



## Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 12:22 AM EDT

PDB ID : 6U7M / pdb\_00006u7m  
EMDB ID : EMD-20673  
Title : Cryo-EM Structure of Helical Lipoprotein Lipase  
Authors : Gunn, K.H.; Wang, F.; Egelman, E.H.; Neher, S.B.  
Deposited on : 2019-09-03  
Resolution : 3.80 Å(reported)  
Based on initial model : 6E7K

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

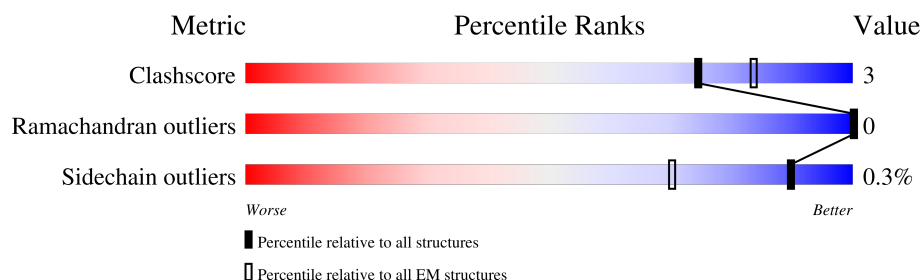
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	478	<div> <div>8%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	B	478	<div> <div>8%</div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
1	C	478	<div> <div>9%</div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
1	D	478	<div> <div>8%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	E	478	<div> <div>8%</div> <div>80%</div> <div>8%</div> <div>13%</div> </div>
1	F	478	<div> <div>8%</div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
1	G	478	<div> <div>8%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	H	478	<div> <div>8%</div> <div>79%</div> <div>9%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	478	
1	J	478	
1	K	478	
1	L	478	
1	M	478	
1	N	478	
1	O	478	
1	P	478	
1	Q	478	
1	R	478	
1	S	478	
1	T	478	
1	U	478	
1	a	478	
1	b	478	
1	c	478	
1	d	478	
1	e	478	
1	f	478	
1	g	478	
1	h	478	
1	i	478	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 99420 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 Lipoprotein lipase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	B	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	C	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	D	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	E	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	F	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	G	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	H	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	I	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	J	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	K	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	L	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	M	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	N	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	O	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	P	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	Q	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		

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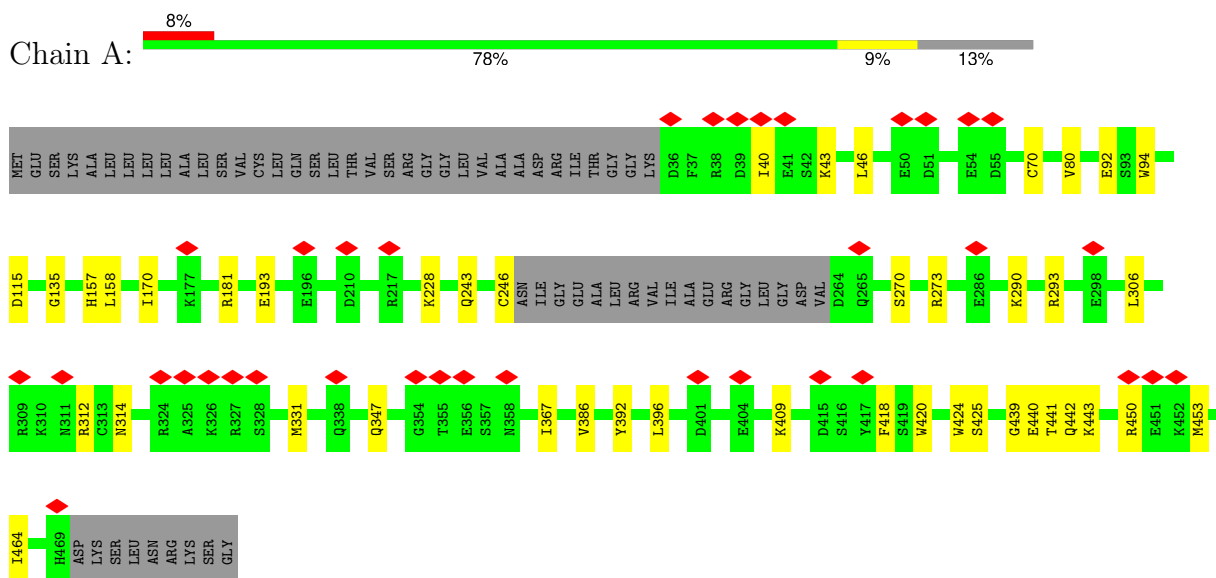
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	S	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	T	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	U	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	a	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	b	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	c	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	d	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	e	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	f	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
1	g	417	Total 3314	C 2114	N 568	O 614	S 18	0	0
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1	i	417	Total 3314	C 2114	N 568	O 614	S 18	0	0

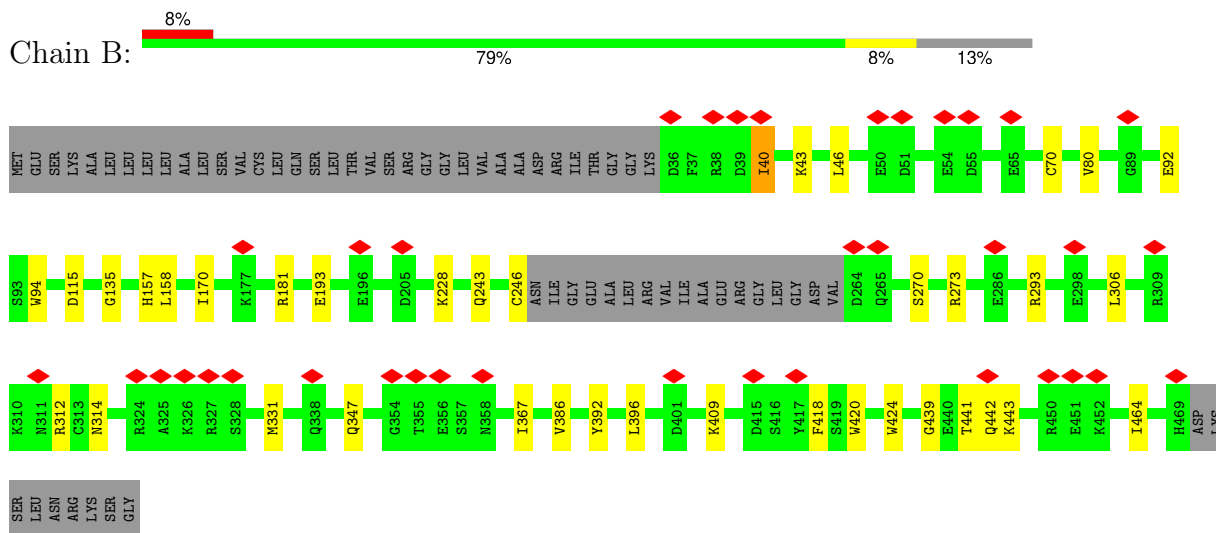
### 3 Residue-property plots

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.

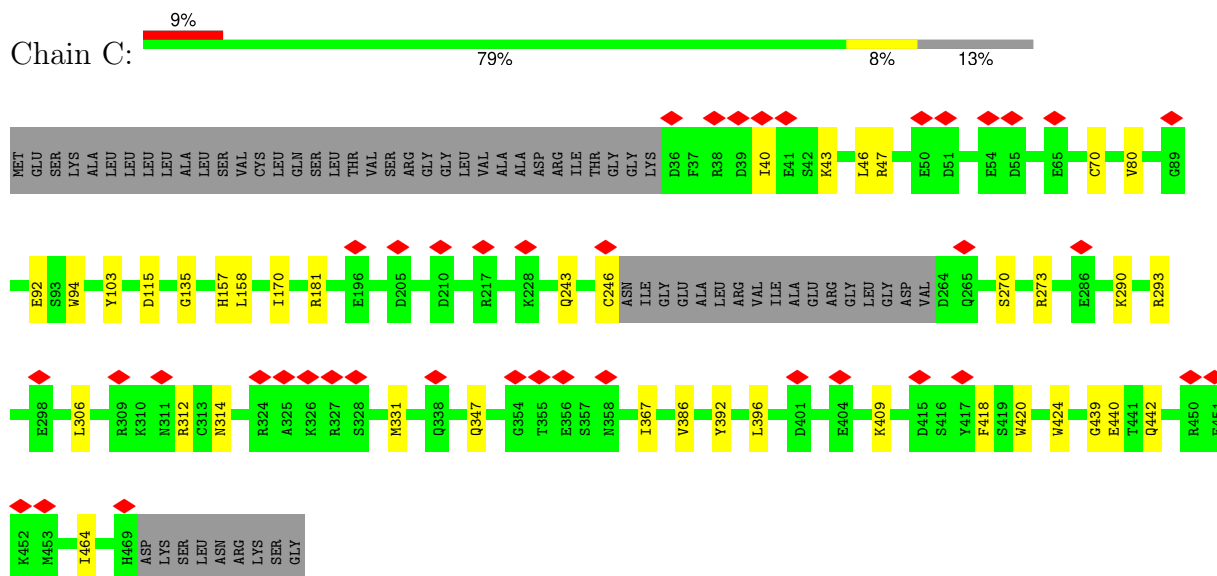
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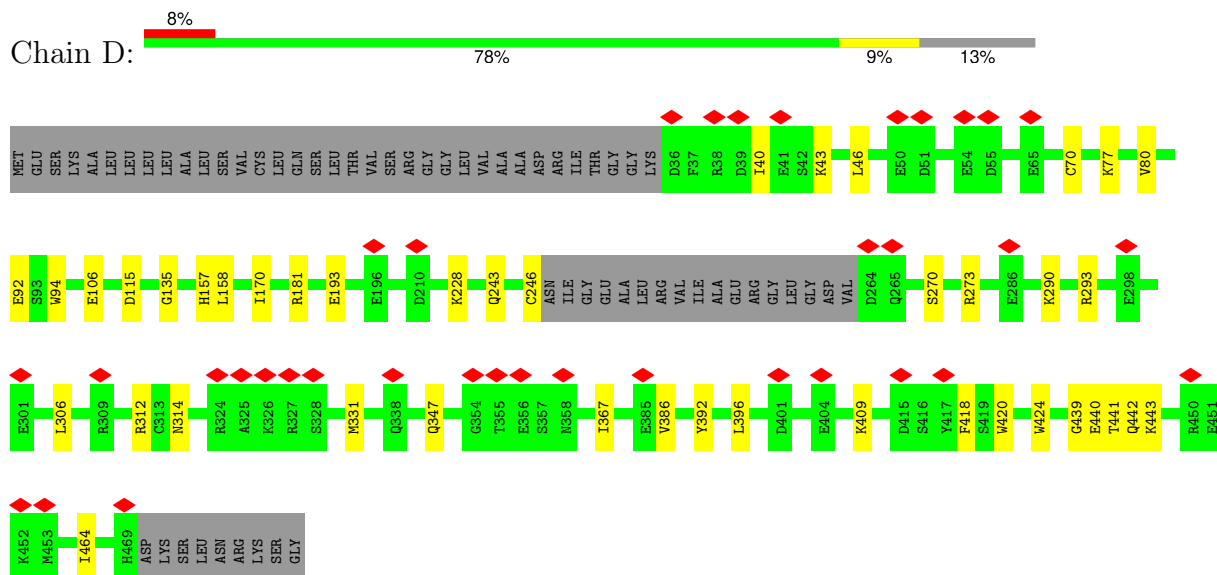
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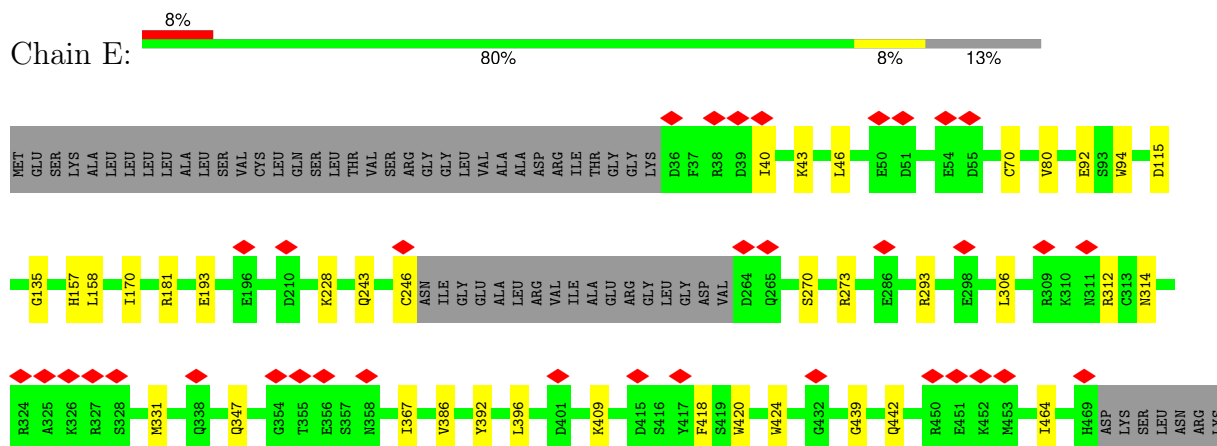
#### • Molecule 1: Lipoprotein lipase



- Molecule 1: Lipoprotein lipase


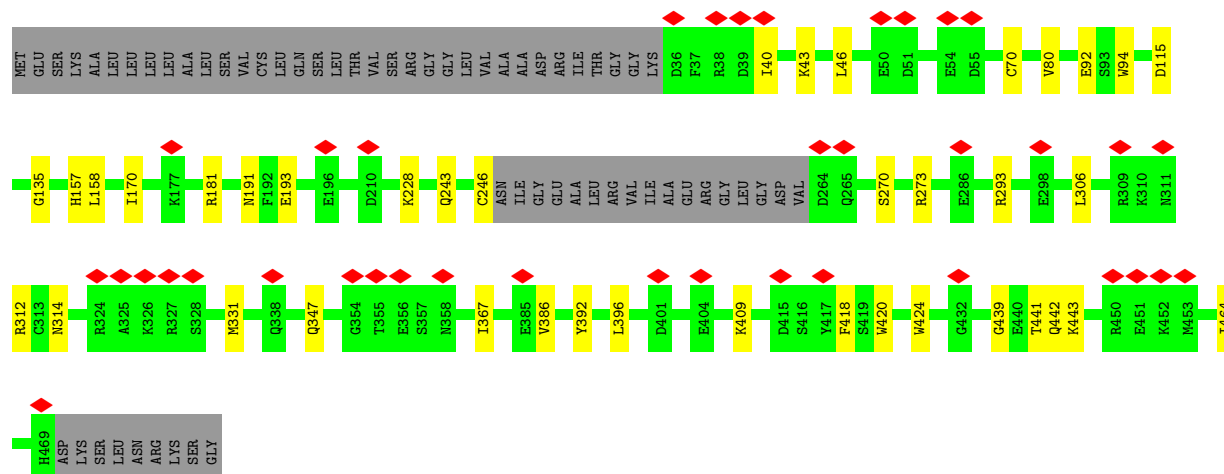


- Molecule 1: Lipoprotein lipase


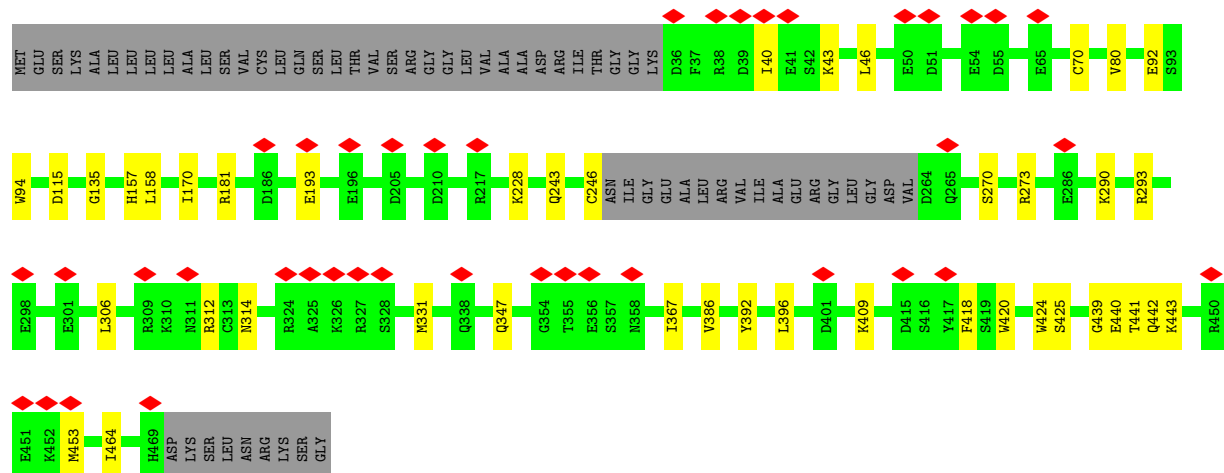


SER  
GLY


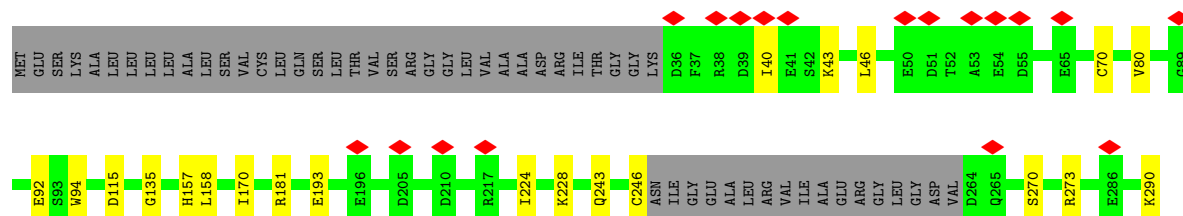
## • Molecule 1: Lipoprotein lipase

Chain F:  8% 79% 8% 13%

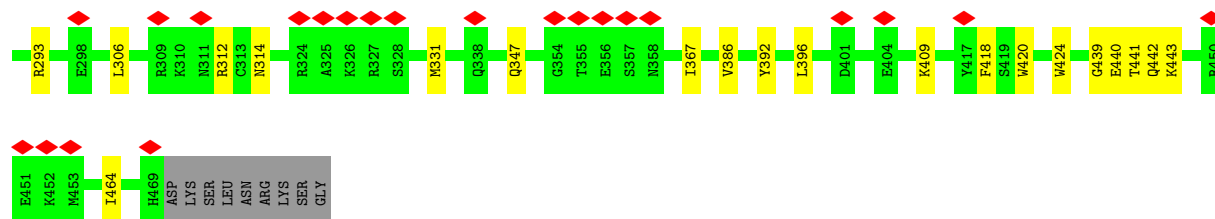
## • Molecule 1: Lipoprotein lipase

Chain G:  8% 78% 9% 13%

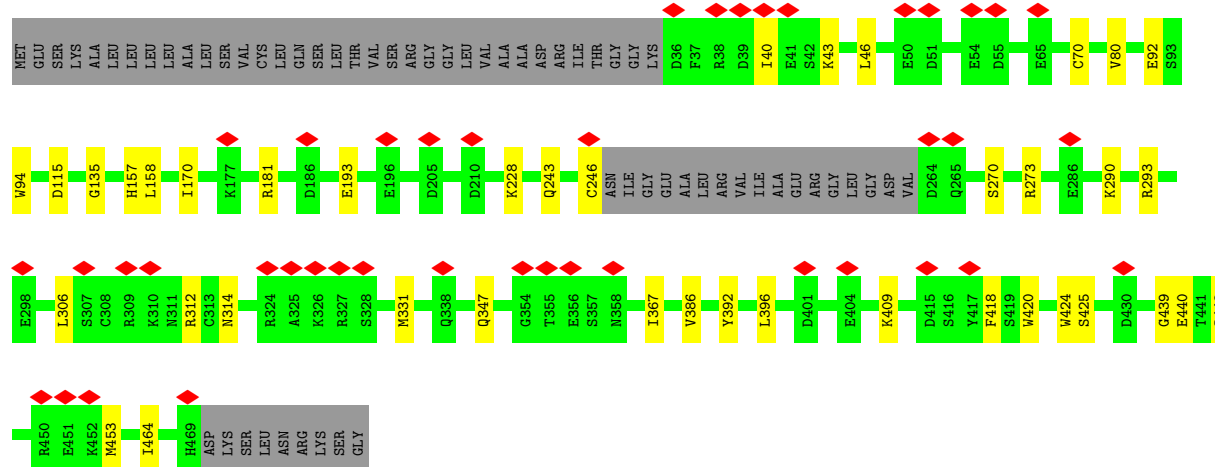
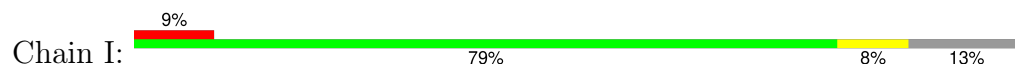
## • Molecule 1: Lipoprotein lipase

Chain H:  8% 79% 9% 13%

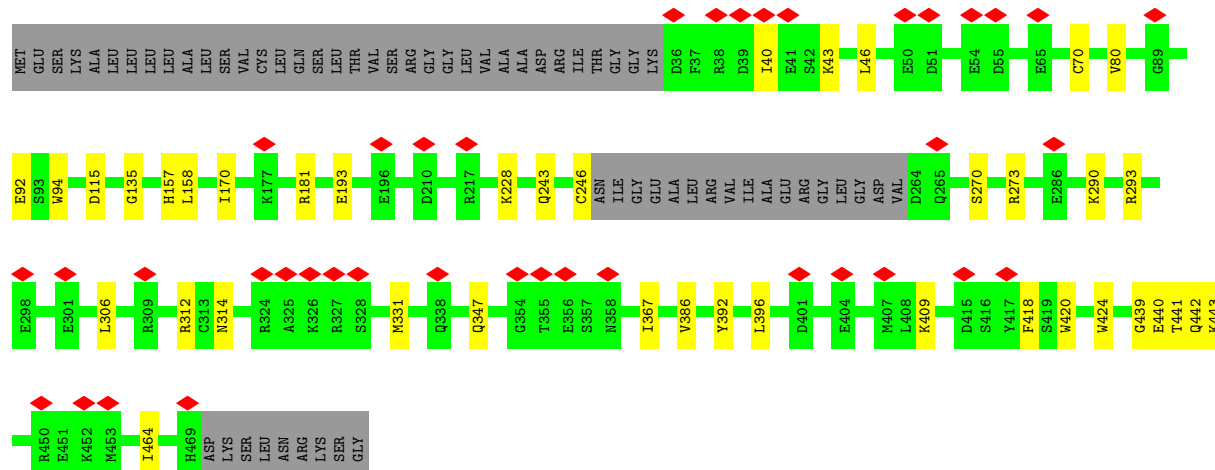
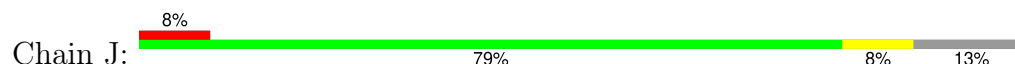




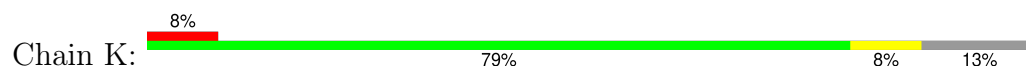
• Molecule 1: Lipoprotein lipase

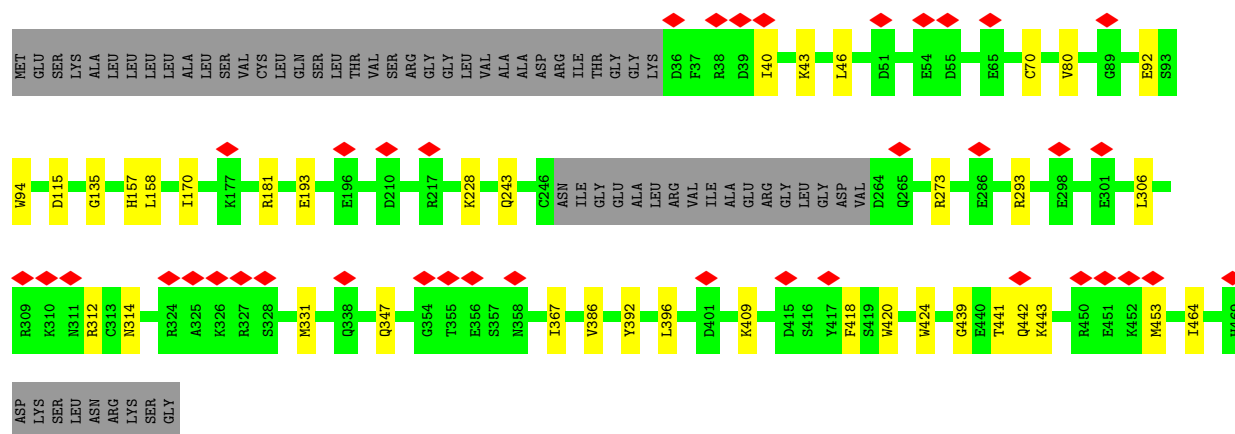


• Molecule 1: Lipoprotein lipase

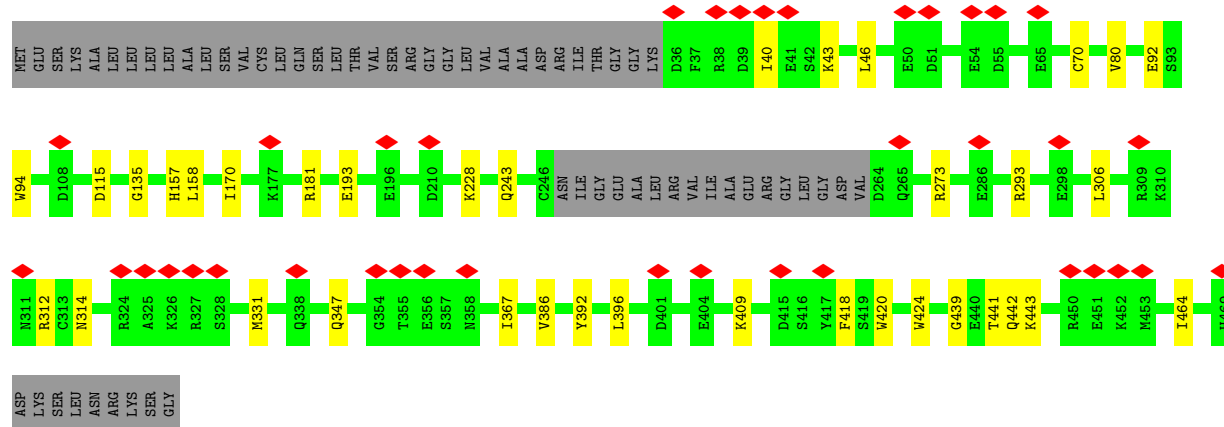
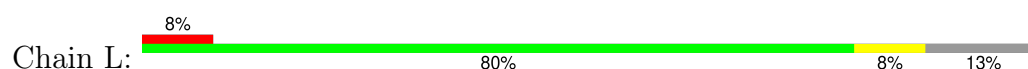


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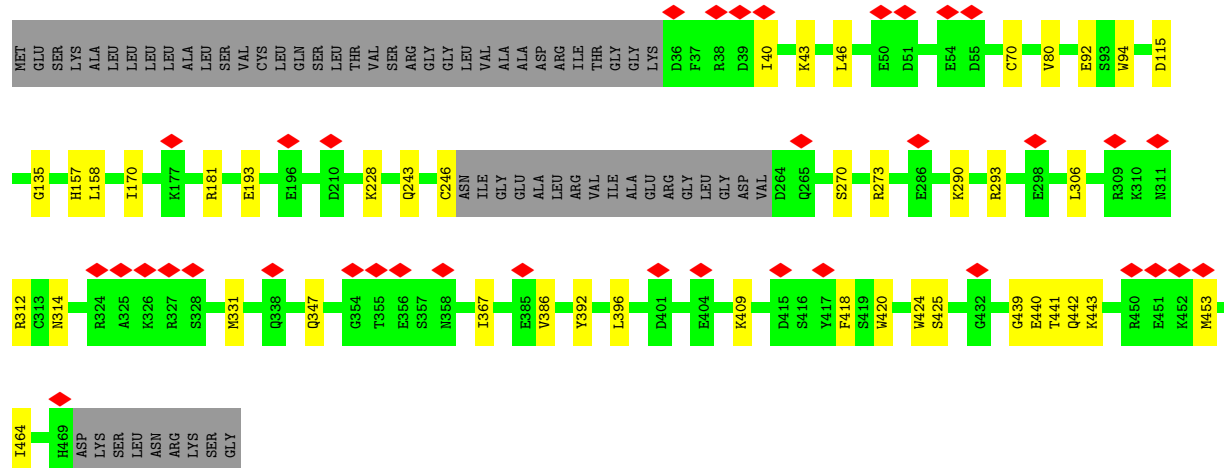
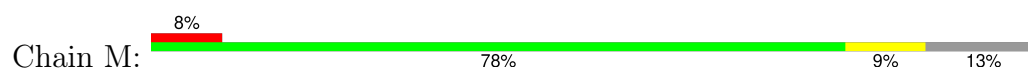




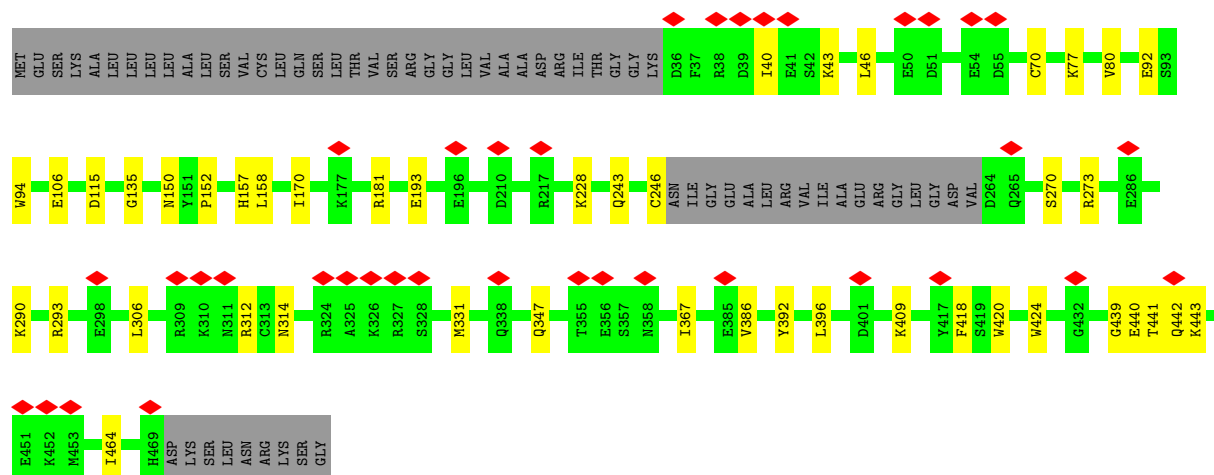
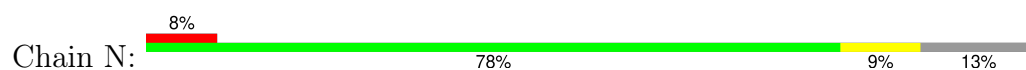
• Molecule 1: Lipoprotein lipase



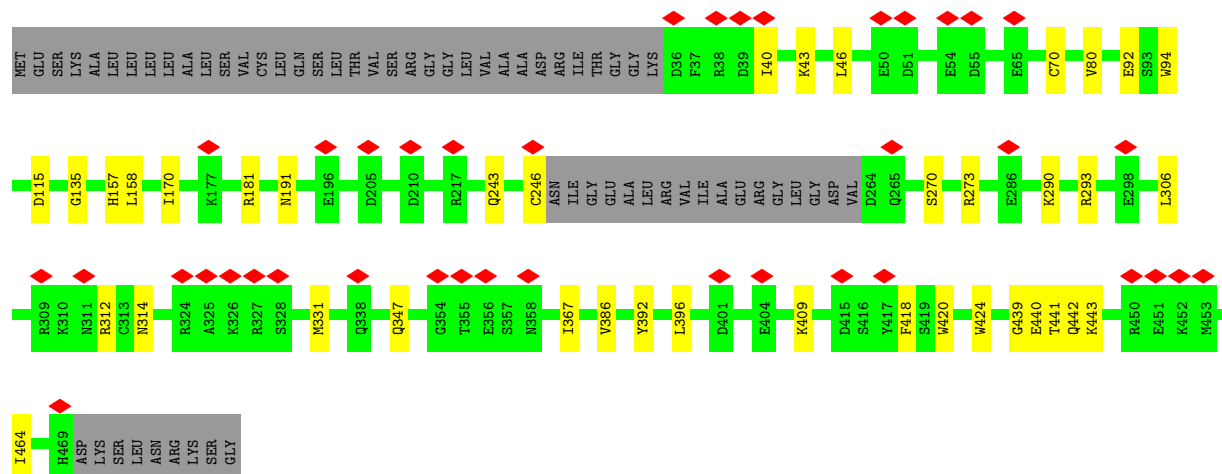
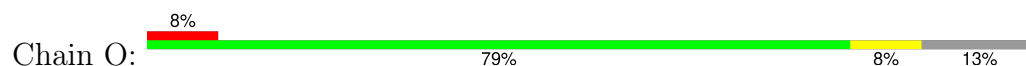
• Molecule 1: Lipoprotein lipase



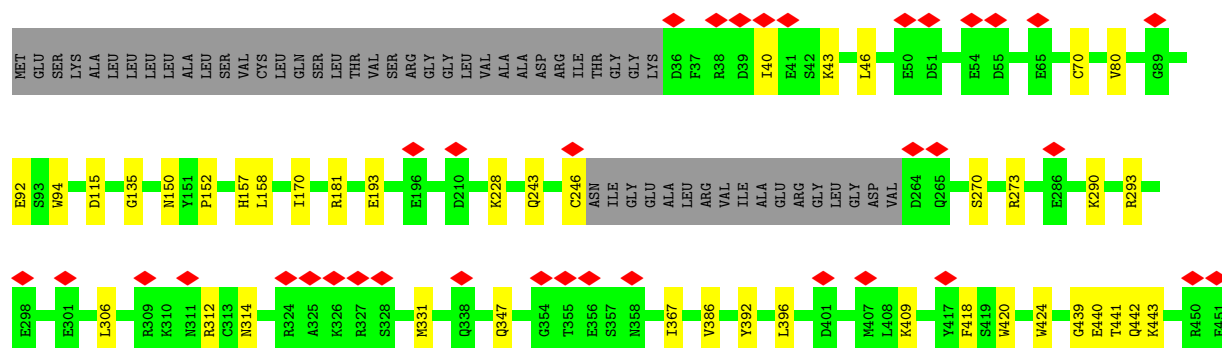
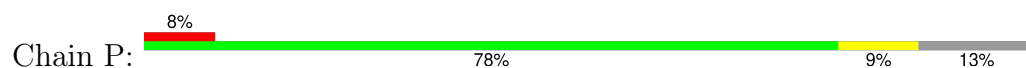
• Molecule 1: Lipoprotein lipase

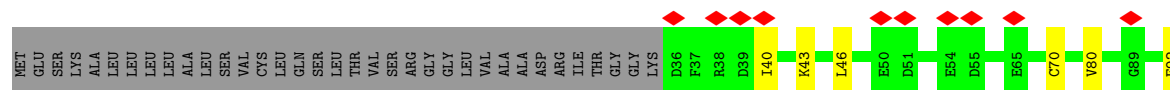


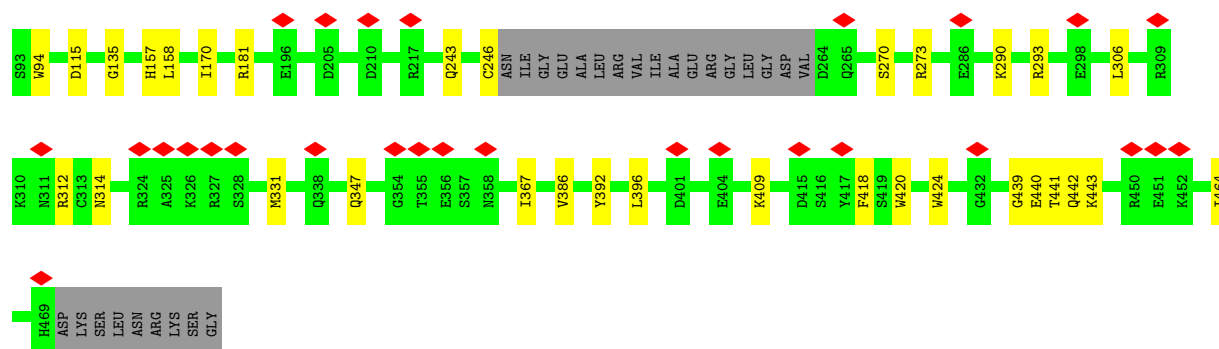
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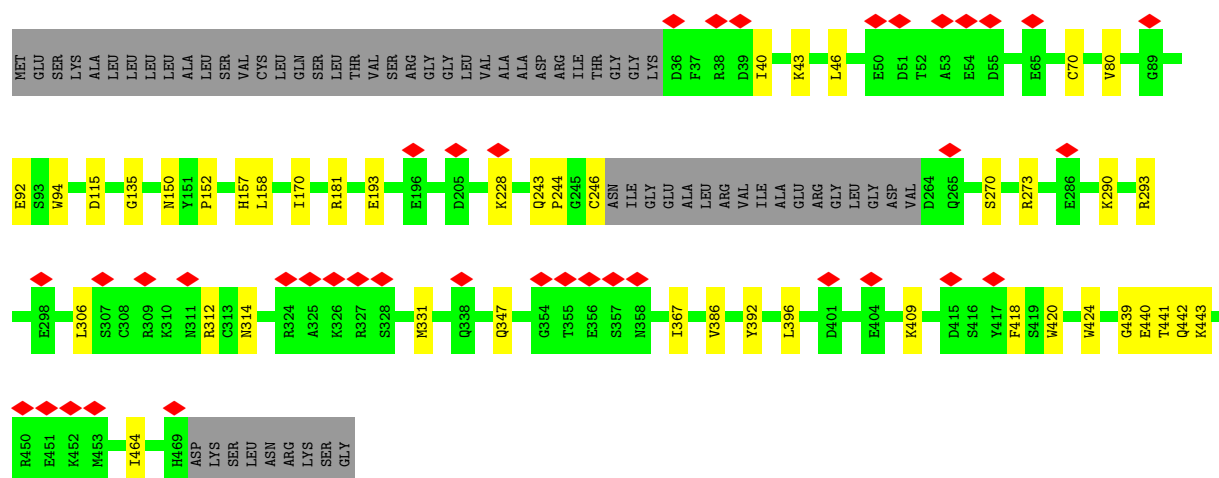
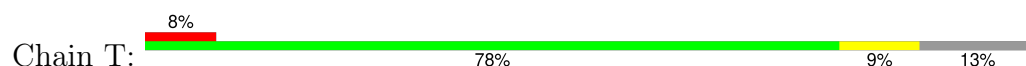
• Molecule 1: Lipoprotein lipase



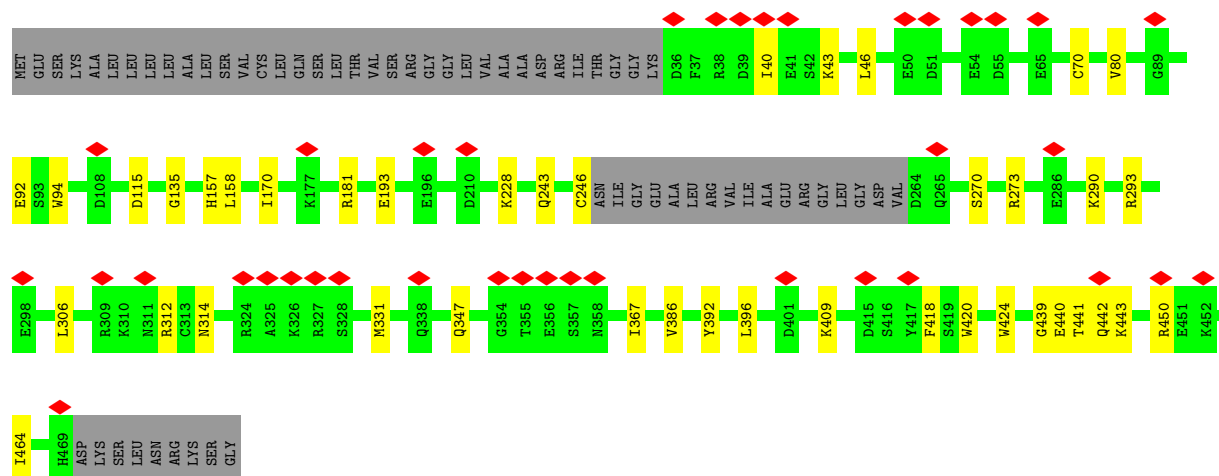
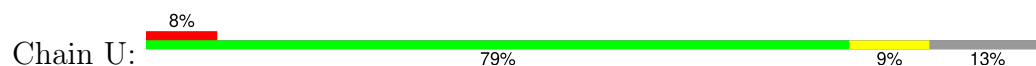




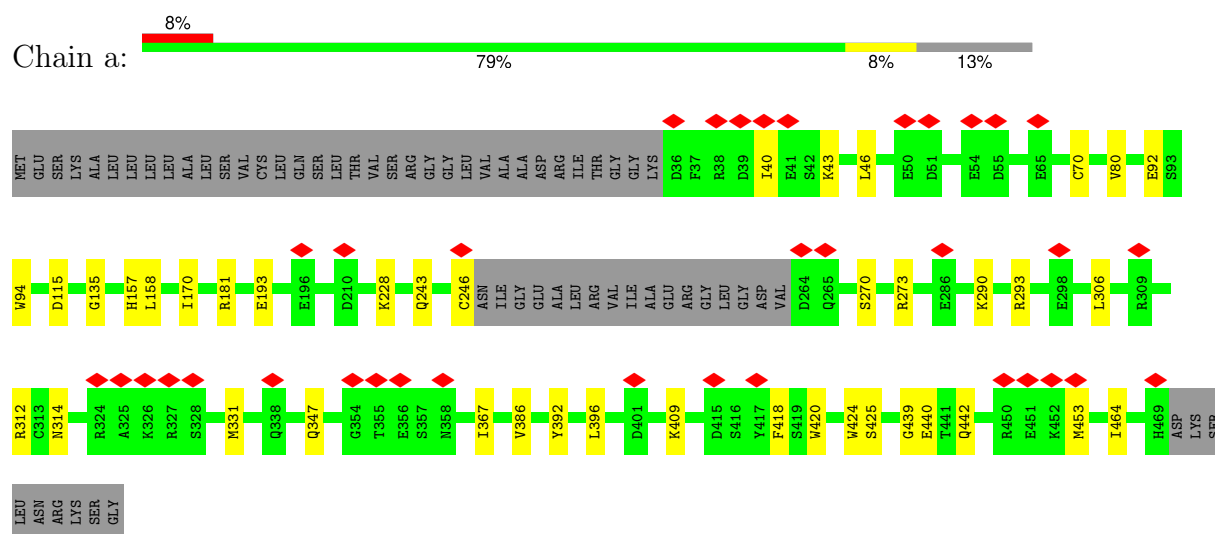
- Molecule 1: Lipoprotein lipase



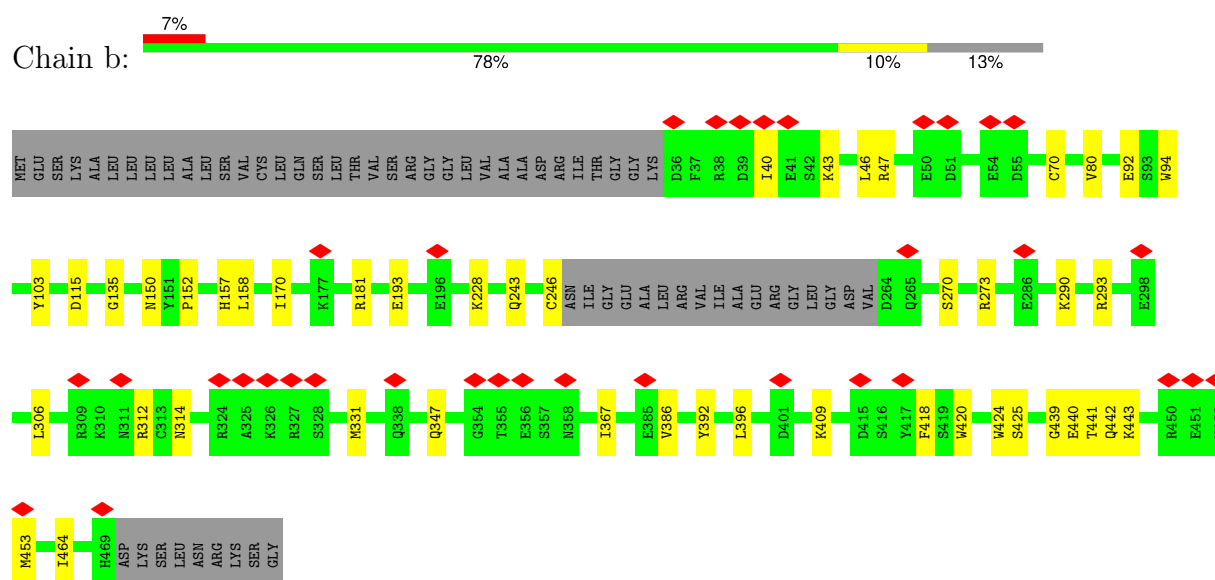
- Molecule 1: Lipoprotein lipase



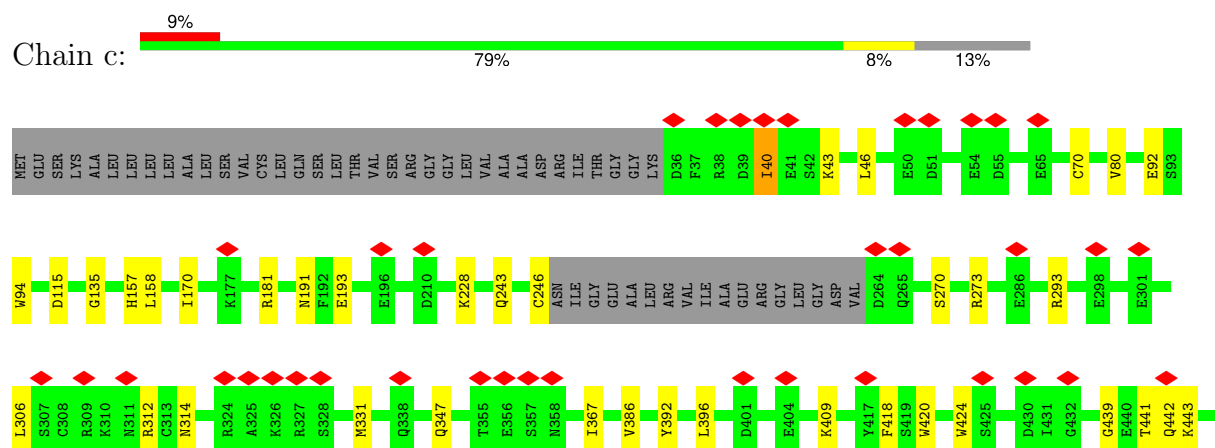
- Molecule 1: Lipoprotein lipase



• Molecule 1: Lipoprotein lipase

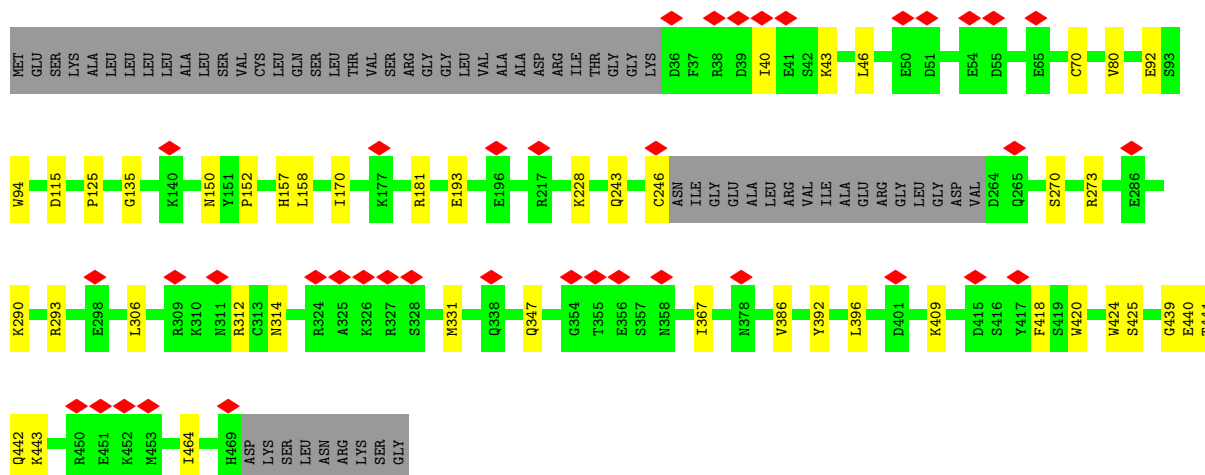
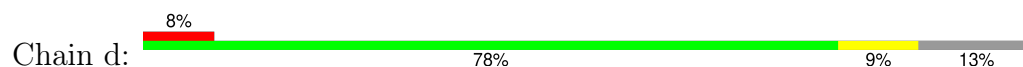


• Molecule 1: Lipoprotein lipase

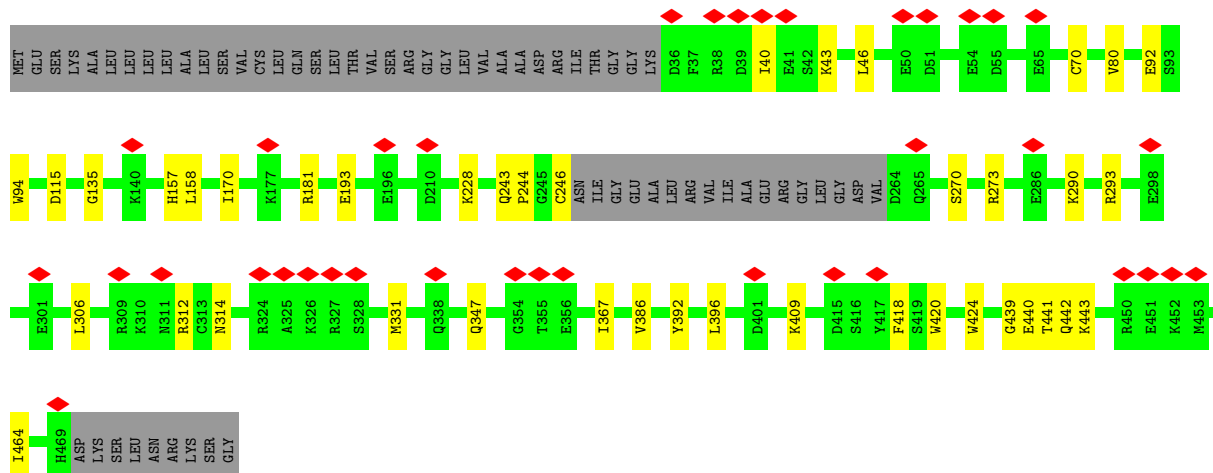
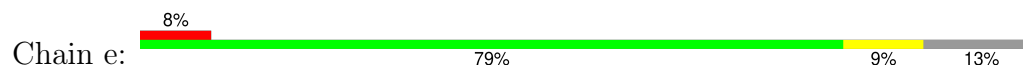




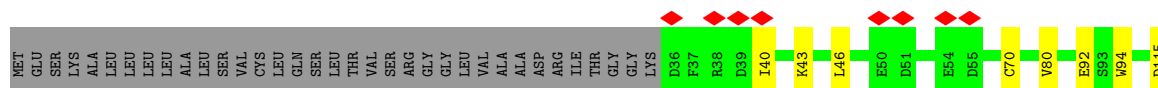
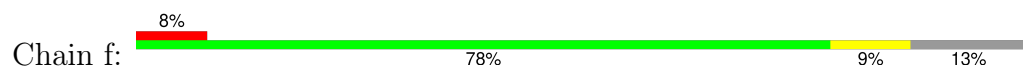
• Molecule 1: Lipoprotein lipase

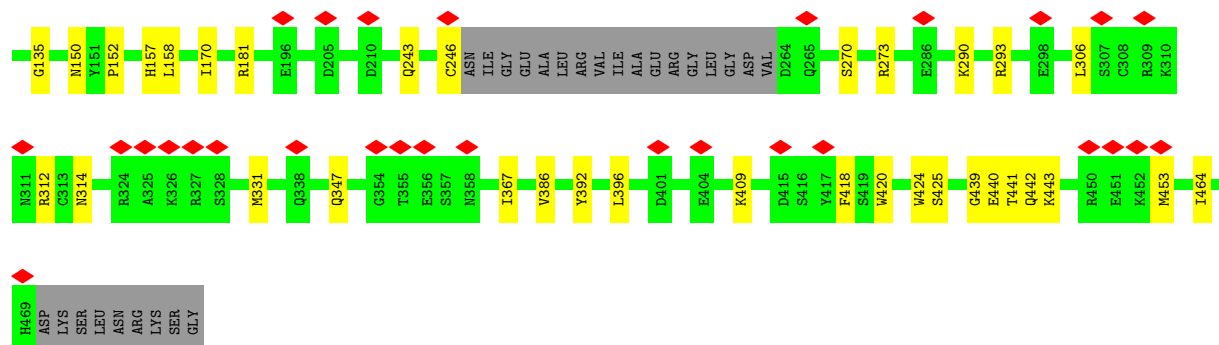


• Molecule 1: Lipoprotein lipase

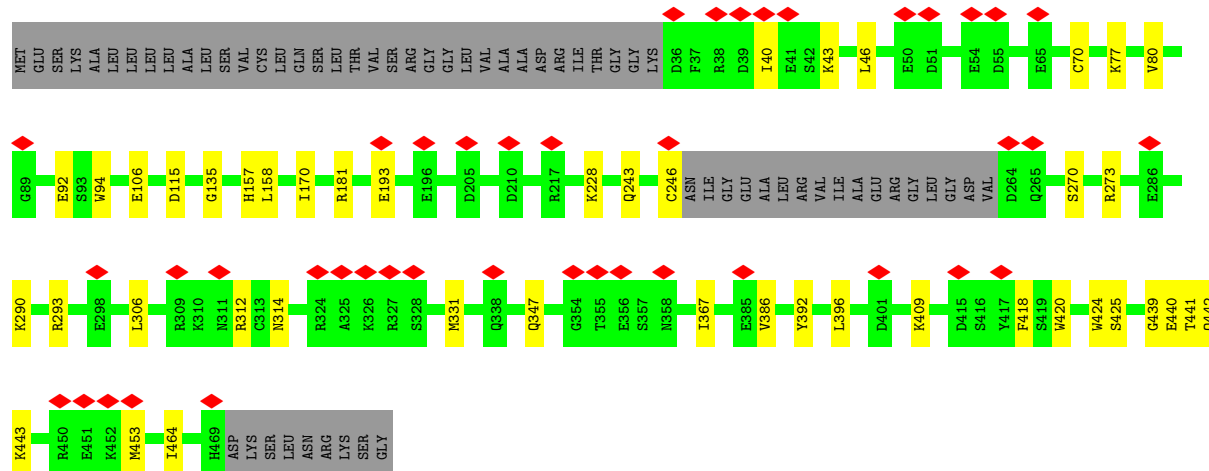
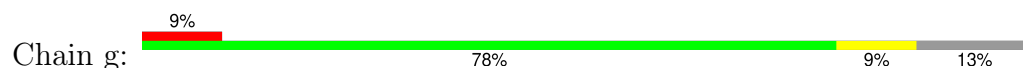


• Molecule 1: Lipoprotein lipase

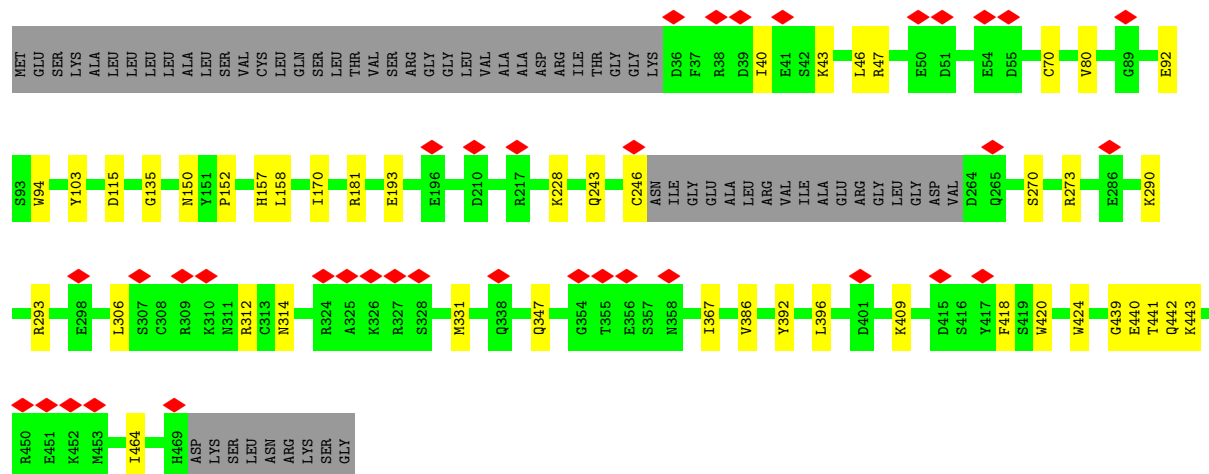
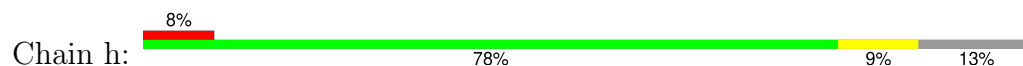




• Molecule 1: Lipoprotein lipase

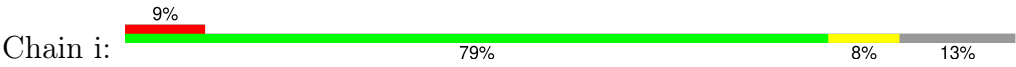


• Molecule 1: Lipoprotein lipase



• Molecule 1: Lipoprotein lipase





MET	GLU	SER	LYS	ALA	LEU	LEU	LEU	ALA	LEU	SER	VAL	CYS	LEU	GLN	SER	LEU	THR	VAL	SER	ARG	GLY	LEU	VAL	ALA	ALA	ASP	ARG	ILE	THR	GLY	LYS	D36	F37	R38	D39	I40	E41	S42	K43	L45	E50	D51	T52	A53	E54	D55	E55	C70	V80	E92
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S93	W94	D115	G135	K140	H157	L158	I170	K177	R181	E193	E196	D205	D210	K228	Q243	C246	ASN	ILE	GLY	ALA	LEU	ARG	VAL	ILE	ALA	GLU	ARG	GLY	LEU	ASP	VAL	D264	Q265	S270	R273	E286	R293	E298
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L306	R309	K310	N311	C313	N314	R324	A325	K326	R327	S328	M331	Q338	Q347	G354	T355	E356	S357	N358	I367	N378	V386	Y392	L396	D401	M407	L408	K409	D415	S416	Y417	F418	S419	W420	W424	G432	G439	E440	T441	Q442	K443
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R450	E451	K452	M453	I464	H469	ASP	LYS	SER	LEU	ASN	ARG	LYS	SER	GLY
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=130.05°, rise=10.88 Å, axial sym=C1	Depositor
Number of segments used	108911	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	46.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	357.7728, 357.7728, 357.7728	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9317, 0.9317, 0.9317	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.19	0/3402	0.47	1/4607 (0.0%)
1	B	0.19	0/3402	0.47	1/4607 (0.0%)
1	C	0.19	0/3402	0.47	1/4607 (0.0%)
1	D	0.19	0/3402	0.47	1/4607 (0.0%)
1	E	0.19	0/3402	0.47	1/4607 (0.0%)
1	F	0.19	0/3402	0.47	1/4607 (0.0%)
1	G	0.19	0/3402	0.47	1/4607 (0.0%)
1	H	0.19	0/3402	0.47	1/4607 (0.0%)
1	I	0.19	0/3402	0.47	1/4607 (0.0%)
1	J	0.19	0/3402	0.47	1/4607 (0.0%)
1	K	0.19	0/3402	0.47	1/4607 (0.0%)
1	L	0.19	0/3402	0.47	1/4607 (0.0%)
1	M	0.19	0/3402	0.47	1/4607 (0.0%)
1	N	0.19	0/3402	0.47	1/4607 (0.0%)
1	O	0.19	0/3402	0.47	1/4607 (0.0%)
1	P	0.19	0/3402	0.47	1/4607 (0.0%)
1	Q	0.19	0/3402	0.47	1/4607 (0.0%)
1	R	0.19	0/3402	0.47	1/4607 (0.0%)
1	S	0.19	0/3402	0.47	1/4607 (0.0%)
1	T	0.19	0/3402	0.47	1/4607 (0.0%)
1	U	0.19	0/3402	0.47	1/4607 (0.0%)
1	a	0.19	0/3402	0.47	1/4607 (0.0%)
1	b	0.19	0/3402	0.47	1/4607 (0.0%)
1	c	0.19	0/3402	0.47	1/4607 (0.0%)
1	d	0.19	0/3402	0.47	1/4607 (0.0%)
1	e	0.19	0/3402	0.47	1/4607 (0.0%)
1	f	0.19	0/3402	0.47	1/4607 (0.0%)
1	g	0.19	0/3402	0.47	1/4607 (0.0%)
1	h	0.19	0/3402	0.47	1/4607 (0.0%)
1	i	0.19	0/3402	0.47	1/4607 (0.0%)
All	All	0.19	0/102060	0.47	30/138210 (0.0%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	424	TRP	CA-CB-CG	5.24	123.55	113.60
1	J	424	TRP	CA-CB-CG	5.24	123.55	113.60
1	L	424	TRP	CA-CB-CG	5.23	123.53	113.60
1	g	424	TRP	CA-CB-CG	5.22	123.53	113.60
1	d	424	TRP	CA-CB-CG	5.22	123.52	113.60
1	G	424	TRP	CA-CB-CG	5.22	123.51	113.60
1	M	424	TRP	CA-CB-CG	5.22	123.51	113.60
1	A	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	D	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	R	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	U	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	S	424	TRP	CA-CB-CG	5.21	123.49	113.60
1	e	424	TRP	CA-CB-CG	5.21	123.49	113.60
1	F	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	I	424	TRP	CA-CB-CG	5.20	123.49	113.60
1	Q	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	a	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	h	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	T	424	TRP	CA-CB-CG	5.20	123.47	113.60
1	c	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	i	424	TRP	CA-CB-CG	5.20	123.47	113.60
1	E	424	TRP	CA-CB-CG	5.20	123.47	113.60
1	N	424	TRP	CA-CB-CG	5.19	123.47	113.60
1	f	424	TRP	CA-CB-CG	5.19	123.47	113.60
1	H	424	TRP	CA-CB-CG	5.19	123.46	113.60
1	C	424	TRP	CA-CB-CG	5.19	123.46	113.60
1	P	424	TRP	CA-CB-CG	5.19	123.46	113.60
1	B	424	TRP	CA-CB-CG	5.18	123.45	113.60
1	K	424	TRP	CA-CB-CG	5.18	123.45	113.60
1	b	424	TRP	CA-CB-CG	5.18	123.44	113.60

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	3314	0	3229	22	0
1	B	3314	0	3229	19	0
1	C	3314	0	3229	18	0
1	D	3314	0	3229	20	0
1	E	3314	0	3229	17	0
1	F	3314	0	3229	19	0
1	G	3314	0	3229	21	0
1	H	3314	0	3229	20	0
1	I	3314	0	3229	20	0
1	J	3314	0	3229	19	0
1	K	3314	0	3229	18	0
1	L	3314	0	3229	17	0
1	M	3314	0	3229	21	0
1	N	3314	0	3229	22	0
1	O	3314	0	3229	19	0
1	P	3314	0	3229	21	0
1	Q	3314	0	3229	18	0
1	R	3314	0	3229	20	0
1	S	3314	0	3229	18	0
1	T	3314	0	3229	22	0
1	U	3314	0	3229	20	0
1	a	3314	0	3229	20	0
1	b	3314	0	3229	24	0
1	c	3314	0	3229	22	0
1	d	3314	0	3229	23	0
1	e	3314	0	3229	20	0
1	f	3314	0	3229	22	0
1	g	3314	0	3229	22	0
1	h	3314	0	3229	22	0
1	i	3314	0	3229	21	0
All	All	99420	0	96870	584	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 3.

All (584) 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:150:ASN:HD22	1:b:152:PRO:HG3	1.57	0.69
1:R:152:PRO:HG3	1:d:150:ASN:HD22	1.59	0.66
1:T:152:PRO:HG3	1:b:150:ASN:HD22	1.63	0.64
1:G:425:SER:HB2	1:a:453:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:150:ASN:HD22	1:f:152:PRO:HG3	1.73	0.54
1:R:150:ASN:HD22	1:d:152:PRO:HG3	1.74	0.53
1:N:152:PRO:HG3	1:h:150:ASN:HD22	1.73	0.53
1:I:439:GLY:O	1:I:442:GLN:NE2	2.42	0.53
1:N:439:GLY:O	1:N:442:GLN:NE2	2.42	0.53
1:O:439:GLY:O	1:O:442:GLN:NE2	2.42	0.53
1:N:150:ASN:HD22	1:h:152:PRO:HG3	1.73	0.53
1:g:439:GLY:O	1:g:442:GLN:NE2	2.42	0.53
1:T:439:GLY:O	1:T:442:GLN:NE2	2.42	0.53
1:f:439:GLY:O	1:f:442:GLN:NE2	2.42	0.53
1:E:439:GLY:O	1:E:442:GLN:NE2	2.42	0.52
1:R:439:GLY:O	1:R:442:GLN:NE2	2.42	0.52
1:S:439:GLY:O	1:S:442:GLN:NE2	2.42	0.52
1:a:439:GLY:O	1:a:442:GLN:NE2	2.42	0.52
1:H:439:GLY:O	1:H:442:GLN:NE2	2.42	0.52
1:J:439:GLY:O	1:J:442:GLN:NE2	2.42	0.52
1:M:439:GLY:O	1:M:442:GLN:NE2	2.42	0.52
1:C:439:GLY:O	1:C:442:GLN:NE2	2.42	0.52
1:G:439:GLY:O	1:G:442:GLN:NE2	2.42	0.52
1:K:439:GLY:O	1:K:442:GLN:NE2	2.42	0.52
1:d:439:GLY:O	1:d:442:GLN:NE2	2.42	0.52
1:A:439:GLY:O	1:A:442:GLN:NE2	2.42	0.52
1:P:439:GLY:O	1:P:442:GLN:NE2	2.42	0.52
1:i:439:GLY:O	1:i:442:GLN:NE2	2.42	0.52
1:D:439:GLY:O	1:D:442:GLN:NE2	2.42	0.52
1:U:439:GLY:O	1:U:442:GLN:NE2	2.42	0.52
1:e:439:GLY:O	1:e:442:GLN:NE2	2.42	0.52
1:F:439:GLY:O	1:F:442:GLN:NE2	2.42	0.52
1:L:439:GLY:O	1:L:442:GLN:NE2	2.42	0.52
1:M:425:SER:HB2	1:f:453:MET:HG2	1.92	0.52
1:c:439:GLY:O	1:c:442:GLN:NE2	2.42	0.52
1:B:439:GLY:O	1:B:442:GLN:NE2	2.42	0.52
1:b:439:GLY:O	1:b:442:GLN:NE2	2.42	0.52
1:h:439:GLY:O	1:h:442:GLN:NE2	2.42	0.52
1:Q:439:GLY:O	1:Q:442:GLN:NE2	2.42	0.52
1:A:425:SER:HB2	1:g:453:MET:HG2	1.92	0.51
1:c:191:ASN:HD22	1:i:450:ARG:NH1	2.08	0.51
1:h:246:CYS:SG	1:h:270:SER:OG	2.67	0.51
1:A:306:LEU:HD12	1:A:347:GLN:HB2	1.93	0.51
1:G:306:LEU:HD12	1:G:347:GLN:HB2	1.93	0.51
1:M:92:GLU:OE1	1:M:94:TRP:NE1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:306:LEU:HD12	1:P:347:GLN:HB2	1.93	0.51
1:e:306:LEU:HD12	1:e:347:GLN:HB2	1.93	0.51
1:e:246:CYS:SG	1:e:270:SER:OG	2.67	0.51
1:f:306:LEU:HD12	1:f:347:GLN:HB2	1.93	0.51
1:D:306:LEU:HD12	1:D:347:GLN:HB2	1.93	0.50
1:J:306:LEU:HD12	1:J:347:GLN:HB2	1.93	0.50
1:S:306:LEU:HD12	1:S:347:GLN:HB2	1.93	0.50
1:f:293:ARG:HD3	1:f:312:ARG:HG2	1.93	0.50
1:M:306:LEU:HD12	1:M:347:GLN:HB2	1.93	0.50
1:O:306:LEU:HD12	1:O:347:GLN:HB2	1.93	0.50
1:P:92:GLU:OE1	1:P:94:TRP:NE1	2.38	0.50
1:P:293:ARG:HD3	1:P:312:ARG:HG2	1.93	0.50
1:U:306:LEU:HD12	1:U:347:GLN:HB2	1.93	0.50
1:b:306:LEU:HD12	1:b:347:GLN:HB2	1.93	0.50
1:d:306:LEU:HD12	1:d:347:GLN:HB2	1.93	0.50
1:E:92:GLU:OE1	1:E:94:TRP:NE1	2.38	0.50
1:S:293:ARG:HD3	1:S:312:ARG:HG2	1.93	0.50
1:I:92:GLU:OE1	1:I:94:TRP:NE1	2.38	0.50
1:a:306:LEU:HD12	1:a:347:GLN:HB2	1.93	0.50
1:A:293:ARG:HD3	1:A:312:ARG:HG2	1.93	0.50
1:B:293:ARG:HD3	1:B:312:ARG:HG2	1.93	0.50
1:F:306:LEU:HD12	1:F:347:GLN:HB2	1.93	0.50
1:Q:306:LEU:HD12	1:Q:347:GLN:HB2	1.93	0.50
1:c:293:ARG:HD3	1:c:312:ARG:HG2	1.93	0.50
1:c:306:LEU:HD12	1:c:347:GLN:HB2	1.93	0.50
1:h:306:LEU:HD12	1:h:347:GLN:HB2	1.93	0.50
1:A:453:MET:HG2	1:g:425:SER:HB2	1.92	0.50
1:C:293:ARG:HD3	1:C:312:ARG:HG2	1.93	0.50
1:G:293:ARG:HD3	1:G:312:ARG:HG2	1.93	0.50
1:I:306:LEU:HD12	1:I:347:GLN:HB2	1.93	0.50
1:R:306:LEU:HD12	1:R:347:GLN:HB2	1.93	0.50
1:C:306:LEU:HD12	1:C:347:GLN:HB2	1.93	0.50
1:E:293:ARG:HD3	1:E:312:ARG:HG2	1.93	0.50
1:D:293:ARG:HD3	1:D:312:ARG:HG2	1.93	0.50
1:J:293:ARG:HD3	1:J:312:ARG:HG2	1.93	0.50
1:i:293:ARG:HD3	1:i:312:ARG:HG2	1.93	0.50
1:H:293:ARG:HD3	1:H:312:ARG:HG2	1.93	0.49
1:L:306:LEU:HD12	1:L:347:GLN:HB2	1.93	0.49
1:N:193:GLU:OE2	1:N:228:LYS:NZ	2.44	0.49
1:R:293:ARG:HD3	1:R:312:ARG:HG2	1.93	0.49
1:T:306:LEU:HD12	1:T:347:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:293:ARG:HD3	1:d:312:ARG:HG2	1.93	0.49
1:K:293:ARG:HD3	1:K:312:ARG:HG2	1.93	0.49
1:b:293:ARG:HD3	1:b:312:ARG:HG2	1.93	0.49
1:K:306:LEU:HD12	1:K:347:GLN:HB2	1.93	0.49
1:L:293:ARG:HD3	1:L:312:ARG:HG2	1.93	0.49
1:T:293:ARG:HD3	1:T:312:ARG:HG2	1.93	0.49
1:U:293:ARG:HD3	1:U:312:ARG:HG2	1.93	0.49
1:i:306:LEU:HD12	1:i:347:GLN:HB2	1.93	0.49
1:G:92:GLU:OE1	1:G:94:TRP:NE1	2.38	0.49
1:H:306:LEU:HD12	1:H:347:GLN:HB2	1.93	0.49
1:M:293:ARG:HD3	1:M:312:ARG:HG2	1.93	0.49
1:N:306:LEU:HD12	1:N:347:GLN:HB2	1.93	0.49
1:O:293:ARG:HD3	1:O:312:ARG:HG2	1.93	0.49
1:a:293:ARG:HD3	1:a:312:ARG:HG2	1.93	0.49
1:g:306:LEU:HD12	1:g:347:GLN:HB2	1.93	0.49
1:G:453:MET:HG2	1:a:425:SER:HB2	1.92	0.49
1:I:193:GLU:OE2	1:I:228:LYS:NZ	2.44	0.49
1:N:293:ARG:HD3	1:N:312:ARG:HG2	1.93	0.49
1:g:293:ARG:HD3	1:g:312:ARG:HG2	1.93	0.49
1:I:293:ARG:HD3	1:I:312:ARG:HG2	1.93	0.49
1:T:193:GLU:OE2	1:T:228:LYS:NZ	2.44	0.49
1:h:293:ARG:HD3	1:h:312:ARG:HG2	1.93	0.49
1:B:306:LEU:HD12	1:B:347:GLN:HB2	1.93	0.49
1:D:193:GLU:OE2	1:D:228:LYS:NZ	2.45	0.49
1:E:306:LEU:HD12	1:E:347:GLN:HB2	1.93	0.49
1:Q:293:ARG:HD3	1:Q:312:ARG:HG2	1.93	0.49
1:T:92:GLU:OE1	1:T:94:TRP:NE1	2.38	0.49
1:h:193:GLU:OE2	1:h:228:LYS:NZ	2.44	0.49
1:E:193:GLU:OE2	1:E:228:LYS:NZ	2.44	0.49
1:e:293:ARG:HD3	1:e:312:ARG:HG2	1.93	0.49
1:F:293:ARG:HD3	1:F:312:ARG:HG2	1.93	0.48
1:J:193:GLU:OE2	1:J:228:LYS:NZ	2.45	0.48
1:c:92:GLU:OE1	1:c:94:TRP:NE1	2.38	0.48
1:M:193:GLU:OE2	1:M:228:LYS:NZ	2.45	0.48
1:i:193:GLU:OE2	1:i:228:LYS:NZ	2.44	0.48
1:K:193:GLU:OE2	1:K:228:LYS:NZ	2.44	0.48
1:P:193:GLU:OE2	1:P:228:LYS:NZ	2.44	0.48
1:c:157:HIS:CE1	1:c:181:ARG:HD3	2.49	0.48
1:g:92:GLU:OE1	1:g:94:TRP:NE1	2.38	0.48
1:i:157:HIS:CE1	1:i:181:ARG:HD3	2.49	0.48
1:A:92:GLU:OE1	1:A:94:TRP:NE1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:HIS:CE1	1:F:181:ARG:HD3	2.49	0.48
1:L:157:HIS:CE1	1:L:181:ARG:HD3	2.49	0.48
1:P:157:HIS:CE1	1:P:181:ARG:HD3	2.49	0.48
1:R:157:HIS:CE1	1:R:181:ARG:HD3	2.49	0.48
1:F:246:CYS:SG	1:F:270:SER:OG	2.67	0.47
1:G:193:GLU:OE2	1:G:228:LYS:NZ	2.44	0.47
1:e:92:GLU:OE1	1:e:94:TRP:NE1	2.38	0.47
1:A:157:HIS:CE1	1:A:181:ARG:HD3	2.49	0.47
1:E:157:HIS:CE1	1:E:181:ARG:HD3	2.49	0.47
1:K:157:HIS:CE1	1:K:181:ARG:HD3	2.49	0.47
1:Q:157:HIS:CE1	1:Q:181:ARG:HD3	2.49	0.47
1:Q:246:CYS:SG	1:Q:270:SER:OG	2.67	0.47
1:d:157:HIS:CE1	1:d:181:ARG:HD3	2.49	0.47
1:e:157:HIS:CE1	1:e:181:ARG:HD3	2.49	0.47
1:B:157:HIS:CE1	1:B:181:ARG:HD3	2.49	0.47
1:D:77:LYS:NZ	1:D:106:GLU:OE1	2.39	0.47
1:J:157:HIS:CE1	1:J:181:ARG:HD3	2.49	0.47
1:U:157:HIS:CE1	1:U:181:ARG:HD3	2.49	0.47
1:i:92:GLU:OE1	1:i:94:TRP:NE1	2.38	0.47
1:G:157:HIS:CE1	1:G:181:ARG:HD3	2.49	0.47
1:b:157:HIS:CE1	1:b:181:ARG:HD3	2.49	0.47
1:h:157:HIS:CE1	1:h:181:ARG:HD3	2.49	0.47
1:T:157:HIS:CE1	1:T:181:ARG:HD3	2.49	0.47
1:g:157:HIS:CE1	1:g:181:ARG:HD3	2.49	0.47
1:B:92:GLU:OE1	1:B:94:TRP:NE1	2.38	0.47
1:C:92:GLU:OE1	1:C:94:TRP:NE1	2.38	0.47
1:H:157:HIS:CE1	1:H:181:ARG:HD3	2.49	0.47
1:N:157:HIS:CE1	1:N:181:ARG:HD3	2.49	0.47
1:O:157:HIS:CE1	1:O:181:ARG:HD3	2.49	0.47
1:a:193:GLU:OE2	1:a:228:LYS:NZ	2.45	0.47
1:e:193:GLU:OE2	1:e:228:LYS:NZ	2.44	0.47
1:A:193:GLU:OE2	1:A:228:LYS:NZ	2.45	0.47
1:D:157:HIS:CE1	1:D:181:ARG:HD3	2.49	0.47
1:L:193:GLU:OE2	1:L:228:LYS:NZ	2.44	0.47
1:a:157:HIS:CE1	1:a:181:ARG:HD3	2.49	0.47
1:I:246:CYS:SG	1:I:270:SER:OG	2.67	0.47
1:N:246:CYS:SG	1:N:270:SER:OG	2.67	0.47
1:g:246:CYS:SG	1:g:270:SER:OG	2.67	0.47
1:T:246:CYS:SG	1:T:270:SER:OG	2.67	0.47
1:I:453:MET:HG2	1:b:425:SER:HB2	1.96	0.46
1:F:193:GLU:OE2	1:F:228:LYS:NZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:191:ASN:HD22	1:i:450:ARG:HH12	1.63	0.46
1:f:157:HIS:CE1	1:f:181:ARG:HD3	2.49	0.46
1:C:246:CYS:SG	1:C:270:SER:OG	2.67	0.46
1:M:157:HIS:CE1	1:M:181:ARG:HD3	2.49	0.46
1:S:157:HIS:CE1	1:S:181:ARG:HD3	2.49	0.46
1:C:157:HIS:CE1	1:C:181:ARG:HD3	2.49	0.46
1:Q:193:GLU:OE2	1:Q:228:LYS:NZ	2.45	0.46
1:b:193:GLU:OE2	1:b:228:LYS:NZ	2.45	0.46
1:I:157:HIS:CE1	1:I:181:ARG:HD3	2.49	0.46
1:M:453:MET:HG2	1:f:425:SER:HB2	1.96	0.46
1:a:246:CYS:SG	1:a:270:SER:OG	2.67	0.46
1:O:246:CYS:SG	1:O:270:SER:OG	2.67	0.46
1:U:92:GLU:OE1	1:U:94:TRP:NE1	2.38	0.46
1:b:92:GLU:OE1	1:b:94:TRP:NE1	2.38	0.46
1:F:92:GLU:OE1	1:F:94:TRP:NE1	2.38	0.46
1:A:246:CYS:SG	1:A:270:SER:OG	2.67	0.45
1:Q:135:GLY:HA3	1:Q:170:ILE:HG23	1.98	0.45
1:d:92:GLU:OE1	1:d:94:TRP:NE1	2.38	0.45
1:H:246:CYS:SG	1:H:270:SER:OG	2.67	0.45
1:h:135:GLY:HA3	1:h:170:ILE:HG23	1.98	0.45
1:K:135:GLY:HA3	1:K:170:ILE:HG23	1.98	0.45
1:b:135:GLY:HA3	1:b:170:ILE:HG23	1.98	0.45
1:i:135:GLY:HA3	1:i:170:ILE:HG23	1.98	0.45
1:I:135:GLY:HA3	1:I:170:ILE:HG23	1.98	0.45
1:T:135:GLY:HA3	1:T:170:ILE:HG23	1.98	0.45
1:U:246:CYS:SG	1:U:270:SER:OG	2.67	0.45
1:d:246:CYS:SG	1:d:270:SER:OG	2.67	0.45
1:F:135:GLY:HA3	1:F:170:ILE:HG23	1.98	0.45
1:O:135:GLY:HA3	1:O:170:ILE:HG23	1.98	0.45
1:A:135:GLY:HA3	1:A:170:ILE:HG23	1.98	0.45
1:H:92:GLU:OE1	1:H:94:TRP:NE1	2.38	0.45
1:L:135:GLY:HA3	1:L:170:ILE:HG23	1.98	0.45
1:P:135:GLY:HA3	1:P:170:ILE:HG23	1.98	0.45
1:c:464:ILE:HD13	1:d:125:PRO:HB2	1.99	0.45
1:E:135:GLY:HA3	1:E:170:ILE:HG23	1.98	0.45
1:N:135:GLY:HA3	1:N:170:ILE:HG23	1.98	0.45
1:R:135:GLY:HA3	1:R:170:ILE:HG23	1.98	0.45
1:e:135:GLY:HA3	1:e:170:ILE:HG23	1.98	0.45
1:C:135:GLY:HA3	1:C:170:ILE:HG23	1.98	0.45
1:G:135:GLY:HA3	1:G:170:ILE:HG23	1.98	0.45
1:c:135:GLY:HA3	1:c:170:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:CYS:SG	1:B:270:SER:OG	2.67	0.45
1:a:135:GLY:HA3	1:a:170:ILE:HG23	1.98	0.45
1:F:43:LYS:NZ	1:F:115:ASP:OD2	2.51	0.45
1:I:425:SER:HB2	1:b:453:MET:HG2	1.98	0.45
1:S:135:GLY:HA3	1:S:170:ILE:HG23	1.98	0.45
1:b:246:CYS:SG	1:b:270:SER:OG	2.67	0.45
1:K:43:LYS:NZ	1:K:115:ASP:OD2	2.51	0.44
1:P:246:CYS:SG	1:P:270:SER:OG	2.67	0.44
1:T:43:LYS:NZ	1:T:115:ASP:OD2	2.51	0.44
1:U:135:GLY:HA3	1:U:170:ILE:HG23	1.98	0.44
1:b:43:LYS:NZ	1:b:115:ASP:OD2	2.51	0.44
1:c:43:LYS:NZ	1:c:115:ASP:OD2	2.51	0.44
1:d:135:GLY:HA3	1:d:170:ILE:HG23	1.98	0.44
1:A:450:ARG:NH1	1:F:191:ASN:HD22	2.15	0.44
1:B:43:LYS:NZ	1:B:115:ASP:OD2	2.50	0.44
1:B:193:GLU:OE2	1:B:228:LYS:NZ	2.45	0.44
1:D:43:LYS:NZ	1:D:115:ASP:OD2	2.51	0.44
1:G:43:LYS:NZ	1:G:115:ASP:OD2	2.51	0.44
1:I:43:LYS:NZ	1:I:115:ASP:OD2	2.50	0.44
1:M:135:GLY:HA3	1:M:170:ILE:HG23	1.98	0.44
1:R:43:LYS:NZ	1:R:115:ASP:OD2	2.51	0.44
1:f:135:GLY:HA3	1:f:170:ILE:HG23	1.98	0.44
1:H:43:LYS:NZ	1:H:115:ASP:OD2	2.51	0.44
1:a:43:LYS:NZ	1:a:115:ASP:OD2	2.51	0.44
1:a:92:GLU:OE1	1:a:94:TRP:NE1	2.38	0.44
1:B:135:GLY:HA3	1:B:170:ILE:HG23	1.98	0.44
1:D:243:GLN:HG3	1:D:273:ARG:HG3	2.00	0.44
1:E:409:LYS:HG2	1:E:464:ILE:HG12	2.00	0.44
1:J:135:GLY:HA3	1:J:170:ILE:HG23	1.98	0.44
1:O:409:LYS:HG2	1:O:464:ILE:HG12	2.00	0.44
1:g:135:GLY:HA3	1:g:170:ILE:HG23	1.98	0.44
1:G:418:PHE:HB3	1:G:420:TRP:HE3	1.83	0.44
1:J:43:LYS:NZ	1:J:115:ASP:OD2	2.51	0.44
1:O:43:LYS:NZ	1:O:115:ASP:OD2	2.51	0.44
1:O:386:VAL:HA	1:O:392:TYR:HE2	1.83	0.44
1:P:418:PHE:HB3	1:P:420:TRP:HE3	1.83	0.44
1:c:409:LYS:HG2	1:c:464:ILE:HG12	2.00	0.44
1:f:43:LYS:NZ	1:f:115:ASP:OD2	2.51	0.44
1:i:409:LYS:HG2	1:i:464:ILE:HG12	2.00	0.44
1:D:135:GLY:HA3	1:D:170:ILE:HG23	1.98	0.44
1:G:246:CYS:SG	1:G:270:SER:OG	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:GLN:HG3	1:H:273:ARG:HG3	2.00	0.44
1:M:43:LYS:NZ	1:M:115:ASP:OD2	2.51	0.44
1:N:386:VAL:HA	1:N:392:TYR:HE2	1.83	0.44
1:O:243:GLN:HG3	1:O:273:ARG:HG3	2.00	0.44
1:S:43:LYS:NZ	1:S:115:ASP:OD2	2.51	0.44
1:T:243:GLN:HG3	1:T:273:ARG:HG3	2.00	0.44
1:U:43:LYS:NZ	1:U:115:ASP:OD2	2.51	0.44
1:c:193:GLU:OE2	1:c:228:LYS:NZ	2.44	0.44
1:f:418:PHE:HB3	1:f:420:TRP:HE3	1.83	0.44
1:g:43:LYS:NZ	1:g:115:ASP:OD2	2.50	0.44
1:g:243:GLN:HG3	1:g:273:ARG:HG3	2.00	0.44
1:i:386:VAL:HA	1:i:392:TYR:HE2	1.83	0.44
1:B:409:LYS:HG2	1:B:464:ILE:HG12	2.00	0.44
1:E:386:VAL:HA	1:E:392:TYR:HE2	1.83	0.44
1:H:135:GLY:HA3	1:H:170:ILE:HG23	1.98	0.44
1:I:243:GLN:HG3	1:I:273:ARG:HG3	2.00	0.44
1:I:409:LYS:HG2	1:I:464:ILE:HG12	2.00	0.44
1:L:386:VAL:HA	1:L:392:TYR:HE2	1.83	0.44
1:M:243:GLN:HG3	1:M:273:ARG:HG3	2.00	0.44
1:N:409:LYS:HG2	1:N:464:ILE:HG12	2.00	0.44
1:P:43:LYS:NZ	1:P:115:ASP:OD2	2.51	0.44
1:Q:386:VAL:HA	1:Q:392:TYR:HE2	1.83	0.44
1:S:418:PHE:HB3	1:S:420:TRP:HE3	1.83	0.44
1:d:43:LYS:NZ	1:d:115:ASP:OD2	2.51	0.44
1:C:43:LYS:NZ	1:C:115:ASP:OD2	2.51	0.44
1:H:409:LYS:HG2	1:H:464:ILE:HG12	2.00	0.44
1:R:409:LYS:HG2	1:R:464:ILE:HG12	2.00	0.44
1:h:386:VAL:HA	1:h:392:TYR:HE2	1.83	0.44
1:C:409:LYS:HG2	1:C:464:ILE:HG12	2.00	0.44
1:K:409:LYS:HG2	1:K:464:ILE:HG12	2.00	0.44
1:L:409:LYS:HG2	1:L:464:ILE:HG12	2.00	0.44
1:O:92:GLU:OE1	1:O:94:TRP:NE1	2.38	0.44
1:T:409:LYS:HG2	1:T:464:ILE:HG12	2.00	0.44
1:T:418:PHE:HB3	1:T:420:TRP:HE3	1.83	0.44
1:a:243:GLN:HG3	1:a:273:ARG:HG3	2.00	0.44
1:a:386:VAL:HA	1:a:392:TYR:HE2	1.83	0.44
1:g:409:LYS:HG2	1:g:464:ILE:HG12	2.00	0.44
1:B:243:GLN:HG3	1:B:273:ARG:HG3	2.00	0.43
1:B:386:VAL:HA	1:B:392:TYR:HE2	1.83	0.43
1:F:409:LYS:HG2	1:F:464:ILE:HG12	2.00	0.43
1:N:43:LYS:NZ	1:N:115:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:409:LYS:HG2	1:U:464:ILE:HG12	2.00	0.43
1:c:243:GLN:HG3	1:c:273:ARG:HG3	2.00	0.43
1:d:409:LYS:HG2	1:d:464:ILE:HG12	2.00	0.43
1:h:43:LYS:NZ	1:h:115:ASP:OD2	2.51	0.43
1:E:43:LYS:NZ	1:E:115:ASP:OD2	2.51	0.43
1:Q:43:LYS:NZ	1:Q:115:ASP:OD2	2.51	0.43
1:S:243:GLN:HG3	1:S:273:ARG:HG3	2.00	0.43
1:e:418:PHE:HB3	1:e:420:TRP:HE3	1.83	0.43
1:g:386:VAL:HA	1:g:392:TYR:HE2	1.83	0.43
1:i:43:LYS:NZ	1:i:115:ASP:OD2	2.51	0.43
1:A:43:LYS:NZ	1:A:115:ASP:OD2	2.51	0.43
1:C:386:VAL:HA	1:C:392:TYR:HE2	1.83	0.43
1:C:418:PHE:HB3	1:C:420:TRP:HE3	1.83	0.43
1:D:92:GLU:OE1	1:D:94:TRP:NE1	2.38	0.43
1:D:386:VAL:HA	1:D:392:TYR:HE2	1.83	0.43
1:D:418:PHE:HB3	1:D:420:TRP:HE3	1.83	0.43
1:J:246:CYS:SG	1:J:270:SER:OG	2.67	0.43
1:J:418:PHE:HB3	1:J:420:TRP:HE3	1.83	0.43
1:P:386:VAL:HA	1:P:392:TYR:HE2	1.83	0.43
1:Q:92:GLU:OE1	1:Q:94:TRP:NE1	2.38	0.43
1:b:418:PHE:HB3	1:b:420:TRP:HE3	1.83	0.43
1:f:243:GLN:HG3	1:f:273:ARG:HG3	2.00	0.43
1:F:418:PHE:HB3	1:F:420:TRP:HE3	1.83	0.43
1:H:193:GLU:OE2	1:H:228:LYS:NZ	2.45	0.43
1:I:386:VAL:HA	1:I:392:TYR:HE2	1.83	0.43
1:J:243:GLN:HG3	1:J:273:ARG:HG3	2.00	0.43
1:K:243:GLN:HG3	1:K:273:ARG:HG3	2.00	0.43
1:L:43:LYS:NZ	1:L:115:ASP:OD2	2.50	0.43
1:O:191:ASN:HD22	1:U:450:ARG:NH1	2.15	0.43
1:Q:409:LYS:HG2	1:Q:464:ILE:HG12	2.00	0.43
1:R:418:PHE:HB3	1:R:420:TRP:HE3	1.83	0.43
1:U:193:GLU:OE2	1:U:228:LYS:NZ	2.45	0.43
1:c:386:VAL:HA	1:c:392:TYR:HE2	1.83	0.43
1:e:43:LYS:NZ	1:e:115:ASP:OD2	2.51	0.43
1:e:243:GLN:HG3	1:e:273:ARG:HG3	2.00	0.43
1:g:418:PHE:HB3	1:g:420:TRP:HE3	1.83	0.43
1:J:386:VAL:HA	1:J:392:TYR:HE2	1.83	0.43
1:M:386:VAL:HA	1:M:392:TYR:HE2	1.83	0.43
1:T:386:VAL:HA	1:T:392:TYR:HE2	1.83	0.43
1:c:246:CYS:SG	1:c:270:SER:OG	2.67	0.43
1:h:409:LYS:HG2	1:h:464:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:418:PHE:HB3	1:i:420:TRP:HE3	1.83	0.43
1:A:386:VAL:HA	1:A:392:TYR:HE2	1.83	0.43
1:A:409:LYS:HG2	1:A:464:ILE:HG12	2.00	0.43
1:B:418:PHE:HB3	1:B:420:TRP:HE3	1.83	0.43
1:H:418:PHE:HB3	1:H:420:TRP:HE3	1.83	0.43
1:a:409:LYS:HG2	1:a:464:ILE:HG12	2.00	0.43
1:b:409:LYS:HG2	1:b:464:ILE:HG12	2.00	0.43
1:d:386:VAL:HA	1:d:392:TYR:HE2	1.83	0.43
1:e:386:VAL:HA	1:e:392:TYR:HE2	1.83	0.43
1:C:243:GLN:HG3	1:C:273:ARG:HG3	2.00	0.43
1:D:409:LYS:HG2	1:D:464:ILE:HG12	2.00	0.43
1:E:246:CYS:SG	1:E:270:SER:OG	2.67	0.43
1:F:243:GLN:HG3	1:F:273:ARG:HG3	2.00	0.43
1:H:386:VAL:HA	1:H:392:TYR:HE2	1.83	0.43
1:P:243:GLN:HG3	1:P:273:ARG:HG3	2.00	0.43
1:R:243:GLN:HG3	1:R:273:ARG:HG3	2.00	0.43
1:S:386:VAL:HA	1:S:392:TYR:HE2	1.83	0.43
1:S:409:LYS:HG2	1:S:464:ILE:HG12	2.00	0.43
1:T:314:ASN:HD22	1:T:331:MET:HE1	1.84	0.43
1:U:386:VAL:HA	1:U:392:TYR:HE2	1.83	0.43
1:c:418:PHE:HB3	1:c:420:TRP:HE3	1.83	0.43
1:i:243:GLN:HG3	1:i:273:ARG:HG3	2.00	0.43
1:D:246:CYS:SG	1:D:270:SER:OG	2.67	0.43
1:G:386:VAL:HA	1:G:392:TYR:HE2	1.83	0.43
1:I:314:ASN:HD22	1:I:331:MET:HE1	1.84	0.43
1:L:314:ASN:HD22	1:L:331:MET:HE1	1.84	0.43
1:P:314:ASN:HD22	1:P:331:MET:HE1	1.84	0.43
1:Q:243:GLN:HG3	1:Q:273:ARG:HG3	2.00	0.43
1:a:314:ASN:HD22	1:a:331:MET:HE1	1.84	0.43
1:e:409:LYS:HG2	1:e:464:ILE:HG12	2.00	0.43
1:f:386:VAL:HA	1:f:392:TYR:HE2	1.83	0.43
1:D:314:ASN:HD22	1:D:331:MET:HE1	1.84	0.43
1:E:243:GLN:HG3	1:E:273:ARG:HG3	2.00	0.43
1:G:409:LYS:HG2	1:G:464:ILE:HG12	2.00	0.43
1:M:246:CYS:SG	1:M:270:SER:OG	2.67	0.43
1:M:314:ASN:HD22	1:M:331:MET:HE1	1.84	0.43
1:M:409:LYS:HG2	1:M:464:ILE:HG12	2.00	0.43
1:P:80:VAL:HB	1:P:158:LEU:HD23	2.01	0.43
1:Q:418:PHE:HB3	1:Q:420:TRP:HE3	1.83	0.43
1:R:386:VAL:HA	1:R:392:TYR:HE2	1.83	0.43
1:c:80:VAL:HB	1:c:158:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:193:GLU:OE2	1:d:228:LYS:NZ	2.45	0.43
1:f:409:LYS:HG2	1:f:464:ILE:HG12	2.00	0.43
1:h:92:GLU:OE1	1:h:94:TRP:NE1	2.38	0.43
1:i:314:ASN:HD22	1:i:331:MET:HE1	1.84	0.43
1:E:314:ASN:HD22	1:E:331:MET:HE1	1.84	0.43
1:F:386:VAL:HA	1:F:392:TYR:HE2	1.83	0.43
1:L:80:VAL:HB	1:L:158:LEU:HD23	2.01	0.43
1:L:418:PHE:HB3	1:L:420:TRP:HE3	1.83	0.43
1:N:243:GLN:HG3	1:N:273:ARG:HG3	2.00	0.43
1:N:418:PHE:HB3	1:N:420:TRP:HE3	1.83	0.43
1:Q:314:ASN:HD22	1:Q:331:MET:HE1	1.84	0.43
1:a:418:PHE:HB3	1:a:420:TRP:HE3	1.83	0.43
1:e:80:VAL:HB	1:e:158:LEU:HD23	2.01	0.43
1:h:314:ASN:HD22	1:h:331:MET:HE1	1.84	0.43
1:A:243:GLN:HG3	1:A:273:ARG:HG3	2.00	0.42
1:E:80:VAL:HB	1:E:158:LEU:HD23	2.01	0.42
1:G:243:GLN:HG3	1:G:273:ARG:HG3	2.00	0.42
1:K:80:VAL:HB	1:K:158:LEU:HD23	2.01	0.42
1:P:152:PRO:HG3	1:f:150:ASN:HD22	1.84	0.42
1:P:409:LYS:HG2	1:P:464:ILE:HG12	2.00	0.42
1:b:80:VAL:HB	1:b:158:LEU:HD23	2.01	0.42
1:d:243:GLN:HG3	1:d:273:ARG:HG3	2.00	0.42
1:h:243:GLN:HG3	1:h:273:ARG:HG3	2.00	0.42
1:h:418:PHE:HB3	1:h:420:TRP:HE3	1.83	0.42
1:i:80:VAL:HB	1:i:158:LEU:HD23	2.01	0.42
1:A:80:VAL:HB	1:A:158:LEU:HD23	2.01	0.42
1:B:80:VAL:HB	1:B:158:LEU:HD23	2.01	0.42
1:F:80:VAL:HB	1:F:158:LEU:HD23	2.01	0.42
1:H:314:ASN:HD22	1:H:331:MET:HE1	1.84	0.42
1:J:80:VAL:HB	1:J:158:LEU:HD23	2.01	0.42
1:J:409:LYS:HG2	1:J:464:ILE:HG12	2.00	0.42
1:K:386:VAL:HA	1:K:392:TYR:HE2	1.83	0.42
1:O:418:PHE:HB3	1:O:420:TRP:HE3	1.83	0.42
1:R:80:VAL:HB	1:R:158:LEU:HD23	2.01	0.42
1:U:243:GLN:HG3	1:U:273:ARG:HG3	2.00	0.42
1:e:314:ASN:HD22	1:e:331:MET:HE1	1.84	0.42
1:E:418:PHE:HB3	1:E:420:TRP:HE3	1.83	0.42
1:F:314:ASN:HD22	1:F:331:MET:HE1	1.84	0.42
1:G:80:VAL:HB	1:G:158:LEU:HD23	2.01	0.42
1:G:314:ASN:HD22	1:G:331:MET:HE1	1.84	0.42
1:I:418:PHE:HB3	1:I:420:TRP:HE3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:GLN:HG3	1:L:273:ARG:HG3	2.00	0.42
1:U:314:ASN:HD22	1:U:331:MET:HE1	1.84	0.42
1:b:314:ASN:HD22	1:b:331:MET:HE1	1.84	0.42
1:A:418:PHE:HB3	1:A:420:TRP:HE3	1.83	0.42
1:B:314:ASN:HD22	1:B:331:MET:HE1	1.84	0.42
1:H:80:VAL:HB	1:H:158:LEU:HD23	2.01	0.42
1:M:418:PHE:HB3	1:M:420:TRP:HE3	1.83	0.42
1:O:367:ILE:HG21	1:O:396:LEU:HD11	2.02	0.42
1:Q:80:VAL:HB	1:Q:158:LEU:HD23	2.01	0.42
1:S:80:VAL:HB	1:S:158:LEU:HD23	2.01	0.42
1:S:246:CYS:SG	1:S:270:SER:OG	2.67	0.42
1:b:367:ILE:HG21	1:b:396:LEU:HD11	2.02	0.42
1:c:314:ASN:HD22	1:c:331:MET:HE1	1.84	0.42
1:d:314:ASN:HD22	1:d:331:MET:HE1	1.84	0.42
1:f:80:VAL:HB	1:f:158:LEU:HD23	2.01	0.42
1:f:246:CYS:SG	1:f:270:SER:OG	2.67	0.42
1:A:367:ILE:HG21	1:A:396:LEU:HD11	2.02	0.42
1:D:80:VAL:HB	1:D:158:LEU:HD23	2.01	0.42
1:I:367:ILE:HG21	1:I:396:LEU:HD11	2.02	0.42
1:K:418:PHE:HB3	1:K:420:TRP:HE3	1.83	0.42
1:M:80:VAL:HB	1:M:158:LEU:HD23	2.01	0.42
1:M:367:ILE:HG21	1:M:396:LEU:HD11	2.02	0.42
1:S:367:ILE:HG21	1:S:396:LEU:HD11	2.02	0.42
1:U:80:VAL:HB	1:U:158:LEU:HD23	2.01	0.42
1:U:418:PHE:HB3	1:U:420:TRP:HE3	1.83	0.42
1:a:367:ILE:HG21	1:a:396:LEU:HD11	2.02	0.42
1:b:386:VAL:HA	1:b:392:TYR:HE2	1.83	0.42
1:d:418:PHE:HB3	1:d:420:TRP:HE3	1.83	0.42
1:e:367:ILE:HG21	1:e:396:LEU:HD11	2.02	0.42
1:f:367:ILE:HG21	1:f:396:LEU:HD11	2.02	0.42
1:g:367:ILE:HG21	1:g:396:LEU:HD11	2.02	0.42
1:h:80:VAL:HB	1:h:158:LEU:HD23	2.01	0.42
1:A:46:LEU:HD23	1:A:70:CYS:HB3	2.02	0.42
1:A:314:ASN:HD22	1:A:331:MET:HE1	1.84	0.42
1:G:367:ILE:HG21	1:G:396:LEU:HD11	2.02	0.42
1:L:92:GLU:OE1	1:L:94:TRP:NE1	2.38	0.42
1:O:314:ASN:HD22	1:O:331:MET:HE1	1.84	0.42
1:R:246:CYS:SG	1:R:270:SER:OG	2.67	0.42
1:b:243:GLN:HG3	1:b:273:ARG:HG3	2.00	0.42
1:d:80:VAL:HB	1:d:158:LEU:HD23	2.01	0.42
1:F:367:ILE:HG21	1:F:396:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:LEU:HD23	1:J:70:CYS:HB3	2.02	0.42
1:J:314:ASN:HD22	1:J:331:MET:HE1	1.84	0.42
1:L:367:ILE:HG21	1:L:396:LEU:HD11	2.02	0.42
1:N:80:VAL:HB	1:N:158:LEU:HD23	2.01	0.42
1:N:314:ASN:HD22	1:N:331:MET:HE1	1.84	0.42
1:T:80:VAL:HB	1:T:158:LEU:HD23	2.01	0.42
1:a:80:VAL:HB	1:a:158:LEU:HD23	2.01	0.42
1:g:80:VAL:HB	1:g:158:LEU:HD23	2.01	0.42
1:h:367:ILE:HG21	1:h:396:LEU:HD11	2.02	0.42
1:C:80:VAL:HB	1:C:158:LEU:HD23	2.01	0.42
1:G:46:LEU:HD23	1:G:70:CYS:HB3	2.02	0.42
1:K:314:ASN:HD22	1:K:331:MET:HE1	1.84	0.42
1:Q:367:ILE:HG21	1:Q:396:LEU:HD11	2.02	0.42
1:R:367:ILE:HG21	1:R:396:LEU:HD11	2.02	0.42
1:U:367:ILE:HG21	1:U:396:LEU:HD11	2.02	0.42
1:d:367:ILE:HG21	1:d:396:LEU:HD11	2.02	0.42
1:e:46:LEU:HD23	1:e:70:CYS:HB3	2.02	0.42
1:C:47:ARG:O	1:C:103:TYR:OH	2.32	0.42
1:C:367:ILE:HG21	1:C:396:LEU:HD11	2.02	0.42
1:N:92:GLU:OE1	1:N:94:TRP:NE1	2.38	0.42
1:O:80:VAL:HB	1:O:158:LEU:HD23	2.02	0.42
1:R:314:ASN:HD22	1:R:331:MET:HE1	1.84	0.42
1:g:314:ASN:HD22	1:g:331:MET:HE1	1.84	0.42
1:D:46:LEU:HD23	1:D:70:CYS:HB3	2.02	0.42
1:F:46:LEU:HD23	1:F:70:CYS:HB3	2.02	0.42
1:I:80:VAL:HB	1:I:158:LEU:HD23	2.01	0.42
1:P:46:LEU:HD23	1:P:70:CYS:HB3	2.01	0.42
1:S:314:ASN:HD22	1:S:331:MET:HE1	1.84	0.42
1:f:314:ASN:HD22	1:f:331:MET:HE1	1.84	0.42
1:g:77:LYS:NZ	1:g:106:GLU:OE1	2.39	0.42
1:B:46:LEU:HD23	1:B:70:CYS:HB3	2.01	0.41
1:C:314:ASN:HD22	1:C:331:MET:HE1	1.84	0.41
1:K:367:ILE:HG21	1:K:396:LEU:HD11	2.02	0.41
1:D:367:ILE:HG21	1:D:396:LEU:HD11	2.02	0.41
1:H:46:LEU:HD23	1:H:70:CYS:HB3	2.02	0.41
1:S:92:GLU:OE1	1:S:94:TRP:NE1	2.38	0.41
1:U:46:LEU:HD23	1:U:70:CYS:HB3	2.02	0.41
1:d:46:LEU:HD23	1:d:70:CYS:HB3	2.02	0.41
1:O:46:LEU:HD23	1:O:70:CYS:HB3	2.02	0.41
1:c:367:ILE:HG21	1:c:396:LEU:HD11	2.02	0.41
1:N:46:LEU:HD23	1:N:70:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:441:THR:HG22	1:P:443:LYS:HG3	2.02	0.41
1:E:367:ILE:HG21	1:E:396:LEU:HD11	2.02	0.41
1:G:441:THR:HG22	1:G:443:LYS:HG3	2.02	0.41
1:I:46:LEU:HD23	1:I:70:CYS:HB3	2.02	0.41
1:J:367:ILE:HG21	1:J:396:LEU:HD11	2.02	0.41
1:K:46:LEU:HD23	1:K:70:CYS:HB3	2.02	0.41
1:N:77:LYS:NZ	1:N:106:GLU:OE1	2.39	0.41
1:R:243:GLN:HA	1:R:244:PRO:HD3	1.94	0.41
1:S:46:LEU:HD23	1:S:70:CYS:HB3	2.02	0.41
1:a:46:LEU:HD23	1:a:70:CYS:HB3	2.02	0.41
1:b:47:ARG:O	1:b:103:TYR:OH	2.32	0.41
1:c:46:LEU:HD23	1:c:70:CYS:HB3	2.02	0.41
1:e:243:GLN:HA	1:e:244:PRO:HD3	1.93	0.41
1:h:46:LEU:HD23	1:h:70:CYS:HB3	2.02	0.41
1:A:441:THR:HG22	1:A:443:LYS:HG3	2.02	0.41
1:Q:46:LEU:HD23	1:Q:70:CYS:HB3	2.02	0.41
1:e:441:THR:HG22	1:e:443:LYS:HG3	2.02	0.41
1:f:46:LEU:HD23	1:f:70:CYS:HB3	2.02	0.41
1:g:46:LEU:HD23	1:g:70:CYS:HB3	2.01	0.41
1:E:46:LEU:HD23	1:E:70:CYS:HB3	2.02	0.41
1:h:47:ARG:O	1:h:103:TYR:OH	2.32	0.41
1:i:367:ILE:HG21	1:i:396:LEU:HD11	2.02	0.41
1:B:367:ILE:HG21	1:B:396:LEU:HD11	2.02	0.41
1:F:441:THR:HG22	1:F:443:LYS:HG3	2.02	0.41
1:H:367:ILE:HG21	1:H:396:LEU:HD11	2.02	0.41
1:J:441:THR:HG22	1:J:443:LYS:HG3	2.02	0.41
1:M:46:LEU:HD23	1:M:70:CYS:HB3	2.01	0.41
1:M:441:THR:HG22	1:M:443:LYS:HG3	2.03	0.41
1:N:367:ILE:HG21	1:N:396:LEU:HD11	2.02	0.41
1:P:367:ILE:HG21	1:P:396:LEU:HD11	2.02	0.41
1:T:46:LEU:HD23	1:T:70:CYS:HB3	2.02	0.41
1:b:441:THR:HG22	1:b:443:LYS:HG3	2.03	0.41
1:h:441:THR:HG22	1:h:443:LYS:HG3	2.02	0.41
1:I:290:LYS:HD3	1:I:440:GLU:HG3	2.03	0.41
1:M:290:LYS:HD3	1:M:440:GLU:HG3	2.03	0.41
1:N:290:LYS:HD3	1:N:440:GLU:HG3	2.03	0.41
1:P:290:LYS:HD3	1:P:440:GLU:HG3	2.03	0.41
1:Q:441:THR:HG22	1:Q:443:LYS:HG3	2.02	0.41
1:R:46:LEU:HD23	1:R:70:CYS:HB3	2.02	0.41
1:T:243:GLN:HA	1:T:244:PRO:HD3	1.94	0.41
1:T:290:LYS:HD3	1:T:440:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:367:ILE:HG21	1:T:396:LEU:HD11	2.02	0.41
1:b:46:LEU:HD23	1:b:70:CYS:HB3	2.02	0.41
1:c:40:ILE:H	1:c:40:ILE:HG13	1.77	0.41
1:f:92:GLU:OE1	1:f:94:TRP:NE1	2.38	0.41
1:f:441:THR:HG22	1:f:443:LYS:HG3	2.02	0.41
1:i:46:LEU:HD23	1:i:70:CYS:HB3	2.02	0.41
1:C:46:LEU:HD23	1:C:70:CYS:HB3	2.02	0.41
1:H:441:THR:HG22	1:H:443:LYS:HG3	2.02	0.41
1:J:290:LYS:HD3	1:J:440:GLU:HG3	2.03	0.41
1:K:92:GLU:OE1	1:K:94:TRP:NE1	2.38	0.41
1:K:453:MET:HG2	1:d:425:SER:HB2	2.03	0.41
1:N:441:THR:HG22	1:N:443:LYS:HG3	2.02	0.41
1:R:92:GLU:OE1	1:R:94:TRP:NE1	2.38	0.41
1:S:290:LYS:HD3	1:S:440:GLU:HG3	2.03	0.41
1:S:441:THR:HG22	1:S:443:LYS:HG3	2.02	0.41
1:f:290:LYS:HD3	1:f:440:GLU:HG3	2.03	0.41
1:g:290:LYS:HD3	1:g:440:GLU:HG3	2.03	0.41
1:C:290:LYS:HD3	1:C:440:GLU:HG3	2.03	0.40
1:K:441:THR:HG22	1:K:443:LYS:HG3	2.02	0.40
1:L:46:LEU:HD23	1:L:70:CYS:HB3	2.02	0.40
1:O:290:LYS:HD3	1:O:440:GLU:HG3	2.03	0.40
1:g:193:GLU:OE2	1:g:228:LYS:NZ	2.45	0.40
1:D:290:LYS:HD3	1:D:440:GLU:HG3	2.03	0.40
1:D:441:THR:HG22	1:D:443:LYS:HG3	2.02	0.40
1:G:290:LYS:HD3	1:G:440:GLU:HG3	2.03	0.40
1:H:290:LYS:HD3	1:H:440:GLU:HG3	2.03	0.40
1:J:92:GLU:OE1	1:J:94:TRP:NE1	2.38	0.40
1:L:441:THR:HG22	1:L:443:LYS:HG3	2.02	0.40
1:U:441:THR:HG22	1:U:443:LYS:HG3	2.02	0.40
1:i:441:THR:HG22	1:i:443:LYS:HG3	2.03	0.40
1:B:40:ILE:H	1:B:40:ILE:HG13	1.77	0.40
1:H:224:ILE:HG21	1:i:418:PHE:HE2	1.87	0.40
1:b:290:LYS:HD3	1:b:440:GLU:HG3	2.03	0.40
1:d:441:THR:HG22	1:d:443:LYS:HG3	2.03	0.40
1:e:290:LYS:HD3	1:e:440:GLU:HG3	2.03	0.40
1:i:246:CYS:SG	1:i:270:SER:OG	2.67	0.40
1:O:441:THR:HG22	1:O:443:LYS:HG3	2.02	0.40
1:T:441:THR:HG22	1:T:443:LYS:HG3	2.03	0.40
1:U:290:LYS:HD3	1:U:440:GLU:HG3	2.03	0.40
1:a:290:LYS:HD3	1:a:440:GLU:HG3	2.03	0.40
1:d:290:LYS:HD3	1:d:440:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:441:THR:HG22	1:g:443:LYS:HG3	2.03	0.40
1:h:290:LYS:HD3	1:h:440:GLU:HG3	2.03	0.40
1:A:290:LYS:HD3	1:A:440:GLU:HG3	2.03	0.40
1:B:441:THR:HG22	1:B:443:LYS:HG3	2.03	0.40
1:R:441:THR:HG22	1:R:443:LYS:HG3	2.02	0.40
1:c:441:THR:HG22	1:c:443:LYS:HG3	2.02	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	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	B	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	C	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	D	413/478 (86%)	377 (91%)	36 (9%)	0	100	100
1	E	413/478 (86%)	380 (92%)	33 (8%)	0	100	100
1	F	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	G	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	H	413/478 (86%)	377 (91%)	36 (9%)	0	100	100
1	I	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	J	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	K	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	L	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	M	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	N	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	O	413/478 (86%)	379 (92%)	34 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	Q	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	R	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	S	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	T	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	U	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	a	413/478 (86%)	380 (92%)	33 (8%)	0	100	100
1	b	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	c	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	d	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	e	413/478 (86%)	380 (92%)	33 (8%)	0	100	100
1	f	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	g	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	h	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	i	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
All	All	12390/14340 (86%)	11364 (92%)	1026 (8%)	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	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	B	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	C	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	D	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	E	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	F	365/413 (88%)	364 (100%)	1 (0%)	91	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	H	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	I	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	J	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	K	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	L	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	M	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	N	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	O	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	P	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	Q	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	R	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	S	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	T	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	U	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	a	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	b	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	c	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	d	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	e	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	f	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	g	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	h	365/413 (88%)	364 (100%)	1 (0%)	91	92
1	i	365/413 (88%)	364 (100%)	1 (0%)	91	92
All	All	10950/12390 (88%)	10920 (100%)	30 (0%)	90	92

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	B	40	ILE
1	C	40	ILE
1	D	40	ILE
1	E	40	ILE

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Mol	Chain	Res	Type
1	F	40	ILE
1	G	40	ILE
1	H	40	ILE
1	I	40	ILE
1	J	40	ILE
1	K	40	ILE
1	L	40	ILE
1	M	40	ILE
1	N	40	ILE
1	O	40	ILE
1	P	40	ILE
1	Q	40	ILE
1	R	40	ILE
1	S	40	ILE
1	T	40	ILE
1	U	40	ILE
1	a	40	ILE
1	b	40	ILE
1	c	40	ILE
1	d	40	ILE
1	e	40	ILE
1	f	40	ILE
1	g	40	ILE
1	h	40	ILE
1	i	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	123	HIS
1	A	166	HIS
1	A	191	ASN
1	A	232	HIS
1	A	265	GLN
1	A	276	HIS
1	A	314	ASN
1	A	338	GLN
1	B	166	HIS
1	B	191	ASN
1	B	265	GLN
1	B	276	HIS

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Mol	Chain	Res	Type
1	B	314	ASN
1	B	338	GLN
1	B	378	ASN
1	B	442	GLN
1	C	83	HIS
1	C	157	HIS
1	C	166	HIS
1	C	232	HIS
1	C	265	GLN
1	C	276	HIS
1	C	314	ASN
1	C	338	GLN
1	C	378	ASN
1	C	442	GLN
1	D	83	HIS
1	D	166	HIS
1	D	191	ASN
1	D	232	HIS
1	D	265	GLN
1	D	276	HIS
1	D	314	ASN
1	D	338	GLN
1	D	378	ASN
1	E	83	HIS
1	E	123	HIS
1	E	166	HIS
1	E	191	ASN
1	E	265	GLN
1	E	276	HIS
1	E	314	ASN
1	E	338	GLN
1	F	123	HIS
1	F	166	HIS
1	F	191	ASN
1	F	232	HIS
1	F	276	HIS
1	F	314	ASN
1	F	338	GLN
1	F	378	ASN
1	F	442	GLN
1	G	123	HIS
1	G	191	ASN

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Mol	Chain	Res	Type
1	G	265	GLN
1	G	276	HIS
1	G	314	ASN
1	G	338	GLN
1	G	378	ASN
1	H	123	HIS
1	H	166	HIS
1	H	191	ASN
1	H	276	HIS
1	H	314	ASN
1	H	338	GLN
1	H	378	ASN
1	I	83	HIS
1	I	123	HIS
1	I	191	ASN
1	I	265	GLN
1	I	276	HIS
1	I	314	ASN
1	I	338	GLN
1	I	378	ASN
1	J	83	HIS
1	J	191	ASN
1	J	265	GLN
1	J	276	HIS
1	J	314	ASN
1	J	338	GLN
1	K	83	HIS
1	K	166	HIS
1	K	191	ASN
1	K	265	GLN
1	K	276	HIS
1	K	314	ASN
1	K	338	GLN
1	K	378	ASN
1	L	83	HIS
1	L	166	HIS
1	L	191	ASN
1	L	232	HIS
1	L	276	HIS
1	L	314	ASN
1	L	338	GLN
1	L	378	ASN

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Mol	Chain	Res	Type
1	L	442	GLN
1	M	191	ASN
1	M	265	GLN
1	M	276	HIS
1	M	314	ASN
1	M	338	GLN
1	N	83	HIS
1	N	150	ASN
1	N	166	HIS
1	N	191	ASN
1	N	265	GLN
1	N	276	HIS
1	N	314	ASN
1	N	338	GLN
1	O	191	ASN
1	O	265	GLN
1	O	276	HIS
1	O	314	ASN
1	O	338	GLN
1	P	83	HIS
1	P	150	ASN
1	P	166	HIS
1	P	191	ASN
1	P	232	HIS
1	P	265	GLN
1	P	276	HIS
1	P	314	ASN
1	P	338	GLN
1	Q	83	HIS
1	Q	166	HIS
1	Q	232	HIS
1	Q	276	HIS
1	Q	314	ASN
1	Q	338	GLN
1	Q	378	ASN
1	R	150	ASN
1	R	166	HIS
1	R	191	ASN
1	R	232	HIS
1	R	265	GLN
1	R	276	HIS
1	R	314	ASN

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Mol	Chain	Res	Type
1	R	338	GLN
1	R	378	ASN
1	S	83	HIS
1	S	213	HIS
1	S	276	HIS
1	S	314	ASN
1	S	338	GLN
1	S	378	ASN
1	T	74	HIS
1	T	150	ASN
1	T	191	ASN
1	T	232	HIS
1	T	276	HIS
1	T	314	ASN
1	T	338	GLN
1	T	378	ASN
1	U	166	HIS
1	U	265	GLN
1	U	276	HIS
1	U	314	ASN
1	U	338	GLN
1	U	442	GLN
1	a	123	HIS
1	a	166	HIS
1	a	191	ASN
1	a	232	HIS
1	a	265	GLN
1	a	276	HIS
1	a	314	ASN
1	a	338	GLN
1	b	123	HIS
1	b	150	ASN
1	b	166	HIS
1	b	191	ASN
1	b	276	HIS
1	b	314	ASN
1	b	338	GLN
1	b	378	ASN
1	b	442	GLN
1	c	123	HIS
1	c	166	HIS
1	c	191	ASN

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Mol	Chain	Res	Type
1	c	232	HIS
1	c	265	GLN
1	c	276	HIS
1	c	314	ASN
1	c	338	GLN
1	c	378	ASN
1	d	74	HIS
1	d	150	ASN
1	d	166	HIS
1	d	265	GLN
1	d	276	HIS
1	d	314	ASN
1	d	338	GLN
1	d	378	ASN
1	e	83	HIS
1	e	123	HIS
1	e	166	HIS
1	e	265	GLN
1	e	276	HIS
1	e	314	ASN
1	e	338	GLN
1	f	123	HIS
1	f	150	ASN
1	f	191	ASN
1	f	276	HIS
1	f	314	ASN
1	f	338	GLN
1	f	378	ASN
1	g	123	HIS
1	g	276	HIS
1	g	314	ASN
1	g	338	GLN
1	g	378	ASN
1	h	83	HIS
1	h	123	HIS
1	h	150	ASN
1	h	166	HIS
1	h	191	ASN
1	h	276	HIS
1	h	314	ASN
1	h	338	GLN
1	h	378	ASN

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Mol	Chain	Res	Type
1	i	83	HIS
1	i	123	HIS
1	i	166	HIS
1	i	232	HIS
1	i	276	HIS
1	i	314	ASN
1	i	338	GLN
1	i	378	ASN
1	i	442	GLN

### 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.

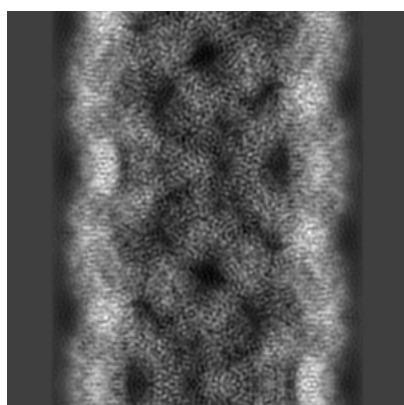
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20673. These allow visual inspection of the internal detail of the map and identification of artifacts.

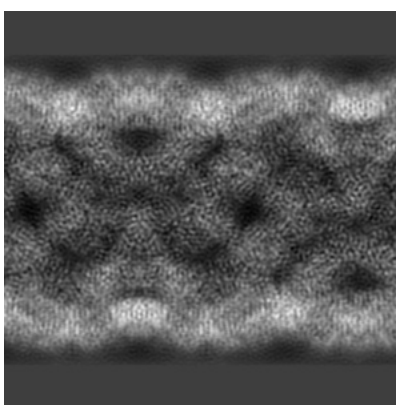
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

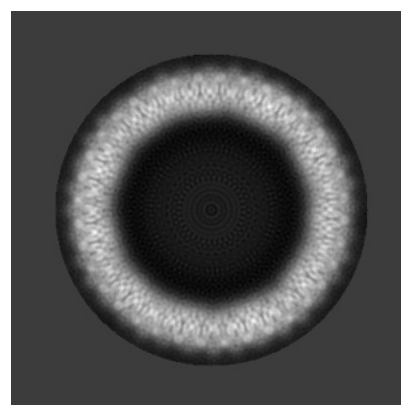
#### 6.1.1 Primary map



X



Y

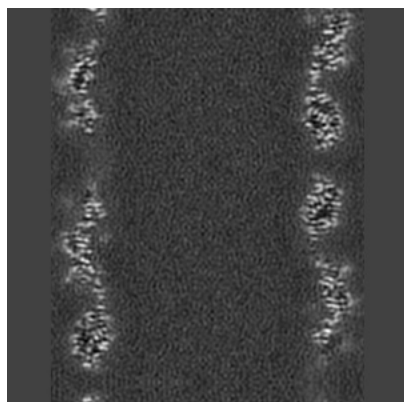


Z

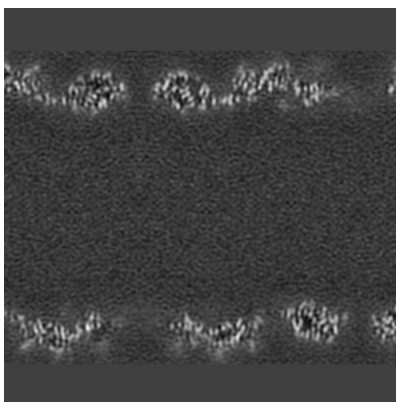
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

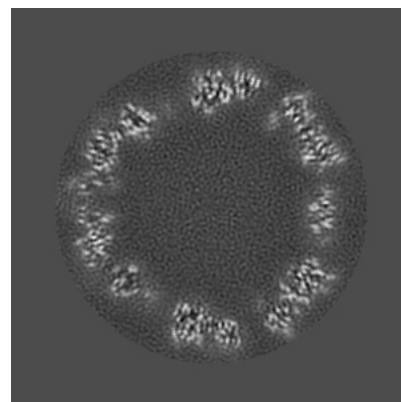
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

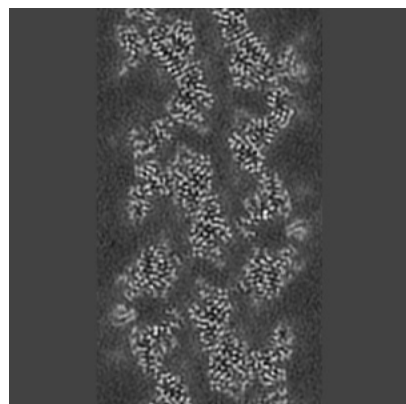


Z Index: 192

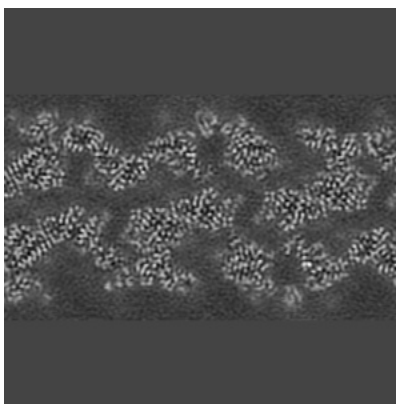
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

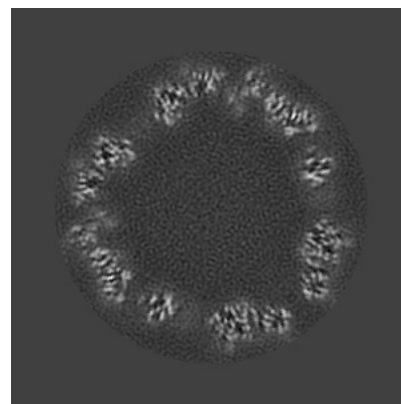
### 6.3.1 Primary map



X Index: 296



Y Index: 296

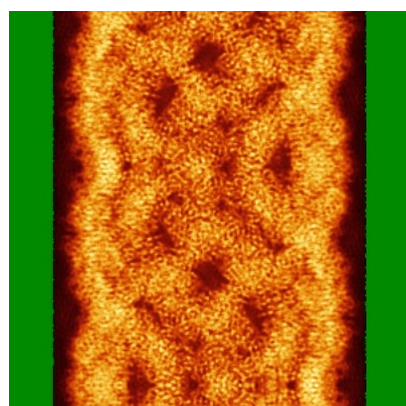


Z Index: 351

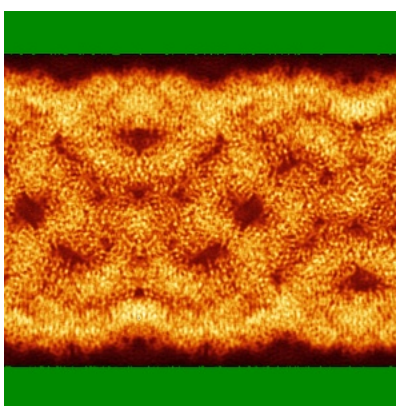
The images above show the largest variance slices of the map in three orthogonal directions.

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

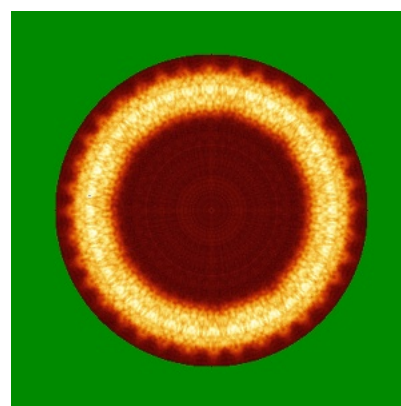
### 6.4.1 Primary map



X



Y

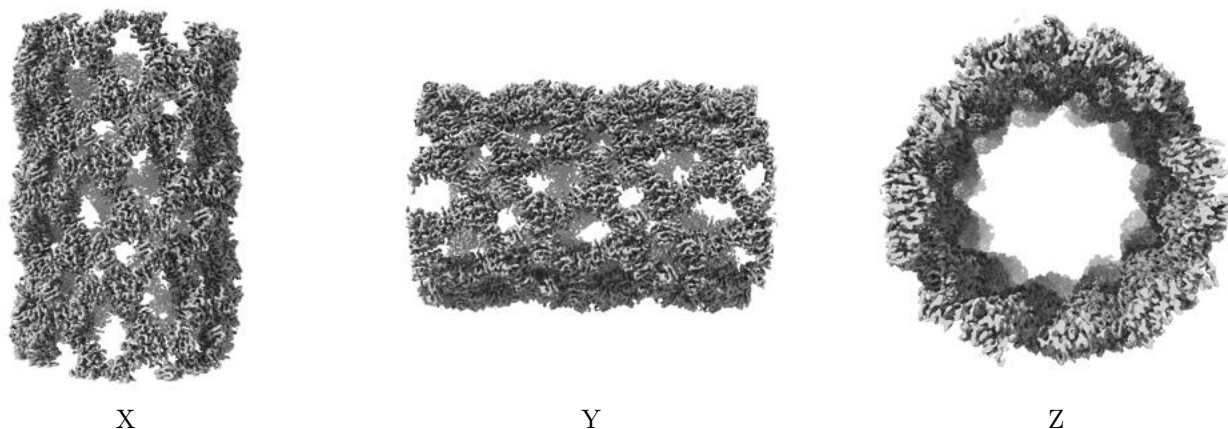


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

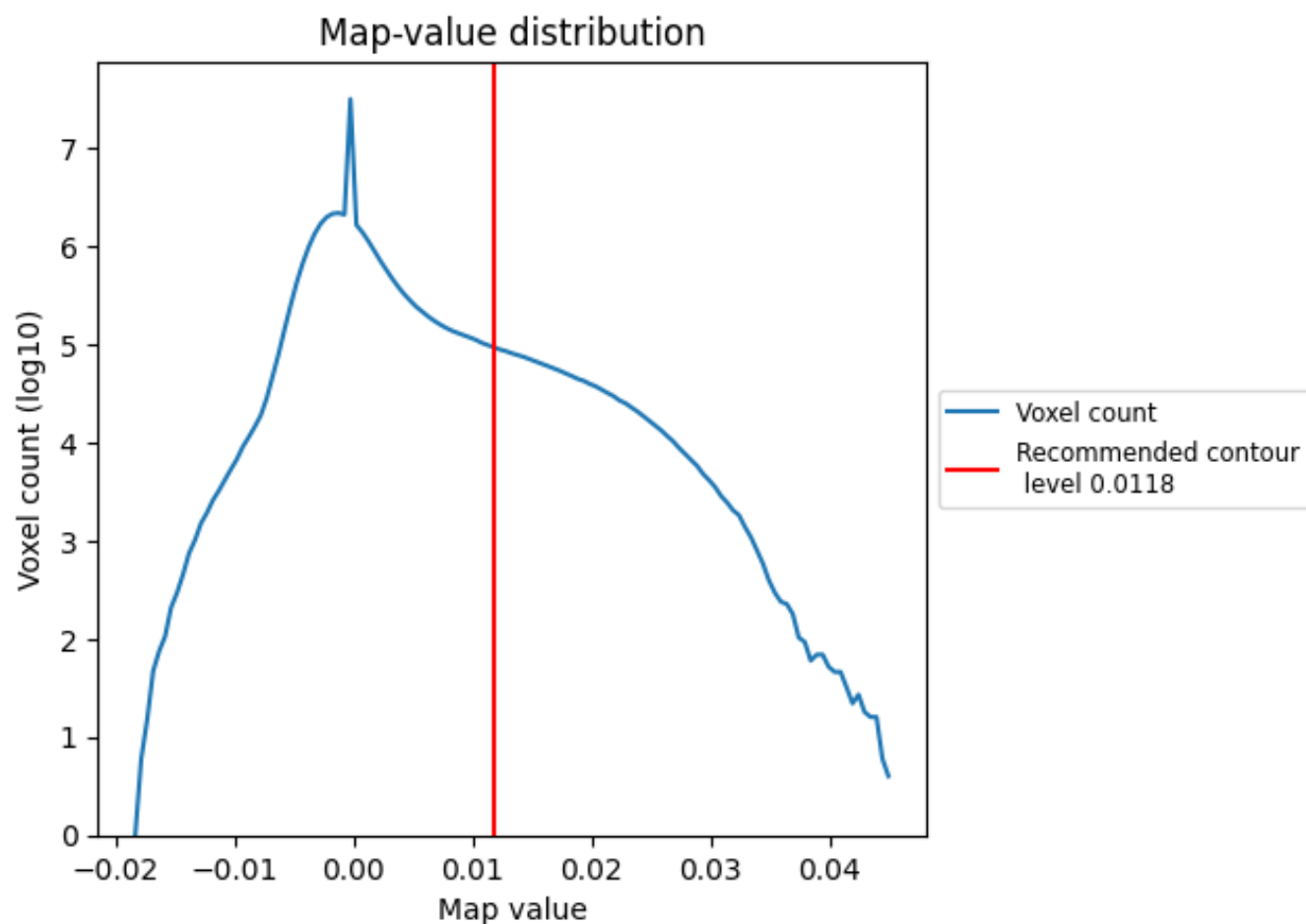
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

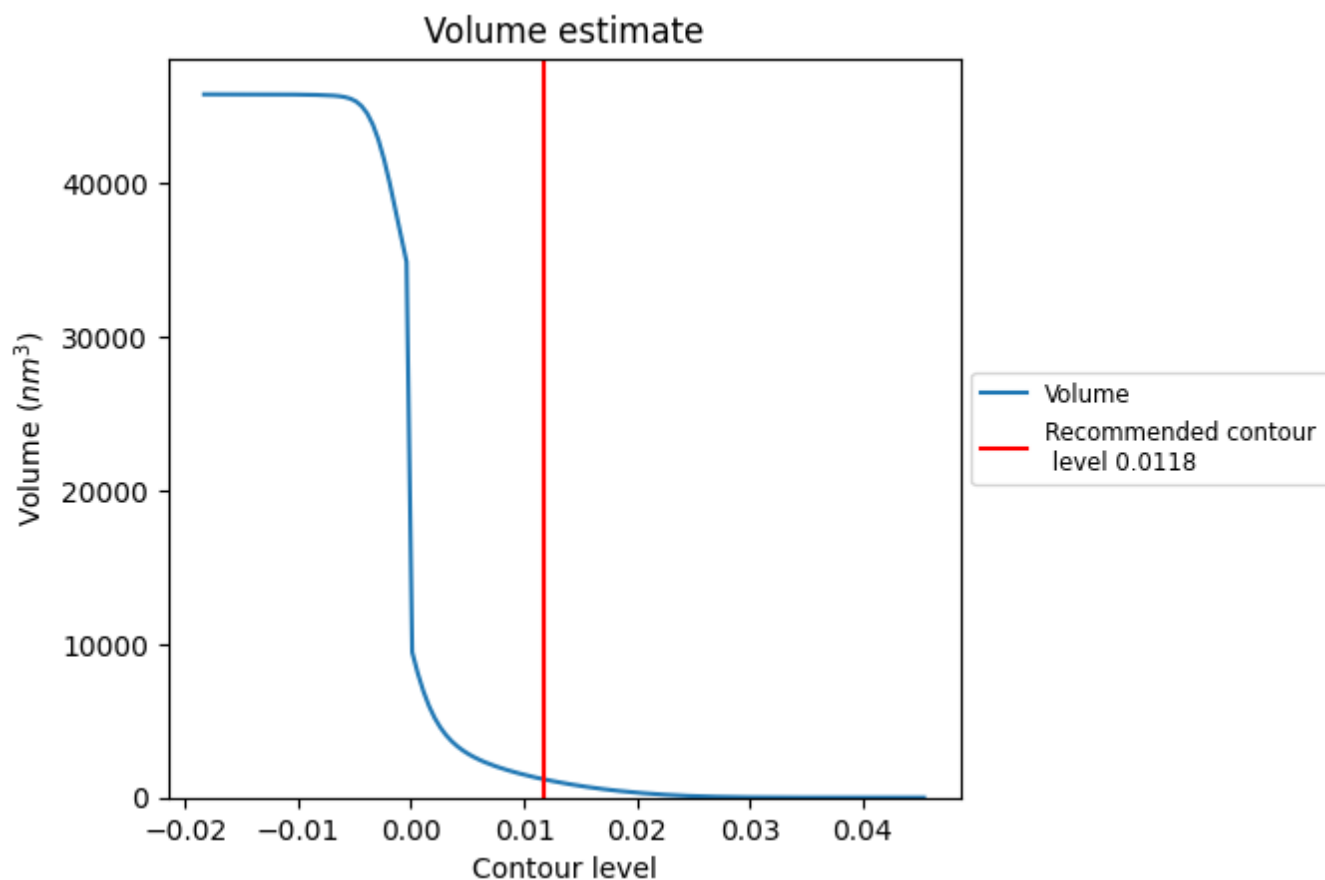
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

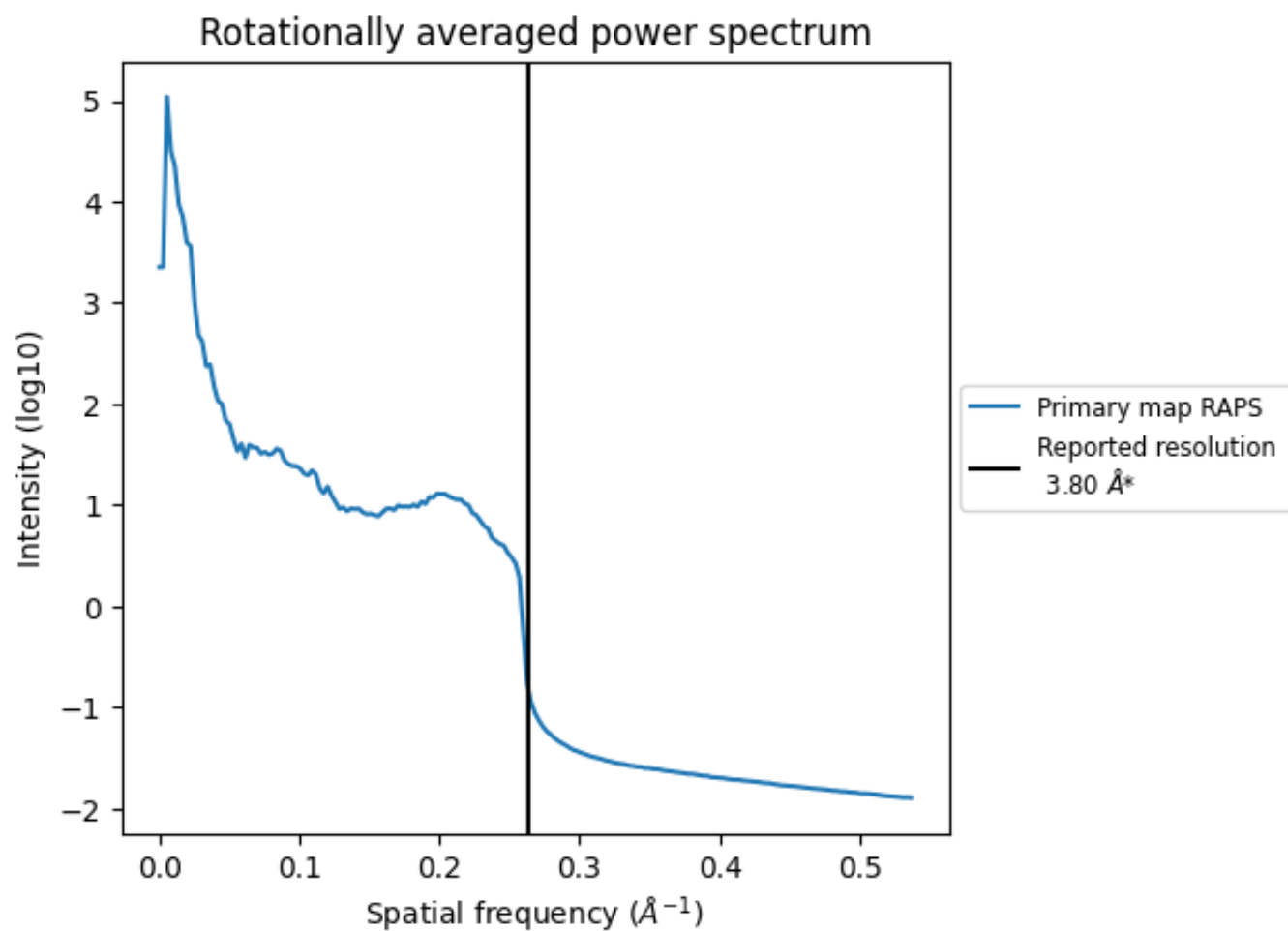
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1186 nm<sup>3</sup>; this corresponds to an approximate mass of 1071 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 0.263 Å<sup>-1</sup>

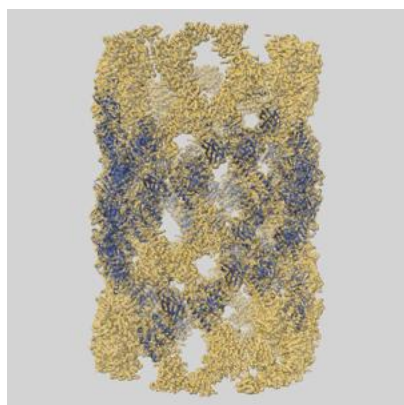
## 8 Fourier-Shell correlation

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

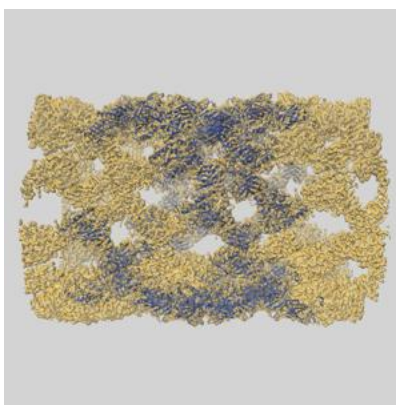
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20673 and PDB model 6U7M. Per-residue inclusion information can be found in section [3](#) on page [6](#).

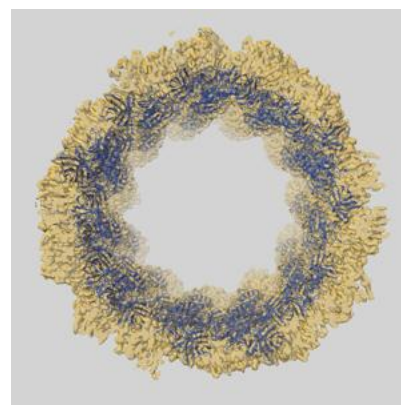
### 9.1 Map-model overlay [i](#)



X



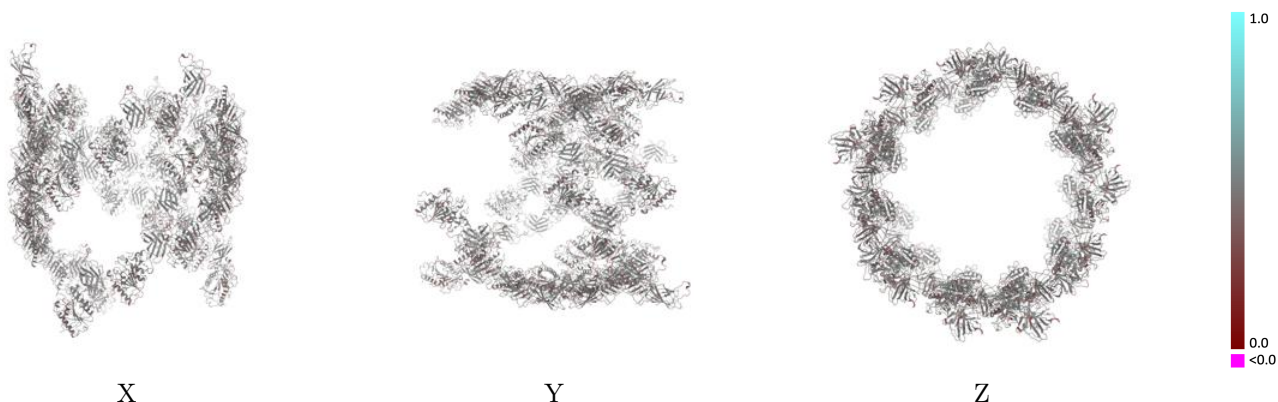
Y



Z

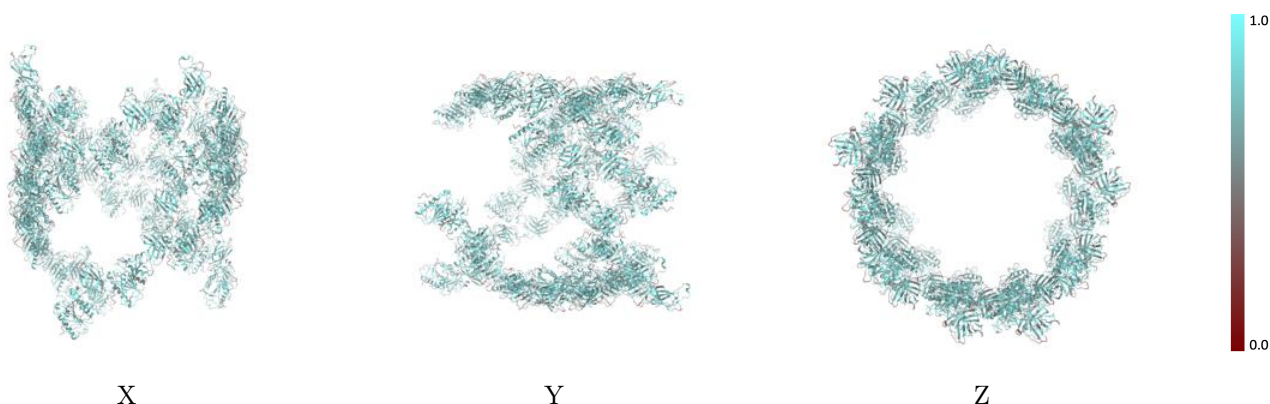
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



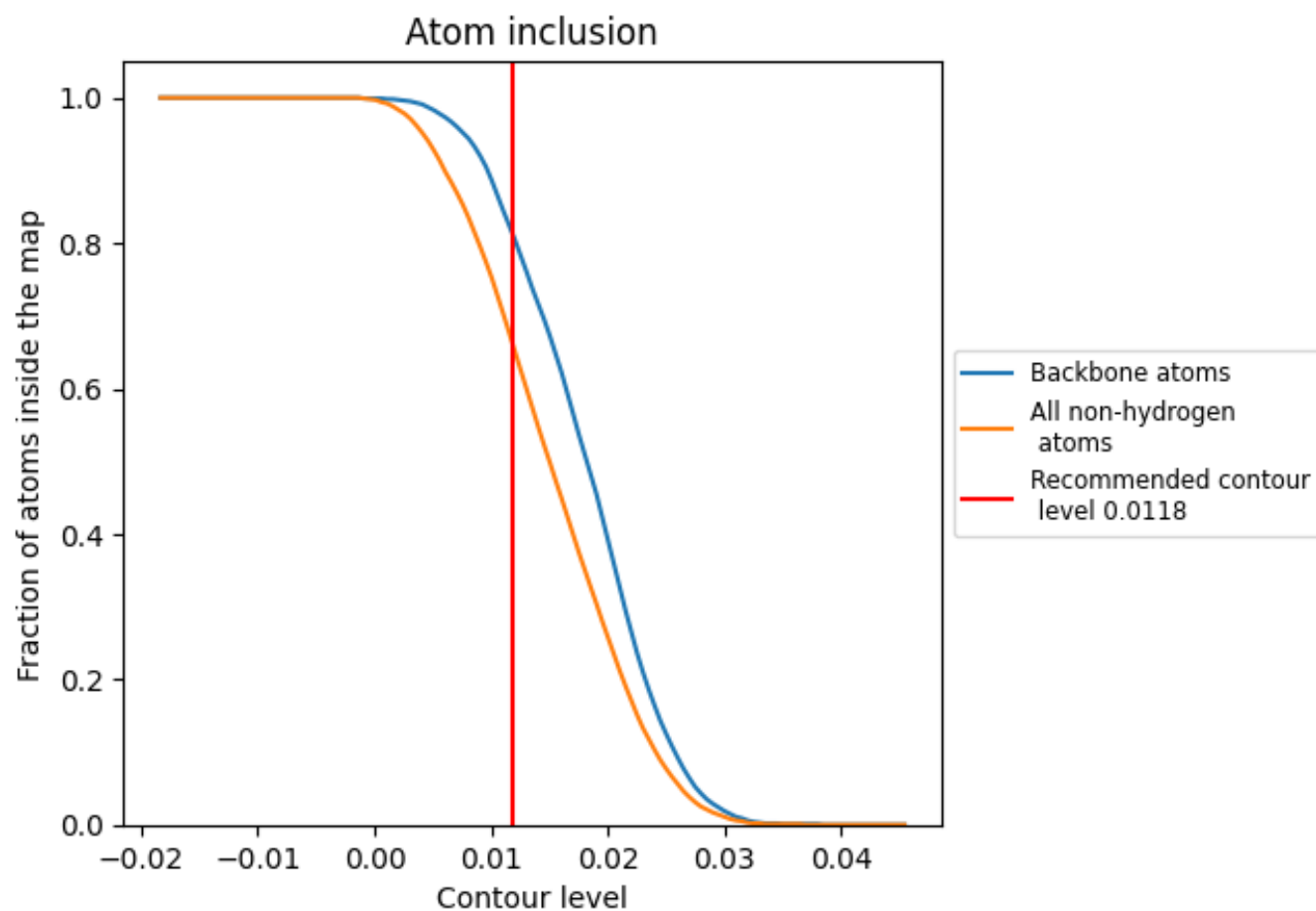
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.4380
A	 0.6640	 0.4400
B	 0.6650	 0.4360
C	 0.6580	 0.4370
D	 0.6640	 0.4390
E	 0.6650	 0.4370
F	 0.6670	 0.4380
G	 0.6630	 0.4390
H	 0.6650	 0.4370
I	 0.6630	 0.4390
J	 0.6670	 0.4410
K	 0.6620	 0.4370
L	 0.6650	 0.4360
M	 0.6610	 0.4370
N	 0.6630	 0.4400
O	 0.6660	 0.4390
P	 0.6640	 0.4370
Q	 0.6620	 0.4390
R	 0.6670	 0.4380
S	 0.6650	 0.4390
T	 0.6580	 0.4360
U	 0.6600	 0.4330
a	 0.6680	 0.4380
b	 0.6640	 0.4380
c	 0.6580	 0.4350
d	 0.6610	 0.4380
e	 0.6690	 0.4380
f	 0.6660	 0.4390
g	 0.6660	 0.4400
h	 0.6640	 0.4360
i	 0.6630	 0.4390

