



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:10 PM UTC

PDB ID : 8CVI / pdb_00008cvi
EMDB ID : EMD-27008
Title : Cryo-EM structure of the supercoiled EPEC H6 flagellar filament core Curly I waveform
Authors : Kreutzberger, M.A.; Chatterjee, S.; Frankel, G.; Egelman, E.H.
Deposited on : 2022-05-18
Resolution : 3.40 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

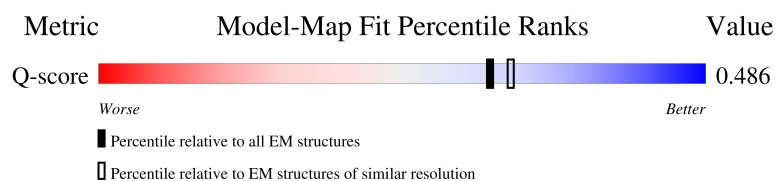
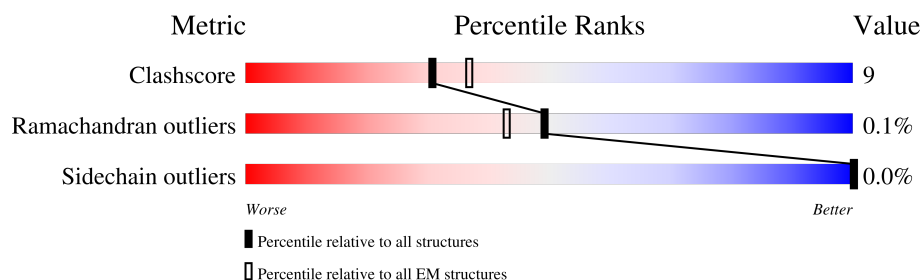
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



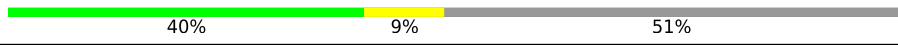
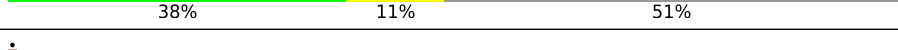
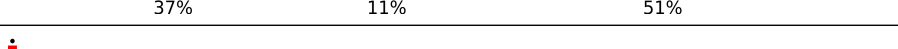
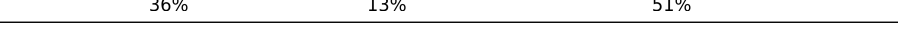
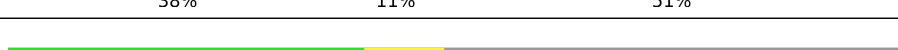
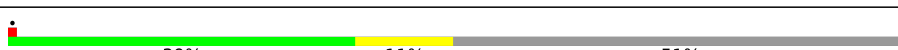
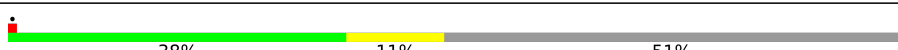
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	548	
1	B	548	
1	C	548	
1	D	548	

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Mol	Chain	Length	Quality of chain
1	E	548	
1	F	548	
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	
1	O	548	
1	P	548	
1	Q	548	
1	R	548	
1	S	548	
1	T	548	
1	U	548	
1	V	548	
1	W	548	
1	X	548	
1	Y	548	
1	Z	548	
1	a	548	
1	b	548	
1	c	548	

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Mol	Chain	Length	Quality of chain
1	d	548	39% 10% 51%
1	e	548	38% 11% 51%
1	f	548	36% 13% 51%
1	g	548	35% 14% 51%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 66030 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.

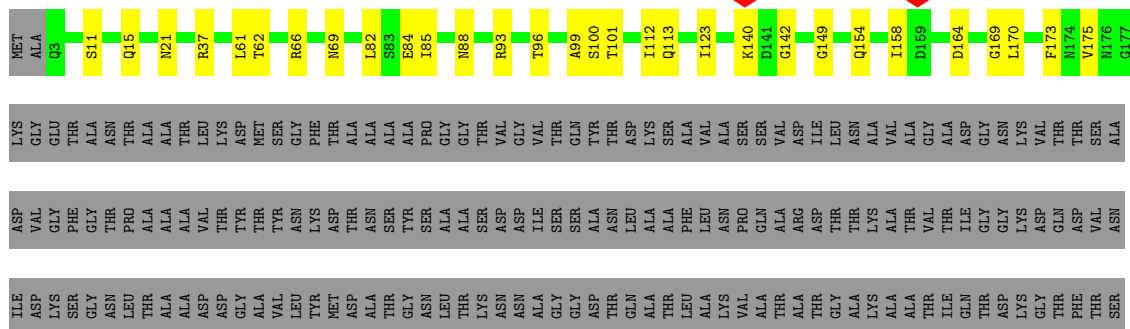
- Molecule 1 is a protein called Flagellin.

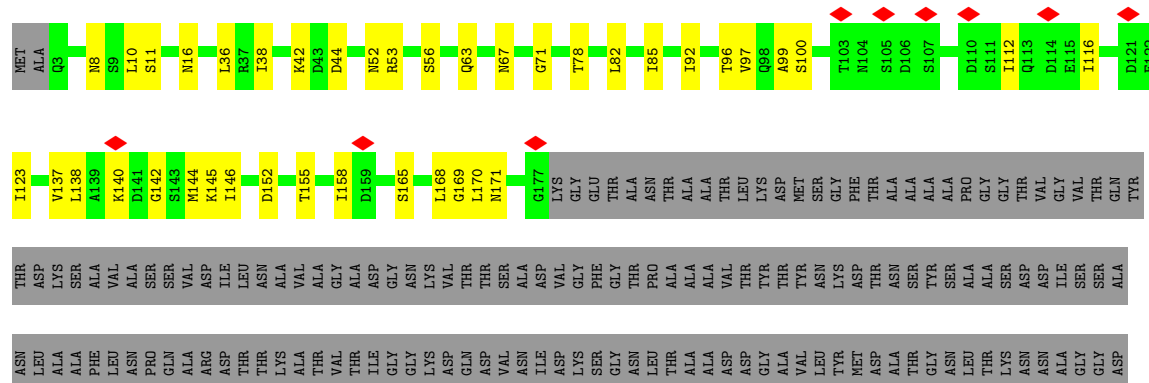
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	267	Total 1985	C 1190	N 363	O 430	S 2	0	0
1	B	267	Total 1985	C 1190	N 363	O 430	S 2	0	0
1	C	267	Total 1985	C 1190	N 363	O 430	S 2	0	0
1	D	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	N	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	X	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	E	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	O	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	Y	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	F	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	P	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	Z	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	G	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	Q	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	a	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	H	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	R	268	Total 1996	C 1196	N 365	O 433	S 2	0	0

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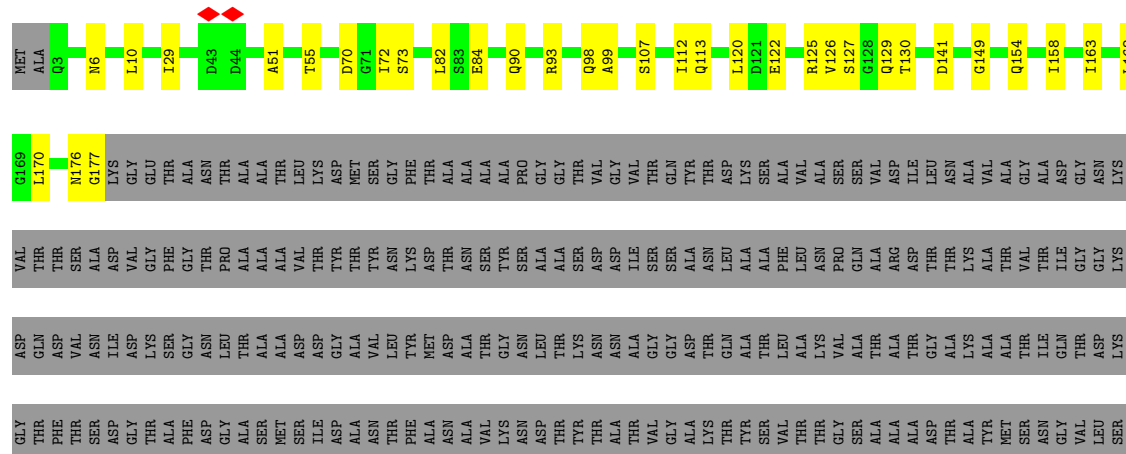
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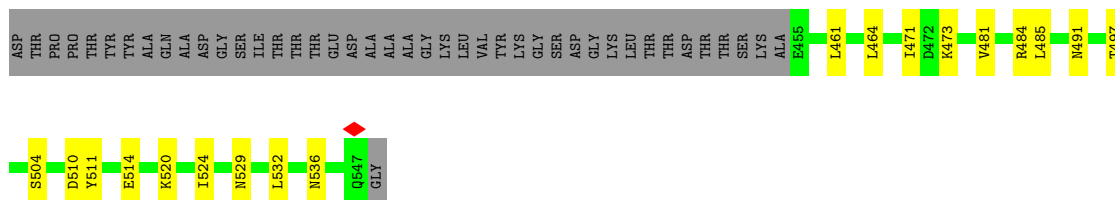
Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	268	Total 1996	C 1196	N 365	O 433	S 2	0	0
1	I	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	S	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	c	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	J	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	T	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	d	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	K	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	U	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	e	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	L	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	V	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	f	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	M	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	W	269	Total 2009	C 1205	N 367	O 435	S 2	1	0
1	g	269	Total 2009	C 1205	N 367	O 435	S 2	1	0



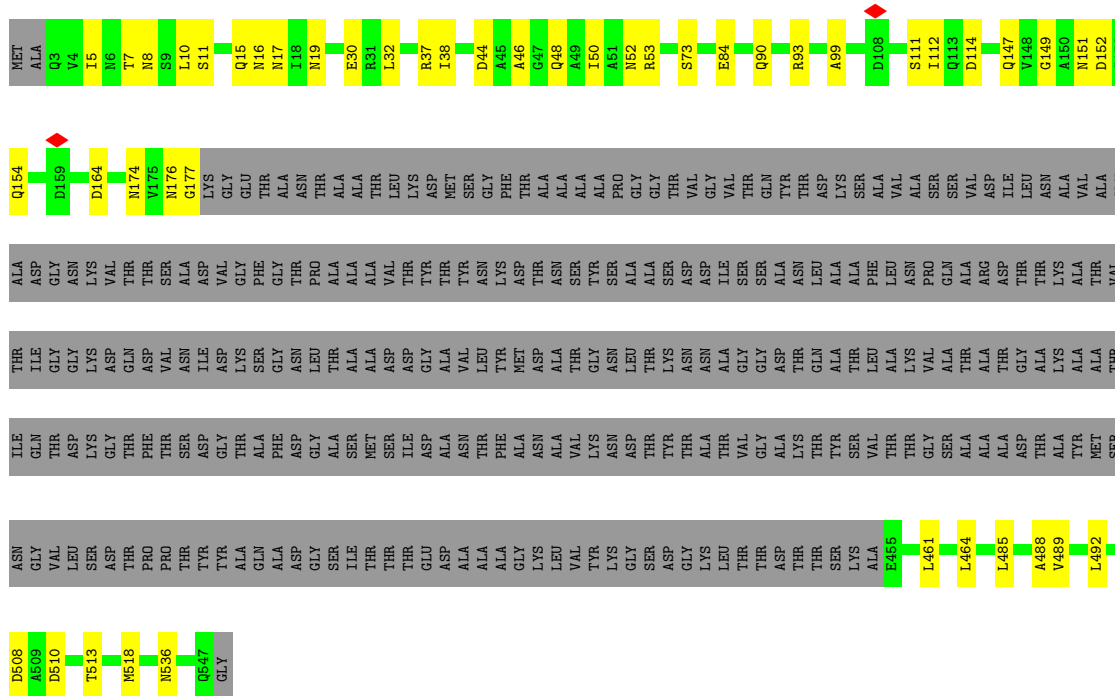
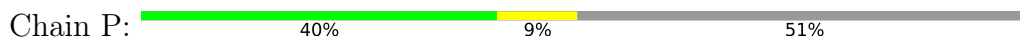




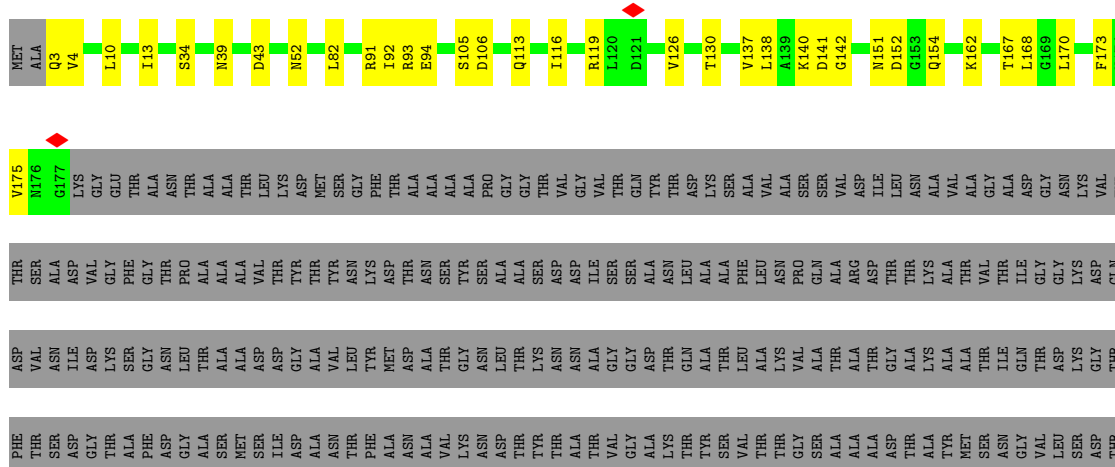




- Molecule 1: Flagellin

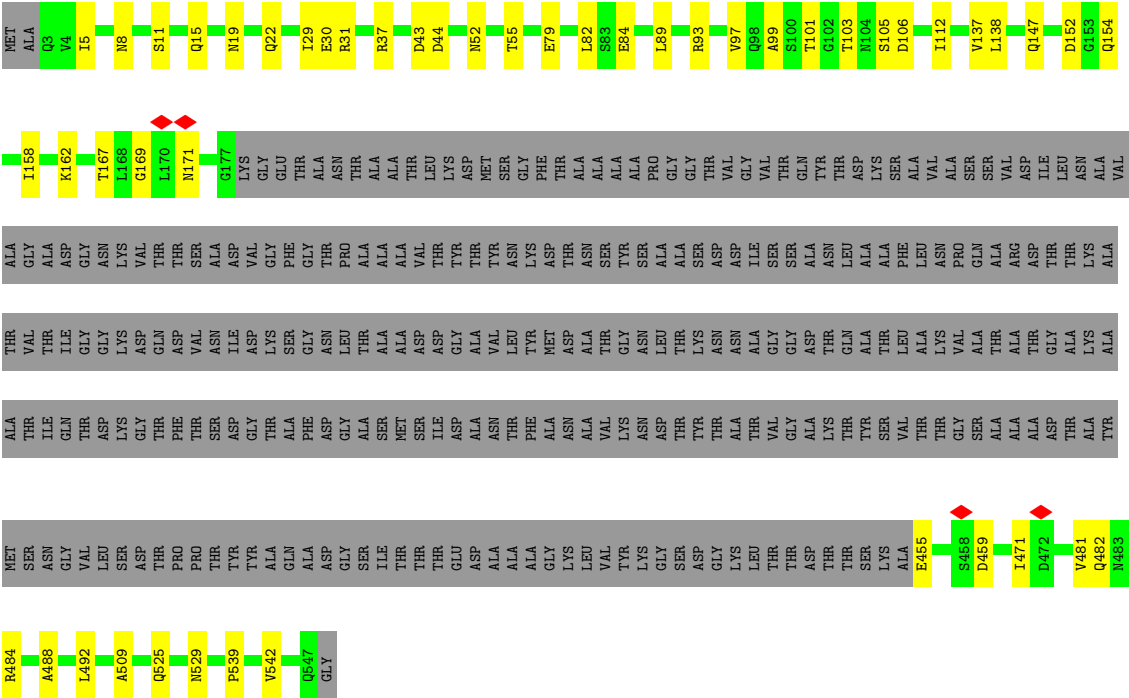
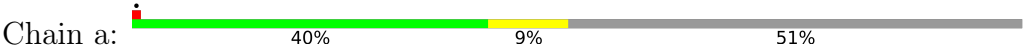


- Molecule 1: Flagellin

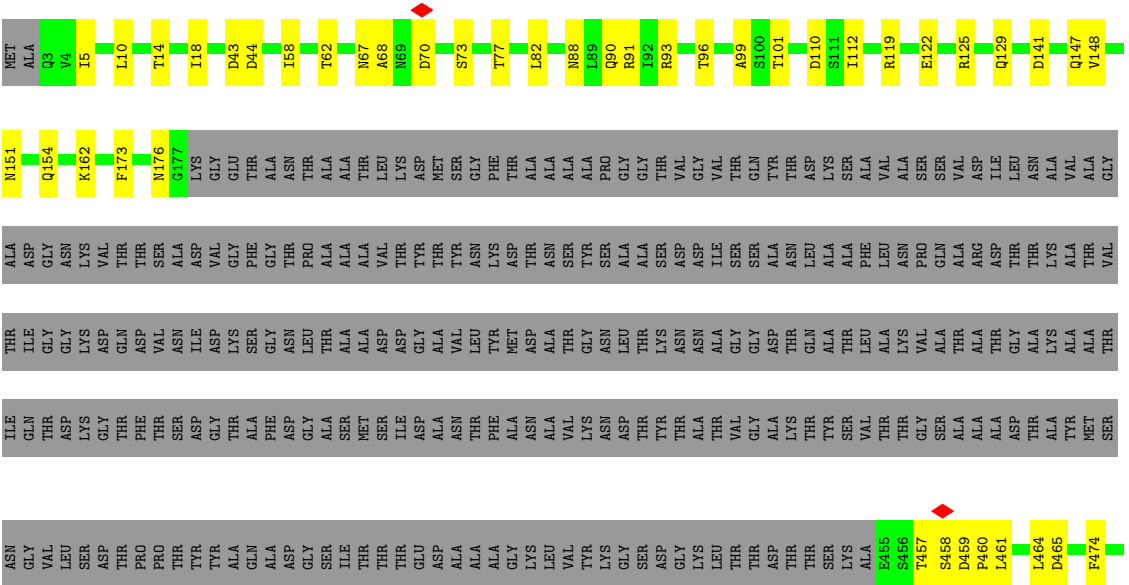
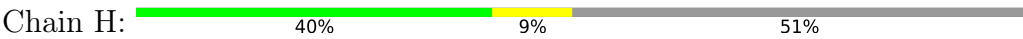




● Molecule 1: Flagellin



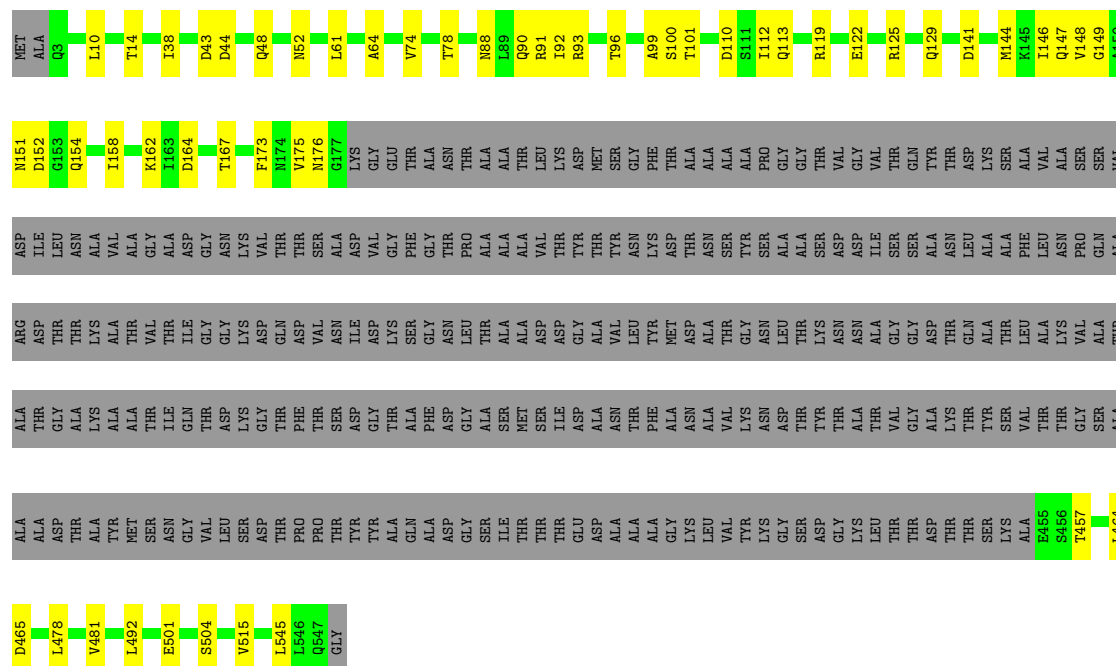
● Molecule 1: Flagellin





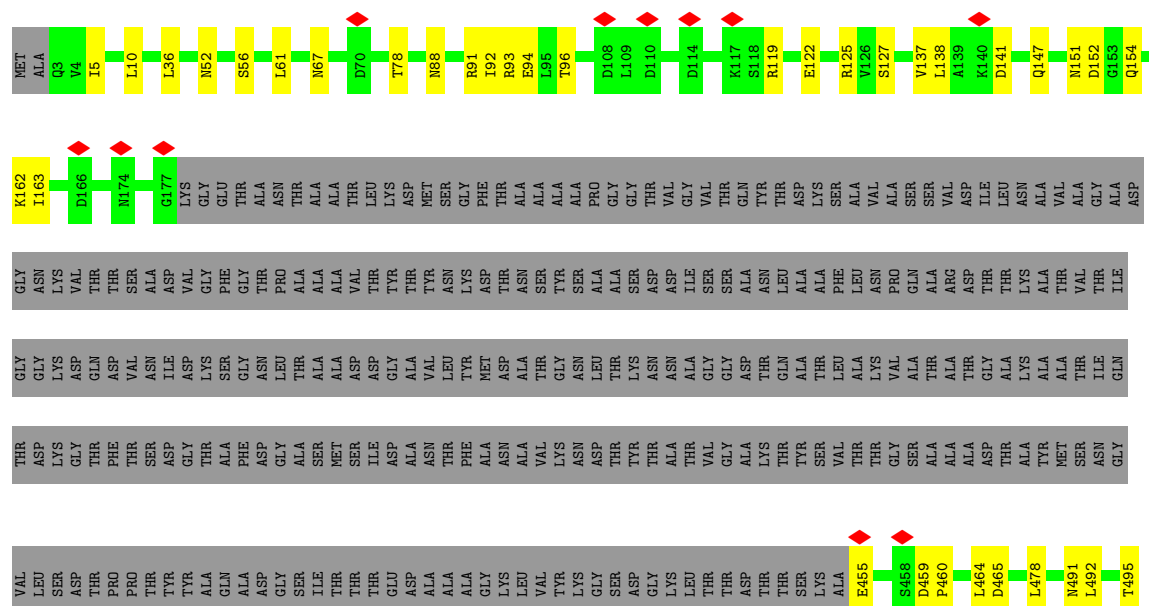
• Molecule 1: Flagellin

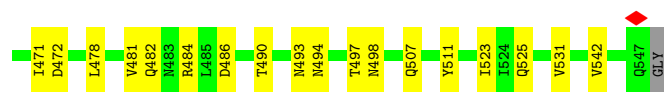
Chain R: 39% 10% 51%



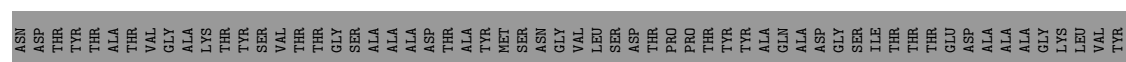
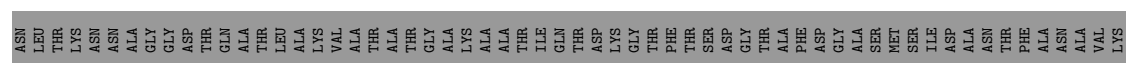
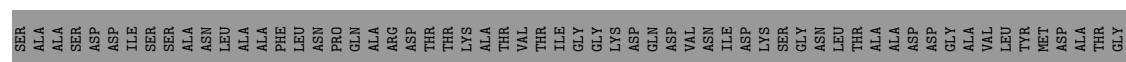
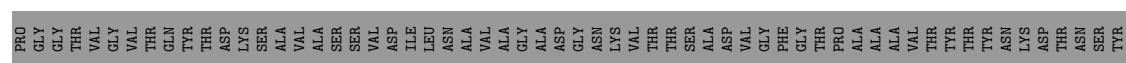
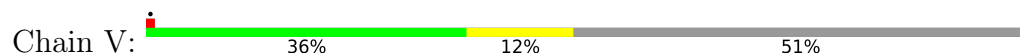
• Molecule 1: Flagellin

Chain b: 41% 7% 51%

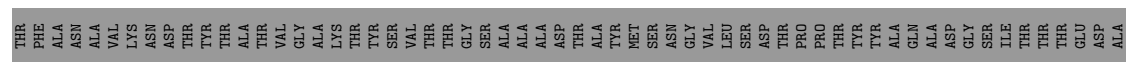
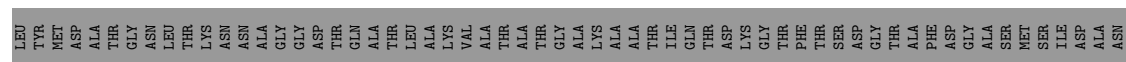
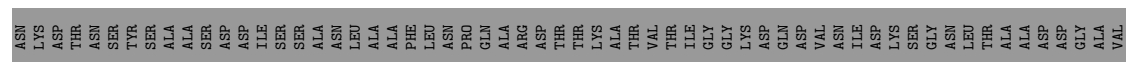
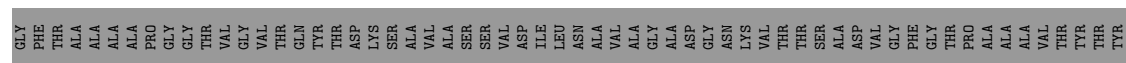
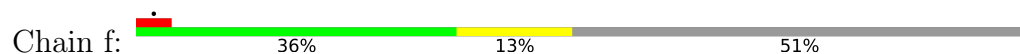


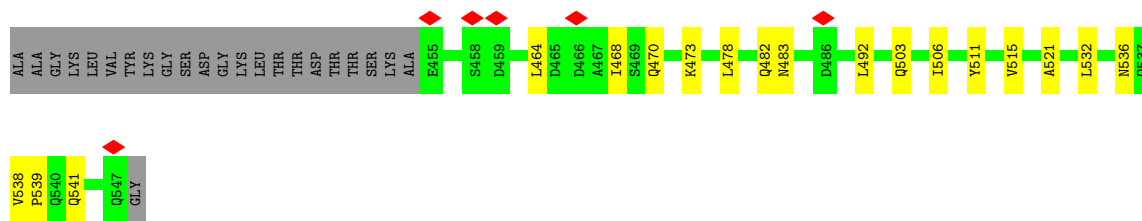


• Molecule 1: Flagellin

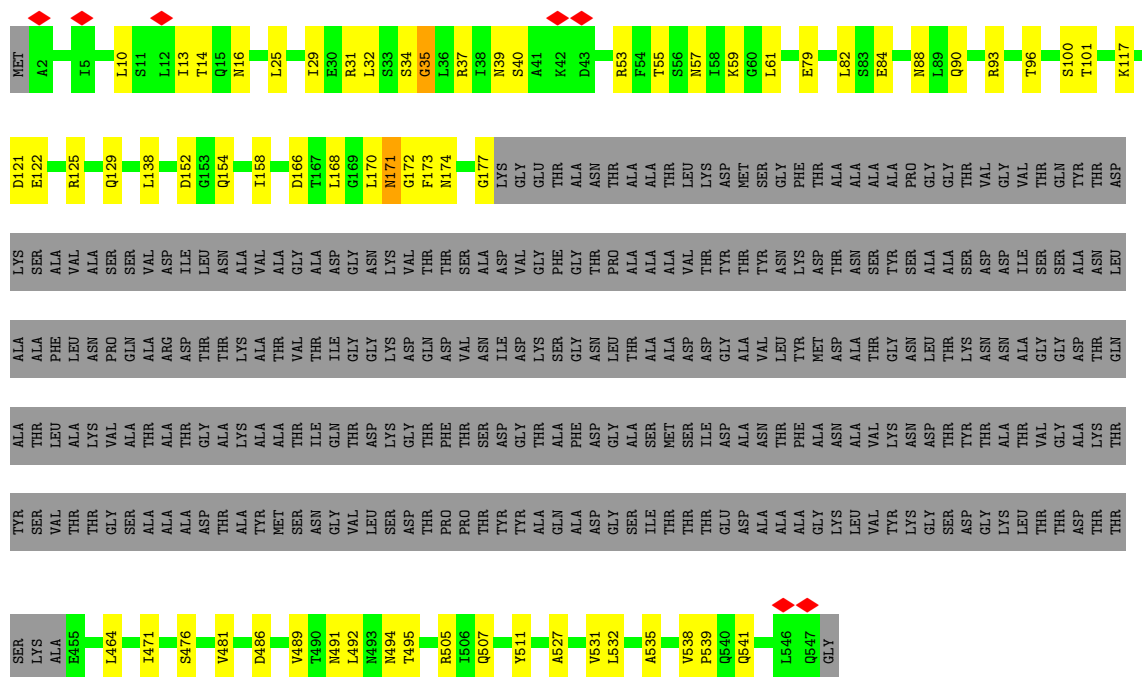
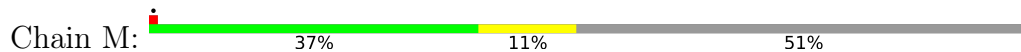


• Molecule 1: Flagellin

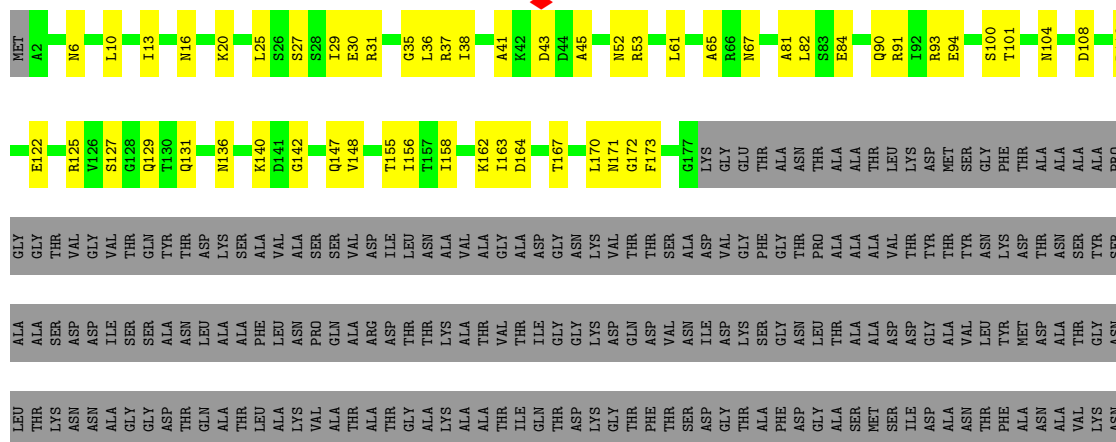
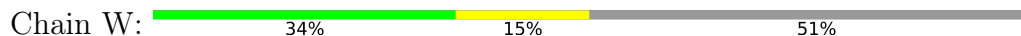


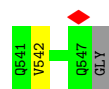


• Molecule 1: Flagellin



• Molecule 1: Flagellin





Chain g:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97477	Depositor
Resolution determination method	FSC 0.33 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.755	Depositor
Minimum map value	-0.525	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.136	Depositor
Map size ($\text{\AA}$)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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	0.13	0/1990	0.32	0/2691
1	B	0.14	0/1990	0.30	0/2691
1	C	0.14	0/1990	0.34	0/2691
1	D	0.13	0/2001	0.29	0/2706
1	E	0.13	0/2001	0.28	0/2706
1	F	0.16	0/2001	0.29	0/2706
1	G	0.14	0/2001	0.30	0/2706
1	H	0.14	0/2001	0.30	0/2706
1	I	0.14	0/2014	0.34	0/2724
1	J	0.14	0/2014	0.36	0/2724
1	K	0.13	0/2014	0.33	0/2724
1	L	0.14	0/2014	0.31	0/2724
1	M	0.15	0/2014	0.36	0/2724
1	N	0.13	0/2001	0.29	0/2706
1	O	0.13	0/2001	0.29	0/2706
1	P	0.14	0/2001	0.28	0/2706
1	Q	0.14	0/2001	0.30	0/2706
1	R	0.14	0/2001	0.29	0/2706
1	S	0.15	0/2014	0.33	0/2724
1	T	0.14	0/2014	0.34	0/2724
1	U	0.15	0/2014	0.36	0/2724
1	V	0.14	0/2014	0.32	0/2724
1	W	0.14	0/2014	0.32	0/2724
1	X	0.12	0/2001	0.29	0/2706
1	Y	0.12	0/2001	0.28	0/2706
1	Z	0.12	0/2001	0.28	0/2706
1	a	0.14	0/2001	0.30	0/2706
1	b	0.12	0/2001	0.26	0/2706
1	c	0.14	0/2014	0.32	0/2724
1	d	0.14	0/2014	0.33	0/2724
1	e	0.14	0/2014	0.34	0/2724
1	f	0.13	0/2014	0.33	0/2724
1	g	0.14	0/2014	0.34	0/2724
All	All	0.14	0/66195	0.31	0/89523

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1
1	V	0	2
1	f	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	538	VAL	Peptide
1	V	40	SER	Peptide
1	V	41	ALA	Peptide
1	f	40	SER	Peptide
1	f	41	ALA	Peptide

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	1985	0	1966	37	0
1	B	1985	0	1966	36	0
1	C	1985	0	1966	49	0
1	D	1996	0	1979	30	0
1	E	1996	0	1979	24	0
1	F	1996	0	1979	44	0
1	G	1996	0	1979	39	0
1	H	1996	0	1979	36	0
1	I	2009	0	1994	34	0
1	J	2009	0	1994	39	0
1	K	2009	0	1994	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2009	0	1994	44	0
1	M	2009	0	1994	45	0
1	N	1996	0	1979	53	0
1	O	1996	0	1979	44	0
1	P	1996	0	1979	35	0
1	Q	1996	0	1979	41	0
1	R	1996	0	1979	37	0
1	S	2009	0	1994	43	0
1	T	2009	0	1994	41	0
1	U	2009	0	1994	53	0
1	V	2009	0	1994	56	0
1	W	2009	0	1994	71	0
1	X	1996	0	1979	41	0
1	Y	1996	0	1979	31	0
1	Z	1996	0	1979	29	0
1	a	1996	0	1979	33	0
1	b	1996	0	1979	30	0
1	c	2009	0	1994	47	0
1	d	2009	0	1994	38	0
1	e	2009	0	1994	48	0
1	f	2009	0	1994	50	0
1	g	2009	0	1994	69	0
All	All	66030	0	65493	1168	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 9.

All (1168) 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:T:34:SER:OG	1:T:39:ASN:ND2	2.12	0.82
1:U:512:ALA:HB2	1:e:545:LEU:HD21	1.64	0.80
1:Y:491:ASN:HB2	1:P:84:GLU:HG2	1.64	0.79
1:g:170:LEU:HD13	1:g:173:PHE:HB2	1.61	0.79
1:O:508:ASP:HB3	1:Y:4:VAL:HG21	1.65	0.78
1:W:35:GLY:O	1:g:6:ASN:ND2	2.18	0.77
1:F:154:GLN:OE1	1:G:129:GLN:NE2	2.17	0.74
1:D:158:ILE:HG12	1:D:481:VAL:HG11	1.68	0.74
1:D:140:LYS:HD2	1:D:142:GLY:H	1.52	0.73
1:P:461:LEU:HB2	1:Z:152:ASP:HB2	1.71	0.72
1:X:99:ALA:HB2	1:X:112:ILE:HD13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:ARG:HG3	1:O:122:GLU:HG3	1.71	0.71
1:f:92:ILE:HG23	1:f:116:ILE:HD12	1.70	0.71
1:X:140:LYS:HG2	1:X:142:GLY:H	1.55	0.71
1:I:497:THR:OG1	1:S:16:ASN:OD1	2.07	0.71
1:X:92:ILE:HD11	1:X:116:ILE:HG23	1.72	0.71
1:d:99:ALA:HB2	1:d:112:ILE:HG21	1.71	0.71
1:A:5:ILE:HG13	1:A:539:PRO:HB2	1.73	0.70
1:N:92:ILE:HD11	1:N:116:ILE:HG23	1.73	0.70
1:J:482:GLN:HB3	1:T:42:LYS:HE3	1.73	0.70
1:L:99:ALA:HB2	1:L:112:ILE:HG21	1.74	0.70
1:O:149:GLY:HA3	1:O:154:GLN:HG3	1.74	0.70
1:M:158:ILE:HG12	1:M:481:VAL:HG11	1.74	0.69
1:V:151:ASN:HD21	1:V:154:GLN:HE21	1.40	0.69
1:J:22:GLN:NE2	1:J:525:GLN:OE1	2.25	0.69
1:C:534:LYS:HA	1:C:537:GLN:HE21	1.57	0.69
1:S:82:LEU:HD12	1:S:471:ILE:HG23	1.74	0.69
1:H:125:ARG:HD2	1:H:129:GLN:HG3	1.74	0.68
1:U:90:GLN:NE2	1:e:52:ASN:OD1	2.27	0.68
1:I:82:LEU:HD21	1:I:471:ILE:HG23	1.74	0.68
1:Y:127:SER:OG	1:Y:163:ILE:O	2.11	0.68
1:O:541:GLN:OE1	1:F:529:ASN:ND2	2.26	0.67
1:f:532:LEU:O	1:f:536:ASN:ND2	2.26	0.67
1:O:88:ASN:ND2	1:O:122:GLU:OE2	2.27	0.67
1:U:101:THR:OG1	1:e:67:ASN:ND2	2.28	0.67
1:e:494:ASN:O	1:e:498:ASN:ND2	2.28	0.67
1:F:504:SER:HB2	1:P:7:THR:HG21	1.76	0.67
1:S:148:VAL:HG21	1:S:156:ILE:HD12	1.77	0.67
1:U:149:GLY:HA3	1:U:154:GLN:HB2	1.75	0.67
1:G:101:THR:HG22	1:Q:147:GLN:HB3	1.77	0.67
1:c:37:ARG:N	1:c:507:GLN:O	2.26	0.67
1:Q:498:ASN:HD22	1:H:77:THR:HA	1.59	0.66
1:L:166:ASP:HA	1:L:171:ASN:HB2	1.77	0.66
1:S:90:GLN:NE2	1:c:56:SER:OG	2.26	0.66
1:f:538:VAL:O	1:f:541:GLN:NE2	2.28	0.66
1:V:541:GLN:HB3	1:W:529:ASN:HD22	1.60	0.66
1:g:147:GLN:HA	1:g:155:THR:HA	1.77	0.66
1:W:37:ARG:NH1	1:W:506:ILE:O	2.27	0.66
1:g:13:ILE:O	1:g:17:ASN:ND2	2.28	0.66
1:g:26:SER:O	1:g:30:GLU:HG2	1.95	0.66
1:M:101:THR:HG22	1:W:147:GLN:H	1.60	0.66
1:F:90:GLN:NE2	1:P:52:ASN:OD1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:82:LEU:HD12	1:a:471:ILE:HG23	1.77	0.65
1:C:491:ASN:HB3	1:N:84:GLU:HG3	1.78	0.65
1:M:125:ARG:NH1	1:M:129:GLN:OE1	2.30	0.65
1:W:127:SER:OG	1:W:163:ILE:O	2.12	0.65
1:A:3:GLN:HE21	1:A:4:VAL:HG12	1.61	0.65
1:B:505:ARG:HD3	1:D:69:ASN:HB3	1.76	0.65
1:c:505:ARG:NH1	1:d:73:SER:OG	2.29	0.65
1:U:37:ARG:NH2	1:U:44:ASP:OD2	2.30	0.65
1:f:5:ILE:HG22	1:f:539:PRO:HB3	1.78	0.65
1:g:61:LEU:HD22	1:g:492:LEU:HD22	1.78	0.65
1:e:158:ILE:HG12	1:e:481:VAL:HG11	1.78	0.65
1:J:99:ALA:HB2	1:J:112:ILE:HG21	1.78	0.65
1:e:22:GLN:NE2	1:e:525:GLN:OE1	2.30	0.65
1:O:63:GLN:NE2	1:O:67:ASN:OD1	2.29	0.64
1:M:174:ASN:ND2	1:M:177:GLY:O	2.30	0.64
1:K:158:ILE:HG12	1:K:481:VAL:HG21	1.80	0.64
1:c:88:ASN:OD1	1:c:119:ARG:NH1	2.29	0.64
1:L:19:ASN:HA	1:L:22:GLN:HE21	1.62	0.64
1:R:92:ILE:HD11	1:R:119:ARG:HB2	1.78	0.64
1:H:173:PHE:O	1:H:457:THR:OG1	2.13	0.64
1:T:147:GLN:NE2	1:T:151:ASN:O	2.32	0.64
1:e:541:GLN:OE1	1:V:529:ASN:ND2	2.30	0.64
1:L:151:ASN:OD1	1:L:154:GLN:NE2	2.31	0.63
1:g:170:LEU:HD12	1:g:171:ASN:H	1.63	0.63
1:P:90:GLN:NE2	1:Z:52:ASN:OD1	2.31	0.63
1:L:101:THR:OG1	1:V:67:ASN:ND2	2.32	0.63
1:K:461:LEU:HB2	1:U:152:ASP:HB2	1.79	0.63
1:V:99:ALA:HB2	1:V:112:ILE:HG21	1.81	0.63
1:g:99:ALA:HB2	1:g:112:ILE:HD13	1.79	0.63
1:Z:140:LYS:HG3	1:Z:142:GLY:H	1.63	0.63
1:O:90:GLN:NE2	1:Y:52:ASN:OD1	2.32	0.63
1:Q:461:LEU:HB2	1:a:152:ASP:HB2	1.80	0.63
1:d:34:SER:OG	1:d:39:ASN:ND2	2.32	0.63
1:J:101:THR:OG1	1:T:67:ASN:ND2	2.32	0.62
1:K:63:GLN:NE2	1:K:67:ASN:OD1	2.32	0.62
1:R:151:ASN:HB3	1:R:154:GLN:HE22	1.64	0.62
1:B:90:GLN:NE2	1:C:52:ASN:OD1	2.32	0.62
1:D:99:ALA:HB2	1:D:112:ILE:HG21	1.82	0.62
1:g:480:ALA:O	1:g:484:ARG:HG3	2.00	0.62
1:N:475:ARG:NH2	1:X:52:ASN:OD1	2.31	0.62
1:G:86:ASN:OD1	1:Q:52:ASN:ND2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:ARG:HA	1:H:464:LEU:HD13	1.81	0.62
1:N:147:GLN:NE2	1:N:151:ASN:O	2.29	0.61
1:O:162:LYS:NZ	1:O:164:ASP:OD2	2.33	0.61
1:c:88:ASN:HB2	1:c:123:ILE:HD11	1.81	0.61
1:U:461:LEU:HB2	1:e:152:ASP:HB2	1.82	0.61
1:e:145:LYS:HG2	1:e:157:THR:HG22	1.82	0.61
1:C:92:ILE:HD11	1:C:119:ARG:HB2	1.82	0.61
1:b:92:ILE:HD11	1:b:119:ARG:HB2	1.82	0.61
1:g:158:ILE:HG12	1:g:481:VAL:HG11	1.83	0.61
1:f:144:MET:HB3	1:f:158:ILE:HB	1.83	0.61
1:g:84:GLU:O	1:g:88:ASN:ND2	2.33	0.61
1:Z:82:LEU:HD12	1:Z:471:ILE:HG23	1.81	0.61
1:b:154:GLN:OE1	1:c:129:GLN:NE2	2.34	0.61
1:T:475:ARG:NH2	1:d:48:GLN:OE1	2.33	0.61
1:J:37:ARG:HG3	1:J:509:ALA:HB2	1.83	0.61
1:d:93:ARG:HB2	1:d:464:LEU:HD22	1.81	0.61
1:I:85:ILE:HG23	1:I:123:ILE:HD12	1.83	0.61
1:g:166:ASP:HA	1:g:171:ASN:HB2	1.82	0.61
1:K:26:SER:O	1:K:30:GLU:HG3	2.01	0.61
1:U:154:GLN:HB3	1:L:129:GLN:HG2	1.83	0.61
1:S:88:ASN:OD1	1:S:119:ARG:NH1	2.33	0.60
1:c:501:GLU:OE2	1:d:76:GLN:NE2	2.34	0.60
1:e:95:LEU:HD12	1:e:112:ILE:HG23	1.82	0.60
1:S:101:THR:HG22	1:c:147:GLN:H	1.67	0.60
1:K:85:ILE:HG23	1:K:123:ILE:HD12	1.81	0.60
1:H:90:GLN:NE2	1:R:52:ASN:OD1	2.34	0.60
1:M:31:ARG:NH1	1:M:37:ARG:O	2.34	0.60
1:C:488:ALA:HB2	1:N:125:ARG:HH22	1.66	0.60
1:G:30:GLU:OE1	1:G:39:ASN:ND2	2.34	0.60
1:B:61:LEU:HD22	1:B:492:LEU:HD22	1.83	0.60
1:T:170:LEU:HB2	1:T:173:PHE:HB2	1.84	0.60
1:X:485:LEU:O	1:X:489:VAL:HG23	2.02	0.60
1:A:99:ALA:HB2	1:A:112:ILE:HG21	1.84	0.60
1:E:90:GLN:NE2	1:O:52:ASN:OD1	2.35	0.60
1:E:99:ALA:HB2	1:E:112:ILE:HG21	1.82	0.60
1:E:149:GLY:HA3	1:E:154:GLN:HG3	1.84	0.60
1:g:69:ASN:HA	1:g:72:ILE:HD12	1.82	0.60
1:C:174:ASN:ND2	1:C:455:GLU:O	2.35	0.60
1:T:99:ALA:HB2	1:T:112:ILE:HG21	1.82	0.60
1:M:166:ASP:HA	1:M:171:ASN:HB2	1.84	0.60
1:S:151:ASN:HB2	1:S:154:GLN:HE22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:VAL:HG23	1:J:138:LEU:HD12	1.84	0.60
1:K:174:ASN:ND2	1:K:177:GLY:O	2.34	0.60
1:f:89:LEU:HD11	1:f:168:LEU:HD21	1.83	0.60
1:g:106:ASP:HA	1:g:109:LEU:HD12	1.83	0.60
1:H:110:ASP:OD1	1:H:176:ASN:ND2	2.34	0.59
1:H:122:GLU:OE2	1:H:125:ARG:NH2	2.35	0.59
1:L:494:ASN:O	1:L:498:ASN:ND2	2.35	0.59
1:S:103:THR:HG22	1:c:133:ASN:HD22	1.66	0.59
1:L:82:LEU:HD12	1:L:471:ILE:HG23	1.83	0.59
1:V:101:THR:HG23	1:f:146:ILE:HA	1.83	0.59
1:Z:491:ASN:HB2	1:a:84:GLU:HG2	1.83	0.59
1:I:36:LEU:HD22	1:I:507:GLN:HG2	1.83	0.59
1:M:101:THR:HG21	1:W:67:ASN:HB3	1.83	0.59
1:M:53:ARG:O	1:M:57:ASN:ND2	2.36	0.59
1:N:144:MET:HB3	1:N:158:ILE:HB	1.83	0.59
1:M:90:GLN:NE2	1:W:52:ASN:OD1	2.35	0.59
1:W:461:LEU:HD13	1:g:152:ASP:HB3	1.84	0.59
1:U:99:ALA:HB2	1:U:112:ILE:HG21	1.84	0.59
1:f:149:GLY:HA3	1:f:154:GLN:HG2	1.83	0.59
1:W:125:ARG:NH1	1:W:129:GLN:OE1	2.35	0.59
1:g:140:LYS:HD3	1:g:142:GLY:H	1.68	0.59
1:A:79:GLU:HG3	1:A:478:LEU:HD23	1.84	0.59
1:A:147:GLN:NE2	1:A:151:ASN:O	2.35	0.59
1:R:113:GLN:HG2	1:R:175:VAL:HG12	1.84	0.59
1:c:158:ILE:HG12	1:c:481:VAL:HG11	1.85	0.59
1:J:55:THR:HA	1:J:58:ILE:HD12	1.85	0.59
1:e:93:ARG:HD3	1:e:464:LEU:HD11	1.85	0.59
1:g:170:LEU:HD12	1:g:171:ASN:N	2.16	0.59
1:F:93:ARG:HA	1:F:464:LEU:HD13	1.85	0.58
1:Z:92:ILE:HD11	1:Z:119:ARG:HB2	1.84	0.58
1:U:69:ASN:O	1:U:72:ILE:HG22	2.02	0.58
1:V:90:GLN:NE2	1:f:52:ASN:OD1	2.36	0.58
1:M:35:GLY:O	1:W:6:ASN:ND2	2.33	0.58
1:O:492:LEU:O	1:O:496:THR:HG23	2.03	0.58
1:b:93:ARG:NH1	1:b:465:ASP:OD1	2.36	0.58
1:J:147:GLN:NE2	1:J:149:GLY:O	2.37	0.58
1:X:491:ASN:HB2	1:Y:84:GLU:HG3	1.85	0.58
1:L:31:ARG:HD3	1:L:37:ARG:HG3	1.85	0.58
1:B:73:SER:HG	1:W:505:ARG:HH22	1.47	0.58
1:C:37:ARG:NH2	1:C:506:ILE:O	2.36	0.58
1:M:61:LEU:HD22	1:M:492:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:460:PRO:HG2	1:W:461:LEU:HD12	1.86	0.58
1:g:125:ARG:NH1	1:g:129:GLN:OE1	2.37	0.58
1:D:85:ILE:HD11	1:D:123:ILE:HG23	1.84	0.58
1:H:151:ASN:HB3	1:H:154:GLN:HE22	1.69	0.58
1:K:125:ARG:NH1	1:K:129:GLN:OE1	2.36	0.58
1:g:27:SER:HB2	1:g:31:ARG:HH21	1.68	0.58
1:D:82:LEU:HD12	1:D:471:ILE:HG23	1.85	0.58
1:N:3:GLN:HG2	1:N:4:VAL:HG23	1.86	0.58
1:S:110:ASP:OD1	1:S:176:ASN:ND2	2.36	0.58
1:F:122:GLU:OE1	1:F:125:ARG:NH2	2.33	0.58
1:Z:93:ARG:HA	1:Z:464:LEU:HD13	1.86	0.58
1:R:88:ASN:OD1	1:R:119:ARG:NH1	2.37	0.58
1:f:170:LEU:HD21	1:f:173:PHE:HD1	1.69	0.58
1:g:5:ILE:HD11	1:g:542:VAL:HG11	1.84	0.58
1:Y:93:ARG:HA	1:Y:464:LEU:HD13	1.85	0.58
1:X:85:ILE:HD11	1:X:123:ILE:HG23	1.86	0.58
1:N:99:ALA:HB2	1:N:112:ILE:HG21	1.86	0.57
1:H:515:VAL:HG21	1:R:545:LEU:HD21	1.84	0.57
1:e:37:ARG:HB2	1:e:509:ALA:H	1.69	0.57
1:R:173:PHE:O	1:R:457:THR:OG1	2.21	0.57
1:A:25:LEU:O	1:A:29:ILE:HG12	2.04	0.57
1:a:99:ALA:HB2	1:a:112:ILE:HG21	1.86	0.57
1:I:110:ASP:OD1	1:I:176:ASN:ND2	2.37	0.57
1:e:3:GLN:OE1	1:V:22:GLN:NE2	2.36	0.57
1:F:51:ALA:O	1:F:55:THR:HG23	2.04	0.57
1:R:149:GLY:HA3	1:R:154:GLN:HG3	1.87	0.57
1:T:29:ILE:HD13	1:T:518:MET:HE2	1.86	0.57
1:A:38:ILE:HD11	1:A:507:GLN:HG2	1.86	0.57
1:f:46:ALA:O	1:f:50:ILE:HG13	2.04	0.57
1:N:492:LEU:O	1:N:496:THR:HG23	2.05	0.57
1:K:137:VAL:HG23	1:K:138:LEU:HD12	1.87	0.57
1:U:91:ARG:NH1	1:U:94:GLU:OE1	2.38	0.57
1:A:108:ASP:OD1	1:W:53:ARG:NH2	2.37	0.57
1:G:25:LEU:O	1:G:29:ILE:HG13	2.05	0.57
1:B:37:ARG:NH2	1:B:506:ILE:O	2.36	0.57
1:F:511:TYR:CE2	1:P:5:ILE:HG12	2.40	0.57
1:P:93:ARG:HA	1:P:464:LEU:HD13	1.86	0.57
1:T:17:ASN:ND2	1:K:33:SER:OG	2.37	0.57
1:N:126:VAL:O	1:N:130:THR:OG1	2.19	0.56
1:e:125:ARG:NH1	1:e:129:GLN:OE1	2.38	0.56
1:L:523:ILE:HD11	1:W:540:GLN:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:65:ALA:HB1	1:W:489:VAL:HG23	1.86	0.56
1:b:93:ARG:HA	1:b:464:LEU:HD13	1.85	0.56
1:J:512:ALA:HB2	1:T:545:LEU:HD13	1.86	0.56
1:M:93:ARG:HA	1:M:464:LEU:HD13	1.87	0.56
1:W:527:ALA:O	1:W:531:VAL:HG23	2.05	0.56
1:Y:99:ALA:HB2	1:Y:112:ILE:HG21	1.87	0.56
1:F:532:LEU:O	1:F:536:ASN:ND2	2.38	0.56
1:Q:99:ALA:HB2	1:Q:112:ILE:HG21	1.88	0.56
1:J:91:ARG:NH1	1:J:94:GLU:OE2	2.39	0.56
1:J:166:ASP:OD1	1:J:171:ASN:ND2	2.39	0.56
1:d:491:ASN:HA	1:d:494:ASN:HD21	1.71	0.56
1:U:505:ARG:HD3	1:L:69:ASN:HB3	1.87	0.56
1:L:125:ARG:HG2	1:L:129:GLN:OE1	2.05	0.56
1:V:93:ARG:HA	1:V:464:LEU:HD13	1.87	0.56
1:V:541:GLN:HB3	1:W:529:ASN:ND2	2.18	0.56
1:X:82:LEU:HD12	1:X:471:ILE:HG23	1.88	0.56
1:F:484:ARG:HH12	1:G:121:ASP:HB3	1.70	0.56
1:J:101:THR:HG22	1:J:103:THR:H	1.71	0.56
1:T:93:ARG:HA	1:T:464:LEU:HD21	1.88	0.56
1:L:158:ILE:HG12	1:L:481:VAL:HG11	1.87	0.56
1:Z:151:ASN:HB3	1:Z:154:GLN:HE22	1.70	0.56
1:e:31:ARG:NH1	1:e:37:ARG:O	2.39	0.56
1:f:31:ARG:HD3	1:f:37:ARG:HG3	1.87	0.56
1:A:26:SER:O	1:A:30:GLU:HG3	2.05	0.56
1:Y:505:ARG:NH1	1:P:73:SER:OG	2.39	0.56
1:G:99:ALA:HB2	1:G:112:ILE:HG21	1.88	0.56
1:U:538:VAL:HG13	1:L:525:GLN:HE22	1.70	0.56
1:f:99:ALA:HB2	1:f:112:ILE:HD13	1.88	0.56
1:Z:113:GLN:HG2	1:Z:175:VAL:HG12	1.87	0.56
1:G:149:GLY:HA3	1:G:154:GLN:HG3	1.88	0.56
1:D:494:ASN:OD1	1:N:16:ASN:ND2	2.38	0.55
1:H:93:ARG:NH1	1:H:465:ASP:OD1	2.38	0.55
1:L:531:VAL:HG11	1:M:32:LEU:HB3	1.88	0.55
1:C:125:ARG:NH1	1:C:129:GLN:OE1	2.39	0.55
1:W:36:LEU:HD12	1:W:507:GLN:HG2	1.89	0.55
1:W:90:GLN:NE2	1:g:52:ASN:OD1	2.39	0.55
1:X:10:LEU:HD23	1:Y:29:ILE:HG21	1.88	0.55
1:X:546:LEU:O	1:X:547:GLN:NE2	2.36	0.55
1:d:158:ILE:HG12	1:d:481:VAL:HG11	1.88	0.55
1:C:472:ASP:OD2	1:C:475:ARG:NH2	2.39	0.55
1:Q:82:LEU:HD12	1:Q:471:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:82:LEU:HD21	1:S:138:LEU:HD21	1.88	0.55
1:K:109:LEU:HB3	1:K:176:ASN:HB3	1.87	0.55
1:e:160:LEU:HA	1:e:474:PHE:HZ	1.71	0.55
1:O:93:ARG:HA	1:O:464:LEU:HD13	1.87	0.55
1:U:31:ARG:NH1	1:U:37:ARG:O	2.39	0.55
1:e:484:ARG:HG3	1:V:122:GLU:HB2	1.88	0.55
1:f:10:LEU:HD21	1:g:29:ILE:HG13	1.89	0.55
1:a:158:ILE:HG12	1:a:481:VAL:HG21	1.88	0.55
1:b:91:ARG:NH1	1:b:94:GLU:OE2	2.40	0.55
1:H:91:ARG:HG2	1:H:119:ARG:NE	2.22	0.55
1:J:497:THR:HG21	1:T:16:ASN:OD1	2.07	0.55
1:Z:43:ASP:N	1:Z:43:ASP:OD1	2.40	0.55
1:a:162:LYS:NZ	1:a:167:THR:OG1	2.39	0.55
1:I:520:LYS:O	1:I:524:ILE:HG13	2.07	0.55
1:C:14:THR:HG21	1:C:532:LEU:HB2	1.88	0.55
1:P:17:ASN:ND2	1:Q:33:SER:OG	2.39	0.55
1:N:140:LYS:HD2	1:N:142:GLY:H	1.70	0.55
1:W:93:ARG:HA	1:W:464:LEU:HD13	1.89	0.55
1:A:456:SER:OG	1:A:457:THR:N	2.40	0.54
1:C:76:GLN:NE2	1:C:482:GLN:OE1	2.39	0.54
1:E:89:LEU:HD12	1:E:471:ILE:HD12	1.89	0.54
1:S:117:LYS:NZ	1:S:121:ASP:OD2	2.40	0.54
1:f:120:LEU:HA	1:f:123:ILE:HD12	1.89	0.54
1:Z:170:LEU:HD22	1:Z:173:PHE:HE1	1.72	0.54
1:H:101:THR:HG22	1:R:147:GLN:HB3	1.88	0.54
1:R:93:ARG:NH1	1:R:465:ASP:OD1	2.40	0.54
1:e:505:ARG:NH1	1:V:73:SER:OG	2.40	0.54
1:N:137:VAL:HG23	1:N:138:LEU:HG	1.89	0.54
1:H:82:LEU:HD21	1:H:474:PHE:CD2	2.42	0.54
1:B:485:LEU:O	1:B:489:VAL:HG23	2.06	0.54
1:N:8:ASN:ND2	1:N:11:SER:OG	2.30	0.54
1:c:92:ILE:HD11	1:c:119:ARG:HB2	1.89	0.54
1:J:486:ASP:HA	1:J:489:VAL:HG12	1.89	0.54
1:A:88:ASN:OD1	1:A:119:ARG:NH1	2.39	0.54
1:N:147:GLN:HA	1:N:155:THR:HG22	1.89	0.54
1:F:497:THR:HG21	1:P:16:ASN:HD21	1.73	0.54
1:c:31:ARG:HD2	1:c:37:ARG:HA	1.88	0.54
1:J:503:GLN:NE2	1:J:507:GLN:OE1	2.41	0.54
1:K:88:ASN:HB2	1:K:123:ILE:HD11	1.89	0.54
1:N:531:VAL:HG11	1:O:32:LEU:HB3	1.90	0.54
1:F:158:ILE:HG12	1:F:481:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:99:ALA:HB2	1:S:112:ILE:HG21	1.90	0.54
1:J:170:LEU:HB2	1:J:173:PHE:HB2	1.89	0.54
1:V:149:GLY:HA3	1:V:154:GLN:HG2	1.90	0.54
1:U:147:GLN:HG2	1:U:155:THR:HG22	1.90	0.54
1:N:79:GLU:OE2	1:N:482:GLN:NE2	2.24	0.54
1:L:93:ARG:NH1	1:L:465:ASP:OD1	2.41	0.54
1:N:53:ARG:NH2	1:E:108:ASP:OD1	2.40	0.54
1:Z:105:SER:OG	1:Z:106:ASP:N	2.41	0.54
1:L:105:SER:OG	1:L:106:ASP:N	2.41	0.54
1:B:125:ARG:NH1	1:B:129:GLN:OE1	2.41	0.53
1:C:485:LEU:O	1:C:489:VAL:HG23	2.08	0.53
1:Q:5:ILE:HG21	1:Q:542:VAL:HG21	1.90	0.53
1:Q:90:GLN:NE2	1:a:52:ASN:OD1	2.41	0.53
1:T:96:THR:O	1:T:100:SER:OG	2.27	0.53
1:Z:92:ILE:HD12	1:Z:116:ILE:HG23	1.89	0.53
1:G:461:LEU:HB2	1:Q:152:ASP:HB2	1.89	0.53
1:H:534:LYS:NZ	1:S:546:LEU:O	2.38	0.53
1:R:96:THR:O	1:R:100:SER:OG	2.27	0.53
1:K:497:THR:HG21	1:U:16:ASN:OD1	2.08	0.53
1:U:176:ASN:OD1	1:U:177:GLY:N	2.41	0.53
1:C:91:ARG:NH1	1:C:94:GLU:OE2	2.41	0.53
1:Q:145:LYS:HG2	1:Q:157:THR:HG22	1.91	0.53
1:f:88:ASN:O	1:f:92:ILE:HG13	2.08	0.53
1:W:140:LYS:HG2	1:W:142:GLY:H	1.73	0.53
1:g:93:ARG:O	1:g:97:VAL:HG23	2.08	0.53
1:F:99:ALA:HB2	1:F:112:ILE:HG21	1.89	0.53
1:L:95:LEU:HD11	1:L:112:ILE:HG12	1.91	0.53
1:M:84:GLU:O	1:M:88:ASN:ND2	2.41	0.53
1:D:173:PHE:O	1:D:457:THR:OG1	2.26	0.53
1:G:43:ASP:OD1	1:G:44:ASP:N	2.41	0.53
1:a:79:GLU:OE1	1:a:482:GLN:NE2	2.41	0.53
1:b:491:ASN:HB2	1:c:84:GLU:HG3	1.90	0.53
1:d:51:ALA:O	1:d:55:THR:HG23	2.08	0.53
1:e:512:ALA:HB1	1:f:532:LEU:HD21	1.91	0.53
1:f:88:ASN:OD1	1:f:119:ARG:NH1	2.38	0.53
1:M:168:LEU:HD11	1:M:471:ILE:HD11	1.89	0.53
1:D:93:ARG:HA	1:D:464:LEU:HD13	1.89	0.53
1:Y:13:ILE:HG21	1:P:30:GLU:HG2	1.91	0.53
1:S:125:ARG:HG2	1:S:129:GLN:OE1	2.09	0.53
1:K:99:ALA:HB2	1:K:112:ILE:HG21	1.91	0.53
1:U:93:ARG:HH12	1:U:461:LEU:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:ILE:HD11	1:L:542:VAL:HG11	1.90	0.53
1:V:105:SER:OG	1:V:106:ASP:N	2.42	0.53
1:O:68:ALA:HB2	1:O:148:VAL:HG12	1.91	0.53
1:Z:13:ILE:HG21	1:a:30:GLU:HG2	1.91	0.53
1:c:122:GLU:OE2	1:c:125:ARG:NH2	2.42	0.53
1:X:145:LYS:NZ	1:X:155:THR:OG1	2.35	0.53
1:Q:145:LYS:HB3	1:Q:155:THR:HG21	1.91	0.53
1:A:125:ARG:NH1	1:A:129:GLN:OE1	2.35	0.52
1:C:6:ASN:HA	1:W:520:LYS:HD2	1.91	0.52
1:C:511:TYR:O	1:C:515:VAL:HG23	2.09	0.52
1:E:105:SER:OG	1:E:106:ASP:N	2.42	0.52
1:Z:137:VAL:HG23	1:Z:138:LEU:HG	1.91	0.52
1:Q:15:GLN:O	1:Q:19:ASN:ND2	2.42	0.52
1:R:101:THR:HG22	1:b:147:GLN:H	1.74	0.52
1:A:503:GLN:NE2	1:A:507:GLN:OE1	2.42	0.52
1:F:82:LEU:HD12	1:F:471:ILE:HG23	1.92	0.52
1:P:15:GLN:O	1:P:19:ASN:ND2	2.42	0.52
1:P:37:ARG:NH1	1:P:44:ASP:OD2	2.40	0.52
1:d:498:ASN:HD22	1:U:77:THR:HA	1.74	0.52
1:U:89:LEU:HD12	1:U:471:ILE:HD12	1.92	0.52
1:e:149:GLY:HA3	1:e:154:GLN:HB2	1.91	0.52
1:N:149:GLY:HA3	1:N:154:GLN:HG3	1.91	0.52
1:X:520:LYS:O	1:X:524:ILE:HG13	2.08	0.52
1:S:531:VAL:HA	1:S:534:LYS:HG2	1.91	0.52
1:V:113:GLN:HE22	1:V:174:ASN:HA	1.74	0.52
1:V:137:VAL:HG23	1:V:138:LEU:HG	1.91	0.52
1:I:96:THR:O	1:I:100:SER:OG	2.27	0.52
1:c:113:GLN:HB2	1:c:176:ASN:HB3	1.91	0.52
1:K:79:GLU:OE2	1:U:40:SER:OG	2.27	0.52
1:X:96:THR:O	1:X:100:SER:OG	2.28	0.52
1:X:505:ARG:O	1:Y:66:ARG:NH2	2.41	0.52
1:E:16:ASN:HA	1:E:19:ASN:HD21	1.75	0.52
1:O:99:ALA:HB2	1:O:112:ILE:HG21	1.91	0.52
1:Z:3:GLN:OE1	1:a:22:GLN:NE2	2.42	0.52
1:R:93:ARG:HA	1:R:464:LEU:HD13	1.90	0.52
1:S:493:ASN:O	1:S:497:THR:HG23	2.09	0.52
1:e:36:LEU:HD23	1:e:508:ASP:HB3	1.92	0.52
1:e:159:ASP:OD2	1:e:159:ASP:N	2.43	0.52
1:M:527:ALA:O	1:M:531:VAL:HG23	2.10	0.52
1:X:531:VAL:HG11	1:Y:32:LEU:HB3	1.91	0.52
1:O:105:SER:OG	1:O:106:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:38:ILE:HG21	1:R:48:GLN:HB2	1.92	0.52
1:T:105:SER:OG	1:T:106:ASP:N	2.42	0.52
1:f:81:ALA:O	1:f:85:ILE:HG13	2.09	0.52
1:B:30:GLU:HG2	1:W:13:ILE:HG21	1.92	0.52
1:M:37:ARG:NH2	1:M:505:ARG:O	2.43	0.52
1:C:487:SER:O	1:C:491:ASN:ND2	2.43	0.52
1:G:90:GLN:NE2	1:Q:52:ASN:OD1	2.40	0.52
1:a:89:LEU:HD12	1:a:471:ILE:HD12	1.90	0.52
1:S:22:GLN:NE2	1:S:525:GLN:OE1	2.40	0.52
1:W:147:GLN:HA	1:W:155:THR:HG22	1.92	0.52
1:X:459:ASP:HB2	1:X:462:ALA:HB3	1.92	0.52
1:I:164:ASP:H	1:I:167:THR:HG22	1.74	0.52
1:T:38[A]:ILE:HG23	1:T:41:ALA:HB2	1.92	0.52
1:T:38[B]:ILE:HG23	1:T:41:ALA:HB2	1.92	0.52
1:d:110:ASP:HA	1:d:176:ASN:HD22	1.75	0.52
1:N:96:THR:HG21	1:N:464:LEU:HD11	1.92	0.52
1:X:525:GLN:O	1:X:529:ASN:ND2	2.43	0.52
1:L:170:LEU:HD11	1:L:457:THR:HG21	1.91	0.52
1:V:25:LEU:HB2	1:V:521:ALA:HB1	1.92	0.52
1:N:494:ASN:OD1	1:X:16:ASN:ND2	2.37	0.51
1:O:147:GLN:HA	1:O:155:THR:HG22	1.92	0.51
1:I:88:ASN:HB2	1:I:123:ILE:HD11	1.92	0.51
1:S:66:ARG:HA	1:S:69:ASN:ND2	2.24	0.51
1:a:484:ARG:HG3	1:R:122:GLU:HB2	1.92	0.51
1:H:88:ASN:OD1	1:H:119:ARG:NH1	2.42	0.51
1:R:61:LEU:HD22	1:R:492:LEU:HD22	1.91	0.51
1:R:144:MET:HE3	1:R:146:ILE:HD11	1.92	0.51
1:W:158:ILE:HG12	1:W:481:VAL:HG11	1.91	0.51
1:A:541:GLN:O	1:A:545:LEU:HG	2.10	0.51
1:X:53:ARG:NH2	1:O:108:ASP:OD1	2.42	0.51
1:O:34:SER:OG	1:O:39:ASN:OD1	2.25	0.51
1:V:82:LEU:HD11	1:V:163:ILE:HD12	1.91	0.51
1:A:164:ASP:OD1	1:A:165:SER:N	2.43	0.51
1:D:149:GLY:HA3	1:D:154:GLN:HG3	1.92	0.51
1:X:8:ASN:OD1	1:X:11:SER:N	2.35	0.51
1:T:104:ASN:HB3	1:T:108:ASP:HB2	1.92	0.51
1:X:38:ILE:HG21	1:X:44:ASP:HB3	1.93	0.51
1:E:149:GLY:O	1:E:154:GLN:NE2	2.43	0.51
1:Y:61:LEU:HD22	1:Y:492:LEU:HD22	1.93	0.51
1:G:58:ILE:O	1:G:62:THR:HG23	2.10	0.51
1:c:66:ARG:HA	1:c:69:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:151:ASN:OD1	1:K:131:GLN:NE2	2.43	0.51
1:U:82:LEU:HD12	1:U:471:ILE:HG23	1.93	0.51
1:C:158:ILE:HG12	1:C:481:VAL:HG11	1.93	0.51
1:b:61:LEU:HD13	1:b:495:THR:HG23	1.93	0.51
1:b:88:ASN:OD1	1:b:119:ARG:NH1	2.43	0.51
1:I:74:VAL:HG22	1:I:132:PHE:CE1	2.46	0.51
1:e:477:SER:O	1:e:481:VAL:HG23	2.09	0.51
1:g:93:ARG:HA	1:g:464:LEU:HD13	1.93	0.51
1:A:131:GLN:HE22	1:M:154:GLN:HE22	1.59	0.51
1:A:162:LYS:NZ	1:A:167:THR:OG1	2.39	0.51
1:P:38:ILE:HD12	1:P:48:GLN:HA	1.93	0.51
1:G:64:ALA:HB3	1:G:492:LEU:HD21	1.93	0.51
1:a:93:ARG:O	1:a:97:VAL:HG23	2.10	0.51
1:R:101:THR:HG21	1:b:67:ASN:HB3	1.93	0.51
1:K:510:ASP:O	1:K:513:THR:OG1	2.23	0.51
1:F:168:LEU:HD11	1:F:471:ILE:HD11	1.93	0.51
1:T:35:GLY:O	1:T:508:ASP:HA	2.11	0.51
1:D:113:GLN:OE1	1:D:175:VAL:N	2.39	0.51
1:S:85:ILE:HG23	1:S:123:ILE:HD12	1.92	0.51
1:f:470:GLN:HA	1:f:473:LYS:NZ	2.25	0.51
1:C:457:THR:HB	1:C:460:PRO:HG3	1.93	0.50
1:U:44:ASP:OD1	1:U:44:ASP:N	2.44	0.50
1:L:472:ASP:OD2	1:V:52:ASN:ND2	2.43	0.50
1:V:158:ILE:HG12	1:V:481:VAL:HG11	1.92	0.50
1:g:38[A]:ILE:HG23	1:g:41:ALA:HB2	1.94	0.50
1:g:38[B]:ILE:HG23	1:g:41:ALA:HB2	1.94	0.50
1:C:5:ILE:HD11	1:W:523:ILE:HD12	1.94	0.50
1:O:515:VAL:HA	1:O:518:MET:HG2	1.93	0.50
1:R:110:ASP:OD1	1:R:176:ASN:ND2	2.39	0.50
1:b:137:VAL:HG23	1:b:138:LEU:HG	1.92	0.50
1:A:527:ALA:O	1:A:531:VAL:HG23	2.12	0.50
1:A:529:ASN:ND2	1:M:541:GLN:HB3	2.25	0.50
1:C:122:GLU:OE2	1:g:484:ARG:HB3	2.11	0.50
1:S:486:ASP:OD1	1:c:42:LYS:NZ	2.44	0.50
1:c:92:ILE:HD12	1:c:116:ILE:HG12	1.93	0.50
1:e:91:ARG:NH1	1:e:94:GLU:OE2	2.44	0.50
1:N:170:LEU:HB2	1:N:173:PHE:HD1	1.77	0.50
1:G:459:ASP:OD1	1:G:459:ASP:N	2.42	0.50
1:Q:459:ASP:OD2	1:Q:459:ASP:N	2.43	0.50
1:d:541:GLN:O	1:d:544:SER:OG	2.27	0.50
1:f:51:ALA:O	1:f:55:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:ARG:HA	1:I:69:ASN:ND2	2.27	0.50
1:I:125:ARG:HG2	1:I:129:GLN:OE1	2.11	0.50
1:T:51:ALA:O	1:T:55:THR:HG23	2.11	0.50
1:d:93:ARG:HA	1:d:96:THR:HG22	1.92	0.50
1:e:154:GLN:HB3	1:V:129:GLN:OE1	2.11	0.50
1:A:32:LEU:HB3	1:M:531:VAL:HG21	1.92	0.50
1:K:485:LEU:O	1:K:489:VAL:HG13	2.11	0.50
1:f:50:ILE:HG12	1:W:108:ASP:OD1	2.12	0.50
1:W:38[A]:ILE:HG22	1:W:41:ALA:H	1.77	0.50
1:A:511:TYR:O	1:A:515:VAL:HG23	2.12	0.50
1:F:141:ASP:OD1	1:F:141:ASP:N	2.44	0.50
1:G:98:GLN:HE21	1:G:112:ILE:HG12	1.75	0.50
1:H:43:ASP:OD1	1:H:44:ASP:N	2.44	0.50
1:c:137:VAL:HG13	1:c:160:LEU:HD13	1.94	0.50
1:V:497:THR:OG1	1:f:16:ASN:OD1	2.26	0.50
1:b:122:GLU:OE2	1:b:125:ARG:NH2	2.29	0.50
1:M:37:ARG:N	1:M:507:GLN:O	2.34	0.50
1:W:82:LEU:HD12	1:W:471:ILE:HG23	1.92	0.50
1:Z:10:LEU:HD13	1:a:29:ILE:HG21	1.93	0.50
1:S:156:ILE:HD13	1:S:484:ARG:HD3	1.93	0.50
1:c:91:ARG:NH1	1:c:94:GLU:OE1	2.45	0.50
1:K:101:THR:HG22	1:K:103:THR:H	1.77	0.50
1:L:125:ARG:NH1	1:L:129:GLN:OE1	2.45	0.50
1:V:95:LEU:HD12	1:V:112:ILE:HG23	1.94	0.50
1:b:10:LEU:HD21	1:c:26:SER:HA	1.94	0.49
1:V:40:SER:O	1:V:42:LYS:N	2.41	0.49
1:g:31:ARG:NH1	1:g:37:ARG:O	2.44	0.49
1:g:64:ALA:HB1	1:g:148:VAL:HA	1.93	0.49
1:D:21:ASN:HD21	1:D:521:ALA:HA	1.77	0.49
1:X:492:LEU:O	1:X:496:THR:HG23	2.12	0.49
1:E:541:GLN:O	1:E:544:SER:OG	2.24	0.49
1:a:43:ASP:OD1	1:a:44:ASP:N	2.44	0.49
1:d:44:ASP:HB3	1:K:91:ARG:HH21	1.76	0.49
1:W:61:LEU:HD22	1:W:492:LEU:HG	1.93	0.49
1:g:40:SER:O	1:g:48:GLN:NE2	2.45	0.49
1:P:53:ARG:NH2	1:G:108:ASP:OD2	2.45	0.49
1:S:88:ASN:HB2	1:S:123:ILE:HD11	1.94	0.49
1:J:37:ARG:H	1:J:508:ASP:N	2.10	0.49
1:W:38[B]:ILE:HG22	1:W:41:ALA:H	1.77	0.49
1:P:99:ALA:HB2	1:P:112:ILE:HG21	1.94	0.49
1:R:91:ARG:HG2	1:R:119:ARG:NE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:GLN:NE2	1:S:56:SER:OG	2.40	0.49
1:c:92:ILE:HG22	1:c:464:LEU:HD21	1.93	0.49
1:W:104:ASN:HB2	1:W:108:ASP:HB3	1.94	0.49
1:g:170:LEU:HD22	1:g:173:PHE:CD1	2.47	0.49
1:F:520:LYS:NZ	1:Q:6:ASN:O	2.36	0.49
1:Q:144:MET:HE3	1:Q:146:ILE:HD11	1.93	0.49
1:I:504:SER:HB2	1:S:7:THR:HG21	1.93	0.49
1:e:531:VAL:HG11	1:V:33:SER:HB3	1.94	0.49
1:R:162:LYS:O	1:R:167:THR:HG21	2.11	0.49
1:g:41:ALA:HB1	1:g:44:ASP:O	2.13	0.49
1:A:43:ASP:OD1	1:A:44:ASP:N	2.45	0.49
1:P:164:ASP:OD1	1:P:164:ASP:N	2.46	0.49
1:a:8:ASN:OD1	1:a:11:SER:N	2.34	0.49
1:c:14:THR:HG23	1:d:33:SER:HB2	1.94	0.49
1:T:147:GLN:NE2	1:T:149:GLY:O	2.43	0.49
1:B:506:ILE:HA	1:D:66:ARG:NH2	2.27	0.49
1:d:37:ARG:HG3	1:d:509:ALA:HB2	1.95	0.49
1:K:93:ARG:HA	1:K:464:LEU:HD13	1.94	0.49
1:X:505:ARG:NH1	1:Y:69:ASN:OD1	2.44	0.49
1:Y:149:GLY:HA3	1:Y:154:GLN:HG3	1.95	0.49
1:a:137:VAL:HG23	1:a:138:LEU:HG	1.95	0.49
1:c:108:ASP:OD1	1:c:108:ASP:N	2.46	0.49
1:f:137:VAL:HG23	1:f:138:LEU:HG	1.95	0.49
1:W:31:ARG:HB2	1:W:514:GLU:HG2	1.94	0.49
1:B:158:ILE:HG12	1:B:481:VAL:HG11	1.93	0.49
1:O:38:ILE:HG21	1:O:44:ASP:HB2	1.94	0.49
1:G:542:VAL:HA	1:G:545:LEU:HD12	1.93	0.49
1:N:170:LEU:HB2	1:N:173:PHE:CD1	2.48	0.48
1:O:89:LEU:HD12	1:O:471:ILE:HD12	1.95	0.48
1:Y:527:ALA:O	1:Y:531:VAL:HG23	2.13	0.48
1:c:140:LYS:HD3	1:c:141:ASP:N	2.27	0.48
1:U:158:ILE:HG12	1:U:481:VAL:HG11	1.95	0.48
1:L:17:ASN:HB3	1:M:34:SER:HB3	1.95	0.48
1:c:57:ASN:O	1:c:61:LEU:HG	2.13	0.48
1:K:19:ASN:HA	1:K:22:GLN:HE21	1.78	0.48
1:g:148:VAL:HB	1:g:492:LEU:HD11	1.96	0.48
1:C:31:ARG:HE	1:C:37:ARG:HG3	1.77	0.48
1:C:78:THR:HB	1:C:478:LEU:HD21	1.94	0.48
1:N:485:LEU:O	1:N:489:VAL:HG13	2.14	0.48
1:K:69:ASN:O	1:K:72:ILE:HG22	2.13	0.48
1:W:81:ALA:O	1:W:84:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:THR:O	1:Q:133:ASN:ND2	2.42	0.48
1:R:141:ASP:OD1	1:R:162:LYS:N	2.45	0.48
1:U:531:VAL:HG11	1:L:33:SER:HB3	1.95	0.48
1:F:127:SER:OG	1:F:163:ILE:O	2.17	0.48
1:G:14:THR:O	1:G:18:ILE:HG13	2.13	0.48
1:c:85:ILE:HG23	1:c:123:ILE:HD12	1.95	0.48
1:J:501:GLU:OE2	1:J:505:ARG:NH2	2.45	0.48
1:K:38[B]:ILE:HD11	1:K:506:ILE:HG22	1.95	0.48
1:V:10:LEU:HD21	1:W:29:ILE:HG13	1.95	0.48
1:B:25:LEU:O	1:B:29:ILE:HG12	2.13	0.48
1:P:149:GLY:HA3	1:P:154:GLN:HG3	1.95	0.48
1:T:505:ARG:HH21	1:K:73:SER:HB3	1.78	0.48
1:L:478:LEU:O	1:L:482:GLN:HG3	2.13	0.48
1:g:53:ARG:O	1:g:57:ASN:ND2	2.36	0.48
1:C:32:LEU:HG	1:C:514:GLU:HB3	1.96	0.48
1:X:71:GLY:HA3	1:X:146:ILE:HD13	1.96	0.48
1:c:511:TYR:O	1:c:515:VAL:HG23	2.13	0.48
1:T:3:GLN:HG3	1:T:4:VAL:H	1.78	0.48
1:W:13:ILE:HA	1:W:16:ASN:HD21	1.78	0.48
1:D:101:THR:HG22	1:N:147:GLN:HB3	1.95	0.48
1:F:461:LEU:HB2	1:P:152:ASP:HB2	1.94	0.48
1:W:511:TYR:O	1:W:515:VAL:HG23	2.14	0.48
1:g:82:LEU:HD12	1:g:471:ILE:HG23	1.96	0.48
1:N:20:LYS:HE3	1:N:20:LYS:HB2	1.71	0.48
1:O:8:ASN:O	1:O:11:SER:OG	2.29	0.48
1:O:505:ARG:HH12	1:F:73:SER:HB3	1.79	0.48
1:Y:8:ASN:O	1:Y:11:SER:OG	2.31	0.48
1:U:165:SER:OG	1:U:170:LEU:O	2.29	0.48
1:V:101:THR:HG22	1:V:103:THR:H	1.79	0.48
1:M:166:ASP:HB3	1:M:171:ASN:ND2	2.28	0.48
1:W:101:THR:HG22	1:g:147:GLN:H	1.79	0.48
1:C:84:GLU:O	1:C:88:ASN:ND2	2.47	0.47
1:X:168:LEU:HD23	1:X:467:ALA:HB1	1.96	0.47
1:P:510:ASP:HB3	1:P:513:THR:HG22	1.94	0.47
1:R:162:LYS:NZ	1:R:164:ASP:OD2	2.46	0.47
1:c:5:ILE:HG22	1:c:539:PRO:HB3	1.96	0.47
1:d:512:ALA:HA	1:d:515:VAL:HB	1.96	0.47
1:U:93:ARG:HA	1:U:464:LEU:HD13	1.96	0.47
1:M:491:ASN:HA	1:M:494:ASN:ND2	2.29	0.47
1:F:149:GLY:O	1:F:154:GLN:NE2	2.46	0.47
1:P:8:ASN:O	1:P:11:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:10:LEU:HD13	1:Q:29:ILE:HG21	1.96	0.47
1:H:10:LEU:O	1:H:14:THR:HG23	2.14	0.47
1:H:483:ASN:OD1	1:I:119:ARG:NH2	2.47	0.47
1:H:486:ASP:OD2	1:H:487:SER:N	2.47	0.47
1:S:523:ILE:HD13	1:d:539:PRO:HB2	1.94	0.47
1:J:122:GLU:OE2	1:J:125:ARG:NH2	2.47	0.47
1:d:139:ALA:O	1:d:140:LYS:HD2	2.14	0.47
1:L:11:SER:OG	1:L:15:GLN:OE1	2.30	0.47
1:g:38[B]:ILE:HG12	1:g:507:GLN:HA	1.95	0.47
1:C:170:LEU:HD23	1:C:173:PHE:HA	1.96	0.47
1:D:517:ASN:HA	1:D:520:LYS:HG2	1.97	0.47
1:E:37:ARG:H	1:E:508:ASP:H	1.60	0.47
1:F:524:ILE:HG12	1:Q:5:ILE:HD12	1.95	0.47
1:P:174:ASN:HD21	1:P:177:GLY:HA2	1.78	0.47
1:f:164:ASP:OD1	1:f:165:SER:N	2.48	0.47
1:f:478:LEU:O	1:f:482:GLN:HG2	2.14	0.47
1:g:38[A]:ILE:HG12	1:g:507:GLN:HA	1.95	0.47
1:g:101:THR:HG22	1:g:103:THR:HG23	1.96	0.47
1:B:78:THR:HB	1:B:478:LEU:HD21	1.96	0.47
1:c:111:SER:O	1:c:115:GLU:HG3	2.14	0.47
1:c:493:ASN:O	1:c:497:THR:HG23	2.15	0.47
1:B:40:SER:OG	1:B:42:LYS:HG2	2.15	0.47
1:X:63:GLN:HE22	1:X:67:ASN:HD21	1.62	0.47
1:Y:113:GLN:OE1	1:Y:175:VAL:N	2.38	0.47
1:G:89:LEU:HD12	1:G:471:ILE:HD12	1.96	0.47
1:J:149:GLY:HA3	1:J:154:GLN:HG3	1.96	0.47
1:U:510:ASP:OD1	1:U:511:TYR:N	2.48	0.47
1:e:105:SER:OG	1:e:106:ASP:N	2.48	0.47
1:e:106:ASP:N	1:e:106:ASP:OD1	2.46	0.47
1:W:27:SER:O	1:W:31:ARG:HG2	2.13	0.47
1:F:497:THR:HG21	1:P:16:ASN:ND2	2.29	0.47
1:b:91:ARG:HG2	1:b:119:ARG:NE	2.30	0.47
1:c:66:ARG:HA	1:c:69:ASN:HD21	1.79	0.47
1:A:90:GLN:NE2	1:B:52:ASN:OD1	2.48	0.47
1:B:122:GLU:HB2	1:W:484:ARG:HG2	1.97	0.47
1:D:62:THR:O	1:D:66:ARG:HG3	2.15	0.47
1:N:82:LEU:HD12	1:N:471:ILE:HG23	1.96	0.47
1:G:15:GLN:O	1:G:19:ASN:ND2	2.47	0.47
1:G:95:LEU:HD11	1:G:115:GLU:HG2	1.97	0.47
1:Q:137:VAL:HG23	1:Q:138:LEU:HG	1.96	0.47
1:H:14:THR:HG22	1:I:33:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:THR:O	1:H:18:ILE:HG13	2.13	0.47
1:b:459:ASP:N	1:b:459:ASP:OD1	2.46	0.47
1:K:38[A]:ILE:HD11	1:K:506:ILE:HG22	1.95	0.47
1:e:147:GLN:HA	1:e:155:THR:HB	1.96	0.47
1:f:483:ASN:HD22	1:g:119:ARG:HH21	1.61	0.47
1:M:117:LYS:NZ	1:M:121:ASP:OD2	2.48	0.47
1:W:82:LEU:HG	1:W:474:PHE:HD2	1.80	0.47
1:g:65:ALA:HB1	1:g:489:VAL:HG23	1.95	0.47
1:g:137:VAL:HG23	1:g:138:LEU:HG	1.96	0.47
1:A:64:ALA:HB1	1:A:148:VAL:HG23	1.95	0.47
1:Z:167:THR:HG23	1:Z:168:LEU:HD12	1.96	0.47
1:G:523:ILE:HG22	1:H:5:ILE:HD11	1.97	0.47
1:b:96:THR:HG21	1:b:460:PRO:HB2	1.97	0.47
1:e:97:VAL:HG12	1:e:461:LEU:HD11	1.95	0.47
1:M:170:LEU:HD23	1:M:173:PHE:HB2	1.97	0.47
1:A:93:ARG:NH1	1:A:461:LEU:HD22	2.29	0.47
1:J:486:ASP:OD2	1:J:487:SER:N	2.47	0.47
1:L:149:GLY:HA3	1:L:154:GLN:HG3	1.97	0.47
1:f:112:ILE:O	1:f:116:ILE:HG12	2.15	0.47
1:A:455:GLU:OE2	1:A:455:GLU:N	2.47	0.47
1:N:461:LEU:HB2	1:X:152:ASP:HB2	1.96	0.47
1:K:104:ASN:HB3	1:K:108:ASP:HB2	1.97	0.47
1:V:92:ILE:HA	1:V:95:LEU:HD23	1.97	0.47
1:Z:91:ARG:O	1:Z:94:GLU:HG3	2.15	0.46
1:R:99:ALA:HB2	1:R:112:ILE:HG21	1.97	0.46
1:K:486:ASP:O	1:K:489:VAL:HG22	2.15	0.46
1:K:508:ASP:HB3	1:U:4:VAL:HG13	1.97	0.46
1:V:19:ASN:O	1:V:22:GLN:HG2	2.15	0.46
1:g:148:VAL:HG23	1:g:148:VAL:O	2.14	0.46
1:A:26:SER:HA	1:M:10:LEU:HD11	1.96	0.46
1:F:126:VAL:O	1:F:130:THR:OG1	2.30	0.46
1:G:158:ILE:HB	1:G:481:VAL:HG21	1.96	0.46
1:S:37:ARG:N	1:S:507:GLN:O	2.44	0.46
1:S:129:GLN:O	1:S:130:THR:OG1	2.33	0.46
1:S:459:ASP:OD1	1:S:459:ASP:N	2.48	0.46
1:J:156:ILE:HD11	1:J:484:ARG:HE	1.80	0.46
1:d:160:LEU:HA	1:d:474:PHE:HZ	1.80	0.46
1:M:152:ASP:OD1	1:M:152:ASP:N	2.42	0.46
1:A:486:ASP:O	1:A:490:THR:HG23	2.15	0.46
1:N:103:THR:HA	1:X:144:MET:HE3	1.98	0.46
1:T:37:ARG:HG3	1:T:509:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:GLN:HG2	1:L:155:THR:HG22	1.97	0.46
1:C:6:ASN:OD1	1:C:6:ASN:N	2.49	0.46
1:P:508:ASP:HB3	1:Z:4:VAL:HG13	1.97	0.46
1:R:43:ASP:OD1	1:R:44:ASP:N	2.47	0.46
1:T:461:LEU:HD13	1:d:152:ASP:HB3	1.98	0.46
1:D:510:ASP:HB2	1:N:3:GLN:HB2	1.96	0.46
1:N:71:GLY:HA3	1:N:146:ILE:HD13	1.97	0.46
1:F:10:LEU:HD11	1:G:29:ILE:HB	1.96	0.46
1:Q:105:SER:N	1:Q:108:ASP:OD1	2.37	0.46
1:a:101:THR:HG22	1:a:103:THR:HG22	1.98	0.46
1:O:520:LYS:O	1:O:524:ILE:HG13	2.16	0.46
1:b:61:LEU:HD22	1:b:492:LEU:HD22	1.97	0.46
1:T:491:ASN:HA	1:T:494:ASN:ND2	2.31	0.46
1:Z:140:LYS:HD3	1:Z:141:ASP:H	1.81	0.46
1:Q:484:ARG:HG3	1:H:122:GLU:HB2	1.97	0.46
1:R:90:GLN:HE22	1:b:56:SER:HB3	1.80	0.46
1:R:122:GLU:OE2	1:R:125:ARG:NH2	2.38	0.46
1:R:501:GLU:O	1:R:504:SER:OG	2.30	0.46
1:c:96:THR:O	1:c:100:SER:OG	2.33	0.46
1:T:127:SER:OG	1:T:163:ILE:O	2.29	0.46
1:U:170:LEU:O	1:U:170:LEU:HD12	2.16	0.46
1:D:82:LEU:O	1:D:85:ILE:HG22	2.15	0.46
1:b:36:LEU:HD22	1:b:507:GLN:HB3	1.97	0.46
1:c:73:SER:HA	1:c:76:GLN:HG2	1.97	0.46
1:T:164:ASP:H	1:T:167:THR:HG22	1.79	0.46
1:K:38[B]:ILE:HD13	1:K:507:GLN:HG2	1.98	0.46
1:V:84:GLU:O	1:V:88:ASN:ND2	2.48	0.46
1:B:86:ASN:HD21	1:C:52:ASN:HD21	1.64	0.46
1:P:46:ALA:O	1:P:50:ILE:HG13	2.16	0.46
1:I:88:ASN:OD1	1:I:119:ARG:NH1	2.49	0.46
1:J:164:ASP:H	1:J:167:THR:HG22	1.81	0.46
1:f:101:THR:HG22	1:f:103:THR:HG23	1.96	0.46
1:D:170:LEU:HB2	1:D:173:PHE:HD1	1.81	0.46
1:N:37:ARG:HE	1:N:38:ILE:HG23	1.81	0.46
1:N:484:ARG:NH1	1:O:121:ASP:OD1	2.49	0.46
1:X:38:ILE:O	1:X:38:ILE:HG13	2.16	0.46
1:G:170:LEU:HB3	1:G:173:PHE:HD1	1.81	0.46
1:I:148:VAL:HG21	1:I:156:ILE:HD12	1.98	0.46
1:f:176:ASN:OD1	1:f:177:GLY:N	2.49	0.46
1:B:106:ASP:OD1	1:B:107:SER:N	2.49	0.45
1:E:89:LEU:HD23	1:E:89:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:176:ASN:OD1	1:P:177:GLY:N	2.46	0.45
1:a:31:ARG:HD3	1:a:37:ARG:HA	1.98	0.45
1:b:141:ASP:OD1	1:b:162:LYS:N	2.49	0.45
1:S:505:ARG:NH1	1:T:69:ASN:OD1	2.49	0.45
1:d:63:GLN:NE2	1:d:67:ASN:OD1	2.42	0.45
1:d:147:GLN:NE2	1:d:149:GLY:O	2.49	0.45
1:d:151:ASN:HB2	1:d:154:GLN:NE2	2.31	0.45
1:L:93:ARG:HA	1:L:464:LEU:HD13	1.98	0.45
1:V:13:ILE:HG21	1:W:30:GLU:OE2	2.16	0.45
1:V:113:GLN:NE2	1:V:174:ASN:HA	2.31	0.45
1:N:534:LYS:HE3	1:O:518:MET:HE1	1.98	0.45
1:Y:68:ALA:O	1:Y:72:ILE:HG13	2.17	0.45
1:F:120:LEU:HD21	1:F:170:LEU:HD23	1.97	0.45
1:G:31:ARG:HD3	1:G:37:ARG:HA	1.97	0.45
1:I:131:GLN:HB3	1:I:136:ASN:ND2	2.31	0.45
1:S:501:GLU:OE1	1:T:76:GLN:NE2	2.37	0.45
1:K:55:THR:HB	1:K:503:GLN:HE22	1.81	0.45
1:C:173:PHE:CZ	1:C:460:PRO:HB3	2.51	0.45
1:a:459:ASP:OD1	1:a:459:ASP:N	2.48	0.45
1:b:151:ASN:OD1	1:b:152:ASP:N	2.47	0.45
1:T:80:GLY:O	1:T:83:SER:OG	2.33	0.45
1:V:94:GLU:OE1	1:f:59:LYS:NZ	2.36	0.45
1:C:43:ASP:OD1	1:C:44:ASP:N	2.49	0.45
1:a:15:GLN:O	1:a:19:ASN:ND2	2.50	0.45
1:R:90:GLN:NE2	1:b:52:ASN:OD1	2.42	0.45
1:S:39:ASN:O	1:S:40:SER:OG	2.34	0.45
1:K:479:GLY:HA3	1:U:41:ALA:O	2.15	0.45
1:U:97:VAL:HG22	1:U:461:LEU:HD21	1.97	0.45
1:f:154:GLN:OE1	1:g:129:GLN:NE2	2.50	0.45
1:W:131:GLN:HB3	1:W:136:ASN:ND2	2.31	0.45
1:N:91:ARG:HG2	1:N:119:ARG:NH2	2.32	0.45
1:Q:539:PRO:O	1:Q:542:VAL:HG22	2.17	0.45
1:b:455:GLU:N	1:b:455:GLU:OE2	2.49	0.45
1:J:147:GLN:HG2	1:J:155:THR:HG22	1.99	0.45
1:C:539:PRO:O	1:C:542:VAL:HG22	2.17	0.45
1:a:154:GLN:CD	1:R:129:GLN:HE22	2.24	0.45
1:K:38[A]:ILE:HD13	1:K:507:GLN:HG2	1.98	0.45
1:e:36:LEU:HA	1:e:508:ASP:HA	1.98	0.45
1:e:487:SER:HB2	1:V:84:GLU:OE2	2.15	0.45
1:X:137:VAL:HG23	1:X:138:LEU:HG	1.97	0.45
1:E:93:ARG:HA	1:E:464:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:43:ASP:OD1	1:Q:44:ASP:N	2.49	0.45
1:V:82:LEU:HD12	1:V:471:ILE:HG23	1.99	0.45
1:g:147:GLN:HB3	1:g:155:THR:HG22	1.99	0.45
1:B:114:ASP:OD1	1:B:115:GLU:N	2.49	0.45
1:N:5:ILE:HG21	1:N:542:VAL:HG21	1.98	0.45
1:N:461:LEU:HA	1:N:464:LEU:HD12	1.98	0.45
1:F:491:ASN:HB2	1:G:84:GLU:CD	2.42	0.45
1:F:511:TYR:HE2	1:P:5:ILE:HG12	1.80	0.45
1:R:515:VAL:HG21	1:b:545:LEU:HD21	1.99	0.45
1:I:505:ARG:NH1	1:J:72:ILE:HD11	2.32	0.45
1:d:53:ARG:NH1	1:K:107:SER:OG	2.50	0.45
1:e:54:PHE:HE1	1:V:133:ASN:HB2	1.82	0.45
1:e:82:LEU:HD11	1:e:474:PHE:HD2	1.81	0.45
1:M:79:GLU:OE2	1:W:41:ALA:HB3	2.16	0.45
1:F:70:ASP:O	1:F:73:SER:OG	2.30	0.45
1:Z:91:ARG:NH1	1:Z:94:GLU:OE2	2.50	0.45
1:T:491:ASN:HA	1:T:494:ASN:HD21	1.82	0.45
1:f:61:LEU:HD22	1:f:492:LEU:HD22	1.98	0.45
1:f:92:ILE:HA	1:f:95:LEU:HD23	1.98	0.45
1:N:37:ARG:HH12	1:O:66:ARG:CZ	2.30	0.45
1:E:70:ASP:O	1:E:73:SER:OG	2.26	0.45
1:G:93:ARG:HA	1:G:464:LEU:HD13	1.99	0.45
1:S:96:THR:O	1:S:100:SER:OG	2.28	0.45
1:c:170:LEU:HD21	1:c:464:LEU:HD12	1.99	0.45
1:U:55:THR:OG1	1:U:503:GLN:OE1	2.31	0.45
1:W:13:ILE:HA	1:W:16:ASN:ND2	2.32	0.45
1:W:100:SER:OG	1:g:147:GLN:NE2	2.49	0.45
1:g:91:ARG:HG2	1:g:119:ARG:CZ	2.47	0.45
1:C:21:ASN:HD22	1:C:524:ILE:HG22	1.81	0.44
1:N:105:SER:OG	1:N:106:ASP:N	2.50	0.44
1:Y:55:THR:OG1	1:Y:503:GLN:OE1	2.34	0.44
1:P:485:LEU:O	1:P:489:VAL:HG23	2.17	0.44
1:Z:170:LEU:HD22	1:Z:173:PHE:CE1	2.50	0.44
1:a:539:PRO:O	1:a:542:VAL:HG22	2.17	0.44
1:H:461:LEU:HB2	1:R:152:ASP:CG	2.41	0.44
1:I:459:ASP:OD1	1:I:459:ASP:N	2.50	0.44
1:K:160:LEU:HA	1:K:474:PHE:HZ	1.83	0.44
1:e:89:LEU:HD11	1:e:168:LEU:HD11	1.98	0.44
1:f:154:GLN:HE22	1:g:129:GLN:CD	2.25	0.44
1:g:8:ASN:O	1:g:11:SER:OG	2.28	0.44
1:g:109:LEU:HA	1:g:112:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ASN:HA	1:E:19:ASN:ND2	2.31	0.44
1:K:147:GLN:NE2	1:K:149:GLY:O	2.46	0.44
1:K:512:ALA:HA	1:K:515:VAL:HB	2.00	0.44
1:U:472:ASP:CG	1:e:52:ASN:HD22	2.24	0.44
1:g:37:ARG:N	1:g:507:GLN:O	2.43	0.44
1:g:86:ASN:HD22	1:g:475:ARG:CZ	2.31	0.44
1:O:505:ARG:NH1	1:F:73:SER:HB3	2.32	0.44
1:Z:141:ASP:OD1	1:Z:162:LYS:N	2.44	0.44
1:H:58:ILE:O	1:H:62:THR:HG23	2.17	0.44
1:S:108:ASP:OD2	1:S:108:ASP:N	2.49	0.44
1:c:99:ALA:HB2	1:c:112:ILE:HG21	1.99	0.44
1:d:491:ASN:HA	1:d:494:ASN:ND2	2.32	0.44
1:W:91:ARG:NH1	1:W:94:GLU:OE2	2.51	0.44
1:W:164:ASP:OD2	1:W:167:THR:HG22	2.17	0.44
1:A:81:ALA:O	1:A:85:ILE:HG13	2.17	0.44
1:X:96:THR:HG21	1:X:464:LEU:HD11	1.98	0.44
1:O:8:ASN:HB3	1:O:11:SER:OG	2.17	0.44
1:Y:492:LEU:O	1:Y:496:THR:HG23	2.17	0.44
1:F:72:ILE:HD11	1:F:485:LEU:HB3	2.00	0.44
1:H:491:ASN:HB2	1:I:84:GLU:HG3	2.00	0.44
1:H:534:LYS:HZ1	1:S:546:LEU:C	2.25	0.44
1:I:99:ALA:HB2	1:I:112:ILE:HG21	1.99	0.44
1:L:101:THR:HG22	1:L:103:THR:H	1.82	0.44
1:V:491:ASN:HB2	1:W:84:GLU:OE1	2.17	0.44
1:f:72:ILE:HG13	1:f:482:GLN:OE1	2.16	0.44
1:M:13:ILE:HA	1:M:16:ASN:ND2	2.33	0.44
1:g:41:ALA:HB3	1:g:48:GLN:NE2	2.32	0.44
1:C:41:ALA:HB2	1:C:48:GLN:NE2	2.33	0.44
1:C:525:GLN:NE2	1:C:529:ASN:OD1	2.46	0.44
1:Q:93:ARG:HA	1:Q:464:LEU:HD13	2.00	0.44
1:H:68:ALA:HB2	1:H:148:VAL:HG12	1.99	0.44
1:I:129:GLN:O	1:I:130:THR:OG1	2.33	0.44
1:S:69:ASN:O	1:S:72:ILE:HG22	2.18	0.44
1:B:99:ALA:HB2	1:B:112:ILE:HG21	1.98	0.44
1:C:164:ASP:OD1	1:C:165:SER:N	2.51	0.44
1:D:505:ARG:HD3	1:E:69:ASN:HB3	1.98	0.44
1:c:129:GLN:O	1:c:130:THR:OG1	2.33	0.44
1:M:170:LEU:C	1:M:172:GLY:H	2.24	0.44
1:g:470:GLN:O	1:g:473:LYS:HG2	2.18	0.44
1:A:122:GLU:OE2	1:A:125:ARG:NH2	2.44	0.44
1:B:537:GLN:HB2	1:B:540:GLN:HE22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:487:SER:OG	1:F:84:GLU:OE2	2.35	0.44
1:Q:164:ASP:H	1:Q:167:THR:HG22	1.83	0.44
1:U:486:ASP:HA	1:U:489:VAL:HG12	1.99	0.44
1:f:511:TYR:O	1:f:515:VAL:HG22	2.17	0.44
1:M:96:THR:O	1:M:100:SER:OG	2.34	0.44
1:W:170:LEU:C	1:W:172:GLY:H	2.26	0.44
1:B:96:THR:O	1:B:100:SER:OG	2.33	0.44
1:C:10:LEU:HD21	1:N:29:ILE:HD12	1.99	0.44
1:D:37:ARG:NH2	1:D:506:ILE:O	2.51	0.44
1:N:482:GLN:HE21	1:X:42:LYS:HB2	1.82	0.44
1:X:165:SER:O	1:X:169:GLY:N	2.49	0.44
1:d:84:GLU:O	1:d:88:ASN:ND2	2.51	0.44
1:V:93:ARG:NH1	1:V:461:LEU:HD22	2.33	0.44
1:f:43:ASP:OD1	1:f:44:ASP:N	2.44	0.44
1:A:492:LEU:O	1:A:496:THR:HG23	2.17	0.44
1:X:78:THR:HB	1:X:478:LEU:HD21	2.00	0.44
1:P:111:SER:HA	1:P:114:ASP:OD2	2.18	0.44
1:E:8:ASN:O	1:E:11:SER:OG	2.36	0.43
1:R:64:ALA:HB1	1:R:148:VAL:HA	2.00	0.43
1:c:86:ASN:HD22	1:c:475:ARG:NH1	2.15	0.43
1:d:129:GLN:O	1:d:130:THR:OG1	2.33	0.43
1:U:8:ASN:O	1:U:11:SER:OG	2.35	0.43
1:U:79:GLU:OE1	1:e:41:ALA:HB3	2.18	0.43
1:U:461:LEU:H	1:U:461:LEU:HD12	1.83	0.43
1:U:501:GLU:OE1	1:U:505:ARG:NH2	2.51	0.43
1:W:170:LEU:O	1:W:172:GLY:N	2.51	0.43
1:C:117:LYS:NZ	1:C:121:ASP:OD2	2.51	0.43
1:Z:126:VAL:O	1:Z:130:THR:OG1	2.29	0.43
1:L:95:LEU:HG	1:L:112:ILE:HG23	1.99	0.43
1:B:108:ASP:HA	1:g:53:ARG:HH22	1.83	0.43
1:C:96:THR:HG21	1:C:464:LEU:HD12	2.00	0.43
1:C:505:ARG:HD3	1:N:69:ASN:HB3	2.00	0.43
1:D:535:ALA:O	1:D:538:VAL:HG22	2.18	0.43
1:E:37:ARG:HB2	1:E:509:ALA:N	2.34	0.43
1:O:10:LEU:HD23	1:F:29:ILE:HG21	1.99	0.43
1:H:141:ASP:OD1	1:H:162:LYS:N	2.52	0.43
1:c:498:ASN:HD22	1:d:77:THR:HA	1.83	0.43
1:V:61:LEU:HD22	1:V:492:LEU:HD22	2.01	0.43
1:M:39:ASN:O	1:M:40:SER:OG	2.32	0.43
1:M:538:VAL:N	1:M:539:PRO:HD2	2.33	0.43
1:A:64:ALA:HB1	1:A:148:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:34:SER:OG	1:Z:39:ASN:OD1	2.28	0.43
1:R:78:THR:HB	1:R:478:LEU:HD21	1.99	0.43
1:b:92:ILE:HD13	1:b:92:ILE:HA	1.86	0.43
1:I:77:THR:HG21	1:I:132:PHE:CD2	2.53	0.43
1:d:3:GLN:CD	1:U:22:GLN:HE22	2.26	0.43
1:e:93:ARG:O	1:e:97:VAL:HG13	2.18	0.43
1:V:3:GLN:HG3	1:V:4:VAL:HG23	2.00	0.43
1:f:464:LEU:O	1:f:468:ILE:HG12	2.18	0.43
1:C:122:GLU:OE2	1:g:484:ARG:NE	2.24	0.43
1:O:518:MET:HG3	1:O:519:SER:N	2.33	0.43
1:F:176:ASN:OD1	1:F:177:GLY:N	2.51	0.43
1:J:54:PHE:HB3	1:J:503:GLN:HB2	1.99	0.43
1:M:14:THR:HG21	1:M:532:LEU:HB2	2.01	0.43
1:M:31:ARG:NH1	1:M:37:ARG:HG2	2.33	0.43
1:C:173:PHE:HZ	1:C:460:PRO:HB3	1.84	0.43
1:G:151:ASN:HB3	1:G:154:GLN:HE22	1.83	0.43
1:b:505:ARG:NH1	1:c:69:ASN:O	2.52	0.43
1:S:89:LEU:HD12	1:S:89:LEU:HA	1.87	0.43
1:V:104:ASN:HB3	1:V:108:ASP:HB2	1.99	0.43
1:V:125:ARG:HG2	1:V:129:GLN:HG3	2.00	0.43
1:W:91:ARG:HG2	1:W:119:ARG:NH2	2.33	0.43
1:B:475:ARG:HG2	1:C:48:GLN:NE2	2.34	0.43
1:D:84:GLU:O	1:D:88:ASN:ND2	2.52	0.43
1:X:169:GLY:C	1:X:170:LEU:HD23	2.44	0.43
1:Y:38:ILE:O	1:Y:38:ILE:HG13	2.18	0.43
1:F:484:ARG:NH1	1:G:121:ASP:HB3	2.33	0.43
1:f:25:LEU:HB2	1:f:521:ALA:HB1	2.00	0.43
1:M:55:THR:O	1:M:59:LYS:HG3	2.18	0.43
1:g:510:ASP:O	1:g:514:GLU:HG2	2.18	0.43
1:B:107:SER:OG	1:g:53:ARG:NH1	2.52	0.43
1:N:78:THR:HB	1:N:478:LEU:HD21	2.00	0.43
1:P:518:MET:HE2	1:P:518:MET:HB3	1.92	0.43
1:G:91:ARG:HG2	1:G:119:ARG:NH2	2.34	0.43
1:Q:542:VAL:HA	1:Q:545:LEU:HD12	2.00	0.43
1:H:505:ARG:NH1	1:I:73:SER:HB2	2.34	0.43
1:R:74:VAL:HG11	1:R:144:MET:HE1	2.01	0.43
1:J:109:LEU:HB3	1:J:176:ASN:HB3	2.00	0.43
1:e:537:GLN:O	1:e:540:GLN:HG2	2.19	0.43
1:L:486:ASP:O	1:L:490:THR:HG23	2.19	0.43
1:V:541:GLN:O	1:V:544:SER:OG	2.27	0.43
1:g:164:ASP:N	1:g:164:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HD21	1:C:457:THR:OG1	2.18	0.43
1:O:511:TYR:HD2	1:Y:542:VAL:HG11	1.83	0.43
1:F:125:ARG:O	1:F:129:GLN:HG2	2.19	0.43
1:b:127:SER:OG	1:b:163:ILE:O	2.27	0.43
1:K:10:LEU:HD12	1:K:10:LEU:H	1.84	0.43
1:e:89:LEU:HD12	1:e:471:ILE:HD12	2.01	0.43
1:T:472:ASP:CG	1:d:52:ASN:HD22	2.27	0.43
1:d:69:ASN:O	1:d:72:ILE:HG12	2.19	0.43
1:K:37:ARG:HA	1:K:509:ALA:HB2	2.01	0.43
1:L:484:ARG:HG2	1:M:122:GLU:HB2	1.99	0.43
1:V:534:LYS:HB2	1:V:534:LYS:HE3	1.86	0.43
1:W:25:LEU:HB2	1:W:521:ALA:HB1	2.00	0.43
1:g:152:ASP:OD1	1:g:152:ASP:N	2.52	0.43
1:B:14:THR:HB	1:B:532:LEU:HD13	2.01	0.42
1:D:169:GLY:C	1:D:170:LEU:HD23	2.44	0.42
1:O:176:ASN:OD1	1:O:177:GLY:N	2.52	0.42
1:a:525:GLN:NE2	1:a:529:ASN:OD1	2.52	0.42
1:H:122:GLU:CD	1:H:125:ARG:HH21	2.25	0.42
1:J:106:ASP:OD1	1:J:107:SER:N	2.52	0.42
1:K:492:LEU:O	1:K:496:THR:OG1	2.30	0.42
1:V:503:GLN:OE1	1:V:507:GLN:NE2	2.52	0.42
1:C:137:VAL:HG23	1:C:138:LEU:HG	2.00	0.42
1:N:538:VAL:HG13	1:O:525:GLN:HE22	1.83	0.42
1:I:69:ASN:HA	1:I:72:ILE:HG22	2.01	0.42
1:c:74:VAL:O	1:c:77:THR:HG22	2.19	0.42
1:c:110:ASP:OD1	1:c:176:ASN:ND2	2.42	0.42
1:d:160:LEU:HA	1:d:474:PHE:CZ	2.55	0.42
1:L:38[A]:ILE:HG22	1:L:41:ALA:H	1.84	0.42
1:L:38[B]:ILE:HG22	1:L:41:ALA:H	1.84	0.42
1:M:492:LEU:HA	1:M:495:THR:HG22	2.01	0.42
1:A:78:THR:HB	1:A:478:LEU:HD21	2.00	0.42
1:B:539:PRO:O	1:B:542:VAL:HG22	2.19	0.42
1:N:177:GLY:O	1:N:456:SER:N	2.52	0.42
1:E:64:ALA:HB1	1:E:148:VAL:HA	2.02	0.42
1:J:120:LEU:HD21	1:J:170:LEU:HD11	2.01	0.42
1:T:129:GLN:O	1:T:130:THR:OG1	2.33	0.42
1:e:3:GLN:HG2	1:e:4:VAL:HG13	2.01	0.42
1:f:145:LYS:HD3	1:f:155:THR:HG21	2.01	0.42
1:g:31:ARG:HD2	1:g:514:GLU:OE2	2.19	0.42
1:N:89:LEU:O	1:N:92:ILE:HG22	2.19	0.42
1:O:46:ALA:O	1:O:50:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:113:GLN:HG2	1:Y:176:ASN:OD1	2.19	0.42
1:Q:158:ILE:HD12	1:Q:481:VAL:HG11	2.01	0.42
1:a:52:ASN:O	1:a:55:THR:HG22	2.19	0.42
1:T:131:GLN:H	1:T:131:GLN:HG3	1.69	0.42
1:d:149:GLY:HA3	1:d:154:GLN:HG3	2.01	0.42
1:W:101:THR:HG21	1:g:67:ASN:HB3	2.01	0.42
1:A:91:ARG:HD2	1:A:91:ARG:HA	1.69	0.42
1:X:144:MET:HB3	1:X:158:ILE:HB	2.01	0.42
1:F:98:GLN:O	1:F:98:GLN:NE2	2.50	0.42
1:I:534:LYS:HD3	1:J:518:MET:HE1	2.01	0.42
1:c:120:LEU:HD11	1:c:173:PHE:CE1	2.54	0.42
1:U:55:THR:O	1:U:59:LYS:HG3	2.18	0.42
1:M:511:TYR:HD2	1:W:542:VAL:HG21	1.85	0.42
1:W:10:LEU:HD12	1:W:10:LEU:H	1.85	0.42
1:W:20:LYS:HE3	1:W:20:LYS:HB2	1.79	0.42
1:N:10:LEU:HD23	1:O:29:ILE:HG21	2.00	0.42
1:X:36:LEU:HD23	1:X:38:ILE:H	1.85	0.42
1:c:459:ASP:OD1	1:c:459:ASP:N	2.53	0.42
1:J:105:SER:OG	1:J:108:ASP:OD2	2.30	0.42
1:e:494:ASN:OD1	1:e:498:ASN:ND2	2.48	0.42
1:M:535:ALA:O	1:M:538:VAL:HG22	2.19	0.42
1:B:72:ILE:HG23	1:B:482:GLN:HE21	1.83	0.42
1:C:92:ILE:HD13	1:C:92:ILE:HA	1.87	0.42
1:X:171:ASN:OD1	1:X:171:ASN:N	2.51	0.42
1:O:83:SER:O	1:O:87:ASN:ND2	2.51	0.42
1:G:165:SER:O	1:G:169:GLY:N	2.42	0.42
1:Q:169:GLY:C	1:Q:171:ASN:H	2.28	0.42
1:J:158:ILE:HG12	1:J:481:VAL:HG11	2.02	0.42
1:W:90:GLN:NE2	1:g:56:SER:OG	2.41	0.42
1:W:91:ARG:HA	1:W:91:ARG:HD2	1.86	0.42
1:W:494:ASN:O	1:W:498:ASN:ND2	2.53	0.42
1:C:74:VAL:HG22	1:C:132:PHE:CD2	2.55	0.42
1:D:11:SER:C	1:D:15:GLN:HE21	2.28	0.42
1:E:520:LYS:HD2	1:F:6:ASN:O	2.19	0.42
1:Y:53:ARG:NH2	1:F:107:SER:OG	2.53	0.42
1:a:5:ILE:CG2	1:a:542:VAL:HG21	2.50	0.42
1:T:472:ASP:OD2	1:d:52:ASN:ND2	2.53	0.42
1:K:511:TYR:HE2	1:U:5:ILE:HG12	1.85	0.42
1:e:8:ASN:HB3	1:e:11:SER:OG	2.19	0.42
1:f:162:LYS:NZ	1:f:164:ASP:HB2	2.34	0.42
1:N:169:GLY:C	1:N:170:LEU:HD23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:97:VAL:HG22	1:X:461:LEU:HD21	2.02	0.42
1:H:70:ASP:O	1:H:73:SER:OG	2.30	0.42
1:I:537:GLN:O	1:I:540:GLN:NE2	2.44	0.42
1:K:539:PRO:O	1:K:542:VAL:HG22	2.19	0.42
1:U:140:LYS:HD3	1:U:141:ASP:H	1.85	0.42
1:L:38[A]:ILE:HG12	1:L:507:GLN:HB3	2.02	0.42
1:L:38[B]:ILE:HG12	1:L:507:GLN:HB3	2.02	0.42
1:f:170:LEU:C	1:f:172:GLY:H	2.28	0.42
1:f:470:GLN:HA	1:f:473:LYS:HZ2	1.84	0.42
1:M:476:SER:HB3	1:W:45:ALA:HB1	2.00	0.42
1:J:511:TYR:HE2	1:T:5:ILE:HG12	1.84	0.42
1:g:95:LEU:HD22	1:g:112:ILE:HG13	2.00	0.42
1:g:122:GLU:OE2	1:g:125:ARG:NE	2.47	0.42
1:B:503:GLN:NE2	1:B:507:GLN:OE1	2.48	0.41
1:D:61:LEU:HD22	1:D:492:LEU:HD22	2.01	0.41
1:D:113:GLN:O	1:D:113:GLN:NE2	2.53	0.41
1:I:86:ASN:HD21	1:S:52:ASN:ND2	2.18	0.41
1:J:93:ARG:HA	1:J:464:LEU:HD13	2.00	0.41
1:K:39:ASN:O	1:K:40:SER:OG	2.33	0.41
1:U:36:LEU:HA	1:U:508:ASP:HA	2.02	0.41
1:U:531:VAL:HG13	1:L:29:ILE:HG23	2.02	0.41
1:e:44:ASP:N	1:e:44:ASP:OD1	2.53	0.41
1:f:148:VAL:HG21	1:f:156:ILE:HG13	2.02	0.41
1:B:538:VAL:N	1:B:539:PRO:CD	2.84	0.41
1:O:89:LEU:HD23	1:O:89:LEU:HA	1.86	0.41
1:G:125:ARG:O	1:G:129:GLN:HG2	2.20	0.41
1:Q:543:LEU:O	1:Q:547:GLN:HG2	2.21	0.41
1:a:455:GLU:OE1	1:a:455:GLU:N	2.53	0.41
1:a:488:ALA:O	1:a:492:LEU:HG	2.20	0.41
1:U:49:ALA:HB1	1:U:53:ARG:HH21	1.84	0.41
1:e:53:ARG:NH1	1:L:108:ASP:OD2	2.36	0.41
1:L:511:TYR:HE2	1:V:5:ILE:HG12	1.85	0.41
1:V:74:VAL:HG11	1:V:144:MET:HE1	2.02	0.41
1:A:148:VAL:HG13	1:A:148:VAL:O	2.19	0.41
1:E:137:VAL:HG23	1:E:138:LEU:HG	2.03	0.41
1:O:19:ASN:HA	1:O:22:GLN:HB2	2.00	0.41
1:G:168:LEU:HD13	1:G:467:ALA:HB1	2.02	0.41
1:b:5:ILE:HD11	1:b:542:VAL:HG21	2.02	0.41
1:K:514:GLU:CD	1:K:514:GLU:H	2.27	0.41
1:e:38[A]:ILE:C	1:e:40:SER:H	2.28	0.41
1:e:38[B]:ILE:C	1:e:40:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:154:GLN:HE22	1:W:129:GLN:CD	2.27	0.41
1:V:154:GLN:HE22	1:W:129:GLN:HG2	1.85	0.41
1:W:148:VAL:HG21	1:W:156:ILE:HG13	2.02	0.41
1:B:142:GLY:O	1:B:160:LEU:HB2	2.20	0.41
1:C:113:GLN:HG2	1:C:176:ASN:ND2	2.35	0.41
1:N:90:GLN:OE1	1:X:56:SER:HB3	2.20	0.41
1:E:25:LEU:HB2	1:E:521:ALA:HB1	2.02	0.41
1:E:77:THR:HG21	1:E:132:PHE:CD1	2.55	0.41
1:Q:55:THR:OG1	1:Q:503:GLN:OE1	2.31	0.41
1:a:37:ARG:HB2	1:a:509:ALA:HB2	2.02	0.41
1:a:105:SER:OG	1:a:106:ASP:N	2.53	0.41
1:H:99:ALA:HB2	1:H:112:ILE:HG21	2.03	0.41
1:b:78:THR:HB	1:b:478:LEU:HD21	2.01	0.41
1:b:501:GLU:OE2	1:c:76:GLN:NE2	2.53	0.41
1:d:35:GLY:O	1:d:36:LEU:HD23	2.20	0.41
1:U:505:ARG:NE	1:L:73:SER:OG	2.46	0.41
1:V:9:SER:O	1:V:13:ILE:HG12	2.20	0.41
1:V:163:ILE:HG23	1:V:168:LEU:HD11	2.02	0.41
1:g:112:ILE:O	1:g:116:ILE:HG12	2.21	0.41
1:D:96:THR:O	1:D:100:SER:OG	2.31	0.41
1:P:8:ASN:ND2	1:P:536:ASN:HA	2.36	0.41
1:U:537:GLN:O	1:U:540:GLN:HG2	2.21	0.41
1:L:493:ASN:O	1:L:497:THR:HG23	2.20	0.41
1:V:152:ASP:OD1	1:V:153:GLY:N	2.51	0.41
1:f:37:ARG:NH2	1:f:506:ILE:O	2.50	0.41
1:f:40:SER:O	1:f:42:LYS:N	2.51	0.41
1:D:495:THR:O	1:D:499:LEU:HD23	2.21	0.41
1:O:96:THR:HG21	1:O:460:PRO:HB2	2.01	0.41
1:Z:458:SER:OG	1:Z:459:ASP:N	2.53	0.41
1:Q:488:ALA:O	1:Q:492:LEU:HG	2.21	0.41
1:d:505:ARG:HD3	1:U:69:ASN:HB3	2.02	0.41
1:U:147:GLN:HA	1:U:155:THR:HG22	2.02	0.41
1:f:152:ASP:OD1	1:f:153:GLY:N	2.49	0.41
1:G:539:PRO:O	1:G:542:VAL:HG22	2.21	0.41
1:Q:36:LEU:O	1:Q:39:ASN:ND2	2.54	0.41
1:Q:68:ALA:HB2	1:Q:148:VAL:HG12	2.02	0.41
1:Q:91:ARG:HG2	1:Q:119:ARG:NH2	2.36	0.41
1:Q:105:SER:OG	1:Q:106:ASP:N	2.51	0.41
1:Q:143:SER:HA	1:Q:159:ASP:HA	2.03	0.41
1:I:464:LEU:HD12	1:I:464:LEU:HA	1.91	0.41
1:S:493:ASN:HB3	1:c:16:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:101:THR:OG1	1:T:102:GLY:N	2.53	0.41
1:K:478:LEU:O	1:K:482:GLN:HG3	2.21	0.41
1:K:511:TYR:HA	1:K:514:GLU:OE2	2.20	0.41
1:W:43:ASP:N	1:W:43:ASP:OD1	2.51	0.41
1:C:86:ASN:HD22	1:C:475:ARG:HH22	1.69	0.41
1:J:511:TYR:C	1:J:513:THR:H	2.28	0.41
1:W:539:PRO:O	1:W:542:VAL:HG12	2.20	0.41
1:g:77:THR:HG21	1:g:132:PHE:CD1	2.56	0.41
1:B:64:ALA:HB1	1:B:148:VAL:HA	2.03	0.41
1:C:99:ALA:HB2	1:C:112:ILE:HG21	2.03	0.41
1:Y:90:GLN:OE1	1:Y:468:ILE:HD13	2.21	0.41
1:Y:170:LEU:HD22	1:Y:173:PHE:HE2	1.86	0.41
1:G:149:GLY:HA3	1:G:154:GLN:CG	2.50	0.41
1:Q:101:THR:HG22	1:a:147:GLN:H	1.86	0.41
1:a:169:GLY:C	1:a:171:ASN:H	2.29	0.41
1:H:96:THR:HG21	1:H:460:PRO:HB2	2.03	0.41
1:R:10:LEU:O	1:R:14:THR:HG23	2.21	0.41
1:K:5:ILE:HG12	1:K:542:VAL:HG21	2.02	0.41
1:U:36:LEU:HB2	1:U:39:ASN:OD1	2.21	0.41
1:U:461:LEU:HD13	1:e:152:ASP:HA	2.03	0.41
1:V:147:GLN:NE2	1:V:149:GLY:O	2.50	0.41
1:V:476:SER:HA	1:f:45:ALA:HB1	2.03	0.41
1:W:519:SER:O	1:W:523:ILE:HG12	2.21	0.41
1:g:82:LEU:HG	1:g:474:PHE:HD2	1.85	0.41
1:A:31:ARG:HE	1:A:37:ARG:HG3	1.86	0.41
1:D:164:ASP:OD1	1:D:164:ASP:N	2.54	0.41
1:E:481:VAL:HA	1:E:484:ARG:HG2	2.03	0.41
1:Y:145:LYS:HD3	1:Y:157:THR:HG23	2.03	0.41
1:F:113:GLN:HG2	1:F:176:ASN:ND2	2.36	0.41
1:Z:485:LEU:HD12	1:Z:485:LEU:HA	1.89	0.41
1:Q:511:TYR:O	1:Q:515:VAL:HG22	2.21	0.41
1:R:158:ILE:HG12	1:R:481:VAL:HG11	2.02	0.41
1:L:40:SER:O	1:L:40:SER:OG	2.33	0.41
1:V:31:ARG:HD3	1:V:37:ARG:HG3	2.03	0.41
1:B:486:ASP:OD2	1:B:487:SER:N	2.54	0.40
1:Y:46:ALA:O	1:Y:50:ILE:HG13	2.21	0.40
1:Y:149:GLY:O	1:Y:154:GLN:NE2	2.54	0.40
1:F:510:ASP:O	1:F:514:GLU:HG2	2.20	0.40
1:P:32:LEU:HA	1:P:32:LEU:HD23	1.84	0.40
1:P:147:GLN:NE2	1:P:151:ASN:O	2.54	0.40
1:Z:168:LEU:HD23	1:Z:467:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LEU:HD21	1:G:474:PHE:HD2	1.86	0.40
1:Q:518:MET:HE2	1:Q:518:MET:HB3	1.93	0.40
1:H:458:SER:OG	1:H:459:ASP:N	2.54	0.40
1:S:69:ASN:HA	1:S:72:ILE:HG22	2.02	0.40
1:S:541:GLN:O	1:S:545:LEU:HB2	2.22	0.40
1:f:55:THR:HG22	1:f:503:GLN:HE22	1.86	0.40
1:W:170:LEU:HD23	1:W:173:PHE:CG	2.56	0.40
1:A:493:ASN:O	1:A:496:THR:OG1	2.30	0.40
1:N:522:GLN:O	1:N:526:GLN:HG3	2.22	0.40
1:F:473:LYS:HE3	1:F:473:LYS:HB3	1.90	0.40
1:S:120:LEU:HD11	1:S:173:PHE:CE1	2.56	0.40
1:T:43:ASP:OD1	1:T:43:ASP:N	2.48	0.40
1:V:484:ARG:HG2	1:W:122:GLU:HB2	2.03	0.40
1:M:82:LEU:HD21	1:M:138:LEU:HD21	2.02	0.40
1:g:113:GLN:HA	1:g:116:ILE:HG12	2.03	0.40
1:B:73:SER:OG	1:W:505:ARG:NH2	2.30	0.40
1:F:72:ILE:HG12	1:F:485:LEU:HD23	2.04	0.40
1:H:67:ASN:HD22	1:H:147:GLN:HB3	1.86	0.40
1:I:70:ASP:O	1:I:74:VAL:HG23	2.21	0.40
1:S:147:GLN:NE2	1:S:151:ASN:O	2.55	0.40
1:c:152:ASP:OD1	1:c:152:ASP:N	2.49	0.40
1:J:25:LEU:HB2	1:J:521:ALA:HB1	2.04	0.40
1:J:104:ASN:HB3	1:J:108:ASP:HB2	2.02	0.40
1:T:141:ASP:OD1	1:T:162:LYS:N	2.34	0.40
1:d:170:LEU:HD23	1:d:170:LEU:H	1.86	0.40
1:M:25:LEU:HD23	1:M:29:ILE:HD13	2.04	0.40
1:W:162:LYS:O	1:W:167:THR:HG21	2.20	0.40
1:B:501:GLU:O	1:B:505:ARG:HG3	2.21	0.40
1:B:511:TYR:HD2	1:C:542:VAL:HG21	1.86	0.40
1:B:511:TYR:O	1:B:515:VAL:HG23	2.21	0.40
1:E:511:TYR:CE2	1:O:5:ILE:HG12	2.56	0.40
1:O:543:LEU:HD12	1:O:546:LEU:HD12	2.03	0.40
1:G:37:ARG:HB2	1:G:509:ALA:HB2	2.03	0.40
1:S:501:GLU:O	1:S:504:SER:OG	2.32	0.40
1:J:160:LEU:HA	1:J:474:PHE:HZ	1.86	0.40
1:L:126:VAL:O	1:L:130:THR:OG1	2.27	0.40
1:N:151:ASN:OD1	1:N:152:ASP:N	2.51	0.40
1:N:475:ARG:O	1:N:479:GLY:N	2.55	0.40
1:X:527:ALA:O	1:X:531:VAL:HG13	2.22	0.40
1:O:5:ILE:HG22	1:O:539:PRO:HB3	2.04	0.40
1:Y:88:ASN:O	1:Y:92:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:520:LYS:O	1:F:524:ILE:HG13	2.22	0.40
1:P:488:ALA:O	1:P:492:LEU:HG	2.22	0.40
1:a:5:ILE:HG21	1:a:542:VAL:HG21	2.04	0.40
1:I:88:ASN:O	1:I:92:ILE:HG13	2.22	0.40
1:I:170:LEU:C	1:I:172:GLY:H	2.30	0.40
1:J:515:VAL:HA	1:J:518:MET:HG2	2.04	0.40
1:T:486:ASP:HA	1:T:489:VAL:HG12	2.03	0.40
1:U:164:ASP:H	1:U:167:THR:HB	1.86	0.40
1:M:486:ASP:HA	1:M:489:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/548 (48%)	248 (94%)	15 (6%)	0	100	100
1	B	263/548 (48%)	253 (96%)	10 (4%)	0	100	100
1	C	263/548 (48%)	253 (96%)	10 (4%)	0	100	100
1	D	264/548 (48%)	257 (97%)	7 (3%)	0	100	100
1	E	264/548 (48%)	259 (98%)	5 (2%)	0	100	100
1	F	264/548 (48%)	253 (96%)	11 (4%)	0	100	100
1	G	264/548 (48%)	255 (97%)	9 (3%)	0	100	100
1	H	264/548 (48%)	257 (97%)	7 (3%)	0	100	100
1	I	266/548 (48%)	248 (93%)	18 (7%)	0	100	100
1	J	266/548 (48%)	251 (94%)	15 (6%)	0	100	100
1	K	266/548 (48%)	252 (95%)	14 (5%)	0	100	100
1	L	266/548 (48%)	259 (97%)	7 (3%)	0	100	100
1	M	266/548 (48%)	254 (96%)	10 (4%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	264/548 (48%)	254 (96%)	10 (4%)	0	100	100
1	O	264/548 (48%)	259 (98%)	5 (2%)	0	100	100
1	P	264/548 (48%)	252 (96%)	12 (4%)	0	100	100
1	Q	264/548 (48%)	253 (96%)	11 (4%)	0	100	100
1	R	264/548 (48%)	254 (96%)	10 (4%)	0	100	100
1	S	266/548 (48%)	250 (94%)	16 (6%)	0	100	100
1	T	266/548 (48%)	253 (95%)	13 (5%)	0	100	100
1	U	266/548 (48%)	248 (93%)	18 (7%)	0	100	100
1	V	266/548 (48%)	257 (97%)	8 (3%)	1 (0%)	30	59
1	W	266/548 (48%)	255 (96%)	10 (4%)	1 (0%)	30	59
1	X	264/548 (48%)	255 (97%)	9 (3%)	0	100	100
1	Y	264/548 (48%)	260 (98%)	4 (2%)	0	100	100
1	Z	264/548 (48%)	254 (96%)	10 (4%)	0	100	100
1	a	264/548 (48%)	252 (96%)	12 (4%)	0	100	100
1	b	264/548 (48%)	258 (98%)	6 (2%)	0	100	100
1	c	266/548 (48%)	248 (93%)	18 (7%)	0	100	100
1	d	266/548 (48%)	255 (96%)	11 (4%)	0	100	100
1	e	266/548 (48%)	249 (94%)	17 (6%)	0	100	100
1	f	266/548 (48%)	255 (96%)	11 (4%)	0	100	100
1	g	266/548 (48%)	250 (94%)	15 (6%)	1 (0%)	30	59
All	All	8739/18084 (48%)	8370 (96%)	364 (4%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	41	ALA
1	W	171	ASN
1	M	35	GLY
1	M	171	ASN
1	g	35	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	224/425 (53%)	224 (100%)	0	100	100
1	B	224/425 (53%)	224 (100%)	0	100	100
1	C	224/425 (53%)	224 (100%)	0	100	100
1	D	226/425 (53%)	226 (100%)	0	100	100
1	E	226/425 (53%)	226 (100%)	0	100	100
1	F	226/425 (53%)	226 (100%)	0	100	100
1	G	226/425 (53%)	226 (100%)	0	100	100
1	H	226/425 (53%)	226 (100%)	0	100	100
1	I	227/425 (53%)	227 (100%)	0	100	100
1	J	227/425 (53%)	227 (100%)	0	100	100
1	K	227/425 (53%)	227 (100%)	0	100	100
1	L	227/425 (53%)	227 (100%)	0	100	100
1	M	227/425 (53%)	227 (100%)	0	100	100
1	N	226/425 (53%)	226 (100%)	0	100	100
1	O	226/425 (53%)	226 (100%)	0	100	100
1	P	226/425 (53%)	226 (100%)	0	100	100
1	Q	226/425 (53%)	226 (100%)	0	100	100
1	R	226/425 (53%)	226 (100%)	0	100	100
1	S	227/425 (53%)	227 (100%)	0	100	100
1	T	227/425 (53%)	227 (100%)	0	100	100
1	U	227/425 (53%)	225 (99%)	2 (1%)	70	76
1	V	227/425 (53%)	227 (100%)	0	100	100
1	W	227/425 (53%)	227 (100%)	0	100	100
1	X	226/425 (53%)	226 (100%)	0	100	100
1	Y	226/425 (53%)	226 (100%)	0	100	100
1	Z	226/425 (53%)	226 (100%)	0	100	100
1	a	226/425 (53%)	226 (100%)	0	100	100
1	b	226/425 (53%)	226 (100%)	0	100	100
1	c	227/425 (53%)	227 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	227/425 (53%)	227 (100%)	0	100	100
1	e	227/425 (53%)	225 (99%)	2 (1%)	70	76
1	f	227/425 (53%)	227 (100%)	0	100	100
1	g	227/425 (53%)	227 (100%)	0	100	100
All	All	7467/14025 (53%)	7463 (100%)	4 (0%)	100	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	38[A]	ILE
1	U	38[B]	ILE
1	e	38[A]	ILE
1	e	38[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (223) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	17	ASN
1	A	19	ASN
1	A	63	GLN
1	A	86	ASN
1	A	90	GLN
1	A	131	GLN
1	A	503	GLN
1	B	17	ASN
1	B	63	GLN
1	B	76	GLN
1	B	86	ASN
1	B	470	GLN
1	B	482	GLN
1	C	3	GLN
1	C	22	GLN
1	C	39	ASN
1	C	48	GLN
1	C	63	GLN
1	C	86	ASN
1	C	88	ASN
1	C	491	ASN
1	C	517	ASN

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Mol	Chain	Res	Type
1	C	537	GLN
1	D	21	ASN
1	D	63	GLN
1	D	67	ASN
1	D	131	GLN
1	D	171	ASN
1	D	176	ASN
1	D	491	ASN
1	D	493	ASN
1	N	522	GLN
1	N	536	ASN
1	X	67	ASN
1	X	69	ASN
1	X	86	ASN
1	X	493	ASN
1	X	494	ASN
1	X	498	ASN
1	X	503	GLN
1	X	525	GLN
1	E	15	GLN
1	E	129	GLN
1	E	136	ASN
1	E	498	ASN
1	E	503	GLN
1	E	507	GLN
1	O	6	ASN
1	O	90	GLN
1	O	525	GLN
1	O	540	GLN
1	Y	16	ASN
1	Y	19	ASN
1	Y	22	GLN
1	Y	491	ASN
1	Y	498	ASN
1	Y	522	GLN
1	F	63	GLN
1	F	147	GLN
1	F	482	GLN
1	F	503	GLN
1	F	547	GLN
1	P	16	ASN
1	P	17	ASN

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Mol	Chain	Res	Type
1	P	48	GLN
1	P	63	GLN
1	P	129	GLN
1	P	174	ASN
1	P	491	ASN
1	P	503	GLN
1	Z	17	ASN
1	Z	98	GLN
1	Z	154	GLN
1	Z	482	GLN
1	Z	494	ASN
1	G	6	ASN
1	G	19	ASN
1	G	98	GLN
1	G	154	GLN
1	G	498	ASN
1	G	503	GLN
1	G	517	ASN
1	G	536	ASN
1	G	547	GLN
1	Q	19	ASN
1	Q	63	GLN
1	Q	76	GLN
1	Q	129	GLN
1	Q	491	ASN
1	Q	498	ASN
1	Q	540	GLN
1	a	3	GLN
1	a	19	ASN
1	a	22	GLN
1	a	48	GLN
1	a	491	ASN
1	a	525	GLN
1	a	529	ASN
1	H	8	ASN
1	H	17	ASN
1	H	63	GLN
1	H	67	ASN
1	H	86	ASN
1	H	526	GLN
1	R	15	GLN
1	R	17	ASN

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Mol	Chain	Res	Type
1	R	129	GLN
1	R	147	GLN
1	R	154	GLN
1	b	90	GLN
1	b	517	ASN
1	b	529	ASN
1	I	21	ASN
1	I	22	GLN
1	I	86	ASN
1	I	136	ASN
1	I	171	ASN
1	I	482	GLN
1	I	525	GLN
1	S	3	GLN
1	S	17	ASN
1	S	21	ASN
1	S	48	GLN
1	S	86	ASN
1	S	90	GLN
1	S	482	GLN
1	S	498	ASN
1	S	507	GLN
1	c	16	ASN
1	c	39	ASN
1	c	52	ASN
1	c	86	ASN
1	c	104	ASN
1	c	147	GLN
1	c	154	GLN
1	c	493	ASN
1	c	498	ASN
1	c	517	ASN
1	c	540	GLN
1	J	39	ASN
1	T	17	ASN
1	T	22	GLN
1	T	39	ASN
1	T	67	ASN
1	T	86	ASN
1	T	90	GLN
1	T	129	GLN
1	T	483	ASN

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Mol	Chain	Res	Type
1	T	491	ASN
1	T	493	ASN
1	T	517	ASN
1	T	541	GLN
1	d	22	GLN
1	d	39	ASN
1	d	129	GLN
1	d	147	GLN
1	d	154	GLN
1	d	517	ASN
1	d	522	GLN
1	d	540	GLN
1	K	19	ASN
1	K	22	GLN
1	K	86	ASN
1	K	537	GLN
1	K	547	GLN
1	U	22	GLN
1	U	52	ASN
1	U	90	GLN
1	U	483	ASN
1	U	525	GLN
1	U	547	GLN
1	e	19	ASN
1	e	52	ASN
1	e	63	GLN
1	e	67	ASN
1	e	86	ASN
1	e	113	GLN
1	e	547	GLN
1	L	69	ASN
1	L	133	ASN
1	L	154	GLN
1	L	171	ASN
1	L	503	GLN
1	L	507	GLN
1	L	525	GLN
1	V	16	ASN
1	V	63	GLN
1	V	67	ASN
1	V	113	GLN
1	V	154	GLN

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Mol	Chain	Res	Type
1	V	491	ASN
1	V	494	ASN
1	V	503	GLN
1	V	507	GLN
1	V	525	GLN
1	f	39	ASN
1	f	63	GLN
1	f	67	ASN
1	f	147	GLN
1	f	493	ASN
1	f	503	GLN
1	f	525	GLN
1	f	537	GLN
1	f	540	GLN
1	M	21	ASN
1	M	131	GLN
1	M	171	ASN
1	M	498	ASN
1	W	57	ASN
1	W	69	ASN
1	W	136	ASN
1	W	526	GLN
1	g	63	GLN
1	g	67	ASN
1	g	69	ASN
1	g	76	GLN
1	g	86	ASN
1	g	104	ASN
1	g	147	GLN
1	g	507	GLN
1	g	522	GLN
1	g	526	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

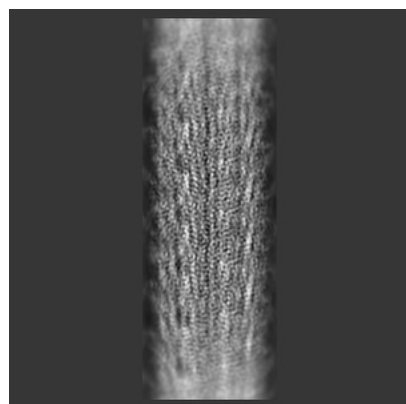
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27008. These allow visual inspection of the internal detail of the map and identification of artifacts.

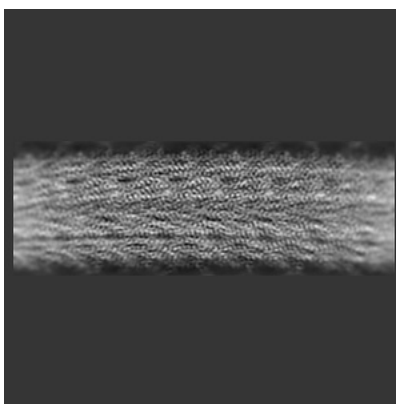
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

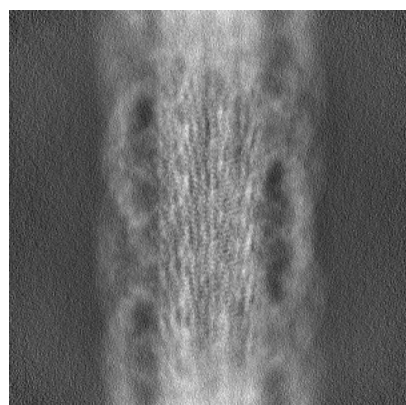


Y

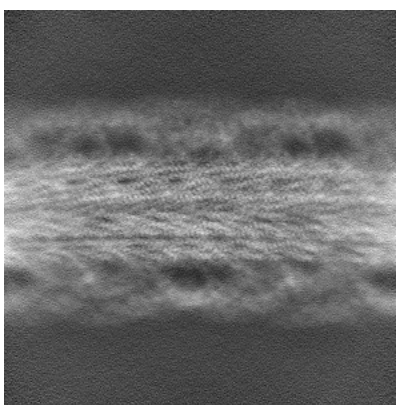


Z

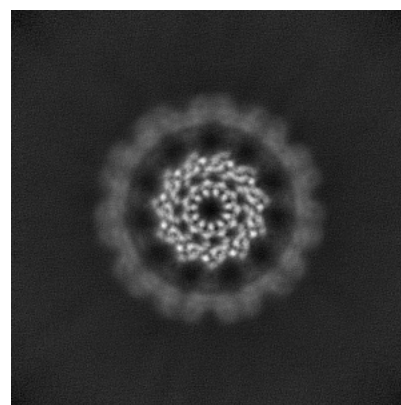
6.1.2 Raw map



X



Y

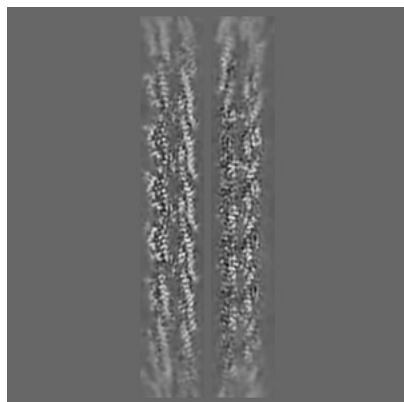


Z

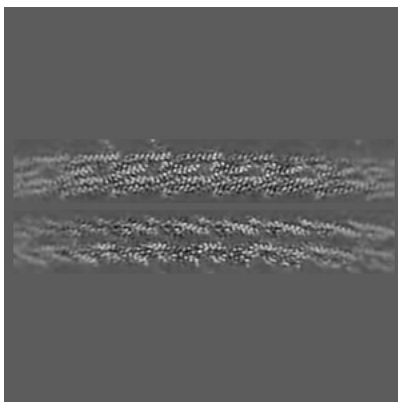
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

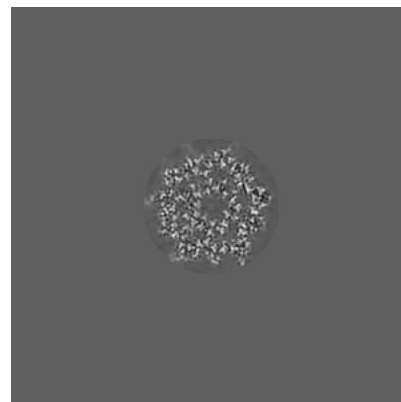
6.2.1 Primary map



X Index: 192

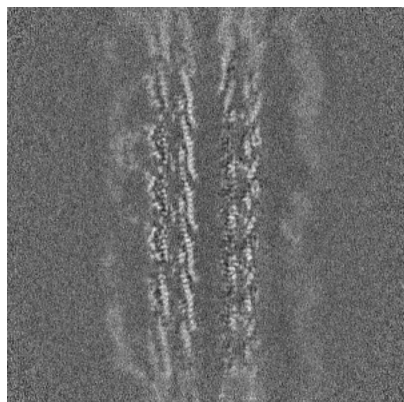


Y Index: 192

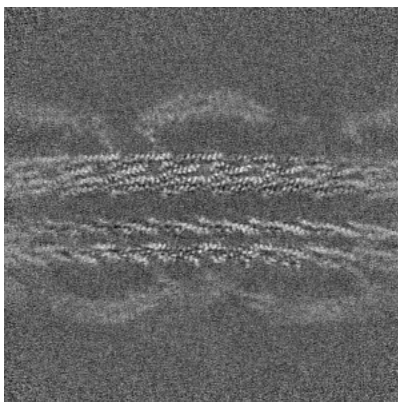


Z Index: 192

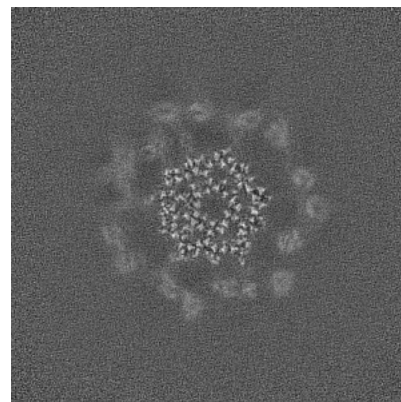
6.2.2 Raw map



X Index: 192



Y Index: 192

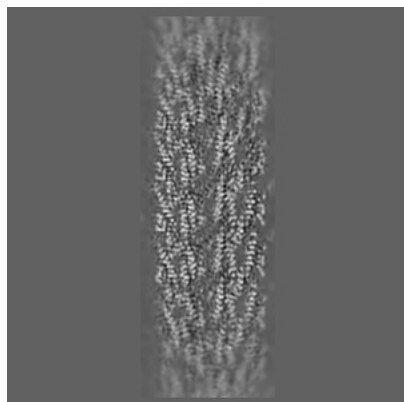


Z Index: 192

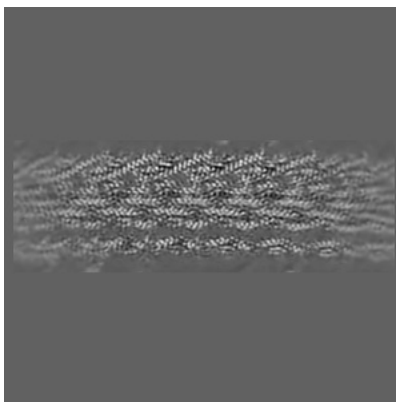
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

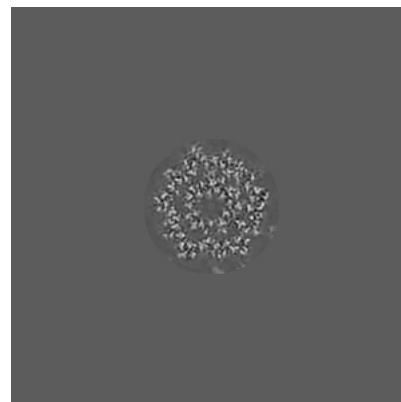
6.3.1 Primary map



X Index: 204

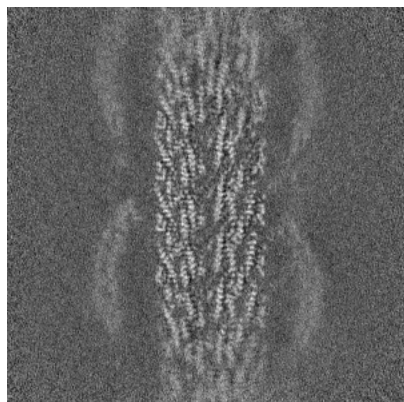


Y Index: 209

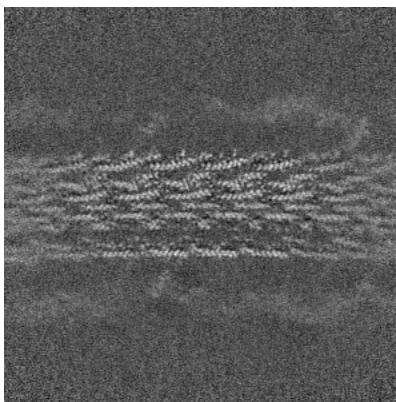


Z Index: 182

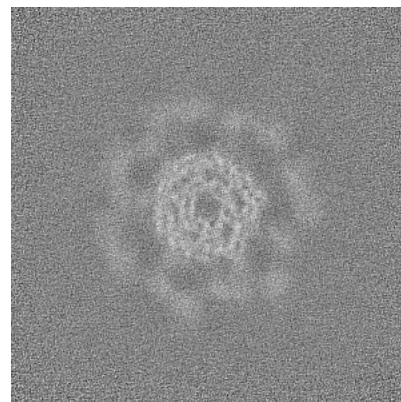
6.3.2 Raw map



X Index: 204



Y Index: 177

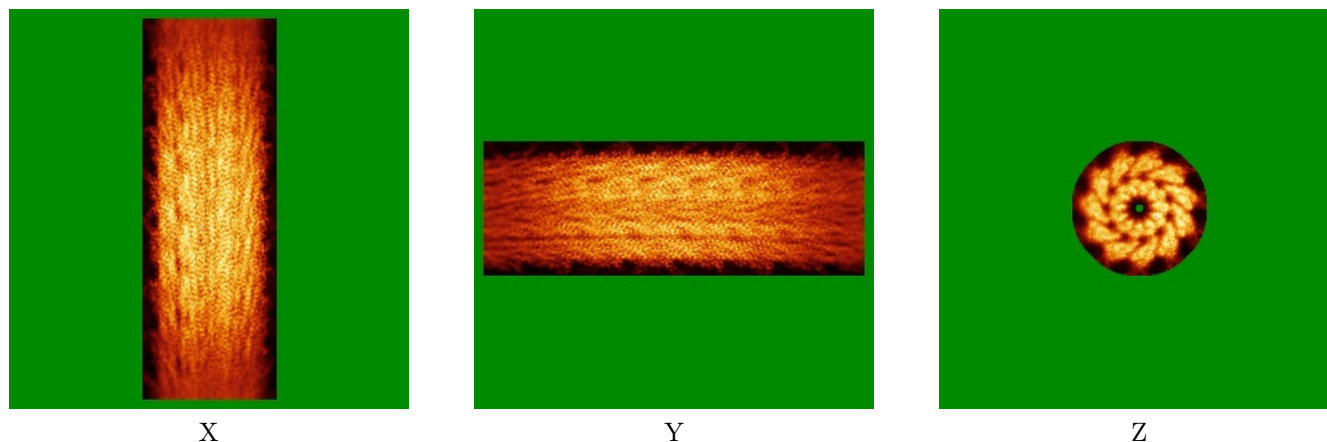


Z Index: 0

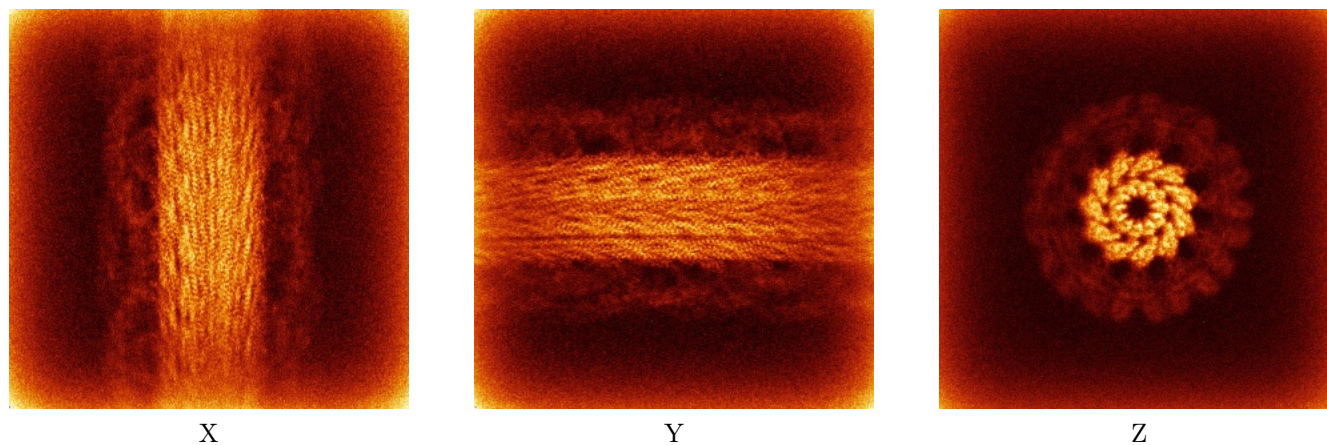
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



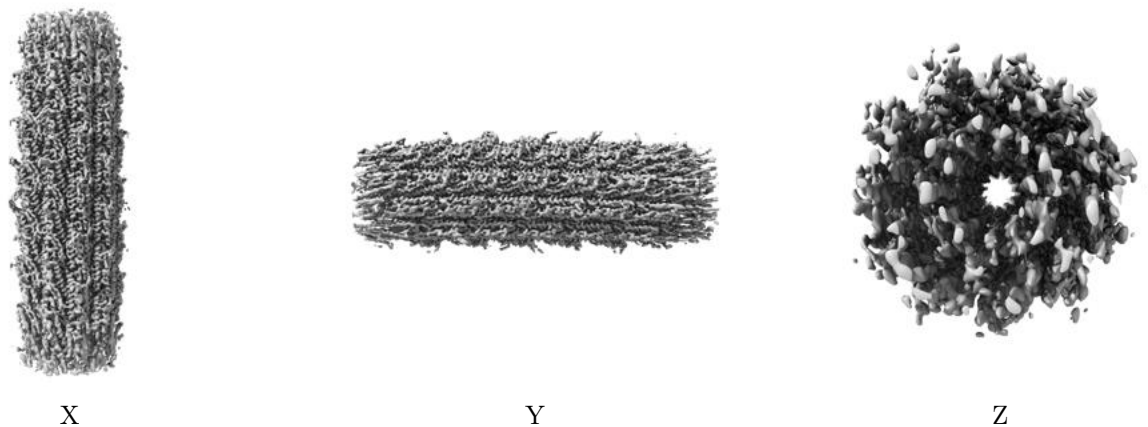
6.4.2 Raw map



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.

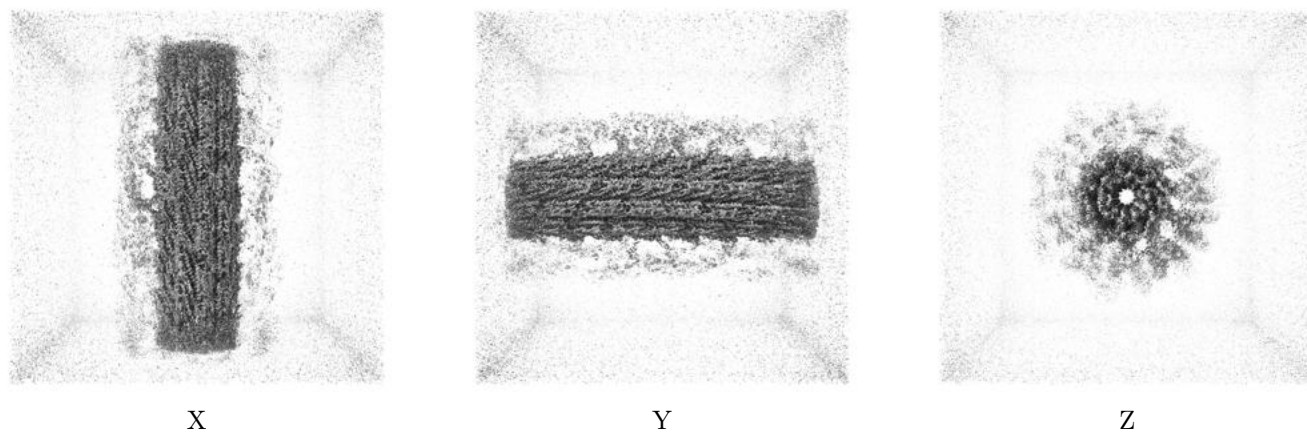
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.136. 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.

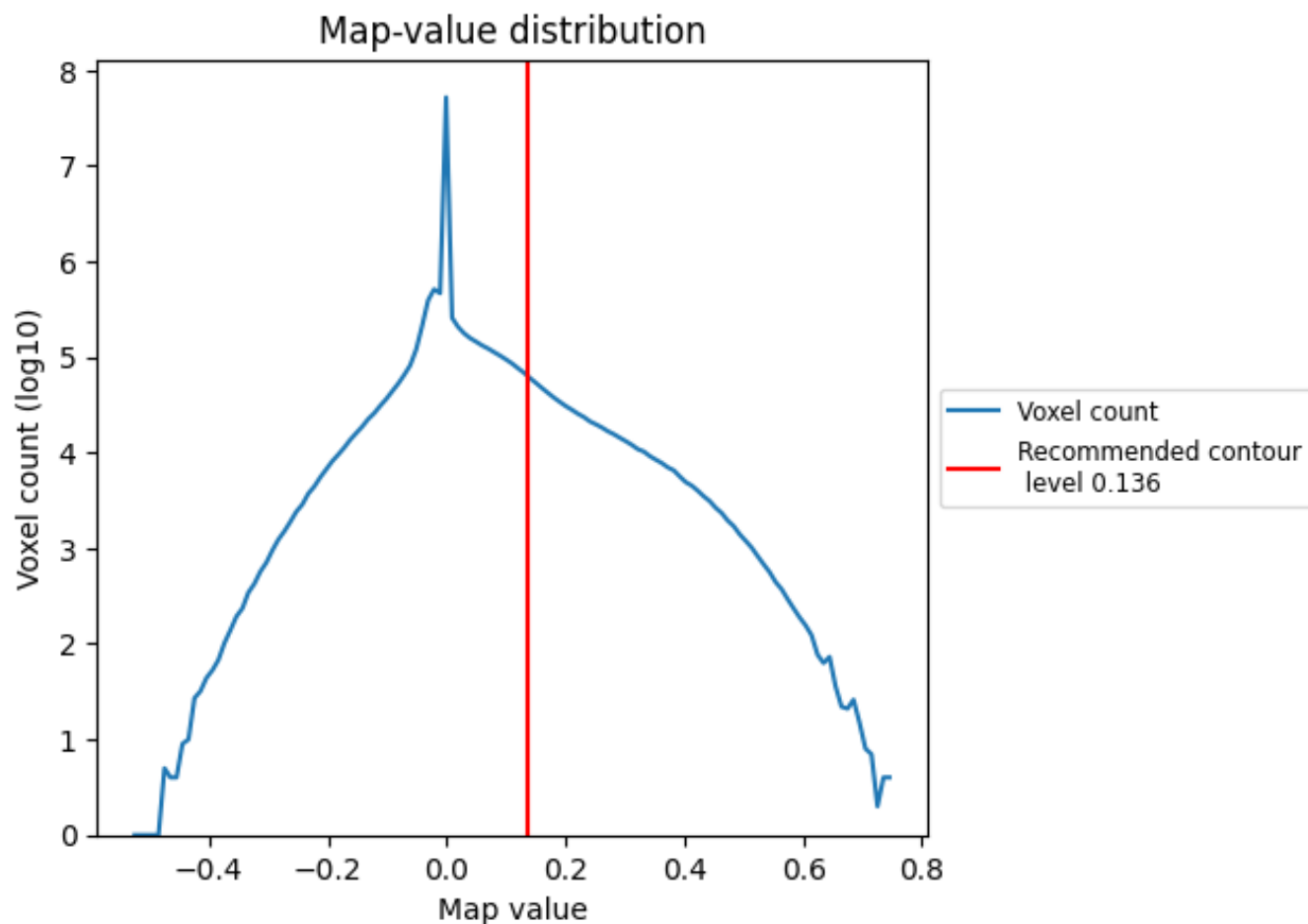
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

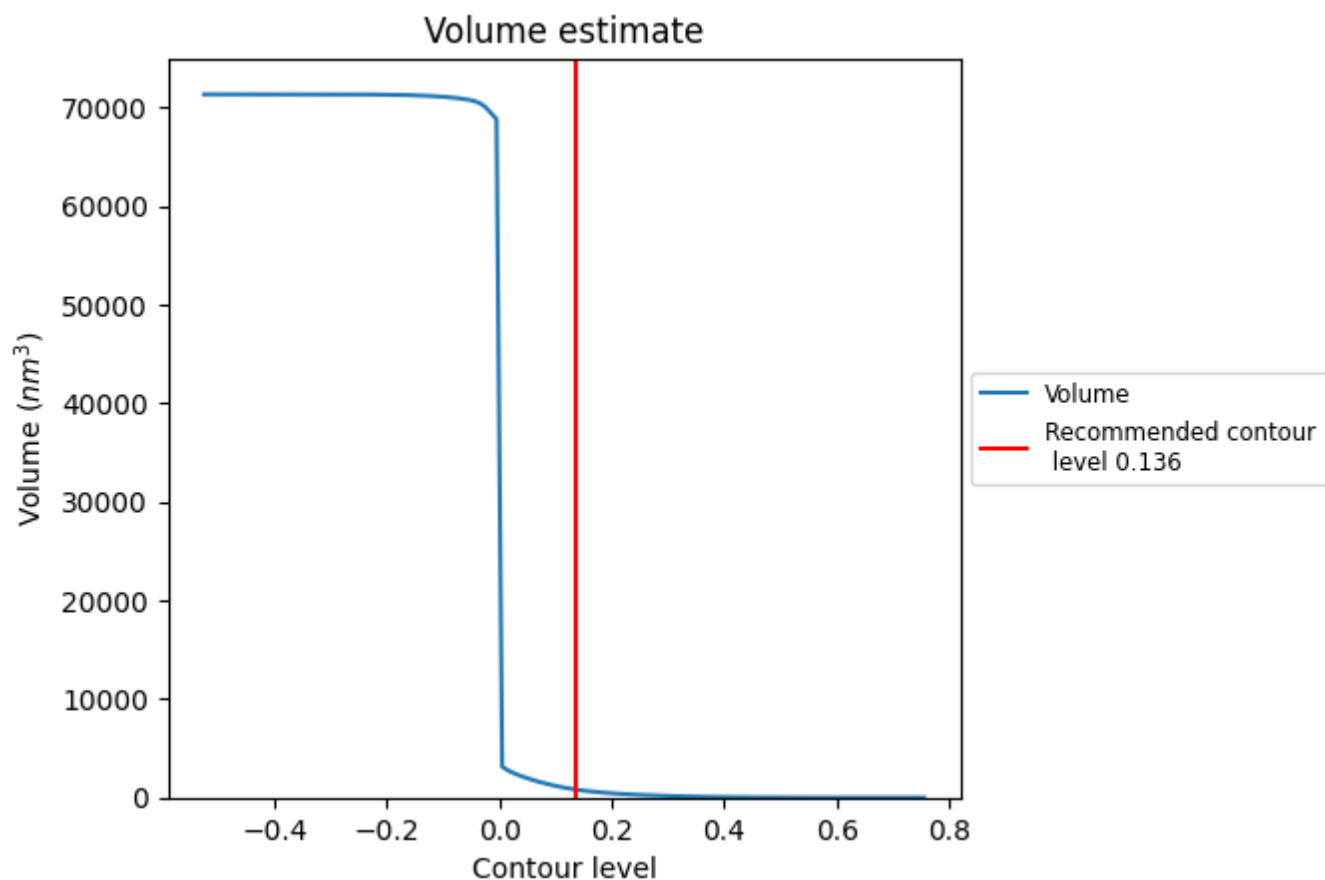
This section contains the results of statistical analysis of the map.

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.

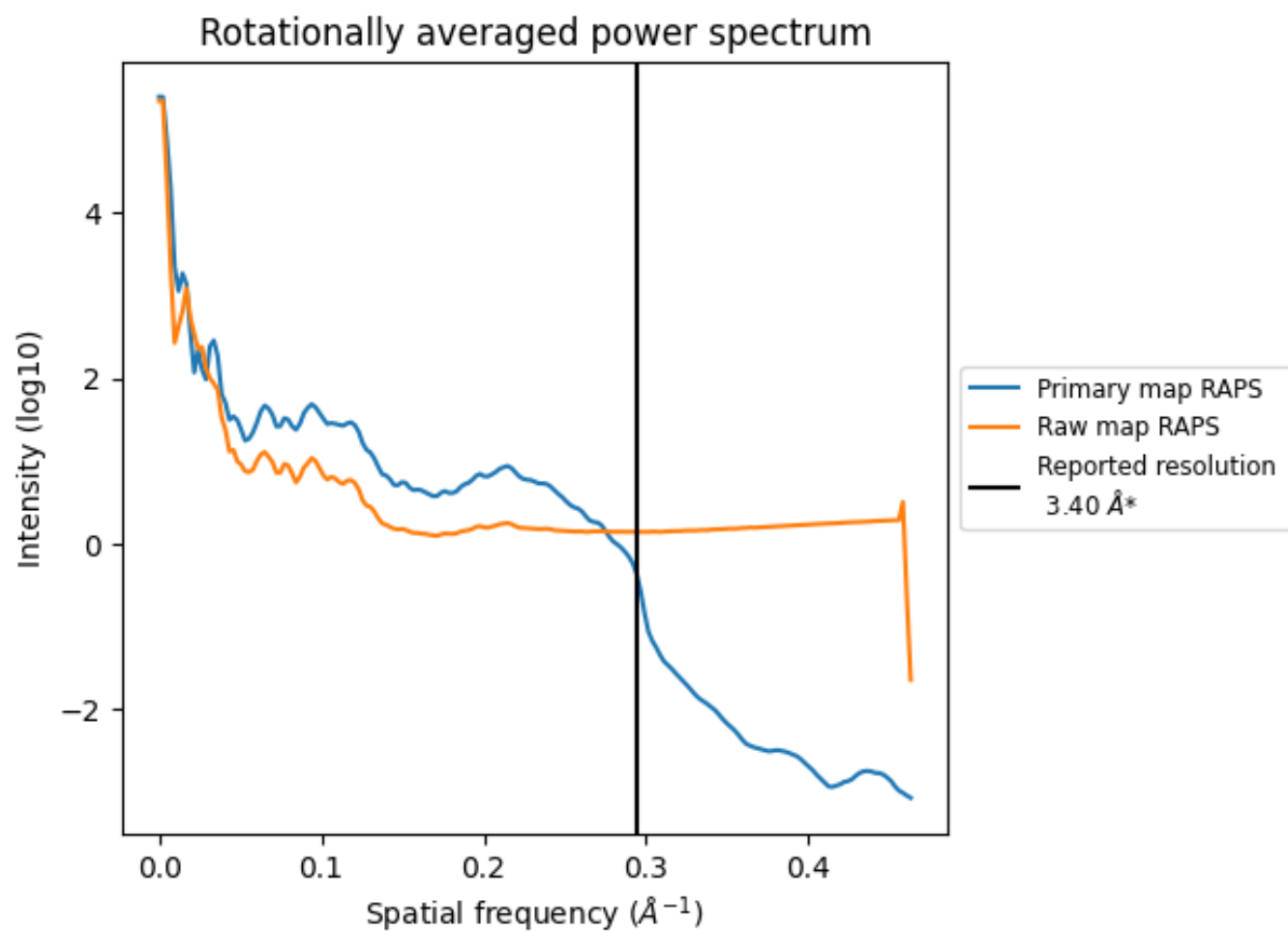
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 811 nm³; this corresponds to an approximate mass of 733 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 ⓘ

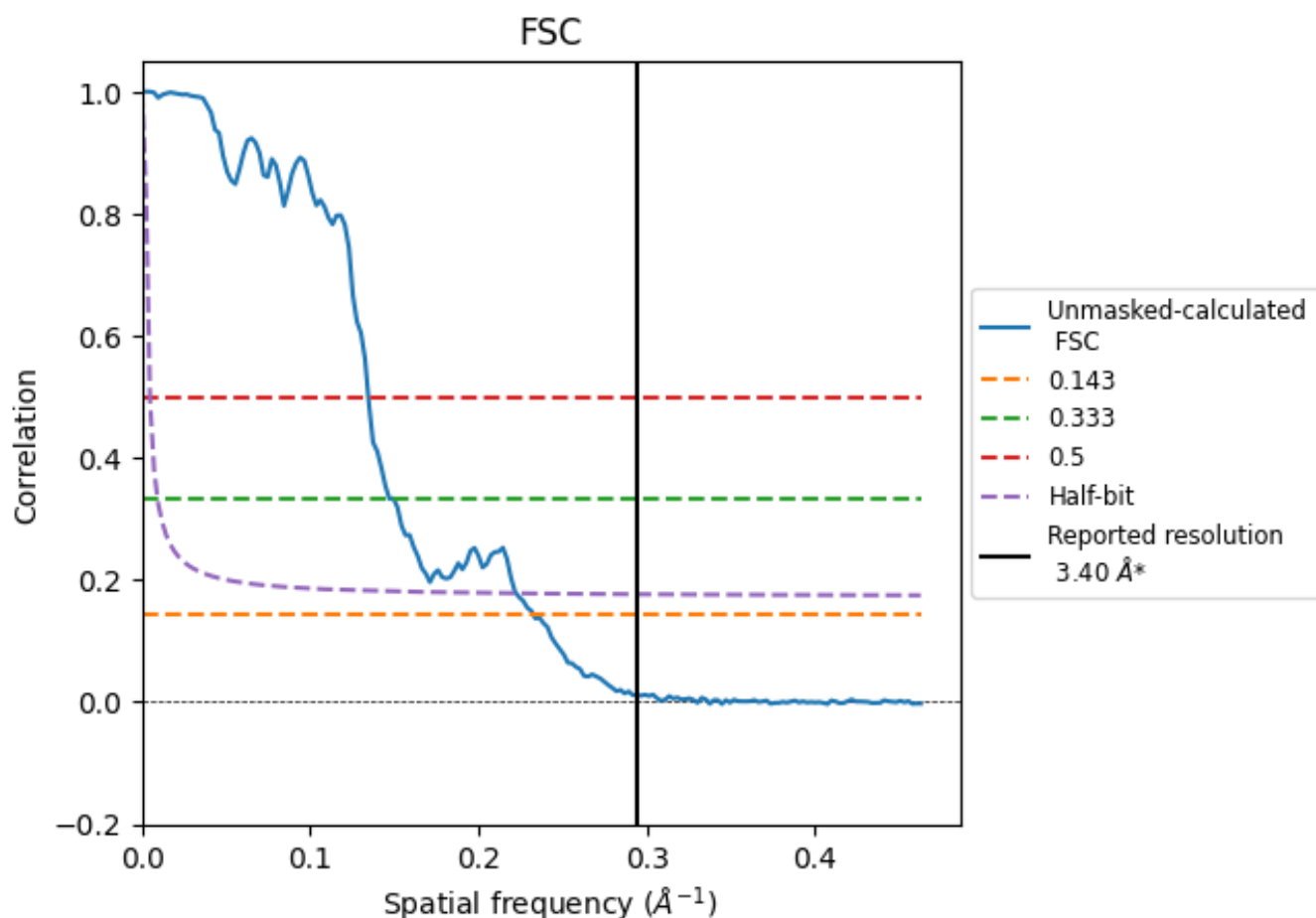


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

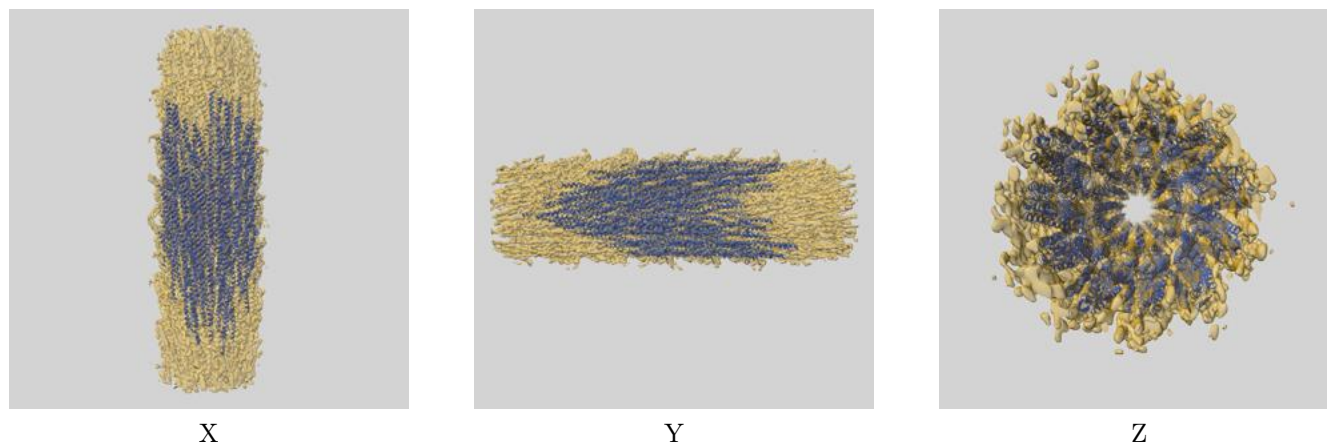
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	0.333
Reported by author	-	-	-	3.40
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	4.30	7.43	4.49	6.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.33 CUT-OFF 6.80 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

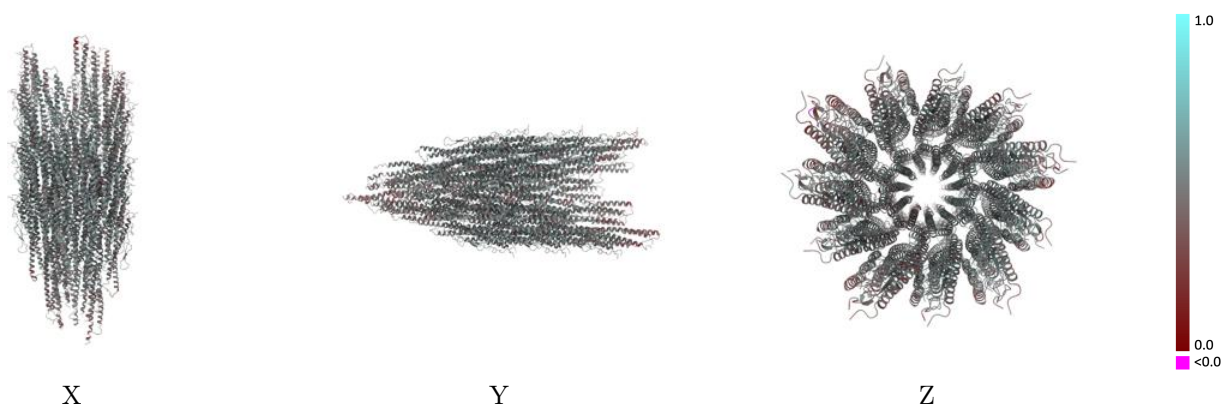
This section contains information regarding the fit between EMDB map EMD-27008 and PDB model 8CVI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



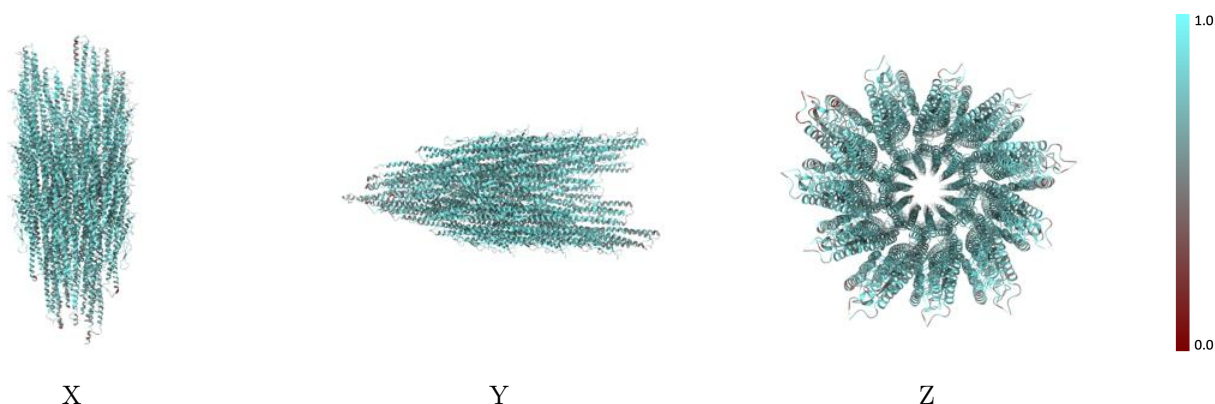
The images above show the 3D surface view of the map at the recommended contour level 0.136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



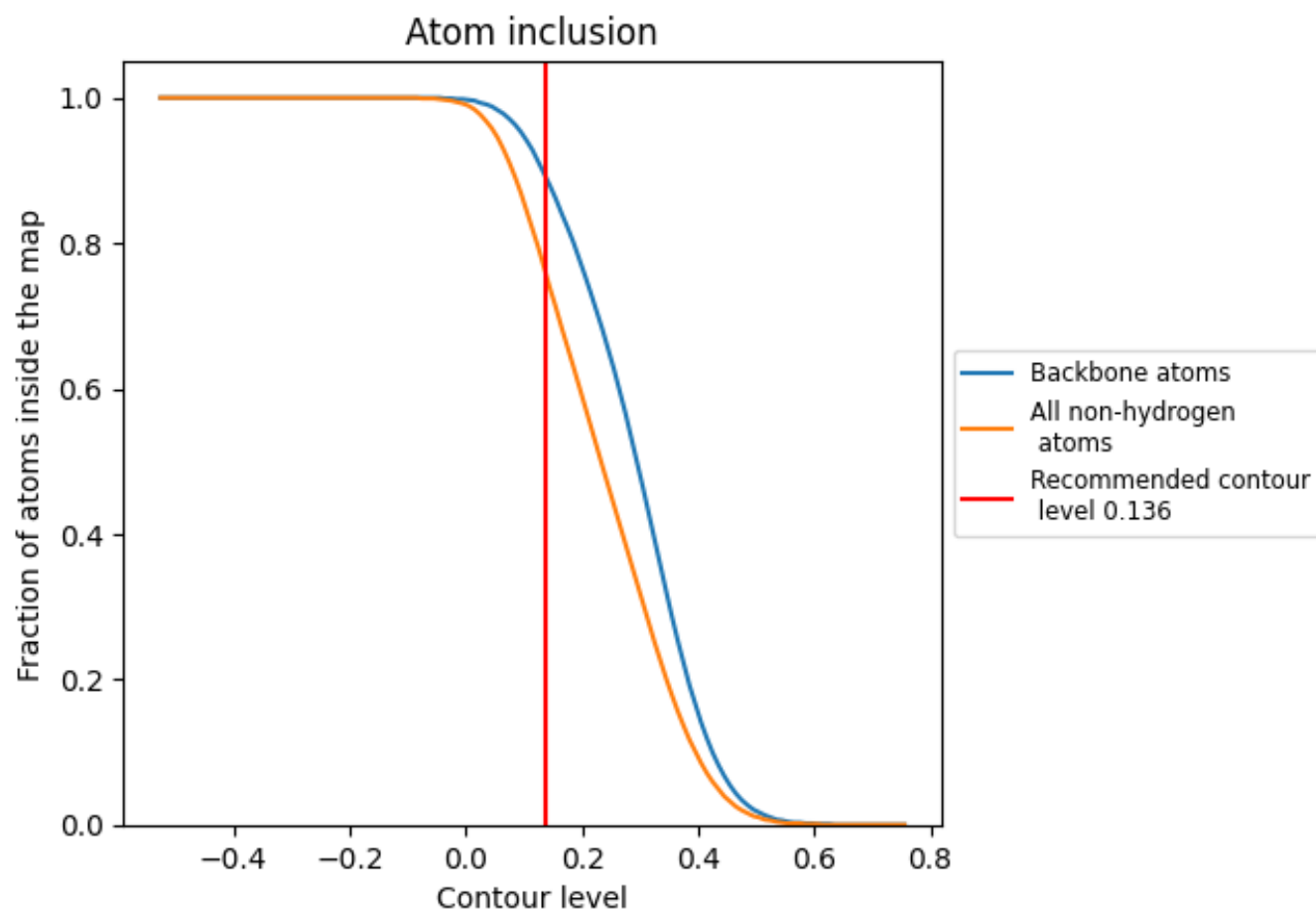
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.136).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 76% 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 (0.136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.4860
A	 0.7460	 0.4760
B	 0.7770	 0.4910
C	 0.7480	 0.4610
D	 0.7640	 0.4870
E	 0.7530	 0.4740
F	 0.7890	 0.5000
G	 0.7680	 0.4920
H	 0.7930	 0.5050
I	 0.7580	 0.4930
J	 0.6880	 0.4420
K	 0.7430	 0.4760
L	 0.7720	 0.4910
M	 0.7500	 0.4900
N	 0.7700	 0.4860
O	 0.7950	 0.5110
P	 0.8040	 0.5140
Q	 0.7930	 0.5110
R	 0.7910	 0.5070
S	 0.7790	 0.4960
T	 0.7720	 0.4940
U	 0.7830	 0.4970
V	 0.7540	 0.4850
W	 0.7720	 0.4920
X	 0.7230	 0.4520
Y	 0.7940	 0.5010
Z	 0.7620	 0.4980
a	 0.7910	 0.5050
b	 0.7490	 0.4740
c	 0.7520	 0.4690
d	 0.7690	 0.4760
e	 0.7430	 0.4700
f	 0.6950	 0.4500
g	 0.7390	 0.4630

