



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 11:14 AM JST

PDB ID : 28EP / pdb_000028ep
EMDB ID : EMD-81689
Title : Proteinase K filament
Authors : Sleutel, M.; Bodson, T.; Remaut, H.
Deposited on : 2026-06-23
Resolution : 3.18 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.dev133
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) : 2.50

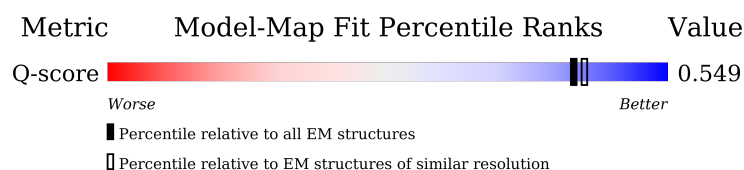
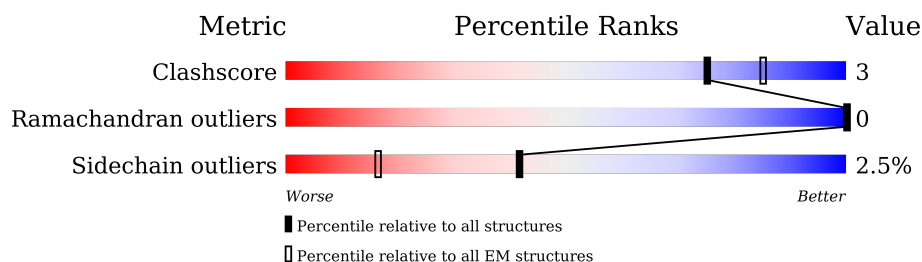
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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.



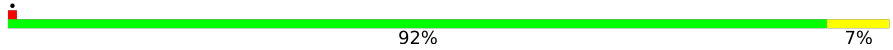
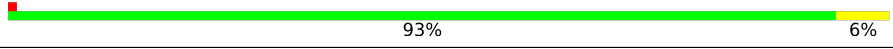
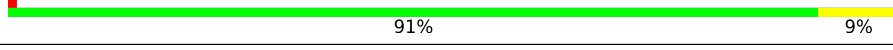
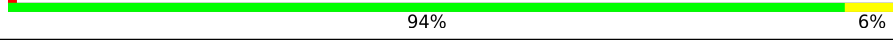
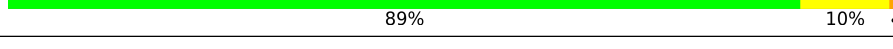
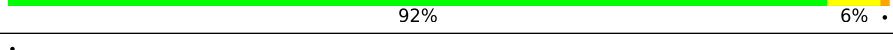
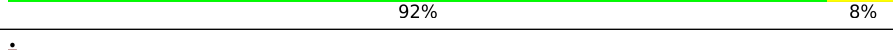
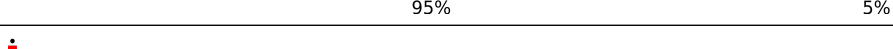
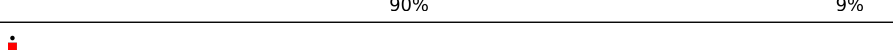
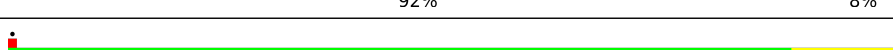
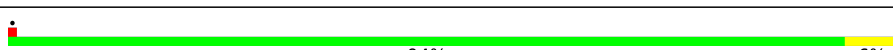
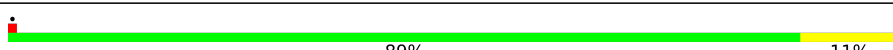
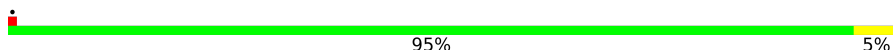
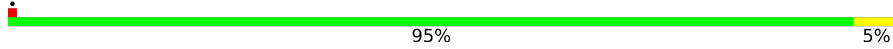
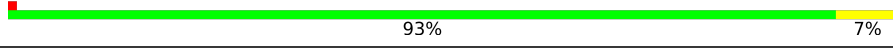
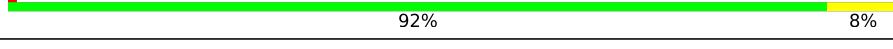
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

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	0	279	
1	1	279	
1	2	279	
1	3	279	

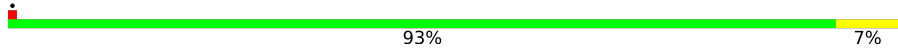
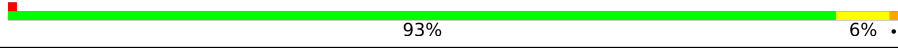
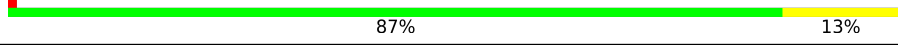
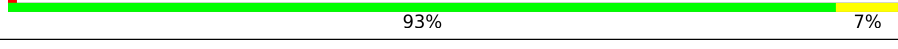
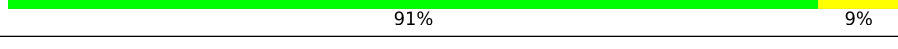
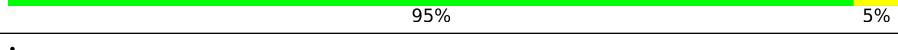
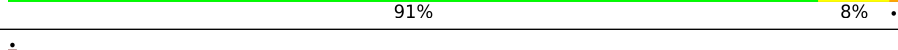
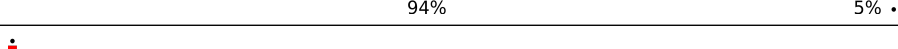
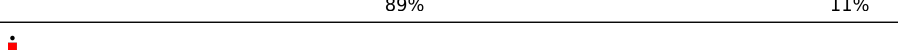
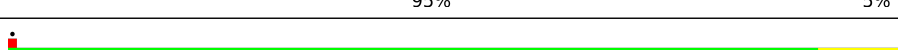
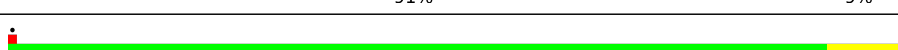
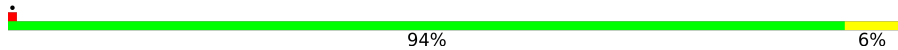
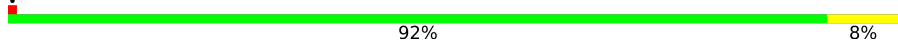
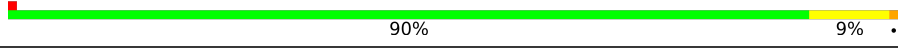
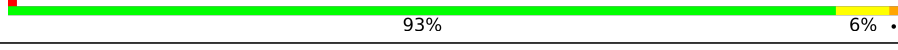
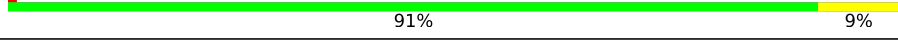
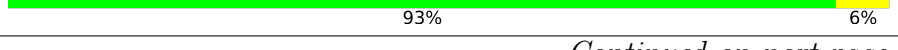
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Mol	Chain	Length	Quality of chain
1	4	279	
1	5	279	
1	6	279	
1	7	279	
1	8	279	
1	9	279	
1	A0	279	
1	A1	279	
1	A2	279	
1	A3	279	
1	A4	279	
1	A5	279	
1	A6	279	
1	A7	279	
1	A8	279	
1	A9	279	
1	AA	279	
1	AB	279	
1	AC	279	
1	AD	279	
1	AE	279	
1	AF	279	
1	AG	279	
1	AH	279	
1	AI	279	

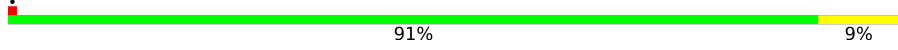
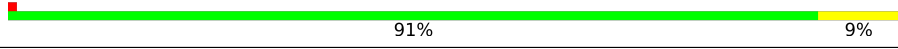
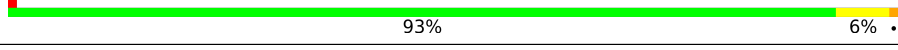
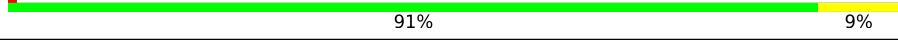
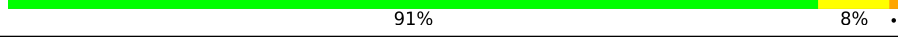
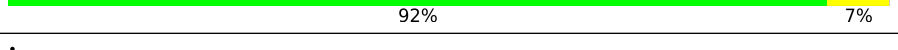
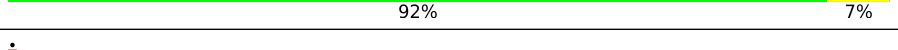
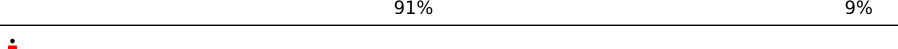
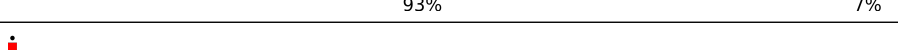
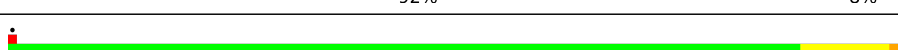
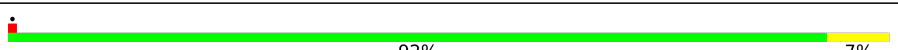
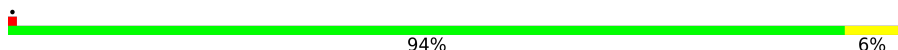
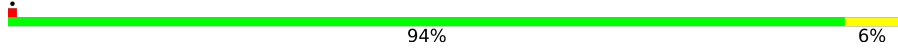
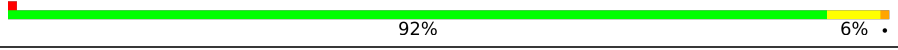
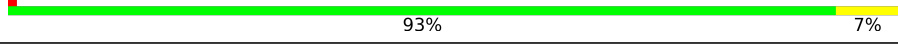
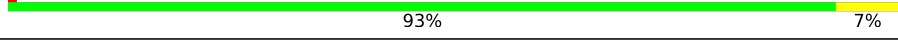
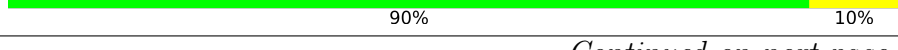
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Mol	Chain	Length	Quality of chain
1	AJ	279	
1	AK	279	
1	AL	279	
1	AM	279	
1	AN	279	
1	AO	279	
1	AP	279	
1	AQ	279	
1	AR	279	
1	AS	279	
1	AT	279	
1	AU	279	
1	AV	279	
1	AW	279	
1	AX	279	
1	AY	279	
1	AZ	279	
1	Aa	279	
1	Ab	279	
1	Ac	279	
1	Ad	279	
1	Ae	279	
1	Af	279	
1	Ag	279	
1	Ah	279	

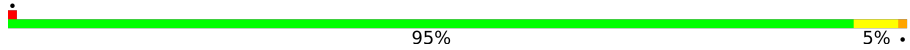
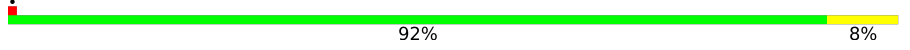
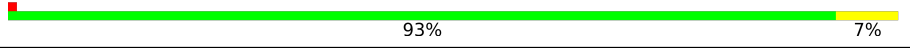
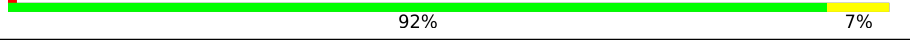
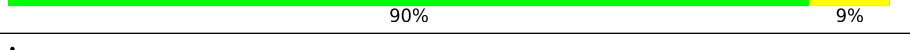
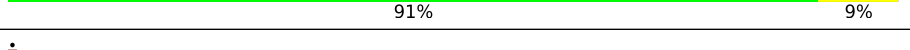
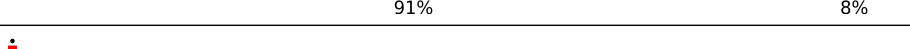
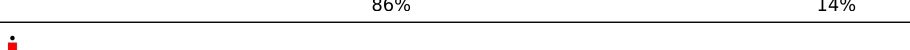
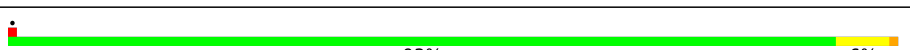
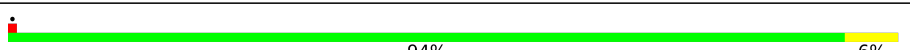
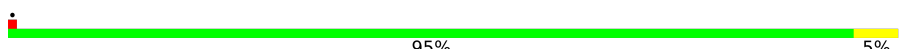
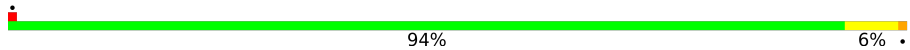
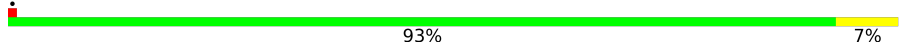
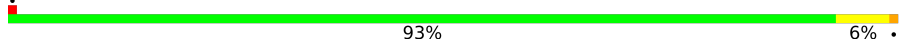
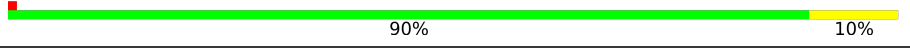
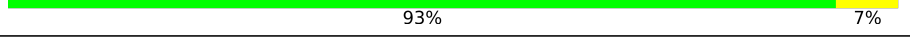
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Mol	Chain	Length	Quality of chain
1	Ai	279	
1	Aj	279	
1	Ak	279	
1	Al	279	
1	Am	279	
1	An	279	
1	Ao	279	
1	Ap	279	
1	Aq	279	
1	Ar	279	
1	As	279	
1	At	279	
1	Au	279	
1	Av	279	
1	Aw	279	
1	Ax	279	
1	Ay	279	
1	Az	279	
1	BA	279	
1	BB	279	
1	BC	279	
1	BD	279	
1	BE	279	
1	BF	279	
1	BG	279	

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Mol	Chain	Length	Quality of chain
1	BH	279	 95% 5%
1	BI	279	 92% 8%
1	BJ	279	 93% 7%
1	BK	279	 91% 8%
1	BL	279	 92% 7%
1	BM	279	 88% 12%
1	BN	279	 90% 9%
1	i	279	 91% 9%
1	j	279	 91% 8%
1	k	279	 86% 14%
1	l	279	 92% 7%
1	m	279	 89% 11%
1	n	279	 95%
1	o	279	 85% 14%
1	p	279	 93% 6%
1	q	279	 94% 6%
1	r	279	 95% 5%
1	s	279	 88% 11%
1	t	279	 94% 6%
1	u	279	 93% 7%
1	v	279	 93% 6%
1	w	279	 90% 10%
1	x	279	 90% 9%
1	y	279	 88% 12%
1	z	279	 93% 7%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 211328 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 Proteinase K.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	j	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	k	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	l	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	m	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	n	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	o	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	p	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	q	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	r	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	s	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	t	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	u	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	v	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	w	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	x	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	y	279	Total 2031	C 1248	N 357	O 416	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	z	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	1	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	2	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	3	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	4	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	5	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	6	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	7	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	8	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	9	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	0	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AA	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AB	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AC	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AD	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AE	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AF	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AG	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AH	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AI	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	AJ	279	Total 2031	C 1248	N 357	O 416	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AK	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AL	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AM	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AN	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AO	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AP	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AQ	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AR	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AS	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AT	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AU	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AV	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AW	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AX	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AY	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	AZ	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Aa	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ab	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ac	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ad	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ae	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Af	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ag	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ah	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ai	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Aj	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ak	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Al	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Am	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	An	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ao	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ap	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Aq	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ar	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	As	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	At	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Au	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Av	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Aw	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ax	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Ay	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	Az	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A2	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A3	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A4	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A5	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A6	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A7	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A8	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A9	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	A0	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BA	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BB	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BC	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BD	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BE	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BF	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BG	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BH	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BI	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BJ	279	Total 2031	C 1248	N 357	O 416	S 10	0	0
1	BK	279	Total 2031	C 1248	N 357	O 416	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BL	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	BM	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		
1	BN	279	Total	C	N	O	S	0	0
			2031	1248	357	416	10		

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	207	ASP	SER	conflict	UNP P06873
j	207	ASP	SER	conflict	UNP P06873
k	207	ASP	SER	conflict	UNP P06873
l	207	ASP	SER	conflict	UNP P06873
m	207	ASP	SER	conflict	UNP P06873
n	207	ASP	SER	conflict	UNP P06873
o	207	ASP	SER	conflict	UNP P06873
p	207	ASP	SER	conflict	UNP P06873
q	207	ASP	SER	conflict	UNP P06873
r	207	ASP	SER	conflict	UNP P06873
s	207	ASP	SER	conflict	UNP P06873
t	207	ASP	SER	conflict	UNP P06873
u	207	ASP	SER	conflict	UNP P06873
v	207	ASP	SER	conflict	UNP P06873
w	207	ASP	SER	conflict	UNP P06873
x	207	ASP	SER	conflict	UNP P06873
y	207	ASP	SER	conflict	UNP P06873
z	207	ASP	SER	conflict	UNP P06873
1	207	ASP	SER	conflict	UNP P06873
2	207	ASP	SER	conflict	UNP P06873
3	207	ASP	SER	conflict	UNP P06873
4	207	ASP	SER	conflict	UNP P06873
5	207	ASP	SER	conflict	UNP P06873
6	207	ASP	SER	conflict	UNP P06873
7	207	ASP	SER	conflict	UNP P06873
8	207	ASP	SER	conflict	UNP P06873
9	207	ASP	SER	conflict	UNP P06873
0	207	ASP	SER	conflict	UNP P06873
AA	207	ASP	SER	conflict	UNP P06873
AB	207	ASP	SER	conflict	UNP P06873
AC	207	ASP	SER	conflict	UNP P06873
AD	207	ASP	SER	conflict	UNP P06873

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Chain	Residue	Modelled	Actual	Comment	Reference
AE	207	ASP	SER	conflict	UNP P06873
AF	207	ASP	SER	conflict	UNP P06873
AG	207	ASP	SER	conflict	UNP P06873
AH	207	ASP	SER	conflict	UNP P06873
AI	207	ASP	SER	conflict	UNP P06873
AJ	207	ASP	SER	conflict	UNP P06873
AK	207	ASP	SER	conflict	UNP P06873
AL	207	ASP	SER	conflict	UNP P06873
AM	207	ASP	SER	conflict	UNP P06873
AN	207	ASP	SER	conflict	UNP P06873
AO	207	ASP	SER	conflict	UNP P06873
AP	207	ASP	SER	conflict	UNP P06873
AQ	207	ASP	SER	conflict	UNP P06873
AR	207	ASP	SER	conflict	UNP P06873
AS	207	ASP	SER	conflict	UNP P06873
AT	207	ASP	SER	conflict	UNP P06873
AU	207	ASP	SER	conflict	UNP P06873
AV	207	ASP	SER	conflict	UNP P06873
AW	207	ASP	SER	conflict	UNP P06873
AX	207	ASP	SER	conflict	UNP P06873
AY	207	ASP	SER	conflict	UNP P06873
AZ	207	ASP	SER	conflict	UNP P06873
Aa	207	ASP	SER	conflict	UNP P06873
Ab	207	ASP	SER	conflict	UNP P06873
Ac	207	ASP	SER	conflict	UNP P06873
Ad	207	ASP	SER	conflict	UNP P06873
Ae	207	ASP	SER	conflict	UNP P06873
Af	207	ASP	SER	conflict	UNP P06873
Ag	207	ASP	SER	conflict	UNP P06873
Ah	207	ASP	SER	conflict	UNP P06873
Ai	207	ASP	SER	conflict	UNP P06873
Aj	207	ASP	SER	conflict	UNP P06873
Ak	207	ASP	SER	conflict	UNP P06873
Al	207	ASP	SER	conflict	UNP P06873
Am	207	ASP	SER	conflict	UNP P06873
An	207	ASP	SER	conflict	UNP P06873
Ao	207	ASP	SER	conflict	UNP P06873
Ap	207	ASP	SER	conflict	UNP P06873
Aq	207	ASP	SER	conflict	UNP P06873
Ar	207	ASP	SER	conflict	UNP P06873
As	207	ASP	SER	conflict	UNP P06873
At	207	ASP	SER	conflict	UNP P06873

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Chain	Residue	Modelled	Actual	Comment	Reference
Au	207	ASP	SER	conflict	UNP P06873
Av	207	ASP	SER	conflict	UNP P06873
Aw	207	ASP	SER	conflict	UNP P06873
Ax	207	ASP	SER	conflict	UNP P06873
Ay	207	ASP	SER	conflict	UNP P06873
Az	207	ASP	SER	conflict	UNP P06873
A1	207	ASP	SER	conflict	UNP P06873
A2	207	ASP	SER	conflict	UNP P06873
A3	207	ASP	SER	conflict	UNP P06873
A4	207	ASP	SER	conflict	UNP P06873
A5	207	ASP	SER	conflict	UNP P06873
A6	207	ASP	SER	conflict	UNP P06873
A7	207	ASP	SER	conflict	UNP P06873
A8	207	ASP	SER	conflict	UNP P06873
A9	207	ASP	SER	conflict	UNP P06873
A0	207	ASP	SER	conflict	UNP P06873
BA	207	ASP	SER	conflict	UNP P06873
BB	207	ASP	SER	conflict	UNP P06873
BC	207	ASP	SER	conflict	UNP P06873
BD	207	ASP	SER	conflict	UNP P06873
BE	207	ASP	SER	conflict	UNP P06873
BF	207	ASP	SER	conflict	UNP P06873
BG	207	ASP	SER	conflict	UNP P06873
BH	207	ASP	SER	conflict	UNP P06873
BI	207	ASP	SER	conflict	UNP P06873
BJ	207	ASP	SER	conflict	UNP P06873
BK	207	ASP	SER	conflict	UNP P06873
BL	207	ASP	SER	conflict	UNP P06873
BM	207	ASP	SER	conflict	UNP P06873
BN	207	ASP	SER	conflict	UNP P06873

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
2	i	1	Total Ca 1 1	0
2	j	1	Total Ca 1 1	0
2	k	1	Total Ca 1 1	0
2	l	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	m	1	Total 1	Ca 1	0
2	n	1	Total 1	Ca 1	0
2	o	1	Total 1	Ca 1	0
2	p	1	Total 1	Ca 1	0
2	q	1	Total 1	Ca 1	0
2	r	1	Total 1	Ca 1	0
2	s	1	Total 1	Ca 1	0
2	t	1	Total 1	Ca 1	0
2	u	1	Total 1	Ca 1	0
2	v	1	Total 1	Ca 1	0
2	w	1	Total 1	Ca 1	0
2	x	1	Total 1	Ca 1	0
2	y	1	Total 1	Ca 1	0
2	z	1	Total 1	Ca 1	0
2	1	1	Total 1	Ca 1	0
2	2	1	Total 1	Ca 1	0
2	3	1	Total 1	Ca 1	0
2	4	1	Total 1	Ca 1	0
2	5	1	Total 1	Ca 1	0
2	6	1	Total 1	Ca 1	0
2	7	1	Total 1	Ca 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	8	1	Total 1	Ca 1	0
2	9	1	Total 1	Ca 1	0
2	0	1	Total 1	Ca 1	0
2	AA	1	Total 1	Ca 1	0
2	AB	1	Total 1	Ca 1	0
2	AC	1	Total 1	Ca 1	0
2	AD	1	Total 1	Ca 1	0
2	AE	1	Total 1	Ca 1	0
2	AF	1	Total 1	Ca 1	0
2	AG	1	Total 1	Ca 1	0
2	AH	1	Total 1	Ca 1	0
2	AI	1	Total 1	Ca 1	0
2	AJ	1	Total 1	Ca 1	0
2	AK	1	Total 1	Ca 1	0
2	AL	1	Total 1	Ca 1	0
2	AM	1	Total 1	Ca 1	0
2	AN	1	Total 1	Ca 1	0
2	AO	1	Total 1	Ca 1	0
2	AP	1	Total 1	Ca 1	0
2	AQ	1	Total 1	Ca 1	0
2	AR	1	Total 1	Ca 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	AS	1	Total 1	Ca 1	0
2	AT	1	Total 1	Ca 1	0
2	AU	1	Total 1	Ca 1	0
2	AV	1	Total 1	Ca 1	0
2	AW	1	Total 1	Ca 1	0
2	AX	1	Total 1	Ca 1	0
2	AY	1	Total 1	Ca 1	0
2	AZ	1	Total 1	Ca 1	0
2	Aa	1	Total 1	Ca 1	0
2	Ab	1	Total 1	Ca 1	0
2	Ac	1	Total 1	Ca 1	0
2	Ad	1	Total 1	Ca 1	0
2	Ae	1	Total 1	Ca 1	0
2	Af	1	Total 1	Ca 1	0
2	Ag	1	Total 1	Ca 1	0
2	Ah	1	Total 1	Ca 1	0
2	Ai	1	Total 1	Ca 1	0
2	Aj	1	Total 1	Ca 1	0
2	Ak	1	Total 1	Ca 1	0
2	Al	1	Total 1	Ca 1	0
2	Am	1	Total 1	Ca 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	An	1	Total 1	Ca 1	0
2	Ao	1	Total 1	Ca 1	0
2	Ap	1	Total 1	Ca 1	0
2	Aq	1	Total 1	Ca 1	0
2	Ar	1	Total 1	Ca 1	0
2	As	1	Total 1	Ca 1	0
2	At	1	Total 1	Ca 1	0
2	Au	1	Total 1	Ca 1	0
2	Av	1	Total 1	Ca 1	0
2	Aw	1	Total 1	Ca 1	0
2	Ax	1	Total 1	Ca 1	0
2	Ay	1	Total 1	Ca 1	0
2	Az	1	Total 1	Ca 1	0
2	A1	1	Total 1	Ca 1	0
2	A2	1	Total 1	Ca 1	0
2	A3	1	Total 1	Ca 1	0
2	A4	1	Total 1	Ca 1	0
2	A5	1	Total 1	Ca 1	0
2	A6	1	Total 1	Ca 1	0
2	A7	1	Total 1	Ca 1	0
2	A8	1	Total 1	Ca 1	0

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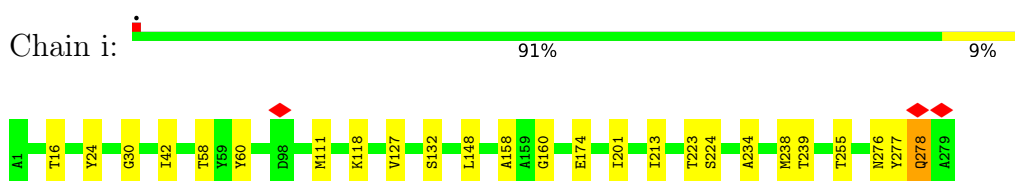
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Mol	Chain	Residues	Atoms		AltConf
2	A9	1	Total 1	Ca 1	0
2	A0	1	Total 1	Ca 1	0
2	BA	1	Total 1	Ca 1	0
2	BB	1	Total 1	Ca 1	0
2	BC	1	Total 1	Ca 1	0
2	BD	1	Total 1	Ca 1	0
2	BE	1	Total 1	Ca 1	0
2	BF	1	Total 1	Ca 1	0
2	BG	1	Total 1	Ca 1	0
2	BH	1	Total 1	Ca 1	0
2	BI	1	Total 1	Ca 1	0
2	BJ	1	Total 1	Ca 1	0
2	BK	1	Total 1	Ca 1	0
2	BL	1	Total 1	Ca 1	0
2	BM	1	Total 1	Ca 1	0
2	BN	1	Total 1	Ca 1	0

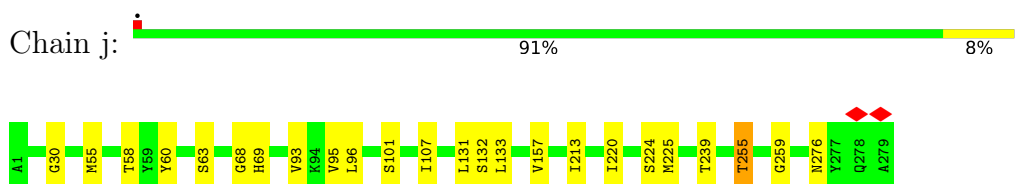
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

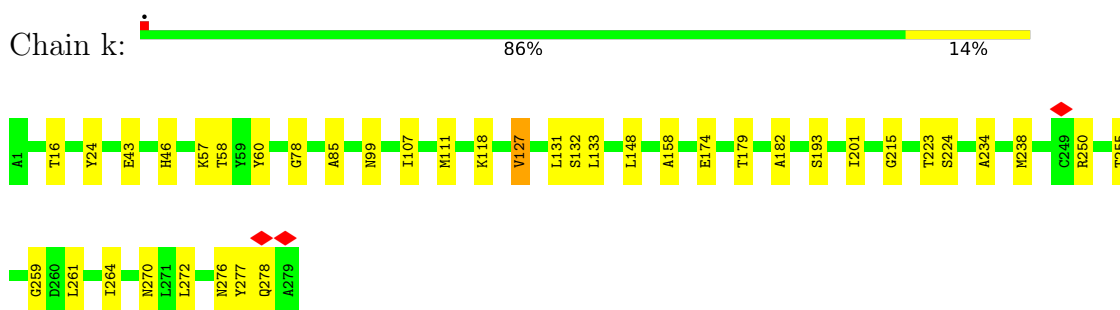
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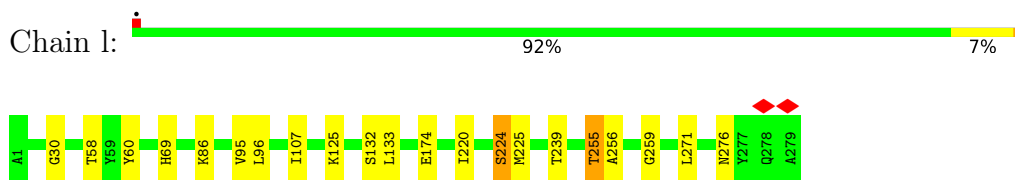
- Molecule 1: Proteinase K



- Molecule 1: Proteinase K

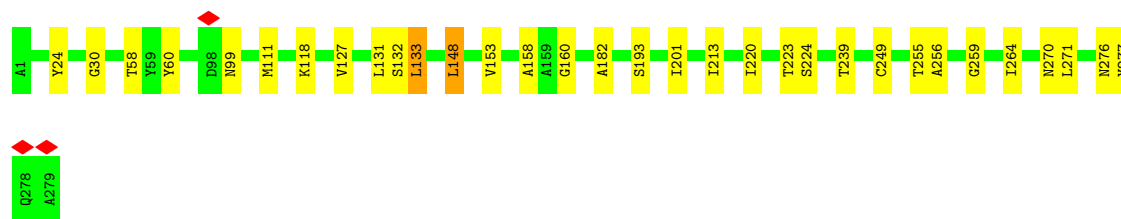


- Molecule 1: Proteinase K



- Molecule 1: Proteinase K

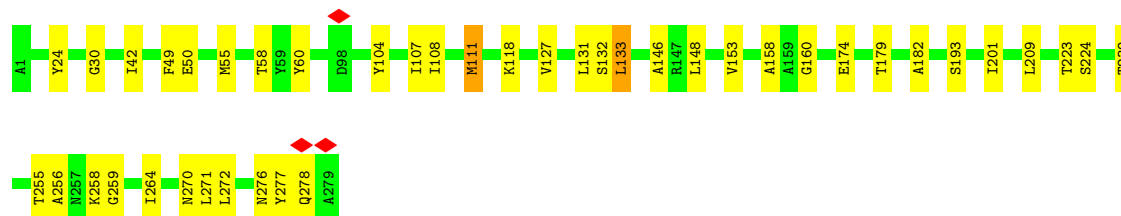
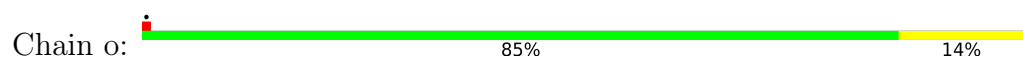




- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



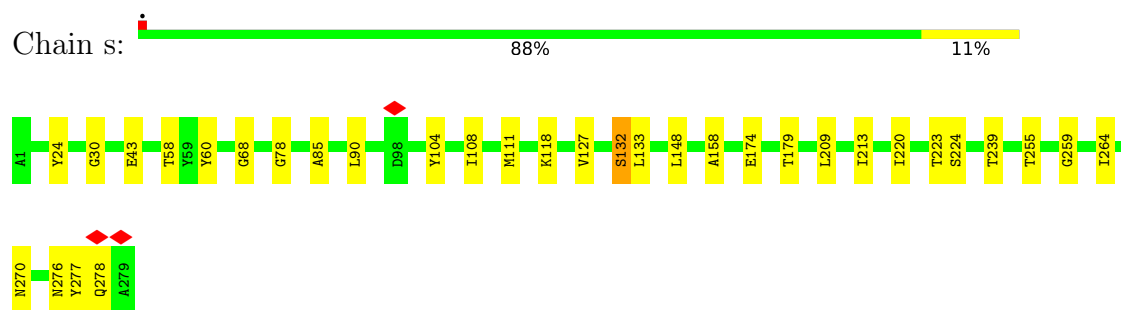
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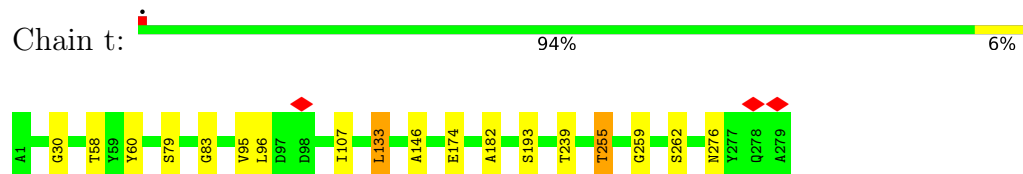
- Molecule 1: Proteinase K



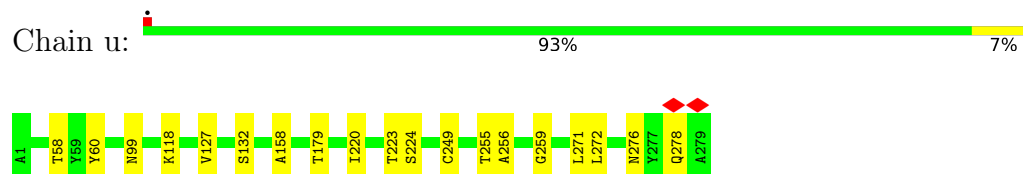
- Molecule 1: Proteinase K



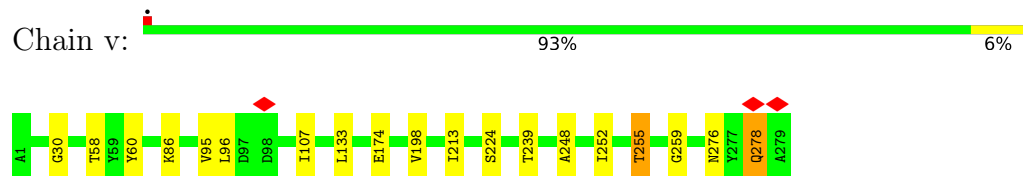
- Molecule 1: Proteinase K



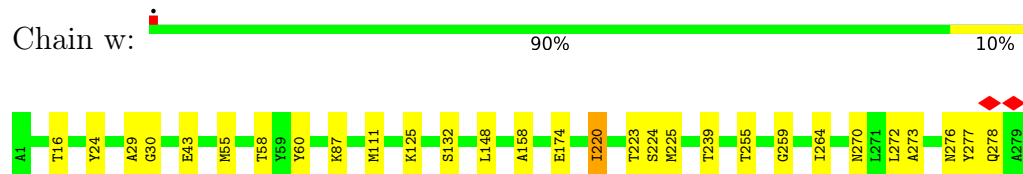
- Molecule 1: Proteinase K



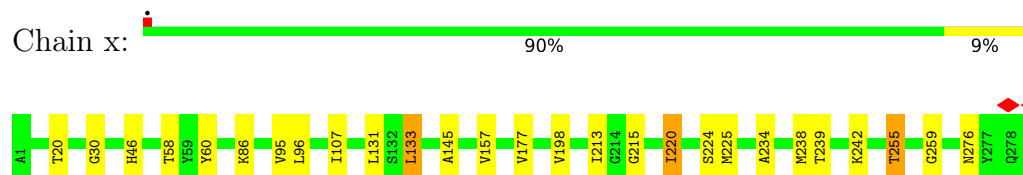
- Molecule 1: Proteinase K



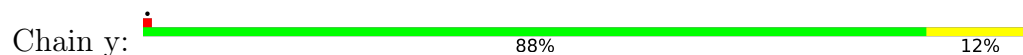
- Molecule 1: Proteinase K

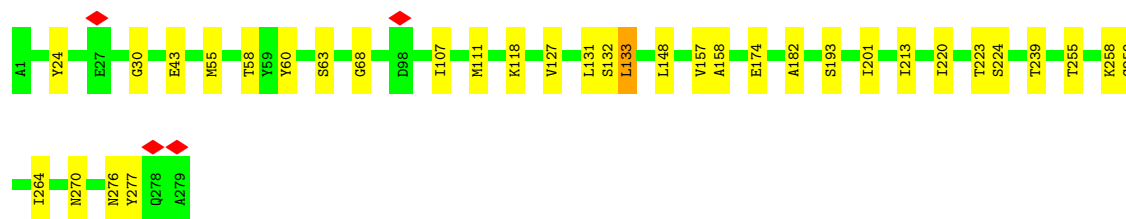


- Molecule 1: Proteinase K



- Molecule 1: Proteinase K

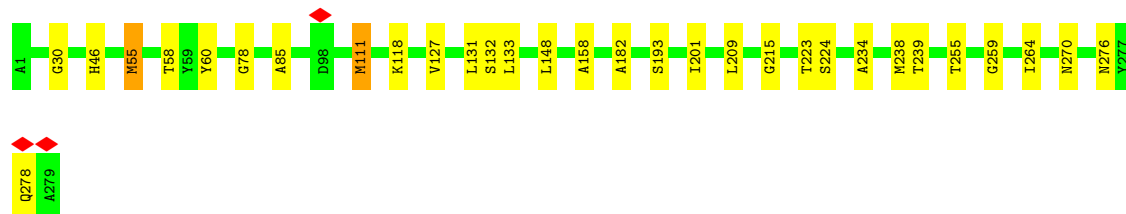
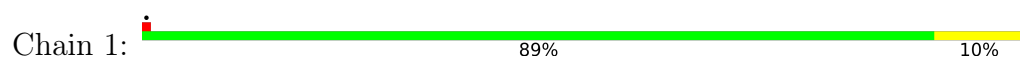




• Molecule 1: Proteinase K



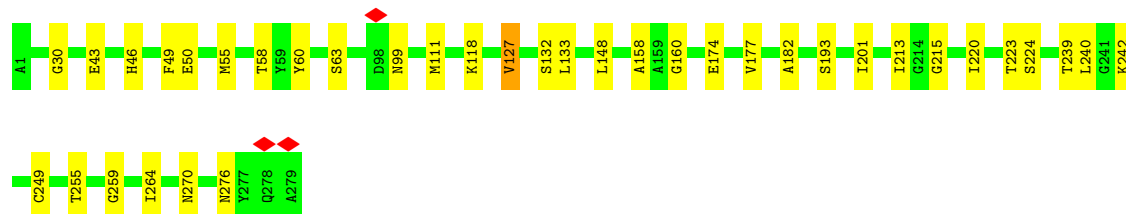
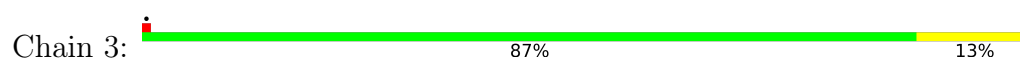
• Molecule 1: Proteinase K



• Molecule 1: Proteinase K



• Molecule 1: Proteinase K

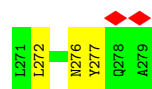
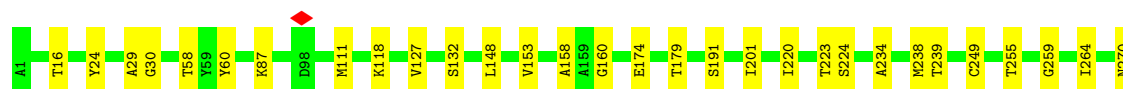
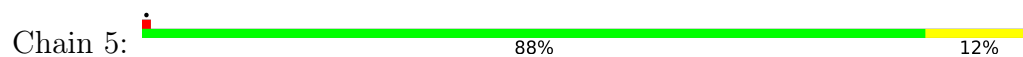


• Molecule 1: Proteinase K





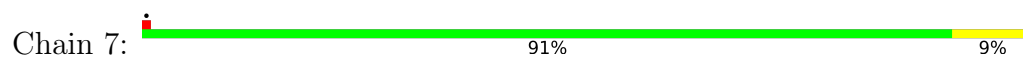
- Molecule 1: Proteinase K



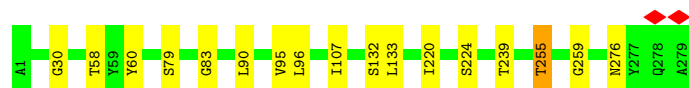
- Molecule 1: Proteinase K



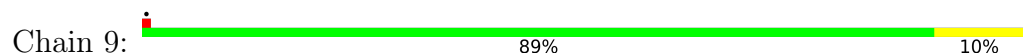
- Molecule 1: Proteinase K



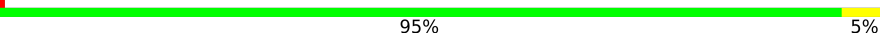
- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K

Chain 0:  95% 5%

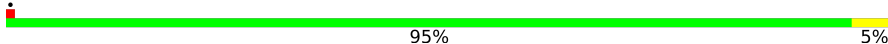


- Molecule 1: Proteinase K

Chain AA:  90% 10%



- Molecule 1: Proteinase K

Chain AB:  95% 5%

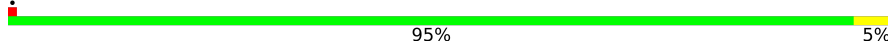


- Molecule 1: Proteinase K

Chain AC:  90% 10%



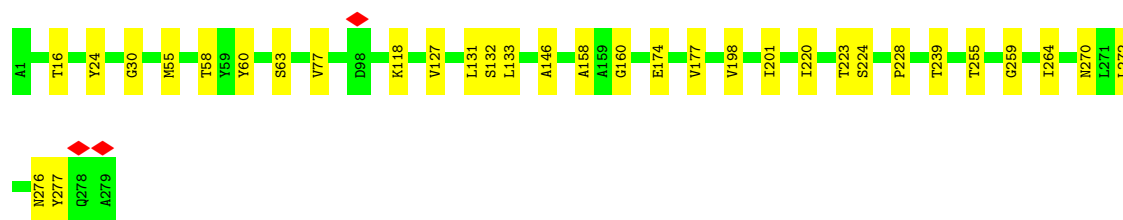
- Molecule 1: Proteinase K

Chain AD:  95% 5%

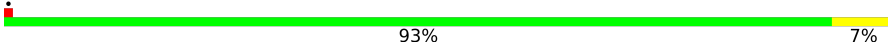


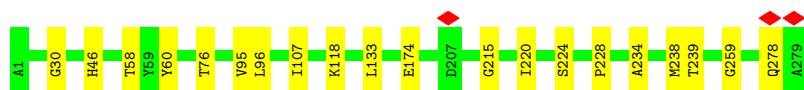
- Molecule 1: Proteinase K

Chain AE:  89% 11%

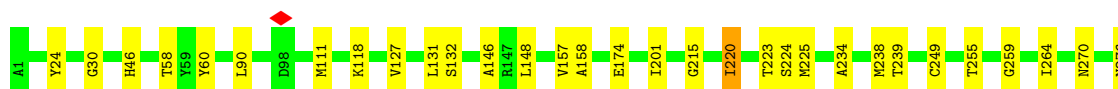


- Molecule 1: Proteinase K

Chain AF:  93% 7%



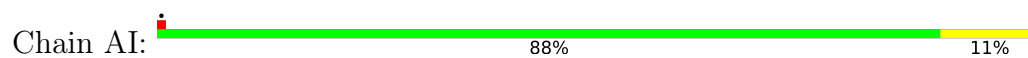
- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



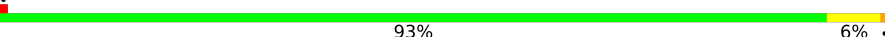
- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



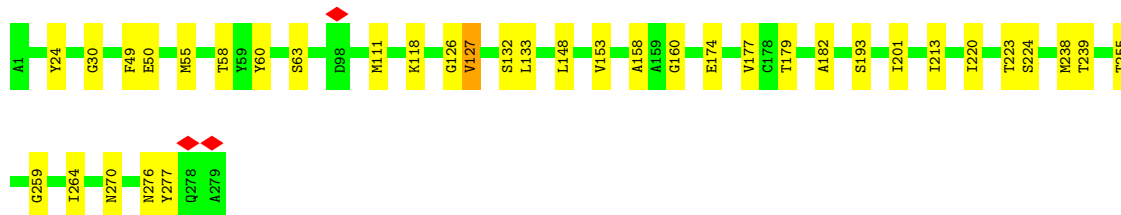
- Molecule 1: Proteinase K

Chain AL:  93% 6%

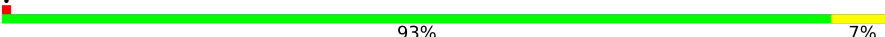


- Molecule 1: Proteinase K

Chain AM:  87% 13%



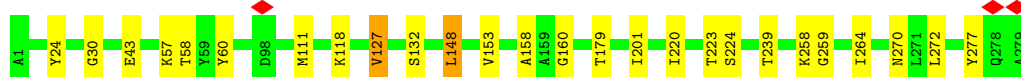
- Molecule 1: Proteinase K

Chain AN:  93% 7%

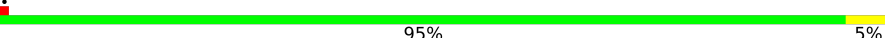


- Molecule 1: Proteinase K

Chain AO:  91% 9%

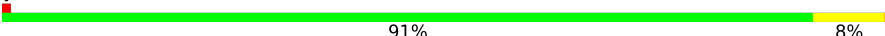


- Molecule 1: Proteinase K

Chain AP:  95% 5%

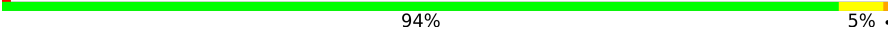


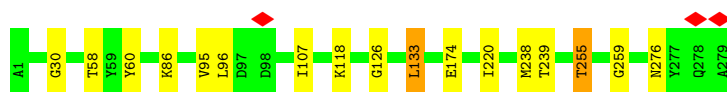
- Molecule 1: Proteinase K

Chain AQ:  91% 8%



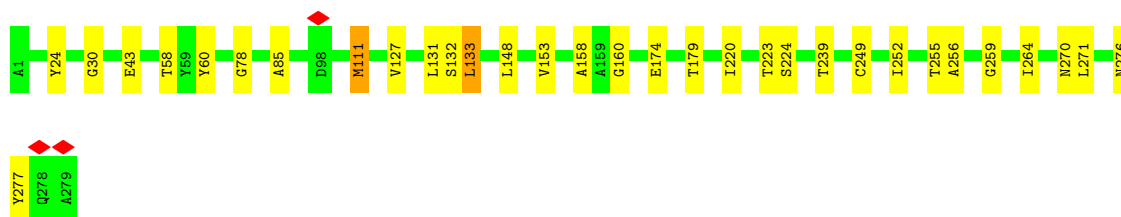
- Molecule 1: Proteinase K

Chain AR:  94% 5%

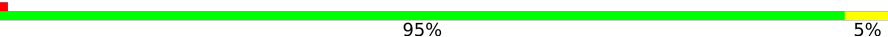


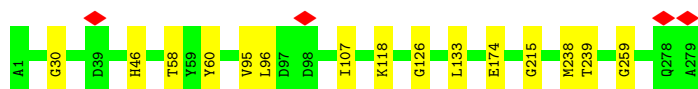
• Molecule 1: Proteinase K

Chain AS:  89% 11%



• Molecule 1: Proteinase K

Chain AT:  95% 5%



• Molecule 1: Proteinase K

Chain AU:  91% 9%



• Molecule 1: Proteinase K

Chain AV:  92% 8%



• Molecule 1: Proteinase K

Chain AW:  89% 10%



• Molecule 1: Proteinase K

Chain AX:  90% 9%



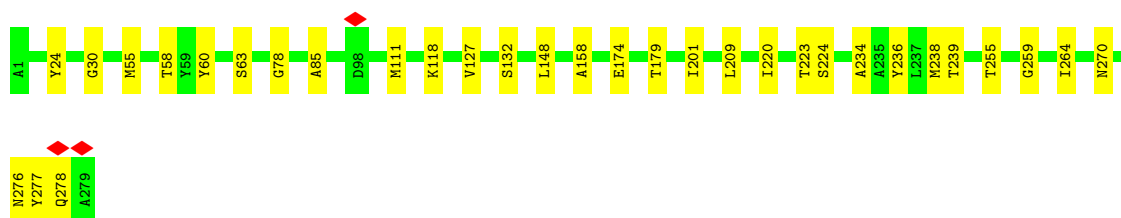
- Molecule 1: Proteinase K



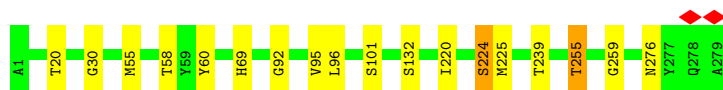
- Molecule 1: Proteinase K



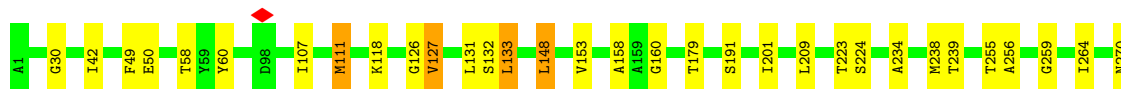
- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K

Chain Ad:  92% 8%



• Molecule 1: Proteinase K

Chain Ae:  90% 9%



• Molecule 1: Proteinase K

Chain Af:  93% 6%

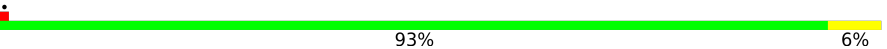


• Molecule 1: Proteinase K

Chain Ag:  91% 9%



• Molecule 1: Proteinase K

Chain Ah:  93% 6%



• Molecule 1: Proteinase K

Chain Ai:  90% 9%

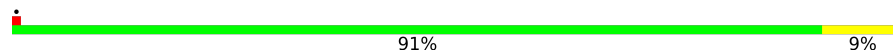


• Molecule 1: Proteinase K

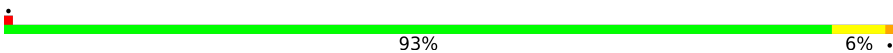
Chain Aj:  91% 9%



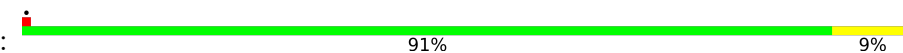
● Molecule 1: Proteinase K

Chain Ak:  91% 9%

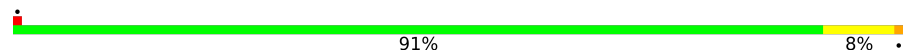
● Molecule 1: Proteinase K

Chain Al:  93% 6%

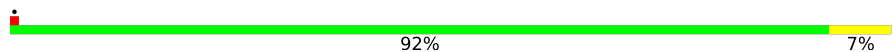
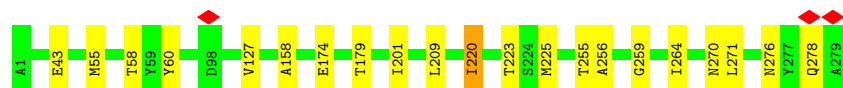
● Molecule 1: Proteinase K

Chain Am:  91% 9%

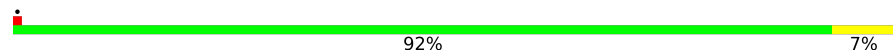
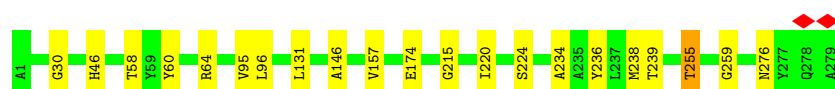
● Molecule 1: Proteinase K

Chain An:  91% 8%

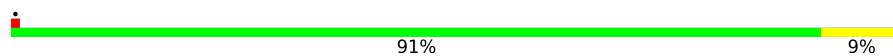
● Molecule 1: Proteinase K

Chain Ao:  92% 7%

● Molecule 1: Proteinase K

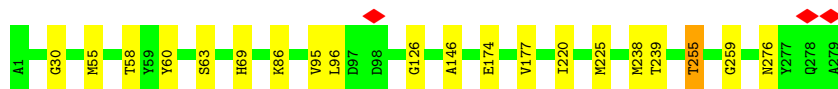
Chain Ap:  92% 7%

● Molecule 1: Proteinase K

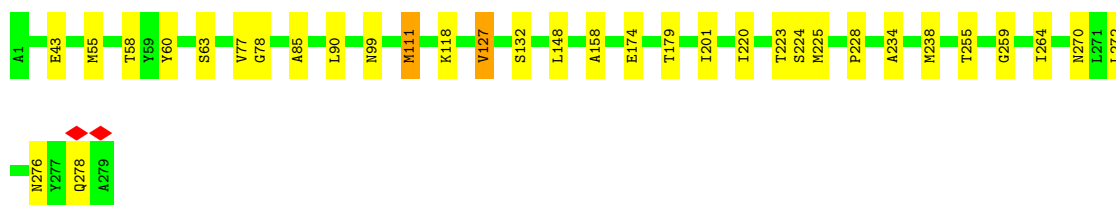
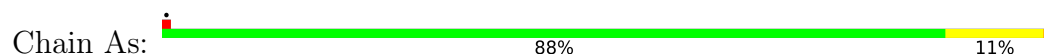
Chain Aq:  91% 9%



- Molecule 1: Proteinase K



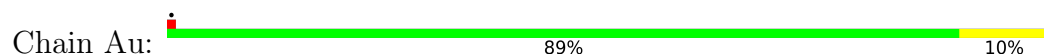
- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



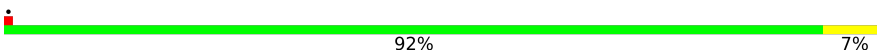
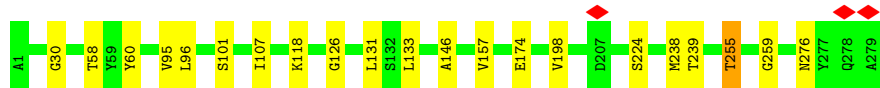
- Molecule 1: Proteinase K



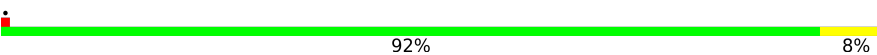
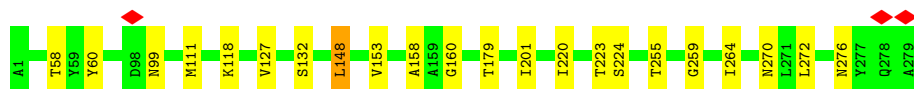
- Molecule 1: Proteinase K



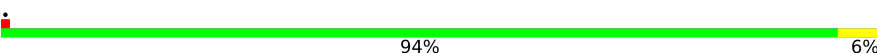
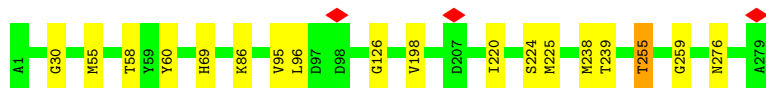
● Molecule 1: Proteinase K

Chain Ax:  92% 7%

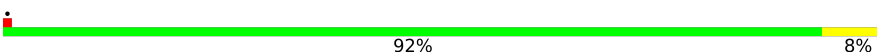
● Molecule 1: Proteinase K

Chain Ay:  92% 8%

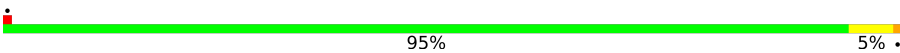
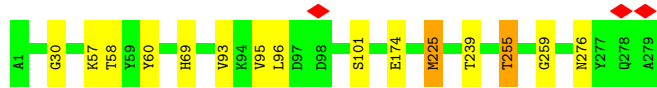
● Molecule 1: Proteinase K

Chain Az:  94% 6%

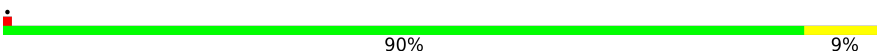
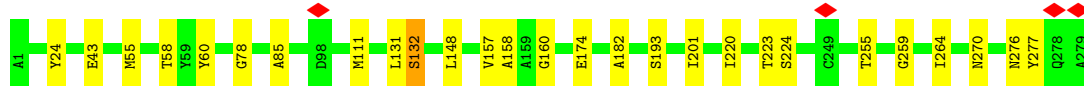
● Molecule 1: Proteinase K

Chain A1:  92% 8%

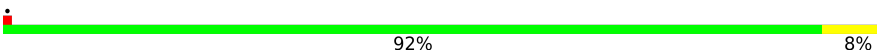
● Molecule 1: Proteinase K

Chain A2:  95% 5%

● Molecule 1: Proteinase K

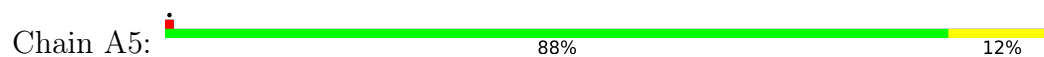
Chain A3:  90% 9%

● Molecule 1: Proteinase K

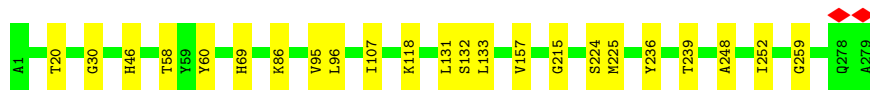
Chain A4:  92% 8%



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



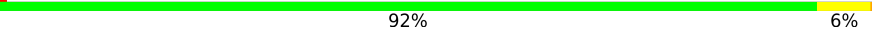
- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



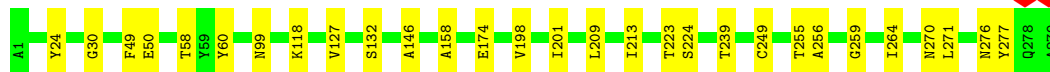
- Molecule 1: Proteinase K

Chain A0:  92% 6%

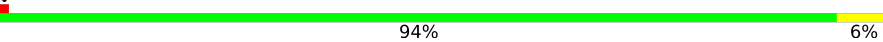


• Molecule 1: Proteinase K

Chain BA:  90% 10%



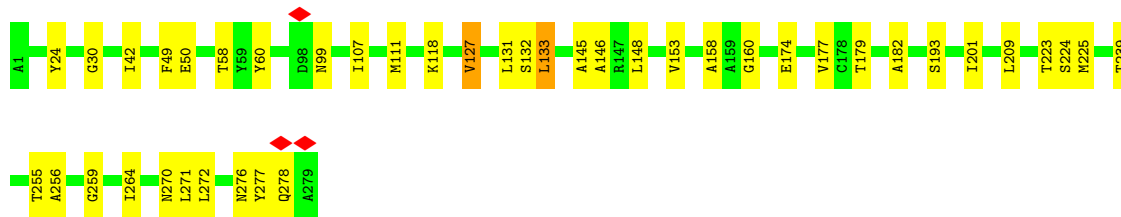
• Molecule 1: Proteinase K

Chain BB:  94% 6%



• Molecule 1: Proteinase K

Chain BC:  85% 14%

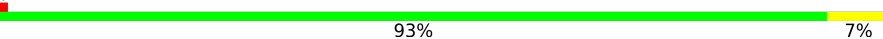


• Molecule 1: Proteinase K

Chain BD:  92% 6%

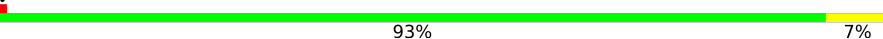


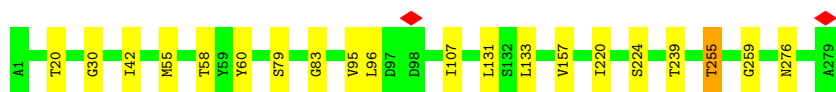
• Molecule 1: Proteinase K

Chain BE:  93% 7%



• Molecule 1: Proteinase K

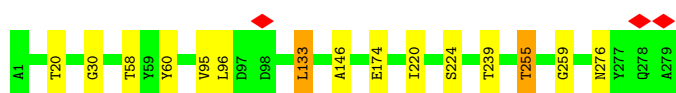
Chain BF:  93% 7%



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K



- Molecule 1: Proteinase K

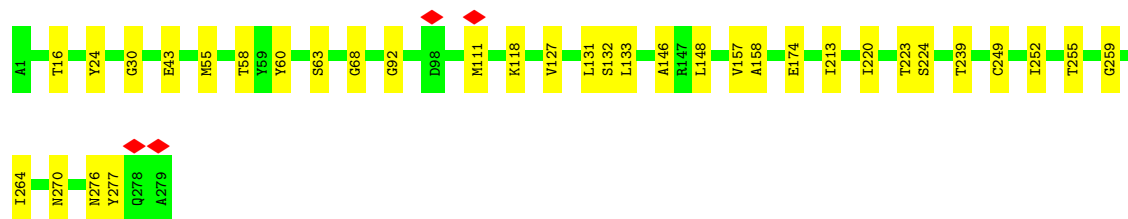


- Molecule 1: Proteinase K



- Molecule 1: Proteinase K

Chain BM:  88% 12%



- Molecule 1: Proteinase K

Chain BN:  90% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-83.72°, rise=8.36 Å, axial sym=C1	Depositor
Number of segments used	55526	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.220	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0457	Depositor
Map size (Å)	568.0, 568.0, 568.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.42, 1.42, 1.42	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0	0.11	0/2070	0.28	0/2813
1	1	0.11	0/2070	0.28	0/2813
1	2	0.10	0/2070	0.27	0/2813
1	3	0.11	0/2070	0.29	0/2813
1	4	0.10	0/2070	0.28	0/2813
1	5	0.11	0/2070	0.28	0/2813
1	6	0.10	0/2070	0.28	0/2813
1	7	0.10	0/2070	0.27	0/2813
1	8	0.10	0/2070	0.27	0/2813
1	9	0.10	0/2070	0.28	0/2813
1	A0	0.11	0/2070	0.29	0/2813
1	A1	0.10	0/2070	0.27	0/2813
1	A2	0.10	0/2070	0.28	0/2813
1	A3	0.10	0/2070	0.28	0/2813
1	A4	0.11	0/2070	0.29	0/2813
1	A5	0.11	0/2070	0.28	0/2813
1	A6	0.10	0/2070	0.27	0/2813
1	A7	0.11	0/2070	0.29	0/2813
1	A8	0.10	0/2070	0.27	0/2813
1	A9	0.11	0/2070	0.28	0/2813
1	AA	0.11	0/2070	0.28	0/2813
1	AB	0.10	0/2070	0.29	0/2813
1	AC	0.11	0/2070	0.30	0/2813
1	AD	0.10	0/2070	0.27	0/2813
1	AE	0.11	0/2070	0.29	0/2813
1	AF	0.11	0/2070	0.31	0/2813
1	AG	0.10	0/2070	0.29	0/2813
1	AH	0.11	0/2070	0.28	0/2813
1	AI	0.11	0/2070	0.28	0/2813
1	AJ	0.10	0/2070	0.28	0/2813
1	AK	0.11	0/2070	0.30	0/2813
1	AL	0.10	0/2070	0.27	0/2813

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AM	0.11	0/2070	0.29	0/2813
1	AN	0.10	0/2070	0.28	0/2813
1	AO	0.10	0/2070	0.27	0/2813
1	AP	0.10	0/2070	0.28	0/2813
1	AQ	0.10	0/2070	0.28	0/2813
1	AR	0.10	0/2070	0.29	0/2813
1	AS	0.11	0/2070	0.29	0/2813
1	AT	0.11	0/2070	0.31	0/2813
1	AU	0.11	0/2070	0.29	0/2813
1	AV	0.10	0/2070	0.28	0/2813
1	AW	0.11	0/2070	0.28	0/2813
1	AX	0.10	0/2070	0.28	0/2813
1	AY	0.11	0/2070	0.28	0/2813
1	AZ	0.11	0/2070	0.28	0/2813
1	Aa	0.11	0/2070	0.29	0/2813
1	Ab	0.10	0/2070	0.27	0/2813
1	Ac	0.11	0/2070	0.29	0/2813
1	Ad	0.10	0/2070	0.27	0/2813
1	Ae	0.11	0/2070	0.30	0/2813
1	Af	0.10	0/2070	0.28	0/2813
1	Ag	0.10	0/2070	0.28	0/2813
1	Ah	0.10	0/2070	0.28	0/2813
1	Ai	0.11	0/2070	0.28	0/2813
1	Aj	0.10	0/2070	0.27	0/2813
1	Ak	0.10	0/2070	0.27	0/2813
1	Al	0.11	0/2070	0.29	0/2813
1	Am	0.10	0/2070	0.28	0/2813
1	An	0.11	0/2070	0.27	0/2813
1	Ao	0.10	0/2070	0.29	0/2813
1	Ap	0.10	0/2070	0.29	0/2813
1	Aq	0.10	0/2070	0.27	0/2813
1	Ar	0.10	0/2070	0.27	0/2813
1	As	0.11	0/2070	0.28	0/2813
1	At	0.10	0/2070	0.28	0/2813
1	Au	0.12	0/2070	0.32	0/2813
1	Av	0.10	0/2070	0.28	0/2813
1	Aw	0.11	0/2070	0.30	0/2813
1	Ax	0.10	0/2070	0.27	0/2813
1	Ay	0.10	0/2070	0.28	0/2813
1	Az	0.10	0/2070	0.27	0/2813
1	BA	0.11	0/2070	0.30	0/2813
1	BB	0.10	0/2070	0.27	0/2813
1	BC	0.12	0/2070	0.30	0/2813

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BD	0.11	0/2070	0.28	0/2813
1	BE	0.10	0/2070	0.28	0/2813
1	BF	0.10	0/2070	0.28	0/2813
1	BG	0.11	0/2070	0.28	0/2813
1	BH	0.10	0/2070	0.27	0/2813
1	BI	0.10	0/2070	0.27	0/2813
1	BJ	0.10	0/2070	0.28	0/2813
1	BK	0.11	0/2070	0.29	0/2813
1	BL	0.10	0/2070	0.27	0/2813
1	BM	0.11	0/2070	0.29	0/2813
1	BN	0.10	0/2070	0.28	0/2813
1	i	0.13	0/2070	0.29	0/2813
1	j	0.10	0/2070	0.27	0/2813
1	k	0.11	0/2070	0.28	0/2813
1	l	0.10	0/2070	0.28	0/2813
1	m	0.10	0/2070	0.27	0/2813
1	n	0.10	0/2070	0.27	0/2813
1	o	0.11	0/2070	0.29	0/2813
1	p	0.10	0/2070	0.28	0/2813
1	q	0.10	0/2070	0.28	0/2813
1	r	0.10	0/2070	0.28	0/2813
1	s	0.11	0/2070	0.28	0/2813
1	t	0.10	0/2070	0.28	0/2813
1	u	0.10	0/2070	0.27	0/2813
1	v	0.12	0/2070	0.30	0/2813
1	w	0.11	0/2070	0.29	0/2813
1	x	0.10	0/2070	0.28	0/2813
1	y	0.11	0/2070	0.28	0/2813
1	z	0.10	0/2070	0.29	0/2813
All	All	0.11	0/215280	0.28	0/292552

There are no bond length outliers.

There are no bond angle outliers.

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	0	2031	0	1934	7	0
1	1	2031	0	1934	19	0
1	2	2031	0	1934	9	0
1	3	2031	0	1934	19	0
1	4	2031	0	1934	9	0
1	5	2031	0	1934	16	0
1	6	2031	0	1934	7	0
1	7	2031	0	1934	13	0
1	8	2031	0	1934	9	0
1	9	2031	0	1934	17	0
1	A0	2031	0	1934	12	0
1	A1	2031	0	1934	12	0
1	A2	2031	0	1934	8	0
1	A3	2031	0	1934	16	0
1	A4	2031	0	1934	10	0
1	A5	2031	0	1934	16	0
1	A6	2031	0	1934	12	0
1	A7	2031	0	1934	19	0
1	A8	2031	0	1934	7	0
1	A9	2031	0	1934	16	0
1	AA	2031	0	1934	13	0
1	AB	2031	0	1934	6	0
1	AC	2031	0	1934	16	0
1	AD	2031	0	1934	5	0
1	AE	2031	0	1934	17	0
1	AF	2031	0	1934	10	0
1	AG	2031	0	1934	17	0
1	AH	2031	0	1934	11	0
1	AI	2031	0	1934	20	0
1	AJ	2031	0	1934	9	0
1	AK	2031	0	1934	19	0
1	AL	2031	0	1934	10	0
1	AM	2031	0	1934	19	0
1	AN	2031	0	1934	8	0
1	AO	2031	0	1934	12	0
1	AP	2031	0	1934	7	0
1	AQ	2031	0	1934	13	0
1	AR	2031	0	1934	9	0
1	AS	2031	0	1934	18	0
1	AT	2031	0	1934	8	0
1	AU	2031	0	1934	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AV	2031	0	1934	11	0
1	AW	2031	0	1934	16	0
1	AX	2031	0	1934	14	0
1	AY	2031	0	1934	16	0
1	AZ	2031	0	1934	12	0
1	Aa	2031	0	1934	18	0
1	Ab	2031	0	1934	8	0
1	Ac	2031	0	1934	18	0
1	Ad	2031	0	1934	11	0
1	Ae	2031	0	1934	13	0
1	Af	2031	0	1934	9	0
1	Ag	2031	0	1934	12	0
1	Ah	2031	0	1934	9	0
1	Ai	2031	0	1934	15	0
1	Aj	2031	0	1934	13	0
1	Ak	2031	0	1934	13	0
1	Al	2031	0	1934	11	0
1	Am	2031	0	1934	14	0
1	An	2031	0	1934	12	0
1	Ao	2031	0	1934	12	0
1	Ap	2031	0	1934	11	0
1	Aq	2031	0	1934	12	0
1	Ar	2031	0	1934	11	0
1	As	2031	0	1934	17	0
1	At	2031	0	1934	10	0
1	Au	2031	0	1934	15	0
1	Av	2031	0	1934	7	0
1	Aw	2031	0	1934	17	0
1	Ax	2031	0	1934	10	0
1	Ay	2031	0	1934	12	0
1	Az	2031	0	1934	8	0
1	BA	2031	0	1934	14	0
1	BB	2031	0	1934	8	0
1	BC	2031	0	1934	23	0
1	BD	2031	0	1934	10	0
1	BE	2031	0	1934	11	0
1	BF	2031	0	1934	9	0
1	BG	2031	0	1934	17	0
1	BH	2031	0	1934	8	0
1	BI	2031	0	1934	12	0
1	BJ	2031	0	1934	9	0
1	BK	2031	0	1934	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BL	2031	0	1934	9	0
1	BM	2031	0	1934	23	0
1	BN	2031	0	1934	12	0
1	i	2031	0	1934	14	0
1	j	2031	0	1934	12	0
1	k	2031	0	1934	22	0
1	l	2031	0	1934	11	0
1	m	2031	0	1934	16	0
1	n	2031	0	1934	7	0
1	o	2031	0	1934	25	0
1	p	2031	0	1934	9	0
1	q	2031	0	1934	10	0
1	r	2031	0	1934	7	0
1	s	2031	0	1934	19	0
1	t	2031	0	1934	10	0
1	u	2031	0	1934	10	0
1	v	2031	0	1934	9	0
1	w	2031	0	1934	18	0
1	x	2031	0	1934	12	0
1	y	2031	0	1934	21	0
1	z	2031	0	1934	10	0
2	0	1	0	0	0	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
2	6	1	0	0	0	0
2	7	1	0	0	0	0
2	8	1	0	0	0	0
2	9	1	0	0	0	0
2	A0	1	0	0	0	0
2	A1	1	0	0	0	0
2	A2	1	0	0	0	0
2	A3	1	0	0	0	0
2	A4	1	0	0	0	0
2	A5	1	0	0	0	0
2	A6	1	0	0	0	0
2	A7	1	0	0	0	0
2	A8	1	0	0	0	0
2	A9	1	0	0	0	0
2	AA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	AD	1	0	0	0	0
2	AE	1	0	0	0	0
2	AF	1	0	0	0	0
2	AG	1	0	0	0	0
2	AH	1	0	0	0	0
2	AI	1	0	0	0	0
2	AJ	1	0	0	0	0
2	AK	1	0	0	0	0
2	AL	1	0	0	0	0
2	AM	1	0	0	0	0
2	AN	1	0	0	0	0
2	AO	1	0	0	0	0
2	AP	1	0	0	0	0
2	AQ	1	0	0	0	0
2	AR	1	0	0	0	0
2	AS	1	0	0	0	0
2	AT	1	0	0	0	0
2	AU	1	0	0	0	0
2	AV	1	0	0	0	0
2	AW	1	0	0	0	0
2	AX	1	0	0	0	0
2	AY	1	0	0	0	0
2	AZ	1	0	0	0	0
2	Aa	1	0	0	0	0
2	Ab	1	0	0	0	0
2	Ac	1	0	0	0	0
2	Ad	1	0	0	0	0
2	Ae	1	0	0	0	0
2	Af	1	0	0	0	0
2	Ag	1	0	0	0	0
2	Ah	1	0	0	0	0
2	Ai	1	0	0	0	0
2	Aj	1	0	0	0	0
2	Ak	1	0	0	0	0
2	Al	1	0	0	0	0
2	Am	1	0	0	0	0
2	An	1	0	0	0	0
2	Ao	1	0	0	0	0
2	Ap	1	0	0	0	0
2	Aq	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ar	1	0	0	0	0
2	As	1	0	0	0	0
2	At	1	0	0	0	0
2	Au	1	0	0	0	0
2	Av	1	0	0	0	0
2	Aw	1	0	0	0	0
2	Ax	1	0	0	0	0
2	Ay	1	0	0	0	0
2	Az	1	0	0	0	0
2	BA	1	0	0	0	0
2	BB	1	0	0	0	0
2	BC	1	0	0	0	0
2	BD	1	0	0	0	0
2	BE	1	0	0	0	0
2	BF	1	0	0	0	0
2	BG	1	0	0	0	0
2	BH	1	0	0	0	0
2	BI	1	0	0	0	0
2	BJ	1	0	0	0	0
2	BK	1	0	0	0	0
2	BL	1	0	0	0	0
2	BM	1	0	0	0	0
2	BN	1	0	0	0	0
2	i	1	0	0	0	0
2	j	1	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	1	0	0	0	0
2	o	1	0	0	0	0
2	p	1	0	0	0	0
2	q	1	0	0	0	0
2	r	1	0	0	0	0
2	s	1	0	0	0	0
2	t	1	0	0	0	0
2	u	1	0	0	0	0
2	v	1	0	0	0	0
2	w	1	0	0	0	0
2	x	1	0	0	0	0
2	y	1	0	0	0	0
2	z	1	0	0	0	0
All	All	211328	0	201136	1272	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 (1272) 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:A4:30:GLY:HA2	1:A4:239:THR:HG21	1.66	0.77
1:BH:255:THR:HG21	1:BH:276:ASN:HD22	1.51	0.76
1:m:132:SER:HB3	1:m:224:SER:HB3	1.68	0.75
1:AK:132:SER:HB3	1:AK:224:SER:HB3	1.70	0.74
1:t:255:THR:HG21	1:t:276:ASN:HD22	1.52	0.73
1:Ah:255:THR:HG21	1:Ah:276:ASN:HD22	1.53	0.73
1:AK:30:GLY:HA2	1:AK:239:THR:HG21	1.70	0.73
1:BA:132:SER:HB3	1:BA:224:SER:HB3	1.71	0.73
1:Ae:132:SER:HB3	1:Ae:224:SER:HB3	1.71	0.72
1:6:255:THR:HG21	1:6:276:ASN:HD22	1.53	0.72
1:At:255:THR:HG21	1:At:276:ASN:HD22	1.53	0.72
1:BD:255:THR:HG21	1:BD:276:ASN:HD22	1.55	0.72
1:BL:255:THR:HG21	1:BL:276:ASN:HD22	1.54	0.72
1:y:132:SER:HB3	1:y:224:SER:HB3	1.72	0.72
1:5:132:SER:HB3	1:5:224:SER:HB3	1.72	0.72
1:An:255:THR:HG21	1:An:276:ASN:HD22	1.54	0.72
1:0:255:THR:HG21	1:0:276:ASN:HD22	1.55	0.71
1:AR:255:THR:HG21	1:AR:276:ASN:HD22	1.53	0.71
1:Ay:111:MET:HG3	1:Ay:148:LEU:HD12	1.72	0.71
1:A4:255:THR:HG21	1:A4:276:ASN:HD22	1.55	0.71
1:n:255:THR:HG21	1:n:276:ASN:HD22	1.55	0.71
1:BJ:255:THR:HG21	1:BJ:276:ASN:HD22	1.54	0.71
1:A2:255:THR:HG21	1:A2:276:ASN:HD22	1.55	0.71
1:x:255:THR:HG21	1:x:276:ASN:HD22	1.56	0.71
1:i:132:SER:HB3	1:i:224:SER:HB3	1.73	0.71
1:AN:255:THR:HG21	1:AN:276:ASN:HD22	1.54	0.71
1:AB:255:THR:HG21	1:AB:276:ASN:HD22	1.55	0.70
1:Ad:255:THR:HG21	1:Ad:276:ASN:HD22	1.56	0.70
1:BN:255:THR:HG21	1:BN:276:ASN:HD22	1.56	0.70
1:p:255:THR:HG21	1:p:276:ASN:HD22	1.56	0.70
1:A9:30:GLY:HA2	1:A9:239:THR:HG21	1.74	0.70
1:Al:255:THR:HG21	1:Al:276:ASN:HD22	1.57	0.69
1:k:131:LEU:HD23	1:k:133:LEU:HD21	1.74	0.69
1:Ab:255:THR:HG21	1:Ab:276:ASN:HD22	1.57	0.69
1:AM:132:SER:HB3	1:AM:224:SER:HB3	1.75	0.69
1:BE:132:SER:HB3	1:BE:224:SER:HB3	1.75	0.69
1:1:133:LEU:HD23	1:1:133:LEU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:255:THR:HG21	1:AP:276:ASN:HD22	1.58	0.69
1:v:255:THR:HG21	1:v:276:ASN:HD22	1.57	0.68
1:Az:255:THR:HG21	1:Az:276:ASN:HD22	1.56	0.68
1:AK:131:LEU:HD23	1:AK:133:LEU:HD21	1.75	0.68
1:AV:255:THR:HG21	1:AV:276:ASN:HD22	1.58	0.68
1:AI:132:SER:HB3	1:AI:224:SER:HB3	1.76	0.68
1:AO:111:MET:HG3	1:AO:148:LEU:HD12	1.75	0.68
1:Ac:132:SER:HB3	1:Ac:224:SER:HB3	1.75	0.68
1:8:255:THR:HG21	1:8:276:ASN:HD22	1.59	0.68
1:AQ:132:SER:HB3	1:AQ:224:SER:HB3	1.74	0.68
1:Ag:132:SER:HB3	1:Ag:224:SER:HB3	1.76	0.68
1:BF:255:THR:HG21	1:BF:276:ASN:HD22	1.57	0.68
1:Al:30:GLY:HA2	1:Al:239:THR:HG21	1.75	0.68
1:Ay:132:SER:HB3	1:Ay:224:SER:HB3	1.76	0.68
1:r:255:THR:HG21	1:r:276:ASN:HD22	1.59	0.67
1:q:132:SER:HB3	1:q:224:SER:HB3	1.76	0.67
1:7:132:SER:HB3	1:7:224:SER:HB3	1.76	0.67
1:AS:131:LEU:HD23	1:AS:133:LEU:HD21	1.75	0.67
1:7:118:LYS:HG3	1:7:127:VAL:HG21	1.77	0.67
1:A3:132:SER:HB3	1:A3:224:SER:HB3	1.76	0.67
1:AI:131:LEU:HD23	1:AI:133:LEU:HD21	1.74	0.67
1:4:255:THR:HG21	1:4:276:ASN:HD22	1.58	0.67
1:AX:255:THR:HG21	1:AX:276:ASN:HD22	1.60	0.67
1:Ai:132:SER:HB3	1:Ai:224:SER:HB3	1.75	0.66
1:Ax:255:THR:HG21	1:Ax:276:ASN:HD22	1.61	0.66
1:BI:132:SER:HB3	1:BI:224:SER:HB3	1.76	0.66
1:AJ:255:THR:HG21	1:AJ:276:ASN:HD22	1.58	0.66
1:v:278:GLN:O	1:v:278:GLN:NE2	2.28	0.66
1:AE:132:SER:HB3	1:AE:224:SER:HB3	1.78	0.66
1:Af:255:THR:HG21	1:Af:276:ASN:HD22	1.61	0.66
1:Ar:255:THR:HG21	1:Ar:276:ASN:HD22	1.59	0.66
1:Ai:118:LYS:HG3	1:Ai:127:VAL:HG21	1.78	0.66
1:A9:132:SER:HB3	1:A9:224:SER:HB3	1.77	0.66
1:j:255:THR:HG21	1:j:276:ASN:HD22	1.60	0.65
1:k:132:SER:HB3	1:k:224:SER:HB3	1.77	0.65
1:2:255:THR:HG21	1:2:276:ASN:HD22	1.61	0.65
1:AE:131:LEU:HD23	1:AE:133:LEU:HD21	1.75	0.65
1:Au:132:SER:HB3	1:Au:224:SER:HB3	1.78	0.65
1:l:255:THR:HG21	1:l:276:ASN:HD22	1.60	0.65
1:AW:131:LEU:HD23	1:AW:133:LEU:HD21	1.78	0.65
1:Ae:111:MET:HG3	1:Ae:148:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BM:133:LEU:HD23	1:BM:133:LEU:H	1.62	0.65
1:u:132:SER:HB3	1:u:224:SER:HB3	1.79	0.65
1:AL:255:THR:HG21	1:AL:276:ASN:HD22	1.62	0.65
1:Ag:131:LEU:HD23	1:Ag:133:LEU:HD21	1.79	0.65
1:Ak:255:THR:HB	1:Ak:276:ASN:HD21	1.62	0.65
1:A7:118:LYS:HG3	1:A7:127:VAL:HG21	1.78	0.65
1:o:118:LYS:HG3	1:o:127:VAL:HG21	1.78	0.65
1:o:132:SER:HB3	1:o:224:SER:HB3	1.78	0.65
1:A1:132:SER:HB3	1:A1:224:SER:HB3	1.78	0.65
1:AA:132:SER:HB3	1:AA:224:SER:HB3	1.79	0.65
1:AE:118:LYS:HG3	1:AE:127:VAL:HG21	1.78	0.65
1:AH:255:THR:HG21	1:AH:276:ASN:HD22	1.61	0.65
1:Aa:132:SER:HB3	1:Aa:224:SER:HB3	1.77	0.65
1:Au:278:GLN:O	1:Au:278:GLN:NE2	2.30	0.65
1:A0:255:THR:HG21	1:A0:276:ASN:HD22	1.60	0.65
1:BC:132:SER:HB3	1:BC:224:SER:HB3	1.79	0.65
1:Ac:111:MET:HG3	1:Ac:148:LEU:HD12	1.78	0.64
1:3:132:SER:HB3	1:3:224:SER:HB3	1.79	0.64
1:i:255:THR:HB	1:i:276:ASN:HD21	1.62	0.64
1:BG:132:SER:HB3	1:BG:224:SER:HB3	1.79	0.64
1:AG:132:SER:HB3	1:AG:224:SER:HB3	1.78	0.64
1:s:118:LYS:HG3	1:s:127:VAL:HG21	1.80	0.64
1:l:118:LYS:HG3	1:l:127:VAL:HG21	1.78	0.64
1:AU:131:LEU:HD23	1:AU:133:LEU:HD21	1.80	0.64
1:Aw:131:LEU:HD23	1:Aw:133:LEU:HD21	1.78	0.64
1:AF:107:ILE:HD13	1:AF:133:LEU:HD22	1.80	0.64
1:AS:132:SER:HB3	1:AS:224:SER:HB3	1.80	0.64
1:BK:132:SER:HB3	1:BK:224:SER:HB3	1.79	0.64
1:z:255:THR:HG21	1:z:276:ASN:HD22	1.63	0.63
1:AG:118:LYS:HG3	1:AG:127:VAL:HG21	1.80	0.63
1:9:132:SER:HB3	1:9:224:SER:HB3	1.81	0.63
1:AK:133:LEU:HD23	1:AK:133:LEU:H	1.63	0.63
1:m:58:THR:HG22	1:m:60:TYR:H	1.63	0.63
1:Aq:132:SER:HB3	1:Aq:224:SER:HB3	1.79	0.63
1:A7:255:THR:HB	1:A7:276:ASN:HD21	1.62	0.63
1:Av:132:SER:HB3	1:Av:224:SER:HB3	1.81	0.63
1:BH:30:GLY:HA2	1:BH:239:THR:HG21	1.79	0.63
1:s:58:THR:HG22	1:s:60:TYR:H	1.64	0.63
1:AE:255:THR:HB	1:AE:276:ASN:HD21	1.62	0.63
1:AI:118:LYS:HG3	1:AI:127:VAL:HG21	1.81	0.63
1:Ac:118:LYS:HG3	1:Ac:127:VAL:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:255:THR:HB	1:AA:276:ASN:HD21	1.64	0.63
1:AW:118:LYS:HG3	1:AW:127:VAL:HG21	1.81	0.63
1:AY:132:SER:HB3	1:AY:224:SER:HB3	1.81	0.63
1:Aq:255:THR:HB	1:Aq:276:ASN:HD21	1.64	0.63
1:BC:107:ILE:HD13	1:BC:133:LEU:HD13	1.81	0.63
1:Aj:30:GLY:HA2	1:Aj:239:THR:HG21	1.81	0.62
1:q:158:ALA:HB1	1:q:223:THR:HG23	1.81	0.62
1:Aw:118:LYS:HG3	1:Aw:127:VAL:HG21	1.80	0.62
1:Ay:118:LYS:HG3	1:Ay:127:VAL:HG21	1.80	0.62
1:BC:118:LYS:HG3	1:BC:127:VAL:HG21	1.80	0.62
1:BG:111:MET:HG3	1:BG:148:LEU:HD12	1.81	0.62
1:BM:132:SER:HB3	1:BM:224:SER:HB3	1.79	0.62
1:AY:111:MET:HG3	1:AY:148:LEU:HD12	1.81	0.62
1:AC:255:THR:HB	1:AC:276:ASN:HD21	1.64	0.62
1:BG:118:LYS:HG3	1:BG:127:VAL:HG21	1.80	0.62
1:k:118:LYS:HG3	1:k:127:VAL:HG21	1.82	0.62
1:AZ:255:THR:HG21	1:AZ:276:ASN:HD22	1.64	0.62
1:9:111:MET:HG3	1:9:148:LEU:HD12	1.82	0.62
1:x:30:GLY:HA2	1:x:239:THR:HG21	1.81	0.62
1:AK:220:ILE:HD11	1:AK:225:MET:HE3	1.82	0.62
1:Ap:255:THR:HG21	1:Ap:276:ASN:HD22	1.65	0.62
1:A4:174:GLU:HB3	1:A4:177:VAL:HG22	1.82	0.62
1:AB:30:GLY:HA2	1:AB:239:THR:HG21	1.81	0.61
1:AI:255:THR:HB	1:AI:276:ASN:HD21	1.65	0.61
1:AO:132:SER:HB3	1:AO:224:SER:HB3	1.82	0.61
1:A7:132:SER:HB3	1:A7:224:SER:HB3	1.82	0.61
1:Ar:30:GLY:HA2	1:Ar:239:THR:HG21	1.81	0.61
1:BG:58:THR:HG22	1:BG:60:TYR:H	1.65	0.61
1:s:255:THR:HB	1:s:276:ASN:HD21	1.65	0.61
1:A9:118:LYS:HG3	1:A9:127:VAL:HG21	1.81	0.61
1:BM:131:LEU:HD23	1:BM:133:LEU:HD21	1.81	0.61
1:A3:255:THR:HB	1:A3:276:ASN:HD21	1.65	0.61
1:9:131:LEU:HD23	1:9:133:LEU:HD21	1.83	0.61
1:AG:255:THR:HB	1:AG:276:ASN:HD21	1.65	0.61
1:AR:58:THR:HG22	1:AR:60:TYR:H	1.64	0.61
1:AW:255:THR:HB	1:AW:276:ASN:HD21	1.66	0.61
1:Ao:255:THR:HB	1:Ao:276:ASN:HD21	1.66	0.61
1:BC:131:LEU:HD23	1:BC:133:LEU:HD21	1.83	0.61
1:BA:255:THR:HB	1:BA:276:ASN:HD21	1.66	0.60
1:y:255:THR:HB	1:y:276:ASN:HD21	1.66	0.60
1:6:107:ILE:HD13	1:6:133:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:30:GLY:HA2	1:An:239:THR:HG21	1.83	0.60
1:i:118:LYS:HG3	1:i:127:VAL:HG21	1.82	0.60
1:AB:126:GLY:HA3	1:AB:238:MET:HE1	1.84	0.60
1:A5:255:THR:HB	1:A5:276:ASN:HD21	1.66	0.60
1:3:118:LYS:HG3	1:3:127:VAL:HG21	1.83	0.60
1:5:111:MET:HG3	1:5:148:LEU:HD12	1.82	0.60
1:AY:255:THR:HB	1:AY:276:ASN:HD21	1.66	0.60
1:A9:255:THR:HB	1:A9:276:ASN:HD21	1.65	0.60
1:Ae:58:THR:HG22	1:Ae:60:TYR:H	1.67	0.60
1:Aa:118:LYS:HG3	1:Aa:127:VAL:HG21	1.82	0.60
1:Aq:118:LYS:HG3	1:Aq:127:VAL:HG21	1.82	0.60
1:BA:118:LYS:HG3	1:BA:127:VAL:HG21	1.84	0.60
1:3:255:THR:HB	1:3:276:ASN:HD21	1.67	0.60
1:Ai:255:THR:HB	1:Ai:276:ASN:HD21	1.66	0.60
1:Aj:126:GLY:HA3	1:Aj:238:MET:HE1	1.84	0.60
1:BL:259:GLY:HA3	1:BM:259:GLY:HA3	1.83	0.60
1:BJ:259:GLY:HA3	1:BK:259:GLY:HA3	1.84	0.59
1:AC:118:LYS:HG3	1:AC:127:VAL:HG21	1.85	0.59
1:Ae:158:ALA:HB1	1:Ae:223:THR:HG23	1.85	0.59
1:1:131:LEU:HD23	1:1:133:LEU:HD21	1.84	0.59
1:AM:118:LYS:HG3	1:AM:127:VAL:HG21	1.84	0.59
1:Ay:255:THR:HB	1:Ay:276:ASN:HD21	1.66	0.59
1:Ae:255:THR:HB	1:Ae:276:ASN:HD21	1.66	0.59
1:Ah:107:ILE:HD13	1:Ah:133:LEU:HD22	1.83	0.59
1:1:111:MET:HG3	1:1:148:LEU:HD12	1.84	0.59
1:m:111:MET:HG3	1:m:148:LEU:HD12	1.84	0.59
1:t:58:THR:HG22	1:t:60:TYR:H	1.68	0.59
1:u:118:LYS:HG3	1:u:127:VAL:HG21	1.85	0.59
1:t:30:GLY:HA2	1:t:239:THR:HG21	1.85	0.59
1:v:58:THR:HG22	1:v:60:TYR:H	1.68	0.58
1:As:118:LYS:HG3	1:As:127:VAL:HG21	1.85	0.58
1:Aw:58:THR:HG22	1:Aw:60:TYR:H	1.67	0.58
1:A5:132:SER:HB3	1:A5:224:SER:HB3	1.85	0.58
1:BK:255:THR:HB	1:BK:276:ASN:HD21	1.67	0.58
1:v:259:GLY:HA3	1:w:259:GLY:HA3	1.83	0.58
1:BE:158:ALA:HB1	1:BE:223:THR:HG23	1.85	0.58
1:1:132:SER:HB3	1:1:224:SER:HB3	1.84	0.58
1:Ap:259:GLY:HA3	1:Aq:259:GLY:HA3	1.85	0.58
1:s:132:SER:HB3	1:s:224:SER:HB3	1.84	0.58
1:x:259:GLY:HA3	1:y:259:GLY:HA3	1.84	0.58
1:6:58:THR:HG22	1:6:60:TYR:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:158:ALA:HB1	1:AA:223:THR:HG23	1.86	0.58
1:AI:158:ALA:HB1	1:AI:223:THR:HG23	1.86	0.58
1:AK:118:LYS:HG3	1:AK:127:VAL:HG21	1.85	0.58
1:AW:132:SER:HB3	1:AW:224:SER:HB3	1.86	0.58
1:Ak:132:SER:HB3	1:Ak:224:SER:HB3	1.84	0.58
1:A8:30:GLY:HA2	1:A8:239:THR:HG21	1.86	0.58
1:AZ:58:THR:HG22	1:AZ:60:TYR:H	1.69	0.58
1:Ag:158:ALA:HB1	1:Ag:223:THR:HG23	1.85	0.58
1:BJ:58:THR:HG22	1:BJ:60:TYR:H	1.69	0.58
1:w:255:THR:HB	1:w:276:ASN:HD21	1.68	0.58
1:AF:259:GLY:HA3	1:AG:259:GLY:HA3	1.85	0.58
1:u:255:THR:HB	1:u:276:ASN:HD21	1.68	0.58
1:5:255:THR:HB	1:5:276:ASN:HD21	1.68	0.58
1:AO:158:ALA:HB1	1:AO:223:THR:HG23	1.86	0.58
1:y:118:LYS:HG3	1:y:127:VAL:HG21	1.85	0.57
1:AQ:158:ALA:HB1	1:AQ:223:THR:HG23	1.86	0.57
1:AQ:255:THR:HB	1:AQ:276:ASN:HD21	1.70	0.57
1:As:132:SER:HB3	1:As:224:SER:HB3	1.84	0.57
1:BM:255:THR:HB	1:BM:276:ASN:HD21	1.69	0.57
1:9:158:ALA:HB1	1:9:223:THR:HG23	1.86	0.57
1:AU:132:SER:HB3	1:AU:224:SER:HB3	1.85	0.57
1:An:259:GLY:HA3	1:Ao:259:GLY:HA3	1.86	0.57
1:o:158:ALA:HB1	1:o:223:THR:HG23	1.85	0.57
1:v:30:GLY:HA2	1:v:239:THR:HG21	1.86	0.57
1:AV:58:THR:HG22	1:AV:60:TYR:H	1.70	0.57
1:AY:58:THR:HG22	1:AY:60:TYR:H	1.69	0.57
1:A6:58:THR:HG22	1:A6:60:TYR:H	1.70	0.57
1:BM:118:LYS:HG3	1:BM:127:VAL:HG21	1.87	0.57
1:i:278:GLN:O	1:i:278:GLN:NE2	2.36	0.57
1:1:255:THR:HB	1:1:276:ASN:HD21	1.69	0.57
1:AM:58:THR:HG22	1:AM:60:TYR:H	1.70	0.57
1:AO:58:THR:HG22	1:AO:60:TYR:H	1.69	0.57
1:BJ:30:GLY:HA2	1:BJ:239:THR:HG21	1.86	0.57
1:x:220:ILE:HD12	1:x:225:MET:HE3	1.86	0.57
1:Ax:259:GLY:HA3	1:Ay:259:GLY:HA3	1.87	0.57
1:A4:259:GLY:HA3	1:A5:259:GLY:HA3	1.86	0.57
1:0:58:THR:HG22	1:0:60:TYR:H	1.69	0.57
1:AD:259:GLY:HA3	1:AE:259:GLY:HA3	1.86	0.57
1:BE:264:ILE:HD11	1:BE:270:ASN:HD22	1.69	0.57
1:BL:58:THR:HG22	1:BL:60:TYR:H	1.69	0.57
1:AO:127:VAL:HB	1:AO:153:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:158:ALA:HB1	1:Ai:223:THR:HG23	1.86	0.56
1:BA:58:THR:HG22	1:BA:60:TYR:H	1.70	0.56
1:BC:158:ALA:HB1	1:BC:223:THR:HG23	1.87	0.56
1:Am:255:THR:HB	1:Am:276:ASN:HD21	1.69	0.56
1:As:255:THR:HB	1:As:276:ASN:HD21	1.70	0.56
1:o:58:THR:HG22	1:o:60:TYR:H	1.69	0.56
1:3:111:MET:HG3	1:3:148:LEU:HD22	1.88	0.56
1:AR:107:ILE:HD13	1:AR:133:LEU:HD22	1.86	0.56
1:Aw:132:SER:HB3	1:Aw:224:SER:HB3	1.88	0.56
1:A3:158:ALA:HB1	1:A3:223:THR:HG23	1.87	0.56
1:BM:111:MET:HG3	1:BM:148:LEU:HD22	1.87	0.56
1:AB:259:GLY:HA3	1:AC:259:GLY:HA3	1.86	0.56
1:Au:111:MET:HG3	1:Au:148:LEU:HD12	1.87	0.56
1:BG:158:ALA:HB1	1:BG:223:THR:HG23	1.88	0.56
1:j:132:SER:HB3	1:j:224:SER:HB3	1.86	0.56
1:Aa:30:GLY:HA2	1:Aa:239:THR:HG21	1.87	0.56
1:Aj:255:THR:HG21	1:Aj:276:ASN:HD22	1.69	0.56
1:Av:58:THR:HG22	1:Av:60:TYR:H	1.71	0.56
1:x:58:THR:HG22	1:x:60:TYR:H	1.71	0.56
1:AE:58:THR:HG22	1:AE:60:TYR:H	1.71	0.56
1:Aa:255:THR:HB	1:Aa:276:ASN:HD21	1.70	0.56
1:Au:118:LYS:HG3	1:Au:127:VAL:HG21	1.87	0.56
1:Au:264:ILE:HD11	1:Au:270:ASN:HD22	1.70	0.56
1:A6:259:GLY:HA3	1:A7:259:GLY:HA3	1.87	0.56
1:8:132:SER:HB3	1:8:224:SER:HB3	1.87	0.56
1:A1:158:ALA:HB1	1:A1:223:THR:HG23	1.88	0.56
1:m:118:LYS:HG3	1:m:127:VAL:HG21	1.88	0.56
1:AN:58:THR:HG22	1:AN:60:TYR:H	1.71	0.56
1:A4:58:THR:HG22	1:A4:60:TYR:H	1.71	0.56
1:A0:259:GLY:HA3	1:BA:259:GLY:HA3	1.88	0.56
1:BK:158:ALA:HB1	1:BK:223:THR:HG23	1.88	0.56
1:AX:58:THR:HG22	1:AX:60:TYR:H	1.71	0.56
1:AY:133:LEU:H	1:AY:133:LEU:HD23	1.71	0.56
1:0:259:GLY:HA3	1:AA:259:GLY:HA3	1.86	0.55
1:Ab:132:SER:HB3	1:Ab:224:SER:HB3	1.87	0.55
1:BB:259:GLY:HA3	1:BC:259:GLY:HA3	1.88	0.55
1:w:111:MET:HG3	1:w:148:LEU:HD22	1.89	0.55
1:Ag:127:VAL:HB	1:Ag:153:VAL:HG22	1.88	0.55
1:Al:58:THR:HG22	1:Al:60:TYR:H	1.72	0.55
1:Ao:58:THR:HG22	1:Ao:60:TYR:H	1.72	0.55
1:Ac:158:ALA:HB1	1:Ac:223:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AV:259:GLY:HA3	1:AW:259:GLY:HA3	1.88	0.55
1:Ay:58:THR:HG22	1:Ay:60:TYR:H	1.71	0.55
1:7:264:ILE:HD11	1:7:270:ASN:HD22	1.72	0.55
1:AH:58:THR:HG22	1:AH:60:TYR:H	1.72	0.55
1:BA:158:ALA:HB1	1:BA:223:THR:HG23	1.89	0.55
1:BI:158:ALA:HB1	1:BI:223:THR:HG23	1.88	0.55
1:AL:132:SER:HB3	1:AL:224:SER:HB3	1.89	0.55
1:l:58:THR:HG22	1:l:60:TYR:H	1.72	0.55
1:4:58:THR:HG22	1:4:60:TYR:H	1.70	0.55
1:Aw:160:GLY:H	1:Aw:223:THR:HG21	1.71	0.55
1:z:259:GLY:HA3	1:1:259:GLY:HA3	1.89	0.55
1:AY:158:ALA:HB1	1:AY:223:THR:HG23	1.89	0.55
1:A9:58:THR:HG22	1:A9:60:TYR:H	1.71	0.55
1:BA:264:ILE:HD11	1:BA:270:ASN:HD22	1.72	0.55
1:x:131:LEU:HB2	1:x:157:VAL:HG12	1.88	0.54
1:AR:259:GLY:HA3	1:AS:259:GLY:HA3	1.89	0.54
1:Ax:131:LEU:HB2	1:Ax:157:VAL:HG12	1.89	0.54
1:5:118:LYS:HG3	1:5:127:VAL:HG21	1.89	0.54
1:AD:58:THR:HG22	1:AD:60:TYR:H	1.72	0.54
1:Ay:158:ALA:HB1	1:Ay:223:THR:HG23	1.88	0.54
1:l:259:GLY:HA3	1:m:259:GLY:HA3	1.90	0.54
1:r:259:GLY:HA3	1:s:259:GLY:HA3	1.88	0.54
1:2:259:GLY:HA3	1:3:259:GLY:HA3	1.88	0.54
1:AP:259:GLY:HA3	1:AQ:259:GLY:HA3	1.88	0.54
1:AX:259:GLY:HA3	1:AY:259:GLY:HA3	1.88	0.54
1:AY:131:LEU:HD23	1:AY:133:LEU:HD21	1.88	0.54
1:Ar:259:GLY:HA3	1:As:259:GLY:HA3	1.88	0.54
1:q:264:ILE:HD11	1:q:270:ASN:HD22	1.71	0.54
1:AG:158:ALA:HB1	1:AG:223:THR:HG23	1.90	0.54
1:Am:132:SER:HB3	1:Am:224:SER:HB3	1.89	0.54
1:Ar:58:THR:HG22	1:Ar:60:TYR:H	1.72	0.54
1:BI:58:THR:HG22	1:BI:60:TYR:H	1.73	0.54
1:4:259:GLY:HA3	1:5:259:GLY:HA3	1.90	0.54
1:A0:30:GLY:HA2	1:A0:239:THR:HG21	1.88	0.54
1:o:160:GLY:H	1:o:223:THR:HG21	1.73	0.54
1:y:111:MET:HG3	1:y:148:LEU:HD22	1.90	0.54
1:A3:111:MET:HG3	1:A3:148:LEU:HD22	1.90	0.54
1:m:264:ILE:HD11	1:m:270:ASN:HD22	1.72	0.54
1:8:259:GLY:HA3	1:9:259:GLY:HA3	1.89	0.54
1:Ay:264:ILE:HD11	1:Ay:270:ASN:HD22	1.73	0.54
1:A7:58:THR:HG22	1:A7:60:TYR:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A8:259:GLY:HA3	1:A9:259:GLY:HA3	1.89	0.54
1:BG:264:ILE:HD11	1:BG:270:ASN:HD22	1.72	0.54
1:k:158:ALA:HB1	1:k:223:THR:HG23	1.89	0.54
1:u:158:ALA:HB1	1:u:223:THR:HG23	1.90	0.54
1:AM:126:GLY:HA3	1:AM:238:MET:HE1	1.90	0.54
1:AS:158:ALA:HB1	1:AS:223:THR:HG23	1.90	0.54
1:AT:259:GLY:HA3	1:AU:259:GLY:HA3	1.89	0.54
1:w:58:THR:HG22	1:w:60:TYR:H	1.73	0.54
1:Ab:259:GLY:HA3	1:Ac:259:GLY:HA3	1.90	0.54
1:Ak:158:ALA:HB1	1:Ak:223:THR:HG23	1.90	0.54
1:j:259:GLY:HA3	1:k:259:GLY:HA3	1.89	0.53
1:s:158:ALA:HB1	1:s:223:THR:HG23	1.90	0.53
1:y:158:ALA:HB1	1:y:223:THR:HG23	1.89	0.53
1:3:158:ALA:HB1	1:3:223:THR:HG23	1.90	0.53
1:AT:58:THR:HG22	1:AT:60:TYR:H	1.74	0.53
1:AY:30:GLY:HA2	1:AY:239:THR:HG21	1.89	0.53
1:AZ:259:GLY:HA3	1:Aa:259:GLY:HA3	1.90	0.53
1:Ac:58:THR:HG22	1:Ac:60:TYR:H	1.73	0.53
1:BF:259:GLY:HA3	1:BG:259:GLY:HA3	1.89	0.53
1:5:158:ALA:HB1	1:5:223:THR:HG23	1.90	0.53
1:AA:58:THR:HG22	1:AA:60:TYR:H	1.72	0.53
1:AM:111:MET:HG3	1:AM:148:LEU:HD22	1.88	0.53
1:AU:255:THR:HB	1:AU:276:ASN:HD21	1.72	0.53
1:AC:58:THR:HG22	1:AC:60:TYR:H	1.73	0.53
1:AS:255:THR:HB	1:AS:276:ASN:HD21	1.72	0.53
1:Az:259:GLY:HA3	1:A1:259:GLY:HA3	1.88	0.53
1:BB:58:THR:HG22	1:BB:60:TYR:H	1.73	0.53
1:Aw:133:LEU:HD23	1:Aw:133:LEU:H	1.72	0.53
1:AQ:264:ILE:HD11	1:AQ:270:ASN:HD22	1.74	0.53
1:A0:58:THR:HG22	1:A0:60:TYR:H	1.73	0.53
1:AK:264:ILE:HD11	1:AK:270:ASN:HD22	1.73	0.53
1:Ao:220:ILE:HD12	1:Ao:225:MET:HE3	1.91	0.53
1:A1:58:THR:HG22	1:A1:60:TYR:H	1.73	0.53
1:BC:255:THR:HB	1:BC:276:ASN:HD21	1.73	0.53
1:BN:30:GLY:HA2	1:BN:239:THR:HG21	1.90	0.53
1:o:264:ILE:HD11	1:o:270:ASN:HD22	1.73	0.53
1:u:58:THR:HG22	1:u:60:TYR:H	1.74	0.53
1:AL:259:GLY:HA3	1:AM:259:GLY:HA3	1.91	0.53
1:Ak:264:ILE:HD11	1:Ak:270:ASN:HD22	1.74	0.53
1:A5:58:THR:HG22	1:A5:60:TYR:H	1.74	0.53
1:AH:259:GLY:HA3	1:AI:259:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:131:LEU:HD23	1:Ac:133:LEU:HD21	1.91	0.52
1:Af:259:GLY:HA3	1:Ag:259:GLY:HA3	1.91	0.52
1:BB:132:SER:HB3	1:BB:224:SER:HB3	1.90	0.52
1:n:58:THR:HG22	1:n:60:TYR:H	1.74	0.52
1:AG:220:ILE:HD12	1:AG:225:MET:HE3	1.91	0.52
1:Aj:107:ILE:HD13	1:Aj:133:LEU:HD22	1.91	0.52
1:Ay:127:VAL:HB	1:Ay:153:VAL:HG22	1.91	0.52
1:i:58:THR:HG22	1:i:60:TYR:H	1.74	0.52
1:9:255:THR:HB	1:9:276:ASN:HD21	1.74	0.52
1:m:158:ALA:HB1	1:m:223:THR:HG23	1.92	0.52
1:AM:158:ALA:HB1	1:AM:223:THR:HG23	1.91	0.52
1:AA:264:ILE:HD11	1:AA:270:ASN:HD22	1.74	0.52
1:l:132:SER:HB3	1:l:224:SER:HB3	1.92	0.52
1:q:58:THR:HG22	1:q:60:TYR:H	1.75	0.52
1:2:126:GLY:HA3	1:2:238:MET:HE1	1.90	0.52
1:Ag:58:THR:HG22	1:Ag:60:TYR:H	1.74	0.52
1:Ah:259:GLY:HA3	1:Ai:259:GLY:HA3	1.90	0.52
1:Ai:127:VAL:HB	1:Ai:153:VAL:HG22	1.91	0.52
1:As:58:THR:HG22	1:As:60:TYR:H	1.74	0.52
1:As:111:MET:HG3	1:As:148:LEU:HD22	1.92	0.52
1:A3:58:THR:HG22	1:A3:60:TYR:H	1.74	0.52
1:i:158:ALA:HB1	1:i:223:THR:HG23	1.92	0.52
1:s:264:ILE:HD11	1:s:270:ASN:HD22	1.74	0.52
1:w:220:ILE:HD12	1:w:225:MET:HE3	1.92	0.52
1:5:58:THR:HG22	1:5:60:TYR:H	1.74	0.52
1:AL:58:THR:HG22	1:AL:60:TYR:H	1.75	0.52
1:AO:264:ILE:HD11	1:AO:270:ASN:HD22	1.75	0.52
1:Al:259:GLY:HA3	1:Am:259:GLY:HA3	1.91	0.52
1:Ao:158:ALA:HB1	1:Ao:223:THR:HG23	1.92	0.52
1:BE:160:GLY:H	1:BE:223:THR:HG21	1.75	0.52
1:k:182:ALA:HB3	1:k:193:SER:HB2	1.92	0.52
1:AI:111:MET:HG3	1:AI:148:LEU:HD22	1.90	0.52
1:AU:158:ALA:HB1	1:AU:223:THR:HG23	1.92	0.52
1:AX:126:GLY:HA3	1:AX:238:MET:HE1	1.91	0.52
1:Aw:255:THR:HB	1:Aw:276:ASN:HD21	1.74	0.52
1:AC:132:SER:HB3	1:AC:224:SER:HB3	1.90	0.52
1:AQ:58:THR:HG22	1:AQ:60:TYR:H	1.75	0.52
1:Aw:264:ILE:HD11	1:Aw:270:ASN:HD22	1.75	0.52
1:BH:58:THR:HG22	1:BH:60:TYR:H	1.74	0.52
1:p:259:GLY:HA3	1:q:259:GLY:HA3	1.91	0.52
1:At:58:THR:HG22	1:At:60:TYR:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:158:ALA:HB1	1:A5:223:THR:HG23	1.91	0.52
1:j:255:THR:HG21	1:j:276:ASN:ND2	2.25	0.51
1:n:259:GLY:HA3	1:o:259:GLY:HA3	1.91	0.51
1:AE:158:ALA:HB1	1:AE:223:THR:HG23	1.91	0.51
1:Ax:146:ALA:HB2	1:Ax:174:GLU:OE1	2.10	0.51
1:t:259:GLY:HA3	1:u:259:GLY:HA3	1.91	0.51
1:AF:58:THR:HG22	1:AF:60:TYR:H	1.76	0.51
1:Ag:264:ILE:HD11	1:Ag:270:ASN:HD22	1.74	0.51
1:Az:30:GLY:HA2	1:Az:239:THR:HG21	1.92	0.51
1:BC:58:THR:HG22	1:BC:60:TYR:H	1.76	0.51
1:p:58:THR:HG22	1:p:60:TYR:H	1.74	0.51
1:7:160:GLY:H	1:7:223:THR:HG21	1.74	0.51
1:BL:131:LEU:HB2	1:BL:157:VAL:HG12	1.91	0.51
1:5:127:VAL:HB	1:5:153:VAL:HG22	1.91	0.51
1:Ah:30:GLY:HA2	1:Ah:239:THR:HG21	1.92	0.51
1:Am:111:MET:HG3	1:Am:148:LEU:HD22	1.93	0.51
1:Aw:158:ALA:HB1	1:Aw:223:THR:HG23	1.90	0.51
1:BH:259:GLY:HA3	1:BI:259:GLY:HA3	1.92	0.51
1:AM:182:ALA:HB3	1:AM:193:SER:HB2	1.92	0.51
1:Ac:107:ILE:HD13	1:Ac:133:LEU:HD13	1.91	0.51
1:Ap:58:THR:HG22	1:Ap:60:TYR:H	1.75	0.51
1:BA:30:GLY:HA2	1:BA:239:THR:HG21	1.93	0.51
1:BE:127:VAL:HB	1:BE:153:VAL:HG22	1.93	0.51
1:Af:58:THR:HG22	1:Af:60:TYR:H	1.76	0.51
1:w:132:SER:HB3	1:w:224:SER:HB3	1.92	0.51
1:3:58:THR:HG22	1:3:60:TYR:H	1.76	0.51
1:AF:278:GLN:N	1:AF:278:GLN:OE1	2.44	0.51
1:AS:58:THR:HG22	1:AS:60:TYR:H	1.76	0.51
1:k:58:THR:HG22	1:k:60:TYR:H	1.76	0.51
1:6:259:GLY:HA3	1:7:259:GLY:HA3	1.92	0.51
1:9:58:THR:HG22	1:9:60:TYR:H	1.76	0.51
1:AK:158:ALA:HB1	1:AK:223:THR:HG23	1.92	0.51
1:Aq:30:GLY:HA2	1:Aq:239:THR:HG21	1.93	0.51
1:A9:234:ALA:O	1:A9:238:MET:HG3	2.10	0.51
1:A0:132:SER:HB3	1:A0:224:SER:HB3	1.92	0.51
1:BG:104:TYR:O	1:BG:108:ILE:HD12	2.11	0.51
1:1:264:ILE:HD11	1:1:270:ASN:HD22	1.75	0.51
1:m:131:LEU:HD23	1:m:133:LEU:HD21	1.93	0.51
1:p:30:GLY:HA2	1:p:239:THR:HG21	1.93	0.51
1:x:234:ALA:O	1:x:238:MET:HG3	2.11	0.51
1:y:55:MET:HE1	1:y:63:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:58:THR:HG22	1:AG:60:TYR:H	1.76	0.51
1:Al:278:GLN:N	1:Al:278:GLN:OE1	2.44	0.51
1:BD:58:THR:HG22	1:BD:60:TYR:H	1.75	0.51
1:k:234:ALA:O	1:k:238:MET:HG3	2.11	0.50
1:l:58:THR:HG22	1:l:60:TYR:H	1.76	0.50
1:Al:58:THR:HG22	1:Al:60:TYR:H	1.75	0.50
1:As:220:ILE:HD11	1:As:225:MET:HE3	1.94	0.50
1:BN:58:THR:HG22	1:BN:60:TYR:H	1.76	0.50
1:Aj:259:GLY:HA3	1:Ak:259:GLY:HA3	1.93	0.50
1:Ax:58:THR:HG22	1:Ax:60:TYR:H	1.76	0.50
1:k:255:THR:HB	1:k:276:ASN:HD21	1.76	0.50
1:AW:58:THR:HG22	1:AW:60:TYR:H	1.77	0.50
1:Aa:158:ALA:HB1	1:Aa:223:THR:HG23	1.93	0.50
1:Ak:58:THR:HG22	1:Ak:60:TYR:H	1.77	0.50
1:A2:58:THR:HG22	1:A2:60:TYR:H	1.76	0.50
1:y:68:GLY:HA2	1:y:213:ILE:HG23	1.94	0.50
1:l:158:ALA:HB1	1:l:223:THR:HG23	1.94	0.50
1:Aq:264:ILE:HD11	1:Aq:270:ASN:HD22	1.76	0.50
1:At:259:GLY:HA3	1:Au:259:GLY:HA3	1.93	0.50
1:A6:132:SER:HB3	1:A6:224:SER:HB3	1.93	0.50
1:8:95:VAL:HG23	1:8:96:LEU:HG	1.94	0.50
1:AG:234:ALA:O	1:AG:238:MET:HG3	2.12	0.50
1:Ae:234:ALA:O	1:Ae:238:MET:HG3	2.11	0.50
1:Am:158:ALA:HB1	1:Am:223:THR:HG23	1.94	0.50
1:A6:95:VAL:HG23	1:A6:96:LEU:HG	1.94	0.50
1:A8:131:LEU:HB2	1:A8:157:VAL:HG12	1.93	0.50
1:A9:158:ALA:HB1	1:A9:223:THR:HG23	1.93	0.50
1:Ab:58:THR:HG22	1:Ab:60:TYR:H	1.77	0.50
1:Ae:264:ILE:HD11	1:Ae:270:ASN:HD22	1.77	0.50
1:BC:264:ILE:HD11	1:BC:270:ASN:HD22	1.76	0.50
1:Az:69:HIS:CE1	1:Az:225:MET:HE1	2.47	0.50
1:6:95:VAL:HG23	1:6:96:LEU:HG	1.94	0.49
1:AG:264:ILE:HD11	1:AG:270:ASN:HD22	1.77	0.49
1:Ac:255:THR:HB	1:Ac:276:ASN:HD21	1.77	0.49
1:2:58:THR:HG22	1:2:60:TYR:H	1.76	0.49
1:3:264:ILE:HD11	1:3:270:ASN:HD22	1.78	0.49
1:AK:182:ALA:HB3	1:AK:193:SER:HB2	1.94	0.49
1:y:182:ALA:HB3	1:y:193:SER:HB2	1.93	0.49
1:y:264:ILE:HD11	1:y:270:ASN:HD22	1.78	0.49
1:AH:255:THR:HG21	1:AH:276:ASN:ND2	2.27	0.49
1:AK:58:THR:HG22	1:AK:60:TYR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:158:ALA:HB1	1:As:223:THR:HG23	1.94	0.49
1:BM:158:ALA:HB1	1:BM:223:THR:HG23	1.93	0.49
1:w:30:GLY:HA2	1:w:239:THR:HG21	1.93	0.49
1:AL:107:ILE:HD13	1:AL:133:LEU:HD22	1.94	0.49
1:AQ:118:LYS:HG3	1:AQ:127:VAL:HG21	1.95	0.49
1:AW:133:LEU:HD23	1:AW:133:LEU:H	1.77	0.49
1:AZ:255:THR:HG21	1:AZ:276:ASN:ND2	2.28	0.49
1:Au:158:ALA:HB1	1:Au:223:THR:HG23	1.94	0.49
1:BE:58:THR:HG22	1:BE:60:TYR:H	1.78	0.49
1:AJ:259:GLY:HA3	1:AK:259:GLY:HA3	1.95	0.49
1:Aj:255:THR:HG21	1:Aj:276:ASN:ND2	2.27	0.49
1:Aq:58:THR:HG22	1:Aq:60:TYR:H	1.77	0.49
1:A0:255:THR:HG21	1:A0:276:ASN:ND2	2.27	0.49
1:BK:58:THR:HG22	1:BK:60:TYR:H	1.76	0.49
1:r:107:ILE:HD13	1:r:133:LEU:HD22	1.93	0.49
1:y:24:TYR:HB3	1:y:277:TYR:HD2	1.78	0.49
1:5:234:ALA:O	1:5:238:MET:HG3	2.11	0.49
1:o:127:VAL:HB	1:o:153:VAL:HG22	1.94	0.49
1:z:30:GLY:HA2	1:z:239:THR:HG21	1.95	0.49
1:AK:174:GLU:OE1	1:AK:174:GLU:HA	2.12	0.49
1:AS:264:ILE:HD11	1:AS:270:ASN:HD22	1.78	0.49
1:Au:118:LYS:HE2	1:Au:118:LYS:HB3	1.58	0.49
1:A1:104:TYR:O	1:A1:108:ILE:HG13	2.12	0.49
1:AE:77:VAL:HG22	1:AE:228:PRO:HB3	1.95	0.49
1:Ad:58:THR:HG22	1:Ad:60:TYR:H	1.78	0.49
1:Am:264:ILE:HD11	1:Am:270:ASN:HD22	1.78	0.49
1:Aq:158:ALA:HB1	1:Aq:223:THR:HG23	1.95	0.49
1:A7:220:ILE:HD12	1:A7:225:MET:HE3	1.94	0.49
1:z:58:THR:HG22	1:z:60:TYR:H	1.77	0.49
1:7:158:ALA:HB1	1:7:223:THR:HG23	1.94	0.49
1:AA:131:LEU:HB2	1:AA:157:VAL:HG12	1.95	0.49
1:AC:158:ALA:HB1	1:AC:223:THR:HG23	1.95	0.49
1:AI:264:ILE:HD11	1:AI:270:ASN:HD22	1.77	0.49
1:AJ:58:THR:HG22	1:AJ:60:TYR:H	1.78	0.49
1:AO:30:GLY:HA2	1:AO:239:THR:HG21	1.94	0.49
1:AF:30:GLY:HA2	1:AF:239:THR:HG21	1.95	0.49
1:AM:55:MET:HE1	1:AM:63:SER:O	2.13	0.49
1:AS:30:GLY:HA2	1:AS:239:THR:HG21	1.95	0.49
1:AW:264:ILE:HD11	1:AW:270:ASN:HD22	1.78	0.49
1:Ap:131:LEU:HB2	1:Ap:157:VAL:HG12	1.94	0.49
1:Ap:146:ALA:HB2	1:Ap:174:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:58:THR:HG22	1:AU:60:TYR:H	1.77	0.49
1:A7:68:GLY:HA2	1:A7:213:ILE:HG23	1.94	0.49
1:BI:264:ILE:HD11	1:BI:270:ASN:HD22	1.77	0.48
1:AU:174:GLU:HA	1:AU:174:GLU:OE1	2.13	0.48
1:BN:234:ALA:O	1:BN:238:MET:HG3	2.13	0.48
1:l:255:THR:HG21	1:l:276:ASN:ND2	2.27	0.48
1:m:30:GLY:HA2	1:m:239:THR:HG21	1.96	0.48
1:q:160:GLY:H	1:q:223:THR:HG21	1.79	0.48
1:Ap:30:GLY:HA2	1:Ap:239:THR:HG21	1.96	0.48
1:A2:95:VAL:HG23	1:A2:96:LEU:HG	1.94	0.48
1:5:30:GLY:HA2	1:5:239:THR:HG21	1.95	0.48
1:AV:30:GLY:HA2	1:AV:239:THR:HG21	1.94	0.48
1:AI:264:ILE:HD11	1:AI:270:ASN:HD22	1.78	0.48
1:BJ:95:VAL:HG23	1:BJ:96:LEU:HG	1.95	0.48
1:AO:160:GLY:H	1:AO:223:THR:HG21	1.78	0.48
1:Aa:234:ALA:O	1:Aa:238:MET:HG3	2.13	0.48
1:Ad:259:GLY:HA3	1:Ae:259:GLY:HA3	1.94	0.48
1:Av:131:LEU:HB2	1:Av:157:VAL:HG12	1.95	0.48
1:A6:30:GLY:HA2	1:A6:239:THR:HG21	1.95	0.48
1:7:58:THR:HG22	1:7:60:TYR:H	1.78	0.48
1:AB:58:THR:HG22	1:AB:60:TYR:H	1.78	0.48
1:AP:58:THR:HG22	1:AP:60:TYR:H	1.78	0.48
1:AY:234:ALA:O	1:AY:238:MET:HG3	2.14	0.48
1:A2:259:GLY:HA3	1:A3:259:GLY:HA3	1.94	0.48
1:BC:111:MET:HG3	1:BC:148:LEU:HD22	1.95	0.48
1:BF:107:ILE:HD13	1:BF:133:LEU:HD22	1.94	0.48
1:y:58:THR:HG22	1:y:60:TYR:H	1.78	0.48
1:1:55:MET:HB2	1:1:55:MET:HE2	1.71	0.48
1:AI:55:MET:HE1	1:AI:63:SER:O	2.14	0.48
1:AT:30:GLY:HA2	1:AT:239:THR:HG21	1.95	0.48
1:AM:264:ILE:HD11	1:AM:270:ASN:HD22	1.78	0.48
1:Al:220:ILE:HD11	1:Al:225:MET:HE3	1.95	0.48
1:Ap:255:THR:HG21	1:Ap:276:ASN:ND2	2.27	0.48
1:BA:118:LYS:HB3	1:BA:118:LYS:HE2	1.57	0.48
1:BC:118:LYS:HB3	1:BC:118:LYS:HE2	1.56	0.48
1:BM:24:TYR:HB3	1:BM:277:TYR:HD2	1.79	0.48
1:i:30:GLY:HA2	1:i:239:THR:HG21	1.96	0.48
1:m:127:VAL:HB	1:m:153:VAL:HG22	1.95	0.48
1:Ar:55:MET:HE1	1:Ar:63:SER:O	2.14	0.48
1:j:107:ILE:HD13	1:j:133:LEU:HD22	1.96	0.48
1:AG:30:GLY:HA2	1:AG:239:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:69:HIS:CE1	1:Aj:225:MET:HE1	2.48	0.48
1:BG:30:GLY:HA2	1:BG:239:THR:HG21	1.96	0.48
1:o:104:TYR:O	1:o:108:ILE:HD12	2.14	0.47
1:z:255:THR:HG21	1:z:276:ASN:ND2	2.27	0.47
1:0:30:GLY:HA2	1:0:239:THR:HG21	1.96	0.47
1:AM:127:VAL:HB	1:AM:153:VAL:HG22	1.96	0.47
1:AR:126:GLY:HA3	1:AR:238:MET:HE1	1.95	0.47
1:A8:107:ILE:HD13	1:A8:133:LEU:HD22	1.97	0.47
1:BM:58:THR:HG22	1:BM:60:TYR:H	1.78	0.47
1:s:174:GLU:OE1	1:s:174:GLU:HA	2.14	0.47
1:3:55:MET:HE1	1:3:63:SER:O	2.14	0.47
1:4:95:VAL:HG23	1:4:96:LEU:HG	1.96	0.47
1:AK:234:ALA:O	1:AK:238:MET:HG3	2.14	0.47
1:AN:259:GLY:HA3	1:AO:259:GLY:HA3	1.95	0.47
1:A1:182:ALA:HB3	1:A1:193:SER:HB2	1.96	0.47
1:A1:264:ILE:HD11	1:A1:270:ASN:HD22	1.79	0.47
1:AZ:256:ALA:HB3	1:AZ:271:LEU:HD22	1.96	0.47
1:At:69:HIS:CE1	1:At:225:MET:HE1	2.49	0.47
1:s:118:LYS:HB3	1:s:118:LYS:HE2	1.57	0.47
1:A8:95:VAL:HG23	1:A8:96:LEU:HG	1.96	0.47
1:BG:174:GLU:HA	1:BG:174:GLU:OE1	2.15	0.47
1:5:264:ILE:HD11	1:5:270:ASN:HD22	1.80	0.47
1:AC:264:ILE:HD11	1:AC:270:ASN:HD22	1.79	0.47
1:AM:118:LYS:HB3	1:AM:118:LYS:HE2	1.56	0.47
1:AY:264:ILE:HD11	1:AY:270:ASN:HD22	1.79	0.47
1:Ad:30:GLY:HA2	1:Ad:239:THR:HG21	1.95	0.47
1:Av:146:ALA:HB2	1:Av:174:GLU:OE2	2.14	0.47
1:A9:182:ALA:HB3	1:A9:193:SER:HB2	1.96	0.47
1:j:55:MET:HE1	1:j:63:SER:O	2.14	0.47
1:s:111:MET:HG3	1:s:148:LEU:HD22	1.96	0.47
1:AZ:107:ILE:HD13	1:AZ:133:LEU:HD22	1.96	0.47
1:An:133:LEU:H	1:An:133:LEU:HD23	1.80	0.47
1:Au:24:TYR:HB3	1:Au:277:TYR:HD2	1.79	0.47
1:A5:30:GLY:HA2	1:A5:239:THR:HG21	1.96	0.47
1:A7:118:LYS:HE2	1:A7:118:LYS:HB3	1.61	0.47
1:2:30:GLY:HA2	1:2:239:THR:HG21	1.97	0.47
1:8:79:SER:H	1:8:83:GLY:HA3	1.79	0.47
1:AR:95:VAL:HG23	1:AR:96:LEU:HG	1.96	0.47
1:An:107:ILE:HD13	1:An:133:LEU:HD13	1.97	0.47
1:A1:118:LYS:HG3	1:A1:127:VAL:HG21	1.97	0.47
1:A7:30:GLY:HA2	1:A7:239:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:69:HIS:CE1	1:BD:225:MET:HE1	2.50	0.47
1:7:255:THR:HB	1:7:276:ASN:HD21	1.79	0.47
1:AH:256:ALA:HB3	1:AH:271:LEU:HD22	1.96	0.47
1:Aa:58:THR:HG22	1:Aa:60:TYR:H	1.78	0.47
1:A3:55:MET:HE2	1:A3:55:MET:HB3	1.74	0.47
1:p:69:HIS:CE1	1:p:225:MET:HE1	2.50	0.47
1:1:30:GLY:HA2	1:1:239:THR:HG21	1.96	0.47
1:2:69:HIS:CE1	1:2:225:MET:HE1	2.50	0.47
1:AH:95:VAL:HG23	1:AH:96:LEU:HG	1.97	0.47
1:AL:30:GLY:HA2	1:AL:239:THR:HG21	1.96	0.47
1:AL:69:HIS:CE1	1:AL:225:MET:HE1	2.50	0.47
1:Aj:79:SER:H	1:Aj:83:GLY:HA3	1.80	0.47
1:Av:259:GLY:HA3	1:Aw:259:GLY:HA3	1.96	0.47
1:A7:158:ALA:HB1	1:A7:223:THR:HG23	1.96	0.47
1:1:118:LYS:HB3	1:1:118:LYS:HE2	1.58	0.46
1:2:255:THR:HG21	1:2:276:ASN:ND2	2.28	0.46
1:AS:111:MET:HG3	1:AS:148:LEU:HD12	1.97	0.46
1:AU:58:THR:HG22	1:AU:60:TYR:H	1.80	0.46
1:Ah:132:SER:HB3	1:Ah:224:SER:HB2	1.96	0.46
1:Ap:95:VAL:HG23	1:Ap:96:LEU:HG	1.97	0.46
1:BC:30:GLY:HA2	1:BC:239:THR:HG21	1.97	0.46
1:o:49:PHE:C	1:o:50:GLU:OE1	2.59	0.46
1:w:55:MET:HE2	1:w:55:MET:HB2	1.78	0.46
1:Ae:30:GLY:HA2	1:Ae:239:THR:HG21	1.97	0.46
1:Aj:58:THR:HG22	1:Aj:60:TYR:H	1.80	0.46
1:Aq:234:ALA:O	1:Aq:238:MET:HG3	2.15	0.46
1:Az:95:VAL:HG23	1:Az:96:LEU:HG	1.96	0.46
1:A3:255:THR:HB	1:A3:276:ASN:ND2	2.30	0.46
1:A5:264:ILE:HD11	1:A5:270:ASN:HD22	1.81	0.46
1:A7:111:MET:HG3	1:A7:148:LEU:HD22	1.97	0.46
1:AE:30:GLY:HA2	1:AE:239:THR:HG21	1.97	0.46
1:AI:24:TYR:HB3	1:AI:277:TYR:HD2	1.80	0.46
1:AK:49:PHE:C	1:AK:50:GLU:OE2	2.58	0.46
1:AW:220:ILE:HD12	1:AW:225:MET:HE3	1.96	0.46
1:Al:255:THR:HG21	1:Al:276:ASN:ND2	2.28	0.46
1:m:118:LYS:HB3	1:m:118:LYS:HE2	1.60	0.46
1:q:111:MET:HG3	1:q:148:LEU:HD12	1.97	0.46
1:u:256:ALA:HB3	1:u:271:LEU:HD22	1.97	0.46
1:9:104:TYR:O	1:9:108:ILE:HG13	2.15	0.46
1:AJ:256:ALA:HB3	1:AJ:271:LEU:HD22	1.98	0.46
1:Al:107:ILE:HD13	1:Al:133:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:126:GLY:HA3	1:A5:238:MET:HE1	1.96	0.46
1:s:30:GLY:HA2	1:s:239:THR:HG21	1.98	0.46
1:AA:146:ALA:HB2	1:AA:174:GLU:OE1	2.16	0.46
1:AI:133:LEU:H	1:AI:133:LEU:HD23	1.81	0.46
1:AZ:30:GLY:HA2	1:AZ:239:THR:HG21	1.98	0.46
1:Az:58:THR:HG22	1:Az:60:TYR:H	1.81	0.46
1:A0:256:ALA:HB3	1:A0:271:LEU:HD22	1.98	0.46
1:Af:255:THR:HG21	1:Af:276:ASN:ND2	2.30	0.46
1:At:107:ILE:HD13	1:At:133:LEU:HD22	1.98	0.46
1:Au:30:GLY:HA2	1:Au:239:THR:HG21	1.98	0.46
1:BK:264:ILE:HD11	1:BK:270:ASN:HD22	1.80	0.46
1:j:58:THR:HG22	1:j:60:TYR:H	1.80	0.46
1:0:107:ILE:HD13	1:0:133:LEU:HD13	1.97	0.46
1:AE:118:LYS:HB3	1:AE:118:LYS:HE2	1.55	0.46
1:AJ:126:GLY:HA3	1:AJ:238:MET:HE1	1.98	0.46
1:AL:255:THR:HG21	1:AL:276:ASN:ND2	2.30	0.46
1:Ah:58:THR:HG22	1:Ah:60:TYR:H	1.81	0.46
1:A9:24:TYR:HB3	1:A9:277:TYR:HD2	1.80	0.46
1:BE:111:MET:HG3	1:BE:148:LEU:HD12	1.97	0.46
1:i:234:ALA:O	1:i:238:MET:HG3	2.16	0.46
1:o:256:ALA:HB3	1:o:271:LEU:HD22	1.98	0.46
1:s:68:GLY:HA2	1:s:213:ILE:HG23	1.97	0.46
1:AC:24:TYR:HB3	1:AC:277:TYR:HD2	1.81	0.46
1:AW:158:ALA:HB1	1:AW:223:THR:HG23	1.98	0.46
1:A4:234:ALA:O	1:A4:238:MET:HG3	2.15	0.46
1:A5:24:TYR:HB3	1:A5:277:TYR:HD2	1.80	0.46
1:BD:259:GLY:HA3	1:BE:259:GLY:HA3	1.97	0.46
1:7:30:GLY:HA2	1:7:239:THR:HG21	1.97	0.46
1:AJ:69:HIS:CE1	1:AJ:225:MET:HE1	2.51	0.46
1:AP:255:THR:HG21	1:AP:276:ASN:ND2	2.29	0.46
1:AZ:126:GLY:HA3	1:AZ:238:MET:HE1	1.98	0.46
1:Ap:234:ALA:O	1:Ap:238:MET:HG3	2.16	0.46
1:4:255:THR:HG21	1:4:276:ASN:ND2	2.30	0.45
1:AH:30:GLY:HA2	1:AH:239:THR:HG21	1.98	0.45
1:AV:234:ALA:O	1:AV:238:MET:HG3	2.16	0.45
1:Ad:95:VAL:HG23	1:Ad:96:LEU:HG	1.98	0.45
1:Al:95:VAL:HG23	1:Al:96:LEU:HG	1.98	0.45
1:As:55:MET:HE1	1:As:63:SER:O	2.16	0.45
1:A4:107:ILE:HD13	1:A4:133:LEU:HD22	1.98	0.45
1:m:256:ALA:HB3	1:m:271:LEU:HD22	1.99	0.45
1:o:182:ALA:HB3	1:o:193:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:30:GLY:HA2	1:AR:239:THR:HG21	1.99	0.45
1:Aa:174:GLU:HA	1:Aa:174:GLU:OE1	2.16	0.45
1:Aa:278:GLN:H	1:Aa:278:GLN:HG3	1.59	0.45
1:y:118:LYS:HE2	1:y:118:LYS:HB3	1.56	0.45
1:Ag:107:ILE:HD13	1:Ag:133:LEU:HD13	1.98	0.45
1:Ai:68:GLY:HA2	1:Ai:213:ILE:HG23	1.98	0.45
1:Aw:118:LYS:HE2	1:Aw:118:LYS:HB3	1.53	0.45
1:BB:64:ARG:HB3	1:BB:64:ARG:NH1	2.31	0.45
1:l:256:ALA:HB3	1:l:271:LEU:HD22	1.99	0.45
1:w:158:ALA:HB1	1:w:223:THR:HG23	1.98	0.45
1:8:58:THR:HG22	1:8:60:TYR:H	1.82	0.45
1:AH:146:ALA:HB2	1:AH:174:GLU:OE1	2.16	0.45
1:AJ:55:MET:HE1	1:AJ:63:SER:O	2.16	0.45
1:AV:95:VAL:HG23	1:AV:96:LEU:HG	1.99	0.45
1:Aa:264:ILE:HD11	1:Aa:270:ASN:HD22	1.82	0.45
1:Am:55:MET:HE1	1:Am:63:SER:O	2.16	0.45
1:BD:30:GLY:HA2	1:BD:239:THR:HG21	1.99	0.45
1:9:118:LYS:HB3	1:9:118:LYS:HE2	1.58	0.45
1:AI:58:THR:HG22	1:AI:60:TYR:H	1.80	0.45
1:AX:107:ILE:HD13	1:AX:133:LEU:HD13	1.99	0.45
1:Al:79:SER:H	1:Al:83:GLY:HA3	1.80	0.45
1:BH:95:VAL:HG23	1:BH:96:LEU:HG	1.98	0.45
1:BM:118:LYS:HB3	1:BM:118:LYS:HE2	1.57	0.45
1:AH:278:GLN:N	1:AH:278:GLN:OE1	2.50	0.45
1:AI:24:TYR:HB3	1:AI:277:TYR:CD2	2.52	0.45
1:AM:49:PHE:C	1:AM:50:GLU:OE2	2.60	0.45
1:AX:30:GLY:HA2	1:AX:239:THR:HG21	1.99	0.45
1:o:30:GLY:HA2	1:o:239:THR:HG21	1.98	0.45
1:s:278:GLN:H	1:s:278:GLN:HG3	1.59	0.45
1:AP:95:VAL:HG23	1:AP:96:LEU:HG	1.99	0.45
1:AS:127:VAL:HB	1:AS:153:VAL:HG22	1.99	0.45
1:An:95:VAL:HG23	1:An:96:LEU:HG	1.99	0.45
1:k:24:TYR:HB3	1:k:277:TYR:HD2	1.82	0.45
1:n:107:ILE:HD13	1:n:133:LEU:HD22	1.99	0.45
1:AF:95:VAL:HG23	1:AF:96:LEU:HG	1.99	0.45
1:AI:107:ILE:HD13	1:AI:133:LEU:HD13	1.99	0.45
1:AU:133:LEU:H	1:AU:133:LEU:HD23	1.82	0.45
1:Ab:55:MET:HG2	1:Ab:92:GLY:O	2.17	0.45
1:A9:264:ILE:HD11	1:A9:270:ASN:HD22	1.82	0.45
1:BM:249:CYS:HA	1:BM:252:ILE:HG13	1.98	0.45
1:y:255:THR:HB	1:y:276:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:78:GLY:HA2	1:Ak:85:ALA:O	2.17	0.45
1:Ar:95:VAL:HG23	1:Ar:96:LEU:HG	1.99	0.45
1:A8:68:GLY:HA2	1:A8:213:ILE:HG23	1.98	0.45
1:BC:160:GLY:H	1:BC:223:THR:HG21	1.82	0.45
1:BF:95:VAL:HG23	1:BF:96:LEU:HG	1.99	0.45
1:l:30:GLY:HA2	1:l:239:THR:HG21	1.99	0.45
1:t:107:ILE:HD13	1:t:133:LEU:HD13	1.99	0.45
1:v:95:VAL:HG23	1:v:96:LEU:HG	1.99	0.45
1:5:160:GLY:H	1:5:223:THR:HG21	1.81	0.45
1:7:118:LYS:HE2	1:7:118:LYS:HB3	1.73	0.45
1:AH:126:GLY:HA3	1:AH:238:MET:HE1	1.99	0.45
1:Ac:127:VAL:HB	1:Ac:153:VAL:HG22	1.98	0.45
1:A2:69:HIS:CE1	1:A2:225:MET:HE1	2.52	0.45
1:A8:58:THR:HG22	1:A8:60:TYR:H	1.82	0.45
1:k:107:ILE:HD13	1:k:133:LEU:HD13	1.99	0.44
1:t:95:VAL:HG23	1:t:96:LEU:HG	1.98	0.44
1:AZ:55:MET:HE1	1:AZ:63:SER:O	2.17	0.44
1:Af:131:LEU:HB2	1:Af:157:VAL:HG12	1.99	0.44
1:Am:58:THR:HG22	1:Am:60:TYR:H	1.81	0.44
1:Av:30:GLY:HA2	1:Av:239:THR:HG21	1.99	0.44
1:BF:58:THR:HG22	1:BF:60:TYR:H	1.81	0.44
1:l:95:VAL:HG23	1:l:96:LEU:HG	1.99	0.44
1:AA:255:THR:HB	1:AA:276:ASN:ND2	2.30	0.44
1:AJ:30:GLY:HA2	1:AJ:239:THR:HG21	1.99	0.44
1:AX:255:THR:HG21	1:AX:276:ASN:ND2	2.31	0.44
1:Aj:95:VAL:HG23	1:Aj:96:LEU:HG	1.99	0.44
1:At:55:MET:HG2	1:At:92:GLY:O	2.18	0.44
1:A5:77:VAL:HG22	1:A5:228:PRO:HB3	1.99	0.44
1:BI:55:MET:HE3	1:BI:55:MET:HB2	1.81	0.44
1:AO:24:TYR:HB3	1:AO:277:TYR:HD2	1.83	0.44
1:AQ:118:LYS:HB3	1:AQ:118:LYS:HE2	1.59	0.44
1:AW:118:LYS:HB3	1:AW:118:LYS:HE2	1.58	0.44
1:Ac:234:ALA:O	1:Ac:238:MET:HG3	2.18	0.44
1:Ae:118:LYS:HB3	1:Ae:118:LYS:HE3	1.74	0.44
1:Af:256:ALA:HB3	1:Af:271:LEU:HD22	1.97	0.44
1:At:95:VAL:HG23	1:At:96:LEU:HG	1.99	0.44
1:BB:95:VAL:HG23	1:BB:96:LEU:HG	1.99	0.44
1:BG:118:LYS:HB3	1:BG:118:LYS:HE2	1.58	0.44
1:v:107:ILE:HD13	1:v:133:LEU:HD22	1.99	0.44
1:8:107:ILE:HD13	1:8:133:LEU:HD22	1.99	0.44
1:AB:95:VAL:HG23	1:AB:96:LEU:HG	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:234:ALA:O	1:AF:238:MET:HG3	2.17	0.44
1:Ab:30:GLY:HA2	1:Ab:239:THR:HG21	1.99	0.44
1:Ak:30:GLY:HA2	1:Ak:239:THR:HG21	2.00	0.44
1:A9:256:ALA:HB3	1:A9:271:LEU:HD22	1.98	0.44
1:BD:278:GLN:N	1:BD:278:GLN:OE1	2.50	0.44
1:BF:42:ILE:O	1:BF:55:MET:HE2	2.17	0.44
1:p:146:ALA:HB2	1:p:174:GLU:OE1	2.17	0.44
1:BC:49:PHE:C	1:BC:50:GLU:OE1	2.61	0.44
1:2:107:ILE:HD13	1:2:133:LEU:HD22	2.00	0.44
1:AV:55:MET:HE3	1:AV:55:MET:HB2	1.83	0.44
1:Ak:118:LYS:HB3	1:Ak:118:LYS:HE2	1.58	0.44
1:Aw:49:PHE:C	1:Aw:50:GLU:OE1	2.61	0.44
1:Ax:30:GLY:HA2	1:Ax:239:THR:HG21	2.00	0.44
1:A7:255:THR:HB	1:A7:276:ASN:ND2	2.30	0.44
1:BH:133:LEU:HD23	1:BH:133:LEU:H	1.83	0.44
1:BK:255:THR:HB	1:BK:276:ASN:ND2	2.33	0.44
1:r:95:VAL:HG23	1:r:96:LEU:HG	1.99	0.44
1:x:145:ALA:HB1	1:x:177:VAL:HG11	2.00	0.44
1:z:256:ALA:HB3	1:z:271:LEU:HD22	1.98	0.44
1:9:264:ILE:HD11	1:9:270:ASN:HD22	1.82	0.44
1:AD:95:VAL:HG23	1:AD:96:LEU:HG	2.00	0.44
1:AQ:131:LEU:HD23	1:AQ:133:LEU:HD21	2.00	0.44
1:Ac:264:ILE:HD11	1:Ac:270:ASN:HD22	1.82	0.44
1:An:58:THR:HG22	1:An:60:TYR:H	1.83	0.44
1:Ax:255:THR:HG21	1:Ax:276:ASN:ND2	2.29	0.44
1:A3:264:ILE:HD11	1:A3:270:ASN:HD22	1.83	0.44
1:A7:174:GLU:HA	1:A7:174:GLU:OE1	2.18	0.44
1:A0:126:GLY:HA3	1:A0:238:MET:HE1	2.00	0.44
1:BF:30:GLY:HA2	1:BF:239:THR:HG21	2.00	0.44
1:BG:127:VAL:HB	1:BG:153:VAL:HG22	2.00	0.44
1:AE:146:ALA:HB2	1:AE:174:GLU:OE2	2.17	0.44
1:Aq:55:MET:HE1	1:Aq:63:SER:O	2.18	0.44
1:A1:118:LYS:HB3	1:A1:118:LYS:HE2	1.58	0.44
1:A7:256:ALA:HB3	1:A7:271:LEU:HD22	2.00	0.44
1:BK:24:TYR:HB3	1:BK:277:TYR:HD2	1.83	0.44
1:BM:255:THR:HB	1:BM:276:ASN:ND2	2.33	0.44
1:BN:95:VAL:HG23	1:BN:96:LEU:HG	2.00	0.44
1:s:78:GLY:HA2	1:s:85:ALA:O	2.18	0.44
1:w:255:THR:HB	1:w:276:ASN:ND2	2.33	0.44
1:AJ:255:THR:HG21	1:AJ:276:ASN:ND2	2.28	0.44
1:AX:95:VAL:HG23	1:AX:96:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:131:LEU:HD23	1:An:133:LEU:HD21	2.00	0.44
1:An:238:MET:HE3	1:An:238:MET:HB3	1.80	0.44
1:As:234:ALA:O	1:As:238:MET:HG3	2.18	0.44
1:A7:43:GLU:HG3	1:A7:43:GLU:O	2.18	0.44
1:BI:256:ALA:HB3	1:BI:271:LEU:HD22	2.00	0.44
1:i:174:GLU:OE1	1:i:174:GLU:HA	2.18	0.43
1:n:256:ALA:HB3	1:n:271:LEU:HD22	1.99	0.43
1:s:104:TYR:O	1:s:108:ILE:HD12	2.18	0.43
1:AA:160:GLY:H	1:AA:223:THR:HG21	1.83	0.43
1:AF:46:HIS:CD2	1:AF:215:GLY:HA2	2.53	0.43
1:AG:111:MET:HG3	1:AG:148:LEU:HD22	2.00	0.43
1:AS:160:GLY:H	1:AS:223:THR:HG21	1.83	0.43
1:AT:126:GLY:HA3	1:AT:238:MET:HE1	2.00	0.43
1:Ao:256:ALA:HB3	1:Ao:271:LEU:HD22	1.99	0.43
1:Ar:146:ALA:HB2	1:Ar:174:GLU:OE2	2.18	0.43
1:Aw:160:GLY:N	1:Aw:223:THR:HG21	2.31	0.43
1:BM:131:LEU:HB2	1:BM:157:VAL:HG12	1.99	0.43
1:2:174:GLU:OE2	1:2:174:GLU:HA	2.17	0.43
1:7:256:ALA:HB3	1:7:271:LEU:HD22	2.00	0.43
1:AT:174:GLU:OE2	1:AT:174:GLU:HA	2.18	0.43
1:Am:30:GLY:HA2	1:Am:239:THR:HG21	2.00	0.43
1:Ax:95:VAL:HG23	1:Ax:96:LEU:HG	2.00	0.43
1:A3:131:LEU:HB2	1:A3:157:VAL:HG12	1.99	0.43
1:i:255:THR:HB	1:i:276:ASN:ND2	2.31	0.43
1:m:255:THR:HB	1:m:276:ASN:HD21	1.82	0.43
1:y:131:LEU:HB2	1:y:157:VAL:HG12	2.01	0.43
1:AC:160:GLY:H	1:AC:223:THR:HG21	1.84	0.43
1:AQ:107:ILE:HD13	1:AQ:133:LEU:HD13	2.00	0.43
1:Aj:55:MET:HE1	1:Aj:63:SER:O	2.18	0.43
1:BC:182:ALA:HB3	1:BC:193:SER:HB2	2.00	0.43
1:o:160:GLY:N	1:o:223:THR:HG21	2.33	0.43
1:p:95:VAL:HG23	1:p:96:LEU:HG	1.99	0.43
1:6:174:GLU:HB3	1:6:177:VAL:HG22	2.00	0.43
1:0:95:VAL:HG23	1:0:96:LEU:HG	1.99	0.43
1:AQ:78:GLY:HA2	1:AQ:85:ALA:O	2.18	0.43
1:AW:30:GLY:HA2	1:AW:239:THR:HG21	2.00	0.43
1:BA:256:ALA:HB3	1:BA:271:LEU:HD22	2.01	0.43
1:k:174:GLU:OE1	1:k:174:GLU:HA	2.18	0.43
1:l:107:ILE:HD13	1:l:133:LEU:HD22	2.00	0.43
1:w:264:ILE:HD11	1:w:270:ASN:HD22	1.83	0.43
1:3:30:GLY:HA2	1:3:239:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:78:GLY:HA2	1:AC:85:ALA:O	2.19	0.43
1:AS:256:ALA:HB3	1:AS:271:LEU:HD22	2.00	0.43
1:AX:46:HIS:CD2	1:AX:215:GLY:HA2	2.54	0.43
1:Ac:118:LYS:HB3	1:Ac:118:LYS:HE2	1.60	0.43
1:Ak:55:MET:HE1	1:Ak:63:SER:O	2.18	0.43
1:Ap:46:HIS:CD2	1:Ap:215:GLY:HA2	2.53	0.43
1:As:174:GLU:OE1	1:As:174:GLU:HA	2.18	0.43
1:BA:49:PHE:C	1:BA:50:GLU:OE1	2.61	0.43
1:BK:174:GLU:HA	1:BK:174:GLU:OE1	2.18	0.43
1:BL:30:GLY:HA2	1:BL:239:THR:HG21	2.00	0.43
1:k:133:LEU:H	1:k:133:LEU:HD23	1.84	0.43
1:l:69:HIS:CE1	1:l:225:MET:HE1	2.54	0.43
1:w:278:GLN:H	1:w:278:GLN:HG3	1.58	0.43
1:1:278:GLN:H	1:1:278:GLN:HG3	1.60	0.43
1:AD:131:LEU:HB2	1:AD:157:VAL:HG12	2.01	0.43
1:AG:24:TYR:HB3	1:AG:277:TYR:HD2	1.84	0.43
1:AM:255:THR:HB	1:AM:276:ASN:ND2	2.33	0.43
1:AS:24:TYR:HB3	1:AS:277:TYR:HD2	1.83	0.43
1:Aa:24:TYR:HB3	1:Aa:277:TYR:HD2	1.83	0.43
1:Af:30:GLY:HA2	1:Af:239:THR:HG21	2.01	0.43
1:Af:95:VAL:HG23	1:Af:96:LEU:HG	1.99	0.43
1:As:264:ILE:HD11	1:As:270:ASN:HD22	1.83	0.43
1:n:255:THR:HG21	1:n:276:ASN:ND2	2.30	0.43
1:4:69:HIS:CE1	1:4:225:MET:HE1	2.54	0.43
1:AM:24:TYR:HB3	1:AM:277:TYR:HD2	1.83	0.43
1:AP:69:HIS:CE1	1:AP:225:MET:HE1	2.54	0.43
1:AS:174:GLU:OE1	1:AS:174:GLU:HA	2.18	0.43
1:AU:182:ALA:HB3	1:AU:193:SER:HB2	2.01	0.43
1:AV:55:MET:SD	1:AV:63:SER:HB2	2.58	0.43
1:Al:46:HIS:CD2	1:Al:215:GLY:HA2	2.54	0.43
1:BF:131:LEU:HB2	1:BF:157:VAL:HG12	2.01	0.43
1:i:111:MET:HG3	1:i:148:LEU:HD22	2.00	0.43
1:j:95:VAL:HG23	1:j:96:LEU:HG	2.01	0.43
1:n:95:VAL:HG23	1:n:96:LEU:HG	2.00	0.43
1:o:131:LEU:HD23	1:o:133:LEU:HD21	2.01	0.43
1:y:107:ILE:HD13	1:y:133:LEU:HD22	2.00	0.43
1:8:30:GLY:HA2	1:8:239:THR:HG21	2.01	0.43
1:AA:77:VAL:HG22	1:AA:228:PRO:HB3	1.99	0.43
1:AI:278:GLN:H	1:AI:278:GLN:HG3	1.59	0.43
1:AN:95:VAL:HG23	1:AN:96:LEU:HG	1.99	0.43
1:AT:95:VAL:HG23	1:AT:96:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:55:MET:HE1	1:Aa:63:SER:O	2.19	0.43
1:Aa:118:LYS:HB3	1:Aa:118:LYS:HE2	1.60	0.43
1:Af:126:GLY:HA3	1:Af:238:MET:HE1	2.01	0.43
1:An:234:ALA:O	1:An:238:MET:HG3	2.18	0.43
1:Au:49:PHE:C	1:Au:50:GLU:OE2	2.62	0.43
1:A7:107:ILE:HD13	1:A7:133:LEU:HD13	2.01	0.43
1:BH:146:ALA:HB2	1:BH:174:GLU:OE1	2.19	0.43
1:s:43:GLU:O	1:s:43:GLU:HG3	2.19	0.43
1:u:278:GLN:H	1:u:278:GLN:HG3	1.59	0.43
1:3:49:PHE:C	1:3:50:GLU:OE1	2.62	0.43
1:AR:174:GLU:OE2	1:AR:174:GLU:HA	2.19	0.43
1:Az:126:GLY:HA3	1:Az:238:MET:HE1	2.01	0.43
1:A9:174:GLU:OE1	1:A9:174:GLU:HA	2.19	0.43
1:BB:107:ILE:HD13	1:BB:133:LEU:HD22	2.01	0.43
1:BC:24:TYR:HB3	1:BC:277:TYR:HD2	1.83	0.43
1:BG:24:TYR:HB3	1:BG:277:TYR:HD2	1.83	0.43
1:o:258:LYS:HB2	1:o:258:LYS:HE2	1.85	0.43
1:r:58:THR:HG22	1:r:60:TYR:H	1.83	0.43
1:9:43:GLU:O	1:9:43:GLU:HG3	2.19	0.43
1:AY:174:GLU:OE2	1:AY:174:GLU:HA	2.19	0.43
1:AY:238:MET:HE3	1:AY:238:MET:HB3	1.88	0.43
1:Ad:255:THR:HG21	1:Ad:276:ASN:ND2	2.31	0.43
1:A5:43:GLU:O	1:A5:43:GLU:HG3	2.19	0.43
1:j:30:GLY:HA2	1:j:239:THR:HG21	2.01	0.42
1:p:131:LEU:HB2	1:p:157:VAL:HG12	2.01	0.42
1:q:31:GLN:HA	1:q:87:LYS:O	2.18	0.42
1:3:240:LEU:HB3	1:3:242:LYS:HD3	2.01	0.42
1:7:160:GLY:N	1:7:223:THR:HG21	2.34	0.42
1:AY:255:THR:HB	1:AY:276:ASN:ND2	2.32	0.42
1:Aq:278:GLN:H	1:Aq:278:GLN:HG3	1.59	0.42
1:Aw:30:GLY:HA2	1:Aw:239:THR:HG21	2.01	0.42
1:A3:24:TYR:HB3	1:A3:277:TYR:HD2	1.83	0.42
1:BK:55:MET:HB2	1:BK:55:MET:HE2	1.76	0.42
1:m:182:ALA:HB3	1:m:193:SER:HB2	2.01	0.42
1:y:43:GLU:O	1:y:43:GLU:HG3	2.19	0.42
1:5:174:GLU:OE2	1:5:174:GLU:HA	2.19	0.42
1:0:278:GLN:CD	1:0:278:GLN:O	2.61	0.42
1:AR:118:LYS:HE3	1:AR:118:LYS:HB3	1.72	0.42
1:AZ:95:VAL:HG23	1:AZ:96:LEU:HG	2.00	0.42
1:Ad:69:HIS:CE1	1:Ad:225:MET:HE1	2.55	0.42
1:Ai:30:GLY:HA2	1:Ai:239:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:278:GLN:H	1:BK:278:GLN:HG3	1.59	0.42
1:4:68:GLY:HA2	1:4:213:ILE:HG23	2.00	0.42
1:AI:255:THR:HB	1:AI:276:ASN:ND2	2.32	0.42
1:AM:30:GLY:HA2	1:AM:239:THR:HG21	2.01	0.42
1:AM:174:GLU:HB3	1:AM:177:VAL:HG22	2.00	0.42
1:AU:30:GLY:HA2	1:AU:239:THR:HG21	2.02	0.42
1:Am:24:TYR:HB3	1:Am:277:TYR:HD2	1.84	0.42
1:Av:69:HIS:CE1	1:Av:225:MET:HE1	2.55	0.42
1:A2:30:GLY:HA2	1:A2:239:THR:HG21	2.01	0.42
1:A6:248:ALA:O	1:A6:252:ILE:HG13	2.19	0.42
1:BC:278:GLN:H	1:BC:278:GLN:HG3	1.59	0.42
1:BE:118:LYS:HE2	1:BE:118:LYS:HB3	1.65	0.42
1:BM:68:GLY:HA2	1:BM:213:ILE:HG23	2.01	0.42
1:k:111:MET:HG3	1:k:148:LEU:HD22	2.02	0.42
1:k:250:ARG:HA	1:k:250:ARG:NE	2.35	0.42
1:o:118:LYS:HB3	1:o:118:LYS:HE2	1.58	0.42
1:y:131:LEU:HD23	1:y:133:LEU:HD21	2.02	0.42
1:5:29:ALA:HB3	1:5:87:LYS:HG2	2.00	0.42
1:AG:46:HIS:CD2	1:AG:215:GLY:HA2	2.54	0.42
1:AI:234:ALA:O	1:AI:238:MET:HG3	2.18	0.42
1:AN:79:SER:H	1:AN:83:GLY:HA3	1.84	0.42
1:AS:133:LEU:HD23	1:AS:133:LEU:H	1.84	0.42
1:Ac:160:GLY:H	1:Ac:223:THR:HG21	1.84	0.42
1:As:278:GLN:H	1:As:278:GLN:HG3	1.60	0.42
1:A3:160:GLY:H	1:A3:223:THR:HG21	1.84	0.42
1:A4:126:GLY:HA3	1:A4:238:MET:HE1	2.01	0.42
1:A5:174:GLU:OE2	1:A5:174:GLU:HA	2.19	0.42
1:BI:278:GLN:H	1:BI:278:GLN:HG3	1.60	0.42
1:BN:255:THR:HG21	1:BN:276:ASN:ND2	2.27	0.42
1:i:24:TYR:HB3	1:i:277:TYR:HD2	1.84	0.42
1:o:107:ILE:HD13	1:o:133:LEU:HD22	2.01	0.42
1:z:238:MET:HB3	1:z:238:MET:HE3	1.84	0.42
1:3:118:LYS:HB3	1:3:118:LYS:HE2	1.55	0.42
1:AE:174:GLU:O	1:AE:177:VAL:HG22	2.20	0.42
1:AM:255:THR:HB	1:AM:276:ASN:HD21	1.85	0.42
1:AN:174:GLU:HB3	1:AN:177:VAL:HG22	2.00	0.42
1:Ah:95:VAL:HG23	1:Ah:96:LEU:HG	2.01	0.42
1:Ao:264:ILE:HD11	1:Ao:270:ASN:HD22	1.84	0.42
1:Aq:255:THR:HB	1:Aq:276:ASN:ND2	2.32	0.42
1:Au:278:GLN:NE2	1:Au:278:GLN:C	2.77	0.42
1:BD:68:GLY:HA2	1:BD:213:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BN:132:SER:HB3	1:BN:224:SER:HB3	2.02	0.42
1:r:131:LEU:HB2	1:r:157:VAL:HG12	2.02	0.42
1:s:24:TYR:HB3	1:s:277:TYR:CD2	2.55	0.42
1:s:255:THR:HB	1:s:276:ASN:ND2	2.32	0.42
1:t:182:ALA:HB3	1:t:193:SER:HB2	2.02	0.42
1:AC:249:CYS:HA	1:AC:252:ILE:HG13	2.00	0.42
1:AE:55:MET:HE1	1:AE:63:SER:O	2.18	0.42
1:AK:77:VAL:HG22	1:AK:228:PRO:HB3	2.00	0.42
1:Ac:126:GLY:HA3	1:Ac:238:MET:HE1	2.01	0.42
1:A3:43:GLU:O	1:A3:43:GLU:HG3	2.19	0.42
1:A7:24:TYR:HB3	1:A7:277:TYR:HD2	1.84	0.42
1:A0:174:GLU:HA	1:A0:174:GLU:OE1	2.20	0.42
1:BM:24:TYR:HB3	1:BM:277:TYR:CD2	2.55	0.42
1:o:111:MET:HG3	1:o:148:LEU:HD22	2.00	0.42
1:3:174:GLU:OE2	1:3:174:GLU:HA	2.19	0.42
1:Aj:182:ALA:HB3	1:Aj:193:SER:HB2	2.02	0.42
1:Ak:278:GLN:H	1:Ak:278:GLN:HG3	1.59	0.42
1:Ao:255:THR:HB	1:Ao:276:ASN:ND2	2.32	0.42
1:Ap:236:TYR:O	1:Ap:239:THR:HG22	2.20	0.42
1:Aw:255:THR:HB	1:Aw:276:ASN:ND2	2.34	0.42
1:A3:78:GLY:HA2	1:A3:85:ALA:O	2.20	0.42
1:A3:174:GLU:HA	1:A3:174:GLU:OE2	2.20	0.42
1:A3:182:ALA:HB3	1:A3:193:SER:HB2	2.02	0.42
1:BD:95:VAL:HG23	1:BD:96:LEU:HG	2.01	0.42
1:BE:160:GLY:N	1:BE:223:THR:HG21	2.33	0.42
1:BM:43:GLU:O	1:BM:43:GLU:HG3	2.19	0.42
1:s:24:TYR:HB3	1:s:277:TYR:HD2	1.84	0.42
1:w:272:LEU:HD23	1:w:273:ALA:N	2.34	0.42
1:x:95:VAL:HG23	1:x:96:LEU:HG	2.01	0.42
1:z:95:VAL:HG23	1:z:96:LEU:HG	2.02	0.42
1:8:255:THR:HG21	1:8:276:ASN:ND2	2.32	0.42
1:Ad:174:GLU:OE2	1:Ad:174:GLU:HA	2.20	0.42
1:Ak:256:ALA:HB3	1:Ak:271:LEU:HD22	2.02	0.42
1:Am:24:TYR:HB3	1:Am:277:TYR:CD2	2.54	0.42
1:A6:46:HIS:CD2	1:A6:215:GLY:HA2	2.55	0.42
1:BA:24:TYR:HB3	1:BA:277:TYR:HD2	1.85	0.42
1:BB:256:ALA:HB3	1:BB:271:LEU:HD22	2.01	0.42
1:i:160:GLY:H	1:i:223:THR:HG21	1.85	0.42
1:l:174:GLU:HA	1:l:174:GLU:OE2	2.20	0.42
1:m:24:TYR:HB3	1:m:277:TYR:HD2	1.84	0.42
1:x:46:HIS:CD2	1:x:215:GLY:HA2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:118:LYS:HB3	1:AC:118:LYS:HE2	1.55	0.42
1:AY:278:GLN:H	1:AY:278:GLN:HG3	1.59	0.42
1:Aa:111:MET:HG3	1:Aa:148:LEU:HD22	2.02	0.42
1:Ab:95:VAL:HG23	1:Ab:96:LEU:HG	2.02	0.42
1:As:43:GLU:O	1:As:43:GLU:HG3	2.20	0.42
1:A2:174:GLU:HA	1:A2:174:GLU:OE2	2.20	0.42
1:A2:255:THR:HG21	1:A2:276:ASN:ND2	2.30	0.42
1:BG:24:TYR:HB3	1:BG:277:TYR:CD2	2.55	0.42
1:BM:264:ILE:HD11	1:BM:270:ASN:HD22	1.84	0.42
1:AK:278:GLN:H	1:AK:278:GLN:HG3	1.59	0.42
1:AZ:131:LEU:HB2	1:AZ:157:VAL:HG12	2.01	0.42
1:Ai:43:GLU:HG3	1:Ai:43:GLU:O	2.20	0.42
1:Ai:160:GLY:H	1:Ai:223:THR:HG21	1.85	0.42
1:Am:255:THR:HB	1:Am:276:ASN:ND2	2.34	0.42
1:A5:8:TRP:CH2	1:A5:204:PRO:HB3	2.55	0.42
1:BC:146:ALA:HB2	1:BC:174:GLU:OE2	2.20	0.42
1:BG:43:GLU:O	1:BG:43:GLU:HG3	2.20	0.42
1:BN:46:HIS:CD2	1:BN:215:GLY:HA2	2.55	0.42
1:v:248:ALA:O	1:v:252:ILE:HG13	2.20	0.41
1:w:24:TYR:HB3	1:w:277:TYR:HD2	1.85	0.41
1:A0:69:HIS:CE1	1:A0:225:MET:HE1	2.55	0.41
1:BJ:107:ILE:HD13	1:BJ:133:LEU:HD22	2.02	0.41
1:BL:95:VAL:HG23	1:BL:96:LEU:HG	2.01	0.41
1:t:79:SER:H	1:t:83:GLY:HA3	1.85	0.41
1:u:118:LYS:HE2	1:u:118:LYS:HB3	1.61	0.41
1:l:234:ALA:O	1:l:238:MET:HG3	2.21	0.41
1:4:30:GLY:HA2	1:4:239:THR:HG21	2.02	0.41
1:9:160:GLY:H	1:9:223:THR:HG21	1.85	0.41
1:AL:95:VAL:HG23	1:AL:96:LEU:HG	2.00	0.41
1:AS:78:GLY:HA2	1:AS:85:ALA:O	2.20	0.41
1:AS:249:CYS:HA	1:AS:252:ILE:HG13	2.02	0.41
1:AX:174:GLU:OE2	1:AX:174:GLU:HA	2.20	0.41
1:Ah:29:ALA:HB3	1:Ah:87:LYS:HG2	2.01	0.41
1:k:46:HIS:CD2	1:k:215:GLY:HA2	2.55	0.41
1:k:118:LYS:HB3	1:k:118:LYS:HE2	1.61	0.41
1:x:242:LYS:HE3	1:x:242:LYS:HB3	1.92	0.41
1:AU:55:MET:HG2	1:AU:92:GLY:O	2.20	0.41
1:Ad:79:SER:H	1:Ad:83:GLY:HA3	1.84	0.41
1:A5:160:GLY:H	1:A5:223:THR:HG21	1.86	0.41
1:A5:272:LEU:HD23	1:A5:273:ALA:H	1.86	0.41
1:A6:131:LEU:HB2	1:A6:157:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:182:ALA:HB3	1:1:193:SER:HB2	2.01	0.41
1:5:24:TYR:HB3	1:5:277:TYR:CD2	2.55	0.41
1:AE:264:ILE:HD11	1:AE:270:ASN:HD22	1.86	0.41
1:AL:55:MET:HE2	1:AL:55:MET:HB3	1.78	0.41
1:AU:43:GLU:O	1:AU:43:GLU:HG3	2.19	0.41
1:Aj:174:GLU:OE2	1:Aj:174:GLU:HA	2.20	0.41
1:Am:238:MET:HE3	1:Am:238:MET:HB3	1.88	0.41
1:Am:250:ARG:HA	1:Am:250:ARG:NE	2.35	0.41
1:k:278:GLN:H	1:k:278:GLN:HG3	1.59	0.41
1:m:160:GLY:H	1:m:223:THR:HG21	1.85	0.41
1:AG:24:TYR:HB3	1:AG:277:TYR:CD2	2.55	0.41
1:AK:255:THR:HB	1:AK:276:ASN:ND2	2.36	0.41
1:AN:69:HIS:CE1	1:AN:225:MET:HE1	2.55	0.41
1:AO:160:GLY:N	1:AO:223:THR:HG21	2.35	0.41
1:AU:264:ILE:HD11	1:AU:270:ASN:HD22	1.86	0.41
1:AY:46:HIS:CD2	1:AY:215:GLY:HA2	2.56	0.41
1:Aa:255:THR:HB	1:Aa:276:ASN:ND2	2.35	0.41
1:As:77:VAL:HG22	1:As:228:PRO:HB3	2.02	0.41
1:BD:146:ALA:HB2	1:BD:174:GLU:OE1	2.20	0.41
1:BL:107:ILE:HD13	1:BL:133:LEU:HD22	2.03	0.41
1:j:131:LEU:HB2	1:j:157:VAL:HG12	2.01	0.41
1:o:146:ALA:HB2	1:o:174:GLU:OE2	2.21	0.41
1:q:160:GLY:N	1:q:223:THR:HG21	2.35	0.41
1:z:236:TYR:O	1:z:239:THR:HG22	2.21	0.41
1:1:46:HIS:CD2	1:1:215:GLY:HA2	2.56	0.41
1:3:174:GLU:HB3	1:3:177:VAL:HG22	2.03	0.41
1:3:182:ALA:HB3	1:3:193:SER:HB2	2.01	0.41
1:5:118:LYS:HB3	1:5:118:LYS:HE2	1.56	0.41
1:9:258:LYS:HE3	1:9:258:LYS:HB2	1.92	0.41
1:AA:30:GLY:HA2	1:AA:239:THR:HG21	2.03	0.41
1:AE:160:GLY:H	1:AE:223:THR:HG21	1.86	0.41
1:AI:160:GLY:H	1:AI:223:THR:HG21	1.85	0.41
1:AI:174:GLU:OE2	1:AI:174:GLU:HA	2.21	0.41
1:AS:43:GLU:O	1:AS:43:GLU:HG3	2.20	0.41
1:Ab:69:HIS:CE1	1:Ab:225:MET:HE1	2.56	0.41
1:Ac:256:ALA:HB3	1:Ac:271:LEU:HD22	2.03	0.41
1:Ag:43:GLU:O	1:Ag:43:GLU:HG3	2.21	0.41
1:Ay:255:THR:HB	1:Ay:276:ASN:ND2	2.32	0.41
1:A1:78:GLY:HA2	1:A1:85:ALA:O	2.21	0.41
1:A5:107:ILE:HD13	1:A5:133:LEU:HD13	2.02	0.41
1:BC:256:ALA:HB3	1:BC:271:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:55:MET:HE1	1:BE:63:SER:O	2.20	0.41
1:BN:236:TYR:O	1:BN:239:THR:HG22	2.21	0.41
1:k:24:TYR:HB3	1:k:277:TYR:CD2	2.56	0.41
1:k:264:ILE:HD11	1:k:270:ASN:HD22	1.85	0.41
1:o:255:THR:HB	1:o:276:ASN:HD21	1.85	0.41
1:o:278:GLN:H	1:o:278:GLN:HG3	1.60	0.41
1:r:174:GLU:OE2	1:r:174:GLU:HA	2.20	0.41
1:t:146:ALA:HB2	1:t:174:GLU:OE1	2.21	0.41
1:z:174:GLU:OE2	1:z:174:GLU:HA	2.20	0.41
1:6:126:GLY:HA3	1:6:238:MET:HE3	2.02	0.41
1:AC:30:GLY:HA2	1:AC:239:THR:HG21	2.03	0.41
1:AQ:160:GLY:H	1:AQ:223:THR:HG21	1.85	0.41
1:AV:126:GLY:HA3	1:AV:238:MET:HE1	2.02	0.41
1:AW:256:ALA:HB3	1:AW:271:LEU:HD22	2.03	0.41
1:AX:131:LEU:HB2	1:AX:157:VAL:HG12	2.01	0.41
1:Ae:24:TYR:HB3	1:Ae:277:TYR:CD2	2.56	0.41
1:Ax:126:GLY:HA3	1:Ax:238:MET:HE3	2.01	0.41
1:BG:160:GLY:H	1:BG:223:THR:HG21	1.86	0.41
1:BL:46:HIS:CD2	1:BL:215:GLY:HA2	2.55	0.41
1:BL:174:GLU:OE2	1:BL:174:GLU:HA	2.20	0.41
1:BN:174:GLU:OE2	1:BN:174:GLU:HA	2.20	0.41
1:i:24:TYR:HB3	1:i:277:TYR:CD2	2.56	0.41
1:q:118:LYS:HB3	1:q:118:LYS:HE2	1.62	0.41
1:x:107:ILE:HD13	1:x:133:LEU:HD22	2.03	0.41
1:7:43:GLU:O	1:7:43:GLU:HG3	2.21	0.41
1:AV:146:ALA:HB2	1:AV:174:GLU:OE2	2.20	0.41
1:AW:174:GLU:HA	1:AW:174:GLU:OE2	2.20	0.41
1:Ar:126:GLY:HA3	1:Ar:238:MET:HE1	2.02	0.41
1:As:78:GLY:HA2	1:As:85:ALA:O	2.21	0.41
1:Ay:118:LYS:HB3	1:Ay:118:LYS:HE2	1.57	0.41
1:A6:224:SER:HB2	1:A6:225:MET:HE2	2.02	0.41
1:A7:248:ALA:O	1:A7:252:ILE:HG13	2.21	0.41
1:BC:24:TYR:HB3	1:BC:277:TYR:CD2	2.56	0.41
1:BM:30:GLY:HA2	1:BM:239:THR:HG21	2.03	0.41
1:BM:146:ALA:HB2	1:BM:174:GLU:OE1	2.21	0.41
1:o:174:GLU:HA	1:o:174:GLU:OE1	2.21	0.41
1:w:29:ALA:HB3	1:w:87:LYS:HG2	2.01	0.41
1:y:30:GLY:HA2	1:y:239:THR:HG21	2.03	0.41
1:1:133:LEU:H	1:1:133:LEU:CD2	2.31	0.41
1:3:43:GLU:HG3	1:3:43:GLU:O	2.21	0.41
1:3:46:HIS:CD2	1:3:215:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:255:THR:HB	1:AE:276:ASN:ND2	2.32	0.41
1:AF:174:GLU:OE2	1:AF:174:GLU:HA	2.20	0.41
1:AH:236:TYR:O	1:AH:239:THR:HG22	2.21	0.41
1:AI:29:ALA:HB3	1:AI:87:LYS:HG2	2.01	0.41
1:AK:255:THR:HB	1:AK:276:ASN:HD21	1.85	0.41
1:AQ:30:GLY:HA2	1:AQ:239:THR:HG21	2.03	0.41
1:AT:107:ILE:HD13	1:AT:133:LEU:HD22	2.03	0.41
1:AV:236:TYR:O	1:AV:239:THR:HG22	2.21	0.41
1:AW:43:GLU:HG3	1:AW:43:GLU:O	2.21	0.41
1:AX:20:THR:HG22	1:AX:22:THR:H	1.86	0.41
1:AX:256:ALA:HB3	1:AX:271:LEU:HD22	2.02	0.41
1:Ah:249:CYS:HA	1:Ah:252:ILE:HG13	2.03	0.41
1:Ao:278:GLN:H	1:Ao:278:GLN:HG3	1.59	0.41
1:Ar:255:THR:HG21	1:Ar:276:ASN:ND2	2.29	0.41
1:At:30:GLY:HA2	1:At:239:THR:HG21	2.02	0.41
1:At:174:GLU:HA	1:At:174:GLU:OE2	2.20	0.41
1:At:248:ALA:O	1:At:252:ILE:HG13	2.21	0.41
1:Ay:160:GLY:H	1:Ay:223:THR:HG21	1.86	0.41
1:A4:69:HIS:CE1	1:A4:225:MET:HE1	2.55	0.41
1:A6:236:TYR:O	1:A6:239:THR:HG22	2.21	0.41
1:A9:24:TYR:HB3	1:A9:277:TYR:CD2	2.55	0.41
1:A9:43:GLU:O	1:A9:43:GLU:HG3	2.20	0.41
1:BC:145:ALA:HB1	1:BC:177:VAL:HG11	2.03	0.41
1:BC:174:GLU:HA	1:BC:174:GLU:OE1	2.21	0.41
1:BH:174:GLU:HA	1:BH:174:GLU:OE2	2.21	0.41
1:BI:118:LYS:HB3	1:BI:118:LYS:HE2	1.60	0.41
1:BJ:248:ALA:O	1:BJ:252:ILE:HG13	2.21	0.41
1:BJ:277:TYR:CE2	1:BJ:279:ALA:HB2	2.55	0.41
1:BK:24:TYR:HB3	1:BK:277:TYR:CD2	2.55	0.41
1:j:69:HIS:CE1	1:j:225:MET:HE1	2.55	0.41
1:k:78:GLY:HA2	1:k:85:ALA:O	2.20	0.41
1:u:255:THR:HB	1:u:276:ASN:ND2	2.34	0.41
1:y:174:GLU:HA	1:y:174:GLU:OE2	2.21	0.41
1:1:78:GLY:HA2	1:1:85:ALA:O	2.21	0.41
1:9:174:GLU:OE2	1:9:174:GLU:HA	2.21	0.41
1:AC:31:GLN:HA	1:AC:87:LYS:O	2.21	0.41
1:AD:174:GLU:OE2	1:AD:174:GLU:HA	2.20	0.41
1:AK:118:LYS:HE2	1:AK:118:LYS:HB3	1.58	0.41
1:AO:43:GLU:HG3	1:AO:43:GLU:O	2.21	0.41
1:Aa:78:GLY:HA2	1:Aa:85:ALA:O	2.21	0.41
1:Ac:49:PHE:C	1:Ac:50:GLU:OE2	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:58:THR:HG23	1:Ad:94:LYS:HD3	2.03	0.41
1:Ag:24:TYR:HB3	1:Ag:277:TYR:HD2	1.86	0.41
1:Ai:118:LYS:HE2	1:Ai:118:LYS:HB3	1.57	0.41
1:Az:55:MET:HE2	1:Az:55:MET:HB2	1.84	0.41
1:A0:118:LYS:HB3	1:A0:118:LYS:HE3	1.88	0.41
1:BA:146:ALA:HB2	1:BA:174:GLU:OE2	2.21	0.41
1:BA:174:GLU:HA	1:BA:174:GLU:OE1	2.21	0.41
1:BK:30:GLY:HA2	1:BK:239:THR:HG21	2.03	0.41
1:BM:174:GLU:HA	1:BM:174:GLU:OE2	2.21	0.41
1:o:24:TYR:HB3	1:o:277:TYR:HD2	1.85	0.40
1:o:55:MET:HE2	1:o:55:MET:HB3	1.84	0.40
1:p:174:GLU:OE2	1:p:174:GLU:HA	2.21	0.40
1:w:24:TYR:HB3	1:w:277:TYR:CD2	2.56	0.40
1:w:174:GLU:OE2	1:w:174:GLU:HA	2.21	0.40
1:AG:131:LEU:HB2	1:AG:157:VAL:HG12	2.02	0.40
1:AN:68:GLY:HA2	1:AN:213:ILE:HG23	2.03	0.40
1:AW:111:MET:HG3	1:AW:148:LEU:HD22	2.03	0.40
1:Ao:55:MET:HE2	1:Ao:55:MET:HB2	1.75	0.40
1:Ar:69:HIS:CE1	1:Ar:225:MET:HE1	2.57	0.40
1:Ar:174:GLU:O	1:Ar:177:VAL:HG22	2.21	0.40
1:Aw:43:GLU:O	1:Aw:43:GLU:HG3	2.21	0.40
1:Ax:107:ILE:HD13	1:Ax:133:LEU:HD22	2.03	0.40
1:A1:108:ILE:HG13	1:A1:108:ILE:H	1.61	0.40
1:A7:264:ILE:HD11	1:A7:270:ASN:HD22	1.86	0.40
1:BF:79:SER:H	1:BF:83:GLY:HA3	1.85	0.40
1:BI:160:GLY:H	1:BI:223:THR:HG21	1.86	0.40
1:BM:55:MET:HE1	1:BM:63:SER:O	2.21	0.40
1:j:68:GLY:HA2	1:j:213:ILE:HG23	2.02	0.40
1:t:174:GLU:HA	1:t:174:GLU:OE2	2.22	0.40
1:v:174:GLU:HA	1:v:174:GLU:OE2	2.22	0.40
1:y:24:TYR:HB3	1:y:277:TYR:CD2	2.54	0.40
1:3:160:GLY:H	1:3:223:THR:HG21	1.87	0.40
1:4:131:LEU:HB2	1:4:157:VAL:HG12	2.03	0.40
1:9:78:GLY:HA2	1:9:85:ALA:O	2.21	0.40
1:AG:278:GLN:H	1:AG:278:GLN:HG3	1.59	0.40
1:AU:78:GLY:HA2	1:AU:85:ALA:O	2.21	0.40
1:AX:238:MET:HE3	1:AX:238:MET:HB3	1.82	0.40
1:Ae:43:GLU:O	1:Ae:43:GLU:HG3	2.21	0.40
1:Ai:78:GLY:HA2	1:Ai:85:ALA:O	2.22	0.40
1:Ak:255:THR:HB	1:Ak:276:ASN:ND2	2.33	0.40
1:An:24:TYR:HB3	1:An:277:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:55:MET:HE1	1:An:63:SER:O	2.21	0.40
1:Ao:43:GLU:O	1:Ao:43:GLU:HG3	2.20	0.40
1:A1:43:GLU:O	1:A1:43:GLU:HG3	2.21	0.40
1:A4:46:HIS:CD2	1:A4:215:GLY:HA2	2.57	0.40
1:A9:111:MET:HG3	1:A9:148:LEU:HD22	2.03	0.40
1:BK:43:GLU:O	1:BK:43:GLU:HG3	2.20	0.40
1:BM:55:MET:HG2	1:BM:92:GLY:O	2.22	0.40
1:BN:238:MET:HE3	1:BN:238:MET:HB3	1.88	0.40
1:BN:248:ALA:O	1:BN:252:ILE:HG13	2.21	0.40
1:w:43:GLU:O	1:w:43:GLU:HG3	2.19	0.40
1:9:146:ALA:HB2	1:9:174:GLU:OE1	2.21	0.40
1:AA:256:ALA:HB3	1:AA:271:LEU:HD22	2.03	0.40
1:AE:24:TYR:HB3	1:AE:277:TYR:CD2	2.56	0.40
1:AZ:79:SER:H	1:AZ:83:GLY:HA3	1.85	0.40
1:Aa:236:TYR:O	1:Aa:239:THR:HG22	2.22	0.40
1:Ag:78:GLY:HA2	1:Ag:85:ALA:O	2.21	0.40
1:Ag:146:ALA:HB2	1:Ag:174:GLU:OE2	2.21	0.40
1:As:118:LYS:HE2	1:As:118:LYS:HB3	1.57	0.40
1:Au:24:TYR:HB3	1:Au:277:TYR:CD2	2.55	0.40
1:Aw:278:GLN:H	1:Aw:278:GLN:HG3	1.61	0.40
1:A6:69:HIS:CE1	1:A6:225:MET:HE1	2.56	0.40
1:BI:43:GLU:HG3	1:BI:43:GLU:O	2.21	0.40
1:BJ:174:GLU:HA	1:BJ:174:GLU:OE2	2.22	0.40
1:k:261:LEU:H	1:k:270:ASN:HD21	1.69	0.40
1:AC:188:ARG:HE	1:AC:188:ARG:HB2	1.68	0.40
1:AF:76:THR:HB	1:AF:228:PRO:HB2	2.02	0.40
1:AP:30:GLY:HA2	1:AP:239:THR:HG21	2.04	0.40
1:AT:46:HIS:CD2	1:AT:215:GLY:HA2	2.56	0.40
1:Ac:30:GLY:HA2	1:Ac:239:THR:HG21	2.04	0.40
1:Ae:160:GLY:H	1:Ae:223:THR:HG21	1.86	0.40
1:Ai:255:THR:HB	1:Ai:276:ASN:ND2	2.34	0.40
1:Ao:174:GLU:HA	1:Ao:174:GLU:OE1	2.21	0.40
1:A6:107:ILE:HD13	1:A6:133:LEU:HD22	2.02	0.40
1:A0:95:VAL:HG23	1:A0:96:LEU:HG	2.02	0.40
1:BG:78:GLY:HA2	1:BG:85:ALA:O	2.21	0.40
1:9:256:ALA:HB3	1:9:271:LEU:HD22	2.04	0.40
1:AC:24:TYR:HB3	1:AC:277:TYR:CD2	2.55	0.40
1:AG:146:ALA:HB2	1:AG:174:GLU:OE2	2.22	0.40
1:AM:160:GLY:H	1:AM:223:THR:HG21	1.86	0.40
1:AU:255:THR:HB	1:AU:276:ASN:ND2	2.37	0.40
1:Ad:256:ALA:HB3	1:Ad:271:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:78:GLY:HA2	1:Au:85:ALA:O	2.22	0.40
1:BB:55:MET:HG2	1:BB:92:GLY:O	2.21	0.40
1:BC:127:VAL:HB	1:BC:153:VAL:HG22	2.02	0.40
1:BD:174:GLU:OE2	1:BD:174:GLU:HA	2.21	0.40
1:BI:78:GLY:HA2	1:BI:85:ALA:O	2.22	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	0	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	1	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	2	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	3	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	4	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	5	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	6	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	7	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	8	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	9	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	A0	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	A1	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	A2	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	A3	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	A4	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	A5	277/279 (99%)	267 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A6	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	A7	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	A8	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	A9	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	AA	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	AB	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	AC	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	AD	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	AE	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	AF	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	AG	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	AH	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	AI	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	AJ	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	AK	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	AL	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	AM	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	AN	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	AO	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	AP	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	AQ	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	AR	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	AS	277/279 (99%)	269 (97%)	8 (3%)	0	100	100
1	AT	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	AU	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	AV	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	AW	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	AX	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	AY	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	AZ	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	Aa	277/279 (99%)	266 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	Ac	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	Ad	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	Ae	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	Af	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	Ag	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	Ah	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	Ai	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	Aj	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	Ak	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	Al	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	Am	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	An	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	Ao	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	Ap	277/279 (99%)	263 (95%)	14 (5%)	0	100	100
1	Aq	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	Ar	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	As	277/279 (99%)	268 (97%)	9 (3%)	0	100	100
1	At	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	Au	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	Av	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	Aw	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	Ax	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	Ay	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	Az	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	BA	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	BB	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	BC	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	BD	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	BE	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	BF	277/279 (99%)	266 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BG	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	BH	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	BI	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	BJ	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	BK	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	BL	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	BM	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	BN	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	i	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	j	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	k	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	l	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	m	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	n	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	o	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	p	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	q	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	r	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	s	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	t	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	u	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	v	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	w	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
1	x	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	y	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
1	z	277/279 (99%)	265 (96%)	12 (4%)	0	100	100
All	All	28808/29016 (99%)	27657 (96%)	1151 (4%)	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	0	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	1	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	2	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	3	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	4	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	5	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	6	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	7	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	8	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	9	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	A0	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	A1	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	A2	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	A3	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	A4	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	A5	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	A6	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	A7	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	A8	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	A9	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AA	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	AB	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AC	213/213 (100%)	211 (99%)	2 (1%)	70	79
1	AD	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AE	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AF	213/213 (100%)	210 (99%)	3 (1%)	59	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AG	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	AH	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	AI	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AJ	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	AK	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AL	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AM	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	AN	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	AO	213/213 (100%)	204 (96%)	9 (4%)	26	56
1	AP	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AQ	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AR	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	AS	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	AT	213/213 (100%)	212 (100%)	1 (0%)	81	83
1	AU	213/213 (100%)	211 (99%)	2 (1%)	70	79
1	AV	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	AW	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	AX	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	AY	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	AZ	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	Aa	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	Ab	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	Ac	213/213 (100%)	203 (95%)	10 (5%)	23	54
1	Ad	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	Ae	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	Af	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	Ag	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	Ah	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	Ai	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	Aj	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	Ak	213/213 (100%)	209 (98%)	4 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Al	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	Am	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	An	213/213 (100%)	205 (96%)	8 (4%)	29	59
1	Ao	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	Ap	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	Aq	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	Ar	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	As	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	At	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	Au	213/213 (100%)	203 (95%)	10 (5%)	23	54
1	Av	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	Aw	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	Ax	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	Ay	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	Az	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	BA	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	BB	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	BC	213/213 (100%)	204 (96%)	9 (4%)	26	56
1	BD	213/213 (100%)	205 (96%)	8 (4%)	29	59
1	BE	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	BF	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	BG	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	BH	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	BI	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	BJ	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	BK	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	BL	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	BM	213/213 (100%)	211 (99%)	2 (1%)	70	79
1	BN	213/213 (100%)	203 (95%)	10 (5%)	23	54
1	i	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	j	213/213 (100%)	209 (98%)	4 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	213/213 (100%)	205 (96%)	8 (4%)	29	59
1	l	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	m	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	n	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	o	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	p	213/213 (100%)	206 (97%)	7 (3%)	33	62
1	q	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	r	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	s	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	t	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	u	213/213 (100%)	208 (98%)	5 (2%)	44	68
1	v	213/213 (100%)	207 (97%)	6 (3%)	38	64
1	w	213/213 (100%)	210 (99%)	3 (1%)	59	74
1	x	213/213 (100%)	205 (96%)	8 (4%)	29	59
1	y	213/213 (100%)	209 (98%)	4 (2%)	50	70
1	z	213/213 (100%)	206 (97%)	7 (3%)	33	62
All	All	22152/22152 (100%)	21599 (98%)	553 (2%)	42	66

All (553) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	i	16	THR
1	i	42	ILE
1	i	201	ILE
1	i	213	ILE
1	i	278	GLN
1	j	93	VAL
1	j	101	SER
1	j	220	ILE
1	j	255	THR
1	k	16	THR
1	k	43	GLU
1	k	57	LYS
1	k	99	ASN
1	k	127	VAL
1	k	179	THR

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Mol	Chain	Res	Type
1	k	201	ILE
1	k	272	LEU
1	l	86	LYS
1	l	125	LYS
1	l	220	ILE
1	l	224	SER
1	l	255	THR
1	m	99	ASN
1	m	133	LEU
1	m	148	LEU
1	m	201	ILE
1	m	213	ILE
1	m	220	ILE
1	m	249	CYS
1	n	220	ILE
1	n	224	SER
1	n	255	THR
1	o	42	ILE
1	o	111	MET
1	o	133	LEU
1	o	179	THR
1	o	201	ILE
1	o	209	LEU
1	o	272	LEU
1	p	90	LEU
1	p	101	SER
1	p	220	ILE
1	p	224	SER
1	p	225	MET
1	p	239	THR
1	p	255	THR
1	q	132	SER
1	q	179	THR
1	q	201	ILE
1	q	220	ILE
1	r	20	THR
1	r	118	LYS
1	r	224	SER
1	r	255	THR
1	s	90	LEU
1	s	132	SER
1	s	133	LEU

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Mol	Chain	Res	Type
1	s	179	THR
1	s	209	LEU
1	s	220	ILE
1	t	133	LEU
1	t	255	THR
1	t	262	SER
1	u	99	ASN
1	u	179	THR
1	u	220	ILE
1	u	249	CYS
1	u	272	LEU
1	v	86	LYS
1	v	198	VAL
1	v	213	ILE
1	v	224	SER
1	v	255	THR
1	v	278	GLN
1	w	16	THR
1	w	125	LYS
1	w	220	ILE
1	x	20	THR
1	x	86	LYS
1	x	133	LEU
1	x	198	VAL
1	x	213	ILE
1	x	220	ILE
1	x	224	SER
1	x	255	THR
1	y	133	LEU
1	y	201	ILE
1	y	220	ILE
1	y	258	LYS
1	z	101	SER
1	z	133	LEU
1	z	154	MET
1	z	220	ILE
1	z	224	SER
1	z	255	THR
1	z	262	SER
1	1	55	MET
1	1	111	MET
1	1	201	ILE

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Mol	Chain	Res	Type
1	1	209	LEU
1	2	20	THR
1	2	86	LYS
1	2	168	ASN
1	2	220	ILE
1	2	224	SER
1	2	255	THR
1	3	99	ASN
1	3	127	VAL
1	3	133	LEU
1	3	201	ILE
1	3	213	ILE
1	3	220	ILE
1	3	249	CYS
1	4	20	THR
1	4	93	VAL
1	4	101	SER
1	4	177	VAL
1	4	220	ILE
1	4	224	SER
1	4	255	THR
1	5	16	THR
1	5	179	THR
1	5	191	SER
1	5	201	ILE
1	5	220	ILE
1	5	249	CYS
1	5	272	LEU
1	6	20	THR
1	6	90	LEU
1	6	118	LYS
1	6	198	VAL
1	6	220	ILE
1	6	224	SER
1	6	255	THR
1	7	57	LYS
1	7	90	LEU
1	7	179	THR
1	7	201	ILE
1	7	209	LEU
1	7	220	ILE
1	8	90	LEU

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Mol	Chain	Res	Type
1	8	220	ILE
1	8	255	THR
1	9	13	ILE
1	9	111	MET
1	9	133	LEU
1	9	179	THR
1	9	201	ILE
1	9	220	ILE
1	9	224	SER
1	0	86	LYS
1	0	224	SER
1	0	255	THR
1	AA	99	ASN
1	AA	201	ILE
1	AA	213	ILE
1	AA	220	ILE
1	AA	249	CYS
1	AA	272	LEU
1	AB	101	SER
1	AB	133	LEU
1	AB	198	VAL
1	AB	224	SER
1	AB	255	THR
1	AC	16	THR
1	AC	220	ILE
1	AD	20	THR
1	AD	93	VAL
1	AD	209	LEU
1	AD	224	SER
1	AD	262	SER
1	AE	16	THR
1	AE	198	VAL
1	AE	201	ILE
1	AE	220	ILE
1	AE	272	LEU
1	AF	118	LYS
1	AF	220	ILE
1	AF	224	SER
1	AG	90	LEU
1	AG	201	ILE
1	AG	220	ILE
1	AG	249	CYS

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Mol	Chain	Res	Type
1	AH	101	SER
1	AH	154	MET
1	AH	209	LEU
1	AH	220	ILE
1	AH	224	SER
1	AH	255	THR
1	AI	43	GLU
1	AI	133	LEU
1	AI	179	THR
1	AI	201	ILE
1	AI	249	CYS
1	AJ	90	LEU
1	AJ	101	SER
1	AJ	198	VAL
1	AJ	220	ILE
1	AJ	224	SER
1	AJ	255	THR
1	AK	127	VAL
1	AK	201	ILE
1	AK	209	LEU
1	AK	249	CYS
1	AK	272	LEU
1	AL	20	THR
1	AL	101	SER
1	AL	220	ILE
1	AL	224	SER
1	AL	255	THR
1	AM	127	VAL
1	AM	133	LEU
1	AM	179	THR
1	AM	201	ILE
1	AM	213	ILE
1	AM	220	ILE
1	AN	20	THR
1	AN	101	SER
1	AN	133	LEU
1	AN	220	ILE
1	AN	255	THR
1	AN	262	SER
1	AO	57	LYS
1	AO	118	LYS
1	AO	127	VAL

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Mol	Chain	Res	Type
1	AO	148	LEU
1	AO	179	THR
1	AO	201	ILE
1	AO	220	ILE
1	AO	258	LYS
1	AO	272	LEU
1	AP	20	THR
1	AP	118	LYS
1	AP	220	ILE
1	AP	224	SER
1	AP	255	THR
1	AQ	99	ASN
1	AQ	133	LEU
1	AQ	148	LEU
1	AQ	179	THR
1	AQ	224	SER
1	AR	86	LYS
1	AR	133	LEU
1	AR	220	ILE
1	AR	255	THR
1	AS	111	MET
1	AS	133	LEU
1	AS	179	THR
1	AS	220	ILE
1	AT	118	LYS
1	AU	16	THR
1	AU	220	ILE
1	AV	101	SER
1	AV	118	LYS
1	AV	213	ILE
1	AV	220	ILE
1	AV	224	SER
1	AV	255	THR
1	AW	16	THR
1	AW	42	ILE
1	AW	90	LEU
1	AW	133	LEU
1	AW	191	SER
1	AW	209	LEU
1	AW	220	ILE
1	AX	101	SER
1	AX	118	LYS

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Mol	Chain	Res	Type
1	AX	198	VAL
1	AX	220	ILE
1	AX	224	SER
1	AX	255	THR
1	AY	16	THR
1	AY	127	VAL
1	AY	148	LEU
1	AY	201	ILE
1	AY	220	ILE
1	AZ	54	GLN
1	AZ	101	SER
1	AZ	118	LYS
1	AZ	220	ILE
1	AZ	224	SER
1	Aa	179	THR
1	Aa	201	ILE
1	Aa	209	LEU
1	Aa	220	ILE
1	Ab	20	THR
1	Ab	101	SER
1	Ab	220	ILE
1	Ab	224	SER
1	Ab	255	THR
1	Ac	42	ILE
1	Ac	111	MET
1	Ac	127	VAL
1	Ac	133	LEU
1	Ac	148	LEU
1	Ac	179	THR
1	Ac	191	SER
1	Ac	201	ILE
1	Ac	209	LEU
1	Ac	272	LEU
1	Ad	20	THR
1	Ad	55	MET
1	Ad	86	LYS
1	Ad	101	SER
1	Ad	220	ILE
1	Ad	224	SER
1	Ad	255	THR
1	Ae	57	LYS
1	Ae	118	LYS

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Mol	Chain	Res	Type
1	Ae	148	LEU
1	Ae	179	THR
1	Ae	201	ILE
1	Ae	213	ILE
1	Ae	249	CYS
1	Af	90	LEU
1	Af	101	SER
1	Af	198	VAL
1	Af	220	ILE
1	Af	224	SER
1	Af	239	THR
1	Af	255	THR
1	Ag	111	MET
1	Ag	118	LYS
1	Ag	127	VAL
1	Ag	133	LEU
1	Ag	179	THR
1	Ag	201	ILE
1	Ag	220	ILE
1	Ah	101	SER
1	Ah	220	ILE
1	Ah	255	THR
1	Ai	111	MET
1	Ai	132	SER
1	Ai	179	THR
1	Ai	201	ILE
1	Ai	220	ILE
1	Ai	272	LEU
1	Aj	90	LEU
1	Aj	101	SER
1	Aj	224	SER
1	Aj	225	MET
1	Aj	255	THR
1	Aj	262	SER
1	Ak	42	ILE
1	Ak	148	LEU
1	Ak	201	ILE
1	Ak	220	ILE
1	Al	118	LYS
1	Al	220	ILE
1	Al	255	THR
1	Am	42	ILE

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Mol	Chain	Res	Type
1	Am	90	LEU
1	Am	111	MET
1	Am	201	ILE
1	Am	220	ILE
1	Am	272	LEU
1	An	20	THR
1	An	86	LYS
1	An	101	SER
1	An	133	LEU
1	An	198	VAL
1	An	213	ILE
1	An	224	SER
1	An	255	THR
1	Ao	127	VAL
1	Ao	179	THR
1	Ao	201	ILE
1	Ao	209	LEU
1	Ao	220	ILE
1	Ap	64	ARG
1	Ap	220	ILE
1	Ap	224	SER
1	Ap	255	THR
1	Aq	16	THR
1	Aq	42	ILE
1	Aq	133	LEU
1	Aq	201	ILE
1	Aq	249	CYS
1	Aq	272	LEU
1	Ar	86	LYS
1	Ar	220	ILE
1	Ar	255	THR
1	As	90	LEU
1	As	99	ASN
1	As	111	MET
1	As	127	VAL
1	As	179	THR
1	As	201	ILE
1	As	272	LEU
1	At	20	THR
1	At	111	MET
1	At	198	VAL
1	At	220	ILE

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Mol	Chain	Res	Type
1	At	224	SER
1	At	255	THR
1	Au	42	ILE
1	Au	57	LYS
1	Au	99	ASN
1	Au	148	LEU
1	Au	179	THR
1	Au	201	ILE
1	Au	213	ILE
1	Au	220	ILE
1	Au	272	LEU
1	Au	278	GLN
1	Av	20	THR
1	Av	198	VAL
1	Av	220	ILE
1	Av	224	SER
1	Aw	179	THR
1	Aw	201	ILE
1	Aw	209	LEU
1	Aw	225	MET
1	Aw	249	CYS
1	Ax	101	SER
1	Ax	118	LYS
1	Ax	198	VAL
1	Ax	224	SER
1	Ax	255	THR
1	Ay	99	ASN
1	Ay	148	LEU
1	Ay	179	THR
1	Ay	201	ILE
1	Ay	220	ILE
1	Ay	272	LEU
1	Az	86	LYS
1	Az	198	VAL
1	Az	220	ILE
1	Az	224	SER
1	Az	255	THR
1	A1	42	ILE
1	A1	179	THR
1	A1	213	ILE
1	A1	220	ILE
1	A1	272	LEU

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Mol	Chain	Res	Type
1	A2	57	LYS
1	A2	93	VAL
1	A2	101	SER
1	A2	225	MET
1	A2	255	THR
1	A3	132	SER
1	A3	201	ILE
1	A3	220	ILE
1	A4	20	THR
1	A4	198	VAL
1	A4	213	ILE
1	A4	224	SER
1	A4	255	THR
1	A5	90	LEU
1	A5	99	ASN
1	A5	127	VAL
1	A5	191	SER
1	A5	220	ILE
1	A5	249	CYS
1	A5	272	LEU
1	A6	20	THR
1	A6	86	LYS
1	A6	118	LYS
1	A7	16	THR
1	A7	111	MET
1	A7	220	ILE
1	A8	93	VAL
1	A8	198	VAL
1	A8	220	ILE
1	A8	224	SER
1	A8	262	SER
1	A9	90	LEU
1	A9	111	MET
1	A9	198	VAL
1	A9	201	ILE
1	A9	213	ILE
1	A0	101	SER
1	A0	118	LYS
1	A0	220	ILE
1	A0	224	SER
1	A0	255	THR
1	BA	99	ASN

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Mol	Chain	Res	Type
1	BA	198	VAL
1	BA	201	ILE
1	BA	209	LEU
1	BA	213	ILE
1	BA	249	CYS
1	BB	101	SER
1	BB	198	VAL
1	BB	220	ILE
1	BC	42	ILE
1	BC	99	ASN
1	BC	127	VAL
1	BC	133	LEU
1	BC	179	THR
1	BC	201	ILE
1	BC	209	LEU
1	BC	225	MET
1	BC	272	LEU
1	BD	20	THR
1	BD	93	VAL
1	BD	101	SER
1	BD	220	ILE
1	BD	224	SER
1	BD	225	MET
1	BD	239	THR
1	BD	255	THR
1	BE	118	LYS
1	BE	179	THR
1	BE	201	ILE
1	BE	220	ILE
1	BF	20	THR
1	BF	220	ILE
1	BF	224	SER
1	BF	255	THR
1	BG	148	LEU
1	BG	179	THR
1	BG	201	ILE
1	BG	209	LEU
1	BH	20	THR
1	BH	133	LEU
1	BH	220	ILE
1	BH	224	SER
1	BH	255	THR

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Mol	Chain	Res	Type
1	BI	99	ASN
1	BI	179	THR
1	BI	201	ILE
1	BI	220	ILE
1	BI	258	LYS
1	BJ	57	LYS
1	BJ	86	LYS
1	BJ	198	VAL
1	BJ	213	ILE
1	BJ	255	THR
1	BK	16	THR
1	BK	55	MET
1	BK	125	LYS
1	BK	201	ILE
1	BK	220	ILE
1	BK	272	LEU
1	BL	86	LYS
1	BL	198	VAL
1	BL	209	LEU
1	BL	213	ILE
1	BL	224	SER
1	BL	255	THR
1	BM	16	THR
1	BM	220	ILE
1	BN	20	THR
1	BN	93	VAL
1	BN	101	SER
1	BN	118	LYS
1	BN	133	LEU
1	BN	154	MET
1	BN	213	ILE
1	BN	220	ILE
1	BN	255	THR
1	BN	262	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
1	i	89	GLN
1	i	276	ASN
1	i	278	GLN
1	j	168	ASN

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Mol	Chain	Res	Type
1	k	69	HIS
1	k	89	GLN
1	k	276	ASN
1	l	54	GLN
1	m	54	GLN
1	n	162	ASN
1	n	276	ASN
1	p	162	ASN
1	p	276	ASN
1	q	69	HIS
1	q	72	HIS
1	q	168	ASN
1	r	69	HIS
1	r	162	ASN
1	r	276	ASN
1	s	229	HIS
1	s	276	ASN
1	t	103	GLN
1	t	162	ASN
1	u	54	GLN
1	u	168	ASN
1	u	276	ASN
1	v	54	GLN
1	v	162	ASN
1	w	162	ASN
1	w	276	ASN
1	x	162	ASN
1	x	276	ASN
1	y	276	ASN
1	z	5	ASN
1	1	276	ASN
1	2	162	ASN
1	3	229	HIS
1	3	276	ASN
1	4	69	HIS
1	4	162	ASN
1	5	72	HIS
1	5	149	GLN
1	5	229	HIS
1	5	276	ASN
1	6	5	ASN
1	6	162	ASN

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Mol	Chain	Res	Type
1	7	54	GLN
1	7	72	HIS
1	7	89	GLN
1	7	276	ASN
1	8	162	ASN
1	8	276	ASN
1	9	276	ASN
1	0	72	HIS
1	0	149	GLN
1	0	162	ASN
1	0	276	ASN
1	AA	72	HIS
1	AA	276	ASN
1	AB	31	GLN
1	AB	162	ASN
1	AB	276	ASN
1	AC	72	HIS
1	AC	229	HIS
1	AC	276	ASN
1	AD	72	HIS
1	AE	31	GLN
1	AE	168	ASN
1	AE	276	ASN
1	AF	5	ASN
1	AG	276	ASN
1	AH	162	ASN
1	AI	276	ASN
1	AJ	162	ASN
1	AK	149	GLN
1	AK	229	HIS
1	AL	162	ASN
1	AM	149	GLN
1	AM	229	HIS
1	AN	31	GLN
1	AN	162	ASN
1	AO	89	GLN
1	AO	149	GLN
1	AO	168	ASN
1	AP	162	ASN
1	AP	229	HIS
1	AP	276	ASN
1	AQ	72	HIS

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Mol	Chain	Res	Type
1	AQ	229	HIS
1	AQ	276	ASN
1	AR	162	ASN
1	AR	276	ASN
1	AS	72	HIS
1	AS	168	ASN
1	AS	276	ASN
1	AU	276	ASN
1	AV	89	GLN
1	AV	162	ASN
1	AV	276	ASN
1	AW	276	ASN
1	AX	162	ASN
1	AY	276	ASN
1	AZ	162	ASN
1	AZ	168	ASN
1	Aa	276	ASN
1	Ab	149	GLN
1	Ab	276	ASN
1	Ac	229	HIS
1	Ac	276	ASN
1	Ad	162	ASN
1	Ae	276	ASN
1	Af	162	ASN
1	Ag	149	GLN
1	Ah	69	HIS
1	Ah	276	ASN
1	Ai	31	GLN
1	Ai	72	HIS
1	Ai	276	ASN
1	Aj	162	ASN
1	Ak	72	HIS
1	Ak	276	ASN
1	Al	72	HIS
1	Al	162	ASN
1	Am	276	ASN
1	An	162	ASN
1	An	276	ASN
1	Ao	276	ASN
1	Ap	5	ASN
1	Ap	89	GLN
1	Ap	229	HIS

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Mol	Chain	Res	Type
1	Aq	276	ASN
1	Ar	276	ASN
1	As	31	GLN
1	As	276	ASN
1	At	5	ASN
1	At	54	GLN
1	At	69	HIS
1	Au	229	HIS
1	Au	278	GLN
1	Av	162	ASN
1	Aw	276	ASN
1	Ax	162	ASN
1	Ay	149	GLN
1	Ay	276	ASN
1	Az	162	ASN
1	Az	276	ASN
1	A1	168	ASN
1	A2	69	HIS
1	A2	162	ASN
1	A2	276	ASN
1	A3	168	ASN
1	A3	276	ASN
1	A4	276	ASN
1	A5	54	GLN
1	A5	276	ASN
1	A6	72	HIS
1	A6	162	ASN
1	A7	276	ASN
1	A8	69	HIS
1	A8	149	GLN
1	A9	276	ASN
1	A0	5	ASN
1	A0	276	ASN
1	BA	54	GLN
1	BA	276	ASN
1	BB	5	ASN
1	BB	69	HIS
1	BB	162	ASN
1	BC	276	ASN
1	BD	276	ASN
1	BE	276	ASN
1	BF	162	ASN

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Mol	Chain	Res	Type
1	BF	276	ASN
1	BG	72	HIS
1	BH	162	ASN
1	BI	168	ASN
1	BI	229	HIS
1	BJ	276	ASN
1	BK	168	ASN
1	BK	276	ASN
1	BL	89	GLN
1	BL	162	ASN
1	BL	276	ASN
1	BM	168	ASN
1	BM	276	ASN
1	BN	5	ASN
1	BN	162	ASN
1	BN	276	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 104 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

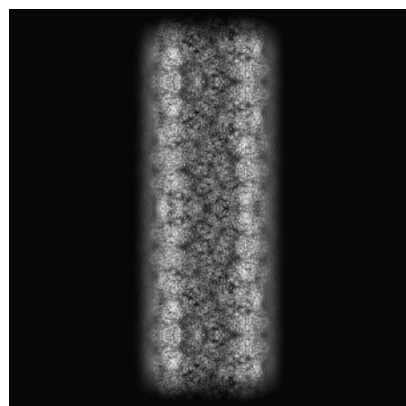
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-81689. These allow visual inspection of the internal detail of the map and identification of artifacts.

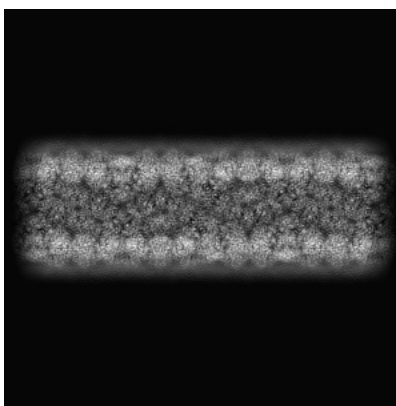
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

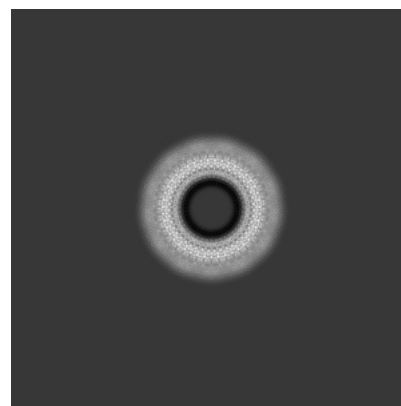
6.1.1 Primary map



X

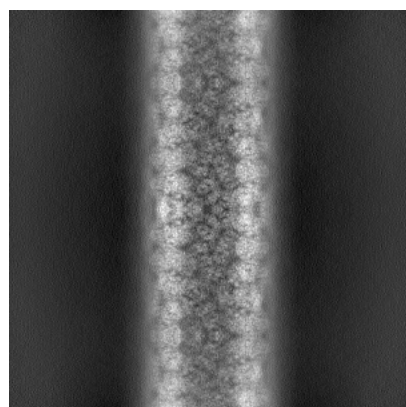


Y

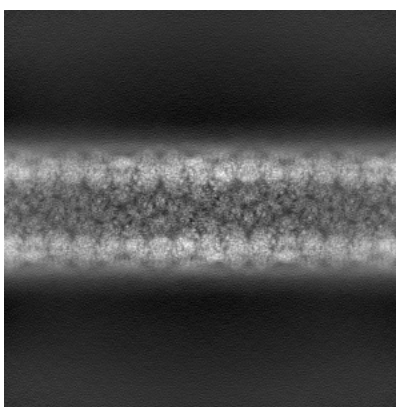


Z

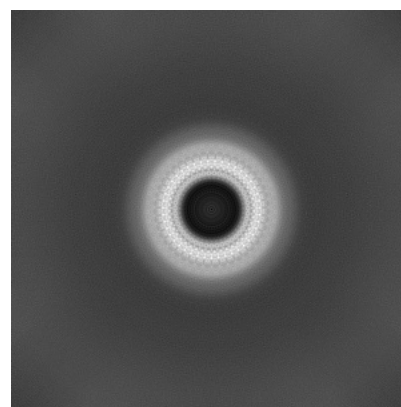
6.1.2 Raw map



X



Y

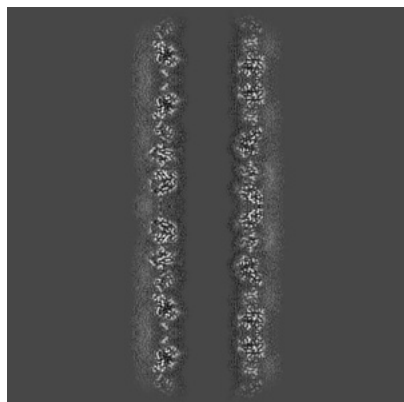


Z

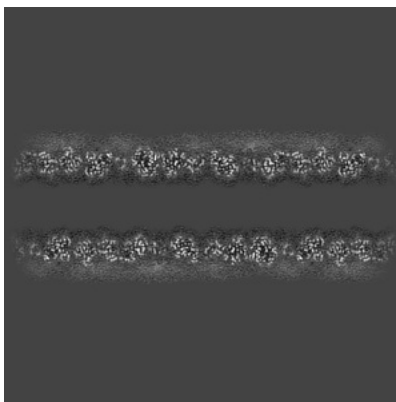
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

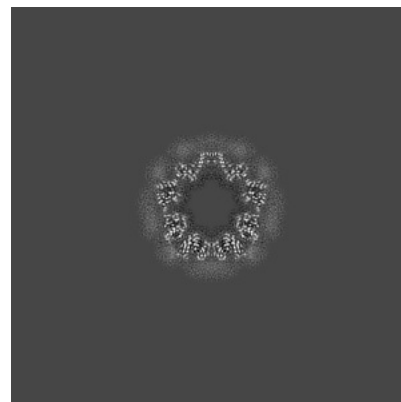
6.2.1 Primary map



X Index: 200

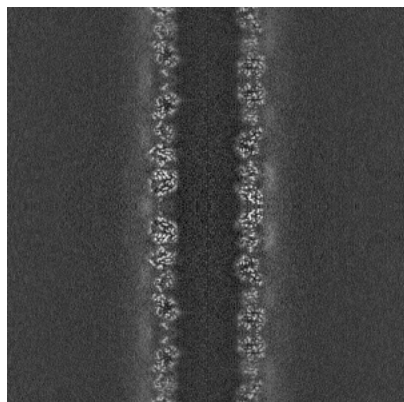


Y Index: 200

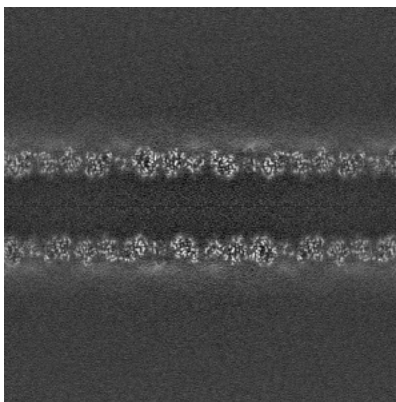


Z Index: 200

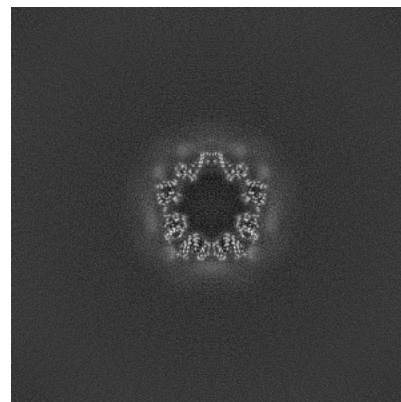
6.2.2 Raw map



X Index: 200



Y Index: 200

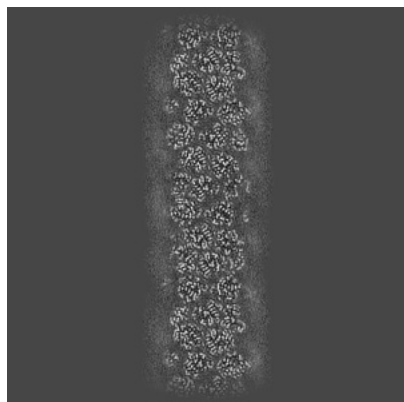


Z Index: 200

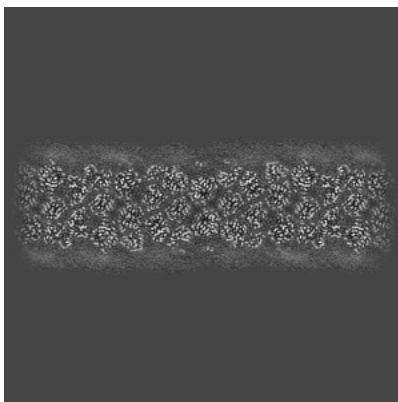
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

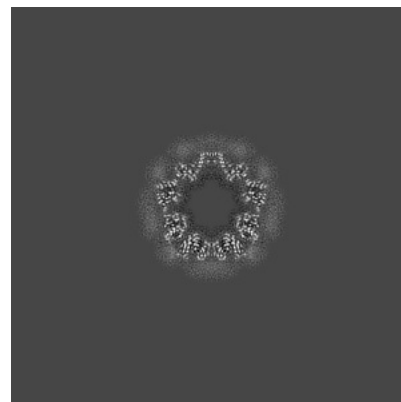
6.3.1 Primary map



X Index: 241

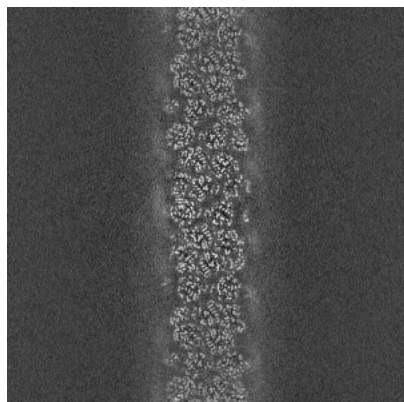


Y Index: 163

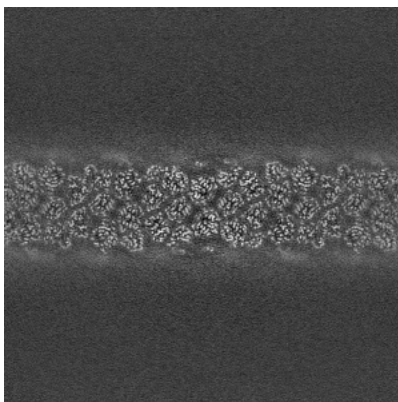


Z Index: 200

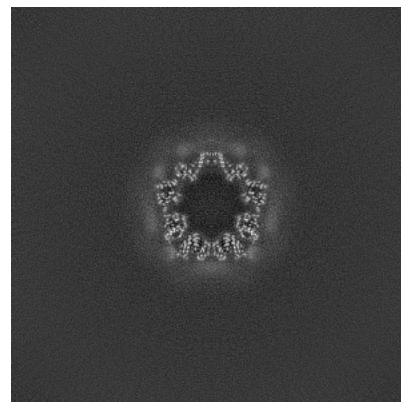
6.3.2 Raw map



X Index: 241



Y Index: 163

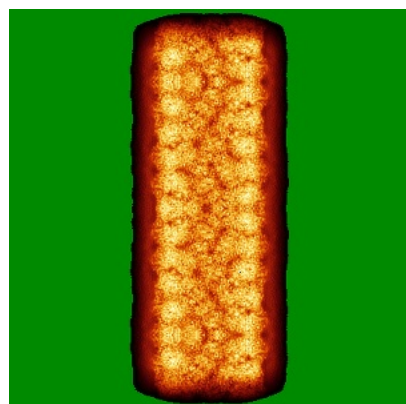


Z Index: 200

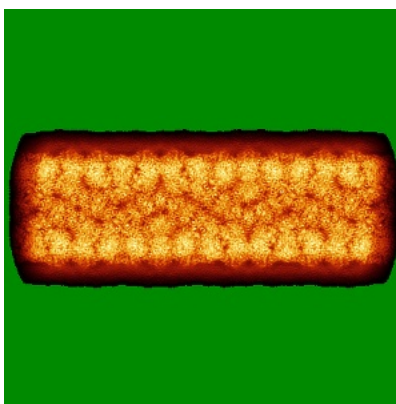
The images above show the largest variance slices of the map in three orthogonal directions.

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

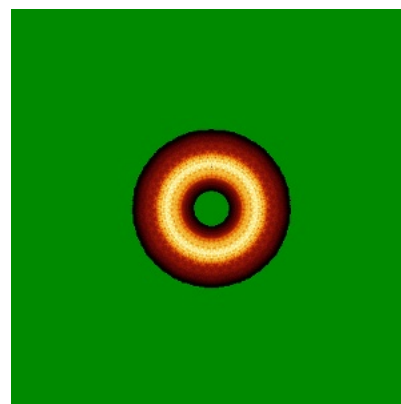
6.4.1 Primary map



X

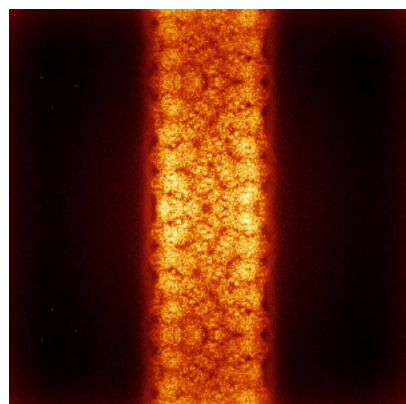


Y

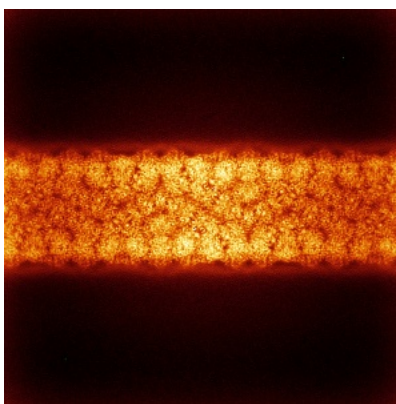


Z

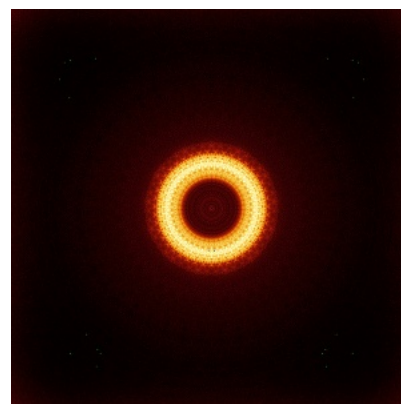
6.4.2 Raw map



X



Y

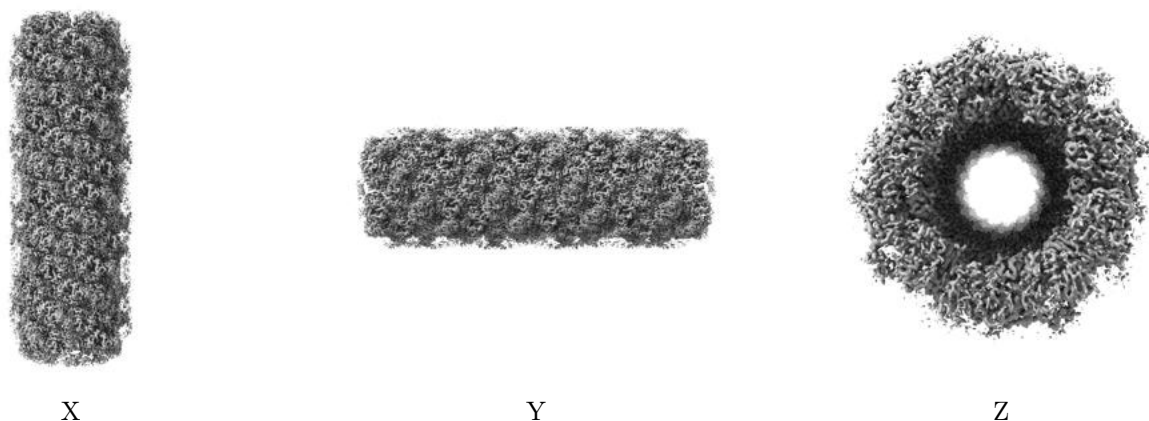


Z

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

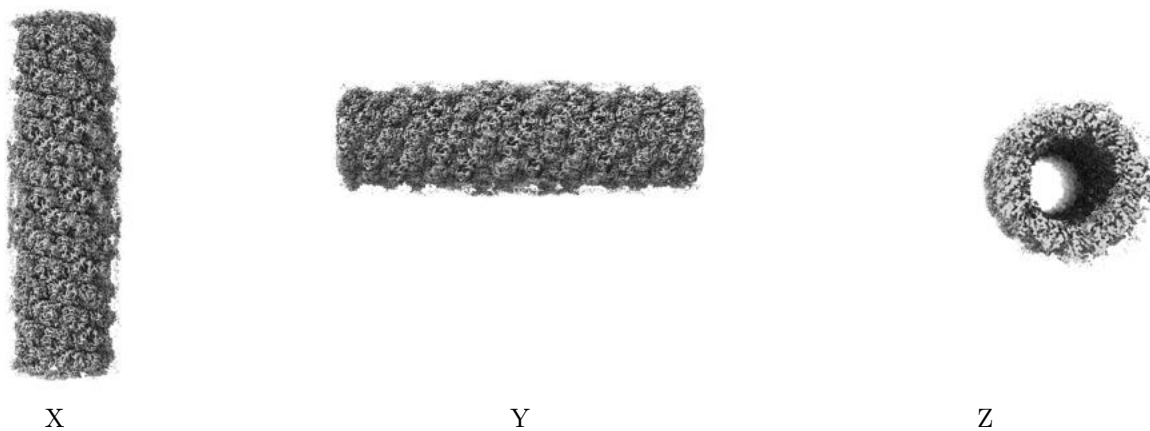
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0457. 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.

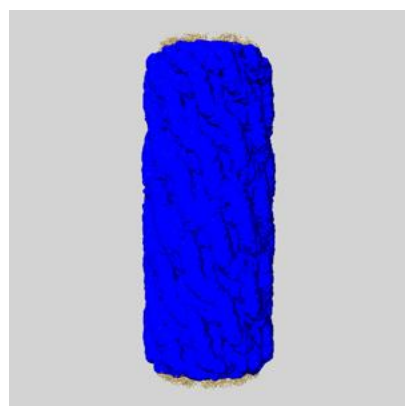
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

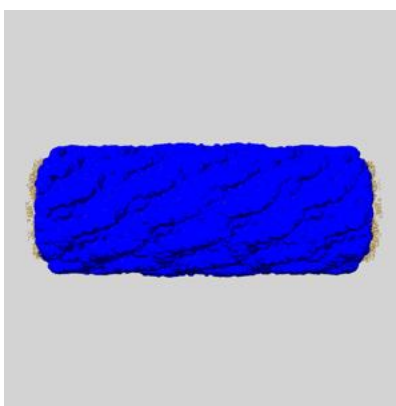
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

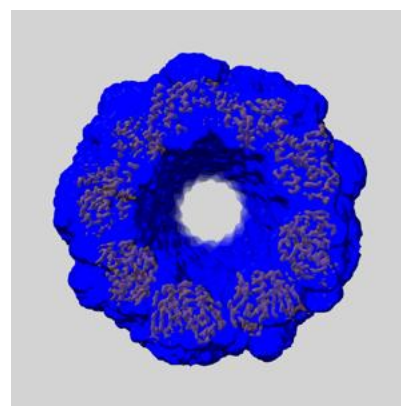
6.6.1 emd_81689_msk_1.map [i](#)



X



Y

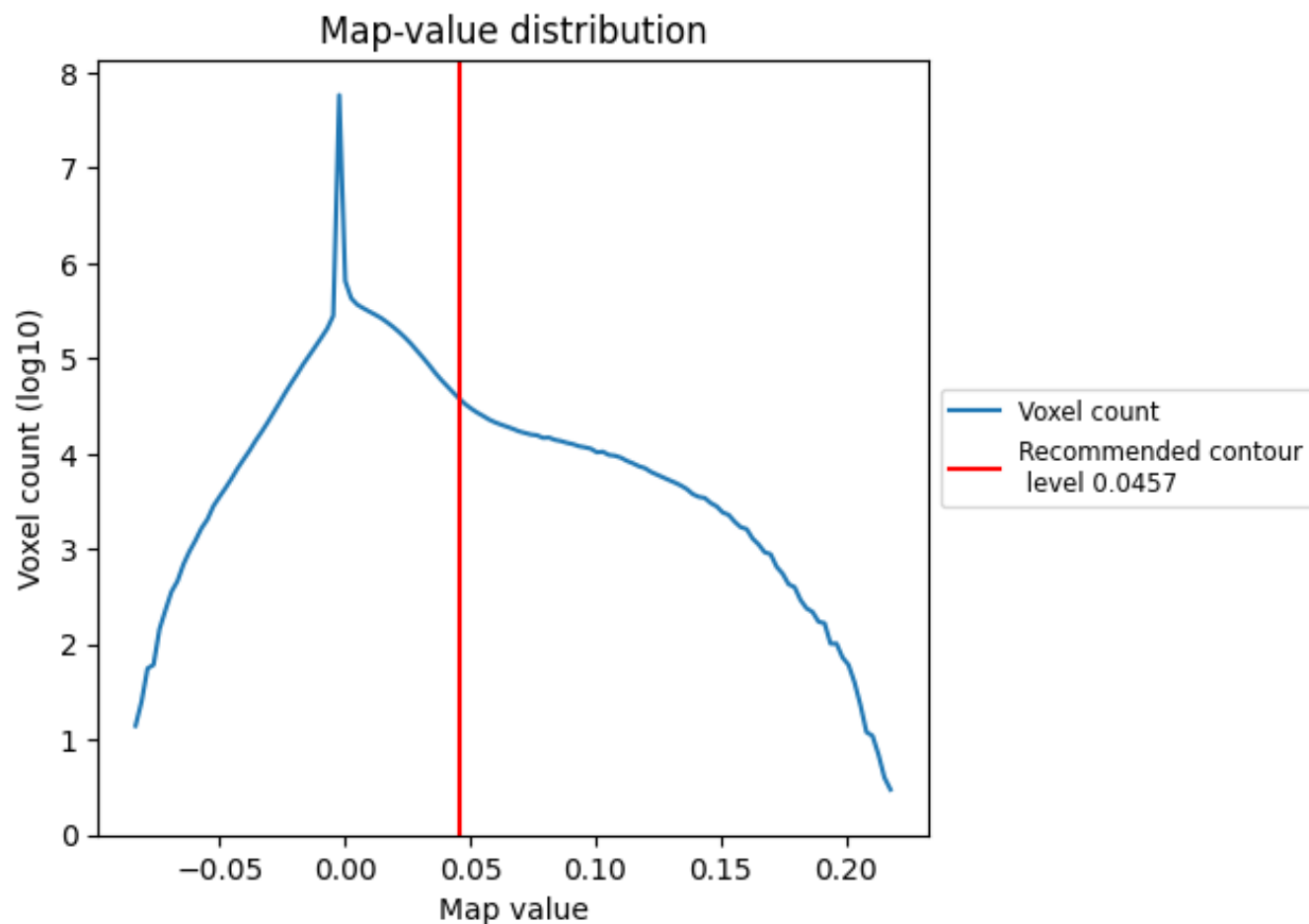


Z

7 Map analysis [i](#)

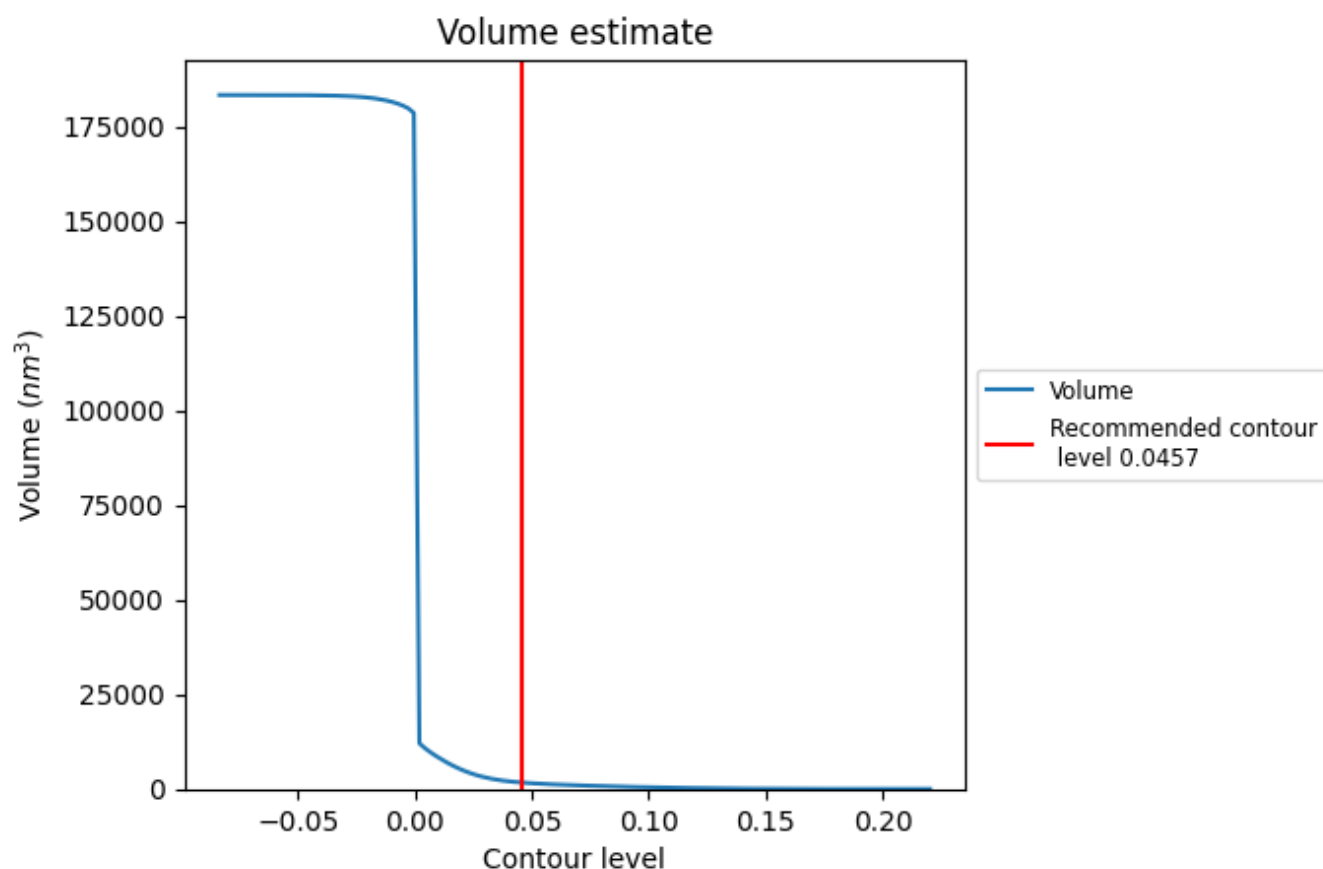
This section contains the results of statistical analysis of the map.

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.

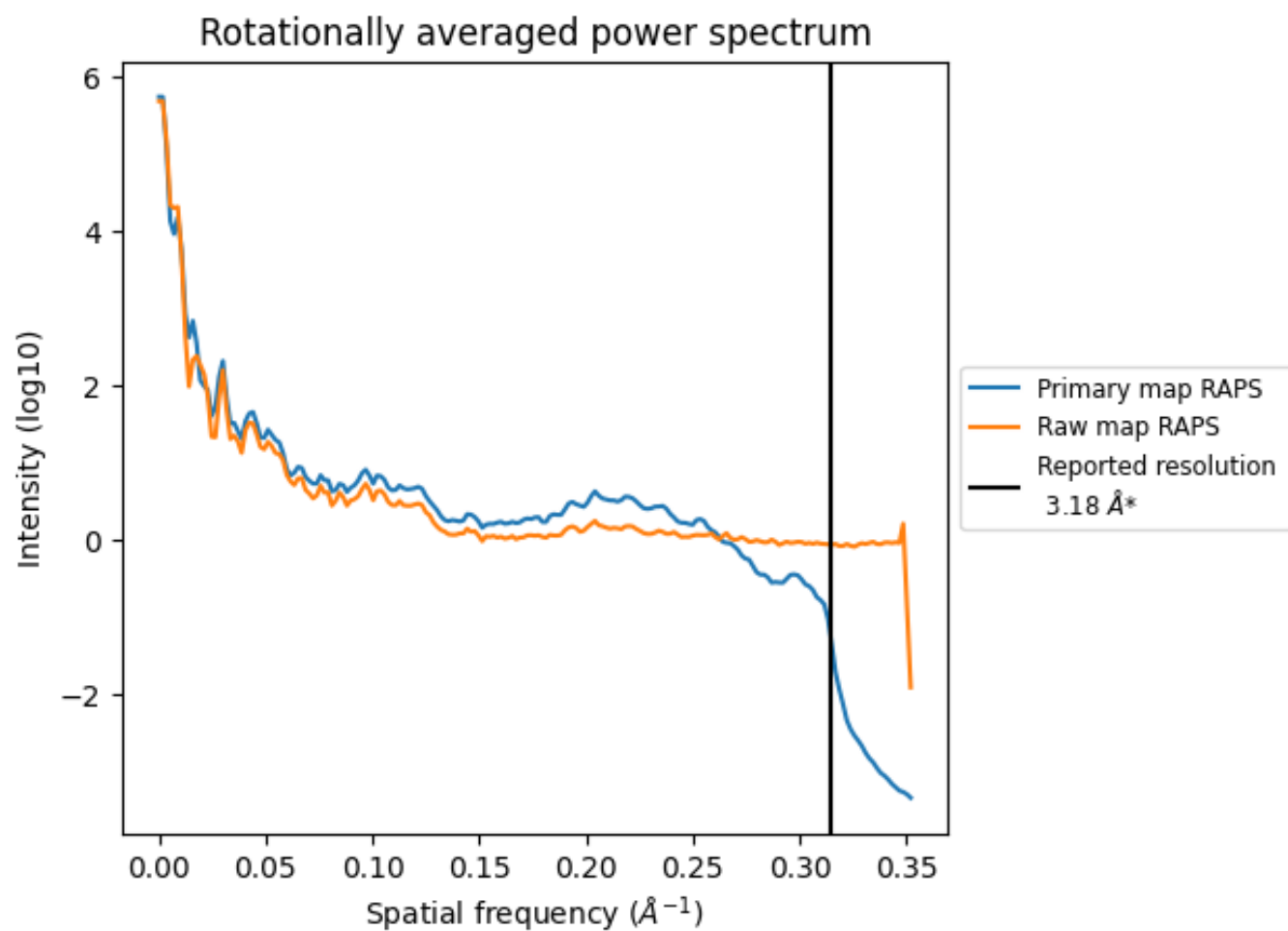
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1690 nm³; this corresponds to an approximate mass of 1527 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 [i](#)

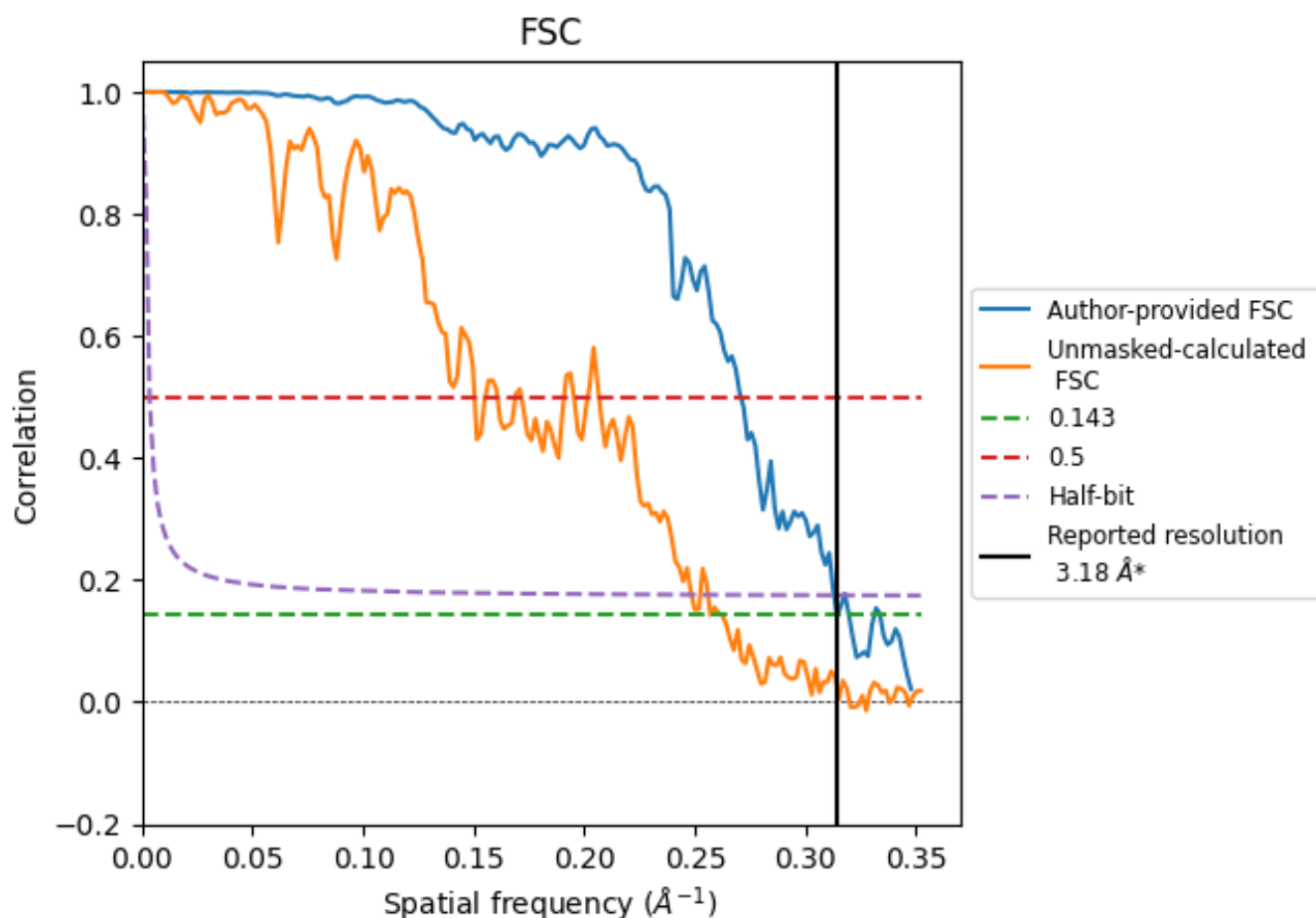


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

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 0.314 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

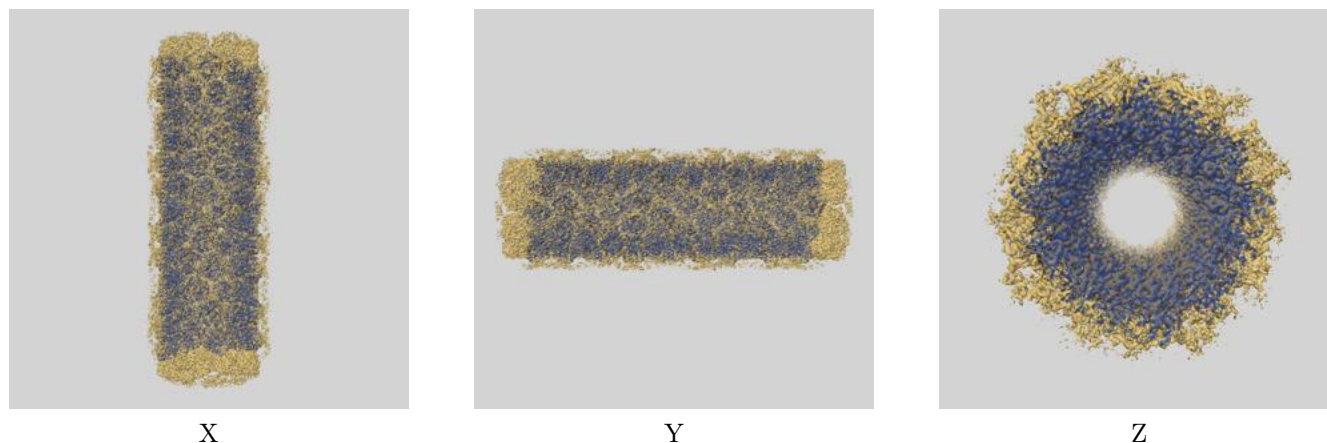
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.69	3.20
Unmasked-calculated*	3.89	6.65	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.18 by more than 10 %

9 Map-model fit [i](#)

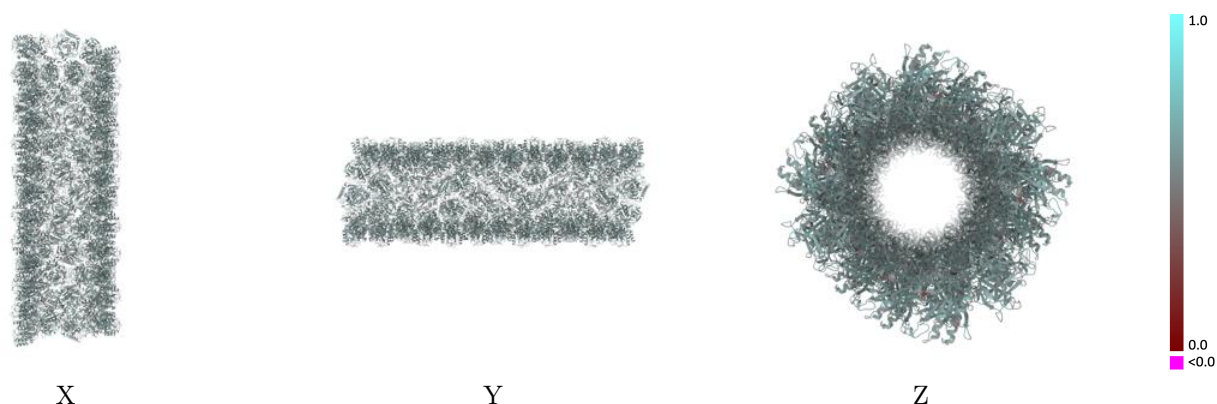
This section contains information regarding the fit between EMDB map EMD-81689 and PDB model 28EP. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



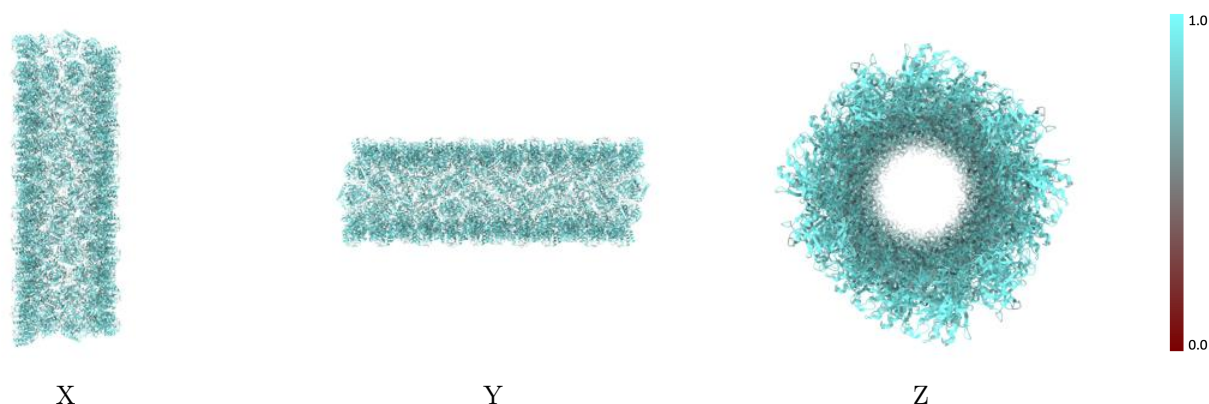
The images above show the 3D surface view of the map at the recommended contour level 0.0457 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



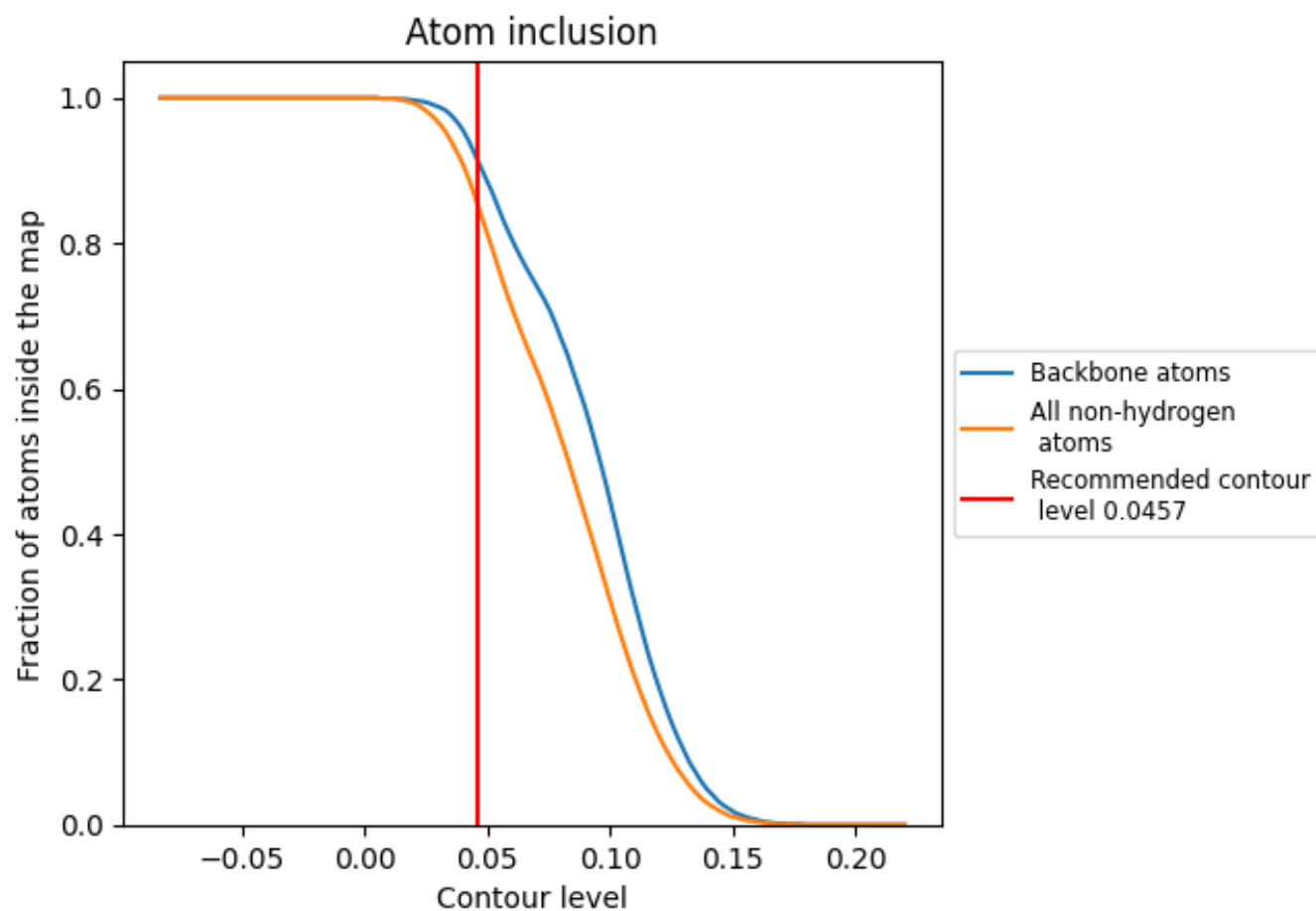
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0457).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.0457) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.5490
0	 0.8510	 0.5480
1	 0.8600	 0.5520
2	 0.8590	 0.5500
3	 0.8590	 0.5490
4	 0.8550	 0.5500
5	 0.8570	 0.5470
6	 0.8530	 0.5510
7	 0.8510	 0.5450
8	 0.8530	 0.5500
9	 0.8520	 0.5450
A0	 0.8640	 0.5510
A1	 0.8530	 0.5450
A2	 0.8490	 0.5500
A3	 0.8510	 0.5460
A4	 0.8510	 0.5510
A5	 0.8560	 0.5480
A6	 0.8630	 0.5530
A7	 0.8560	 0.5460
A8	 0.8640	 0.5490
A9	 0.8610	 0.5500
AA	 0.8550	 0.5460
AB	 0.8600	 0.5500
AC	 0.8530	 0.5450
AD	 0.8550	 0.5520
AE	 0.8530	 0.5490
AF	 0.8570	 0.5500
AG	 0.8570	 0.5480
AH	 0.8660	 0.5520
AI	 0.8590	 0.5510
AJ	 0.8590	 0.5510
AK	 0.8620	 0.5460
AL	 0.8620	 0.5510
AM	 0.8590	 0.5490
AN	 0.8550	 0.5510



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Chain	Atom inclusion	Q-score
AO	 0.8490	 0.5470
AP	 0.8570	 0.5480
AQ	 0.8550	 0.5450
AR	 0.8480	 0.5490
AS	 0.8530	 0.5470
AT	 0.8560	 0.5500
AU	 0.8570	 0.5490
AV	 0.8530	 0.5500
AW	 0.8540	 0.5490
AX	 0.8630	 0.5490
AY	 0.8610	 0.5490
AZ	 0.8610	 0.5520
Aa	 0.8590	 0.5480
Ab	 0.8620	 0.5530
Ac	 0.8590	 0.5480
Ad	 0.8590	 0.5540
Ae	 0.8580	 0.5470
Af	 0.8530	 0.5500
Ag	 0.8560	 0.5460
Ah	 0.8500	 0.5460
Ai	 0.8570	 0.5450
Aj	 0.8580	 0.5500
Ak	 0.8510	 0.5450
Al	 0.8540	 0.5500
Am	 0.8560	 0.5490
An	 0.8570	 0.5510
Ao	 0.8630	 0.5490
Ap	 0.8640	 0.5520
Aq	 0.8590	 0.5480
Ar	 0.8560	 0.5510
As	 0.8560	 0.5480
At	 0.8580	 0.5490
Au	 0.8520	 0.5500
Av	 0.8600	 0.5520
Aw	 0.8530	 0.5480
Ax	 0.8570	 0.5470
Ay	 0.8430	 0.5470
Az	 0.8580	 0.5470
BA	 0.8590	 0.5490
BB	 0.8590	 0.5530
BC	 0.8570	 0.5480
BD	 0.8560	 0.5520

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Chain	Atom inclusion	Q-score
BE	 0.8510	 0.5450
BF	 0.8510	 0.5470
BG	 0.8510	 0.5460
BH	 0.8520	 0.5490
BI	 0.8530	 0.5450
BJ	 0.8530	 0.5500
BK	 0.8580	 0.5470
BL	 0.8550	 0.5520
BM	 0.8560	 0.5470
BN	 0.8550	 0.5480
i	 0.8550	 0.5460
j	 0.8610	 0.5490
k	 0.8580	 0.5500
l	 0.8600	 0.5510
m	 0.8510	 0.5480
n	 0.8540	 0.5510
o	 0.8550	 0.5480
p	 0.8510	 0.5510
q	 0.8460	 0.5450
r	 0.8490	 0.5460
s	 0.8520	 0.5450
t	 0.8590	 0.5510
u	 0.8570	 0.5480
v	 0.8550	 0.5520
w	 0.8610	 0.5480
x	 0.8580	 0.5530
y	 0.8600	 0.5480
z	 0.8540	 0.5480