



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:21 PM UTC

PDB ID : 8WLI / pdb_00008wli
EMDB ID : EMD-37620
Title : Cryo-EM structure of the MS ring (C34) within the flagellar motor-hook complex in the CCW state
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-30
Resolution : 3.20 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

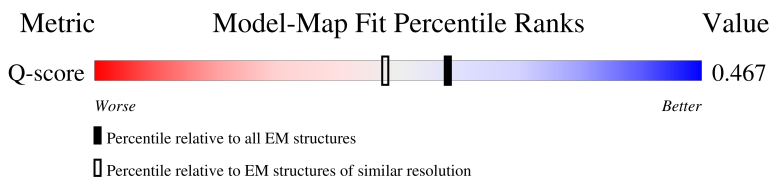
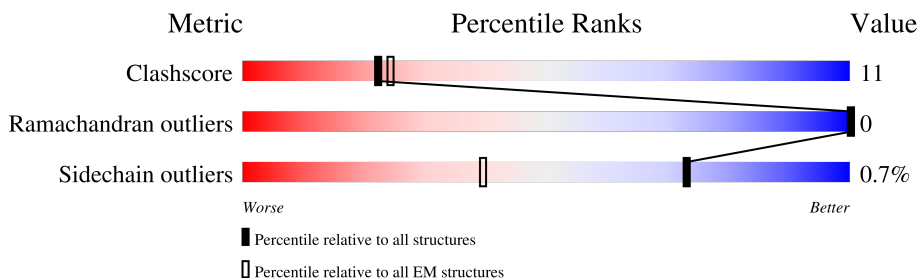
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



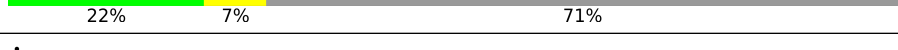
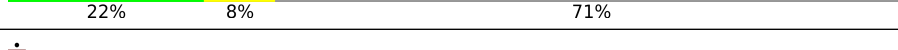
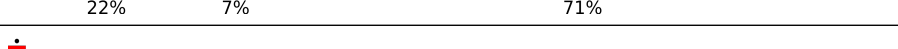
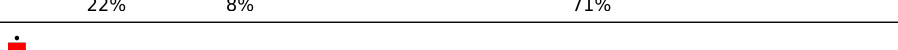
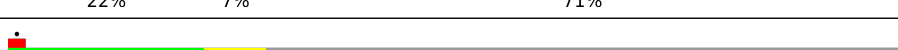
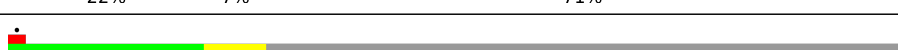
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	A	560	 23% 6% 71%
1	B	560	 22% 7% 71%
1	C	560	 22% 7% 71%
1	D	560	 22% 7% 71%

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Mol	Chain	Length	Quality of chain
1	E	560	
1	F	560	
1	G	560	
1	H	560	
1	I	560	
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	U	560	
1	V	560	
1	W	560	
1	X	560	
1	Y	560	
1	Z	560	
1	a	560	
1	b	560	
1	c	560	

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Mol	Chain	Length	Quality of chain
1	d	560	22%7%71%
1	e	560	22%7%71%
1	f	560	23%6%71%
1	g	560	22%7%71%
1	h	560	22%7%71%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 43350 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	B	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	C	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	D	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	E	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	F	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	G	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	H	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	I	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	J	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	K	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	L	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	M	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	N	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	O	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	P	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	Q	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

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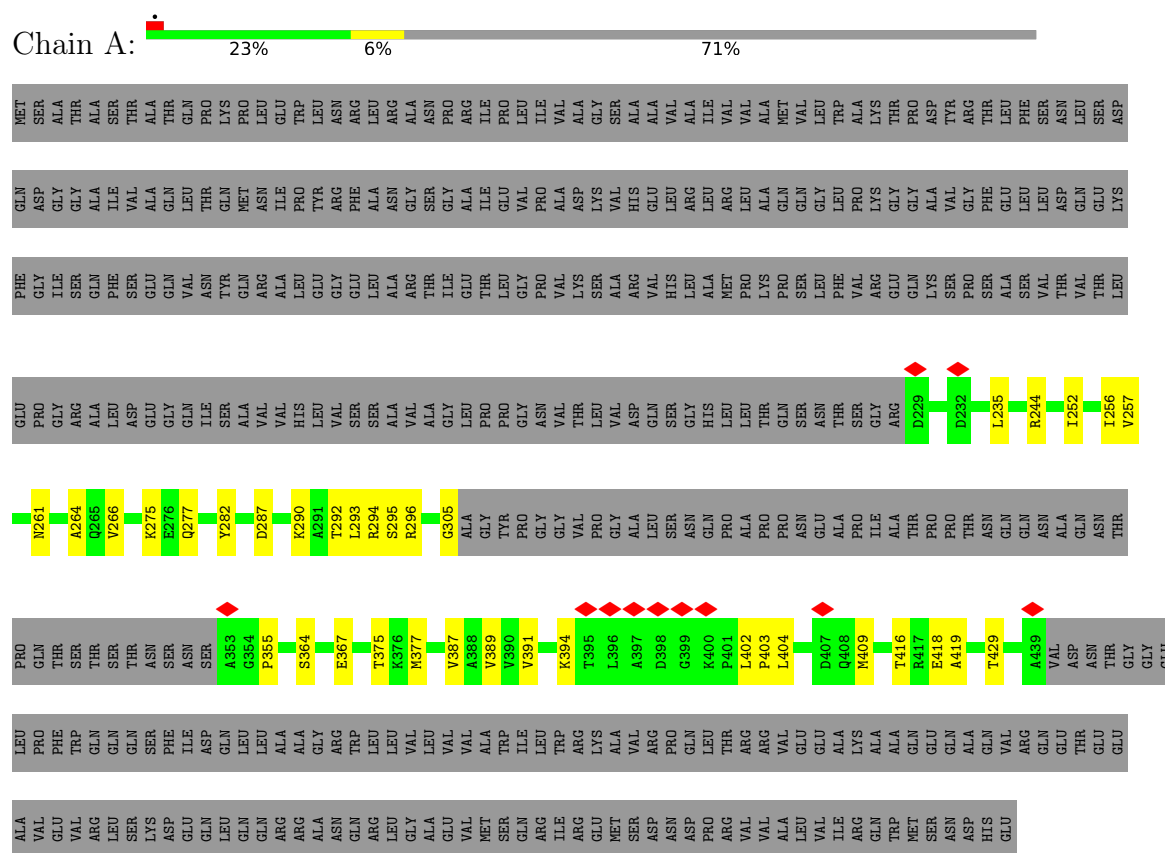
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	S	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	T	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	U	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	V	164	Total 1275	C 776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

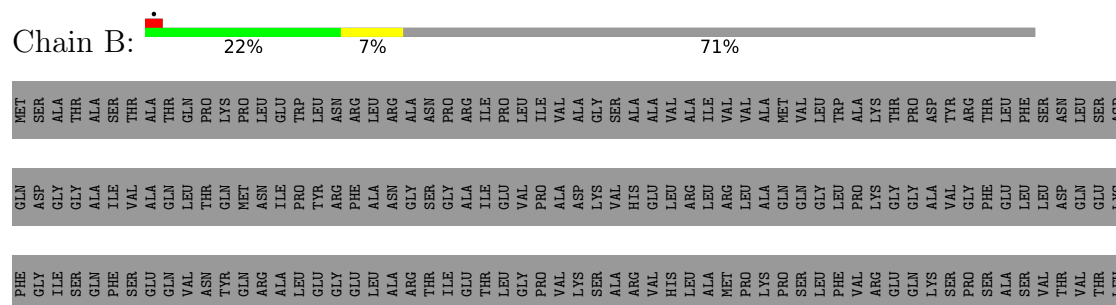
3 Residue-property plots

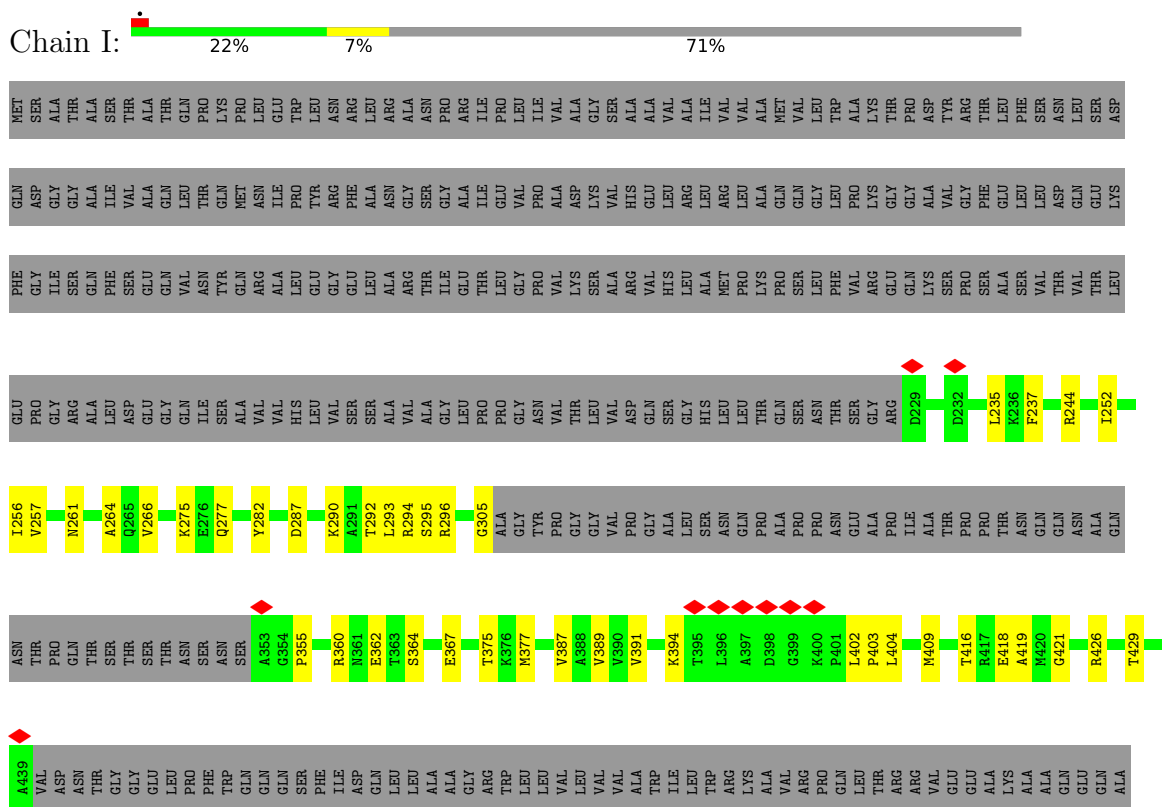
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





HIS	GLN	VAL	ARG	GLN	GLU	THR	GLU	GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	ARG	ARG	ALA	ASN	GLN	ARG	LEU	GLY	ALA	GLU	VAL	MET	SER	GLN	ARG	ARG	TLE	ARG	GLU	MET	SER	ASP	ASN	ASP	PRO	ARG	VAL	VAL	ALA	LEU	VAL	TLE	ARG	GLN	THR	MET	SER	ASN	ASP
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- Molecule 1: Flagellar M-ring protein

[illegible][illegible]

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

GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	VAL	VAL	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	LEU	ASP	VAL	GLN	SER	GLY	HIS	LEU	LEU	THR	GLN	SER	ASN	THR	SER	GLY	ARG	D229	D231	D232	L235	R244	I252
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V257	N261	A264	G265	V266	K275	E276	Q277	Y282	D287	K290	G291	T292	L293	R294	S295	R296	G305	ALA	GLY	TYR	PRO	PRO	GLY	GLY	VAL	PRO	PRO	GLY	GLY	ALA	LEU	SER	ASN	ASN	GLN	PRO	PRO	ALA	ALA	ALA	PRO	PRO	PRO	ASN	ASN	GLN	GLY	ALA	THR	PRO	PRO	PRO	PRO	ASN	ASN	GLN	ALA	ALA	GLN	SVS
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[illegible]

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



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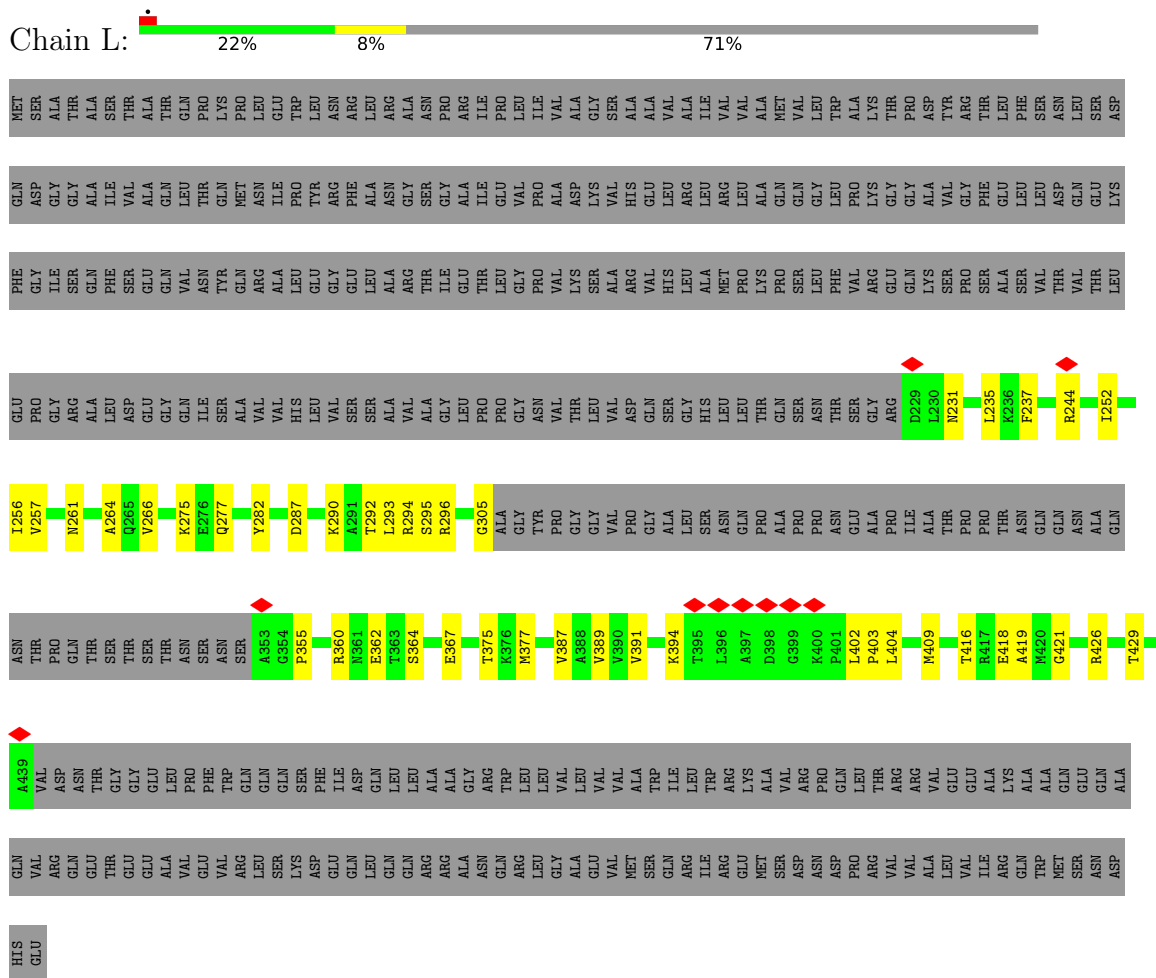
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PHE GLY ILE SER GLN PHE SER GLU GLN VAL TYR GLN ARG ALA LEU GLU GLY GLU LEU LEU THR LEU GLY GLY VAL LYS SER SER ARG ARG HIS LEU LEU MET MET PRO PRO PRO SER PHE VAL VAL ARG ARG GLU GLN LYS SER SER PRO PRO SER ALA ALA THR THR VAL VAL THR THR LEU

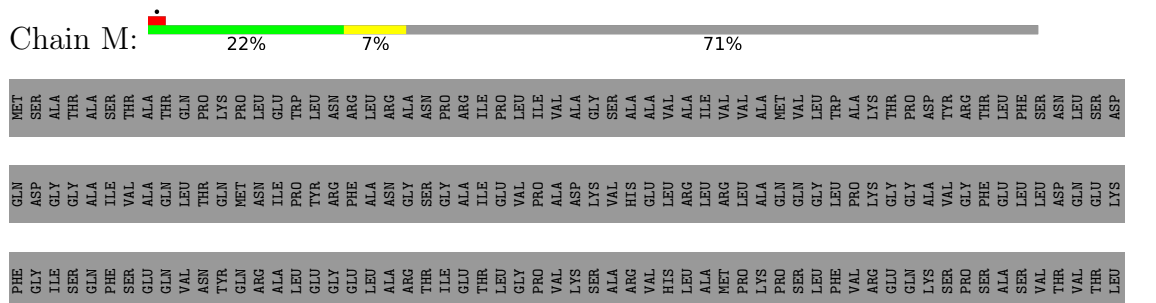
GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	VAL	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	VAL	ASP	GLN	SER	SER	HIS	LEU	LEU	THR	GLN	SER	ASN	THR	SER	GLY	ARG	D229	L230	M231	D232	L235	K236	F237	R244
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K266
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A284
G265
V266
Z276
K275
Q277
Y282
D287
K290
A291
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L293
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S295
E296
G305
ALA GLY TYR PRO GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ILE ALA THR PRO THR ASN GLN GLN ASN ALA

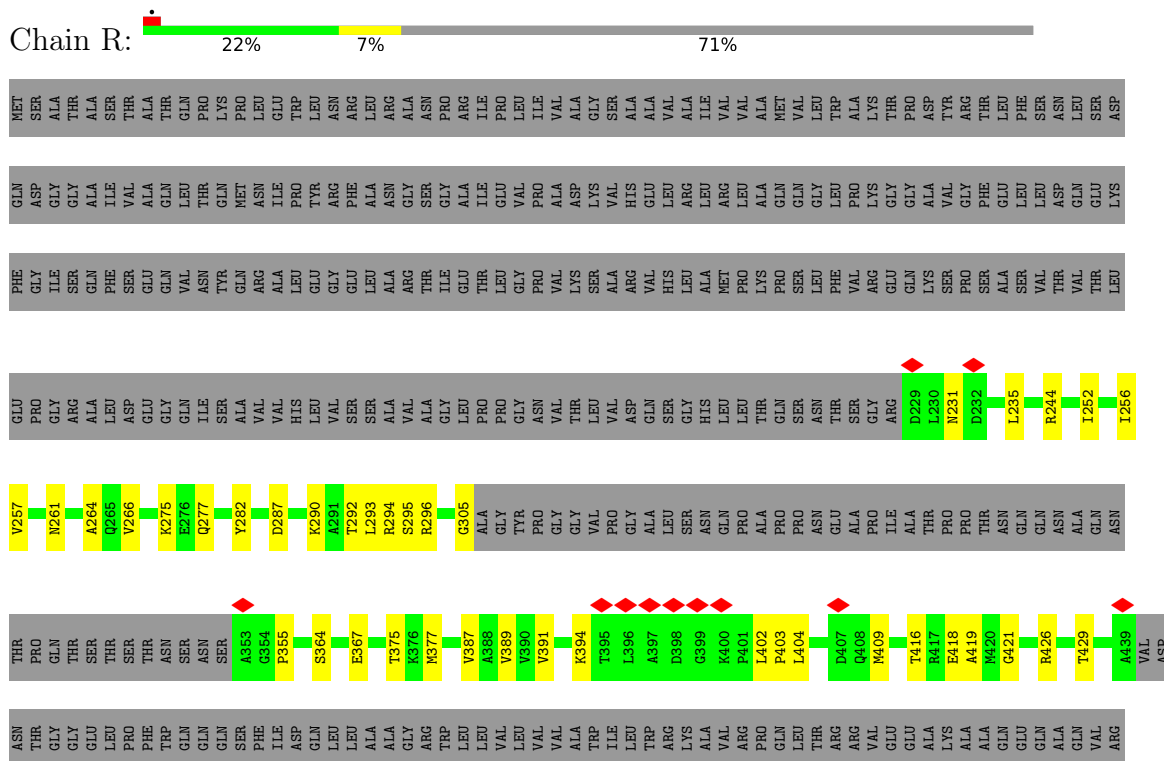
- Molecule 1: Flagellar M-ring protein



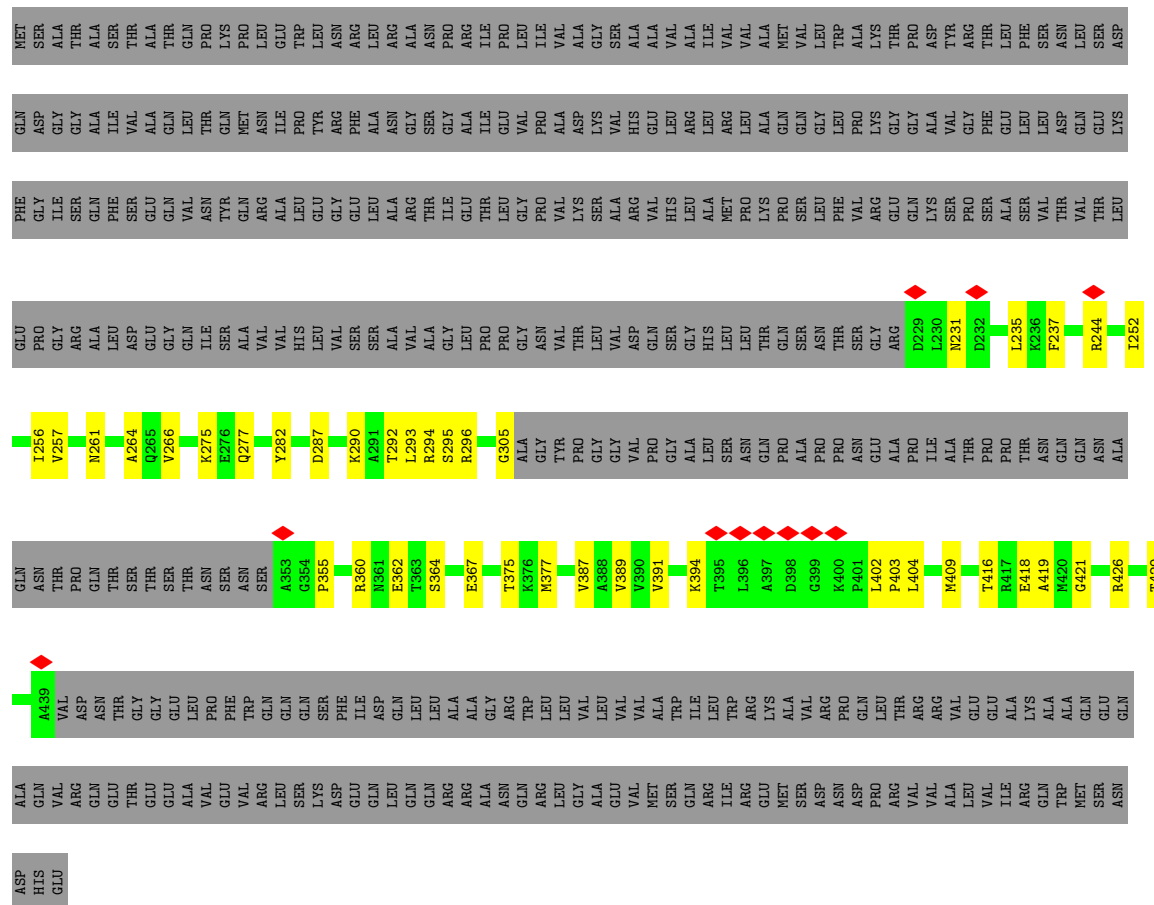
- Molecule 1: Flagellar M-ring protein



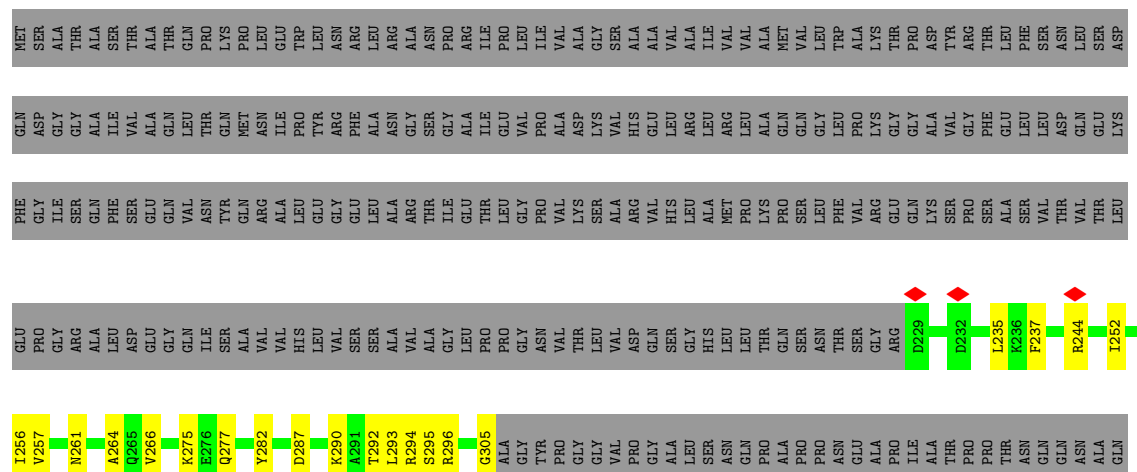


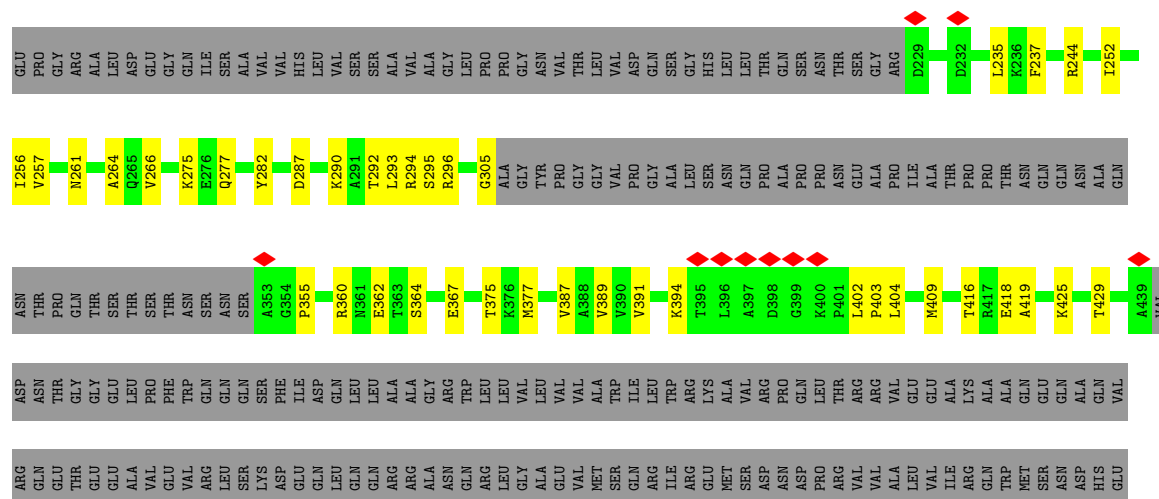


Chain S: 22% 8% 71%

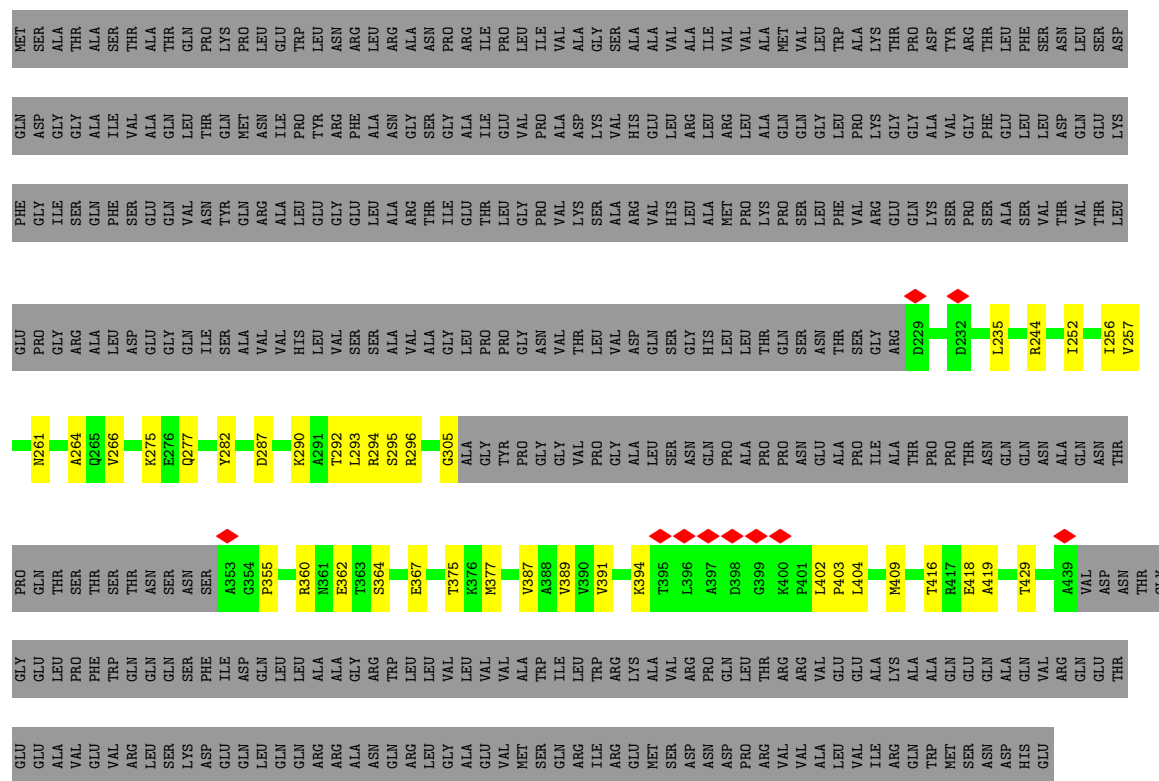


Chain T: 22% 7% 71%

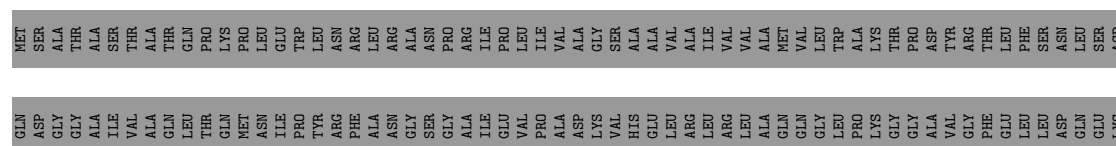


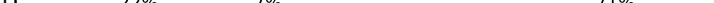


• Molecule 1: Flagellar M-ring protein



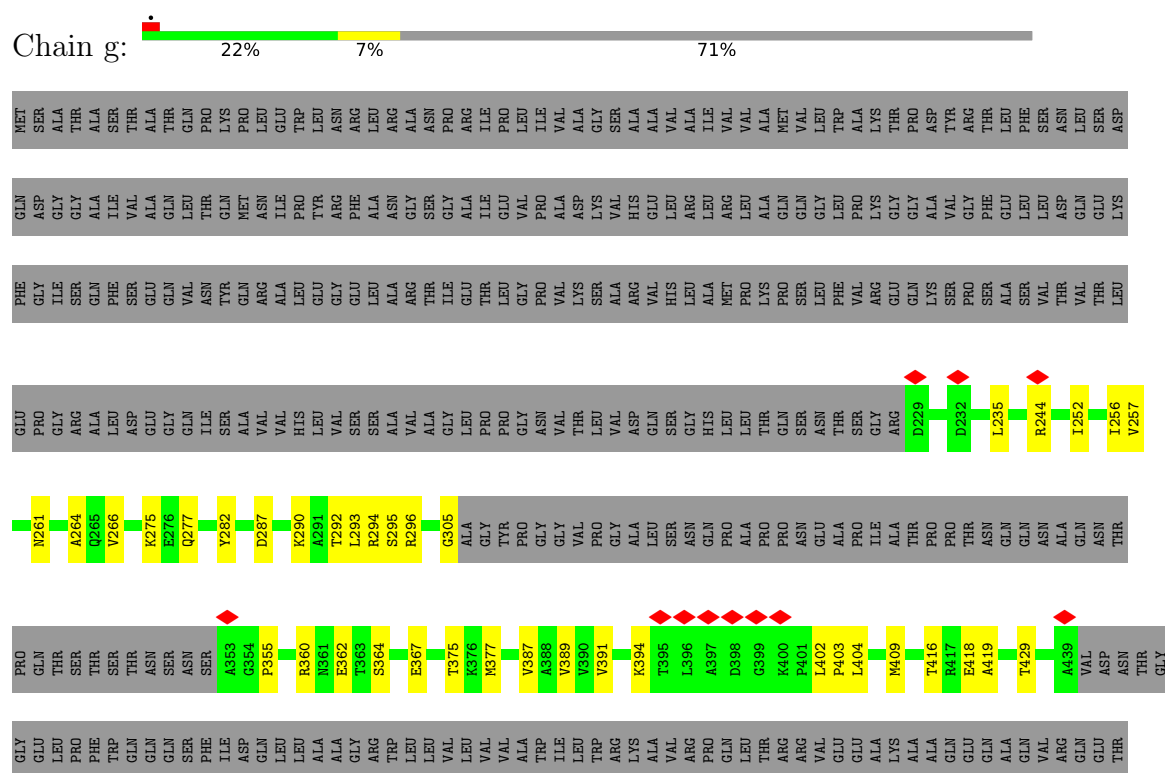
• Molecule 1: Flagellar M-ring protein



Chain b:  22% 7% 71%







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● Molecule 1: Flagellar M-ring protein



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GLY
VAL
THR
LEU
VAL
VAL
GLN
ASP
SER
GLY
HIS
LEU
THR
THR
GLN
SER
ASN
THR
THR
SER
ARG
D229
D232
L235
R244
I252
I256
V257

N261
A264
Q265
V266
K275
E276
Q277
Y282
D287
K290
A291
T292
L293
R294
S295
R296
G305
ALA
GLY
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PRO
GLY
GLY
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A353
G354
P355
R360
A361
E362
T363
S364
E367
T375
R376
K377
V387
A388
V389
V390
V391
K394
T395
L396
A397
D398
G399
K400
P401
L402
P403
L404
M409
T416
R417
E418
A419
T429
A439
VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	11858	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.271	Depositor
Minimum map value	-2.836	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	681.984, 681.984, 681.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332, 1.332, 1.332	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/1289	0.44	1/1741 (0.1%)
1	B	0.22	0/1289	0.44	1/1741 (0.1%)
1	C	0.22	0/1289	0.44	1/1741 (0.1%)
1	D	0.22	0/1289	0.44	1/1741 (0.1%)
1	E	0.22	0/1289	0.44	1/1741 (0.1%)
1	F	0.22	0/1289	0.44	1/1741 (0.1%)
1	G	0.22	0/1289	0.44	1/1741 (0.1%)
1	H	0.22	0/1289	0.44	1/1741 (0.1%)
1	I	0.22	0/1289	0.44	1/1741 (0.1%)
1	J	0.22	0/1289	0.44	1/1741 (0.1%)
1	K	0.22	0/1289	0.44	1/1741 (0.1%)
1	L	0.22	0/1289	0.44	1/1741 (0.1%)
1	M	0.22	0/1289	0.44	1/1741 (0.1%)
1	N	0.22	0/1289	0.44	1/1741 (0.1%)
1	O	0.22	0/1289	0.44	1/1741 (0.1%)
1	P	0.22	0/1289	0.44	1/1741 (0.1%)
1	Q	0.22	0/1289	0.44	1/1741 (0.1%)
1	R	0.22	0/1289	0.44	1/1741 (0.1%)
1	S	0.22	0/1289	0.44	1/1741 (0.1%)
1	T	0.22	0/1289	0.44	1/1741 (0.1%)
1	U	0.22	0/1289	0.44	1/1741 (0.1%)
1	V	0.22	0/1289	0.44	1/1741 (0.1%)
1	W	0.22	0/1289	0.44	1/1741 (0.1%)
1	X	0.22	0/1289	0.44	1/1741 (0.1%)
1	Y	0.22	0/1289	0.44	1/1741 (0.1%)
1	Z	0.22	0/1289	0.44	1/1741 (0.1%)
1	a	0.22	0/1289	0.44	1/1741 (0.1%)
1	b	0.22	0/1289	0.44	1/1741 (0.1%)
1	c	0.22	0/1289	0.44	1/1741 (0.1%)
1	d	0.22	0/1289	0.44	1/1741 (0.1%)
1	e	0.22	0/1289	0.44	1/1741 (0.1%)
1	f	0.22	0/1289	0.44	1/1741 (0.1%)
1	g	0.22	0/1289	0.44	1/1741 (0.1%)
1	h	0.22	0/1289	0.44	1/1741 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.22	0/43826	0.44	34/59194 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	261	ASN	N-CA-C	-5.38	106.57	113.02
1	X	261	ASN	N-CA-C	-5.38	106.57	113.02
1	M	261	ASN	N-CA-C	-5.37	106.57	113.02
1	d	261	ASN	N-CA-C	-5.37	106.57	113.02
1	P	261	ASN	N-CA-C	-5.37	106.58	113.02
1	g	261	ASN	N-CA-C	-5.37	106.58	113.02
1	A	261	ASN	N-CA-C	-5.36	106.59	113.02
1	C	261	ASN	N-CA-C	-5.36	106.58	113.02
1	R	261	ASN	N-CA-C	-5.36	106.59	113.02
1	T	261	ASN	N-CA-C	-5.36	106.58	113.02
1	I	261	ASN	N-CA-C	-5.36	106.59	113.02
1	Z	261	ASN	N-CA-C	-5.36	106.59	113.02
1	J	261	ASN	N-CA-C	-5.36	106.59	113.02
1	N	261	ASN	N-CA-C	-5.36	106.59	113.02
1	a	261	ASN	N-CA-C	-5.36	106.59	113.02
1	e	261	ASN	N-CA-C	-5.36	106.59	113.02
1	F	261	ASN	N-CA-C	-5.36	106.59	113.02
1	Q	261	ASN	N-CA-C	-5.36	106.59	113.02
1	W	261	ASN	N-CA-C	-5.36	106.59	113.02
1	h	261	ASN	N-CA-C	-5.36	106.59	113.02
1	B	261	ASN	N-CA-C	-5.35	106.60	113.02
1	O	261	ASN	N-CA-C	-5.35	106.60	113.02
1	S	261	ASN	N-CA-C	-5.35	106.60	113.02
1	f	261	ASN	N-CA-C	-5.35	106.60	113.02
1	L	261	ASN	N-CA-C	-5.34	106.61	113.02
1	c	261	ASN	N-CA-C	-5.34	106.61	113.02
1	E	261	ASN	N-CA-C	-5.34	106.61	113.02
1	H	261	ASN	N-CA-C	-5.34	106.61	113.02
1	K	261	ASN	N-CA-C	-5.34	106.61	113.02
1	V	261	ASN	N-CA-C	-5.34	106.61	113.02
1	Y	261	ASN	N-CA-C	-5.34	106.61	113.02
1	b	261	ASN	N-CA-C	-5.34	106.61	113.02
1	D	261	ASN	N-CA-C	-5.31	106.64	113.02
1	U	261	ASN	N-CA-C	-5.31	106.64	113.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1275	0	1254	36	0
1	B	1275	0	1254	38	0
1	C	1275	0	1254	40	0
1	D	1275	0	1254	39	0
1	E	1275	0	1254	38	0
1	F	1275	0	1254	39	0
1	G	1275	0	1254	38	0
1	H	1275	0	1254	39	0
1	I	1275	0	1254	40	0
1	J	1275	0	1254	38	0
1	K	1275	0	1254	39	0
1	L	1275	0	1254	40	0
1	M	1275	0	1254	39	0
1	N	1275	0	1254	40	0
1	O	1275	0	1254	39	0
1	P	1275	0	1254	38	0
1	Q	1275	0	1254	37	0
1	R	1275	0	1254	38	0
1	S	1275	0	1254	40	0
1	T	1275	0	1254	37	0
1	U	1275	0	1254	39	0
1	V	1275	0	1254	39	0
1	W	1275	0	1254	37	0
1	X	1275	0	1254	40	0
1	Y	1275	0	1254	38	0
1	Z	1275	0	1254	37	0
1	a	1275	0	1254	38	0
1	b	1275	0	1254	40	0
1	c	1275	0	1254	38	0
1	d	1275	0	1254	39	0
1	e	1275	0	1254	39	0
1	f	1275	0	1254	37	0
1	g	1275	0	1254	37	0
1	h	1275	0	1254	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	43350	0	42636	978	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 (978) 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:b:391:VAL:HG21	1:b:409:MET:HE1	1.78	0.66
1:d:391:VAL:HG21	1:d:409:MET:HE1	1.78	0.66
1:C:391:VAL:HG21	1:C:409:MET:HE1	1.78	0.66
1:G:391:VAL:HG21	1:G:409:MET:HE1	1.78	0.66
1:X:391:VAL:HG21	1:X:409:MET:HE1	1.78	0.66
1:Z:391:VAL:HG21	1:Z:409:MET:HE1	1.78	0.66
1:c:391:VAL:HG21	1:c:409:MET:HE1	1.78	0.66
1:e:391:VAL:HG21	1:e:409:MET:HE1	1.78	0.66
1:f:391:VAL:HG21	1:f:409:MET:HE1	1.78	0.66
1:g:391:VAL:HG21	1:g:409:MET:HE1	1.78	0.66
1:h:391:VAL:HG21	1:h:409:MET:HE1	1.78	0.66
1:A:391:VAL:HG21	1:A:409:MET:HE1	1.78	0.66
1:B:391:VAL:HG21	1:B:409:MET:HE1	1.78	0.66
1:D:391:VAL:HG21	1:D:409:MET:HE1	1.78	0.66
1:E:391:VAL:HG21	1:E:409:MET:HE1	1.78	0.66
1:F:391:VAL:HG21	1:F:409:MET:HE1	1.78	0.66
1:I:391:VAL:HG21	1:I:409:MET:HE1	1.78	0.66
1:W:391:VAL:HG21	1:W:409:MET:HE1	1.78	0.66
1:a:391:VAL:HG21	1:a:409:MET:HE1	1.78	0.66
1:K:391:VAL:HG21	1:K:409:MET:HE1	1.78	0.66
1:M:391:VAL:HG21	1:M:409:MET:HE1	1.78	0.66
1:T:391:VAL:HG21	1:T:409:MET:HE1	1.78	0.66
1:U:391:VAL:HG21	1:U:409:MET:HE1	1.78	0.66
1:V:391:VAL:HG21	1:V:409:MET:HE1	1.78	0.66
1:Y:391:VAL:HG21	1:Y:409:MET:HE1	1.78	0.66
1:H:391:VAL:HG21	1:H:409:MET:HE1	1.78	0.66
1:J:391:VAL:HG21	1:J:409:MET:HE1	1.78	0.66
1:L:391:VAL:HG21	1:L:409:MET:HE1	1.78	0.66
1:O:391:VAL:HG21	1:O:409:MET:HE1	1.78	0.66
1:Q:391:VAL:HG21	1:Q:409:MET:HE1	1.78	0.66
1:N:391:VAL:HG21	1:N:409:MET:HE1	1.78	0.66
1:P:391:VAL:HG21	1:P:409:MET:HE1	1.78	0.66
1:R:391:VAL:HG21	1:R:409:MET:HE1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:391:VAL:HG21	1:S:409:MET:HE1	1.78	0.66
1:L:389:VAL:HG21	1:L:416:THR:HG21	1.79	0.65
1:A:389:VAL:HG21	1:A:416:THR:HG21	1.79	0.65
1:C:389:VAL:HG21	1:C:416:THR:HG21	1.79	0.65
1:N:389:VAL:HG21	1:N:416:THR:HG21	1.79	0.65
1:g:389:VAL:HG21	1:g:416:THR:HG21	1.79	0.65
1:E:235:LEU:HD22	1:F:244:ARG:HH12	1.62	0.65
1:H:389:VAL:HG21	1:H:416:THR:HG21	1.79	0.65
1:J:389:VAL:HG21	1:J:416:THR:HG21	1.79	0.65
1:O:389:VAL:HG21	1:O:416:THR:HG21	1.79	0.65
1:P:389:VAL:HG21	1:P:416:THR:HG21	1.79	0.65
1:d:389:VAL:HG21	1:d:416:THR:HG21	1.79	0.65
1:e:389:VAL:HG21	1:e:416:THR:HG21	1.79	0.65
1:f:389:VAL:HG21	1:f:416:THR:HG21	1.79	0.65
1:h:389:VAL:HG21	1:h:416:THR:HG21	1.79	0.65
1:C:235:LEU:HD22	1:D:244:ARG:HH12	1.62	0.65
1:E:389:VAL:HG21	1:E:416:THR:HG21	1.79	0.65
1:G:235:LEU:HD22	1:H:244:ARG:HH12	1.62	0.65
1:G:389:VAL:HG21	1:G:416:THR:HG21	1.79	0.65
1:A:235:LEU:HD22	1:B:244:ARG:HH12	1.62	0.65
1:D:389:VAL:HG21	1:D:416:THR:HG21	1.79	0.65
1:I:235:LEU:HD22	1:J:244:ARG:HH12	1.62	0.65
1:M:389:VAL:HG21	1:M:416:THR:HG21	1.79	0.65
1:Q:389:VAL:HG21	1:Q:416:THR:HG21	1.79	0.65
1:R:389:VAL:HG21	1:R:416:THR:HG21	1.79	0.65
1:S:389:VAL:HG21	1:S:416:THR:HG21	1.79	0.65
1:X:235:LEU:HD22	1:Y:244:ARG:HH12	1.62	0.65
1:Z:235:LEU:HD22	1:a:244:ARG:HH12	1.62	0.65
1:b:389:VAL:HG21	1:b:416:THR:HG21	1.79	0.65
1:c:389:VAL:HG21	1:c:416:THR:HG21	1.79	0.65
1:F:389:VAL:HG21	1:F:416:THR:HG21	1.79	0.64
1:I:389:VAL:HG21	1:I:416:THR:HG21	1.79	0.64
1:K:389:VAL:HG21	1:K:416:THR:HG21	1.79	0.64
1:V:235:LEU:HD22	1:W:244:ARG:HH12	1.62	0.64
1:Z:389:VAL:HG21	1:Z:416:THR:HG21	1.79	0.64
1:g:235:LEU:HD22	1:h:244:ARG:HH12	1.62	0.64
1:B:389:VAL:HG21	1:B:416:THR:HG21	1.79	0.64
1:T:389:VAL:HG21	1:T:416:THR:HG21	1.79	0.64
1:U:389:VAL:HG21	1:U:416:THR:HG21	1.79	0.64
1:X:389:VAL:HG21	1:X:416:THR:HG21	1.79	0.64
1:a:389:VAL:HG21	1:a:416:THR:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:235:LEU:HD22	1:c:244:ARG:HH12	1.62	0.64
1:K:235:LEU:HD22	1:L:244:ARG:HH12	1.62	0.64
1:V:389:VAL:HG21	1:V:416:THR:HG21	1.79	0.64
1:W:389:VAL:HG21	1:W:416:THR:HG21	1.79	0.64
1:T:235:LEU:HD22	1:U:244:ARG:HH12	1.62	0.64
1:Y:389:VAL:HG21	1:Y:416:THR:HG21	1.79	0.64
1:d:235:LEU:HD22	1:e:244:ARG:HH12	1.62	0.64
1:e:235:LEU:HD22	1:f:244:ARG:HH12	1.62	0.64
1:M:235:LEU:HD22	1:N:244:ARG:HH12	1.62	0.64
1:c:235:LEU:HD22	1:d:244:ARG:HH12	1.62	0.64
1:N:235:LEU:HD22	1:O:244:ARG:HH12	1.62	0.64
1:O:235:LEU:HD22	1:P:244:ARG:HH12	1.62	0.64
1:a:235:LEU:HD22	1:b:244:ARG:HH12	1.62	0.64
1:f:235:LEU:HD22	1:g:244:ARG:HH12	1.62	0.64
1:P:235:LEU:HD22	1:Q:244:ARG:HH12	1.62	0.64
1:R:235:LEU:HD22	1:S:244:ARG:HH12	1.62	0.64
1:S:394:LYS:HE3	1:S:394:LYS:HA	1.80	0.64
1:U:394:LYS:HE3	1:U:394:LYS:HA	1.80	0.64
1:A:244:ARG:HH12	1:h:235:LEU:HD22	1.62	0.64
1:Q:235:LEU:HD22	1:R:244:ARG:HH12	1.62	0.64
1:S:235:LEU:HD22	1:T:244:ARG:HH12	1.62	0.64
1:S:287:ASP:HB3	1:S:290:LYS:HE2	1.80	0.64
1:Y:235:LEU:HD22	1:Z:244:ARG:HH12	1.62	0.64
1:Y:394:LYS:HE3	1:Y:394:LYS:HA	1.80	0.64
1:h:287:ASP:HB3	1:h:290:LYS:HE2	1.80	0.64
1:U:235:LEU:HD22	1:V:244:ARG:HH12	1.62	0.64
1:W:235:LEU:HD22	1:X:244:ARG:HH12	1.62	0.64
1:W:394:LYS:HE3	1:W:394:LYS:HA	1.80	0.64
1:Z:394:LYS:HE3	1:Z:394:LYS:HA	1.80	0.64
1:g:287:ASP:HB3	1:g:290:LYS:HE2	1.80	0.64
1:F:287:ASP:HB3	1:F:290:LYS:HE2	1.80	0.64
1:L:287:ASP:HB3	1:L:290:LYS:HE2	1.80	0.64
1:M:287:ASP:HB3	1:M:290:LYS:HE2	1.80	0.64
1:X:394:LYS:HE3	1:X:394:LYS:HA	1.80	0.64
1:b:394:LYS:HA	1:b:394:LYS:HE3	1.80	0.64
1:B:235:LEU:HD22	1:C:244:ARG:HH12	1.62	0.63
1:E:287:ASP:HB3	1:E:290:LYS:HE2	1.80	0.63
1:N:394:LYS:HE3	1:N:394:LYS:HA	1.80	0.63
1:P:394:LYS:HE3	1:P:394:LYS:HA	1.80	0.63
1:Q:394:LYS:HA	1:Q:394:LYS:HE3	1.80	0.63
1:R:287:ASP:HB3	1:R:290:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:394:LYS:HE3	1:R:394:LYS:HA	1.80	0.63
1:V:394:LYS:HA	1:V:394:LYS:HE3	1.80	0.63
1:O:394:LYS:HA	1:O:394:LYS:HE3	1.80	0.63
1:T:287:ASP:HB3	1:T:290:LYS:HE2	1.80	0.63
1:T:394:LYS:HE3	1:T:394:LYS:HA	1.80	0.63
1:a:394:LYS:HE3	1:a:394:LYS:HA	1.80	0.63
1:c:287:ASP:HB3	1:c:290:LYS:HE2	1.80	0.63
1:A:287:ASP:HB3	1:A:290:LYS:HE2	1.80	0.63
1:D:235:LEU:HD22	1:E:244:ARG:HH12	1.62	0.63
1:G:287:ASP:HB3	1:G:290:LYS:HE2	1.80	0.63
1:L:394:LYS:HE3	1:L:394:LYS:HA	1.80	0.63
1:N:287:ASP:HB3	1:N:290:LYS:HE2	1.80	0.63
1:X:287:ASP:HB3	1:X:290:LYS:HE2	1.80	0.63
1:d:394:LYS:HE3	1:d:394:LYS:HA	1.80	0.63
1:F:235:LEU:HD22	1:G:244:ARG:HH12	1.62	0.63
1:J:235:LEU:HD22	1:K:244:ARG:HH12	1.62	0.63
1:L:235:LEU:HD22	1:M:244:ARG:HH12	1.62	0.63
1:b:287:ASP:HB3	1:b:290:LYS:HE2	1.80	0.63
1:D:287:ASP:HB3	1:D:290:LYS:HE2	1.80	0.63
1:H:235:LEU:HD22	1:I:244:ARG:HH12	1.62	0.63
1:W:287:ASP:HB3	1:W:290:LYS:HE2	1.80	0.63
1:c:394:LYS:HE3	1:c:394:LYS:HA	1.80	0.63
1:g:235:LEU:HB3	1:h:244:ARG:HH22	1.64	0.63
1:K:287:ASP:HB3	1:K:290:LYS:HE2	1.80	0.63
1:Q:287:ASP:HB3	1:Q:290:LYS:HE2	1.80	0.63
1:f:287:ASP:HB3	1:f:290:LYS:HE2	1.80	0.63
1:f:394:LYS:HE3	1:f:394:LYS:HA	1.80	0.63
1:I:235:LEU:HB3	1:J:244:ARG:HH22	1.64	0.63
1:J:394:LYS:HA	1:J:394:LYS:HE3	1.80	0.63
1:M:394:LYS:HE3	1:M:394:LYS:HA	1.80	0.63
1:Y:287:ASP:HB3	1:Y:290:LYS:HE2	1.80	0.63
1:B:235:LEU:HB3	1:C:244:ARG:HH22	1.64	0.63
1:D:235:LEU:HB3	1:E:244:ARG:HH22	1.64	0.63
1:G:235:LEU:HB3	1:H:244:ARG:HH22	1.64	0.63
1:L:235:LEU:HB3	1:M:244:ARG:HH22	1.64	0.63
1:N:235:LEU:HB3	1:O:244:ARG:HH22	1.64	0.63
1:b:235:LEU:HB3	1:c:244:ARG:HH22	1.64	0.63
1:e:235:LEU:HB3	1:f:244:ARG:HH22	1.64	0.63
1:Q:235:LEU:HB3	1:R:244:ARG:HH22	1.64	0.63
1:d:287:ASP:HB3	1:d:290:LYS:HE2	1.80	0.63
1:H:287:ASP:HB3	1:H:290:LYS:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:394:LYS:HE3	1:K:394:LYS:HA	1.80	0.62
1:O:287:ASP:HB3	1:O:290:LYS:HE2	1.80	0.62
1:U:287:ASP:HB3	1:U:290:LYS:HE2	1.80	0.62
1:a:287:ASP:HB3	1:a:290:LYS:HE2	1.80	0.62
1:e:394:LYS:HE3	1:e:394:LYS:HA	1.80	0.62
1:B:287:ASP:HB3	1:B:290:LYS:HE2	1.80	0.62
1:H:394:LYS:HE3	1:H:394:LYS:HA	1.80	0.62
1:h:394:LYS:HE3	1:h:394:LYS:HA	1.80	0.62
1:T:235:LEU:HB3	1:U:244:ARG:HH22	1.64	0.62
1:Y:235:LEU:HB3	1:Z:244:ARG:HH22	1.64	0.62
1:d:235:LEU:HB3	1:e:244:ARG:HH22	1.64	0.62
1:B:394:LYS:HE3	1:B:394:LYS:HA	1.80	0.62
1:O:235:LEU:HB3	1:P:244:ARG:HH22	1.64	0.62
1:V:287:ASP:HB3	1:V:290:LYS:HE2	1.80	0.62
1:g:394:LYS:HA	1:g:394:LYS:HE3	1.80	0.62
1:A:235:LEU:HB3	1:B:244:ARG:HH22	1.64	0.62
1:F:235:LEU:HB3	1:G:244:ARG:HH22	1.64	0.62
1:J:235:LEU:HB3	1:K:244:ARG:HH22	1.64	0.62
1:K:235:LEU:HB3	1:L:244:ARG:HH22	1.64	0.62
1:V:235:LEU:HB3	1:W:244:ARG:HH22	1.64	0.62
1:A:244:ARG:HH22	1:h:235:LEU:HB3	1.64	0.62
1:C:287:ASP:HB3	1:C:290:LYS:HE2	1.80	0.62
1:D:394:LYS:HE3	1:D:394:LYS:HA	1.80	0.62
1:E:235:LEU:HB3	1:F:244:ARG:HH22	1.64	0.62
1:F:394:LYS:HE3	1:F:394:LYS:HA	1.80	0.62
1:J:287:ASP:HB3	1:J:290:LYS:HE2	1.80	0.62
1:W:235:LEU:HB3	1:X:244:ARG:HH22	1.64	0.62
1:I:394:LYS:HE3	1:I:394:LYS:HA	1.80	0.62
1:Z:235:LEU:HB3	1:a:244:ARG:HH22	1.64	0.62
1:Z:287:ASP:HB3	1:Z:290:LYS:HE2	1.80	0.62
1:e:287:ASP:HB3	1:e:290:LYS:HE2	1.80	0.62
1:G:394:LYS:HE3	1:G:394:LYS:HA	1.80	0.62
1:S:235:LEU:HB3	1:T:244:ARG:HH22	1.64	0.62
1:A:394:LYS:HE3	1:A:394:LYS:HA	1.80	0.62
1:C:394:LYS:HE3	1:C:394:LYS:HA	1.80	0.62
1:P:287:ASP:HB3	1:P:290:LYS:HE2	1.80	0.62
1:P:235:LEU:HB3	1:Q:244:ARG:HH22	1.64	0.62
1:a:235:LEU:HB3	1:b:244:ARG:HH22	1.64	0.62
1:E:394:LYS:HA	1:E:394:LYS:HE3	1.80	0.61
1:C:235:LEU:HB3	1:D:244:ARG:HH22	1.64	0.61
1:I:287:ASP:HB3	1:I:290:LYS:HE2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:235:LEU:HB3	1:S:244:ARG:HH22	1.64	0.61
1:c:235:LEU:HB3	1:d:244:ARG:HH22	1.64	0.61
1:U:235:LEU:HB3	1:V:244:ARG:HH22	1.64	0.61
1:X:235:LEU:HB3	1:Y:244:ARG:HH22	1.64	0.61
1:Z:277:GLN:HB3	1:Z:377:MET:HE1	1.83	0.61
1:f:235:LEU:HB3	1:g:244:ARG:HH22	1.64	0.61
1:H:235:LEU:HB3	1:I:244:ARG:HH22	1.64	0.61
1:M:235:LEU:HB3	1:N:244:ARG:HH22	1.64	0.61
1:Y:277:GLN:HB3	1:Y:377:MET:HE1	1.83	0.61
1:a:277:GLN:HB3	1:a:377:MET:HE1	1.83	0.61
1:c:277:GLN:HB3	1:c:377:MET:HE1	1.83	0.61
1:X:277:GLN:HB3	1:X:377:MET:HE1	1.83	0.61
1:b:277:GLN:HB3	1:b:377:MET:HE1	1.83	0.61
1:d:277:GLN:HB3	1:d:377:MET:HE1	1.83	0.61
1:W:277:GLN:HB3	1:W:377:MET:HE1	1.83	0.61
1:e:277:GLN:HB3	1:e:377:MET:HE1	1.83	0.61
1:g:277:GLN:HB3	1:g:377:MET:HE1	1.83	0.61
1:U:277:GLN:HB3	1:U:377:MET:HE1	1.83	0.60
1:V:277:GLN:HB3	1:V:377:MET:HE1	1.83	0.60
1:f:277:GLN:HB3	1:f:377:MET:HE1	1.83	0.60
1:h:277:GLN:HB3	1:h:377:MET:HE1	1.83	0.60
1:T:277:GLN:HB3	1:T:377:MET:HE1	1.83	0.60
1:A:277:GLN:HB3	1:A:377:MET:HE1	1.83	0.60
1:B:277:GLN:HB3	1:B:377:MET:HE1	1.83	0.60
1:S:277:GLN:HB3	1:S:377:MET:HE1	1.83	0.60
1:C:277:GLN:HB3	1:C:377:MET:HE1	1.83	0.60
1:H:277:GLN:HB3	1:H:377:MET:HE1	1.83	0.60
1:M:277:GLN:HB3	1:M:377:MET:HE1	1.83	0.60
1:D:277:GLN:HB3	1:D:377:MET:HE1	1.83	0.60
1:I:277:GLN:HB3	1:I:377:MET:HE1	1.83	0.60
1:Q:277:GLN:HB3	1:Q:377:MET:HE1	1.83	0.59
1:R:277:GLN:HB3	1:R:377:MET:HE1	1.83	0.59
1:G:277:GLN:HB3	1:G:377:MET:HE1	1.83	0.59
1:P:402:LEU:HD12	1:P:403:PRO:HD2	1.84	0.59
1:L:277:GLN:HB3	1:L:377:MET:HE1	1.83	0.59
1:N:277:GLN:HB3	1:N:377:MET:HE1	1.83	0.59
1:A:402:LEU:HD12	1:A:403:PRO:HD2	1.84	0.59
1:M:402:LEU:HD12	1:M:403:PRO:HD2	1.84	0.59
1:N:402:LEU:HD12	1:N:403:PRO:HD2	1.84	0.59
1:S:402:LEU:HD12	1:S:403:PRO:HD2	1.84	0.59
1:c:402:LEU:HD12	1:c:403:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:GLN:HB3	1:F:377:MET:HE1	1.83	0.59
1:O:277:GLN:HB3	1:O:377:MET:HE1	1.83	0.59
1:Q:402:LEU:HD12	1:Q:403:PRO:HD2	1.84	0.59
1:T:402:LEU:HD12	1:T:403:PRO:HD2	1.84	0.59
1:h:402:LEU:HD12	1:h:403:PRO:HD2	1.84	0.59
1:B:402:LEU:HD12	1:B:403:PRO:HD2	1.84	0.59
1:L:402:LEU:HD12	1:L:403:PRO:HD2	1.84	0.59
1:O:402:LEU:HD12	1:O:403:PRO:HD2	1.84	0.59
1:P:277:GLN:HB3	1:P:377:MET:HE1	1.83	0.59
1:E:277:GLN:HB3	1:E:377:MET:HE1	1.83	0.59
1:b:402:LEU:HD12	1:b:403:PRO:HD2	1.84	0.59
1:d:402:LEU:HD12	1:d:403:PRO:HD2	1.84	0.59
1:J:402:LEU:HD12	1:J:403:PRO:HD2	1.84	0.59
1:K:402:LEU:HD12	1:K:403:PRO:HD2	1.84	0.59
1:R:402:LEU:HD12	1:R:403:PRO:HD2	1.84	0.59
1:I:402:LEU:HD12	1:I:403:PRO:HD2	1.84	0.59
1:J:277:GLN:HB3	1:J:377:MET:HE1	1.83	0.59
1:V:402:LEU:HD12	1:V:403:PRO:HD2	1.84	0.59
1:W:377:MET:SD	1:W:377:MET:N	2.76	0.59
1:g:402:LEU:HD12	1:g:403:PRO:HD2	1.84	0.59
1:K:277:GLN:HB3	1:K:377:MET:HE1	1.83	0.58
1:U:377:MET:SD	1:U:377:MET:N	2.76	0.58
1:U:402:LEU:HD12	1:U:403:PRO:HD2	1.84	0.58
1:W:402:LEU:HD12	1:W:403:PRO:HD2	1.84	0.58
1:Y:377:MET:N	1:Y:377:MET:SD	2.76	0.58
1:S:377:MET:SD	1:S:377:MET:N	2.76	0.58
1:U:305:GLY:HA3	1:U:355:PRO:HG2	1.86	0.58
1:a:377:MET:SD	1:a:377:MET:N	2.76	0.58
1:F:402:LEU:HD12	1:F:403:PRO:HD2	1.84	0.58
1:Z:305:GLY:HA3	1:Z:355:PRO:HG2	1.86	0.58
1:e:252:ILE:HD11	1:e:419:ALA:HB2	1.85	0.58
1:e:402:LEU:HD12	1:e:403:PRO:HD2	1.84	0.58
1:Q:377:MET:SD	1:Q:377:MET:N	2.76	0.58
1:V:305:GLY:HA3	1:V:355:PRO:HG2	1.86	0.58
1:d:252:ILE:HD11	1:d:419:ALA:HB2	1.85	0.58
1:f:252:ILE:HD11	1:f:419:ALA:HB2	1.85	0.58
1:E:377:MET:SD	1:E:377:MET:N	2.76	0.58
1:G:402:LEU:HD12	1:G:403:PRO:HD2	1.84	0.58
1:Z:252:ILE:HD11	1:Z:419:ALA:HB2	1.85	0.58
1:a:305:GLY:HA3	1:a:355:PRO:HG2	1.86	0.58
1:c:377:MET:SD	1:c:377:MET:N	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:LEU:HD12	1:E:403:PRO:HD2	1.84	0.58
1:H:402:LEU:HD12	1:H:403:PRO:HD2	1.84	0.58
1:O:305:GLY:HA3	1:O:355:PRO:HG2	1.86	0.58
1:O:377:MET:SD	1:O:377:MET:N	2.76	0.58
1:P:305:GLY:HA3	1:P:355:PRO:HG2	1.86	0.58
1:R:377:MET:SD	1:R:377:MET:N	2.76	0.58
1:T:305:GLY:HA3	1:T:355:PRO:HG2	1.86	0.58
1:X:402:LEU:HD12	1:X:403:PRO:HD2	1.84	0.58
1:Y:252:ILE:HD11	1:Y:419:ALA:HB2	1.85	0.58
1:B:377:MET:SD	1:B:377:MET:N	2.76	0.58
1:C:402:LEU:HD12	1:C:403:PRO:HD2	1.84	0.58
1:G:377:MET:SD	1:G:377:MET:N	2.76	0.58
1:P:377:MET:SD	1:P:377:MET:N	2.76	0.58
1:T:377:MET:N	1:T:377:MET:SD	2.76	0.58
1:X:252:ILE:HD11	1:X:419:ALA:HB2	1.85	0.58
1:a:402:LEU:HD12	1:a:403:PRO:HD2	1.84	0.58
1:B:252:ILE:HD11	1:B:419:ALA:HB2	1.85	0.58
1:C:252:ILE:HD11	1:C:419:ALA:HB2	1.85	0.58
1:Q:305:GLY:HA3	1:Q:355:PRO:HG2	1.86	0.58
1:V:377:MET:SD	1:V:377:MET:N	2.76	0.58
1:f:305:GLY:HA3	1:f:355:PRO:HG2	1.86	0.58
1:C:377:MET:N	1:C:377:MET:SD	2.76	0.58
1:L:252:ILE:HD11	1:L:419:ALA:HB2	1.85	0.58
1:M:377:MET:SD	1:M:377:MET:N	2.76	0.58
1:O:252:ILE:HD11	1:O:419:ALA:HB2	1.85	0.58
1:Y:305:GLY:HA3	1:Y:355:PRO:HG2	1.86	0.58
1:Z:402:LEU:HD12	1:Z:403:PRO:HD2	1.84	0.58
1:e:377:MET:SD	1:e:377:MET:N	2.76	0.58
1:h:377:MET:SD	1:h:377:MET:N	2.76	0.58
1:I:252:ILE:HD11	1:I:419:ALA:HB2	1.85	0.58
1:J:252:ILE:HD11	1:J:419:ALA:HB2	1.85	0.58
1:J:377:MET:SD	1:J:377:MET:N	2.76	0.58
1:M:252:ILE:HD11	1:M:419:ALA:HB2	1.85	0.58
1:N:377:MET:SD	1:N:377:MET:N	2.76	0.58
1:c:252:ILE:HD11	1:c:419:ALA:HB2	1.85	0.58
1:e:305:GLY:HA3	1:e:355:PRO:HG2	1.86	0.58
1:f:402:LEU:HD12	1:f:403:PRO:HD2	1.84	0.58
1:W:305:GLY:HA3	1:W:355:PRO:HG2	1.86	0.57
1:X:377:MET:SD	1:X:377:MET:N	2.76	0.57
1:Y:402:LEU:HD12	1:Y:403:PRO:HD2	1.84	0.57
1:a:252:ILE:HD11	1:a:419:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:305:GLY:HA3	1:b:355:PRO:HG2	1.86	0.57
1:A:252:ILE:HD11	1:A:419:ALA:HB2	1.85	0.57
1:D:377:MET:SD	1:D:377:MET:N	2.76	0.57
1:K:252:ILE:HD11	1:K:419:ALA:HB2	1.85	0.57
1:P:252:ILE:HD11	1:P:419:ALA:HB2	1.85	0.57
1:Z:377:MET:SD	1:Z:377:MET:N	2.76	0.57
1:A:377:MET:SD	1:A:377:MET:N	2.76	0.57
1:J:305:GLY:HA3	1:J:355:PRO:HG2	1.86	0.57
1:K:305:GLY:HA3	1:K:355:PRO:HG2	1.86	0.57
1:K:377:MET:SD	1:K:377:MET:N	2.76	0.57
1:N:305:GLY:HA3	1:N:355:PRO:HG2	1.86	0.57
1:S:305:GLY:HA3	1:S:355:PRO:HG2	1.86	0.57
1:g:252:ILE:HD11	1:g:419:ALA:HB2	1.85	0.57
1:g:305:GLY:HA3	1:g:355:PRO:HG2	1.86	0.57
1:D:402:LEU:HD12	1:D:403:PRO:HD2	1.84	0.57
1:N:252:ILE:HD11	1:N:419:ALA:HB2	1.85	0.57
1:R:252:ILE:HD11	1:R:419:ALA:HB2	1.85	0.57
1:T:252:ILE:HD11	1:T:419:ALA:HB2	1.85	0.57
1:b:377:MET:SD	1:b:377:MET:N	2.76	0.57
1:d:305:GLY:HA3	1:d:355:PRO:HG2	1.86	0.57
1:g:377:MET:SD	1:g:377:MET:N	2.76	0.57
1:D:252:ILE:HD11	1:D:419:ALA:HB2	1.85	0.57
1:H:252:ILE:HD11	1:H:419:ALA:HB2	1.85	0.57
1:I:305:GLY:HA3	1:I:355:PRO:HG2	1.86	0.57
1:L:377:MET:SD	1:L:377:MET:N	2.76	0.57
1:Q:252:ILE:HD11	1:Q:419:ALA:HB2	1.85	0.57
1:R:305:GLY:HA3	1:R:355:PRO:HG2	1.86	0.57
1:S:252:ILE:HD11	1:S:419:ALA:HB2	1.85	0.57
1:W:252:ILE:HD11	1:W:419:ALA:HB2	1.85	0.57
1:D:305:GLY:HA3	1:D:355:PRO:HG2	1.86	0.57
1:I:377:MET:SD	1:I:377:MET:N	2.76	0.57
1:L:305:GLY:HA3	1:L:355:PRO:HG2	1.86	0.57
1:d:377:MET:SD	1:d:377:MET:N	2.76	0.57
1:F:252:ILE:HD11	1:F:419:ALA:HB2	1.85	0.57
1:G:252:ILE:HD11	1:G:419:ALA:HB2	1.85	0.57
1:X:305:GLY:HA3	1:X:355:PRO:HG2	1.86	0.57
1:C:305:GLY:HA3	1:C:355:PRO:HG2	1.86	0.57
1:E:305:GLY:HA3	1:E:355:PRO:HG2	1.86	0.57
1:f:377:MET:SD	1:f:377:MET:N	2.76	0.57
1:b:252:ILE:HD11	1:b:419:ALA:HB2	1.85	0.57
1:U:252:ILE:HD11	1:U:419:ALA:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:305:GLY:HA3	1:c:355:PRO:HG2	1.86	0.56
1:B:305:GLY:HA3	1:B:355:PRO:HG2	1.86	0.56
1:E:252:ILE:HD11	1:E:419:ALA:HB2	1.85	0.56
1:h:252:ILE:HD11	1:h:419:ALA:HB2	1.85	0.56
1:h:305:GLY:HA3	1:h:355:PRO:HG2	1.86	0.56
1:F:377:MET:SD	1:F:377:MET:N	2.76	0.56
1:F:305:GLY:HA3	1:F:355:PRO:HG2	1.86	0.56
1:H:305:GLY:HA3	1:H:355:PRO:HG2	1.86	0.56
1:V:252:ILE:HD11	1:V:419:ALA:HB2	1.85	0.56
1:M:305:GLY:HA3	1:M:355:PRO:HG2	1.86	0.56
1:G:305:GLY:HA3	1:G:355:PRO:HG2	1.86	0.56
1:H:377:MET:SD	1:H:377:MET:N	2.76	0.56
1:A:305:GLY:HA3	1:A:355:PRO:HG2	1.86	0.56
1:D:264:ALA:HB2	1:D:389:VAL:HG13	1.89	0.55
1:F:264:ALA:HB2	1:F:389:VAL:HG13	1.89	0.55
1:I:264:ALA:HB2	1:I:389:VAL:HG13	1.89	0.55
1:L:264:ALA:HB2	1:L:389:VAL:HG13	1.89	0.55
1:M:264:ALA:HB2	1:M:389:VAL:HG13	1.89	0.55
1:U:264:ALA:HB2	1:U:389:VAL:HG13	1.89	0.55
1:G:264:ALA:HB2	1:G:389:VAL:HG13	1.89	0.55
1:P:264:ALA:HB2	1:P:389:VAL:HG13	1.89	0.55
1:R:264:ALA:HB2	1:R:389:VAL:HG13	1.89	0.55
1:S:264:ALA:HB2	1:S:389:VAL:HG13	1.89	0.55
1:J:264:ALA:HB2	1:J:389:VAL:HG13	1.89	0.55
1:O:264:ALA:HB2	1:O:389:VAL:HG13	1.89	0.55
1:A:264:ALA:HB2	1:A:389:VAL:HG13	1.89	0.55
1:V:264:ALA:HB2	1:V:389:VAL:HG13	1.89	0.55
1:X:264:ALA:HB2	1:X:389:VAL:HG13	1.89	0.55
1:A:409:MET:HA	1:A:409:MET:HE2	1.89	0.55
1:B:409:MET:HE2	1:B:409:MET:HA	1.89	0.55
1:C:264:ALA:HB2	1:C:389:VAL:HG13	1.89	0.55
1:D:409:MET:HE2	1:D:409:MET:HA	1.89	0.55
1:E:409:MET:HE2	1:E:409:MET:HA	1.89	0.55
1:C:409:MET:HA	1:C:409:MET:HE2	1.89	0.55
1:h:409:MET:HA	1:h:409:MET:HE2	1.89	0.55
1:F:409:MET:HA	1:F:409:MET:HE2	1.89	0.54
1:a:264:ALA:HB2	1:a:389:VAL:HG13	1.89	0.54
1:f:264:ALA:HB2	1:f:389:VAL:HG13	1.89	0.54
1:g:409:MET:HE2	1:g:409:MET:HA	1.89	0.54
1:G:409:MET:HE2	1:G:409:MET:HA	1.89	0.54
1:c:264:ALA:HB2	1:c:389:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:409:MET:HA	1:H:409:MET:HE2	1.89	0.54
1:J:409:MET:HA	1:J:409:MET:HE2	1.89	0.54
1:d:264:ALA:HB2	1:d:389:VAL:HG13	1.89	0.54
1:f:409:MET:HE2	1:f:409:MET:HA	1.89	0.54
1:I:409:MET:HE2	1:I:409:MET:HA	1.89	0.54
1:K:409:MET:HE2	1:K:409:MET:HA	1.89	0.54
1:Z:264:ALA:HB2	1:Z:389:VAL:HG13	1.89	0.54
1:e:409:MET:HA	1:e:409:MET:HE2	1.89	0.54
1:h:264:ALA:HB2	1:h:389:VAL:HG13	1.89	0.54
1:L:409:MET:HE2	1:L:409:MET:HA	1.89	0.54
1:Y:264:ALA:HB2	1:Y:389:VAL:HG13	1.89	0.54
1:g:264:ALA:HB2	1:g:389:VAL:HG13	1.89	0.54
1:d:409:MET:HE2	1:d:409:MET:HA	1.89	0.54
1:B:264:ALA:HB2	1:B:389:VAL:HG13	1.89	0.54
1:E:264:ALA:HB2	1:E:389:VAL:HG13	1.89	0.54
1:M:409:MET:HA	1:M:409:MET:HE2	1.89	0.54
1:V:409:MET:HE2	1:V:409:MET:HA	1.89	0.54
1:W:264:ALA:HB2	1:W:389:VAL:HG13	1.89	0.54
1:Q:264:ALA:HB2	1:Q:389:VAL:HG13	1.89	0.54
1:c:409:MET:HA	1:c:409:MET:HE2	1.89	0.54
1:N:264:ALA:HB2	1:N:389:VAL:HG13	1.89	0.54
1:N:409:MET:HE2	1:N:409:MET:HA	1.89	0.54
1:H:264:ALA:HB2	1:H:389:VAL:HG13	1.89	0.53
1:K:264:ALA:HB2	1:K:389:VAL:HG13	1.89	0.53
1:S:409:MET:HE2	1:S:409:MET:HA	1.89	0.53
1:T:264:ALA:HB2	1:T:389:VAL:HG13	1.89	0.53
1:X:409:MET:HE2	1:X:409:MET:HA	1.89	0.53
1:b:409:MET:HE2	1:b:409:MET:HA	1.89	0.53
1:O:409:MET:HA	1:O:409:MET:HE2	1.89	0.53
1:a:409:MET:HE2	1:a:409:MET:HA	1.89	0.53
1:b:264:ALA:HB2	1:b:389:VAL:HG13	1.89	0.53
1:P:409:MET:HE2	1:P:409:MET:HA	1.89	0.53
1:Y:409:MET:HA	1:Y:409:MET:HE2	1.89	0.53
1:e:264:ALA:HB2	1:e:389:VAL:HG13	1.89	0.53
1:U:409:MET:HE2	1:U:409:MET:HA	1.89	0.53
1:Z:409:MET:HE2	1:Z:409:MET:HA	1.89	0.53
1:Q:409:MET:HE2	1:Q:409:MET:HA	1.89	0.53
1:S:293:LEU:HD21	1:S:364:SER:HB3	1.91	0.53
1:U:293:LEU:HD21	1:U:364:SER:HB3	1.91	0.53
1:L:293:LEU:HD21	1:L:364:SER:HB3	1.91	0.53
1:N:293:LEU:HD21	1:N:364:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:293:LEU:HD21	1:Q:364:SER:HB3	1.91	0.53
1:T:409:MET:HA	1:T:409:MET:HE2	1.89	0.53
1:E:429:THR:OG1	1:F:418:GLU:OE2	2.27	0.53
1:H:429:THR:OG1	1:I:418:GLU:OE2	2.27	0.53
1:J:429:THR:OG1	1:K:418:GLU:OE2	2.27	0.53
1:M:429:THR:OG1	1:N:418:GLU:OE2	2.27	0.53
1:P:293:LEU:HD21	1:P:364:SER:HB3	1.91	0.53
1:R:293:LEU:HD21	1:R:364:SER:HB3	1.91	0.53
1:R:409:MET:HA	1:R:409:MET:HE2	1.89	0.53
1:W:293:LEU:HD21	1:W:364:SER:HB3	1.91	0.53
1:G:429:THR:OG1	1:H:418:GLU:OE2	2.27	0.52
1:O:293:LEU:HD21	1:O:364:SER:HB3	1.91	0.52
1:V:293:LEU:HD21	1:V:364:SER:HB3	1.91	0.52
1:X:293:LEU:HD21	1:X:364:SER:HB3	1.91	0.52
1:Z:293:LEU:HD21	1:Z:364:SER:HB3	1.91	0.52
1:J:293:LEU:HD21	1:J:364:SER:HB3	1.91	0.52
1:K:429:THR:OG1	1:L:418:GLU:OE2	2.27	0.52
1:W:409:MET:HA	1:W:409:MET:HE2	1.89	0.52
1:Y:293:LEU:HD21	1:Y:364:SER:HB3	1.92	0.52
1:b:293:LEU:HD21	1:b:364:SER:HB3	1.91	0.52
1:K:293:LEU:HD21	1:K:364:SER:HB3	1.91	0.52
1:W:429:THR:OG1	1:X:418:GLU:OE2	2.27	0.52
1:Y:429:THR:OG1	1:Z:418:GLU:OE2	2.27	0.52
1:B:429:THR:OG1	1:C:418:GLU:OE2	2.27	0.52
1:M:293:LEU:HD21	1:M:364:SER:HB3	1.91	0.52
1:T:293:LEU:HD21	1:T:364:SER:HB3	1.91	0.52
1:D:429:THR:OG1	1:E:418:GLU:OE2	2.27	0.52
1:H:293:LEU:HD21	1:H:364:SER:HB3	1.92	0.52
1:P:429:THR:OG1	1:Q:418:GLU:OE2	2.27	0.52
1:a:293:LEU:HD21	1:a:364:SER:HB3	1.91	0.52
1:d:293:LEU:HD21	1:d:364:SER:HB3	1.91	0.52
1:I:293:LEU:HD21	1:I:364:SER:HB3	1.91	0.52
1:a:429:THR:OG1	1:b:418:GLU:OE2	2.27	0.52
1:b:429:THR:OG1	1:c:418:GLU:OE2	2.27	0.52
1:c:293:LEU:HD21	1:c:364:SER:HB3	1.91	0.52
1:d:429:THR:OG1	1:e:418:GLU:OE2	2.27	0.52
1:F:293:LEU:HD21	1:F:364:SER:HB3	1.91	0.52
1:G:293:LEU:HD21	1:G:364:SER:HB3	1.91	0.52
1:N:429:THR:OG1	1:O:418:GLU:OE2	2.27	0.52
1:U:429:THR:OG1	1:V:418:GLU:OE2	2.27	0.52
1:Z:429:THR:OG1	1:a:418:GLU:OE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:293:LEU:HD21	1:f:364:SER:HB3	1.91	0.52
1:D:293:LEU:HD21	1:D:364:SER:HB3	1.91	0.52
1:L:429:THR:OG1	1:M:418:GLU:OE2	2.27	0.52
1:h:293:LEU:HD21	1:h:364:SER:HB3	1.91	0.52
1:A:429:THR:OG1	1:B:418:GLU:OE2	2.27	0.52
1:B:293:LEU:HD21	1:B:364:SER:HB3	1.91	0.52
1:E:293:LEU:HD21	1:E:364:SER:HB3	1.91	0.52
1:F:429:THR:OG1	1:G:418:GLU:OE2	2.27	0.52
1:f:429:THR:OG1	1:g:418:GLU:OE2	2.27	0.52
1:C:293:LEU:HD21	1:C:364:SER:HB3	1.91	0.51
1:C:429:THR:OG1	1:D:418:GLU:OE2	2.27	0.51
1:O:429:THR:OG1	1:P:418:GLU:OE2	2.27	0.51
1:e:293:LEU:HD21	1:e:364:SER:HB3	1.91	0.51
1:g:293:LEU:HD21	1:g:364:SER:HB3	1.91	0.51
1:g:429:THR:OG1	1:h:418:GLU:OE2	2.27	0.51
1:I:429:THR:OG1	1:J:418:GLU:OE2	2.27	0.51
1:Q:429:THR:OG1	1:R:418:GLU:OE2	2.27	0.51
1:S:429:THR:OG1	1:T:418:GLU:OE2	2.27	0.51
1:c:429:THR:OG1	1:d:418:GLU:OE2	2.27	0.51
1:A:293:LEU:HD21	1:A:364:SER:HB3	1.91	0.51
1:P:256:ILE:HG13	1:P:257:VAL:N	2.26	0.51
1:X:429:THR:OG1	1:Y:418:GLU:OE2	2.27	0.51
1:b:256:ILE:HG13	1:b:257:VAL:N	2.26	0.51
1:d:256:ILE:HG13	1:d:257:VAL:N	2.26	0.51
1:A:418:GLU:OE2	1:h:429:THR:OG1	2.27	0.51
1:B:256:ILE:HG13	1:B:257:VAL:N	2.26	0.51
1:M:256:ILE:HG13	1:M:257:VAL:N	2.26	0.51
1:S:256:ILE:HG13	1:S:257:VAL:N	2.26	0.51
1:Z:256:ILE:HG13	1:Z:257:VAL:N	2.26	0.51
1:g:256:ILE:HG13	1:g:257:VAL:N	2.26	0.51
1:J:256:ILE:HG13	1:J:257:VAL:N	2.26	0.51
1:T:429:THR:OG1	1:U:418:GLU:OE2	2.27	0.51
1:V:429:THR:OG1	1:W:418:GLU:OE2	2.27	0.51
1:X:256:ILE:HG13	1:X:257:VAL:N	2.26	0.51
1:E:256:ILE:HG13	1:E:257:VAL:N	2.26	0.51
1:R:429:THR:OG1	1:S:418:GLU:OE2	2.27	0.51
1:V:256:ILE:HG13	1:V:257:VAL:N	2.26	0.51
1:A:256:ILE:HG13	1:A:257:VAL:N	2.26	0.51
1:D:256:ILE:HG13	1:D:257:VAL:N	2.26	0.51
1:G:256:ILE:HG13	1:G:257:VAL:N	2.26	0.51
1:R:256:ILE:HG13	1:R:257:VAL:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:256:ILE:HG13	1:T:257:VAL:N	2.26	0.51
1:f:256:ILE:HG13	1:f:257:VAL:N	2.26	0.51
1:F:256:ILE:HG13	1:F:257:VAL:N	2.26	0.51
1:c:256:ILE:HG13	1:c:257:VAL:N	2.26	0.51
1:H:256:ILE:HG13	1:H:257:VAL:N	2.26	0.51
1:L:256:ILE:HG13	1:L:257:VAL:N	2.26	0.50
1:N:256:ILE:HG13	1:N:257:VAL:N	2.26	0.50
1:O:256:ILE:HG13	1:O:257:VAL:N	2.26	0.50
1:V:235:LEU:HB3	1:W:244:ARG:NH2	2.27	0.50
1:Y:235:LEU:HB3	1:Z:244:ARG:NH2	2.27	0.50
1:b:235:LEU:HB3	1:c:244:ARG:NH2	2.27	0.50
1:e:429:THR:OG1	1:f:418:GLU:OE2	2.27	0.50
1:K:256:ILE:HG13	1:K:257:VAL:N	2.26	0.50
1:Q:256:ILE:HG13	1:Q:257:VAL:N	2.26	0.50
1:S:235:LEU:HB3	1:T:244:ARG:NH2	2.27	0.50
1:W:256:ILE:HG13	1:W:257:VAL:N	2.26	0.50
1:e:235:LEU:HB3	1:f:244:ARG:NH2	2.27	0.50
1:P:235:LEU:HB3	1:Q:244:ARG:NH2	2.27	0.50
1:A:244:ARG:NH2	1:h:235:LEU:HB3	2.27	0.50
1:Y:256:ILE:HG13	1:Y:257:VAL:N	2.26	0.50
1:h:256:ILE:HG13	1:h:257:VAL:N	2.26	0.50
1:U:256:ILE:HG13	1:U:257:VAL:N	2.26	0.50
1:a:256:ILE:HG13	1:a:257:VAL:N	2.26	0.50
1:C:256:ILE:HG13	1:C:257:VAL:N	2.26	0.50
1:M:235:LEU:HB3	1:N:244:ARG:NH2	2.27	0.50
1:N:235:LEU:HB3	1:O:244:ARG:NH2	2.27	0.50
1:U:235:LEU:HB3	1:V:244:ARG:NH2	2.27	0.50
1:e:256:ILE:HG13	1:e:257:VAL:N	2.26	0.50
1:K:235:LEU:HB3	1:L:244:ARG:NH2	2.27	0.50
1:X:235:LEU:HB3	1:Y:244:ARG:NH2	2.27	0.50
1:a:235:LEU:HB3	1:b:244:ARG:NH2	2.27	0.50
1:g:235:LEU:HB3	1:h:244:ARG:NH2	2.27	0.50
1:B:235:LEU:HB3	1:C:244:ARG:NH2	2.27	0.49
1:C:235:LEU:HB3	1:D:244:ARG:NH2	2.27	0.49
1:G:294:ARG:HD2	1:G:367:GLU:OE1	2.12	0.49
1:H:294:ARG:HD2	1:H:367:GLU:OE1	2.12	0.49
1:I:256:ILE:HG13	1:I:257:VAL:N	2.26	0.49
1:R:235:LEU:HB3	1:S:244:ARG:NH2	2.27	0.49
1:d:235:LEU:HB3	1:e:244:ARG:NH2	2.27	0.49
1:A:294:ARG:HD2	1:A:367:GLU:OE1	2.12	0.49
1:E:235:LEU:HB3	1:F:244:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:LEU:HB3	1:I:244:ARG:NH2	2.27	0.49
1:N:294:ARG:HD2	1:N:367:GLU:OE1	2.12	0.49
1:F:294:ARG:HD2	1:F:367:GLU:OE1	2.12	0.49
1:I:294:ARG:HD2	1:I:367:GLU:OE1	2.12	0.49
1:M:294:ARG:HD2	1:M:367:GLU:OE1	2.12	0.49
1:h:294:ARG:HD2	1:h:367:GLU:OE1	2.12	0.49
1:B:294:ARG:HD2	1:B:367:GLU:OE1	2.12	0.49
1:J:235:LEU:HB3	1:K:244:ARG:NH2	2.27	0.49
1:O:294:ARG:HD2	1:O:367:GLU:OE1	2.12	0.49
1:U:367:GLU:HA	1:V:294:ARG:HH21	1.78	0.49
1:A:367:GLU:HA	1:B:294:ARG:HH21	1.78	0.49
1:F:235:LEU:HB3	1:G:244:ARG:NH2	2.27	0.49
1:K:294:ARG:HD2	1:K:367:GLU:OE1	2.12	0.49
1:L:294:ARG:HD2	1:L:367:GLU:OE1	2.12	0.49
1:O:235:LEU:HB3	1:P:244:ARG:NH2	2.27	0.49
1:R:367:GLU:HA	1:S:294:ARG:HH21	1.78	0.49
1:E:294:ARG:HD2	1:E:367:GLU:OE1	2.12	0.49
1:H:367:GLU:HA	1:I:294:ARG:HH21	1.78	0.49
1:J:294:ARG:HD2	1:J:367:GLU:OE1	2.13	0.49
1:b:367:GLU:HA	1:c:294:ARG:HH21	1.78	0.49
1:D:294:ARG:HD2	1:D:367:GLU:OE1	2.13	0.49
1:D:367:GLU:HA	1:E:294:ARG:HH21	1.78	0.49
1:E:367:GLU:HA	1:F:294:ARG:HH21	1.78	0.49
1:H:266:VAL:HG22	1:H:387:VAL:HG22	1.95	0.49
1:J:367:GLU:HA	1:K:294:ARG:HH21	1.78	0.49
1:M:367:GLU:HA	1:N:294:ARG:HH21	1.78	0.49
1:O:367:GLU:HA	1:P:294:ARG:HH21	1.78	0.49
1:U:266:VAL:HG22	1:U:387:VAL:HG22	1.95	0.49
1:Z:367:GLU:HA	1:a:294:ARG:HH21	1.78	0.49
1:a:266:VAL:HG22	1:a:387:VAL:HG22	1.95	0.49
1:e:367:GLU:HA	1:f:294:ARG:HH21	1.78	0.49
1:f:367:GLU:HA	1:g:294:ARG:HH21	1.78	0.49
1:g:294:ARG:HD2	1:g:367:GLU:OE1	2.12	0.49
1:C:294:ARG:HD2	1:C:367:GLU:OE1	2.12	0.49
1:G:266:VAL:HG22	1:G:387:VAL:HG22	1.95	0.49
1:M:266:VAL:HG22	1:M:387:VAL:HG22	1.95	0.49
1:N:266:VAL:HG22	1:N:387:VAL:HG22	1.95	0.49
1:T:266:VAL:HG22	1:T:387:VAL:HG22	1.95	0.49
1:W:367:GLU:HA	1:X:294:ARG:HH21	1.78	0.49
1:Z:266:VAL:HG22	1:Z:387:VAL:HG22	1.95	0.49
1:c:294:ARG:HD2	1:c:367:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:LEU:HB3	1:H:244:ARG:NH2	2.27	0.49
1:I:367:GLU:HA	1:J:294:ARG:HH21	1.78	0.49
1:L:367:GLU:HA	1:M:294:ARG:HH21	1.78	0.49
1:P:294:ARG:HD2	1:P:367:GLU:OE1	2.12	0.49
1:T:294:ARG:HD2	1:T:367:GLU:OE1	2.12	0.49
1:X:367:GLU:HA	1:Y:294:ARG:HH21	1.78	0.49
1:b:294:ARG:HD2	1:b:367:GLU:OE1	2.12	0.49
1:O:266:VAL:HG22	1:O:387:VAL:HG22	1.95	0.48
1:P:367:GLU:HA	1:Q:294:ARG:HH21	1.78	0.48
1:U:294:ARG:HD2	1:U:367:GLU:OE1	2.13	0.48
1:V:266:VAL:HG22	1:V:387:VAL:HG22	1.95	0.48
1:a:367:GLU:HA	1:b:294:ARG:HH21	1.78	0.48
1:I:266:VAL:HG22	1:I:387:VAL:HG22	1.95	0.48
1:L:266:VAL:HG22	1:L:387:VAL:HG22	1.95	0.48
1:S:294:ARG:HD2	1:S:367:GLU:OE1	2.12	0.48
1:a:294:ARG:HD2	1:a:367:GLU:OE1	2.13	0.48
1:b:266:VAL:HG22	1:b:387:VAL:HG22	1.95	0.48
1:c:367:GLU:HA	1:d:294:ARG:HH21	1.78	0.48
1:B:266:VAL:HG22	1:B:387:VAL:HG22	1.95	0.48
1:B:367:GLU:HA	1:C:294:ARG:HH21	1.78	0.48
1:C:266:VAL:HG22	1:C:387:VAL:HG22	1.95	0.48
1:F:266:VAL:HG22	1:F:387:VAL:HG22	1.95	0.48
1:S:266:VAL:HG22	1:S:387:VAL:HG22	1.95	0.48
1:V:294:ARG:HD2	1:V:367:GLU:OE1	2.12	0.48
1:d:294:ARG:HD2	1:d:367:GLU:OE1	2.12	0.48
1:f:266:VAL:HG22	1:f:387:VAL:HG22	1.95	0.48
1:A:294:ARG:HH21	1:h:367:GLU:HA	1.78	0.48
1:Q:294:ARG:HD2	1:Q:367:GLU:OE1	2.12	0.48
1:S:367:GLU:HA	1:T:294:ARG:HH21	1.78	0.48
1:T:367:GLU:HA	1:U:294:ARG:HH21	1.78	0.48
1:Y:266:VAL:HG22	1:Y:387:VAL:HG22	1.95	0.48
1:e:266:VAL:HG22	1:e:387:VAL:HG22	1.95	0.48
1:D:235:LEU:HB3	1:E:244:ARG:NH2	2.27	0.48
1:G:367:GLU:HA	1:H:294:ARG:HH21	1.78	0.48
1:K:367:GLU:HA	1:L:294:ARG:HH21	1.78	0.48
1:L:235:LEU:HB3	1:M:244:ARG:NH2	2.27	0.48
1:W:294:ARG:HD2	1:W:367:GLU:OE1	2.12	0.48
1:X:294:ARG:HD2	1:X:367:GLU:OE1	2.12	0.48
1:Y:294:ARG:HD2	1:Y:367:GLU:OE1	2.12	0.48
1:Y:367:GLU:HA	1:Z:294:ARG:HH21	1.78	0.48
1:R:294:ARG:HD2	1:R:367:GLU:OE1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:294:ARG:HD2	1:Z:367:GLU:OE1	2.12	0.48
1:f:294:ARG:HD2	1:f:367:GLU:OE1	2.12	0.48
1:g:266:VAL:HG22	1:g:387:VAL:HG22	1.95	0.48
1:A:266:VAL:HG22	1:A:387:VAL:HG22	1.95	0.48
1:P:266:VAL:HG22	1:P:387:VAL:HG22	1.95	0.48
1:W:266:VAL:HG22	1:W:387:VAL:HG22	1.95	0.48
1:D:266:VAL:HG22	1:D:387:VAL:HG22	1.95	0.48
1:Q:367:GLU:HA	1:R:294:ARG:HH21	1.78	0.48
1:e:294:ARG:HD2	1:e:367:GLU:OE1	2.12	0.48
1:A:235:LEU:HB3	1:B:244:ARG:NH2	2.27	0.48
1:F:367:GLU:HA	1:G:294:ARG:HH21	1.78	0.48
1:c:266:VAL:HG22	1:c:387:VAL:HG22	1.95	0.48
1:F:296:ARG:HH11	1:F:296:ARG:HG2	1.79	0.48
1:J:266:VAL:HG22	1:J:387:VAL:HG22	1.95	0.48
1:K:266:VAL:HG22	1:K:387:VAL:HG22	1.95	0.48
1:R:266:VAL:HG22	1:R:387:VAL:HG22	1.95	0.48
1:T:235:LEU:HB3	1:U:244:ARG:NH2	2.27	0.48
1:W:235:LEU:HB3	1:X:244:ARG:NH2	2.27	0.48
1:d:266:VAL:HG22	1:d:387:VAL:HG22	1.95	0.48
1:Q:296:ARG:HG2	1:Q:296:ARG:HH11	1.79	0.47
1:V:367:GLU:HA	1:W:294:ARG:HH21	1.78	0.47
1:Z:235:LEU:HB3	1:a:244:ARG:NH2	2.27	0.47
1:d:367:GLU:HA	1:e:294:ARG:HH21	1.78	0.47
1:f:235:LEU:HB3	1:g:244:ARG:NH2	2.27	0.47
1:C:367:GLU:HA	1:D:294:ARG:HH21	1.78	0.47
1:E:266:VAL:HG22	1:E:387:VAL:HG22	1.95	0.47
1:N:296:ARG:HG2	1:N:296:ARG:HH11	1.79	0.47
1:Y:296:ARG:HG2	1:Y:296:ARG:HH11	1.79	0.47
1:c:235:LEU:HB3	1:d:244:ARG:NH2	2.27	0.47
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.80	0.47
1:C:296:ARG:HG2	1:C:296:ARG:HH11	1.80	0.47
1:I:296:ARG:HG2	1:I:296:ARG:HH11	1.79	0.47
1:T:296:ARG:HG2	1:T:296:ARG:HH11	1.80	0.47
1:V:296:ARG:HG2	1:V:296:ARG:HH11	1.80	0.47
1:b:296:ARG:HG2	1:b:296:ARG:HH11	1.79	0.47
1:g:367:GLU:HA	1:h:294:ARG:HH21	1.78	0.47
1:D:296:ARG:HG2	1:D:296:ARG:HH11	1.79	0.47
1:Q:235:LEU:HB3	1:R:244:ARG:NH2	2.27	0.47
1:X:266:VAL:HG22	1:X:387:VAL:HG22	1.95	0.47
1:d:296:ARG:HG2	1:d:296:ARG:HH11	1.79	0.47
1:I:235:LEU:HB3	1:J:244:ARG:NH2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:296:ARG:HH11	1:K:296:ARG:HG2	1.79	0.47
1:L:296:ARG:HG2	1:L:296:ARG:HH11	1.79	0.47
1:N:367:GLU:HA	1:O:294:ARG:HH21	1.78	0.47
1:a:296:ARG:HH11	1:a:296:ARG:HG2	1.80	0.47
1:c:296:ARG:HH11	1:c:296:ARG:HG2	1.79	0.47
1:f:296:ARG:HH11	1:f:296:ARG:HG2	1.80	0.47
1:h:266:VAL:HG22	1:h:387:VAL:HG22	1.95	0.47
1:S:296:ARG:HG2	1:S:296:ARG:HH11	1.80	0.47
1:A:244:ARG:HH22	1:h:235:LEU:CB	2.28	0.47
1:C:235:LEU:CB	1:D:244:ARG:HH22	2.28	0.47
1:H:296:ARG:HG2	1:H:296:ARG:HH11	1.79	0.47
1:M:235:LEU:CB	1:N:244:ARG:HH22	2.28	0.47
1:Q:266:VAL:HG22	1:Q:387:VAL:HG22	1.95	0.47
1:R:235:LEU:CB	1:S:244:ARG:HH22	2.28	0.47
1:U:235:LEU:CB	1:V:244:ARG:HH22	2.28	0.47
1:W:296:ARG:HH11	1:W:296:ARG:HG2	1.79	0.47
1:Z:235:LEU:CB	1:a:244:ARG:HH22	2.28	0.47
1:c:235:LEU:CB	1:d:244:ARG:HH22	2.28	0.47
1:e:296:ARG:HG2	1:e:296:ARG:HH11	1.79	0.47
1:f:235:LEU:CB	1:g:244:ARG:HH22	2.28	0.47
1:E:235:LEU:CB	1:F:244:ARG:HH22	2.28	0.47
1:H:235:LEU:CB	1:I:244:ARG:HH22	2.28	0.47
1:O:235:LEU:CB	1:P:244:ARG:HH22	2.28	0.47
1:O:296:ARG:HG2	1:O:296:ARG:HH11	1.80	0.47
1:U:296:ARG:HG2	1:U:296:ARG:HH11	1.79	0.47
1:X:296:ARG:HG2	1:X:296:ARG:HH11	1.79	0.47
1:g:296:ARG:HG2	1:g:296:ARG:HH11	1.79	0.47
1:J:235:LEU:CB	1:K:244:ARG:HH22	2.28	0.47
1:L:282:TYR:HB3	1:M:292:THR:HG21	1.97	0.47
1:h:296:ARG:HH11	1:h:296:ARG:HG2	1.79	0.47
1:B:296:ARG:HG2	1:B:296:ARG:HH11	1.80	0.47
1:G:282:TYR:HB3	1:H:292:THR:HG21	1.97	0.47
1:G:296:ARG:HG2	1:G:296:ARG:HH11	1.79	0.47
1:I:282:TYR:HB3	1:J:292:THR:HG21	1.97	0.47
1:P:296:ARG:HH11	1:P:296:ARG:HG2	1.79	0.47
1:W:235:LEU:CB	1:X:244:ARG:HH22	2.28	0.47
1:e:235:LEU:CB	1:f:244:ARG:HH22	2.28	0.47
1:Z:296:ARG:HG2	1:Z:296:ARG:HH11	1.79	0.46
1:J:282:TYR:HB3	1:K:292:THR:HG21	1.97	0.46
1:R:296:ARG:HH11	1:R:296:ARG:HG2	1.80	0.46
1:T:235:LEU:CB	1:U:244:ARG:HH22	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:TYR:HB3	1:E:292:THR:HG21	1.97	0.46
1:E:296:ARG:HG2	1:E:296:ARG:HH11	1.80	0.46
1:O:282:TYR:HB3	1:P:292:THR:HG21	1.97	0.46
1:B:235:LEU:CB	1:C:244:ARG:HH22	2.28	0.46
1:Y:282:TYR:HB3	1:Z:292:THR:HG21	1.97	0.46
1:Z:282:TYR:HB3	1:a:292:THR:HG21	1.97	0.46
1:a:282:TYR:HB3	1:b:292:THR:HG21	1.97	0.46
1:b:282:TYR:HB3	1:c:292:THR:HG21	1.97	0.46
1:F:282:TYR:HB3	1:G:292:THR:HG21	1.97	0.46
1:N:282:TYR:HB3	1:O:292:THR:HG21	1.97	0.46
1:c:282:TYR:HB3	1:d:292:THR:HG21	1.97	0.46
1:G:235:LEU:CB	1:H:244:ARG:HH22	2.28	0.46
1:L:235:LEU:CB	1:M:244:ARG:HH22	2.28	0.46
1:M:296:ARG:HH11	1:M:296:ARG:HG2	1.79	0.46
1:Q:235:LEU:CB	1:R:244:ARG:HH22	2.28	0.46
1:Q:282:TYR:HB3	1:R:292:THR:HG21	1.97	0.46
1:b:235:LEU:CB	1:c:244:ARG:HH22	2.28	0.46
1:J:296:ARG:HG2	1:J:296:ARG:HH11	1.80	0.46
1:W:282:TYR:HB3	1:X:292:THR:HG21	1.97	0.46
1:X:282:TYR:HB3	1:Y:292:THR:HG21	1.97	0.46
1:A:282:TYR:HB3	1:B:292:THR:HG21	1.97	0.46
1:E:282:TYR:HB3	1:F:292:THR:HG21	1.97	0.46
1:K:282:TYR:HB3	1:L:292:THR:HG21	1.97	0.46
1:d:282:TYR:HB3	1:e:292:THR:HG21	1.97	0.46
1:e:282:TYR:HB3	1:f:292:THR:HG21	1.97	0.46
1:B:282:TYR:HB3	1:C:292:THR:HG21	1.97	0.46
1:f:282:TYR:HB3	1:g:292:THR:HG21	1.97	0.46
1:M:282:TYR:HB3	1:N:292:THR:HG21	1.97	0.46
1:R:282:TYR:HB3	1:S:292:THR:HG21	1.97	0.46
1:V:282:TYR:HB3	1:W:292:THR:HG21	1.97	0.46
1:Y:235:LEU:CB	1:Z:244:ARG:HH22	2.28	0.45
1:g:235:LEU:CB	1:h:244:ARG:HH22	2.28	0.45
1:T:282:TYR:HB3	1:U:292:THR:HG21	1.97	0.45
1:U:282:TYR:HB3	1:V:292:THR:HG21	1.97	0.45
1:C:282:TYR:HB3	1:D:292:THR:HG21	1.97	0.45
1:H:282:TYR:HB3	1:I:292:THR:HG21	1.97	0.45
1:g:282:TYR:HB3	1:h:292:THR:HG21	1.97	0.45
1:A:292:THR:HG21	1:h:282:TYR:HB3	1.97	0.45
1:V:235:LEU:CB	1:W:244:ARG:HH22	2.28	0.45
1:D:235:LEU:CB	1:E:244:ARG:HH22	2.28	0.45
1:N:235:LEU:CB	1:O:244:ARG:HH22	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:LEU:CB	1:J:244:ARG:HH22	2.28	0.45
1:S:282:TYR:HB3	1:T:292:THR:HG21	1.97	0.45
1:P:282:TYR:HB3	1:Q:292:THR:HG21	1.97	0.45
1:d:235:LEU:CB	1:e:244:ARG:HH22	2.28	0.44
1:S:235:LEU:CB	1:T:244:ARG:HH22	2.28	0.44
1:A:235:LEU:CB	1:B:244:ARG:HH22	2.28	0.44
1:a:235:LEU:CB	1:b:244:ARG:HH22	2.28	0.44
1:F:235:LEU:CB	1:G:244:ARG:HH22	2.28	0.43
1:K:235:LEU:CB	1:L:244:ARG:HH22	2.28	0.43
1:b:275:LYS:HG2	1:c:375:THR:HG23	2.01	0.43
1:K:275:LYS:HG2	1:L:375:THR:HG23	2.01	0.43
1:N:275:LYS:HG2	1:O:375:THR:HG23	2.01	0.43
1:O:275:LYS:HG2	1:P:375:THR:HG23	2.01	0.43
1:P:235:LEU:CB	1:Q:244:ARG:HH22	2.28	0.43
1:Q:275:LYS:HG2	1:R:375:THR:HG23	2.01	0.43
1:c:275:LYS:HG2	1:d:375:THR:HG23	2.01	0.43
1:P:275:LYS:HG2	1:Q:375:THR:HG23	2.01	0.43
1:R:275:LYS:HG2	1:S:375:THR:HG23	2.01	0.43
1:U:275:LYS:HG2	1:V:375:THR:HG23	2.01	0.43
1:V:275:LYS:HG2	1:W:375:THR:HG23	2.01	0.43
1:Y:275:LYS:HG2	1:Z:375:THR:HG23	2.01	0.43
1:e:275:LYS:HG2	1:f:375:THR:HG23	2.01	0.43
1:J:275:LYS:HG2	1:K:375:THR:HG23	2.01	0.43
1:L:275:LYS:HG2	1:M:375:THR:HG23	2.01	0.43
1:X:275:LYS:HG2	1:Y:375:THR:HG23	2.01	0.43
1:Z:275:LYS:HG2	1:a:375:THR:HG23	2.01	0.43
1:a:275:LYS:HG2	1:b:375:THR:HG23	2.01	0.43
1:f:275:LYS:HG2	1:g:375:THR:HG23	2.01	0.43
1:S:275:LYS:HG2	1:T:375:THR:HG23	2.01	0.43
1:f:290:LYS:HE3	1:f:290:LYS:HB2	1.93	0.43
1:A:275:LYS:HG2	1:B:375:THR:HG23	2.01	0.43
1:D:275:LYS:HG2	1:E:375:THR:HG23	2.01	0.43
1:H:275:LYS:HG2	1:I:375:THR:HG23	2.01	0.43
1:M:275:LYS:HG2	1:N:375:THR:HG23	2.01	0.43
1:T:275:LYS:HG2	1:U:375:THR:HG23	2.01	0.43
1:W:275:LYS:HG2	1:X:375:THR:HG23	2.01	0.43
1:X:235:LEU:CB	1:Y:244:ARG:HH22	2.28	0.43
1:A:375:THR:HG23	1:h:275:LYS:HG2	2.01	0.43
1:G:275:LYS:HG2	1:H:375:THR:HG23	2.01	0.43
1:I:275:LYS:HG2	1:J:375:THR:HG23	2.01	0.43
1:d:275:LYS:HG2	1:e:375:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:275:LYS:HG2	1:h:375:THR:HG23	2.01	0.43
1:B:275:LYS:HG2	1:C:375:THR:HG23	2.01	0.42
1:E:275:LYS:HG2	1:F:375:THR:HG23	2.01	0.42
1:C:275:LYS:HG2	1:D:375:THR:HG23	2.01	0.42
1:D:296:ARG:HG2	1:D:296:ARG:NH1	2.35	0.42
1:P:296:ARG:HG2	1:P:296:ARG:NH1	2.35	0.42
1:Q:296:ARG:HG2	1:Q:296:ARG:NH1	2.35	0.42
1:d:296:ARG:HG2	1:d:296:ARG:NH1	2.35	0.42
1:e:296:ARG:HG2	1:e:296:ARG:NH1	2.35	0.42
1:E:296:ARG:HG2	1:E:296:ARG:NH1	2.35	0.42
1:F:275:LYS:HG2	1:G:375:THR:HG23	2.01	0.42
1:J:296:ARG:HG2	1:J:296:ARG:NH1	2.35	0.42
1:c:296:ARG:HG2	1:c:296:ARG:NH1	2.35	0.42
1:f:296:ARG:HG2	1:f:296:ARG:NH1	2.35	0.42
1:H:235:LEU:HD13	1:I:244:ARG:HH22	1.85	0.42
1:K:296:ARG:HG2	1:K:296:ARG:NH1	2.35	0.42
1:M:235:LEU:HD13	1:N:244:ARG:HH22	1.85	0.42
1:V:296:ARG:HG2	1:V:296:ARG:NH1	2.35	0.42
1:W:235:LEU:HD13	1:X:244:ARG:HH22	1.85	0.42
1:Z:235:LEU:HD13	1:a:244:ARG:HH22	1.85	0.42
1:b:296:ARG:HG2	1:b:296:ARG:NH1	2.35	0.42
1:g:296:ARG:HG2	1:g:296:ARG:NH1	2.35	0.42
1:h:296:ARG:HG2	1:h:296:ARG:NH1	2.35	0.42
1:E:235:LEU:HD13	1:F:244:ARG:HH22	1.85	0.42
1:F:296:ARG:HG2	1:F:296:ARG:NH1	2.35	0.42
1:I:290:LYS:HE3	1:I:290:LYS:HB2	1.93	0.42
1:U:296:ARG:HG2	1:U:296:ARG:NH1	2.35	0.42
1:W:296:ARG:HG2	1:W:296:ARG:NH1	2.35	0.42
1:a:296:ARG:HG2	1:a:296:ARG:NH1	2.35	0.42
1:C:296:ARG:HG2	1:C:296:ARG:NH1	2.35	0.42
1:I:296:ARG:HG2	1:I:296:ARG:NH1	2.35	0.42
1:O:296:ARG:HG2	1:O:296:ARG:NH1	2.35	0.42
1:R:235:LEU:HD13	1:S:244:ARG:HH22	1.85	0.42
1:U:235:LEU:HD13	1:V:244:ARG:HH22	1.85	0.42
1:Z:296:ARG:HG2	1:Z:296:ARG:NH1	2.35	0.42
1:b:235:LEU:HD13	1:c:244:ARG:HH22	1.85	0.42
1:A:244:ARG:HH22	1:h:235:LEU:HD13	1.85	0.42
1:B:404:LEU:HD22	1:B:409:MET:HE3	2.02	0.42
1:C:290:LYS:HE3	1:C:290:LYS:HB2	1.93	0.42
1:K:235:LEU:HD13	1:L:244:ARG:HH22	1.85	0.42
1:L:296:ARG:HG2	1:L:296:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:235:LEU:HD13	1:Q:244:ARG:HH22	1.85	0.42
1:R:296:ARG:HG2	1:R:296:ARG:NH1	2.35	0.42
1:e:235:LEU:HD13	1:f:244:ARG:HH22	1.85	0.42
1:h:404:LEU:HD22	1:h:409:MET:HE3	2.02	0.42
1:A:296:ARG:HG2	1:A:296:ARG:NH1	2.35	0.42
1:A:404:LEU:HD22	1:A:409:MET:HE3	2.02	0.42
1:C:235:LEU:HD13	1:D:244:ARG:HH22	1.85	0.42
1:C:404:LEU:HD22	1:C:409:MET:HE3	2.02	0.42
1:J:235:LEU:HD13	1:K:244:ARG:HH22	1.85	0.42
1:Q:235:LEU:HD13	1:R:244:ARG:HH22	1.85	0.42
1:T:235:LEU:HD13	1:U:244:ARG:HH22	1.85	0.42
1:D:404:LEU:HD22	1:D:409:MET:HE3	2.02	0.42
1:O:290:LYS:HE3	1:O:290:LYS:HB2	1.93	0.42
1:c:235:LEU:HD13	1:d:244:ARG:HH22	1.85	0.42
1:g:404:LEU:HD22	1:g:409:MET:HE3	2.02	0.42
1:B:235:LEU:HD13	1:C:244:ARG:HH22	1.85	0.41
1:E:404:LEU:HD22	1:E:409:MET:HE3	2.02	0.41
1:F:235:LEU:HD13	1:G:244:ARG:HH22	1.85	0.41
1:O:235:LEU:HD13	1:P:244:ARG:HH22	1.85	0.41
1:P:421:GLY:O	1:P:426:ARG:NH2	2.51	0.41
1:Q:421:GLY:O	1:Q:426:ARG:NH2	2.51	0.41
1:R:421:GLY:O	1:R:426:ARG:NH2	2.51	0.41
1:T:296:ARG:HG2	1:T:296:ARG:NH1	2.35	0.41
1:Y:235:LEU:HD13	1:Z:244:ARG:HH22	1.85	0.41
1:f:404:LEU:HD22	1:f:409:MET:HE3	2.02	0.41
1:H:296:ARG:HG2	1:H:296:ARG:NH1	2.35	0.41
1:N:296:ARG:HG2	1:N:296:ARG:NH1	2.35	0.41
1:O:421:GLY:O	1:O:426:ARG:NH2	2.51	0.41
1:U:290:LYS:HE3	1:U:290:LYS:HB2	1.93	0.41
1:b:290:LYS:HE3	1:b:290:LYS:HB2	1.93	0.41
1:d:404:LEU:HD22	1:d:409:MET:HE3	2.02	0.41
1:e:404:LEU:HD22	1:e:409:MET:HE3	2.02	0.41
1:F:404:LEU:HD22	1:F:409:MET:HE3	2.02	0.41
1:G:404:LEU:HD22	1:G:409:MET:HE3	2.02	0.41
1:X:235:LEU:HD13	1:Y:244:ARG:HH22	1.85	0.41
1:X:296:ARG:HG2	1:X:296:ARG:NH1	2.35	0.41
1:g:235:LEU:HD13	1:h:244:ARG:HH22	1.85	0.41
1:G:296:ARG:HG2	1:G:296:ARG:NH1	2.35	0.41
1:M:296:ARG:HG2	1:M:296:ARG:NH1	2.35	0.41
1:N:421:GLY:O	1:N:426:ARG:NH2	2.51	0.41
1:B:296:ARG:HG2	1:B:296:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:LEU:HD13	1:H:244:ARG:HH22	1.85	0.41
1:H:404:LEU:HD22	1:H:409:MET:HE3	2.02	0.41
1:S:421:GLY:O	1:S:426:ARG:NH2	2.51	0.41
1:b:404:LEU:HD22	1:b:409:MET:HE3	2.02	0.41
1:I:235:LEU:HD13	1:J:244:ARG:HH22	1.85	0.41
1:P:404:LEU:HD22	1:P:409:MET:HE3	2.02	0.41
1:S:235:LEU:HD13	1:T:244:ARG:HH22	1.85	0.41
1:S:296:ARG:HG2	1:S:296:ARG:NH1	2.35	0.41
1:c:404:LEU:HD22	1:c:409:MET:HE3	2.02	0.41
1:I:404:LEU:HD22	1:I:409:MET:HE3	2.02	0.41
1:N:235:LEU:HD13	1:O:244:ARG:HH22	1.85	0.41
1:T:421:GLY:O	1:T:426:ARG:NH2	2.51	0.41
1:X:429:THR:HG1	1:Y:418:GLU:CD	2.29	0.41
1:Y:296:ARG:HG2	1:Y:296:ARG:NH1	2.35	0.41
1:a:404:LEU:HD22	1:a:409:MET:HE3	2.02	0.41
1:d:235:LEU:HD13	1:e:244:ARG:HH22	1.85	0.41
1:d:429:THR:HG1	1:e:418:GLU:CD	2.29	0.41
1:f:235:LEU:HD13	1:g:244:ARG:HH22	1.85	0.41
1:M:421:GLY:O	1:M:426:ARG:NH2	2.51	0.41
1:S:404:LEU:HD22	1:S:409:MET:HE3	2.02	0.41
1:Z:404:LEU:HD22	1:Z:409:MET:HE3	2.02	0.41
1:A:235:LEU:HD13	1:B:244:ARG:HH22	1.85	0.41
1:G:231:ASN:HB3	1:H:237:PHE:CE1	2.56	0.41
1:J:231:ASN:HB3	1:K:237:PHE:CE1	2.56	0.41
1:J:404:LEU:HD22	1:J:409:MET:HE3	2.02	0.41
1:K:231:ASN:HB3	1:L:237:PHE:CE1	2.56	0.41
1:L:235:LEU:HD13	1:M:244:ARG:HH22	1.85	0.41
1:M:404:LEU:HD22	1:M:409:MET:HE3	2.02	0.41
1:N:404:LEU:HD22	1:N:409:MET:HE3	2.02	0.41
1:V:235:LEU:HD13	1:W:244:ARG:HH22	1.85	0.41
1:b:231:ASN:HB3	1:c:237:PHE:CE1	2.56	0.41
1:F:231:ASN:HB3	1:G:237:PHE:CE1	2.56	0.41
1:L:231:ASN:HB3	1:M:237:PHE:CE1	2.56	0.41
1:M:231:ASN:HB3	1:N:237:PHE:CE1	2.56	0.41
1:N:231:ASN:HB3	1:O:237:PHE:CE1	2.56	0.41
1:O:231:ASN:HB3	1:P:237:PHE:CE1	2.56	0.41
1:R:404:LEU:HD22	1:R:409:MET:HE3	2.02	0.41
1:U:404:LEU:HD22	1:U:409:MET:HE3	2.02	0.41
1:X:404:LEU:HD22	1:X:409:MET:HE3	2.02	0.41
1:Y:404:LEU:HD22	1:Y:409:MET:HE3	2.02	0.41
1:C:231:ASN:HB3	1:D:237:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ARG:NH1	1:C:362:GLU:OE1	2.55	0.40
1:D:235:LEU:HD13	1:E:244:ARG:HH22	1.85	0.40
1:D:425:LYS:HE3	1:D:425:LYS:HB3	1.96	0.40
1:F:360:ARG:NH1	1:F:362:GLU:OE1	2.55	0.40
1:I:360:ARG:NH1	1:I:362:GLU:OE1	2.55	0.40
1:K:404:LEU:HD22	1:K:409:MET:HE3	2.02	0.40
1:a:231:ASN:HB3	1:b:237:PHE:CE1	2.56	0.40
1:a:235:LEU:HD13	1:b:244:ARG:HH22	1.85	0.40
1:c:231:ASN:HB3	1:d:237:PHE:CE1	2.56	0.40
1:h:360:ARG:NH1	1:h:362:GLU:OE1	2.55	0.40
1:L:421:GLY:O	1:L:426:ARG:NH2	2.51	0.40
1:U:421:GLY:O	1:U:426:ARG:NH2	2.51	0.40
1:V:360:ARG:NH1	1:V:362:GLU:OE1	2.55	0.40
1:Y:360:ARG:NH1	1:Y:362:GLU:OE1	2.55	0.40
1:Z:290:LYS:HE3	1:Z:290:LYS:HB2	1.93	0.40
1:d:360:ARG:NH1	1:d:362:GLU:OE1	2.55	0.40
1:e:360:ARG:NH1	1:e:362:GLU:OE1	2.55	0.40
1:B:231:ASN:HB3	1:C:237:PHE:CE1	2.56	0.40
1:E:231:ASN:HB3	1:F:237:PHE:CE1	2.56	0.40
1:J:421:GLY:O	1:J:426:ARG:NH2	2.51	0.40
1:L:404:LEU:HD22	1:L:409:MET:HE3	2.02	0.40
1:Q:404:LEU:HD22	1:Q:409:MET:HE3	2.02	0.40
1:V:231:ASN:HB3	1:W:237:PHE:CE1	2.56	0.40
1:X:360:ARG:NH1	1:X:362:GLU:OE1	2.55	0.40
1:a:360:ARG:NH1	1:a:362:GLU:OE1	2.55	0.40
1:b:360:ARG:NH1	1:b:362:GLU:OE1	2.55	0.40
1:g:360:ARG:NH1	1:g:362:GLU:OE1	2.55	0.40
1:D:231:ASN:HB3	1:E:237:PHE:CE1	2.56	0.40
1:I:421:GLY:O	1:I:426:ARG:NH2	2.51	0.40
1:L:360:ARG:NH1	1:L:362:GLU:OE1	2.55	0.40
1:R:231:ASN:HB3	1:S:237:PHE:CE1	2.56	0.40
1:S:231:ASN:HB3	1:T:237:PHE:CE1	2.56	0.40
1:V:404:LEU:HD22	1:V:409:MET:HE3	2.02	0.40
1:B:360:ARG:NH1	1:B:362:GLU:OE1	2.55	0.40
1:H:231:ASN:HB3	1:I:237:PHE:CE1	2.56	0.40
1:H:421:GLY:O	1:H:426:ARG:NH2	2.51	0.40
1:K:421:GLY:O	1:K:426:ARG:NH2	2.51	0.40
1:N:360:ARG:NH1	1:N:362:GLU:OE1	2.55	0.40
1:S:360:ARG:NH1	1:S:362:GLU:OE1	2.55	0.40
1:U:231:ASN:HB3	1:V:237:PHE:CE1	2.56	0.40
1:W:231:ASN:HB3	1:X:237:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:425:LYS:HE3	1:X:425:LYS:HB3	1.97	0.40
1:e:290:LYS:HE3	1:e:290:LYS:HB2	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	B	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	C	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	D	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	E	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	F	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	G	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	H	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	I	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	J	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	K	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	L	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	M	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	N	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	O	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	P	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	Q	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	R	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	T	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	U	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	V	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	W	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	X	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	Y	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	Z	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	a	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	b	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	c	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	d	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	e	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	f	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	g	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	h	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
All	All	5440/19040 (29%)	5372 (99%)	68 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	B	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	C	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	D	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	E	141/467 (30%)	140 (99%)	1 (1%)	76	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	G	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	H	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	I	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	J	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	K	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	L	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	M	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	N	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	O	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	P	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	Q	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	R	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	S	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	T	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	U	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	V	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	W	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	X	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	Y	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	Z	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	a	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	b	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	c	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	d	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	e	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	f	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	g	141/467 (30%)	140 (99%)	1 (1%)	76	83
1	h	141/467 (30%)	140 (99%)	1 (1%)	76	83
All	All	4794/15878 (30%)	4760 (99%)	34 (1%)	73	83

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	B	295	SER
1	C	295	SER
1	D	295	SER
1	E	295	SER
1	F	295	SER
1	G	295	SER
1	H	295	SER
1	I	295	SER
1	J	295	SER
1	K	295	SER
1	L	295	SER
1	M	295	SER
1	N	295	SER
1	O	295	SER
1	P	295	SER
1	Q	295	SER
1	R	295	SER
1	S	295	SER
1	T	295	SER
1	U	295	SER
1	V	295	SER
1	W	295	SER
1	X	295	SER
1	Y	295	SER
1	Z	295	SER
1	a	295	SER
1	b	295	SER
1	c	295	SER
1	d	295	SER
1	e	295	SER
1	f	295	SER
1	g	295	SER
1	h	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (270) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	234	GLN
1	A	297	GLN
1	A	303	GLN
1	A	374	HIS

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Mol	Chain	Res	Type
1	A	378	ASN
1	A	434	ASN
1	B	231	ASN
1	B	234	GLN
1	B	297	GLN
1	B	303	GLN
1	B	374	HIS
1	B	378	ASN
1	B	434	ASN
1	C	231	ASN
1	C	234	GLN
1	C	281	HIS
1	C	297	GLN
1	C	303	GLN
1	C	374	HIS
1	C	378	ASN
1	C	434	ASN
1	D	231	ASN
1	D	234	GLN
1	D	297	GLN
1	D	303	GLN
1	D	374	HIS
1	D	378	ASN
1	D	434	ASN
1	E	231	ASN
1	E	234	GLN
1	E	281	HIS
1	E	297	GLN
1	E	303	GLN
1	E	374	HIS
1	E	378	ASN
1	E	434	ASN
1	F	231	ASN
1	F	234	GLN
1	F	297	GLN
1	F	303	GLN
1	F	374	HIS
1	F	378	ASN
1	F	434	ASN
1	G	231	ASN
1	G	234	GLN
1	G	297	GLN

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Mol	Chain	Res	Type
1	G	303	GLN
1	G	374	HIS
1	G	378	ASN
1	G	434	ASN
1	H	231	ASN
1	H	234	GLN
1	H	281	HIS
1	H	297	GLN
1	H	303	GLN
1	H	374	HIS
1	H	378	ASN
1	H	434	ASN
1	I	231	ASN
1	I	234	GLN
1	I	297	GLN
1	I	303	GLN
1	I	374	HIS
1	I	378	ASN
1	I	431	ASN
1	I	434	ASN
1	J	231	ASN
1	J	234	GLN
1	J	281	HIS
1	J	297	GLN
1	J	303	GLN
1	J	374	HIS
1	J	378	ASN
1	J	434	ASN
1	K	231	ASN
1	K	234	GLN
1	K	281	HIS
1	K	297	GLN
1	K	303	GLN
1	K	374	HIS
1	K	378	ASN
1	K	431	ASN
1	K	434	ASN
1	L	231	ASN
1	L	234	GLN
1	L	281	HIS
1	L	297	GLN
1	L	303	GLN

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Mol	Chain	Res	Type
1	L	374	HIS
1	L	378	ASN
1	L	434	ASN
1	M	231	ASN
1	M	234	GLN
1	M	281	HIS
1	M	297	GLN
1	M	303	GLN
1	M	374	HIS
1	M	378	ASN
1	M	431	ASN
1	M	434	ASN
1	N	231	ASN
1	N	234	GLN
1	N	281	HIS
1	N	297	GLN
1	N	303	GLN
1	N	374	HIS
1	N	378	ASN
1	N	431	ASN
1	N	434	ASN
1	O	231	ASN
1	O	234	GLN
1	O	281	HIS
1	O	297	GLN
1	O	303	GLN
1	O	374	HIS
1	O	378	ASN
1	O	434	ASN
1	P	231	ASN
1	P	234	GLN
1	P	297	GLN
1	P	303	GLN
1	P	374	HIS
1	P	378	ASN
1	P	431	ASN
1	P	434	ASN
1	Q	231	ASN
1	Q	234	GLN
1	Q	297	GLN
1	Q	303	GLN
1	Q	374	HIS

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Mol	Chain	Res	Type
1	Q	378	ASN
1	Q	431	ASN
1	Q	434	ASN
1	R	231	ASN
1	R	234	GLN
1	R	281	HIS
1	R	297	GLN
1	R	303	GLN
1	R	374	HIS
1	R	378	ASN
1	R	431	ASN
1	R	434	ASN
1	S	231	ASN
1	S	234	GLN
1	S	297	GLN
1	S	303	GLN
1	S	374	HIS
1	S	378	ASN
1	S	431	ASN
1	S	434	ASN
1	T	231	ASN
1	T	234	GLN
1	T	281	HIS
1	T	297	GLN
1	T	303	GLN
1	T	374	HIS
1	T	378	ASN
1	T	431	ASN
1	T	434	ASN
1	U	231	ASN
1	U	234	GLN
1	U	281	HIS
1	U	297	GLN
1	U	303	GLN
1	U	374	HIS
1	U	378	ASN
1	U	431	ASN
1	U	434	ASN
1	V	231	ASN
1	V	234	GLN
1	V	281	HIS
1	V	297	GLN

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

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Mol	Chain	Res	Type
1	b	234	GLN
1	b	297	GLN
1	b	303	GLN
1	b	374	HIS
1	b	378	ASN
1	b	431	ASN
1	b	434	ASN
1	c	231	ASN
1	c	234	GLN
1	c	281	HIS
1	c	297	GLN
1	c	303	GLN
1	c	374	HIS
1	c	378	ASN
1	c	431	ASN
1	c	434	ASN
1	d	231	ASN
1	d	234	GLN
1	d	281	HIS
1	d	297	GLN
1	d	303	GLN
1	d	374	HIS
1	d	378	ASN
1	d	431	ASN
1	d	434	ASN
1	e	231	ASN
1	e	234	GLN
1	e	281	HIS
1	e	297	GLN
1	e	303	GLN
1	e	374	HIS
1	e	378	ASN
1	e	434	ASN
1	f	231	ASN
1	f	234	GLN
1	f	297	GLN
1	f	303	GLN
1	f	374	HIS
1	f	378	ASN
1	f	431	ASN
1	f	434	ASN
1	g	231	ASN

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Mol	Chain	Res	Type
1	g	234	GLN
1	g	297	GLN
1	g	303	GLN
1	g	374	HIS
1	g	378	ASN
1	g	434	ASN
1	h	231	ASN
1	h	234	GLN
1	h	297	GLN
1	h	303	GLN
1	h	374	HIS
1	h	378	ASN
1	h	434	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.

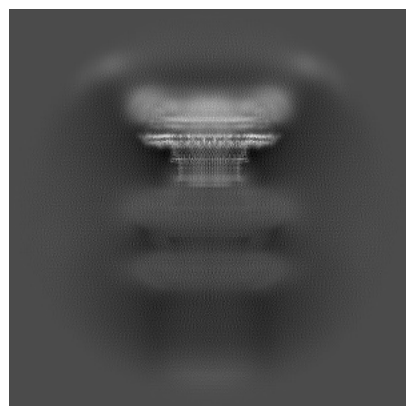
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37620. These allow visual inspection of the internal detail of the map and identification of artifacts.

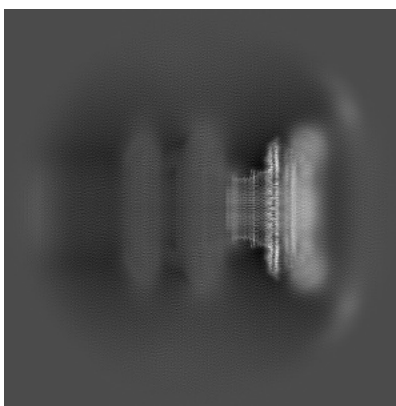
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

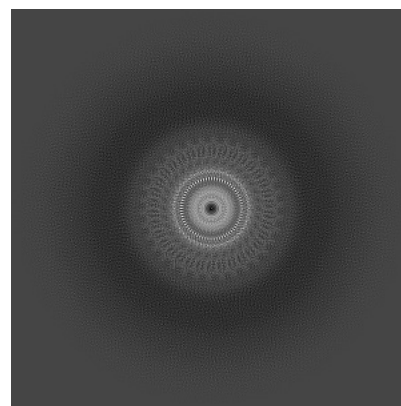
6.1.1 Primary map



X

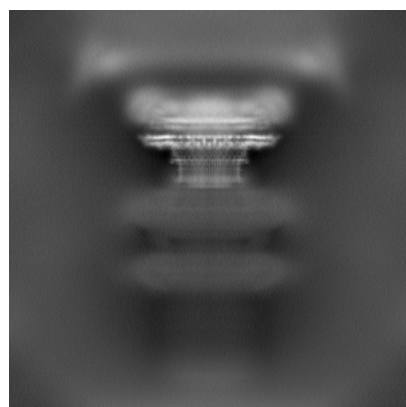


Y

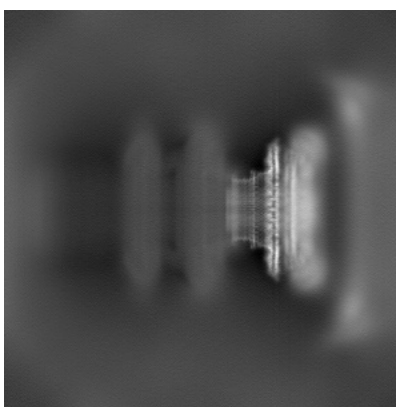


Z

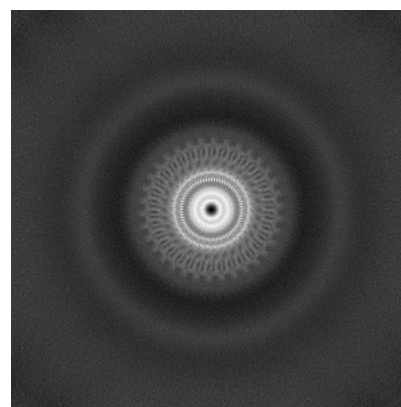
6.1.2 Raw map



X



Y

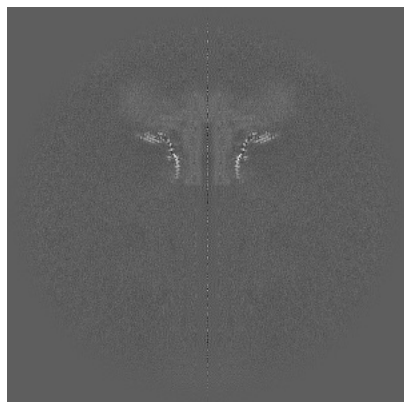


Z

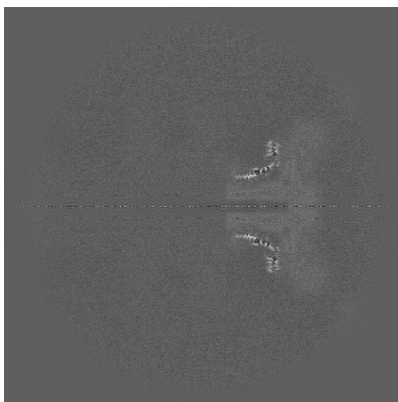
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

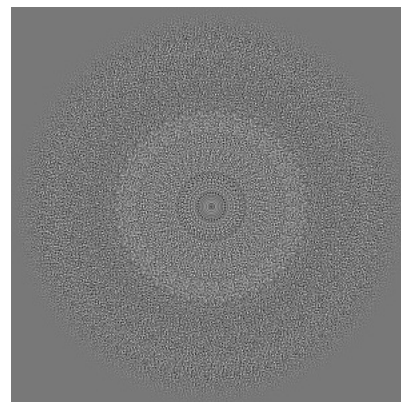
6.2.1 Primary map



X Index: 256

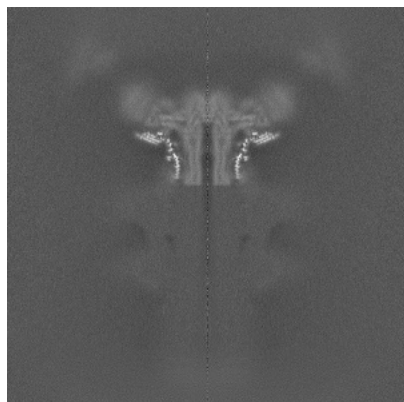


Y Index: 256

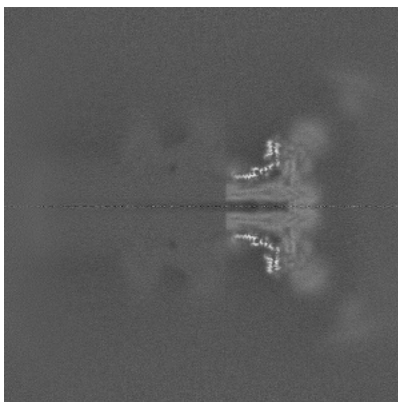


Z Index: 256

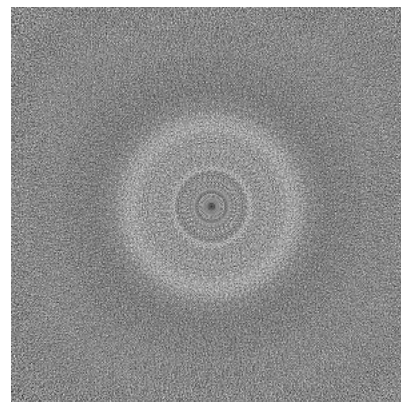
6.2.2 Raw map



X Index: 256



Y Index: 256

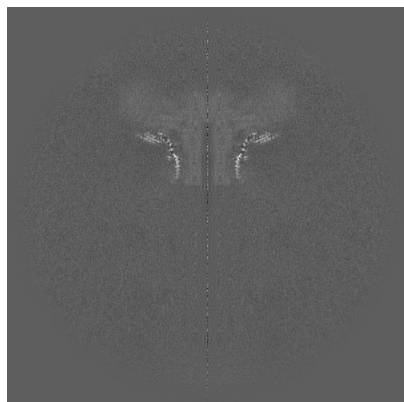


Z Index: 256

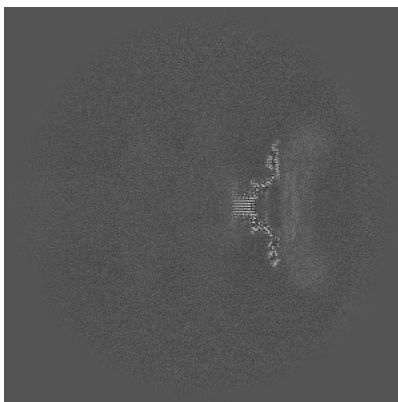
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

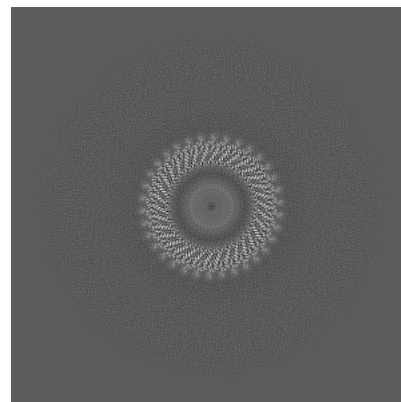
6.3.1 Primary map



X Index: 256

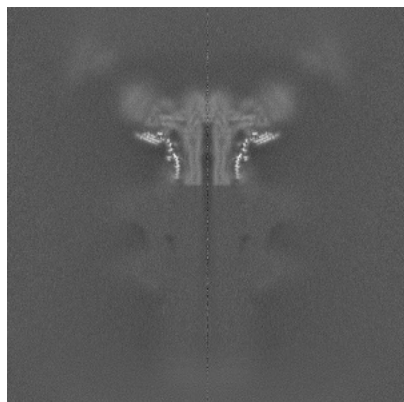


Y Index: 294

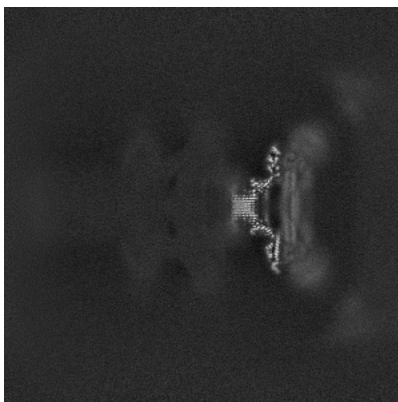


Z Index: 348

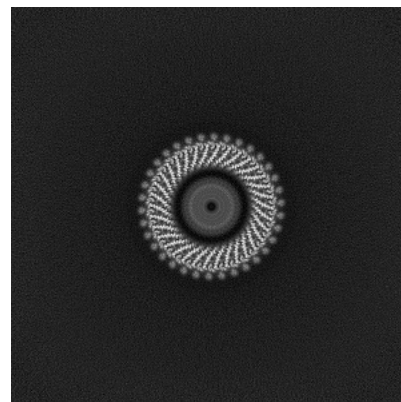
6.3.2 Raw map



X Index: 256



Y Index: 218

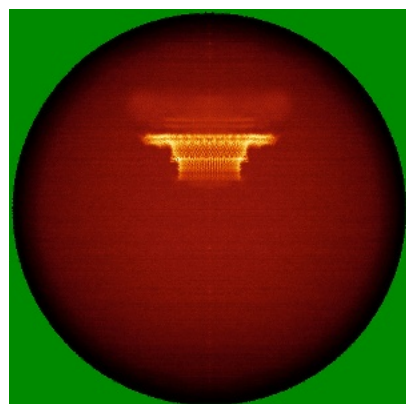


Z Index: 349

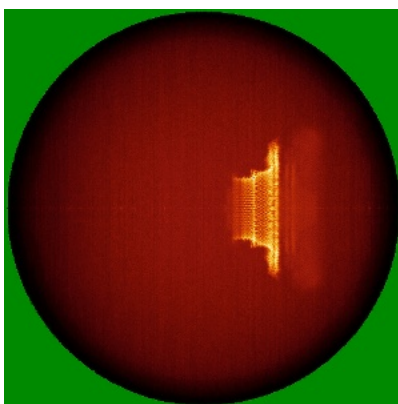
The images above show the largest variance slices of the map in three orthogonal directions.

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

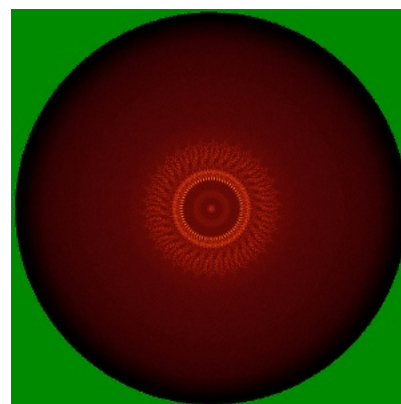
6.4.1 Primary map



X

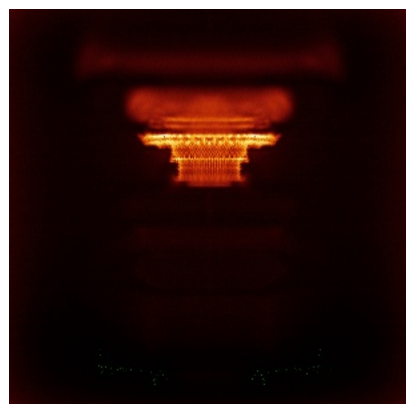


Y

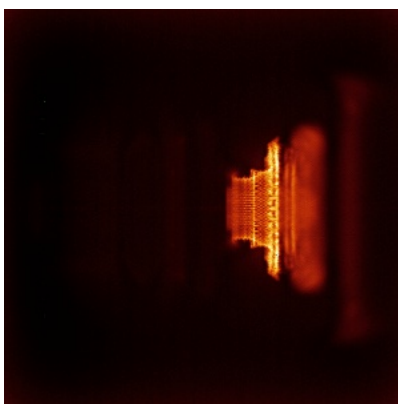


Z

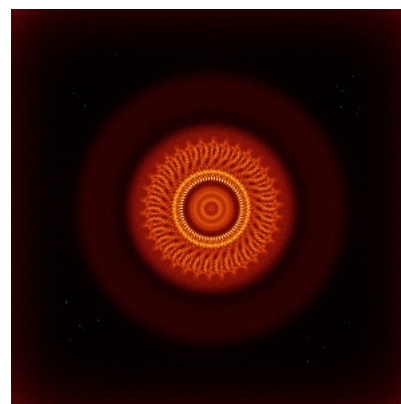
6.4.2 Raw map



X



Y

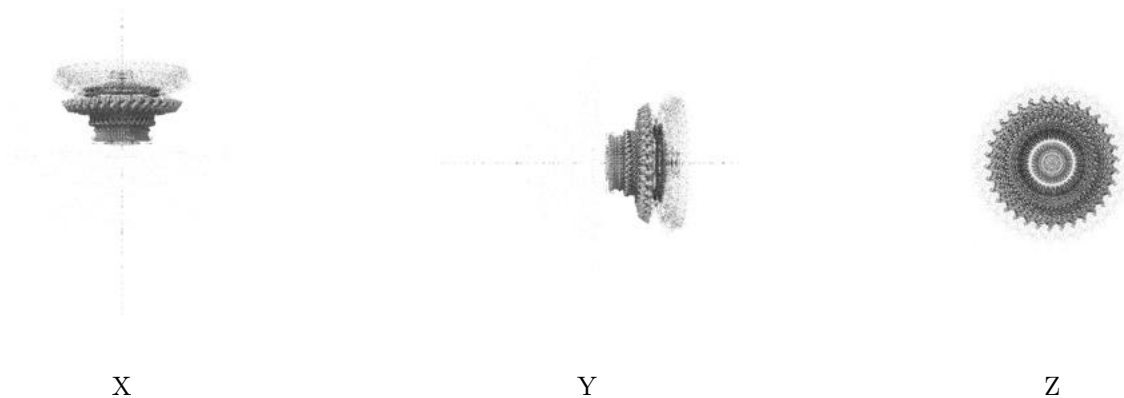


Z

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

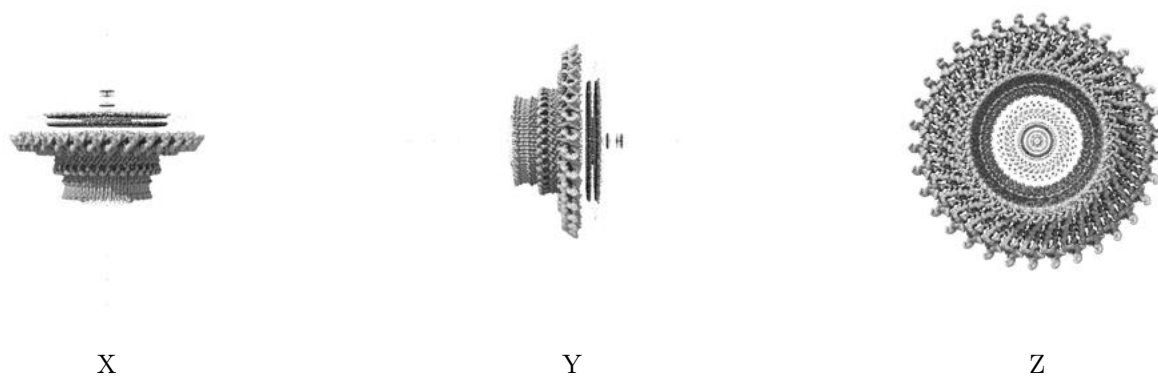
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

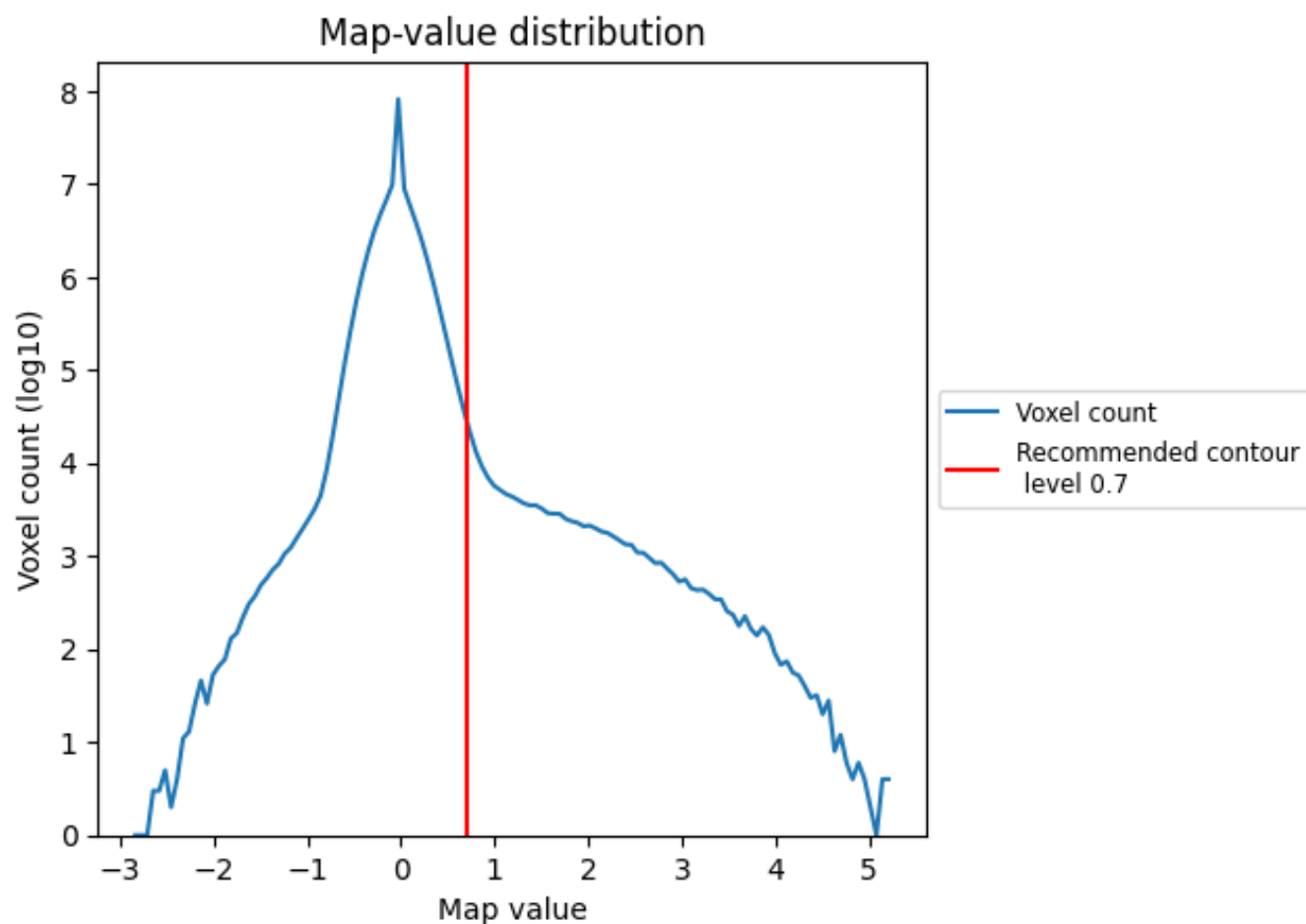
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

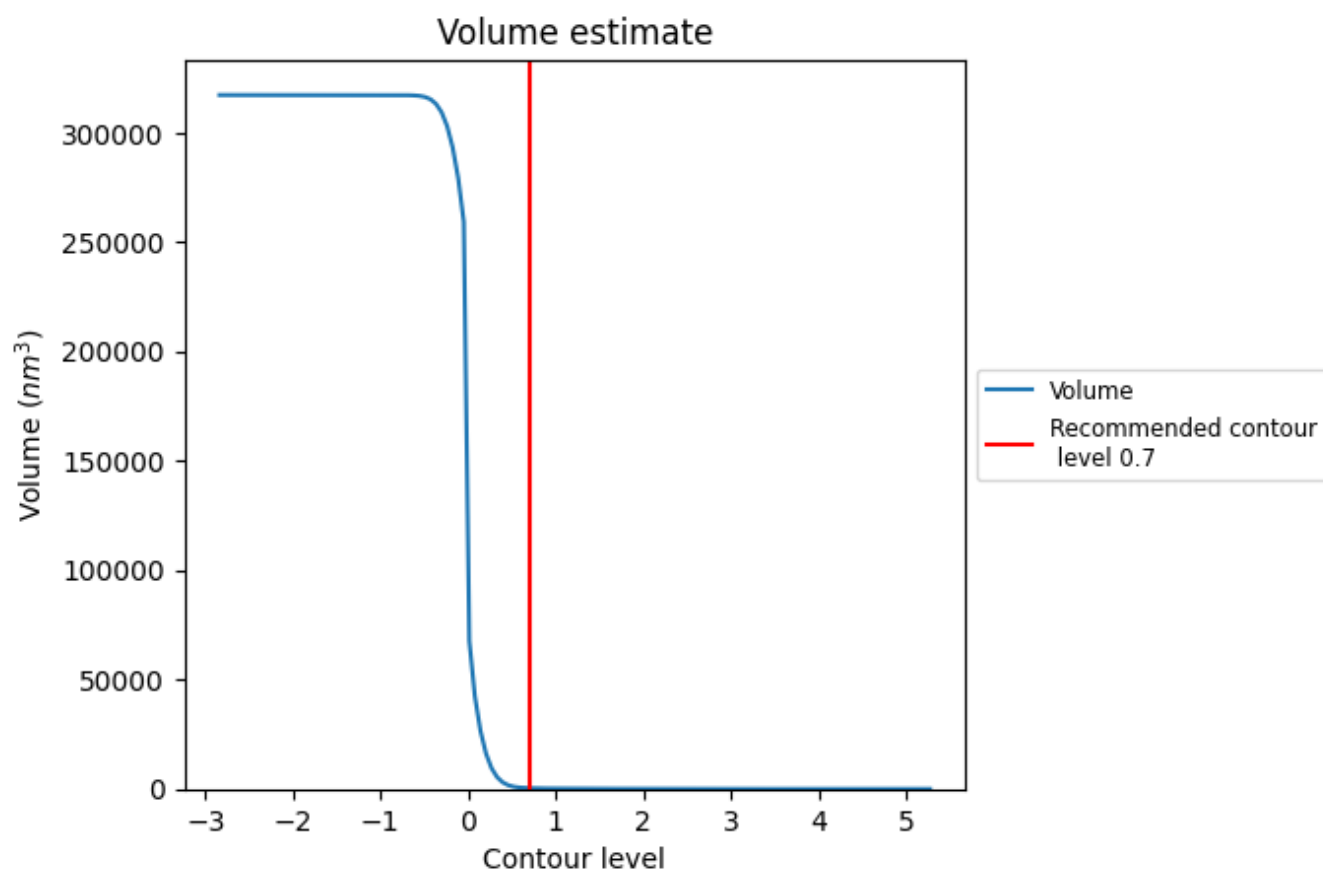
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

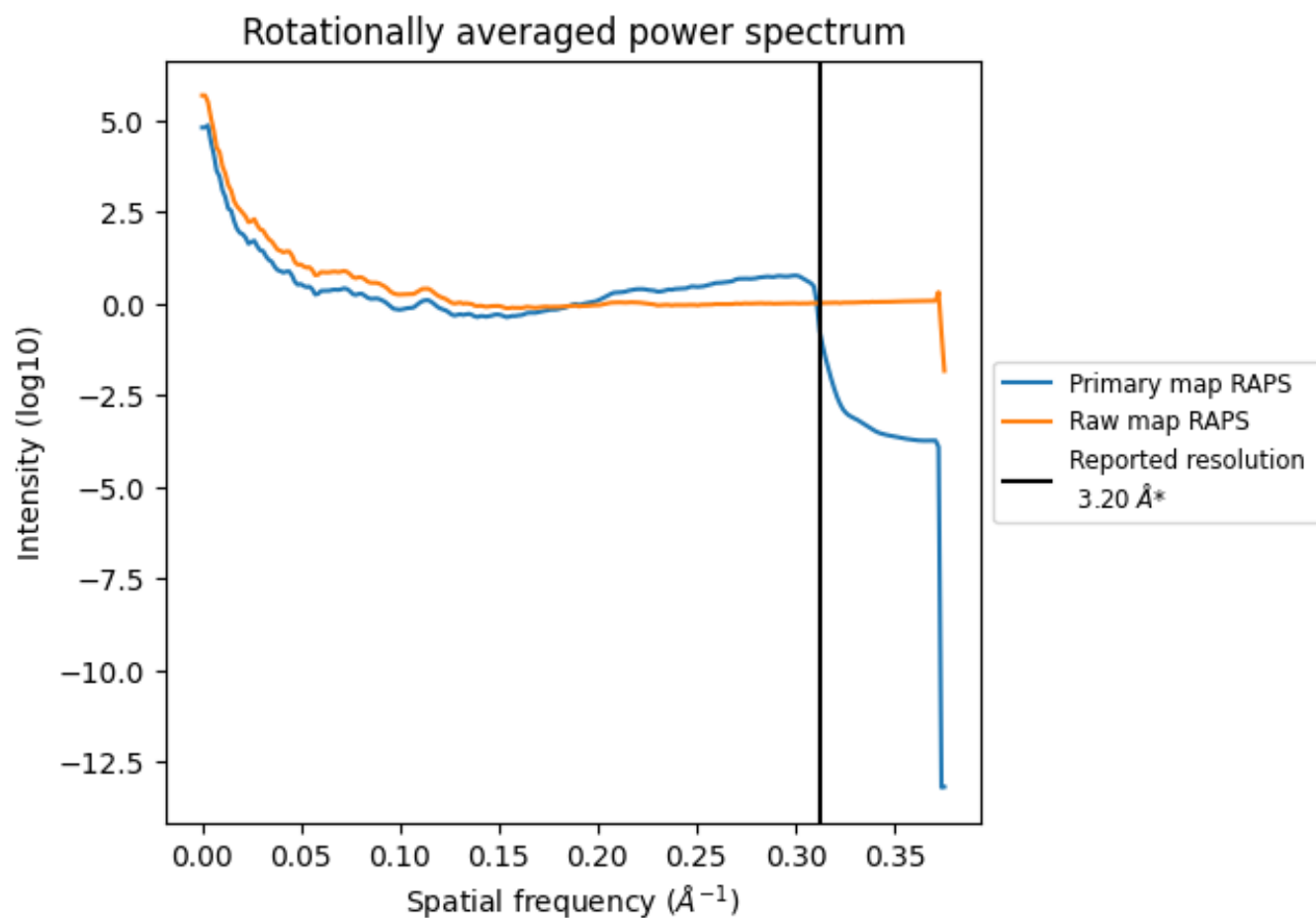
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm^3 ; this corresponds to an approximate mass of 327 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 ⓘ

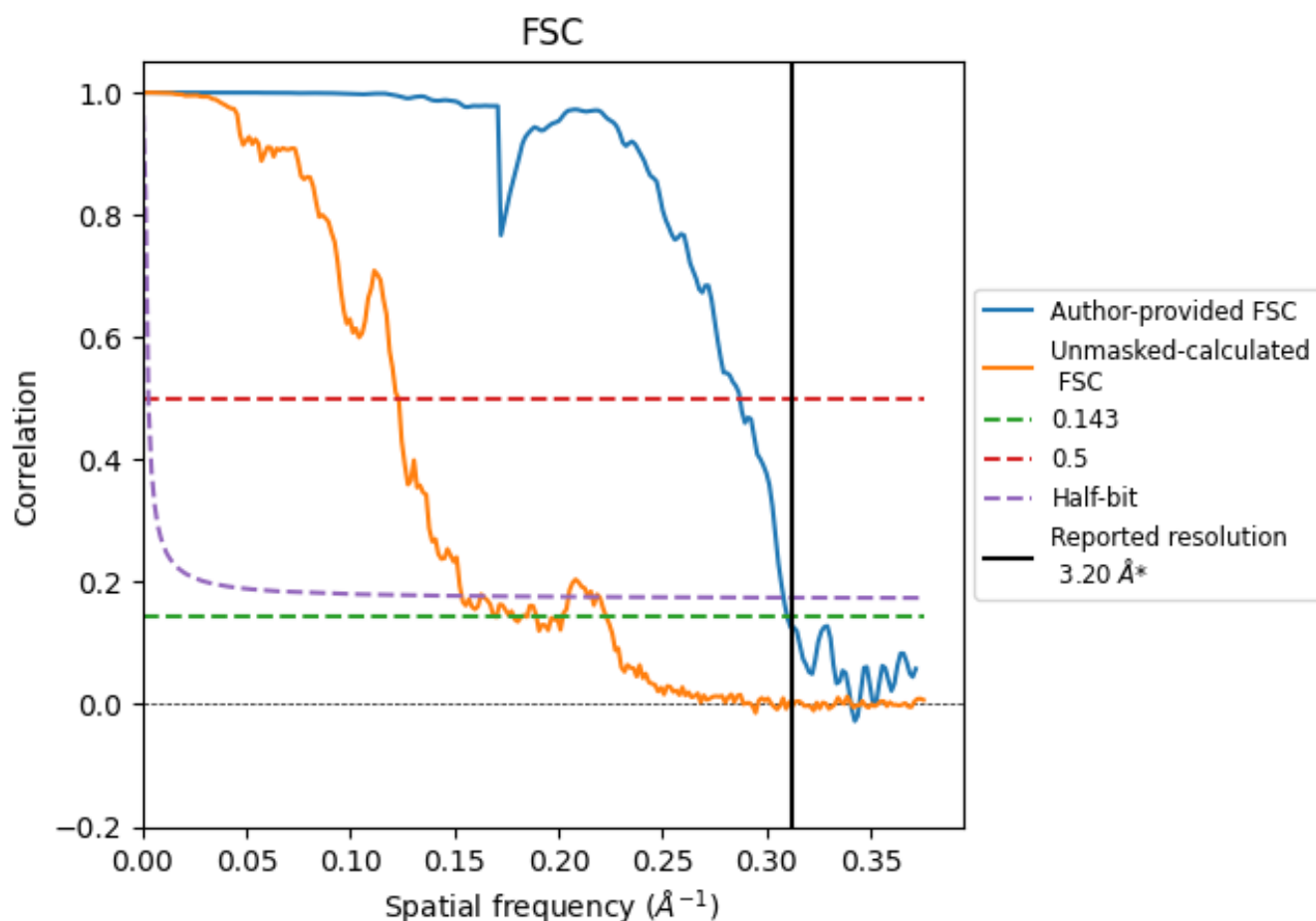


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

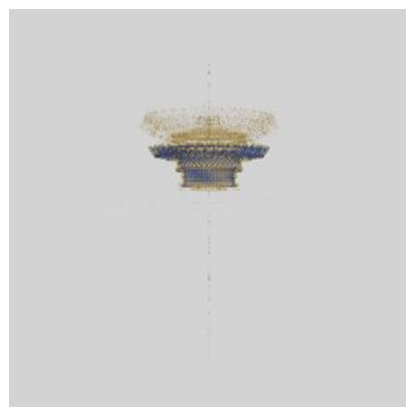
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.48	3.25
Unmasked-calculated*	5.89	8.12	6.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.89 differs from the reported value 3.2 by more than 10 %

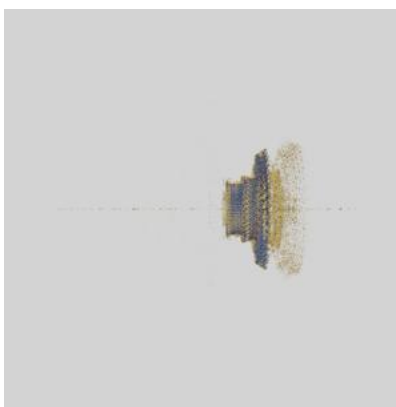
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37620 and PDB model 8WLI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

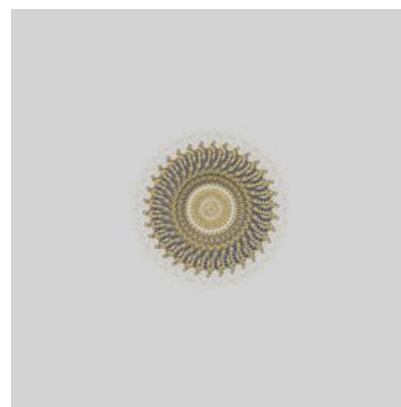
9.1 Map-model overlay [i](#)



X



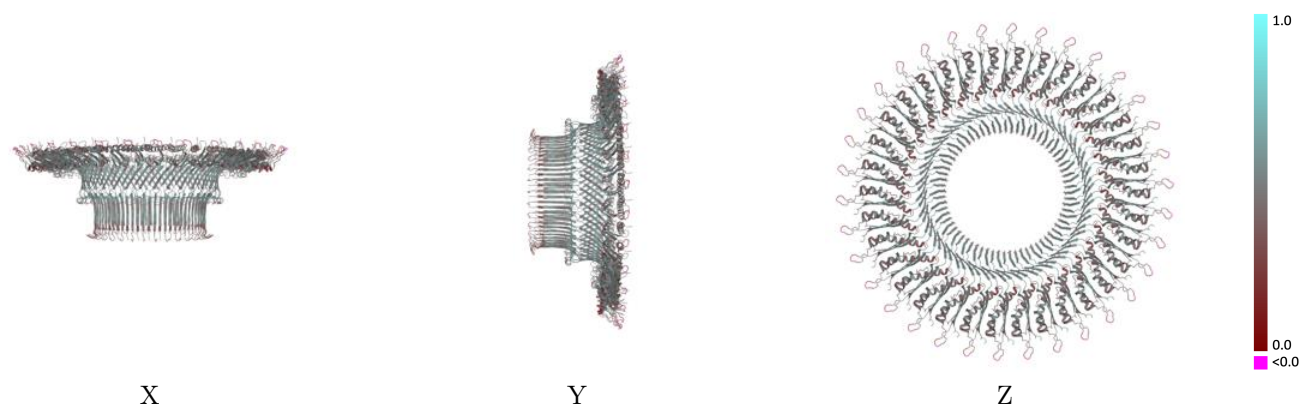
Y



Z

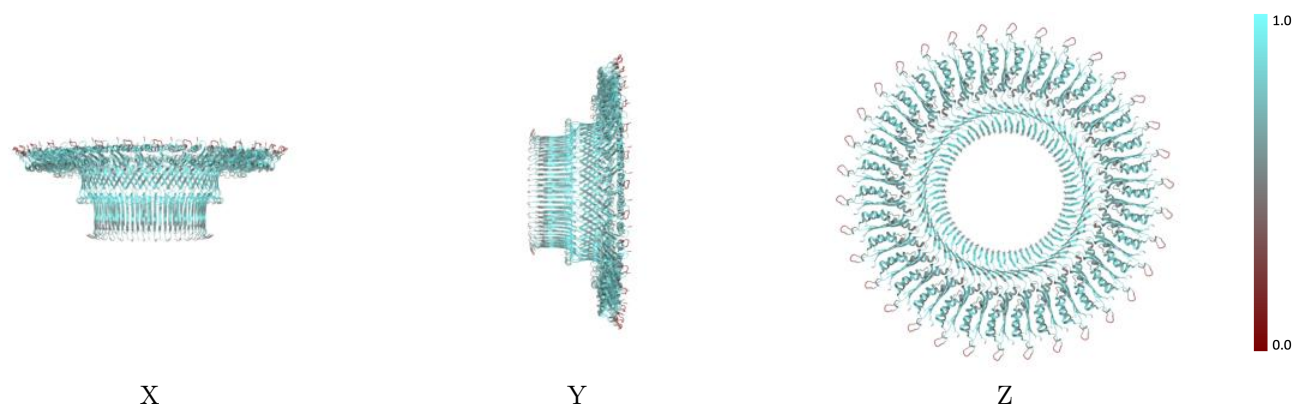
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



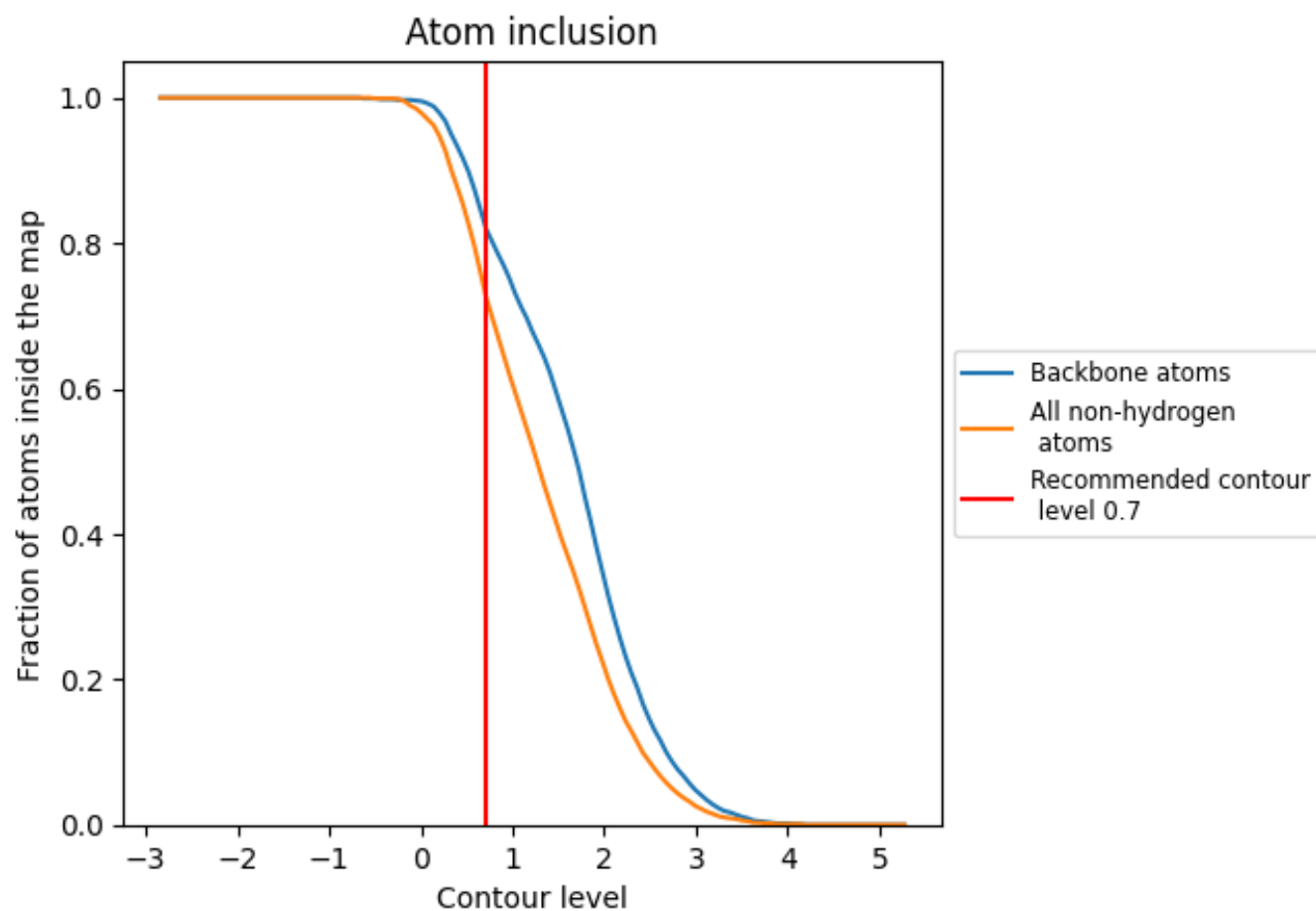
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 73% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.4670
A	 0.7360	 0.4670
B	 0.7340	 0.4630
C	 0.7320	 0.4650
D	 0.7320	 0.4650
E	 0.7300	 0.4690
F	 0.7330	 0.4670
G	 0.7340	 0.4670
H	 0.7280	 0.4690
I	 0.7400	 0.4670
J	 0.7340	 0.4680
K	 0.7280	 0.4670
L	 0.7270	 0.4640
M	 0.7290	 0.4660
N	 0.7330	 0.4660
O	 0.7310	 0.4640
P	 0.7290	 0.4680
Q	 0.7320	 0.4660
R	 0.7360	 0.4690
S	 0.7340	 0.4650
T	 0.7320	 0.4670
U	 0.7320	 0.4670
V	 0.7300	 0.4690
W	 0.7330	 0.4690
X	 0.7340	 0.4670
Y	 0.7280	 0.4700
Z	 0.7400	 0.4660
a	 0.7340	 0.4670
b	 0.7280	 0.4660
c	 0.7270	 0.4650
d	 0.7290	 0.4660
e	 0.7330	 0.4650
f	 0.7310	 0.4650
g	 0.7290	 0.4690
h	 0.7320	 0.4640

