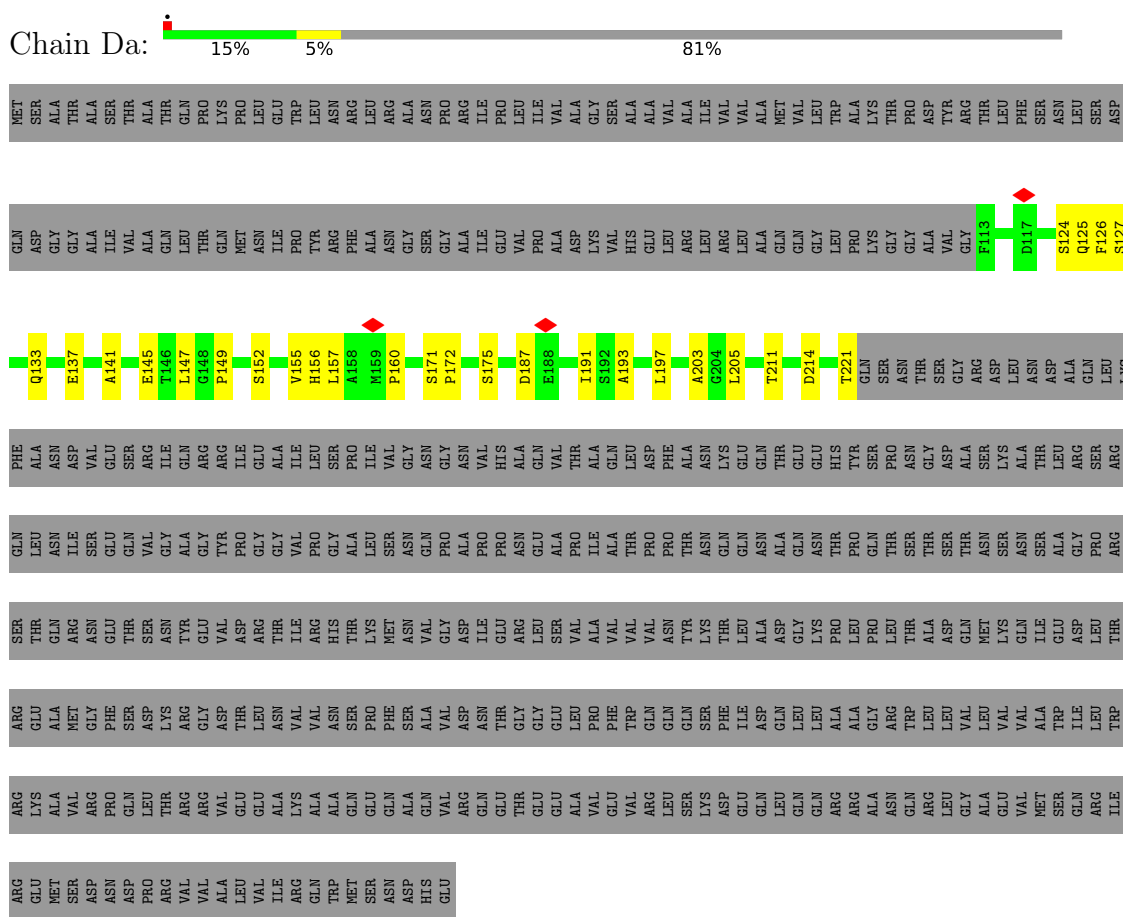
- Molecule 3 is a protein called FliE helix 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	GF	18	Total	C	N	O	0	0
			90	54	18	18		
3	GG	18	Total	C	N	O	0	0
			90	54	18	18		
3	GH	18	Total	C	N	O	0	0
			90	54	18	18		
3	GI	15	Total	C	N	O	0	0
			75	45	15	15		
3	GJ	18	Total	C	N	O	0	0
			90	54	18	18		
3	GK	18	Total	C	N	O	0	0
			90	54	18	18		

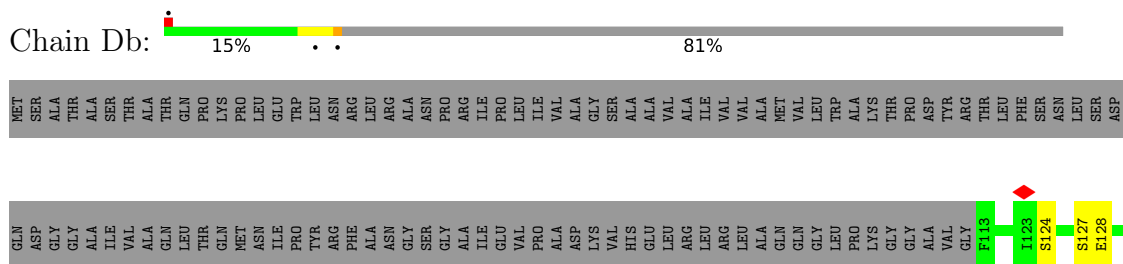
3 Residue-property plots

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 M-ring protein



- Molecule 1: Flagellar M-ring protein

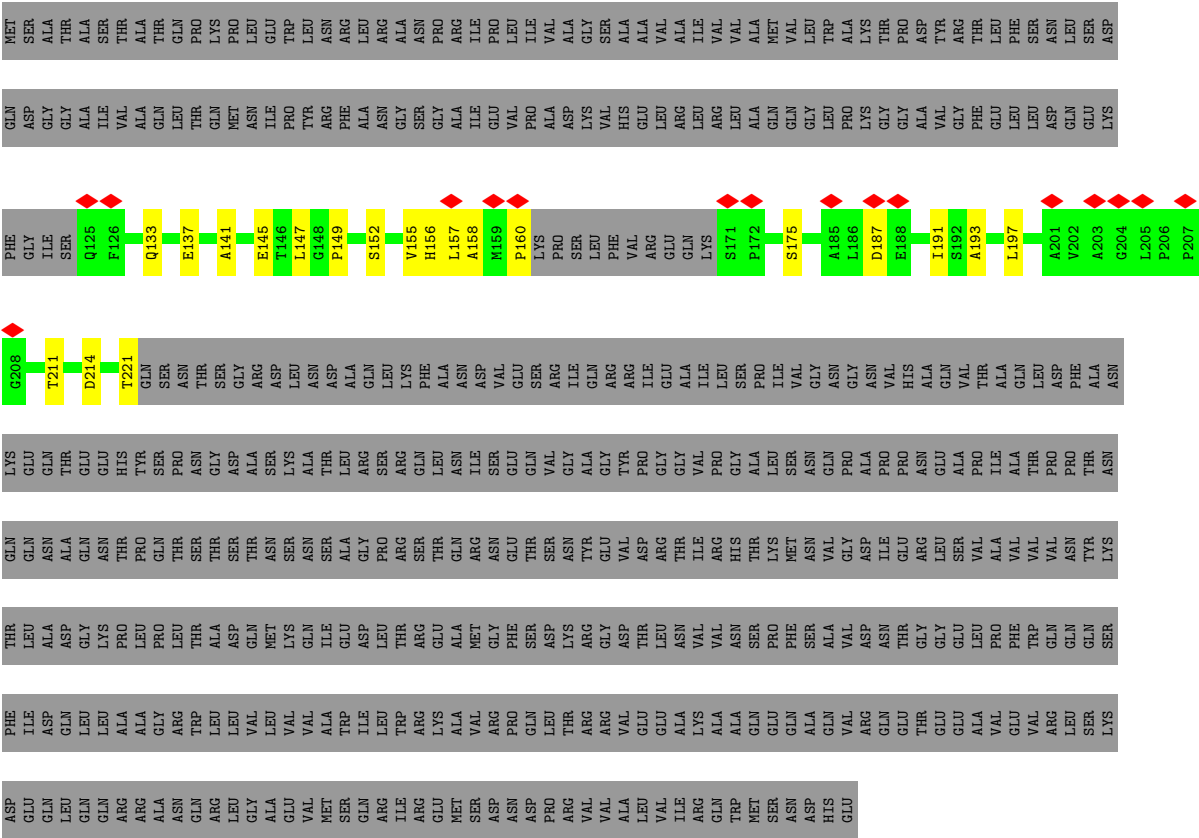




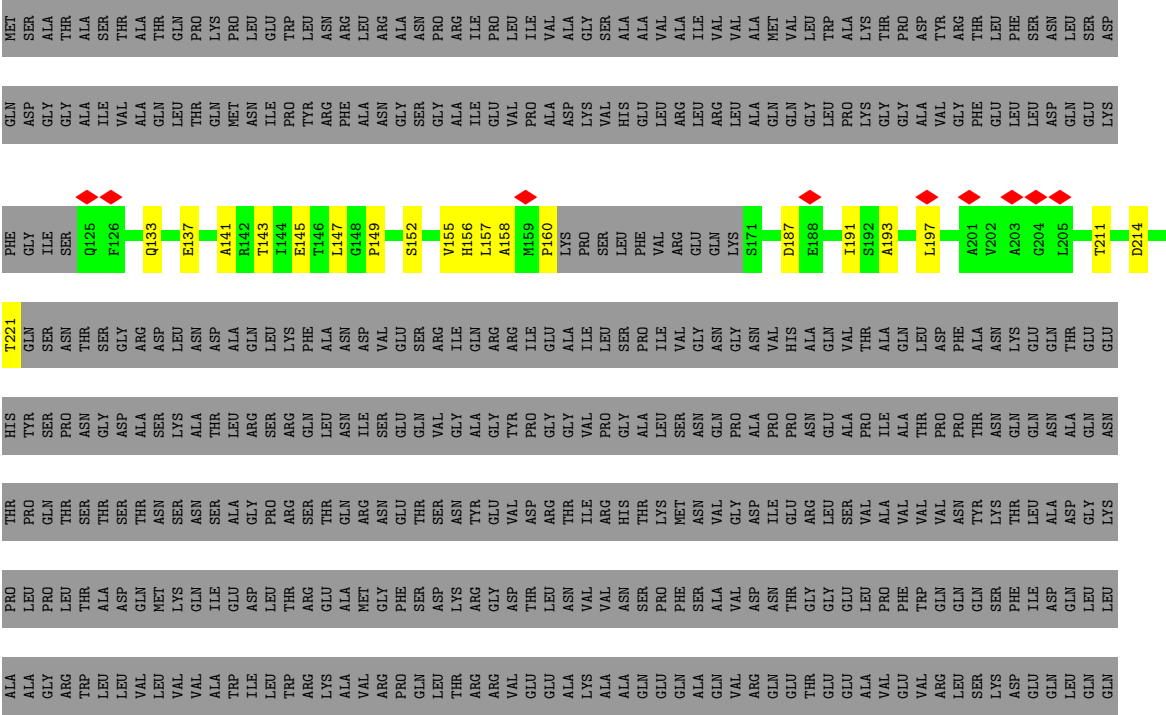


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• Molecule 1: Flagellar M-ring protein



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

● Molecule 1: Flagellar M-ring protein

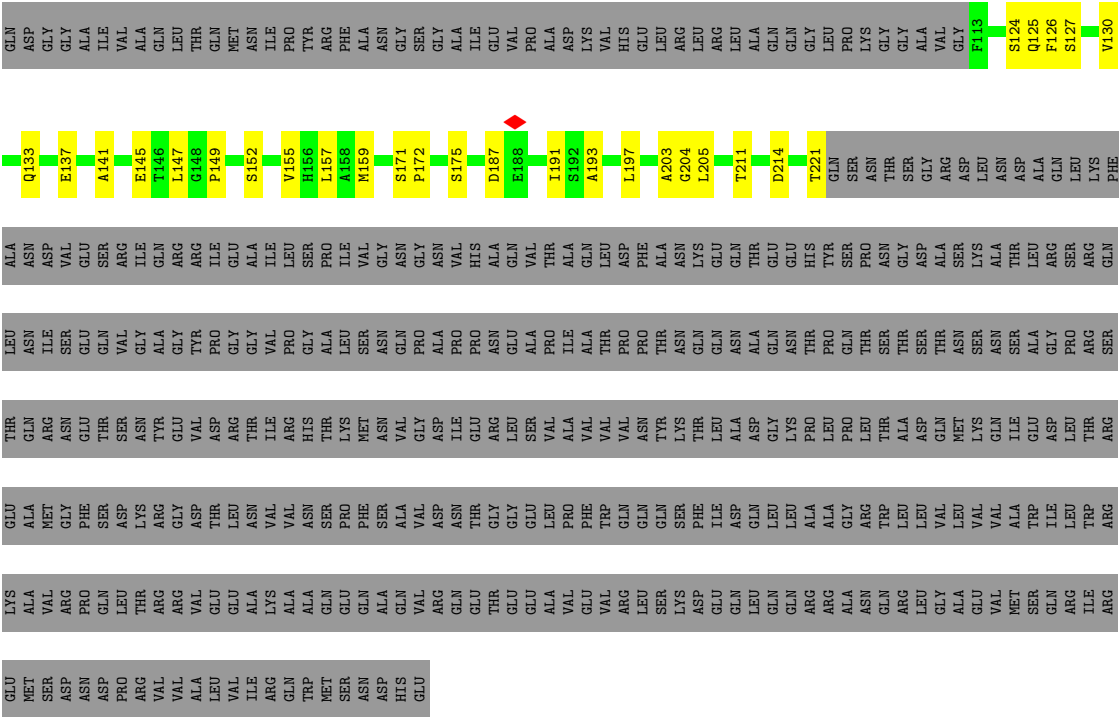


ARG	LEU	LEU	ARG	GLY	VAL	VAL	GLU	VAL	GLN	THR	ASP	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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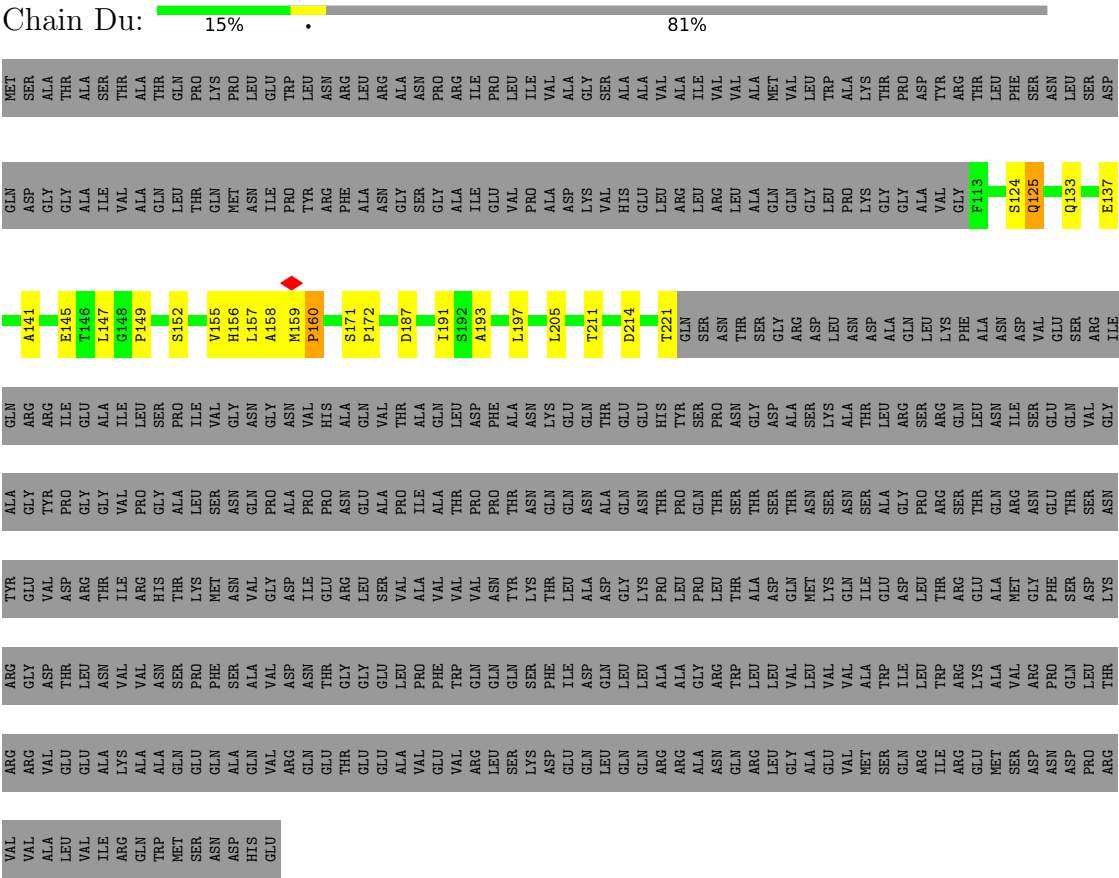
● Molecule 1: Flagellar M-ring protein



MET	SER	ALA	THR	ALA	SER	THR	ALA	GLN	PRO	LYS	PRO	LEU	GLU	TRP	ILE	ARG	LEU	ALA	ARG	LEU	VAL	ALA	GLY	SER	ALA	ALA	VAL	VAL	ALA	GLY	SER	ASP	GLY	THR	ALA	GLN	THR	ASP															
GLN	ASP	GLY	GLY	ALA	VAL	ILE	VAL	GLN	THR	GLN	MET	ASN	GLU	TRP	TYR	PHE	ALA	ASN	GLY	GLY	ALA	ILE	GLU	VAL	GLN	PRO	ALA	ASP	LYS	VAL	HIS	GLU	GLU	LEU	ARG	LEU	ARG	VAL	ALA	GLN	GLY	LEU	TRP	LYS	THR	THR	PHE	ASN	LEU	SER	ASP		
Q125	F126	S127	E128	Q129	V130	E137	A141	E145	T146	L147	G148	P149	S152	V155	H156	L157	A158	M159	P160	S171	P172	S175	D187	I191	S192	A193	L197	A201	T211	D214	T221	GLN	SER	ASN	THR	GLY	ASP	GLY	ARG	ASP	LYS	LEU	ASN	THR	ALA	GLY	LEU						
LYS	PHE	ALA	ASN	VAL	GLU	SER	ARG	GLY	GLN	ARG	ILE	GLU	ILE	VAL	GLY	SER	PRO	LEU	VAL	PRO	ASN	GLY	ASN	VAL	THR	ALA	THR	ASN	LYS	GLU	GLN	GLU	GLU	GLY	THR	PRO	THR	GLY	ASP	ALA	SER	GLY	ALA	SER	LYS	LEU	ASN	THR	ILE	GLU	ASP	GLY	PRO
ARG	GLN	LEU	ILE	ILE	GLU	GLN	VAL	GLY	ALA	TYR	GLY	GLY	PRO	ALA	THR	HIS	LEU	SER	GLY	ALA	PRO	GLY	VAL	ILE	ALA	VAL	PRO	THR	ASN	GLN	GLY	LYS	PRO	THR	PRO	THR	GLN	THR	THR	ALA	SER	GLY	THR	THR	GLN	LYS	THR	ALA	GLY	ASP	LEU		
ARG	SER	THR	GLN	ASN	THR	THR	ASN	THR	TYR	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		



● Molecule 1: Flagellar M-ring protein



● Molecule 1: Flagellar M-ring protein



[illegible]

- Molecule 1: Flagellar M-ring protein



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

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S243	K244	R247	R248	I249	I252	N261	Q265	V266	K275	S289	K290	V304	GLY	ALA	ALA	GLY	TYR	PRO	GLY	GLY	VAL	PRO	PRO	GLY	ALA	ALA	LEU	SER	ASN	ASN	GLN	PRO	PRO	ALA	PRO	PRO	PRO	ASN	GLY	GLU	ALA	ALA	PRO	ILE	THR	ALA	THR	PRO	PRO	PRO	THR	THR	PRO	GLN	GLN	GLN	ASN	ASN	PRO	THR	PRO	GLN	THR
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SER	THR	THR	THR	ASN	SER	ASN	SER	ALA	GLY	P355	T358	Q359	L385	S386	P387	A388	P389	N392	Y393	Z394	THR	LEU	ALA	LEU	ASP	GLY	LYS	PRO	L402	E413	D414	R417	M420	K425	D428	M431	V432	S438	ALA	VAL	ASP	ASN	THR	GLY	GLY	LEU	PRO	PRO	THR	THR
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GLN GLN GLN SER PHE TLE ASP GLN GLN LEU LEU ALA ALA GLY ARG TRP TRP LEU LEU VAL VAL LEU VAL VAL ALA ALA TRP TRP TLE LEU TRP ARG TRP LYS VAL VAL ARG PRO GLN LEU LEU THR ARG ARG VAL VAL GLU GLU ALA ALA LYS GLN ALA ALA GLN GLN ALA GLN VAL ARG ARG GLN GLN THR GLU GLU ALA VAL VAL VAL

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

- Molecule 1: Flagellar M-ring protein

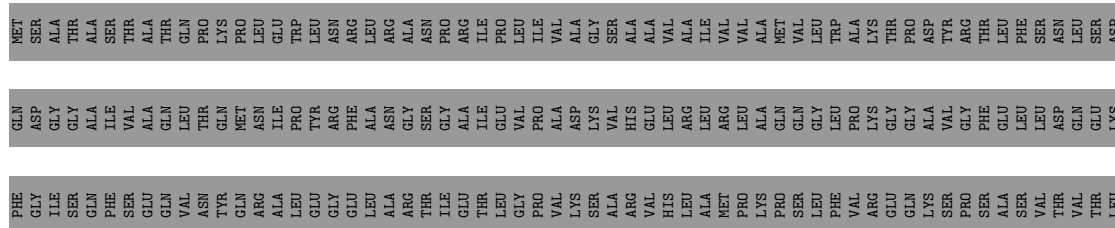
[illegible]

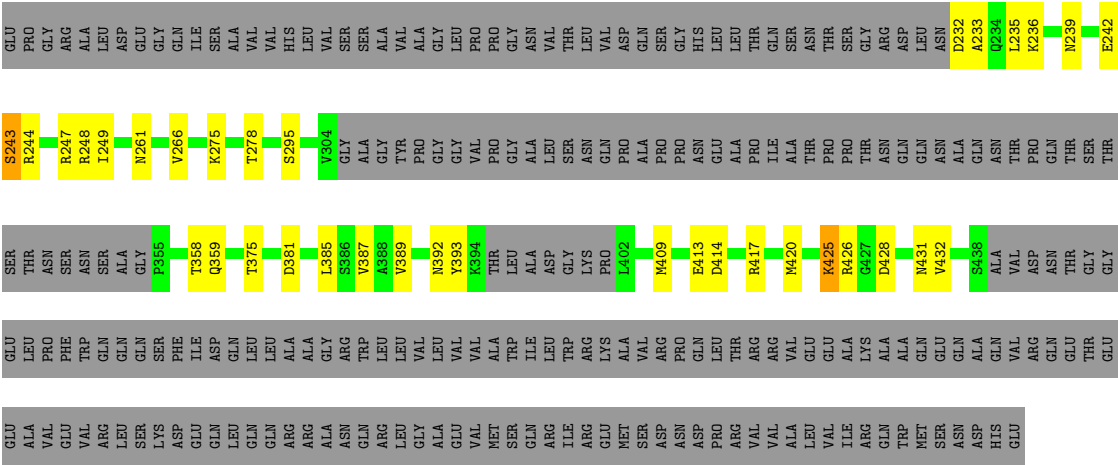
GLN ASP GLY GLY ALA ALA ALA LEU THR GLN MET ASN ILE TYR PRO ARG ALA ALA ASN ASN SER GLY ALA ILE GLU VAL VAL PRO PRO ALA ASP LYS HIS HIS VAL GLU LEU ARG ARG ARG LEU LEU GLN GLN GLY LEU LEU PRO PRO LYS GLY GLY VAL VAL GLY PHE GLU LEU LEU LEU ASP GLN GLY LYS

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

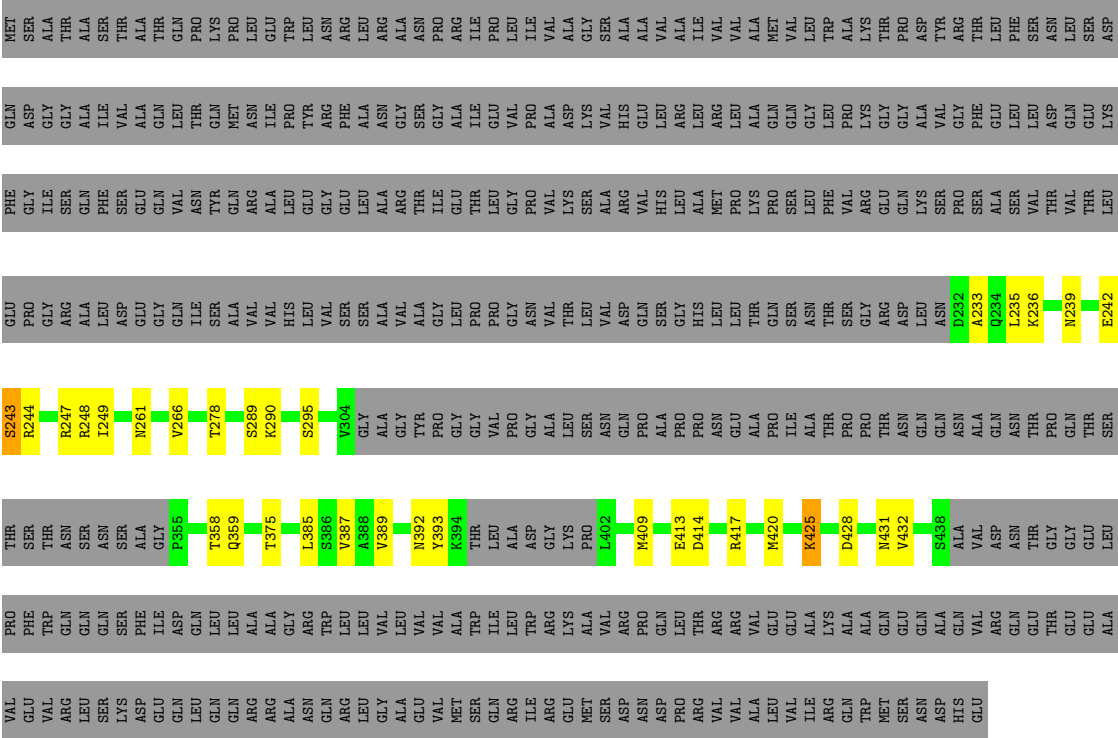
GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	LEU	HIS	LEU	VAL	SER	SER	ALA	ALA	VAL	VAL	GLY	LEU	PRO	PRO	ASN	GLN	ASP	GLN	SER	GLN	GLY	HIS	LEU	LEU	THR	THR	SER	SER	GLY	ARG	ASP	LEU	LEU	ASN	ASN	D232	D233	D234	D235	D236	D237	D238	D239	D240
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------

S243	R244	R247	R248	I249	I252	R259	R260	R261	R265	R266	K275	I278	S289	K290	S304	G304	GLY	ALA	GLY	GLY	TYR	PRO	GLY	GLY	VAL	VAL	PRO	PRO	GLY	ALA	ALA	LEU	SER	SER	ASN	ASN	GLN	PRO	PRO	ALA	ALA	ALA	ILE	ALA	ALA	THR	PRO	PRO	THR	ASN	ASN	GLN	GLN	ASN	ALA	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

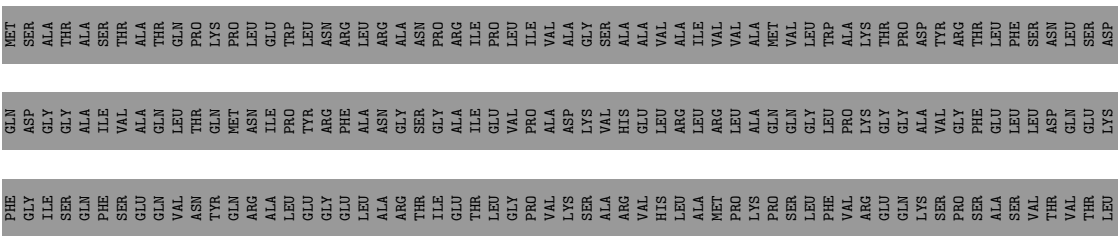


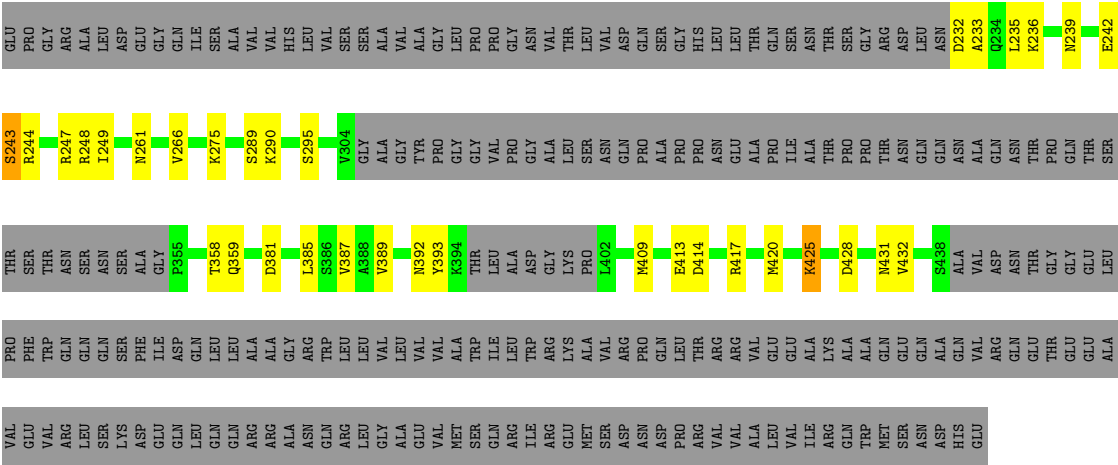


• Molecule 1: Flagellar M-ring protein

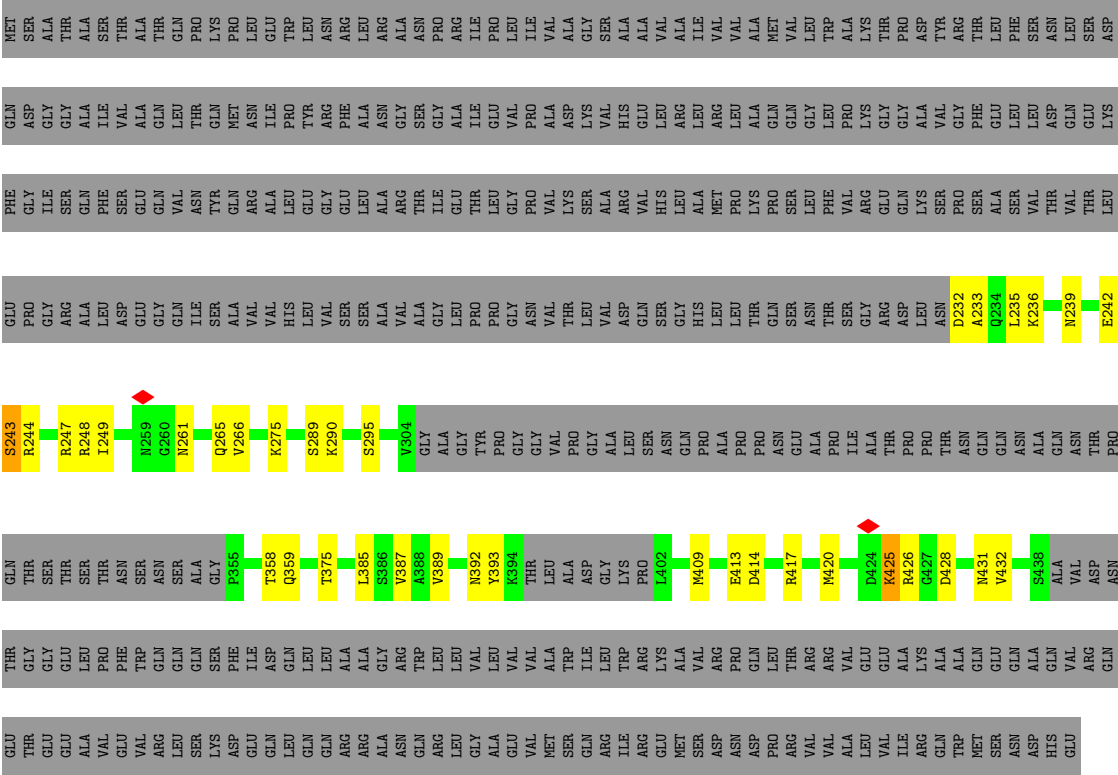


• Molecule 1: Flagellar M-ring protein

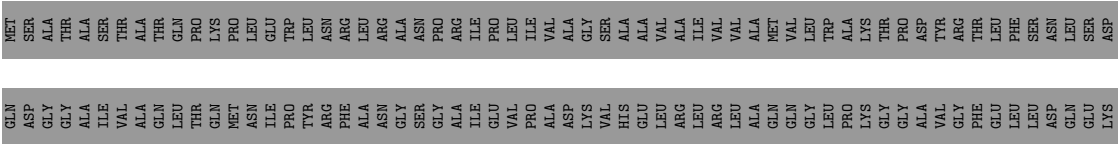




● Molecule 1: Flagellar M-ring protein



● Molecule 1: Flagellar M-ring protein



ARG	GLN	THR	ASP	THR	S243		GLU	PHE	GLN	MET
GLN	GLU	THR	ASN	SER	R244		PRO	GLY	ASP	SER
THR	GLU	THR	THR	THR	R247		GLY	ILE	GLY	ALA
GLU	GLY	SER	GLY	THR	R248		ALA	GLN	ALA	ALA
GLU	GLU	ASN	GLU	ASN	L249		LEU	PHE	ILE	SER
ALA	GLU	SER	LEU	SER			ASP	SER	VAL	THR
VAL	PRO	ASN	PRO	ASN	T252		GLU	GLU	GLN	ALA
GLU	GLU	SER	PHE	SER	N261		GLY	VAL	LEU	GLN
VAL	VAL	ALA	ALA	GLY	V266		ILE	ASN	THR	PRO
ARG	GLN	P355	GLN	GLY			SER	TYR	GLN	LYS
LEU	GLN		GLN				ALA	GLN	MET	PRO
SER			GLN				ALA	GLN	MET	PRO
LYS	SER	T358	SER	THR	R275		VAL	ARG	ASN	LEU
ASP	PHE	Q359	PHE	Q359			VAL	ILE	ILE	TRP
GLU	GLU	ILE	ILE	ILE	S289		HIS	LEU	PRO	GLN
GLN	GLN	I372	ASP	I372	K290		LEU	GLY	TYR	LEU
LEU	GLN		GLN	GLN	Z295		VAL	GLY	ARG	ASN
GLN	LEU	T375	LEU	T375			SER	GLU	PHE	ARG
GLN	LEU		LEU				SER	GLU	ALA	LEU
ARG	ALA	G380	ALA	G380	V304		VAL	ARG	ASN	ARG
ARG	ARG	D381	ALA	D381	GLY		ALA	ARG	GLY	ALA
ALA	GLY		GLY		ALA		GLY	THR	SER	ASN
ASN	ARG	L385	ARG	L385	GLY		ALA	ILE	GLY	PRO
GLN	TRP	S386	TRP	S386	TYR		LEU	GLU	ALA	ARG
LEU	LEU	V387	LEU	V387	PRO		PRO	THR	ILE	ILE
ARG	LEU	A388	LEU	A388	GLY		PRO	LEU	GLU	PRO
GLY	VAL	V389	VAL	V389	GLY		ASN	GLY	VAL	LEU
ALA	LEU		LEU		VAL		GLN	VAL	PRO	ILE
GLU	VAL	N392	VAL	N392	PRO		VAL	VAL	ALA	VAL
VAL	VAL	Y393	VAL	Y393	GLY		THR	LYS	ASP	GLY
MET	ALA	K394	ALA	K394	ALA		LEU	SER	LYS	ALA
SER	SER	THR	TRP	THR	LEU		SER	ARG	VAL	SER
GLN	ILE		ILE		ALA		ASN	VAL	HIS	ALA
ARG	LEU		LEU		GLN		GLN	VAL	GLU	ALA
ILE	TRP		TRP		ASN		SER	HIS	LEU	VAL
ARG	ARG	ASP	ARG	ASP	PRO		GLY	LEU	ARG	ALA
GLU	GLU	LYS	LYS	GLY	ALA		HIS	ALA	LEU	ILE
MET	ALA	PRO	ALA	PRO	PRO		LEU	MET	ARG	ILE
SER	VAL	L402	VAL	L402	PRO		LEU	PRO	LEU	VAL
ASP	ARG		ARG		ASN		THR	LYS	ALA	VAL
ASN	PRO	M409	PRO	M409	GLU		GLN	PRO	GLN	MET
ASP	GLN		GLN		ALA		SER	SER	GLN	VAL
PRO	LEU	E413	LEU	E413	PRO		ASN	LEU	GLY	LEU
ARG	THR	D414	THR	D414	ILE		THR	PHE	LEU	TRP
VAL	ARG		ARG		ALA		SER	VAL	PRO	ALA
VAL	VAL	R417	ARG	R417	THR		GLY	ARG	LYS	LYS
ALA	VAL		VAL		PRO		ARG	GLU	GLY	THR
LEU	LEU	M420	GLU	M420	PRO		ASP	GLN	GLY	PRO
ILE	GLU		GLU		THR		LEU	LYS	ALA	ASP
VAL	ILE		ALA		THR		ASN	SER	VAL	TYR
ARG	ARG	K425	LYS	K425	GLN		ASN	PRO	GLY	ARG
GLN	ALA		ALA		GLN		D232	SER	PHE	THR
TRP	ALA	D428	ALA	D428	ASN		A234	ALA	GLU	LEU
MET	GLN		GLN		ALA		K236	SER	LEU	PHE
SER	GLU	N431	GLU	N431	ALA		L236	VAL	LEU	SER
ASN	GLN	V432	GLN	V432	GLN		THR	THR	ASP	ASN
ASP	ALA	S438	ALA	S438	ASN		N239	VAL	GLM</	

Chain Cq: 22% 5% 73%

LEU	LEU	P355	R247	GLU	PHE	GLN	MET
LEU	ALA	T358	R248	GLY	GLY	ASP	SER
ALA	ALA	Q359	I249	ARG	IIE	GLY	THR
GLY	ARG	Q265	Q265	ALA	GLN	ALA	SER
ARG	ARG	T375	V266	LEU	PHE	IIE	THR
TRP				ASP	SER	VAL	
LEU	LEU	D381	S295	GLU	GLU	ALA	GLN
LEU	LEU	L385	V304	GLY	GLN	LEU	THR
LEU	VAL	S386	GLY	IIE	ASN	THR	LYS
VAL	VAL	V387	ALA	SER	TYR	GLN	PRO
VAL	VAL	A388	GLY	ALA	GLN	MET	PRO
ALA	ALA	V389	TYR	VAL	ALA	ASN	GLN
ILE	ILE	N392	GLY	HIS	ALA	LEU	GLN
LEU	LEU	Y393	GLY	LEU	GLU	PRO	TRP
TRP	TRP	V394	VAL	VAL	GLY	TYR	LEU
ARG	ARG	THR	PRO	SER	GLU	ARG	ASN
LYS	LYS	LEU	GLY	SER	GLU	PHE	ARG
ALA	ALA	ALA	GLY	ALA	ALA	LEU	LEU
VAL	VAL	ASP	LEU	VAL	ASP	GLN	ARG
ARG	ARG	GLY	SER	ALA	THR	GLY	ASN
VAL	VAL	LYS	ASN	ALA	IIE	ASN	PRO
VAL	VAL	PRO	GLN	LEU	GLU	ALA	ASN
LEU	LEU	L402	PRO	PRO	THR	ILE	PRO
ARG	ARG	E413	ALA	PRO	LEU	GLU	LEU
VAL	VAL	D414	PRO	GLY	GLY	VAL	LEU
ALA	ALA	VAL	ASN	ASN	VAL	ALA	ILE
GLU	GLU	R417	GLU	THR	VAL	ALA	VAL
VAL	VAL	ALA	ALA	LEU	LYS	ASP	ALA
ILE	ILE	M420	PRO	VAL	ALA	VAL	ALA
ALA	ALA	D428	ALA	GLN	VAL	GLU	ALA
ALA	ALA	THR	THR	SER	HIS	LEU	VAL
GLN	GLN	M431	PRO	GLY	LEU	ARG	ALA
GLU	GLU	V432	PRO	HIS	ALA	LEU	ILE
GLN	GLN	THR	THR	LEU	MET	ARG	VAL
ASP	ASP	S438	ASN	LEU	PRO	LEU	VAL
ALA	ALA	ALA	GLN	THR	LYS	ALA	VAL
GLN	GLN	VAL	GLN	GLN	PRO	GLN	MET
VAL	VAL	ARG	ASN	SER	ASN	GLN	VAL
ARG	ARG	ASN	ALA	ASN	LEU	GLY	LEU
GLN	GLN	THR	GLN	THR	PHE	LEU	TRP
THR	THR	GLY	ASN	SER	VAL	PRO	ALA
GLU	GLU	GLY	THR	GLY	ARG	LYS	LYS
ALA	ALA	LEU	PRO	ARG	GLU	GLY	THR
VAL	VAL	PHE	THR	ASN	GLN	ASP	PRO
VAL	VAL	TRP	THR	LEU	PRO	GLY	TYR
ARG	ARG	GLN	SER	D232	SER	PHE	THR
LEU	LEU	GLN	THR	D233	ALA	GLU	LEU
SER	SER	GLN	ASN	K236	SER	LEU	PHE
LYS	LYS	SER	SER	THR	VAL	LEU	SER
ASP	ASP	PHE	ASN	E242	THR	ASN	ASN
GLU	GLU	ILE	SER	S243	VAL	GLN	LEU
GLN	GLN	ASP	ALA	R244	THR	GLU	SER
ILE	ILE	GLN	GLY		THR	YS	THR

- Molecule 1: Flagellar M-ring protein

Chain Cr:

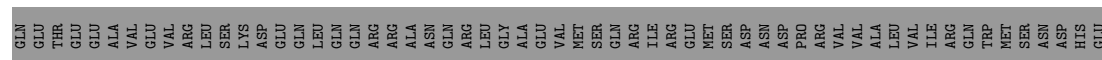


VAL	PRO	SER	GLU	S243	GLU	PHE	GLN	MET
GLU	PHE	THR	PRO	R244	PRO	GLY	ASP	THR
VAL	TRP	SER	GLY		GLY	ILE	GLY	SER
ARG	GLN	THR	ARG	R247	ARG	SER	ALA	ALA
LEU	GLN	ASN	ALA	R248	ALA	GLN	ALA	THR
SER	GLN	SER	LEU	I249	ASP	PHE	ILE	SER
LYS	SER	ASN	ASP			SER	VAL	THR
ASP	PHE	SER	GLU	I262	GLU	GLU	ALA	ALA
GLU	ILE	ALA	GLY		GLY	GLN	LEU	GLN
GLN	ASP	GLY	GLN	N261	GLN	VAL	LEU	THR
LEU	GLN	P355	ILE		ILE	ASN	THR	PRO
GLN	LEU		SER	V266	SER	TYR	GLN	LYS
GLN	LEU	T358	ALA		ALA	GLN	MET	PRO
ARG	ALA	Q359	VAL	K275	VAL	ARG	ASN	PRO
ARG	ALA	E276	VAL		VAL	ALA	ILE	GLU
ALA	GLY	D381	HIS	S289	HIS	LEU	PRO	TRP
ASN	ARG		LEU	K290	LEU	GLU	TYR	LEU
GLN	TRP	L385	VAL		VAL	GLY	ARG	ASN
ARG	LEU	S386	SER	V304	SER	GLU	PHE	ARG
LEU	LEU	V387	SER	GLY	SER	LEU	ALA	ASN
GLY	VAL	A388	ALA		ALA	ALA	ASN	ARG
ALA	LEU	V389	VAL	GLY	VAL	ARG	GLY	ALA
GLU	VAL		ALA	GLY	ALA	THR	SER	ASN
VAL	VAL	N392	GLY	TYR	GLY	ILE	GLY	PRO
MET	ALA	Y393	LEU	PRO	LEU	GLU	ALA	ARG
SER	TRP	K394	PRO	GLY	PRO	THR	ILE	PRO
GLN	ILE	THR	PRO	GLY	PRO	GLU	GLU	GLU
ILE	LEU	LEU	VAL	VAL	ASN	GLY	VAL	LEU
TRP	TRP	ALA	ASN	PRO	ASN	PRO	PRO	ILE
ARG	ARG	ASP	VAL	GLY	VAL	VAL	ALA	VAL
GLU	LYS	GLY	THR	ALA	THR	LYS	ASP	GLY
MET	ALA	LYS	PRO	SER	LEU	SER	LYS	ALA
SER	VAL	VAL	ARG	LEU	ARG	VAL	VAL	SER
ASP	ARG	L402	ASN	ASN	ASP	ARG	HIS	ALA
ASN	PRO		GLN	GLN	GLN	VAL	GLU	ALA
ASP	GLN	E413	SER	PRO	SER	HIS	LEU	VAL
PRO	LEU	D414	ALA	GLY	GLY	LEU	ARG	VAL
ARG	THR		HIS	HIS	ALA	ILE	ILE	GLY
VAL	ARG	R417	PRO	LEU	MET	ARG	ARG	VAL
VAL	ARG		ASN	LEU	PRO	LEU	VAL	VAL
ALA	VAL	M420	THR	THR	LYS	ALA	ALA	VAL
LEU	GLU		GLN	GLN	PRO	PRO	GLN	LEU
VAL	GLU	K425	SER	PRO	SER	SER	GLN	VAL
ILE	ALA	R426	ASN	ILE	ASN	LEU	GLY	VAL
ARG	LYS	G427	THR	ALA	THR	PHE	LEU	TRP
GLN	ALA	D428	SER	SER	SER	VAL	PRO	LYS
TRP	ALA		GLY	GLY	ARG	ARG	LYS	THR
MET	GLN	M431	ARG	PRO	ARG	GLU	GLY	THR
SER	GLU	V432	ASP	THR	ASP	GLN	GLY	PRO
ASN	GLN		ASN	ASN	LEU	VAL	ALA	ASP
ASP	ALA	S438	ASN	ASN	VAL	VAL	VAL	THR
HIS	GLN	ALA	GLN	D232	PRO	GLY	GLY	ARG
GLU	VAL	VAL	ASN	A233	SER	PHE	GLY	THR
	ARG	ASP	ALA	Q234	ALA	GLU	GLU	LEU
	GLN	ASN	GLN	L235	SER	LEU	LEU	PHE
	GLU	THR	ASN	K236	VAL	SER	SER	ASN
	THR	GLY	THR		THR	THR	ASP	ASN
	GLU	GLY	PRO	N239	VAL	VAL	GLN	SER
	GLU	GLU	GLN		THR	THR	GLU	SER

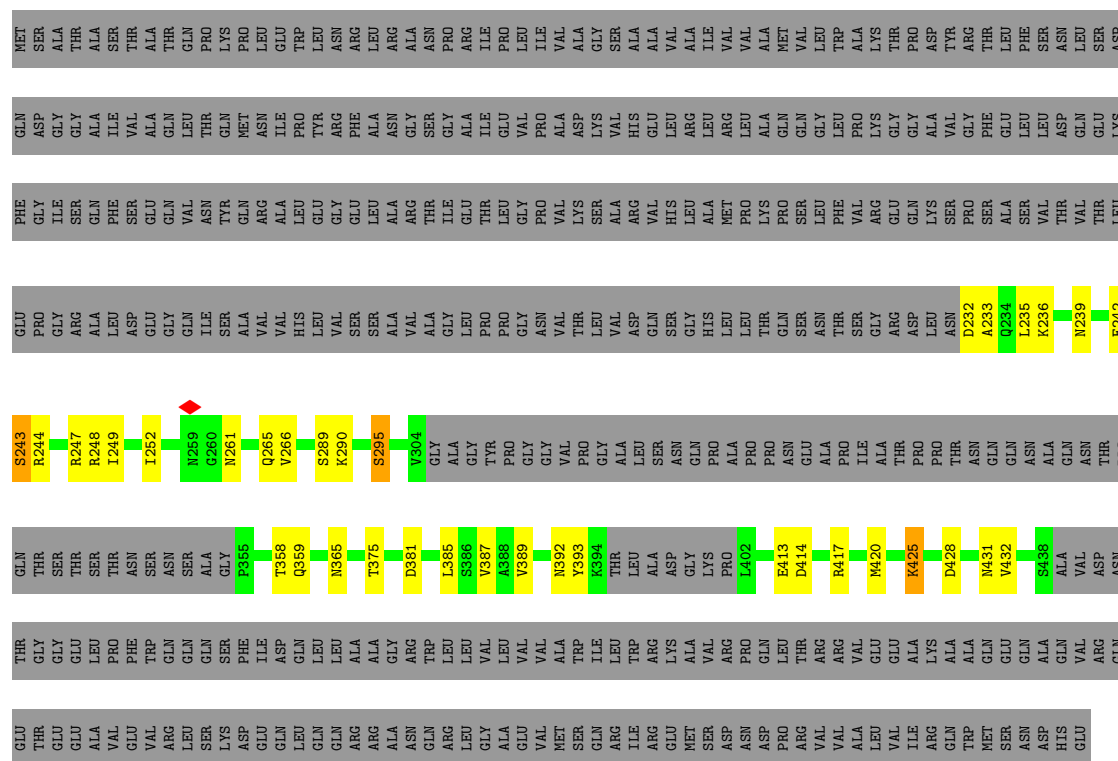
- Molecule 1: Flagellar M-ring protein

Chain Cs:

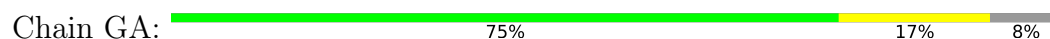
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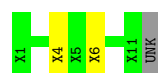
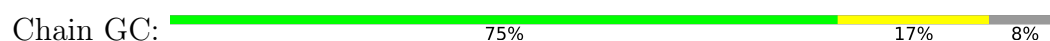
- Molecule 1: Flagellar M-ring protein



- Molecule 2: FlgB-Dc loop



- Molecule 2: FlgB-Dc loop



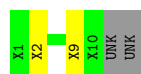
- Molecule 2: FlgB-Dc loop

Chain GE:  67% 33%



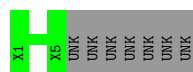
- Molecule 2: FlgB-Dc loop

Chain GD:  67% 17% 17%



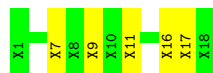
- Molecule 2: FlgB-Dc loop

Chain GB:  42% 58%



- Molecule 3: FliE helix 1

Chain GF:  72% 28%



- Molecule 3: FliE helix 1

Chain GG:  94% 6%



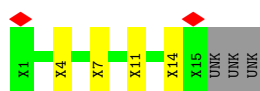
- Molecule 3: FliE helix 1

Chain GH:  78% 22%



- Molecule 3: FliE helix 1

Chain GI:  11% 61% 22% 17%



- Molecule 3: FliE helix 1

Chain GJ:  83% 17%



- Molecule 3: FliE helix 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52714	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.123	Depositor
Minimum map value	-0.372	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	669.184, 669.184, 669.184	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	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	Ca	0.25	0/1197	0.41	0/1613
1	Cb	0.25	0/1197	0.41	0/1613
1	Cc	0.25	0/1197	0.41	0/1613
1	Cd	0.25	0/1197	0.41	0/1613
1	Ce	0.25	0/1197	0.41	0/1613
1	Cf	0.25	0/1197	0.41	0/1613
1	Ch	0.25	0/1197	0.41	0/1613
1	Ci	0.25	0/1197	0.41	0/1613
1	Cj	0.25	0/1197	0.41	0/1613
1	Ck	0.25	0/1197	0.41	0/1613
1	Cl	0.25	0/1197	0.41	0/1613
1	Cm	0.25	0/1197	0.41	0/1613
1	Cn	0.25	0/1197	0.41	0/1613
1	Co	0.25	0/1197	0.41	0/1613
1	Cp	0.25	0/1197	0.41	0/1613
1	Cq	0.25	0/1197	0.41	0/1613
1	Cr	0.25	0/1197	0.41	0/1613
1	Cs	0.25	0/1197	0.41	0/1613
1	Ct	0.25	0/1197	0.41	0/1613
1	Cu	0.25	0/1197	0.41	0/1613
1	Cv	0.25	0/1197	0.41	0/1613
1	Cw	0.25	0/1197	0.41	0/1613
1	Cx	0.25	0/1197	0.41	0/1613
1	Cy	0.25	0/1197	0.41	0/1613
1	Cz	0.25	0/1197	0.41	0/1613
1	Da	0.55	0/756	0.79	0/1036
1	Db	0.91	3/756 (0.4%)	1.26	5/1036 (0.5%)
1	Dc	0.59	0/756	0.76	0/1036
1	Dd	0.58	0/756	0.86	2/1036 (0.2%)
1	De	0.44	0/705	0.57	0/963
1	Df	0.90	3/697 (0.4%)	1.24	5/954 (0.5%)
1	Dg	0.37	0/646	0.50	0/881
1	Dh	0.37	0/646	0.50	0/881
1	Di	0.37	0/646	0.50	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Dj	0.37	0/646	0.50	0/881
1	Dk	0.38	0/646	0.50	0/881
1	DI	0.37	0/646	0.50	0/881
1	Dm	0.37	0/646	0.50	0/881
1	Dn	0.37	0/646	0.50	0/881
1	Do	0.44	0/697	0.59	1/954 (0.1%)
1	Dp	0.56	0/756	0.82	0/1036
1	Dq	0.62	0/756	0.99	4/1036 (0.4%)
1	Dr	0.76	1/756 (0.1%)	1.02	2/1036 (0.2%)
1	Ds	0.77	1/756 (0.1%)	1.15	4/1036 (0.4%)
1	Dt	0.56	0/756	0.80	0/1036
1	Du	0.60	0/756	0.94	5/1036 (0.5%)
1	Dv	0.59	0/756	0.80	0/1036
1	Dw	0.60	0/756	0.88	1/1036 (0.1%)
1	Ea	0.25	0/1197	0.41	0/1613
1	Eb	0.25	0/1197	0.41	0/1613
1	Ec	0.25	0/1197	0.41	0/1613
1	Ed	0.25	0/1197	0.41	0/1613
1	Ee	0.25	0/1197	0.41	0/1613
1	Ef	0.25	0/1197	0.41	0/1613
1	Eg	0.25	0/1197	0.41	0/1613
1	Fh	0.25	0/1197	0.41	0/1613
1	cg	0.25	0/1197	0.41	0/1613
All	All	0.37	8/57037 (0.0%)	0.56	29/77193 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Db	160	PRO	N-CA	17.48	1.69	1.47
1	Df	160	PRO	N-CA	17.46	1.69	1.47
1	Dr	171	SER	C-N	13.99	1.50	1.33
1	Ds	171	SER	C-N	13.59	1.50	1.33
1	Df	171	SER	C-N	7.39	1.51	1.33
1	Db	171	SER	C-N	7.01	1.50	1.33
1	Db	159	MET	C-N	5.12	1.45	1.33
1	Df	159	MET	C-N	5.10	1.45	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ds	171	SER	CA-C-N	17.94	138.28	120.52
1	Ds	171	SER	C-N-CA	17.94	138.28	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Db	159	MET	CA-C-N	17.44	141.63	119.84
1	Db	159	MET	C-N-CA	17.44	141.63	119.84
1	Df	159	MET	CA-C-N	17.10	141.21	119.84
1	Df	159	MET	C-N-CA	17.10	141.21	119.84
1	Dr	171	SER	CA-C-N	15.33	137.41	120.85
1	Dr	171	SER	C-N-CA	15.33	137.41	120.85
1	Db	171	SER	CA-C-N	14.40	137.84	119.84
1	Db	171	SER	C-N-CA	14.40	137.84	119.84
1	Df	171	SER	CA-C-N	13.21	136.35	119.84
1	Df	171	SER	C-N-CA	13.21	136.35	119.84
1	Dq	160	PRO	N-CA-CB	-11.98	90.67	103.25
1	Dd	160	PRO	N-CA-CB	-11.34	91.34	103.25
1	Df	160	PRO	CA-N-CD	-11.04	96.54	112.00
1	Db	160	PRO	CA-N-CD	-10.87	96.78	112.00
1	Dw	160	PRO	N-CA-CB	-9.52	93.25	103.25
1	Ds	160	PRO	N-CA-CB	-8.84	93.97	103.25
1	Dq	160	PRO	CB-CA-C	-8.44	97.64	111.56
1	Du	124	SER	CA-C-N	6.74	129.20	120.44
1	Du	124	SER	C-N-CA	6.74	129.20	120.44
1	Du	125	GLN	CA-C-N	6.59	129.41	120.44
1	Du	125	GLN	C-N-CA	6.59	129.41	120.44
1	Dq	160	PRO	N-CA-C	6.38	125.62	112.47
1	Du	160	PRO	N-CA-CB	-6.22	96.72	103.25
1	Ds	160	PRO	CA-N-CD	-5.42	104.41	112.00
1	Dq	161	LYS	CA-C-O	-5.33	116.80	120.47
1	Do	160	PRO	N-CA-CB	-5.07	97.93	103.25
1	Dd	160	PRO	CA-N-CD	-5.00	105.00	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ca	1185	0	1167	27	0
1	Cb	1185	0	1167	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Cc	1185	0	1167	29	0
1	Cd	1185	0	1167	30	0
1	Ce	1185	0	1167	27	0
1	Cf	1185	0	1167	30	0
1	Ch	1185	0	1167	27	0
1	Ci	1185	0	1167	24	0
1	Cj	1185	0	1167	24	0
1	Ck	1185	0	1167	28	0
1	Cl	1185	0	1167	30	0
1	Cm	1185	0	1167	35	0
1	Cn	1185	0	1167	34	0
1	Co	1185	0	1167	28	0
1	Cp	1185	0	1167	29	0
1	Cq	1185	0	1167	21	0
1	Cr	1185	0	1167	25	0
1	Cs	1185	0	1167	27	0
1	Ct	1185	0	1167	32	0
1	Cu	1185	0	1167	32	0
1	Cv	1185	0	1167	26	0
1	Cw	1185	0	1167	25	0
1	Cx	1185	0	1167	26	0
1	Cy	1185	0	1167	28	0
1	Cz	1185	0	1167	28	0
1	Da	746	0	689	22	0
1	Db	746	0	689	21	0
1	Dc	746	0	689	26	0
1	Dd	746	0	689	15	0
1	De	696	0	669	12	0
1	Df	687	0	664	23	0
1	Dg	637	0	644	10	0
1	Dh	637	0	644	11	0
1	Di	637	0	644	13	0
1	Dj	637	0	644	18	0
1	Dk	637	0	644	13	0
1	Dl	637	0	644	9	0
1	Dm	637	0	644	13	0
1	Dn	637	0	644	15	0
1	Do	687	0	664	14	0
1	Dp	746	0	689	16	0
1	Dq	746	0	689	26	0
1	Dr	746	0	689	15	0
1	Ds	746	0	689	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Dt	746	0	689	35	0
1	Du	746	0	689	21	0
1	Dv	746	0	689	30	0
1	Dw	746	0	689	23	0
1	Ea	1185	0	1167	32	0
1	Eb	1185	0	1167	22	0
1	Ec	1185	0	1167	28	0
1	Ed	1185	0	1167	29	0
1	Ee	1185	0	1167	26	0
1	Ef	1185	0	1167	24	0
1	Eg	1185	0	1167	23	0
1	Fh	1185	0	1167	31	0
1	cg	1185	0	1167	26	0
2	GA	55	0	14	4	0
2	GB	25	0	7	0	0
2	GC	55	0	14	2	0
2	GD	50	0	12	3	0
2	GE	60	0	15	4	0
3	GF	90	0	20	9	0
3	GG	90	0	20	1	0
3	GH	90	0	20	10	0
3	GI	75	0	17	7	0
3	GJ	90	0	20	4	0
3	GK	90	0	20	2	0
All	All	57178	0	55274	1135	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 11.

All (1135) 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:Db:160:PRO:N	1:Db:160:PRO:CA	1.69	1.41
1:Df:160:PRO:N	1:Df:160:PRO:CA	1.69	1.31
3:GH:8:UNK:CB	1:Ct:372:ILE:HG21	1.86	1.06
3:GH:15:UNK:CB	1:Cs:372:ILE:HG21	1.85	1.05
1:Db:124:SER:CB	1:Db:127:SER:HB3	1.90	1.01
1:Di:156:HIS:CE1	1:Dj:143:THR:HG21	1.96	1.01
1:Dv:133:GLN:HG3	1:Dv:159:MET:HE2	1.46	0.98
1:Dj:156:HIS:CE1	1:Dk:143:THR:HG21	2.00	0.96
3:GI:7:UNK:CB	1:Cn:372:ILE:HG21	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dt:159:MET:SD	1:Dt:159:MET:N	2.41	0.92
1:Ca:414:ASP:OD2	1:Fh:431:ASN:ND2	2.03	0.92
1:Df:172:PRO:HG3	1:Df:204:GLY:O	1.70	0.92
1:Di:156:HIS:NE2	1:Dj:143:THR:HG21	1.85	0.91
1:Cn:431:ASN:ND2	1:Co:414:ASP:OD2	2.05	0.90
1:Eg:431:ASN:ND2	1:Fh:414:ASP:OD2	2.04	0.90
3:GH:15:UNK:CB	1:Cs:372:ILE:HD13	2.03	0.88
1:Eb:431:ASN:ND2	1:Ed:414:ASP:OD2	2.06	0.88
1:Da:171:SER:HB2	1:Da:172:PRO:HD3	1.53	0.88
1:Cq:431:ASN:ND2	1:Cr:414:ASP:OD2	2.06	0.87
1:Ef:431:ASN:ND2	1:Eg:414:ASP:OD2	2.08	0.86
1:Cs:431:ASN:ND2	1:Ct:414:ASP:OD2	2.07	0.86
1:Cc:431:ASN:ND2	1:Cd:414:ASP:OD2	2.08	0.86
3:GF:16:UNK:CB	1:Ee:372:ILE:HG21	2.05	0.85
1:Cf:431:ASN:ND2	1:cg:414:ASP:OD2	2.09	0.84
1:Dt:159:MET:HE2	1:Dt:159:MET:O	1.77	0.84
1:Df:172:PRO:HG2	1:Df:205:LEU:HA	1.60	0.83
1:Cz:431:ASN:ND2	1:Ea:414:ASP:OD2	2.11	0.83
3:GF:17:UNK:O	1:Ed:374:HIS:CE1	2.31	0.83
1:Cm:431:ASN:ND2	1:Cn:414:ASP:OD2	2.12	0.82
1:Ck:431:ASN:ND2	1:Cl:414:ASP:OD2	2.12	0.82
1:Da:171:SER:HB2	1:Da:172:PRO:CD	2.09	0.82
3:GI:14:UNK:CB	1:Cm:372:ILE:HG21	2.09	0.82
1:Cw:431:ASN:ND2	1:Cx:414:ASP:OD2	2.12	0.82
1:Cu:431:ASN:ND2	1:Cv:414:ASP:OD2	2.12	0.82
1:Dj:156:HIS:NE2	1:Dk:143:THR:HG21	1.93	0.82
1:Cl:431:ASN:ND2	1:Cm:414:ASP:OD2	2.13	0.81
3:GF:17:UNK:CB	1:Ed:276:GLU:OE1	2.28	0.81
1:Ch:431:ASN:ND2	1:Ci:414:ASP:OD2	2.14	0.81
1:Cj:431:ASN:ND2	1:Ck:414:ASP:OD2	2.14	0.81
1:Ce:431:ASN:ND2	1:Cf:414:ASP:OD2	2.14	0.80
1:Cx:431:ASN:ND2	1:Cy:414:ASP:OD2	2.14	0.80
1:Ci:431:ASN:ND2	1:Cj:414:ASP:OD2	2.15	0.80
1:Ed:431:ASN:ND2	1:Ee:414:ASP:OD2	2.15	0.80
1:Dr:134:ARG:NH1	1:Ds:116:LEU:CB	2.44	0.80
1:Ea:431:ASN:ND2	1:Ec:414:ASP:OD2	2.15	0.80
1:Dd:125:GLN:O	1:Dd:125:GLN:NE2	2.15	0.79
3:GJ:2:UNK:CB	1:Ce:372:ILE:HD12	2.13	0.79
1:Cb:431:ASN:ND2	1:Cc:414:ASP:OD2	2.15	0.78
1:Cv:431:ASN:ND2	1:Cw:414:ASP:OD2	2.16	0.78
1:Dq:158:ALA:HB2	1:Dr:200:SER:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cd:431:ASN:ND2	1:Ce:414:ASP:OD2	2.17	0.77
1:Cs:389:VAL:HB	1:Cs:432:VAL:HG12	1.67	0.77
1:Cv:389:VAL:HB	1:Cv:432:VAL:HG12	1.67	0.77
1:Ea:389:VAL:HB	1:Ea:432:VAL:HG12	1.67	0.77
1:Cx:389:VAL:HB	1:Cx:432:VAL:HG12	1.67	0.77
1:Cp:389:VAL:HB	1:Cp:432:VAL:HG12	1.67	0.77
1:Cq:389:VAL:HB	1:Cq:432:VAL:HG12	1.67	0.77
1:Ed:389:VAL:HB	1:Ed:432:VAL:HG12	1.67	0.77
1:Cy:389:VAL:HB	1:Cy:432:VAL:HG12	1.67	0.76
2:GE:10:UNK:CB	1:Fh:365:ASN:CG	2.58	0.76
1:Cr:431:ASN:ND2	1:Cs:414:ASP:OD2	2.18	0.76
1:Ck:389:VAL:HB	1:Ck:432:VAL:HG12	1.67	0.76
1:Eg:389:VAL:HB	1:Eg:432:VAL:HG12	1.67	0.76
1:Eb:389:VAL:HB	1:Eb:432:VAL:HG12	1.67	0.76
1:Df:171:SER:HB2	1:Df:172:PRO:HD2	1.68	0.76
1:Ch:389:VAL:HB	1:Ch:432:VAL:HG12	1.67	0.76
1:Ct:389:VAL:HB	1:Ct:432:VAL:HG12	1.67	0.76
1:Ct:431:ASN:ND2	1:Cu:414:ASP:OD2	2.18	0.76
1:Cu:389:VAL:HB	1:Cu:432:VAL:HG12	1.67	0.76
1:Cm:389:VAL:HB	1:Cm:432:VAL:HG12	1.67	0.76
1:Ee:431:ASN:ND2	1:Ef:414:ASP:OD2	2.19	0.76
1:Ef:389:VAL:HB	1:Ef:432:VAL:HG12	1.67	0.76
1:Cb:389:VAL:HB	1:Cb:432:VAL:HG12	1.67	0.76
1:Ec:389:VAL:HB	1:Ec:432:VAL:HG12	1.67	0.76
1:Ce:389:VAL:HB	1:Ce:432:VAL:HG12	1.67	0.76
1:Co:431:ASN:ND2	1:Cp:414:ASP:OD2	2.19	0.76
1:Cj:389:VAL:HB	1:Cj:432:VAL:HG12	1.67	0.75
3:GI:7:UNK:CB	1:Cn:372:ILE:CG2	2.64	0.75
1:Cy:431:ASN:ND2	1:Cz:414:ASP:OD2	2.18	0.75
1:Cr:389:VAL:HB	1:Cr:432:VAL:HG12	1.67	0.75
1:Dd:124:SER:C	1:Dd:126:PHE:H	1.94	0.75
1:Ca:389:VAL:HB	1:Ca:432:VAL:HG12	1.67	0.75
1:Cd:389:VAL:HB	1:Cd:432:VAL:HG12	1.67	0.75
1:cg:389:VAL:HB	1:cg:432:VAL:HG12	1.67	0.75
1:cg:431:ASN:ND2	1:Ch:414:ASP:OD2	2.20	0.75
1:Dw:172:PRO:HG2	1:Dw:205:LEU:HA	1.69	0.75
1:Cw:389:VAL:HB	1:Cw:432:VAL:HG12	1.67	0.75
1:Co:389:VAL:HB	1:Co:432:VAL:HG12	1.67	0.75
1:Ee:389:VAL:HB	1:Ee:432:VAL:HG12	1.67	0.75
2:GE:11:UNK:O	2:GE:12:UNK:C	2.35	0.74
1:Cl:389:VAL:HB	1:Cl:432:VAL:HG12	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ci:389:VAL:HB	1:Ci:432:VAL:HG12	1.67	0.74
1:Fh:389:VAL:HB	1:Fh:432:VAL:HG12	1.67	0.74
1:Cf:389:VAL:HB	1:Cf:432:VAL:HG12	1.67	0.74
1:Dq:160:PRO:HD3	1:Dq:172:PRO:HB3	1.70	0.74
1:Ds:126:PHE:CE2	1:Ds:130:VAL:HG21	2.23	0.74
1:Cc:389:VAL:HB	1:Cc:432:VAL:HG12	1.67	0.74
1:Cp:431:ASN:ND2	1:Cq:414:ASP:OD2	2.20	0.74
2:GE:5:UNK:O	1:Fh:295:SER:OG	2.05	0.73
1:Dt:171:SER:HB3	1:Dt:172:PRO:HD3	1.69	0.73
2:GA:6:UNK:CB	1:Ea:365:ASN:ND2	2.52	0.73
1:Dv:160:PRO:HD3	1:Dv:172:PRO:HB3	1.70	0.72
3:GK:15:UNK:CB	1:Ch:278:THR:HG21	2.19	0.72
1:Du:158:ALA:HB2	1:Dv:200:SER:O	1.90	0.71
1:Dc:124:SER:C	1:Dc:126:PHE:H	1.96	0.71
3:GJ:3:UNK:CB	1:Cd:374:HIS:CE1	2.74	0.70
3:GF:17:UNK:O	1:Ed:374:HIS:HE1	1.74	0.69
1:Dq:133:GLN:HB2	1:Dq:159:MET:CE	2.23	0.69
3:GH:15:UNK:CB	1:Cs:372:ILE:CD1	2.71	0.69
1:Dt:126:PHE:CE2	1:Dt:130:VAL:HG21	2.27	0.69
1:Dt:171:SER:HB3	1:Dt:172:PRO:HD2	1.74	0.68
1:Dv:133:GLN:HB2	1:Dv:159:MET:HE1	1.77	0.67
1:Ca:431:ASN:ND2	1:Cb:414:ASP:OD2	2.27	0.67
1:Dg:160:PRO:HG3	1:Dh:203:ALA:HB1	1.75	0.67
1:Dp:159:MET:HA	1:Dp:172:PRO:HB3	1.76	0.66
1:Dw:126:PHE:O	1:Dw:128:GLU:N	2.28	0.66
1:Di:156:HIS:CE1	1:Dj:143:THR:CG2	2.78	0.65
1:Co:242:GLU:OE1	1:Cp:248:ARG:NH2	2.29	0.65
1:Dt:171:SER:CB	1:Dt:172:PRO:CD	2.73	0.65
2:GE:10:UNK:CB	1:Fh:365:ASN:OD1	2.45	0.64
1:Dw:126:PHE:C	1:Dw:128:GLU:H	2.04	0.64
3:GH:1:UNK:CB	1:Cu:372:ILE:HG21	2.28	0.63
1:Eg:242:GLU:OE1	1:Fh:248:ARG:NH2	2.31	0.63
1:Dc:124:SER:O	1:Dc:126:PHE:N	2.31	0.63
1:Dk:211:THR:HA	1:Dk:221:THR:HG21	1.81	0.63
1:Dj:156:HIS:HE2	1:Dk:143:THR:HG21	1.61	0.63
1:Co:275:LYS:HG2	1:Cp:375:THR:HG23	1.80	0.63
1:Df:211:THR:HA	1:Df:221:THR:HG21	1.81	0.62
1:Dh:211:THR:HA	1:Dh:221:THR:HG21	1.81	0.62
3:GH:8:UNK:CB	1:Ct:372:ILE:HD13	2.29	0.62
1:Du:211:THR:HA	1:Du:221:THR:HG21	1.81	0.62
1:Db:211:THR:HA	1:Db:221:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dj:211:THR:HA	1:Dj:221:THR:HG21	1.81	0.62
1:Dd:124:SER:C	1:Dd:126:PHE:N	2.55	0.62
1:Di:211:THR:HA	1:Di:221:THR:HG21	1.81	0.62
1:Dg:211:THR:HA	1:Dg:221:THR:HG21	1.81	0.62
1:Dl:211:THR:HA	1:Dl:221:THR:HG21	1.81	0.62
1:Dm:211:THR:HA	1:Dm:221:THR:HG21	1.81	0.62
1:Dq:211:THR:HA	1:Dq:221:THR:HG21	1.81	0.62
1:Dw:211:THR:HA	1:Dw:221:THR:HG21	1.81	0.62
1:Dj:145:GLU:HG2	1:Dj:152:SER:HA	1.82	0.62
1:Dk:145:GLU:HG2	1:Dk:152:SER:HA	1.82	0.62
1:Dm:145:GLU:HG2	1:Dm:152:SER:HA	1.82	0.62
1:Dh:145:GLU:HG2	1:Dh:152:SER:HA	1.82	0.61
1:Dn:211:THR:HA	1:Dn:221:THR:HG21	1.81	0.61
1:Dc:211:THR:HA	1:Dc:221:THR:HG21	1.81	0.61
1:Di:145:GLU:HG2	1:Di:152:SER:HA	1.82	0.61
1:Dp:211:THR:HA	1:Dp:221:THR:HG21	1.81	0.61
1:Dv:211:THR:HA	1:Dv:221:THR:HG21	1.81	0.61
1:Da:211:THR:HA	1:Da:221:THR:HG21	1.81	0.61
1:Dl:145:GLU:HG2	1:Dl:152:SER:HA	1.82	0.61
3:Gi:14:UNK:CB	1:cm:372:ILE:CG2	2.78	0.61
1:Df:172:PRO:CG	1:Df:205:LEU:HA	2.29	0.61
1:Ds:211:THR:HA	1:Ds:221:THR:HG21	1.81	0.61
1:Dg:145:GLU:HG2	1:Dg:152:SER:HA	1.82	0.61
1:Do:211:THR:HA	1:Do:221:THR:HG21	1.81	0.61
1:Dq:133:GLN:HB2	1:Dq:159:MET:HE1	1.82	0.61
1:Dr:211:THR:HA	1:Dr:221:THR:HG21	1.81	0.61
1:Dd:211:THR:HA	1:Dd:221:THR:HG21	1.81	0.61
1:Dn:145:GLU:HG2	1:Dn:152:SER:HA	1.82	0.61
1:Dt:211:THR:HA	1:Dt:221:THR:HG21	1.81	0.61
3:GH:16:UNK:CB	1:Cr:276:GLU:OE1	2.48	0.61
1:Dr:145:GLU:HG2	1:Dr:152:SER:HA	1.82	0.61
1:Da:145:GLU:HG2	1:Da:152:SER:HA	1.82	0.61
1:Do:145:GLU:HG2	1:Do:152:SER:HA	1.82	0.61
1:Dq:172:PRO:O	1:Dq:205:LEU:HD13	2.01	0.61
1:Di:214:ASP:OD1	1:Di:214:ASP:N	2.34	0.60
1:Dp:145:GLU:HG2	1:Dp:152:SER:HA	1.82	0.60
1:Dc:145:GLU:HG2	1:Dc:152:SER:HA	1.82	0.60
1:Dt:145:GLU:HG2	1:Dt:152:SER:HA	1.82	0.60
1:Dv:145:GLU:HG2	1:Dv:152:SER:HA	1.82	0.60
1:Co:233:ALA:HA	1:Co:236:LYS:HD3	1.83	0.60
1:De:145:GLU:HG2	1:De:152:SER:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dl:214:ASP:OD1	1:Dl:214:ASP:N	2.35	0.60
1:Df:214:ASP:N	1:Df:214:ASP:OD1	2.35	0.60
1:Du:145:GLU:HG2	1:Du:152:SER:HA	1.82	0.60
1:Ca:275:LYS:HG2	1:Cb:375:THR:HG23	1.83	0.60
1:Cq:233:ALA:HA	1:Cq:236:LYS:HD3	1.83	0.60
1:Cm:233:ALA:HA	1:Cm:236:LYS:HD3	1.83	0.60
1:Cs:233:ALA:HA	1:Cs:236:LYS:HD3	1.83	0.60
1:Ct:233:ALA:HA	1:Ct:236:LYS:HD3	1.83	0.60
1:Dq:145:GLU:HG2	1:Dq:152:SER:HA	1.82	0.60
1:Dv:133:GLN:HB2	1:Dv:159:MET:CE	2.30	0.60
1:Ci:261:ASN:HB3	1:Ci:392:ASN:HB3	1.84	0.60
1:Cm:232:ASP:OD1	1:Cm:232:ASP:N	2.34	0.60
1:Cn:232:ASP:N	1:Cn:232:ASP:OD1	2.34	0.60
1:Co:232:ASP:OD1	1:Co:232:ASP:N	2.34	0.60
1:Cp:233:ALA:HA	1:Cp:236:LYS:HD3	1.83	0.60
1:Cr:233:ALA:HA	1:Cr:236:LYS:HD3	1.83	0.60
1:Df:145:GLU:HG2	1:Df:152:SER:HA	1.82	0.60
1:Dg:214:ASP:N	1:Dg:214:ASP:OD1	2.35	0.60
1:Ds:145:GLU:HG2	1:Ds:152:SER:HA	1.82	0.60
1:Cf:261:ASN:HB3	1:Cf:392:ASN:HB3	1.84	0.60
1:Cj:232:ASP:N	1:Cj:232:ASP:OD1	2.34	0.60
1:Ck:232:ASP:OD1	1:Ck:232:ASP:N	2.34	0.60
1:Cl:232:ASP:OD1	1:Cl:232:ASP:N	2.34	0.60
1:Cl:233:ALA:HA	1:Cl:236:LYS:HD3	1.83	0.60
1:Cl:261:ASN:HB3	1:Cl:392:ASN:HB3	1.84	0.60
1:Co:261:ASN:HB3	1:Co:392:ASN:HB3	1.84	0.60
1:Db:145:GLU:HG2	1:Db:152:SER:HA	1.82	0.60
1:Dh:214:ASP:OD1	1:Dh:214:ASP:N	2.34	0.60
1:Dm:214:ASP:OD1	1:Dm:214:ASP:N	2.35	0.60
1:Dw:145:GLU:HG2	1:Dw:152:SER:HA	1.83	0.60
1:Cj:233:ALA:HA	1:Cj:236:LYS:HD3	1.83	0.60
1:Ck:233:ALA:HA	1:Ck:236:LYS:HD3	1.84	0.60
1:Cn:233:ALA:HA	1:Cn:236:LYS:HD3	1.83	0.60
1:Cp:232:ASP:OD1	1:Cp:232:ASP:N	2.34	0.60
1:Cr:261:ASN:HB3	1:Cr:392:ASN:HB3	1.84	0.60
1:Cv:233:ALA:HA	1:Cv:236:LYS:HD3	1.83	0.60
1:Cc:261:ASN:HB3	1:Cc:392:ASN:HB3	1.84	0.59
1:Ch:232:ASP:OD1	1:Ch:232:ASP:N	2.34	0.59
1:Cq:232:ASP:OD1	1:Cq:232:ASP:N	2.34	0.59
1:Cr:232:ASP:N	1:Cr:232:ASP:OD1	2.34	0.59
1:Cu:233:ALA:HA	1:Cu:236:LYS:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dc:172:PRO:HG2	1:Dc:205:LEU:HA	1.84	0.59
1:cg:232:ASP:OD1	1:cg:232:ASP:N	2.34	0.59
1:Ca:242:GLU:OE1	1:Cb:248:ARG:NH2	2.35	0.59
1:Ch:233:ALA:HA	1:Ch:236:LYS:HD3	1.84	0.59
1:Ci:233:ALA:HA	1:Ci:236:LYS:HD3	1.84	0.59
1:Cs:232:ASP:OD1	1:Cs:232:ASP:N	2.34	0.59
1:Cx:233:ALA:HA	1:Cx:236:LYS:HD3	1.83	0.59
1:Dv:133:GLN:CG	1:Dv:159:MET:HE2	2.26	0.59
1:Cf:232:ASP:N	1:Cf:232:ASP:OD1	2.34	0.59
1:cg:261:ASN:HB3	1:cg:392:ASN:HB3	1.84	0.59
1:Cm:261:ASN:HB3	1:Cm:392:ASN:HB3	1.84	0.59
1:Cu:261:ASN:HB3	1:Cu:392:ASN:HB3	1.84	0.59
1:Dc:214:ASP:N	1:Dc:214:ASP:OD1	2.35	0.59
1:Dq:214:ASP:OD1	1:Dq:214:ASP:N	2.35	0.59
1:Ca:233:ALA:HA	1:Ca:236:LYS:HD3	1.84	0.59
1:Cf:233:ALA:HA	1:Cf:236:LYS:HD3	1.83	0.59
1:Ch:261:ASN:HB3	1:Ch:392:ASN:HB3	1.84	0.59
1:Cj:261:ASN:HB3	1:Cj:392:ASN:HB3	1.84	0.59
1:Cn:261:ASN:HB3	1:Cn:392:ASN:HB3	1.84	0.59
1:Cp:358:THR:HG22	1:Cp:359:GLN:H	1.68	0.59
1:Cw:233:ALA:HA	1:Cw:236:LYS:HD3	1.84	0.59
1:Cx:358:THR:HG22	1:Cx:359:GLN:H	1.68	0.59
1:Ef:233:ALA:HA	1:Ef:236:LYS:HD3	1.83	0.59
1:Cd:261:ASN:HB3	1:Cd:392:ASN:HB3	1.84	0.59
1:Ck:261:ASN:HB3	1:Ck:392:ASN:HB3	1.84	0.59
1:Ck:358:THR:HG22	1:Ck:359:GLN:H	1.68	0.59
1:Cm:358:THR:HG22	1:Cm:359:GLN:H	1.68	0.59
1:Cp:261:ASN:HB3	1:Cp:392:ASN:HB3	1.84	0.59
1:Ct:232:ASP:OD1	1:Ct:232:ASP:N	2.34	0.59
1:Cw:358:THR:HG22	1:Cw:359:GLN:H	1.68	0.59
1:Cz:233:ALA:HA	1:Cz:236:LYS:HD3	1.83	0.59
1:Eb:233:ALA:HA	1:Eb:236:LYS:HD3	1.83	0.59
1:Eb:358:THR:HG22	1:Eb:359:GLN:H	1.68	0.59
1:Dn:214:ASP:OD1	1:Dn:214:ASP:N	2.35	0.59
1:Ce:232:ASP:N	1:Ce:232:ASP:OD1	2.34	0.59
1:cg:233:ALA:HA	1:cg:236:LYS:HD3	1.83	0.59
1:Cl:358:THR:HG22	1:Cl:359:GLN:H	1.68	0.59
1:Ct:358:THR:HG22	1:Ct:359:GLN:H	1.68	0.59
1:Dp:124:SER:CB	1:Dp:127:SER:HB3	2.33	0.59
1:Dr:214:ASP:OD1	1:Dr:214:ASP:N	2.34	0.59
1:Du:214:ASP:OD1	1:Du:214:ASP:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cq:358:THR:HG22	1:Cq:359:GLN:H	1.68	0.59
1:Cr:358:THR:HG22	1:Cr:359:GLN:H	1.68	0.59
1:Ct:261:ASN:HB3	1:Ct:392:ASN:HB3	1.84	0.59
1:Fh:261:ASN:HB3	1:Fh:392:ASN:HB3	1.84	0.59
1:Do:214:ASP:N	1:Do:214:ASP:OD1	2.34	0.59
2:GD:9:UNK:CA	1:Cf:363:THR:HG21	2.33	0.59
1:Ca:261:ASN:HB3	1:Ca:392:ASN:HB3	1.84	0.59
1:Cd:232:ASP:OD1	1:Cd:232:ASP:N	2.34	0.59
1:Cf:358:THR:HG22	1:Cf:359:GLN:H	1.68	0.59
1:Cs:358:THR:HG22	1:Cs:359:GLN:H	1.68	0.59
1:Cx:261:ASN:HB3	1:Cx:392:ASN:HB3	1.84	0.59
1:Cy:233:ALA:HA	1:Cy:236:LYS:HD3	1.83	0.59
1:Ec:358:THR:HG22	1:Ec:359:GLN:H	1.68	0.59
1:Ef:261:ASN:HB3	1:Ef:392:ASN:HB3	1.84	0.59
1:Dd:214:ASP:OD1	1:Dd:214:ASP:N	2.35	0.59
1:Dp:171:SER:HB2	1:Dp:172:PRO:HD2	1.85	0.59
1:Dv:158:ALA:HB2	1:Dw:200:SER:O	2.02	0.59
1:Dw:214:ASP:N	1:Dw:214:ASP:OD1	2.35	0.59
1:Cd:233:ALA:HA	1:Cd:236:LYS:HD3	1.84	0.59
1:Ce:358:THR:HG22	1:Ce:359:GLN:H	1.68	0.59
1:Ci:358:THR:HG22	1:Ci:359:GLN:H	1.68	0.59
1:Cv:232:ASP:N	1:Cv:232:ASP:OD1	2.34	0.59
1:Cw:261:ASN:HB3	1:Cw:392:ASN:HB3	1.84	0.59
1:Cs:261:ASN:HB3	1:Cs:392:ASN:HB3	1.84	0.58
1:Cv:358:THR:HG22	1:Cv:359:GLN:H	1.68	0.58
1:Cz:358:THR:HG22	1:Cz:359:GLN:H	1.68	0.58
1:Eb:261:ASN:HB3	1:Eb:392:ASN:HB3	1.84	0.58
1:Db:171:SER:HB3	1:Db:172:PRO:HD2	1.84	0.58
1:De:214:ASP:OD1	1:De:214:ASP:N	2.34	0.58
3:GF:9:UNK:CB	1:Ef:372:ILE:HG21	2.33	0.58
1:Cc:232:ASP:OD1	1:Cc:232:ASP:N	2.34	0.58
1:Ce:233:ALA:HA	1:Ce:236:LYS:HD3	1.83	0.58
1:Cz:261:ASN:HB3	1:Cz:392:ASN:HB3	1.84	0.58
1:Ea:233:ALA:HA	1:Ea:236:LYS:HD3	1.83	0.58
1:Ea:358:THR:HG22	1:Ea:359:GLN:H	1.68	0.58
1:Ec:233:ALA:HA	1:Ec:236:LYS:HD3	1.83	0.58
1:Ed:358:THR:HG22	1:Ed:359:GLN:H	1.68	0.58
1:Fh:358:THR:HG22	1:Fh:359:GLN:H	1.68	0.58
1:Dd:124:SER:O	1:Dd:126:PHE:N	2.36	0.58
1:cg:358:THR:HG22	1:cg:359:GLN:H	1.68	0.58
1:Cj:358:THR:HG22	1:Cj:359:GLN:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cw:232:ASP:OD1	1:Cw:232:ASP:N	2.34	0.58
1:Ed:233:ALA:HA	1:Ed:236:LYS:HD3	1.83	0.58
1:Eg:233:ALA:HA	1:Eg:236:LYS:HD3	1.83	0.58
1:Fh:233:ALA:HA	1:Fh:236:LYS:HD3	1.83	0.58
1:Cb:232:ASP:N	1:Cb:232:ASP:OD1	2.34	0.58
1:Cb:233:ALA:HA	1:Cb:236:LYS:HD3	1.83	0.58
1:Cs:242:GLU:OE1	1:Ct:248:ARG:NH2	2.37	0.58
1:Cy:358:THR:HG22	1:Cy:359:GLN:H	1.68	0.58
1:Dt:214:ASP:OD1	1:Dt:214:ASP:N	2.35	0.58
1:Dv:214:ASP:OD1	1:Dv:214:ASP:N	2.35	0.58
2:GC:4:UNK:O	1:Cl:365:ASN:OD1	2.20	0.58
1:Ca:232:ASP:N	1:Ca:232:ASP:OD1	2.34	0.58
1:Ca:358:THR:HG22	1:Ca:359:GLN:H	1.68	0.58
1:Ee:233:ALA:HA	1:Ee:236:LYS:HD3	1.83	0.58
1:Ee:261:ASN:HB3	1:Ee:392:ASN:HB3	1.84	0.58
1:Dp:214:ASP:OD1	1:Dp:214:ASP:N	2.34	0.58
3:GK:8:UNK:CB	1:Ci:278:THR:HG21	2.33	0.58
1:Cb:261:ASN:HB3	1:Cb:392:ASN:HB3	1.84	0.58
1:Cc:233:ALA:HA	1:Cc:236:LYS:HD3	1.83	0.58
1:Cx:232:ASP:OD1	1:Cx:232:ASP:N	2.34	0.58
1:Eg:358:THR:HG22	1:Eg:359:GLN:H	1.68	0.58
1:Cy:232:ASP:OD1	1:Cy:232:ASP:N	2.34	0.58
1:Da:214:ASP:OD1	1:Da:214:ASP:N	2.34	0.58
1:Cc:358:THR:HG22	1:Cc:359:GLN:H	1.68	0.58
1:Ea:261:ASN:HB3	1:Ea:392:ASN:HB3	1.84	0.58
1:Dn:156:HIS:NE2	1:Do:143:THR:HG21	2.19	0.58
1:Cb:358:THR:HG22	1:Cb:359:GLN:H	1.68	0.58
1:Cd:358:THR:HG22	1:Cd:359:GLN:H	1.68	0.58
1:Cn:358:THR:HG22	1:Cn:359:GLN:H	1.68	0.58
1:Cu:358:THR:HG22	1:Cu:359:GLN:H	1.68	0.58
1:Cz:232:ASP:N	1:Cz:232:ASP:OD1	2.34	0.58
1:Cv:261:ASN:HB3	1:Cv:392:ASN:HB3	1.84	0.58
1:Df:171:SER:HB2	1:Df:172:PRO:CD	2.34	0.57
1:Df:172:PRO:CG	1:Df:204:GLY:O	2.50	0.57
1:Ea:232:ASP:OD1	1:Ea:232:ASP:N	2.34	0.57
1:Ec:261:ASN:HB3	1:Ec:392:ASN:HB3	1.84	0.57
1:Ef:232:ASP:N	1:Ef:232:ASP:OD1	2.34	0.57
1:Ch:358:THR:HG22	1:Ch:359:GLN:H	1.68	0.57
1:Dn:141:ALA:HB2	1:Dn:155:VAL:HG12	1.87	0.57
1:Ec:232:ASP:N	1:Ec:232:ASP:OD1	2.34	0.57
1:Ed:232:ASP:OD1	1:Ed:232:ASP:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ed:261:ASN:HB3	1:Ed:392:ASN:HB3	1.84	0.57
1:Ee:232:ASP:OD1	1:Ee:232:ASP:N	2.34	0.57
1:Ee:358:THR:HG22	1:Ee:359:GLN:H	1.68	0.57
1:Dp:141:ALA:HB2	1:Dp:155:VAL:HG12	1.87	0.57
1:Ds:214:ASP:N	1:Ds:214:ASP:OD1	2.34	0.57
1:Eb:232:ASP:N	1:Eb:232:ASP:OD1	2.34	0.57
1:Da:141:ALA:HB2	1:Da:155:VAL:HG12	1.87	0.57
1:Dd:141:ALA:HB2	1:Dd:155:VAL:HG12	1.87	0.57
1:Du:156:HIS:NE2	1:Dv:143:THR:HG21	2.20	0.57
1:Dv:125:GLN:O	1:Dv:128:GLU:CB	2.53	0.57
1:Cy:261:ASN:HB3	1:Cy:392:ASN:HB3	1.84	0.57
1:Dj:214:ASP:N	1:Dj:214:ASP:OD1	2.34	0.57
1:Dv:141:ALA:HB2	1:Dv:155:VAL:HG12	1.87	0.57
1:Eg:261:ASN:HB3	1:Eg:392:ASN:HB3	1.84	0.57
1:De:141:ALA:HB2	1:De:155:VAL:HG12	1.87	0.57
1:Dr:141:ALA:HB2	1:Dr:155:VAL:HG12	1.87	0.57
1:Dt:141:ALA:HB2	1:Dt:155:VAL:HG12	1.87	0.57
1:Dc:141:ALA:HB2	1:Dc:155:VAL:HG12	1.87	0.57
1:Df:141:ALA:HB2	1:Df:155:VAL:HG12	1.87	0.57
1:Ef:358:THR:HG22	1:Ef:359:GLN:H	1.68	0.57
1:Df:172:PRO:HG3	1:Df:204:GLY:C	2.29	0.56
1:Dh:158:ALA:O	1:Dh:160:PRO:HD3	2.05	0.56
1:Di:158:ALA:O	1:Di:160:PRO:HD3	2.05	0.56
3:GI:4:UNK:CB	1:Cn:374:HIS:CE1	2.88	0.56
1:Dc:208:GLY:C	1:Dc:209:ASN:HD22	2.13	0.56
1:Dl:158:ALA:O	1:Dl:160:PRO:HD3	2.05	0.56
1:Dm:158:ALA:O	1:Dm:160:PRO:HD3	2.05	0.56
1:Ds:126:PHE:C	1:Ds:128:GLU:H	2.13	0.56
1:Cq:242:GLU:OE1	1:Cr:248:ARG:NH2	2.39	0.56
1:Dg:158:ALA:O	1:Dg:160:PRO:HD3	2.05	0.56
1:Dm:141:ALA:HB2	1:Dm:155:VAL:HG12	1.87	0.56
1:Ds:126:PHE:O	1:Ds:128:GLU:N	2.38	0.56
1:Dw:126:PHE:C	1:Dw:128:GLU:N	2.61	0.56
1:Dw:141:ALA:HB2	1:Dw:155:VAL:HG12	1.87	0.56
1:Db:141:ALA:HB2	1:Db:155:VAL:HG12	1.87	0.56
1:Dn:158:ALA:O	1:Dn:160:PRO:HD3	2.05	0.56
1:Du:171:SER:HB3	1:Du:172:PRO:HD2	1.87	0.56
1:Dj:158:ALA:O	1:Dj:160:PRO:HD3	2.05	0.56
1:Dk:214:ASP:N	1:Dk:214:ASP:OD1	2.35	0.56
1:Do:141:ALA:HB2	1:Do:155:VAL:HG12	1.87	0.56
1:Di:141:ALA:HB2	1:Di:155:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dl:141:ALA:HB2	1:Dl:155:VAL:HG12	1.87	0.56
1:Dp:126:PHE:CE2	1:Dp:130:VAL:HG21	2.41	0.56
1:Dq:171:SER:HB2	1:Dq:172:PRO:HD2	1.88	0.56
1:Cy:413:GLU:OE2	1:Cy:417:ARG:NH2	2.39	0.56
1:Cz:413:GLU:OE2	1:Cz:417:ARG:NH2	2.39	0.56
1:Dc:124:SER:C	1:Dc:126:PHE:N	2.58	0.56
1:Dq:141:ALA:HB2	1:Dq:155:VAL:HG12	1.87	0.56
2:GD:9:UNK:CB	1:Cf:363:THR:HG21	2.36	0.56
1:Cx:413:GLU:OE2	1:Cx:417:ARG:NH2	2.39	0.56
1:Ea:413:GLU:OE2	1:Ea:417:ARG:NH2	2.39	0.56
1:Eb:413:GLU:OE2	1:Eb:417:ARG:NH2	2.39	0.56
1:Ec:413:GLU:OE2	1:Ec:417:ARG:NH2	2.39	0.56
1:Ed:413:GLU:OE2	1:Ed:417:ARG:NH2	2.39	0.56
1:Ee:413:GLU:OE2	1:Ee:417:ARG:NH2	2.39	0.56
1:Ef:413:GLU:OE2	1:Ef:417:ARG:NH2	2.39	0.56
1:De:158:ALA:O	1:De:160:PRO:HD3	2.05	0.55
1:Dg:141:ALA:HB2	1:Dg:155:VAL:HG12	1.87	0.55
1:Ds:141:ALA:HB2	1:Ds:155:VAL:HG12	1.87	0.55
1:Du:141:ALA:HB2	1:Du:155:VAL:HG12	1.87	0.55
1:Du:172:PRO:HG2	1:Du:205:LEU:HA	1.87	0.55
1:Dv:125:GLN:O	1:Dv:128:GLU:HB3	2.06	0.55
1:Ca:413:GLU:OE2	1:Ca:417:ARG:NH2	2.39	0.55
1:Cb:413:GLU:OE2	1:Cb:417:ARG:NH2	2.39	0.55
1:Eg:413:GLU:OE2	1:Eg:417:ARG:NH2	2.39	0.55
1:Dt:172:PRO:HD3	1:Dt:204:GLY:O	2.06	0.55
1:Cc:242:GLU:OE1	1:Cd:248:ARG:NH2	2.40	0.55
1:Cc:413:GLU:OE2	1:Cc:417:ARG:NH2	2.39	0.55
1:Cw:413:GLU:OE2	1:Cw:417:ARG:NH2	2.39	0.55
1:Fh:413:GLU:OE2	1:Fh:417:ARG:NH2	2.39	0.55
1:Cd:413:GLU:OE2	1:Cd:417:ARG:NH2	2.39	0.55
1:Cu:413:GLU:OE2	1:Cu:417:ARG:NH2	2.39	0.55
1:Cv:413:GLU:OE2	1:Cv:417:ARG:NH2	2.39	0.55
1:Eb:242:GLU:OE1	1:Ed:248:ARG:NH2	2.39	0.55
1:Dj:141:ALA:HB2	1:Dj:155:VAL:HG12	1.87	0.55
1:Dv:156:HIS:CE1	1:Dw:143:THR:HG21	2.41	0.55
1:Cf:242:GLU:OE1	1:cg:248:ARG:NH2	2.39	0.55
1:Eg:275:LYS:HG2	1:Fh:375:THR:HG23	1.87	0.55
1:Ct:413:GLU:OE2	1:Ct:417:ARG:NH2	2.39	0.55
1:Dh:141:ALA:HB2	1:Dh:155:VAL:HG12	1.87	0.55
1:Dq:160:PRO:HG3	1:Dq:172:PRO:HA	1.89	0.55
3:GF:16:UNK:CB	1:Ee:372:ILE:HD13	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cd:289:SER:OG	1:Cd:290:LYS:NZ	2.40	0.55
1:Ce:413:GLU:OE2	1:Ce:417:ARG:NH2	2.39	0.55
1:Cr:413:GLU:OE2	1:Cr:417:ARG:NH2	2.39	0.55
1:Cu:242:GLU:OE1	1:Cv:248:ARG:NH2	2.39	0.55
1:Ed:289:SER:OG	1:Ed:290:LYS:NZ	2.40	0.55
1:Eg:289:SER:OG	1:Eg:290:LYS:NZ	2.40	0.55
1:Dj:133:GLN:NE2	1:Dj:137:GLU:OE2	2.40	0.55
1:Dk:141:ALA:HB2	1:Dk:155:VAL:HG12	1.87	0.55
1:Ca:289:SER:OG	1:Ca:290:LYS:NZ	2.40	0.55
1:Cb:289:SER:OG	1:Cb:290:LYS:NZ	2.40	0.55
1:Cf:413:GLU:OE2	1:Cf:417:ARG:NH2	2.39	0.55
1:cg:289:SER:OG	1:cg:290:LYS:NZ	2.40	0.55
1:Co:413:GLU:OE2	1:Co:417:ARG:NH2	2.39	0.55
1:Da:156:HIS:NE2	1:Db:143:THR:HG21	2.21	0.54
1:Dk:133:GLN:NE2	1:Dk:137:GLU:OE2	2.41	0.54
1:Cm:413:GLU:OE2	1:Cm:417:ARG:NH2	2.39	0.54
1:Cq:413:GLU:OE2	1:Cq:417:ARG:NH2	2.39	0.54
1:Dg:133:GLN:NE2	1:Dg:137:GLU:OE2	2.40	0.54
1:Dl:133:GLN:NE2	1:Dl:137:GLU:OE2	2.41	0.54
1:Ds:160:PRO:HB3	1:Dt:203:ALA:HB1	1.89	0.54
1:Dw:172:PRO:CG	1:Dw:205:LEU:HA	2.35	0.54
1:cg:413:GLU:OE2	1:cg:417:ARG:NH2	2.39	0.54
1:Ch:413:GLU:OE2	1:Ch:417:ARG:NH2	2.39	0.54
1:Cl:413:GLU:OE2	1:Cl:417:ARG:NH2	2.39	0.54
1:Cn:413:GLU:OE2	1:Cn:417:ARG:NH2	2.39	0.54
1:Cp:413:GLU:OE2	1:Cp:417:ARG:NH2	2.39	0.54
1:Df:133:GLN:NE2	1:Df:137:GLU:OE2	2.40	0.54
3:GJ:3:UNK:CB	1:Cd:374:HIS:HE1	2.20	0.54
1:Ci:413:GLU:OE2	1:Ci:417:ARG:NH2	2.39	0.54
1:Cj:413:GLU:OE2	1:Cj:417:ARG:NH2	2.39	0.54
1:Ck:413:GLU:OE2	1:Ck:417:ARG:NH2	2.39	0.54
1:Cp:289:SER:OG	1:Cp:290:LYS:NZ	2.40	0.54
1:Cr:289:SER:OG	1:Cr:290:LYS:NZ	2.40	0.54
1:Ec:266:VAL:HG12	1:Ec:387:VAL:HG22	1.89	0.54
1:Db:133:GLN:NE2	1:Db:137:GLU:OE2	2.40	0.54
1:Di:133:GLN:NE2	1:Di:137:GLU:OE2	2.41	0.54
1:Cf:289:SER:OG	1:Cf:290:LYS:NZ	2.40	0.54
1:Ci:289:SER:OG	1:Ci:290:LYS:NZ	2.40	0.54
1:Cj:289:SER:OG	1:Cj:290:LYS:NZ	2.40	0.54
1:Ck:266:VAL:HG12	1:Ck:387:VAL:HG22	1.89	0.54
1:Cn:289:SER:OG	1:Cn:290:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ct:289:SER:OG	1:Ct:290:LYS:NZ	2.40	0.54
1:Cz:242:GLU:OE1	1:Ea:248:ARG:NH2	2.40	0.54
1:Cs:289:SER:OG	1:Cs:290:LYS:NZ	2.40	0.54
1:Cu:289:SER:OG	1:Cu:290:LYS:NZ	2.40	0.54
1:Cv:289:SER:OG	1:Cv:290:LYS:NZ	2.40	0.54
1:Cw:266:VAL:HG12	1:Cw:387:VAL:HG22	1.89	0.54
1:Ea:289:SER:OG	1:Ea:290:LYS:NZ	2.40	0.54
1:Ec:289:SER:OG	1:Ec:290:LYS:NZ	2.40	0.54
1:Ee:289:SER:OG	1:Ee:290:LYS:NZ	2.40	0.54
1:Dm:133:GLN:NE2	1:Dm:137:GLU:OE2	2.40	0.54
1:Ca:249:ILE:HD11	1:Ca:420:MET:HG3	1.90	0.54
1:Cd:249:ILE:HD11	1:Cd:420:MET:HG3	1.90	0.54
1:Cl:289:SER:OG	1:Cl:290:LYS:NZ	2.40	0.54
1:Cn:266:VAL:HG12	1:Cn:387:VAL:HG22	1.89	0.54
1:Cs:249:ILE:HD11	1:Cs:420:MET:HG3	1.90	0.54
1:Cv:249:ILE:HD11	1:Cv:420:MET:HG3	1.90	0.54
1:Cw:289:SER:OG	1:Cw:290:LYS:NZ	2.40	0.54
1:Cy:249:ILE:HD11	1:Cy:420:MET:HG3	1.90	0.54
1:Ea:249:ILE:HD11	1:Ea:420:MET:HG3	1.90	0.54
1:Ea:266:VAL:HG12	1:Ea:387:VAL:HG22	1.89	0.54
1:Ef:289:SER:OG	1:Ef:290:LYS:NZ	2.40	0.54
1:Eg:266:VAL:HG12	1:Eg:387:VAL:HG22	1.89	0.54
1:Dt:172:PRO:HG2	1:Dt:205:LEU:HB2	1.90	0.54
1:cg:249:ILE:HD11	1:cg:420:MET:HG3	1.90	0.54
1:Ch:266:VAL:HG12	1:Ch:387:VAL:HG22	1.89	0.54
1:Cx:289:SER:OG	1:Cx:290:LYS:NZ	2.40	0.54
1:Cy:289:SER:OG	1:Cy:290:LYS:NZ	2.40	0.54
1:Eb:266:VAL:HG12	1:Eb:387:VAL:HG22	1.89	0.54
1:Ed:249:ILE:HD11	1:Ed:420:MET:HG3	1.90	0.54
2:GA:6:UNK:CB	1:Ea:365:ASN:HD21	2.20	0.54
1:Co:289:SER:OG	1:Co:290:LYS:NZ	2.40	0.54
1:Cp:249:ILE:HD11	1:Cp:420:MET:HG3	1.90	0.54
1:Ef:249:ILE:HD11	1:Ef:420:MET:HG3	1.90	0.54
1:cg:266:VAL:HG12	1:cg:387:VAL:HG22	1.89	0.54
1:Cj:249:ILE:HD11	1:Cj:420:MET:HG3	1.90	0.54
1:Cm:249:ILE:HD11	1:Cm:420:MET:HG3	1.90	0.54
1:Cm:289:SER:OG	1:Cm:290:LYS:NZ	2.40	0.54
1:Co:266:VAL:HG12	1:Co:387:VAL:HG22	1.89	0.54
1:Cq:266:VAL:HG12	1:Cq:387:VAL:HG22	1.89	0.54
1:Cz:289:SER:OG	1:Cz:290:LYS:NZ	2.40	0.54
1:Ee:232:ASP:O	1:Ee:236:LYS:NZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ef:266:VAL:HG12	1:Ef:387:VAL:HG22	1.89	0.54
1:Eg:249:ILE:HD11	1:Eg:420:MET:HG3	1.90	0.54
1:Fh:266:VAL:HG12	1:Fh:387:VAL:HG22	1.89	0.54
1:Fh:289:SER:OG	1:Fh:290:LYS:NZ	2.40	0.54
1:Dc:209:ASN:HD22	1:Dc:209:ASN:N	2.05	0.54
1:Df:172:PRO:O	1:Df:205:LEU:CD1	2.56	0.54
1:Cc:289:SER:OG	1:Cc:290:LYS:NZ	2.40	0.54
1:Ce:266:VAL:HG12	1:Ce:387:VAL:HG22	1.89	0.54
1:Cj:266:VAL:HG12	1:Cj:387:VAL:HG22	1.89	0.54
1:Cl:266:VAL:HG12	1:Cl:387:VAL:HG22	1.89	0.54
1:Cm:266:VAL:HG12	1:Cm:387:VAL:HG22	1.89	0.54
1:Cv:266:VAL:HG12	1:Cv:387:VAL:HG22	1.89	0.54
1:Cx:266:VAL:HG12	1:Cx:387:VAL:HG22	1.89	0.54
1:Dh:133:GLN:NE2	1:Dh:137:GLU:OE2	2.41	0.53
1:Dt:172:PRO:HG2	1:Dt:205:LEU:HA	1.91	0.53
1:Cf:249:ILE:HD11	1:Cf:420:MET:HG3	1.90	0.53
1:Ee:275:LYS:HG2	1:Ef:375:THR:HG23	1.90	0.53
1:Dn:133:GLN:NE2	1:Dn:137:GLU:OE2	2.41	0.53
1:Du:133:GLN:NE2	1:Du:137:GLU:OE2	2.41	0.53
1:Dw:172:PRO:HG2	1:Dw:205:LEU:CA	2.37	0.53
1:Cc:249:ILE:HD11	1:Cc:420:MET:HG3	1.90	0.53
1:Ci:249:ILE:HD11	1:Ci:420:MET:HG3	1.90	0.53
1:Ck:289:SER:OG	1:Ck:290:LYS:NZ	2.40	0.53
1:Cu:249:ILE:HD11	1:Cu:420:MET:HG3	1.90	0.53
1:Ec:249:ILE:HD11	1:Ec:420:MET:HG3	1.90	0.53
1:Dv:160:PRO:HD3	1:Dv:172:PRO:CB	2.39	0.53
1:Dv:160:PRO:CD	1:Dv:172:PRO:HB3	2.38	0.53
1:Cb:249:ILE:HD11	1:Cb:420:MET:HG3	1.90	0.53
1:Cr:249:ILE:HD11	1:Cr:420:MET:HG3	1.90	0.53
1:Db:158:ALA:HB2	1:Dc:200:SER:O	2.08	0.53
1:Dc:133:GLN:NE2	1:Dc:137:GLU:OE2	2.41	0.53
1:Dq:133:GLN:HB2	1:Dq:159:MET:HE2	1.88	0.53
1:Ci:266:VAL:HG12	1:Ci:387:VAL:HG22	1.89	0.53
1:Eb:249:ILE:HD11	1:Eb:420:MET:HG3	1.90	0.53
1:Eb:289:SER:OG	1:Eb:290:LYS:NZ	2.40	0.53
1:Cm:242:GLU:OE1	1:Cn:248:ARG:NH2	2.42	0.53
1:Cr:266:VAL:HG12	1:Cr:387:VAL:HG22	1.89	0.53
1:Ds:133:GLN:NE2	1:Ds:137:GLU:OE2	2.40	0.53
1:Cb:242:GLU:OE1	1:Cc:248:ARG:NH2	2.42	0.53
1:Cd:266:VAL:HG12	1:Cd:387:VAL:HG22	1.89	0.53
1:Co:249:ILE:HD11	1:Co:420:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cp:266:VAL:HG12	1:Cp:387:VAL:HG22	1.89	0.53
1:Ct:249:ILE:HD11	1:Ct:420:MET:HG3	1.90	0.53
1:Ct:266:VAL:HG12	1:Ct:387:VAL:HG22	1.89	0.53
1:Dt:133:GLN:NE2	1:Dt:137:GLU:OE2	2.40	0.53
1:Cb:266:VAL:HG12	1:Cb:387:VAL:HG22	1.89	0.53
1:Ce:249:ILE:HD11	1:Ce:420:MET:HG3	1.90	0.53
1:Cf:266:VAL:HG12	1:Cf:387:VAL:HG22	1.89	0.53
1:Ed:266:VAL:HG12	1:Ed:387:VAL:HG22	1.89	0.53
1:Cq:249:ILE:HD11	1:Cq:420:MET:HG3	1.90	0.53
1:Cw:249:ILE:HD11	1:Cw:420:MET:HG3	1.90	0.53
1:Fh:249:ILE:HD11	1:Fh:420:MET:HG3	1.90	0.53
1:Ch:249:ILE:HD11	1:Ch:420:MET:HG3	1.90	0.53
1:Cs:266:VAL:HG12	1:Cs:387:VAL:HG22	1.89	0.53
1:Cy:266:VAL:HG12	1:Cy:387:VAL:HG22	1.89	0.53
1:Cz:266:VAL:HG12	1:Cz:387:VAL:HG22	1.89	0.53
1:De:133:GLN:NE2	1:De:137:GLU:OE2	2.41	0.53
3:GI:4:UNK:CB	1:Cn:374:HIS:ND1	2.72	0.53
1:Ck:249:ILE:HD11	1:Ck:420:MET:HG3	1.90	0.53
1:Cn:249:ILE:HD11	1:Cn:420:MET:HG3	1.90	0.53
1:Ee:249:ILE:HD11	1:Ee:420:MET:HG3	1.90	0.53
1:Ee:266:VAL:HG12	1:Ee:387:VAL:HG22	1.89	0.53
1:Do:133:GLN:NE2	1:Do:137:GLU:OE2	2.41	0.52
1:Dq:172:PRO:O	1:Dq:205:LEU:CD1	2.57	0.52
1:Dv:133:GLN:NE2	1:Dv:137:GLU:OE2	2.41	0.52
1:Ca:266:VAL:HG12	1:Ca:387:VAL:HG22	1.89	0.52
1:Cc:266:VAL:HG12	1:Cc:387:VAL:HG22	1.89	0.52
1:Db:159:MET:SD	1:Db:202:VAL:HG13	2.50	0.52
1:Cl:242:GLU:OE1	1:Cm:248:ARG:NH2	2.42	0.52
1:Dr:133:GLN:NE2	1:Dr:137:GLU:OE2	2.41	0.52
1:Cu:266:VAL:HG12	1:Cu:387:VAL:HG22	1.89	0.52
1:De:125:GLN:O	1:De:128:GLU:HB3	2.10	0.52
1:Dw:133:GLN:NE2	1:Dw:137:GLU:OE2	2.41	0.52
1:Cl:239:ASN:O	1:Cl:243:SER:OG	2.28	0.52
1:Cu:239:ASN:O	1:Cu:243:SER:OG	2.28	0.52
1:Cw:385:LEU:N	1:Cw:428:ASP:OD1	2.41	0.52
1:Cz:239:ASN:O	1:Cz:243:SER:OG	2.28	0.52
3:GJ:17:UNK:CB	1:Cb:278:THR:OG1	2.58	0.52
1:Da:133:GLN:NE2	1:Da:137:GLU:OE2	2.41	0.52
1:Cm:239:ASN:O	1:Cm:243:SER:OG	2.28	0.52
1:Cs:385:LEU:N	1:Cs:428:ASP:OD1	2.41	0.52
1:Cv:239:ASN:O	1:Cv:243:SER:OG	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Co:265:GLN:HG3	1:Cp:252:ILE:HB	1.91	0.52
1:Ct:385:LEU:N	1:Ct:428:ASP:OD1	2.41	0.52
1:Ct:392:ASN:OD1	1:Ct:393:TYR:N	2.43	0.52
1:Cy:392:ASN:OD1	1:Cy:393:TYR:N	2.43	0.52
1:Cz:385:LEU:N	1:Cz:428:ASP:OD1	2.41	0.52
1:Ed:392:ASN:OD1	1:Ed:393:TYR:N	2.43	0.52
1:Cb:392:ASN:OD1	1:Cb:393:TYR:N	2.43	0.52
1:cg:242:GLU:OE1	1:Ch:248:ARG:NH2	2.43	0.52
1:Ch:239:ASN:O	1:Ch:243:SER:OG	2.28	0.52
1:Ck:242:GLU:OE1	1:Cl:248:ARG:NH2	2.43	0.52
1:Ck:392:ASN:OD1	1:Ck:393:TYR:N	2.43	0.52
1:Cn:392:ASN:OD1	1:Cn:393:TYR:N	2.43	0.52
1:Cq:392:ASN:OD1	1:Cq:393:TYR:N	2.43	0.52
1:Cr:239:ASN:O	1:Cr:243:SER:OG	2.28	0.52
1:Cv:392:ASN:OD1	1:Cv:393:TYR:N	2.43	0.52
1:Dv:156:HIS:NE2	1:Dw:143:THR:HG21	2.24	0.52
1:cg:239:ASN:O	1:cg:243:SER:OG	2.28	0.52
1:Ch:392:ASN:OD1	1:Ch:393:TYR:N	2.43	0.52
1:Co:392:ASN:OD1	1:Co:393:TYR:N	2.43	0.52
1:Cp:235:LEU:HB3	1:Cq:244:ARG:HH22	1.75	0.52
1:Ec:392:ASN:OD1	1:Ec:393:TYR:N	2.43	0.52
1:Dq:133:GLN:NE2	1:Dq:137:GLU:OE2	2.41	0.51
1:Dt:159:MET:H	1:Dt:159:MET:CE	2.22	0.51
1:Ce:392:ASN:OD1	1:Ce:393:TYR:N	2.43	0.51
1:Cl:392:ASN:OD1	1:Cl:393:TYR:N	2.43	0.51
1:Cw:392:ASN:OD1	1:Cw:393:TYR:N	2.43	0.51
1:Ea:239:ASN:O	1:Ea:243:SER:OG	2.28	0.51
1:Ea:392:ASN:OD1	1:Ea:393:TYR:N	2.43	0.51
1:Ed:239:ASN:O	1:Ed:243:SER:OG	2.28	0.51
1:Ee:239:ASN:O	1:Ee:243:SER:OG	2.28	0.51
1:Ci:239:ASN:O	1:Ci:243:SER:OG	2.28	0.51
1:Ci:392:ASN:OD1	1:Ci:393:TYR:N	2.43	0.51
1:Cp:385:LEU:N	1:Cp:428:ASP:OD1	2.41	0.51
1:Ee:392:ASN:OD1	1:Ee:393:TYR:N	2.43	0.51
1:Cn:239:ASN:O	1:Cn:243:SER:OG	2.28	0.51
1:Fh:392:ASN:OD1	1:Fh:393:TYR:N	2.43	0.51
1:Cb:239:ASN:O	1:Cb:243:SER:OG	2.28	0.51
1:Cc:239:ASN:O	1:Cc:243:SER:OG	2.28	0.51
1:Cr:392:ASN:OD1	1:Cr:393:TYR:N	2.43	0.51
1:Cs:392:ASN:OD1	1:Cs:393:TYR:N	2.43	0.51
1:Cw:239:ASN:O	1:Cw:243:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ef:239:ASN:O	1:Ef:243:SER:OG	2.28	0.51
1:Du:147:LEU:O	1:Du:149:PRO:HD2	2.11	0.51
1:Cc:392:ASN:OD1	1:Cc:393:TYR:N	2.43	0.51
1:Db:147:LEU:O	1:Db:149:PRO:HD2	2.11	0.51
3:Gi:11:UNK:CB	1:Cm:374:HIS:CE1	2.93	0.51
1:Cf:239:ASN:O	1:Cf:243:SER:OG	2.28	0.51
1:Ci:242:GLU:OE1	1:Cj:248:ARG:NH2	2.44	0.51
1:Cq:385:LEU:N	1:Cq:428:ASP:OD1	2.41	0.51
1:Cx:385:LEU:N	1:Cx:428:ASP:OD1	2.41	0.51
1:Ea:385:LEU:N	1:Ea:428:ASP:OD1	2.41	0.51
1:Ec:232:ASP:O	1:Ec:236:LYS:NZ	2.38	0.51
1:Df:147:LEU:O	1:Df:149:PRO:HD2	2.11	0.51
1:Di:147:LEU:O	1:Di:149:PRO:HD2	2.11	0.51
1:Ca:244:ARG:HH22	1:Fh:235:LEU:HB3	1.75	0.51
1:Ch:275:LYS:HG2	1:Ci:375:THR:HG23	1.93	0.51
1:Cp:392:ASN:OD1	1:Cp:393:TYR:N	2.43	0.51
1:Cx:392:ASN:OD1	1:Cx:393:TYR:N	2.43	0.51
1:Ef:392:ASN:OD1	1:Ef:393:TYR:N	2.43	0.51
1:De:147:LEU:O	1:De:149:PRO:HD2	2.11	0.51
1:Dt:172:PRO:HG2	1:Dt:205:LEU:CB	2.40	0.51
1:Cx:242:GLU:OE1	1:Cy:248:ARG:NH2	2.43	0.51
1:Cz:392:ASN:OD1	1:Cz:393:TYR:N	2.43	0.51
1:Dq:147:LEU:O	1:Dq:149:PRO:HD2	2.11	0.51
1:Ca:392:ASN:OD1	1:Ca:393:TYR:N	2.43	0.51
1:Dl:147:LEU:O	1:Dl:149:PRO:HD2	2.11	0.51
1:Dt:159:MET:N	1:Dt:159:MET:CE	2.73	0.51
1:Dv:147:LEU:O	1:Dv:149:PRO:HD2	2.11	0.51
1:Cd:239:ASN:O	1:Cd:243:SER:OG	2.28	0.51
1:Cs:239:ASN:O	1:Cs:243:SER:OG	2.28	0.51
1:Cu:392:ASN:OD1	1:Cu:393:TYR:N	2.43	0.51
1:Eb:392:ASN:OD1	1:Eb:393:TYR:N	2.43	0.51
1:Ec:239:ASN:O	1:Ec:243:SER:OG	2.28	0.51
1:Ec:385:LEU:N	1:Ec:428:ASP:OD1	2.41	0.51
1:Dt:159:MET:N	1:Dt:159:MET:HE2	2.26	0.50
1:Dw:147:LEU:O	1:Dw:149:PRO:HD2	2.11	0.50
1:Cd:392:ASN:OD1	1:Cd:393:TYR:N	2.43	0.50
1:Ch:242:GLU:OE1	1:Ci:248:ARG:NH2	2.44	0.50
1:Cj:239:ASN:O	1:Cj:243:SER:OG	2.28	0.50
1:Cm:392:ASN:OD1	1:Cm:393:TYR:N	2.43	0.50
1:Dc:147:LEU:O	1:Dc:149:PRO:HD2	2.11	0.50
1:Ds:147:LEU:O	1:Ds:149:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ca:244:ARG:HH12	1:Fh:235:LEU:HB3	1.76	0.50
1:Cj:392:ASN:OD1	1:Cj:393:TYR:N	2.43	0.50
1:Cu:385:LEU:N	1:Cu:428:ASP:OD1	2.41	0.50
1:Cw:242:GLU:OE1	1:Cx:248:ARG:NH2	2.43	0.50
1:Da:147:LEU:O	1:Da:149:PRO:HD2	2.11	0.50
1:Dc:156:HIS:NE2	1:Dd:143:THR:HG21	2.27	0.50
1:Dg:147:LEU:O	1:Dg:149:PRO:HD2	2.11	0.50
1:Dn:147:LEU:O	1:Dn:149:PRO:HD2	2.11	0.50
1:cg:392:ASN:OD1	1:cg:393:TYR:N	2.43	0.50
1:Ch:244:ARG:O	1:Ch:247:ARG:HG3	2.12	0.50
1:Cm:385:LEU:N	1:Cm:428:ASP:OD1	2.41	0.50
1:Cu:244:ARG:O	1:Cu:247:ARG:HG3	2.12	0.50
1:Cv:275:LYS:HG2	1:Cw:375:THR:HG23	1.93	0.50
1:Dr:147:LEU:O	1:Dr:149:PRO:HD2	2.11	0.50
1:Dt:147:LEU:O	1:Dt:149:PRO:HD2	2.11	0.50
1:Ce:244:ARG:O	1:Ce:247:ARG:HG3	2.12	0.50
1:Cn:244:ARG:O	1:Cn:247:ARG:HG3	2.12	0.50
1:Co:385:LEU:N	1:Co:428:ASP:OD1	2.41	0.50
1:Cq:244:ARG:O	1:Cq:247:ARG:HG3	2.12	0.50
1:Cw:244:ARG:O	1:Cw:247:ARG:HG3	2.12	0.50
1:Ed:385:LEU:N	1:Ed:428:ASP:OD1	2.41	0.50
1:Eg:239:ASN:O	1:Eg:243:SER:OG	2.28	0.50
1:Dj:147:LEU:O	1:Dj:149:PRO:HD2	2.11	0.50
1:Ds:126:PHE:C	1:Ds:128:GLU:N	2.67	0.50
2:GD:2:UNK:CB	1:Cf:365:ASN:CG	2.84	0.50
1:Cc:244:ARG:O	1:Cc:247:ARG:HG3	2.12	0.50
1:Cf:244:ARG:O	1:Cf:247:ARG:HG3	2.12	0.50
1:Ci:244:ARG:O	1:Ci:247:ARG:HG3	2.12	0.50
1:Ck:244:ARG:O	1:Ck:247:ARG:HG3	2.12	0.50
1:Cr:244:ARG:O	1:Cr:247:ARG:HG3	2.12	0.50
1:Cz:244:ARG:O	1:Cz:247:ARG:HG3	2.12	0.50
1:Ef:385:LEU:N	1:Ef:428:ASP:OD1	2.41	0.50
1:Cn:242:GLU:OE1	1:Co:248:ARG:NH2	2.45	0.50
1:Co:244:ARG:O	1:Co:247:ARG:HG3	2.12	0.50
1:Ct:244:ARG:O	1:Ct:247:ARG:HG3	2.12	0.50
1:Cx:244:ARG:O	1:Cx:247:ARG:HG3	2.12	0.50
1:Fh:244:ARG:O	1:Fh:247:ARG:HG3	2.12	0.50
1:Ca:239:ASN:O	1:Ca:243:SER:OG	2.28	0.50
1:Cl:244:ARG:O	1:Cl:247:ARG:HG3	2.12	0.50
1:Co:239:ASN:O	1:Co:243:SER:OG	2.28	0.50
1:Eb:244:ARG:O	1:Eb:247:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Do:147:LEU:O	1:Do:149:PRO:HD2	2.11	0.50
1:Dq:125:GLN:NE2	1:Dq:129:GLN:OE1	2.45	0.50
1:Cn:385:LEU:N	1:Cn:428:ASP:OD1	2.41	0.50
1:Eb:375:THR:HG23	1:Ec:275:LYS:HG2	1.93	0.50
1:Dk:147:LEU:O	1:Dk:149:PRO:HD2	2.11	0.50
1:Dp:147:LEU:O	1:Dp:149:PRO:HD2	2.11	0.50
1:Cb:244:ARG:O	1:Cb:247:ARG:HG3	2.12	0.50
1:Cx:239:ASN:O	1:Cx:243:SER:OG	2.28	0.50
1:Df:172:PRO:O	1:Df:205:LEU:HD13	2.11	0.49
1:Dr:134:ARG:HH12	1:Ds:116:LEU:CB	2.20	0.49
1:Ef:244:ARG:O	1:Ef:247:ARG:HG3	2.12	0.49
1:Dh:147:LEU:O	1:Dh:149:PRO:HD2	2.11	0.49
1:Dm:147:LEU:O	1:Dm:149:PRO:HD2	2.11	0.49
1:Cj:385:LEU:N	1:Cj:428:ASP:OD1	2.41	0.49
1:Cl:385:LEU:N	1:Cl:428:ASP:OD1	2.41	0.49
1:Ee:385:LEU:N	1:Ee:428:ASP:OD1	2.41	0.49
1:Dd:147:LEU:O	1:Dd:149:PRO:HD2	2.11	0.49
1:Cr:385:LEU:N	1:Cr:428:ASP:OD1	2.41	0.49
1:Cd:242:GLU:OE1	1:Ce:248:ARG:NH2	2.45	0.49
1:Dw:172:PRO:O	1:Dw:205:LEU:CD1	2.60	0.49
1:Cb:275:LYS:HG2	1:Cc:375:THR:HG23	1.94	0.49
1:cg:275:LYS:HG2	1:Ch:375:THR:HG23	1.94	0.49
1:Cj:244:ARG:O	1:Cj:247:ARG:HG3	2.12	0.49
1:Cm:244:ARG:O	1:Cm:247:ARG:HG3	2.12	0.49
1:Cp:235:LEU:HB3	1:Cq:244:ARG:NH2	2.26	0.49
1:Cv:242:GLU:OE1	1:Cw:248:ARG:NH2	2.45	0.49
1:Eb:239:ASN:O	1:Eb:243:SER:OG	2.28	0.49
1:Ec:244:ARG:O	1:Ec:247:ARG:HG3	2.12	0.49
1:Eg:385:LEU:N	1:Eg:428:ASP:OD1	2.41	0.49
1:Ce:385:LEU:N	1:Ce:428:ASP:OD1	2.41	0.49
1:cg:244:ARG:O	1:cg:247:ARG:HG3	2.12	0.49
1:Ci:235:LEU:HB3	1:Cj:244:ARG:HH22	1.77	0.49
1:Cs:275:LYS:HG2	1:Ct:375:THR:HG23	1.93	0.49
1:Cz:275:LYS:HG2	1:Ea:375:THR:HG23	1.93	0.49
1:Ea:242:GLU:OE1	1:Ec:248:ARG:NH2	2.45	0.49
1:Ee:242:GLU:OE1	1:Ef:248:ARG:NH2	2.45	0.49
1:Db:172:PRO:O	1:Db:205:LEU:HD13	2.12	0.49
1:Ca:244:ARG:O	1:Ca:247:ARG:HG3	2.12	0.49
1:Fh:239:ASN:O	1:Fh:243:SER:OG	2.28	0.49
1:Ck:239:ASN:O	1:Ck:243:SER:OG	2.28	0.49
1:Cp:244:ARG:O	1:Cp:247:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Eg:244:ARG:O	1:Eg:247:ARG:HG3	2.12	0.49
1:Eg:265:GLN:HG3	1:Fh:252:ILE:HB	1.94	0.49
1:Ca:385:LEU:N	1:Ca:428:ASP:OD1	2.41	0.49
1:Cf:275:LYS:HG2	1:cg:375:THR:HG23	1.93	0.49
1:Ck:385:LEU:N	1:Ck:428:ASP:OD1	2.41	0.49
1:Cr:242:GLU:OE1	1:Cs:248:ARG:NH2	2.46	0.49
1:Ct:239:ASN:O	1:Ct:243:SER:OG	2.28	0.49
1:Cy:244:ARG:O	1:Cy:247:ARG:HG3	2.12	0.49
1:Cy:385:LEU:N	1:Cy:428:ASP:OD1	2.41	0.49
1:Ed:244:ARG:O	1:Ed:247:ARG:HG3	2.12	0.49
1:cg:385:LEU:N	1:cg:428:ASP:OD1	2.41	0.49
1:Ci:385:LEU:N	1:Ci:428:ASP:OD1	2.41	0.49
1:Cp:242:GLU:OE1	1:Cq:248:ARG:NH2	2.46	0.49
1:Cs:244:ARG:O	1:Cs:247:ARG:HG3	2.12	0.49
1:Cv:244:ARG:O	1:Cv:247:ARG:HG3	2.12	0.49
1:Cd:385:LEU:N	1:Cd:428:ASP:OD1	2.41	0.48
1:Cj:242:GLU:OE1	1:Ck:248:ARG:NH2	2.45	0.48
1:Ed:275:LYS:HG2	1:Ee:375:THR:HG23	1.94	0.48
1:Cc:275:LYS:HG2	1:Cd:375:THR:HG23	1.95	0.48
1:Cd:244:ARG:O	1:Cd:247:ARG:HG3	2.12	0.48
1:Ct:242:GLU:OE1	1:Cu:248:ARG:NH2	2.46	0.48
1:Fh:385:LEU:N	1:Fh:428:ASP:OD1	2.41	0.48
1:Cb:385:LEU:N	1:Cb:428:ASP:OD1	2.41	0.48
1:Ce:275:LYS:HG2	1:Cf:375:THR:HG23	1.94	0.48
1:Ch:385:LEU:N	1:Ch:428:ASP:OD1	2.41	0.48
1:Cd:425:LYS:HE3	1:Cd:425:LYS:HB3	1.71	0.48
1:Ef:232:ASP:O	1:Ef:236:LYS:NZ	2.38	0.48
1:Dt:159:MET:HE2	1:Dt:159:MET:CA	2.43	0.48
1:Ce:425:LYS:HE3	1:Ce:425:LYS:HB3	1.71	0.48
1:Cp:239:ASN:O	1:Cp:243:SER:OG	2.28	0.48
1:Cw:425:LYS:HE3	1:Cw:425:LYS:HB3	1.71	0.48
1:Cx:275:LYS:HG2	1:Cy:375:THR:HG23	1.95	0.48
1:Ed:242:GLU:OE1	1:Ee:248:ARG:NH2	2.46	0.48
1:Db:159:MET:HG2	1:Db:172:PRO:HB3	1.94	0.48
1:Dt:172:PRO:CG	1:Dt:205:LEU:HA	2.44	0.48
1:Cv:385:LEU:N	1:Cv:428:ASP:OD1	2.41	0.48
1:Cy:275:LYS:HG2	1:Cz:375:THR:HG23	1.95	0.48
1:Ea:275:LYS:HG2	1:Ec:375:THR:HG23	1.95	0.48
1:Cc:385:LEU:N	1:Cc:428:ASP:OD1	2.41	0.48
1:Cc:425:LYS:HE3	1:Cc:425:LYS:HB3	1.71	0.48
1:Cf:385:LEU:N	1:Cf:428:ASP:OD1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cy:239:ASN:O	1:Cy:243:SER:OG	2.28	0.48
1:Du:156:HIS:CE1	1:Dv:143:THR:HG21	2.48	0.48
1:Db:124:SER:O	1:Db:128:GLU:N	2.46	0.48
1:Df:171:SER:CB	1:Df:172:PRO:HD2	2.42	0.48
1:Dt:172:PRO:HG2	1:Dt:205:LEU:HD13	1.96	0.48
1:Db:172:PRO:O	1:Db:205:LEU:CD1	2.62	0.47
1:Ct:235:LEU:HB3	1:Cu:244:ARG:HH22	1.79	0.47
1:Cw:275:LYS:HG2	1:Cx:375:THR:HG23	1.95	0.47
1:Df:175:SER:O	1:Df:175:SER:OG	2.32	0.47
1:Dp:160:PRO:HD2	1:Dp:172:PRO:HD3	1.95	0.47
1:Cf:425:LYS:HE3	1:Cf:425:LYS:HB3	1.72	0.47
1:Da:124:SER:C	1:Da:126:PHE:H	2.22	0.47
1:Dq:125:GLN:NE2	1:Dq:129:GLN:HE22	2.13	0.47
1:Ci:235:LEU:HB3	1:Cj:244:ARG:NH2	2.28	0.47
1:Ca:244:ARG:NH2	1:Fh:235:LEU:HB3	2.30	0.47
1:Cz:425:LYS:HE3	1:Cz:425:LYS:HB3	1.71	0.47
1:Dq:133:GLN:HG3	1:Dq:159:MET:HE2	1.95	0.47
1:Du:158:ALA:CB	1:Dv:200:SER:O	2.61	0.47
1:Cb:425:LYS:HE3	1:Cb:425:LYS:HB3	1.71	0.47
1:Dc:175:SER:O	1:Dc:175:SER:OG	2.32	0.47
3:GH:1:UNK:N	1:Cu:372:ILE:HD12	2.30	0.47
1:cg:425:LYS:HE3	1:cg:425:LYS:HB3	1.71	0.47
1:Cj:275:LYS:HG2	1:Ck:375:THR:HG23	1.96	0.47
1:Ck:235:LEU:HB3	1:Cl:244:ARG:HH22	1.80	0.47
1:Cl:275:LYS:HG2	1:Cm:375:THR:HG23	1.95	0.47
1:Cn:235:LEU:HB3	1:Co:244:ARG:HH22	1.78	0.47
1:Co:235:LEU:HB3	1:Cp:244:ARG:NH1	2.29	0.47
1:Ed:425:LYS:HE3	1:Ed:425:LYS:HB3	1.71	0.47
1:Cu:425:LYS:HB3	1:Cu:425:LYS:HE3	1.71	0.47
1:Cv:425:LYS:HB3	1:Cv:425:LYS:HE3	1.71	0.47
1:Dm:156:HIS:CE1	1:Dn:143:THR:HG21	2.50	0.47
1:Da:124:SER:C	1:Da:126:PHE:N	2.71	0.46
1:Dd:125:GLN:NE2	1:Dd:125:GLN:C	2.73	0.46
3:GH:8:UNK:CB	1:Ct:372:ILE:CD1	2.93	0.46
1:Ca:425:LYS:HE3	1:Ca:425:LYS:HB3	1.71	0.46
1:Da:124:SER:CB	1:Da:127:SER:HB3	2.45	0.46
1:Ca:235:LEU:HB3	1:Cb:244:ARG:NH1	2.31	0.46
1:Ct:425:LYS:HB3	1:Ct:425:LYS:HE3	1.71	0.46
1:Dv:113:PHE:N	1:Dv:135:ALA:HB1	2.30	0.46
1:Dr:171:SER:HA	1:Dr:172:PRO:HD3	1.73	0.46
1:Do:175:SER:O	1:Do:175:SER:OG	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cp:275:LYS:HG2	1:Cq:375:THR:HG23	1.97	0.46
1:Cr:275:LYS:HG2	1:Cs:375:THR:HG23	1.97	0.46
1:Cd:235:LEU:HB3	1:Ce:244:ARG:HH22	1.80	0.46
1:Cr:235:LEU:HB3	1:Cs:244:ARG:HH22	1.81	0.46
1:Cd:275:LYS:HG2	1:Ce:375:THR:HG23	1.97	0.46
1:Ch:425:LYS:HE3	1:Ch:425:LYS:HB3	1.71	0.46
1:Cs:425:LYS:HE3	1:Cs:425:LYS:HB3	1.71	0.46
1:Eb:275:LYS:HG2	1:Ed:375:THR:HG23	1.97	0.46
3:GG:5:UNK:CB	1:Cz:278:THR:HG21	2.46	0.46
1:Ca:244:ARG:NH1	1:Fh:235:LEU:HB3	2.31	0.46
1:Cs:265:GLN:HG3	1:Ct:252:ILE:HB	1.98	0.46
1:Db:159:MET:HA	1:Db:160:PRO:HD3	1.72	0.45
1:Dr:125:GLN:O	1:Dr:128:GLU:HB3	2.16	0.45
1:Du:172:PRO:O	1:Du:205:LEU:CD1	2.64	0.45
3:GF:16:UNK:CB	1:Ee:372:ILE:CD1	2.94	0.45
3:GF:7:UNK:O	3:GF:11:UNK:N	2.49	0.45
1:Ck:235:LEU:HB3	1:Cl:244:ARG:NH2	2.31	0.45
1:Cy:425:LYS:HE3	1:Cy:425:LYS:HB3	1.71	0.45
1:Dc:113:PHE:N	1:Dc:135:ALA:HB1	2.32	0.45
1:Dc:158:ALA:HB2	1:Dd:200:SER:O	2.17	0.45
1:Dq:113:PHE:N	1:Dq:135:ALA:HB1	2.31	0.45
1:Ca:248:ARG:NH2	1:Fh:242:GLU:OE1	2.49	0.45
1:Ck:275:LYS:HG2	1:Cl:375:THR:HG23	1.97	0.45
1:Cm:235:LEU:HB3	1:Cn:244:ARG:HH22	1.81	0.45
1:Cn:235:LEU:HB3	1:Co:244:ARG:NH2	2.31	0.45
1:Da:125:GLN:C	1:Da:125:GLN:NE2	2.75	0.45
1:Dc:172:PRO:O	1:Dc:205:LEU:CD1	2.65	0.45
1:Dd:175:SER:O	1:Dd:175:SER:OG	2.32	0.45
1:Df:171:SER:CB	1:Df:172:PRO:CD	2.95	0.45
1:Dj:156:HIS:CE1	1:Dk:143:THR:CG2	2.86	0.45
1:Dq:133:GLN:CG	1:Dq:159:MET:HE2	2.47	0.45
1:Dr:175:SER:O	1:Dr:175:SER:OG	2.32	0.45
1:Cr:425:LYS:HE3	1:Cr:425:LYS:HB3	1.71	0.45
1:Dm:156:HIS:NE2	1:Dn:143:THR:HG21	2.32	0.45
1:Cd:235:LEU:HB3	1:Ce:244:ARG:NH2	2.32	0.45
1:Cp:235:LEU:HB3	1:Cq:244:ARG:NH1	2.32	0.45
1:Dc:172:PRO:HG2	1:Dc:205:LEU:CA	2.46	0.45
1:Dn:158:ALA:HB2	1:Do:200:SER:O	2.17	0.45
1:Ci:425:LYS:HE3	1:Ci:425:LYS:HB3	1.71	0.45
1:Cn:235:LEU:HB3	1:Co:244:ARG:HH12	1.81	0.45
1:Ct:235:LEU:HB3	1:Cu:244:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dg:175:SER:O	1:Dg:175:SER:OG	2.32	0.45
1:Ct:275:LYS:HG2	1:Cu:375:THR:HG23	1.98	0.45
1:Dt:159:MET:HE2	1:Dt:159:MET:C	2.40	0.45
1:Du:160:PRO:HB3	1:Dv:203:ALA:HB1	1.99	0.45
1:Cy:235:LEU:HB3	1:Cz:244:ARG:NH2	2.32	0.45
1:Cu:265:GLN:HG3	1:Cv:252:ILE:HB	1.99	0.44
1:Eb:265:GLN:HG3	1:Ed:252:ILE:HB	1.98	0.44
1:Dq:171:SER:OG	1:Dq:209:ASN:ND2	2.50	0.44
1:Ca:265:GLN:HG3	1:Cb:252:ILE:HB	1.99	0.44
1:Cp:235:LEU:HB3	1:Cq:244:ARG:HH12	1.82	0.44
1:Ef:275:LYS:HG2	1:Eg:375:THR:HG23	1.98	0.44
1:Ck:425:LYS:HE3	1:Ck:425:LYS:HB3	1.71	0.44
1:Cy:235:LEU:HB3	1:Cz:244:ARG:HH22	1.81	0.44
1:Da:160:PRO:HG3	1:Da:171:SER:O	2.18	0.44
1:Di:175:SER:O	1:Di:175:SER:OG	2.32	0.44
1:Dt:172:PRO:HG2	1:Dt:205:LEU:CA	2.47	0.44
1:Cj:425:LYS:HE3	1:Cj:425:LYS:HB3	1.71	0.44
1:Cl:425:LYS:HE3	1:Cl:425:LYS:HB3	1.71	0.44
1:Cm:275:LYS:HG2	1:Cn:375:THR:HG23	1.98	0.44
1:Eb:425:LYS:HE3	1:Eb:425:LYS:HB3	1.72	0.44
1:Fh:425:LYS:HE3	1:Fh:425:LYS:HB3	1.71	0.44
1:Ds:171:SER:HA	1:Ds:172:PRO:HD3	1.69	0.44
2:GA:6:UNK:CB	1:Ea:365:ASN:CG	2.90	0.44
1:Cq:265:GLN:HG3	1:Cr:252:ILE:HB	1.99	0.44
1:Dc:156:HIS:CE1	1:Dd:143:THR:HG21	2.53	0.44
1:Dd:125:GLN:C	1:Dd:125:GLN:CD	2.86	0.44
1:Do:172:PRO:HD2	1:Do:204:GLY:O	2.17	0.44
1:Ca:252:ILE:HB	1:Fh:265:GLN:HG3	1.98	0.44
1:Cm:425:LYS:HE3	1:Cm:425:LYS:HB3	1.72	0.44
1:Cn:425:LYS:HE3	1:Cn:425:LYS:HB3	1.71	0.44
1:Dc:172:PRO:O	1:Dc:205:LEU:HD13	2.18	0.44
1:Dt:125:GLN:CD	1:Dt:125:GLN:C	2.85	0.44
1:Du:125:GLN:CD	1:Du:125:GLN:C	2.86	0.44
1:Dw:172:PRO:HG3	1:Dw:204:GLY:C	2.43	0.44
1:Du:172:PRO:O	1:Du:205:LEU:HD13	2.18	0.43
1:Cm:235:LEU:HB3	1:Cn:244:ARG:NH2	2.32	0.43
1:Cr:235:LEU:HB3	1:Cs:244:ARG:NH2	2.32	0.43
1:Dm:175:SER:O	1:Dm:175:SER:OG	2.32	0.43
1:Cx:426:ARG:NH2	1:Cx:428:ASP:OD2	2.47	0.43
1:Ea:235:LEU:HB3	1:Ec:244:ARG:HH22	1.82	0.43
1:Ea:235:LEU:HB3	1:Ec:244:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cl:235:LEU:HB3	1:Cm:244:ARG:HH22	1.83	0.43
1:Da:175:SER:O	1:Da:175:SER:OG	2.32	0.43
1:Dt:172:PRO:CD	1:Dt:204:GLY:O	2.65	0.43
1:Dt:172:PRO:O	1:Dt:205:LEU:CD1	2.66	0.43
1:Dw:125:GLN:C	1:Dw:125:GLN:CD	2.85	0.43
1:Cn:235:LEU:HB3	1:Co:244:ARG:NH1	2.33	0.43
1:Co:426:ARG:NH2	1:Co:428:ASP:OD2	2.47	0.43
1:Cz:235:LEU:HB3	1:Ea:244:ARG:HH22	1.84	0.43
1:Da:156:HIS:CE1	1:Db:143:THR:HG21	2.54	0.43
1:Dc:172:PRO:CG	1:Dc:205:LEU:HA	2.49	0.43
1:Dn:156:HIS:CE1	1:Do:143:THR:HG21	2.54	0.43
1:Dw:171:SER:OG	1:Dw:209:ASN:ND2	2.52	0.43
1:Cc:235:LEU:HB3	1:Cd:244:ARG:NH2	2.34	0.43
1:Ce:265:GLN:HG3	1:Cf:252:ILE:HB	2.01	0.43
1:Co:425:LYS:HB3	1:Co:425:LYS:HE3	1.71	0.43
1:Cp:425:LYS:HE3	1:Cp:425:LYS:HB3	1.71	0.43
1:Ed:235:LEU:HB3	1:Ee:244:ARG:HH22	1.83	0.43
1:Da:203:ALA:HB1	1:Dw:160:PRO:HB3	1.99	0.43
1:Db:175:SER:O	1:Db:175:SER:OG	2.32	0.43
1:De:175:SER:O	1:De:175:SER:OG	2.32	0.43
1:Dp:175:SER:O	1:Dp:175:SER:OG	2.32	0.43
1:Cc:265:GLN:HG3	1:Cd:252:ILE:HB	2.00	0.43
1:Eg:235:LEU:HB3	1:Fh:244:ARG:NH2	2.34	0.43
1:Dt:157:LEU:HB2	1:Dt:159:MET:SD	2.58	0.43
1:Cw:394:LYS:HB3	1:Cw:394:LYS:HE2	1.84	0.43
1:Cs:235:LEU:HB3	1:Ct:244:ARG:NH2	2.33	0.43
1:Ec:426:ARG:NH2	1:Ec:428:ASP:OD2	2.47	0.43
1:Du:137:GLU:HG2	1:Du:157:LEU:HG	2.01	0.42
2:GC:6:UNK:CB	1:Cm:294:ARG:HD2	2.49	0.42
1:Cx:425:LYS:HE3	1:Cx:425:LYS:HB3	1.71	0.42
1:Ca:235:LEU:HB3	1:Cb:244:ARG:HH12	1.83	0.42
1:Cb:235:LEU:HB3	1:Cc:244:ARG:HH22	1.84	0.42
1:Eg:235:LEU:HB3	1:Fh:244:ARG:NH1	2.34	0.42
1:Db:137:GLU:HG2	1:Db:157:LEU:HG	2.02	0.42
1:Df:137:GLU:HG2	1:Df:157:LEU:HG	2.01	0.42
1:Ds:137:GLU:HG2	1:Ds:157:LEU:HG	2.02	0.42
1:Dt:172:PRO:HG2	1:Dt:205:LEU:CD1	2.50	0.42
1:Dw:172:PRO:HG3	1:Dw:204:GLY:O	2.18	0.42
1:Ce:235:LEU:HB3	1:Cf:244:ARG:NH1	2.34	0.42
1:Cu:235:LEU:HB3	1:Cv:244:ARG:NH1	2.34	0.42
1:Cx:235:LEU:HB3	1:Cy:244:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dc:137:GLU:HG2	1:Dc:157:LEU:HG	2.02	0.42
1:Dr:137:GLU:HG2	1:Dr:157:LEU:HG	2.02	0.42
1:Du:159:MET:HA	1:Du:160:PRO:HD3	1.91	0.42
1:Dv:137:GLU:HG2	1:Dv:157:LEU:HG	2.02	0.42
1:Cc:426:ARG:NH2	1:Cc:428:ASP:OD2	2.47	0.42
1:Ch:235:LEU:HB3	1:Ci:244:ARG:HH22	1.84	0.42
1:Cj:235:LEU:HB3	1:Ck:244:ARG:HH22	1.84	0.42
1:Ck:409:MET:HE3	1:Ck:409:MET:HB3	1.95	0.42
1:Cn:265:GLN:HG3	1:Co:252:ILE:HB	2.01	0.42
1:Co:277:GLN:HA	1:Cp:372:ILE:O	2.20	0.42
1:Do:137:GLU:HG2	1:Do:157:LEU:HG	2.02	0.42
1:Cu:235:LEU:HB3	1:Cv:244:ARG:NH2	2.34	0.42
1:Ee:277:GLN:HA	1:Ef:372:ILE:O	2.20	0.42
1:Df:172:PRO:C	1:Df:205:LEU:HD13	2.44	0.42
1:Dn:137:GLU:HG2	1:Dn:157:LEU:HG	2.02	0.42
1:Dt:172:PRO:O	1:Dt:205:LEU:HD13	2.20	0.42
1:Cb:235:LEU:HB3	1:Cc:244:ARG:NH2	2.34	0.42
1:Ce:235:LEU:HB3	1:Cf:244:ARG:HH12	1.85	0.42
1:Cf:235:LEU:HB3	1:cg:244:ARG:NH1	2.35	0.42
1:Cz:235:LEU:HB3	1:Ea:244:ARG:NH2	2.33	0.42
1:Fh:232:ASP:O	1:Fh:236:LYS:NZ	2.38	0.42
1:Dq:137:GLU:HG2	1:Dq:157:LEU:HG	2.02	0.42
1:Dw:137:GLU:HG2	1:Dw:157:LEU:HG	2.02	0.42
1:Ce:426:ARG:NH2	1:Ce:428:ASP:OD2	2.47	0.42
1:Cj:381:ASP:OD1	1:Cj:381:ASP:N	2.53	0.42
1:Cl:381:ASP:OD1	1:Cl:381:ASP:N	2.53	0.42
1:Cu:235:LEU:HB3	1:Cv:244:ARG:HH12	1.85	0.42
1:Df:159:MET:HA	1:Df:160:PRO:HD3	1.79	0.42
3:GF:17:UNK:O	1:Ed:374:HIS:ND1	2.53	0.42
1:Cc:235:LEU:HB3	1:Cd:244:ARG:HH22	1.84	0.42
1:Cn:426:ARG:NH2	1:Cn:428:ASP:OD2	2.47	0.42
1:Co:381:ASP:OD1	1:Co:381:ASP:N	2.53	0.42
1:Cs:235:LEU:HB3	1:Ct:244:ARG:HH22	1.84	0.42
1:Da:160:PRO:CG	1:Da:171:SER:O	2.68	0.42
1:Dd:137:GLU:HG2	1:Dd:157:LEU:HG	2.01	0.42
1:Dk:137:GLU:HG2	1:Dk:157:LEU:HG	2.02	0.42
1:Do:217:GLY:HA2	1:Dp:193:ALA:HB1	2.02	0.42
1:Cz:265:GLN:HG3	1:Ea:252:ILE:HB	2.00	0.42
1:Ed:381:ASP:OD1	1:Ed:381:ASP:N	2.53	0.42
1:Ee:381:ASP:OD1	1:Ee:381:ASP:N	2.53	0.42
1:Eg:425:LYS:HE3	1:Eg:425:LYS:HB3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dj:137:GLU:HG2	1:Dj:157:LEU:HG	2.02	0.42
1:Ce:235:LEU:HB3	1:Cf:244:ARG:NH2	2.35	0.42
1:Cl:235:LEU:HB3	1:Cm:244:ARG:NH2	2.34	0.42
1:Cm:265:GLN:HG3	1:Cn:252:ILE:HB	2.02	0.42
1:Cm:381:ASP:OD1	1:Cm:381:ASP:N	2.53	0.42
1:Ct:235:LEU:HB3	1:Cu:244:ARG:HH12	1.85	0.42
1:Cz:394:LYS:HB3	1:Cz:394:LYS:HE2	1.84	0.42
1:Ef:426:ARG:NH2	1:Ef:428:ASP:OD2	2.47	0.42
1:Cr:381:ASP:OD1	1:Cr:381:ASP:N	2.53	0.41
1:Ct:409:MET:HE3	1:Ct:409:MET:HB3	1.96	0.41
1:Cv:394:LYS:HB3	1:Cv:394:LYS:HE2	1.84	0.41
1:Cw:409:MET:HE3	1:Cw:409:MET:HB3	1.95	0.41
1:Ea:381:ASP:OD1	1:Ea:381:ASP:N	2.53	0.41
1:Eb:244:ARG:HH22	1:Ec:235:LEU:HB3	1.85	0.41
1:Ec:381:ASP:OD1	1:Ec:381:ASP:N	2.53	0.41
1:Ec:425:LYS:HE3	1:Ec:425:LYS:HB3	1.71	0.41
1:Fh:381:ASP:OD1	1:Fh:381:ASP:N	2.53	0.41
1:Dc:209:ASN:N	1:Dc:209:ASN:ND2	2.67	0.41
1:Cb:426:ARG:NH2	1:Cb:428:ASP:OD2	2.47	0.41
1:cg:235:LEU:HB3	1:Ch:244:ARG:NH2	2.35	0.41
1:Cr:426:ARG:NH2	1:Cr:428:ASP:OD2	2.47	0.41
1:Ef:265:GLN:HG3	1:Eg:252:ILE:HB	2.02	0.41
1:Dt:193:ALA:O	1:Dt:197:LEU:HB2	2.21	0.41
1:Du:160:PRO:O	1:Du:160:PRO:CD	2.68	0.41
1:Ce:235:LEU:HB3	1:Cf:244:ARG:HH22	1.85	0.41
1:Ch:381:ASP:OD1	1:Ch:381:ASP:N	2.53	0.41
1:Ch:426:ARG:NH2	1:Ch:428:ASP:OD2	2.47	0.41
1:Cp:381:ASP:OD1	1:Cp:381:ASP:N	2.53	0.41
1:Cu:381:ASP:OD1	1:Cu:381:ASP:N	2.53	0.41
1:Cu:394:LYS:HB3	1:Cu:394:LYS:HE2	1.84	0.41
1:Cx:381:ASP:OD1	1:Cx:381:ASP:N	2.53	0.41
1:Cy:381:ASP:OD1	1:Cy:381:ASP:N	2.53	0.41
1:Cy:409:MET:HE3	1:Cy:409:MET:HB3	1.95	0.41
1:Eb:244:ARG:NH2	1:Ec:235:LEU:HB3	2.35	0.41
1:De:137:GLU:HG2	1:De:157:LEU:HG	2.02	0.41
1:Di:193:ALA:O	1:Di:197:LEU:HB2	2.21	0.41
1:Dj:175:SER:O	1:Dj:175:SER:OG	2.32	0.41
1:Dm:193:ALA:O	1:Dm:197:LEU:HB2	2.21	0.41
1:Dp:193:ALA:O	1:Dp:197:LEU:HB2	2.21	0.41
1:Dq:193:ALA:O	1:Dq:197:LEU:HB2	2.21	0.41
1:Dr:193:ALA:O	1:Dr:197:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dv:193:ALA:O	1:Dv:197:LEU:HB2	2.21	0.41
1:Cd:235:LEU:HB3	1:Ce:244:ARG:HH12	1.86	0.41
1:Cv:381:ASP:OD1	1:Cv:381:ASP:N	2.53	0.41
1:Da:137:GLU:HG2	1:Da:157:LEU:HG	2.01	0.41
1:Dj:193:ALA:O	1:Dj:197:LEU:HB2	2.21	0.41
1:Dn:193:ALA:O	1:Dn:197:LEU:HB2	2.21	0.41
1:Dv:175:SER:O	1:Dv:175:SER:OG	2.32	0.41
1:cg:235:LEU:HB3	1:Ch:244:ARG:HH22	1.85	0.41
1:Cm:409:MET:HE3	1:Cm:409:MET:HB3	1.95	0.41
1:Ct:394:LYS:HB3	1:Ct:394:LYS:HE2	1.84	0.41
1:Cu:235:LEU:HB3	1:Cv:244:ARG:HH22	1.85	0.41
1:Cx:394:LYS:HB3	1:Cx:394:LYS:HE2	1.84	0.41
1:Eb:235:LEU:HB3	1:Ed:244:ARG:NH2	2.36	0.41
1:Dg:137:GLU:HG2	1:Dg:157:LEU:HG	2.02	0.41
1:Dh:137:GLU:HG2	1:Dh:157:LEU:HG	2.02	0.41
1:Dh:193:ALA:O	1:Dh:197:LEU:HB2	2.21	0.41
1:Di:137:GLU:HG2	1:Di:157:LEU:HG	2.02	0.41
1:Ds:160:PRO:O	1:Ds:160:PRO:HD2	2.20	0.41
1:Dw:193:ALA:O	1:Dw:197:LEU:HB2	2.21	0.41
1:Cj:409:MET:HE3	1:Cj:409:MET:HB3	1.95	0.41
1:Cw:235:LEU:HB3	1:Cx:244:ARG:HH22	1.85	0.41
1:Cw:426:ARG:NH2	1:Cw:428:ASP:OD2	2.47	0.41
1:Cx:409:MET:HE3	1:Cx:409:MET:HB3	1.95	0.41
1:Da:193:ALA:O	1:Da:197:LEU:HB2	2.21	0.41
1:Dl:137:GLU:HG2	1:Dl:157:LEU:HG	2.02	0.41
1:Dl:193:ALA:O	1:Dl:197:LEU:HB2	2.21	0.41
1:Dm:137:GLU:HG2	1:Dm:157:LEU:HG	2.02	0.41
1:Dp:125:GLN:O	1:Dp:128:GLU:CB	2.69	0.41
1:Dt:124:SER:CB	1:Dt:127:SER:HB3	2.51	0.41
1:Du:193:ALA:O	1:Du:197:LEU:HB2	2.21	0.41
3:GH:1:UNK:HA	1:Cu:372:ILE:HD12	2.03	0.41
1:Cc:381:ASP:OD1	1:Cc:381:ASP:N	2.53	0.41
1:Cf:235:LEU:HB3	1:cg:244:ARG:NH2	2.35	0.41
1:Cy:394:LYS:HB3	1:Cy:394:LYS:HE2	1.84	0.41
1:Cy:235:LEU:HB3	1:Cz:244:ARG:HH12	1.86	0.41
1:Cz:235:LEU:HB3	1:Ea:244:ARG:NH1	2.36	0.41
1:Cz:409:MET:HE3	1:Cz:409:MET:HB3	1.96	0.41
1:Da:172:PRO:HG2	1:Da:205:LEU:HB2	2.03	0.41
1:Db:193:ALA:O	1:Db:197:LEU:HB2	2.21	0.41
1:Dk:193:ALA:O	1:Dk:197:LEU:HB2	2.21	0.41
2:GA:11:UNK:HA	1:Ec:365:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ch:235:LEU:HB3	1:Ci:244:ARG:NH2	2.35	0.41
1:Ch:409:MET:HE3	1:Ch:409:MET:HB3	1.96	0.41
1:Ck:235:LEU:HB3	1:Cl:244:ARG:HH12	1.86	0.41
1:Cl:235:LEU:HB3	1:Cm:244:ARG:HH12	1.86	0.41
1:Cn:381:ASP:OD1	1:Cn:381:ASP:N	2.53	0.41
1:Cp:409:MET:HE3	1:Cp:409:MET:HB3	1.96	0.41
1:Eg:426:ARG:NH2	1:Eg:428:ASP:OD2	2.47	0.41
1:De:125:GLN:O	1:De:128:GLU:CB	2.69	0.41
1:Df:193:ALA:O	1:Df:197:LEU:HB2	2.21	0.41
1:Dp:137:GLU:HG2	1:Dp:157:LEU:HG	2.02	0.41
1:Dt:187:ASP:O	1:Dt:191:ILE:HG12	2.21	0.41
1:Dv:125:GLN:O	1:Dv:128:GLU:N	2.43	0.41
1:Ck:426:ARG:NH2	1:Ck:428:ASP:OD2	2.47	0.41
1:Cq:381:ASP:OD1	1:Cq:381:ASP:N	2.53	0.41
1:Cy:235:LEU:HB3	1:Cz:244:ARG:NH1	2.36	0.41
1:Eb:232:ASP:O	1:Eb:236:LYS:NZ	2.38	0.41
1:Ed:235:LEU:HB3	1:Ee:244:ARG:NH2	2.35	0.41
1:Da:187:ASP:O	1:Da:191:ILE:HG12	2.21	0.40
1:Dh:187:ASP:O	1:Dh:191:ILE:HG12	2.21	0.40
1:Dq:187:ASP:O	1:Dq:191:ILE:HG12	2.21	0.40
1:Dt:175:SER:O	1:Dt:175:SER:OG	2.32	0.40
1:Dv:187:ASP:O	1:Dv:191:ILE:HG12	2.21	0.40
1:Cf:235:LEU:HB3	1:cg:244:ARG:HH12	1.85	0.40
1:Ck:265:GLN:HG3	1:Cl:252:ILE:HB	2.03	0.40
1:Cl:265:GLN:HG3	1:Cm:252:ILE:HB	2.03	0.40
1:Cm:235:LEU:HB3	1:Cn:244:ARG:NH1	2.36	0.40
1:Ea:394:LYS:HB3	1:Ea:394:LYS:HE2	1.84	0.40
1:Ef:235:LEU:HB3	1:Eg:244:ARG:NH2	2.36	0.40
1:Dc:187:ASP:O	1:Dc:191:ILE:HG12	2.21	0.40
1:Dj:187:ASP:O	1:Dj:191:ILE:HG12	2.21	0.40
1:Du:187:ASP:O	1:Du:191:ILE:HG12	2.21	0.40
1:Cb:265:GLN:HG3	1:Cc:252:ILE:HB	2.03	0.40
1:Ci:409:MET:HE3	1:Ci:409:MET:HB3	1.95	0.40
1:Cm:235:LEU:HB3	1:Cn:244:ARG:HH12	1.86	0.40
1:Cu:426:ARG:NH2	1:Cu:428:ASP:OD2	2.47	0.40
1:Cx:235:LEU:HB3	1:Cy:244:ARG:NH2	2.35	0.40
1:Ea:235:LEU:HB3	1:Ec:244:ARG:HH12	1.86	0.40
1:Db:187:ASP:O	1:Db:191:ILE:HG12	2.21	0.40
1:De:193:ALA:O	1:De:197:LEU:HB2	2.21	0.40
1:Dk:187:ASP:O	1:Dk:191:ILE:HG12	2.21	0.40
1:Dn:187:ASP:O	1:Dn:191:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Do:160:PRO:O	1:Do:160:PRO:CD	2.70	0.40
1:Dq:123:ILE:O	1:Dq:125:GLN:N	2.54	0.40
1:Dq:171:SER:HB2	1:Dq:172:PRO:CD	2.51	0.40
1:Dv:172:PRO:HG2	1:Dv:205:LEU:HB2	2.04	0.40
1:Cf:235:LEU:HB3	1:cg:244:ARG:HH22	1.86	0.40
1:Ck:235:LEU:HB3	1:Cl:244:ARG:NH1	2.35	0.40
1:De:187:ASP:O	1:De:191:ILE:HG12	2.21	0.40
1:Dm:187:ASP:O	1:Dm:191:ILE:HG12	2.21	0.40
1:Dr:187:ASP:O	1:Dr:191:ILE:HG12	2.21	0.40
1:Ct:381:ASP:OD1	1:Ct:381:ASP:N	2.53	0.40
1:Ea:235:LEU:HB3	1:Ec:244:ARG:NH1	2.37	0.40
1:Dc:193:ALA:O	1:Dc:197:LEU:HB2	2.21	0.40
1:Dp:187:ASP:O	1:Dp:191:ILE:HG12	2.21	0.40
1:Ds:113:PHE:N	1:Ds:135:ALA:HB1	2.36	0.40
1:Cc:287:ASP:OD1	1:Cc:288:ALA:N	2.55	0.40
1:Cd:235:LEU:HB3	1:Ce:244:ARG:NH1	2.36	0.40
1:Cd:287:ASP:OD1	1:Cd:288:ALA:N	2.55	0.40
1:Cw:381:ASP:OD1	1:Cw:381:ASP:N	2.53	0.40
1:Ea:426:ARG:NH2	1:Ea:428:ASP:OD2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	Cf	15/467 (3%)	14 (93%)	1 (7%)	15	37
1	Ch	133/467 (28%)	130 (98%)	3 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ci	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Cj	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Ck	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Cl	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Cm	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Cn	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Co	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Cp	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Cq	72/467 (15%)	70 (97%)	2 (3%)	38	59
1	Cs	36/467 (8%)	34 (94%)	2 (6%)	19	41
1	Cx	74/467 (16%)	73 (99%)	1 (1%)	59	71
1	Cy	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Cz	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Dr	15/467 (3%)	15 (100%)	0	100	100
1	Ea	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Eb	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Ec	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Ed	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Ee	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Ef	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Eg	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	Fh	133/467 (28%)	130 (98%)	3 (2%)	44	63
1	cg	111/467 (24%)	109 (98%)	2 (2%)	51	67
All	All	2850/11675 (24%)	2785 (98%)	65 (2%)	44	63

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Cf	425	LYS
1	cg	243	SER
1	cg	295	SER
1	Ch	243	SER
1	Ch	295	SER
1	Ch	425	LYS

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Mol	Chain	Res	Type
1	Ci	243	SER
1	Ci	295	SER
1	Ci	425	LYS
1	Cj	243	SER
1	Cj	295	SER
1	Cj	425	LYS
1	Ck	243	SER
1	Ck	295	SER
1	Ck	425	LYS
1	Cl	243	SER
1	Cl	295	SER
1	Cl	425	LYS
1	Cm	243	SER
1	Cm	295	SER
1	Cm	425	LYS
1	Cn	243	SER
1	Cn	295	SER
1	Cn	425	LYS
1	Co	243	SER
1	Co	295	SER
1	Co	425	LYS
1	Cp	243	SER
1	Cp	295	SER
1	Cp	425	LYS
1	Cq	243	SER
1	Cq	295	SER
1	Cs	243	SER
1	Cs	295	SER
1	Cx	425	LYS
1	Cy	243	SER
1	Cy	295	SER
1	Cy	425	LYS
1	Cz	243	SER
1	Cz	295	SER
1	Cz	425	LYS
1	Ea	243	SER
1	Ea	295	SER
1	Ea	425	LYS
1	Eb	243	SER
1	Eb	295	SER
1	Eb	425	LYS
1	Ec	243	SER

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Mol	Chain	Res	Type
1	Ec	295	SER
1	Ec	425	LYS
1	Ed	243	SER
1	Ed	295	SER
1	Ed	425	LYS
1	Ee	243	SER
1	Ee	295	SER
1	Ee	425	LYS
1	Ef	243	SER
1	Ef	295	SER
1	Ef	425	LYS
1	Eg	243	SER
1	Eg	295	SER
1	Eg	425	LYS
1	Fh	243	SER
1	Fh	295	SER
1	Fh	425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	cg	281	HIS
1	Ch	281	HIS
1	Ch	361	ASN
1	Ci	281	HIS
1	Ci	361	ASN
1	Cj	281	HIS
1	Cj	411	GLN
1	Ck	281	HIS
1	Cl	281	HIS
1	Cl	361	ASN
1	Cm	281	HIS
1	Cn	281	HIS
1	Cn	361	ASN
1	Co	281	HIS
1	Cp	281	HIS
1	Cp	361	ASN
1	Cp	411	GLN
1	Cq	281	HIS
1	Cy	281	HIS
1	Cy	361	ASN
1	Cz	281	HIS

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Mol	Chain	Res	Type
1	Ea	281	HIS
1	Ea	361	ASN
1	Ea	365	ASN
1	Ec	281	HIS
1	Ed	281	HIS
1	Ed	361	ASN
1	Ed	374	HIS
1	Ee	281	HIS
1	Ee	361	ASN
1	Ef	281	HIS
1	Eg	281	HIS
1	Eg	365	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

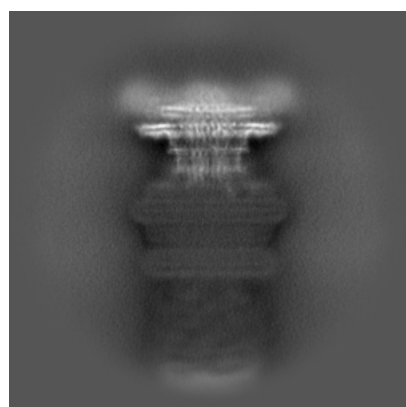
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31007. These allow visual inspection of the internal detail of the map and identification of artifacts.

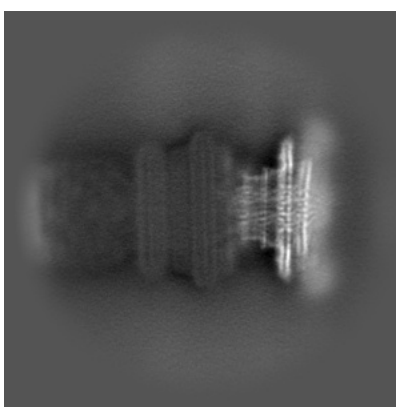
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

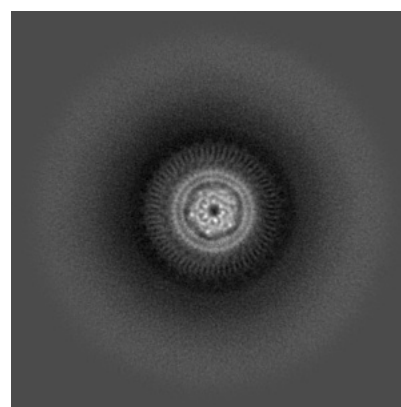
6.1.1 Primary map



X



Y

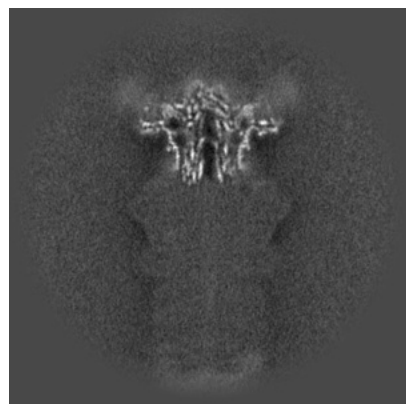


Z

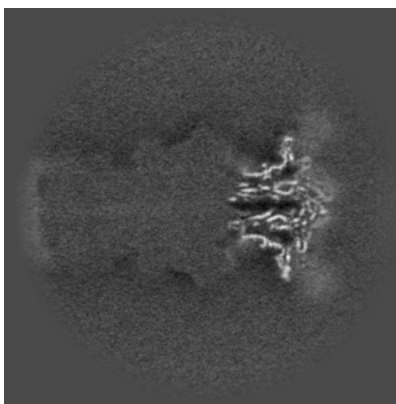
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

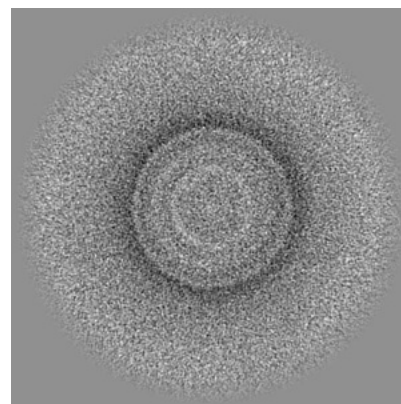
6.2.1 Primary map



X Index: 256



Y Index: 256

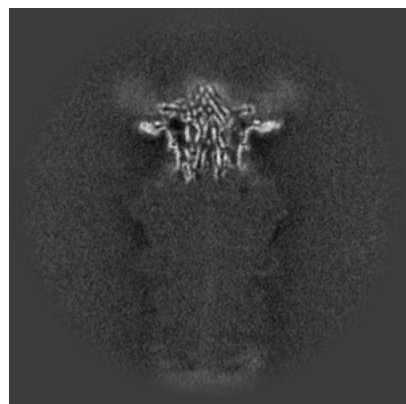


Z Index: 256

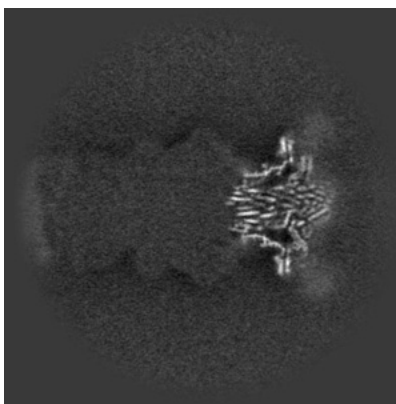
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

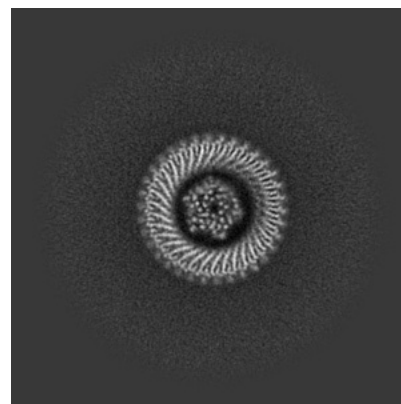
6.3.1 Primary map



X Index: 251



Y Index: 247

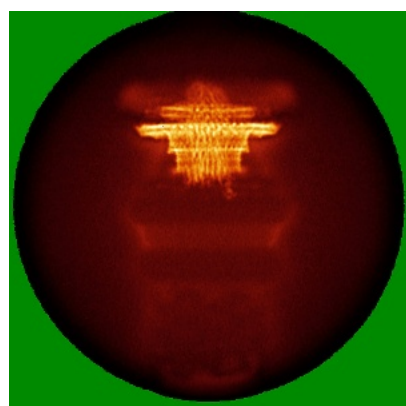


Z Index: 364

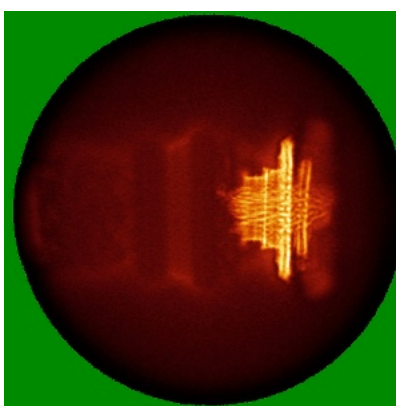
The images above show the largest variance slices of the map in three orthogonal directions.

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

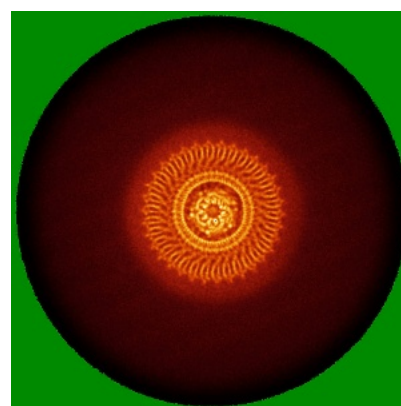
6.4.1 Primary map



X



Y

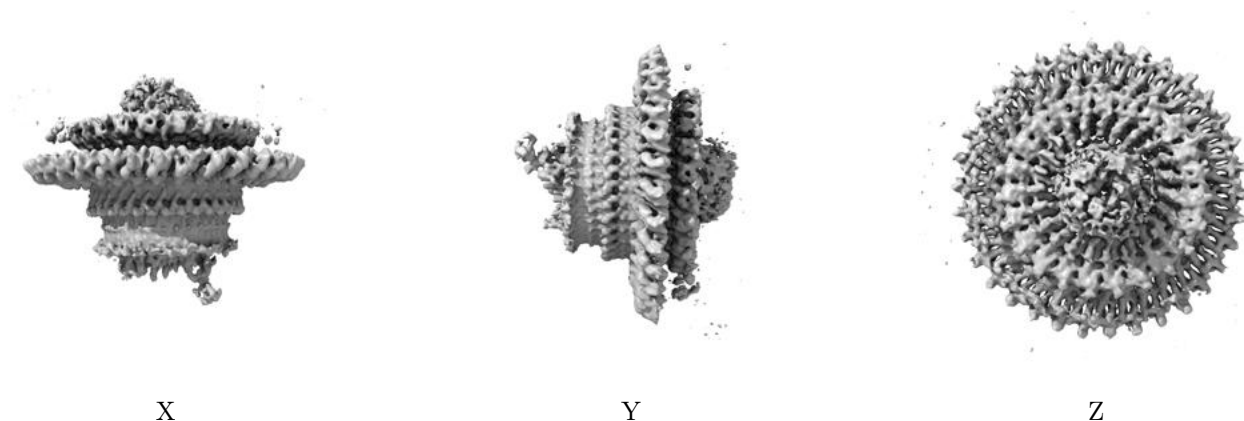


Z

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 0.238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

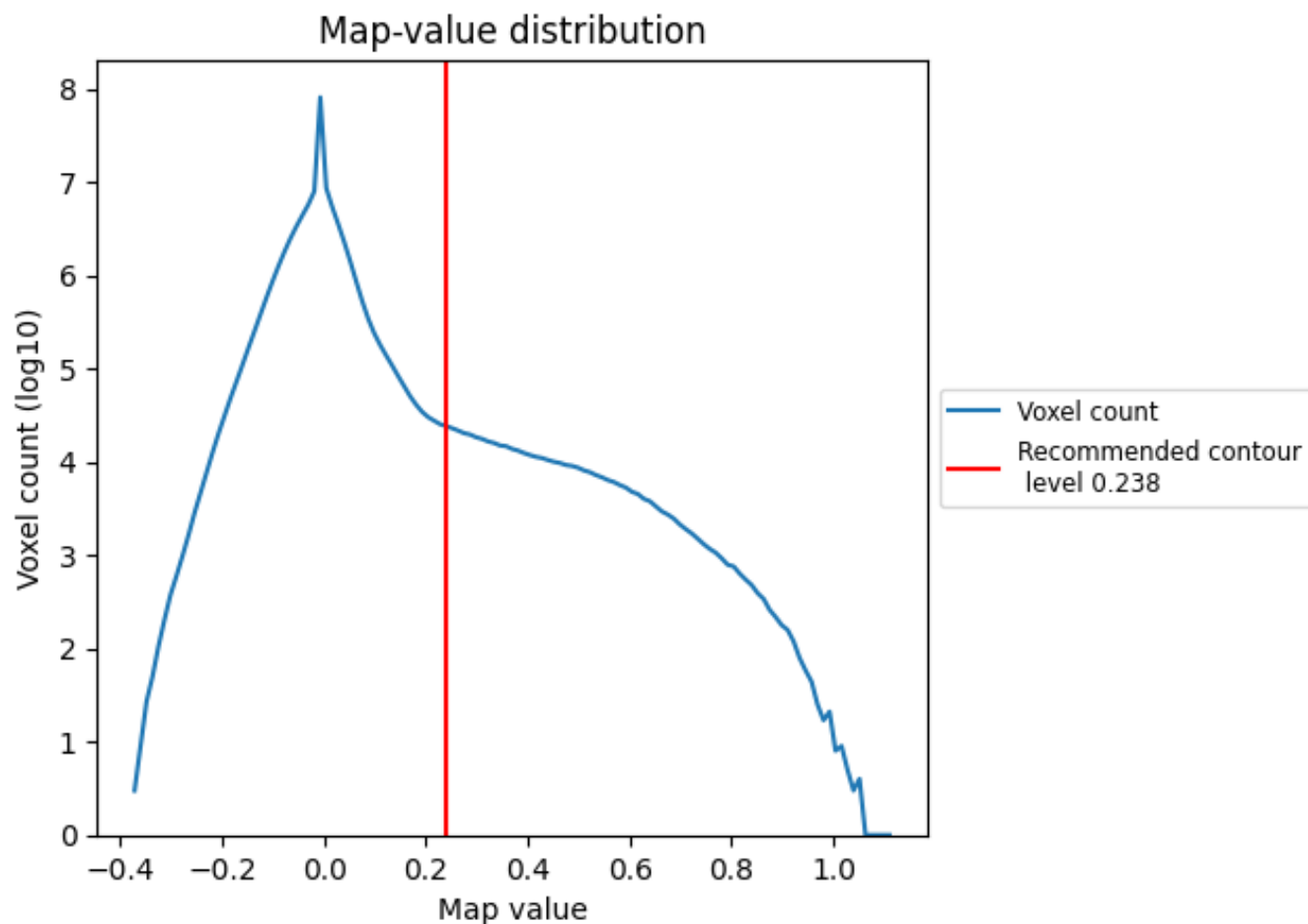
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

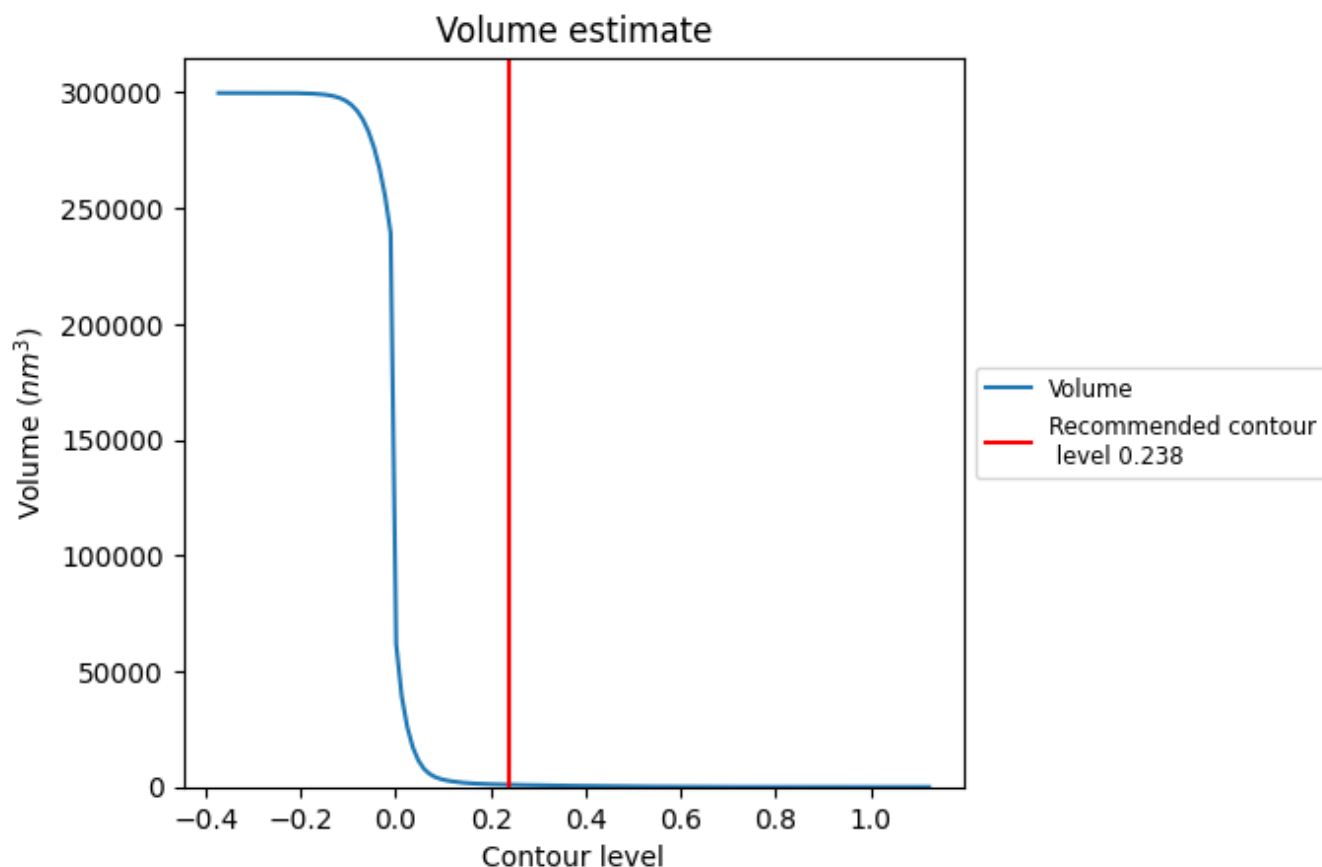
This section contains the results of statistical analysis of the map.

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.

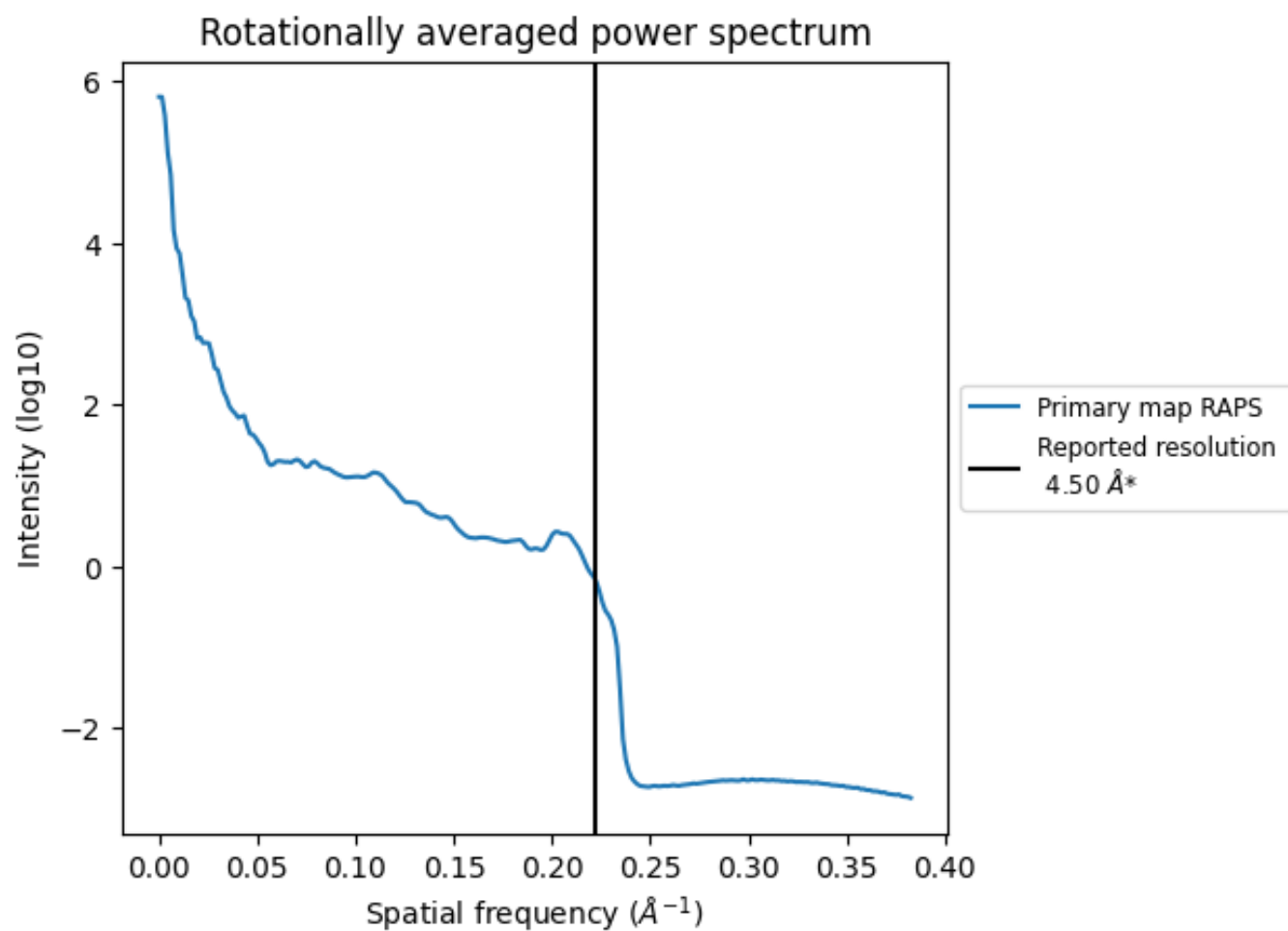
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 982 nm^3 ; this corresponds to an approximate mass of 887 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 0.222 Å⁻¹

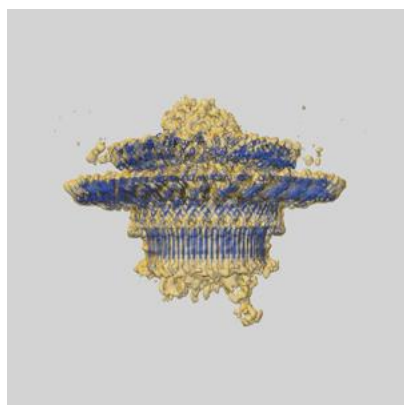
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

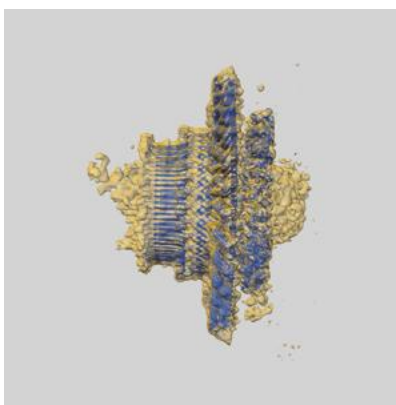
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31007 and PDB model 7E81. Per-residue inclusion information can be found in section [3](#) on page [10](#).

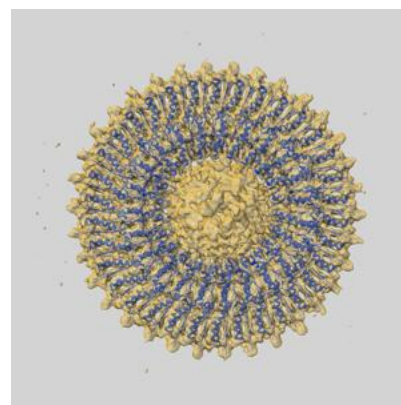
9.1 Map-model overlay [i](#)



X



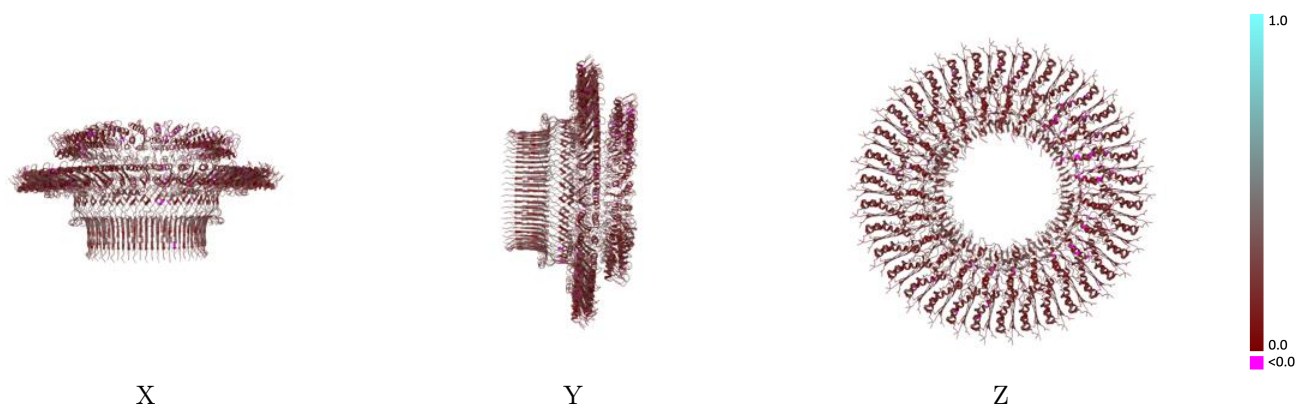
Y



Z

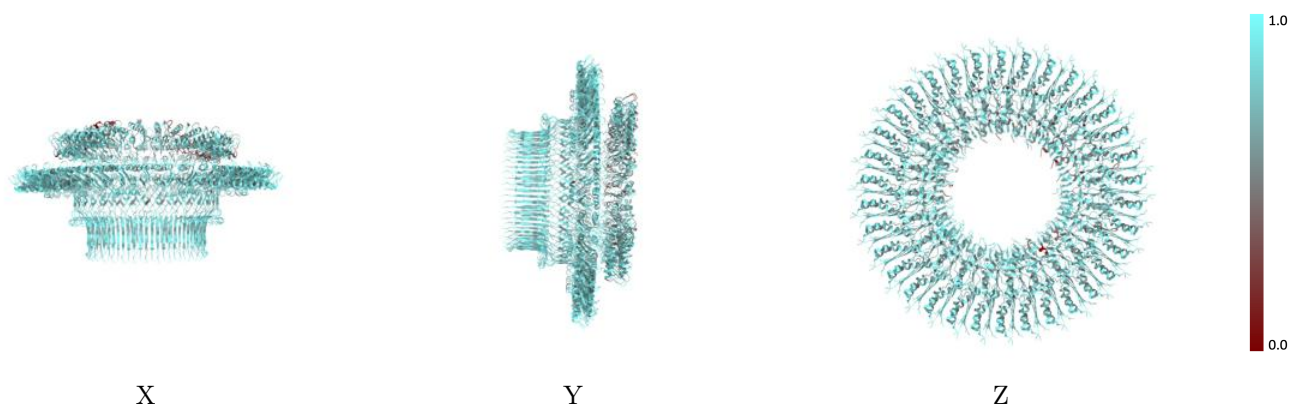
The images above show the 3D surface view of the map at the recommended contour level 0.238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



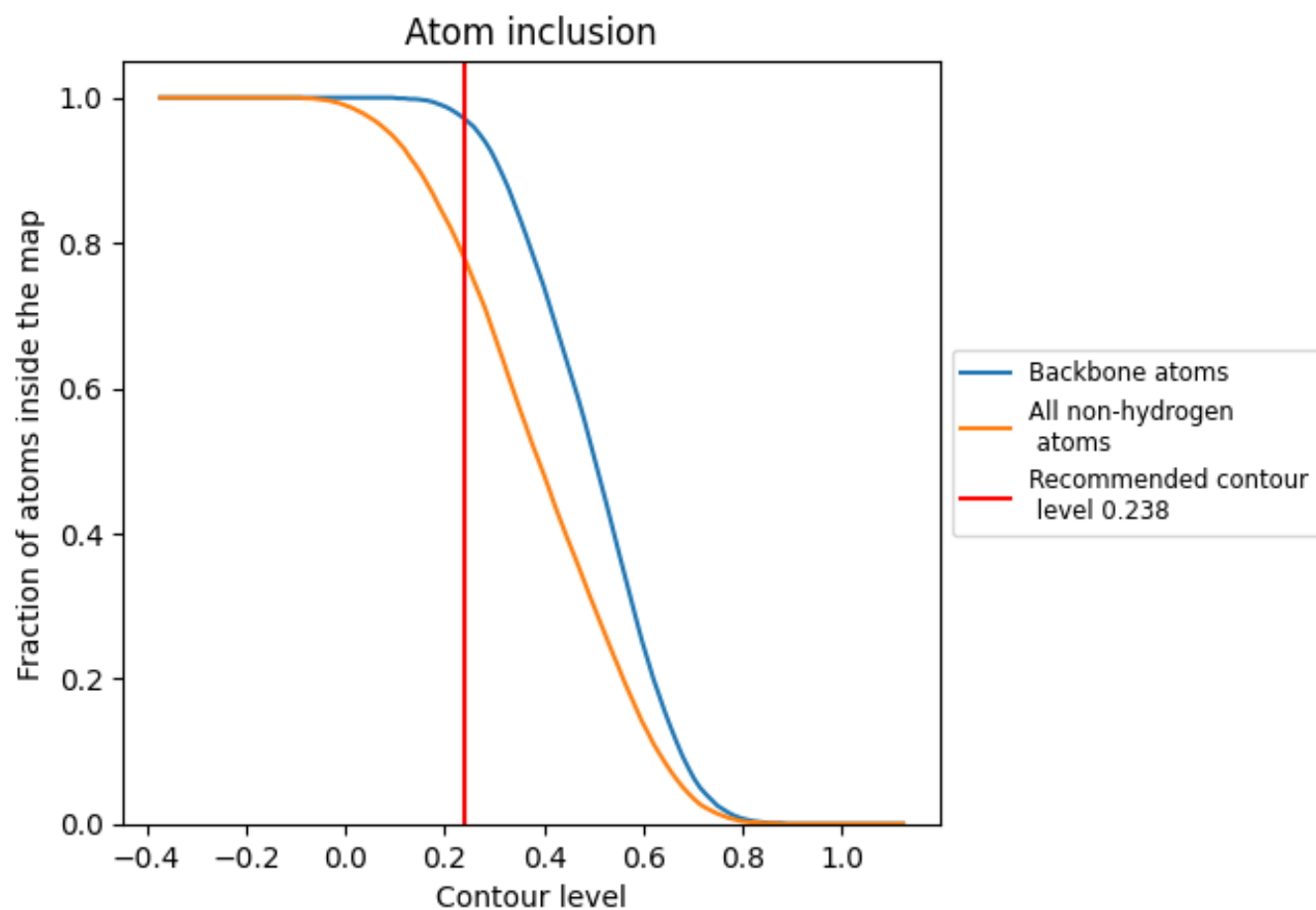
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.238).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 78% 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 (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.2350
Ca	 0.8060	 0.2360
Cb	 0.8030	 0.2450
Cc	 0.8070	 0.2380
Cd	 0.8160	 0.2420
Ce	 0.8070	 0.2310
Cf	 0.8040	 0.2370
Ch	 0.8070	 0.2360
Ci	 0.8030	 0.2450
Cj	 0.8040	 0.2490
Ck	 0.8000	 0.2470
Cl	 0.7980	 0.2440
Cm	 0.7960	 0.2500
Cn	 0.7920	 0.2400
Co	 0.8070	 0.2450
Cp	 0.7880	 0.2390
Cq	 0.7930	 0.2240
Cr	 0.8020	 0.2320
Cs	 0.7890	 0.2310
Ct	 0.8070	 0.2370
Cu	 0.8070	 0.2390
Cv	 0.8120	 0.2440
Cw	 0.8070	 0.2480
Cx	 0.8070	 0.2460
Cy	 0.8030	 0.2410
Cz	 0.8190	 0.2530
Da	 0.7650	 0.2190
Db	 0.7680	 0.2250
Dc	 0.7460	 0.2260
Dd	 0.7100	 0.2090
De	 0.7020	 0.2110
Df	 0.7270	 0.1850
Dg	 0.7330	 0.1780
Dh	 0.6880	 0.1570
Di	 0.6320	 0.1730



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Chain	Atom inclusion	Q-score
Dj	 0.6230	 0.1630
Dk	 0.6500	 0.1750
Dl	 0.6310	 0.1630
Dm	 0.6130	 0.1790
Dn	 0.6720	 0.1880
Do	 0.6890	 0.2070
Dp	 0.7450	 0.2260
Dq	 0.7570	 0.2460
Dr	 0.7450	 0.2330
Ds	 0.7560	 0.2490
Dt	 0.7900	 0.2440
Du	 0.7790	 0.2500
Dv	 0.7690	 0.2300
Dw	 0.7800	 0.2340
Ea	 0.8190	 0.2600
Eb	 0.8140	 0.2520
Ec	 0.8110	 0.2520
Ed	 0.8100	 0.2520
Ee	 0.8000	 0.2590
Ef	 0.8170	 0.2570
Eg	 0.8020	 0.2540
Fh	 0.8030	 0.2460
GA	 0.9090	 0.4060
GB	 0.9200	 0.4010
GC	 0.8910	 0.3930
GD	 0.8800	 0.3640
GE	 0.9330	 0.4570
GF	 0.8670	 0.3010
GG	 0.8780	 0.3500
GH	 0.8560	 0.3180
GI	 0.7470	 0.2920
GJ	 0.9330	 0.2640
GK	 0.8560	 0.3030
cg	 0.8020	 0.2340