



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:40 AM UTC

PDB ID : 9HAU / pdb_00009hau
EMDB ID : EMD-52007
Title : pT=3 virus-like particle of ssRNA phage Hubei14 coat protein
Authors : Kalnins, G.
Deposited on : 2024-11-05
Resolution : 2.90 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

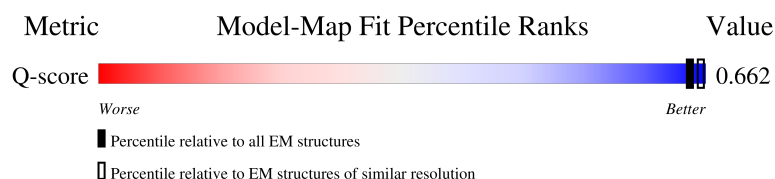
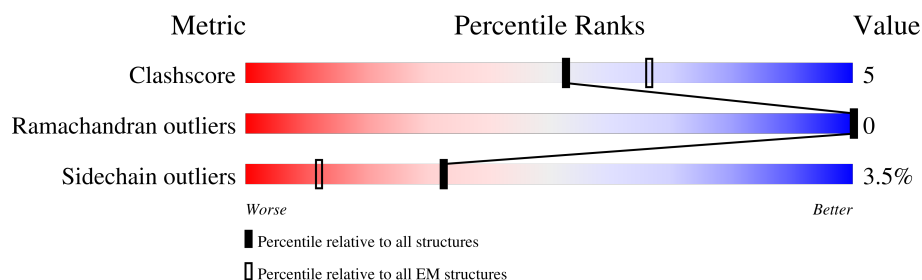
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	AA	117	9% 84% 15% .
1	AC	117	10% 86% 14%
1	AD	117	10% 75% 22% .
1	AE	117	9% 85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AG	117	9% 79% 20%
1	AH	117	11% 81% 18%
1	AI	117	9% 92% 8%
1	AK	117	10% 85% 15%
1	AL	117	12% 79% 20%
1	AM	117	9% 85% 15%
1	AO	117	10% 86% 14%
1	AP	117	10% 75% 22%
1	AQ	117	9% 85% 15%
1	AS	117	10% 80% 19%
1	AT	117	11% 82% 15%
1	AU	117	9% 88% 12%
1	AW	117	9% 85% 15%
1	AX	117	11% 80% 19%
1	AY	117	9% 89% 11%
1	BA	117	10% 86% 14%
1	BB	117	12% 83% 16%
1	BC	117	9% 85% 14%
1	BE	117	10% 85% 15%
1	BF	117	10% 75% 22%
1	BG	117	9% 87% 13%
1	BI	117	10% 82% 18%
1	BJ	117	11% 82% 15%
1	BK	117	9% 91% 9%
1	BM	117	10% 86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BN	117	12% 83% 16%
1	BO	117	9% 85% 15%
1	BQ	117	9% 86% 14%
1	BR	117	11% 80% 19%
1	BS	117	9% 83% 17%
1	BU	117	9% 83% 16%
1	BV	117	11% 77% 22%
1	BW	117	9% 88% 12%
1	BY	117	10% 83% 17%
1	BZ	117	11% 85% 13%
1	CA	117	9% 91% 9%
1	CC	117	10% 85% 15%
1	CD	117	12% 81% 18%
1	CE	117	9% 87% 13%
1	CG	117	9% 87% 13%
1	CH	117	11% 78% 21%
1	CI	117	9% 88% 12%
1	CK	117	10% 83% 17%
1	CL	117	11% 85% 14%
1	CM	117	9% 82% 17%
1	CO	117	9% 82% 17%
1	CP	117	11% 80% 19%
1	CQ	117	9% 84% 15%
1	CS	117	10% 87% 13%
1	CT	117	10% 81% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CU	117	9% 85% 15%
1	CW	117	9% 87% 13%
1	CX	117	11% 78% 21%
1	CY	117	9% 89% 11%
1	DA	117	10% 81% 19%
1	DB	117	11% 80% 17%
1	DC	117	9% 83% 16%
1	DE	117	9% 81% 18%
1	DF	117	11% 84% 16%
1	DG	117	9% 85% 15%
1	DI	117	9% 89% 11%
1	DJ	117	11% 79% 21%
1	DK	117	9% 84% 15%
1	DM	117	10% 85% 15%
1	DN	117	10% 79% 19%
1	DO	117	9% 91% 9%
1	DQ	117	10% 87% 13%
1	DR	117	12% 85% 15%
1	DS	117	9% 87% 13%
1	DU	117	9% 81% 18%
1	DV	117	11% 79% 20%
1	DW	117	9% 85% 15%
1	DY	117	9% 87% 13%
1	DZ	117	11% 80% 19%
1	EA	117	9% 85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EC	117	
1	ED	117	
1	EE	117	
1	EG	117	
1	EH	117	
1	EI	117	
1	EK	117	
1	EL	117	
1	EM	117	
1	EO	117	
1	EP	117	
1	EQ	117	
1	ES	117	
1	ET	117	
1	EU	117	
1	EW	117	
1	EX	117	
1	EY	117	
1	FA	117	
1	FB	117	
1	FC	117	
1	FE	117	
1	FF	117	
1	FG	117	
1	FI	117	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FJ	117	11% 79% 20%
1	FK	117	9% 88% 12%
1	FM	117	10% 84% 16%
1	FN	117	11% 84% 14%
1	FO	117	9% 84% 16%
1	FQ	117	9% 79% 21%
1	FR	117	11% 82% 18%
1	FS	117	9% 85% 14%
1	FU	117	10% 83% 17%
1	FV	117	10% 75% 23%
1	FW	117	9% 86% 14%
1	FY	117	9% 85% 15%
1	FZ	117	10% 85% 14%
1	GA	117	9% 84% 16%
1	GC	117	10% 80% 20%
1	GD	117	11% 83% 17%
1	GE	117	8% 83% 17%
1	GG	117	10% 83% 17%
1	GH	117	11% 78% 21%
1	GI	117	9% 87% 12%
1	GK	117	10% 89% 11%
1	GL	117	12% 85% 13%
1	GM	117	9% 90% 10%
1	GO	117	9% 86% 14%
1	GP	117	10% 84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	GQ	117	9% 85% 15%
1	GS	117	10% 82% 18%
1	GT	117	11% 82% 17%
1	GU	117	8% 84% 16%
1	GW	117	10% 81% 19%
1	GX	117	11% 79% 20%
1	GY	117	9% 90% 10%
1	HA	117	9% 85% 15%
1	HB	117	10% 84% 15%
1	HC	117	9% 87% 12%
1	HE	117	10% 87% 13%
1	HF	117	12% 85% 13%
1	HG	117	9% 84% 16%
1	HI	117	10% 84% 16%
1	HJ	117	10% 79% 20%
1	HK	117	8% 83% 17%
1	HM	117	10% 82% 18%
1	HN	117	11% 77% 21%
1	HO	117	9% 90% 10%
1	HQ	117	9% 86% 14%
1	HR	117	10% 85% 15%
1	HS	117	9% 85% 15%
1	HU	117	10% 84% 16%
1	HV	117	12% 85% 14%
1	HW	117	8% 83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	HY	117	10% 82% 18%
1	HZ	117	11% 77% 21%
1	IA	117	9% 83% 17%
1	IC	117	10% 84% 16%
1	ID	117	10% 78% 21%
1	IE	117	9% 85% 15%
1	IG	117	10% 82% 18%
1	IH	117	11% 82% 17%
1	II	117	9% 85% 14%
1	IK	117	10% 85% 15%
1	IL	117	12% 88% 11%
1	IM	117	8% 85% 15%
1	IO	117	10% 81% 19%
1	IP	117	11% 79% 20%
1	IQ	117	9% 85% 15%
1	IS	117	10% 84% 16%
1	IT	117	10% 75% 22%
1	IU	117	9% 85% 14%
1	IW	117	10% 83% 17%
1	IX	117	12% 88% 11%
1	IY	117	9% 87% 13%
1	JA	117	10% 82% 18%
1	JB	117	11% 82% 17%
1	JC	117	9% 89% 11%
1	JE	117	9% 85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	JF	117	10% 84% 15%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 156420 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AC	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AD	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AE	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AG	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AH	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AI	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AK	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AL	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AM	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AO	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AP	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AQ	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AS	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AT	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AU	117	Total	C	N	O	S	0	0
			869	541	154	171	3		
1	AW	117	Total	C	N	O	S	0	0
			869	541	154	171	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AX	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	AY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BB	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BF	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BG	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BI	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BJ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BK	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BN	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BR	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BS	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BV	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	BY	117	Total 869	C 541	N 154	O 171	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BZ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CD	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CG	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CH	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CI	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CK	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CL	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CP	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CS	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CT	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CX	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	CY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DA	117	Total 869	C 541	N 154	O 171	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DB	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DF	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DG	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DI	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DJ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DK	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DN	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DR	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DS	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DV	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	DZ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EC	117	Total 869	C 541	N 154	O 171	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	ED	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EG	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EH	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EI	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EK	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EL	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EP	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	ES	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	ET	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EX	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	EY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FB	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FE	117	Total 869	C 541	N 154	O 171	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	FF	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FG	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FI	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FJ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FK	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FN	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FR	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FS	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FV	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	FZ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GD	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GG	117	Total 869	C 541	N 154	O 171	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	GH	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GI	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GK	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GL	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GP	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GS	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GT	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GX	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	GY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HB	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HF	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HG	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HI	117	Total 869	C 541	N 154	O 171	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	HJ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HK	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HN	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HR	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HS	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HV	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	HZ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	ID	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IG	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IH	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	II	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IK	117	Total 869	C 541	N 154	O 171	S 3	0	0

Continued on next page...

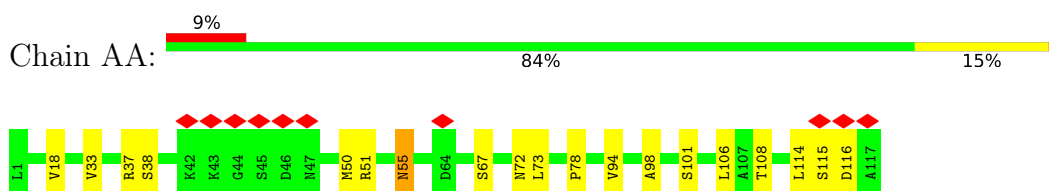
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	IL	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IM	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IO	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IP	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IQ	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IS	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IT	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IU	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IW	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IX	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	IY	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	JA	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	JB	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	JC	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	JE	117	Total 869	C 541	N 154	O 171	S 3	0	0
1	JF	117	Total 869	C 541	N 154	O 171	S 3	0	0

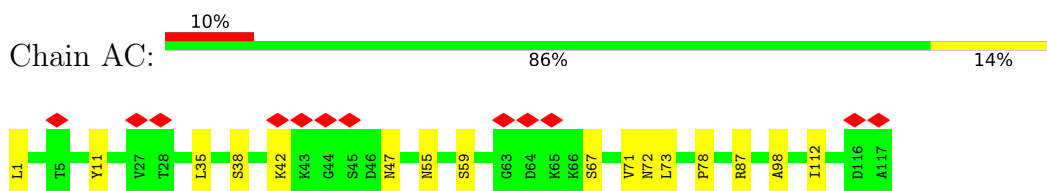
3 Residue-property plots [i](#)

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.

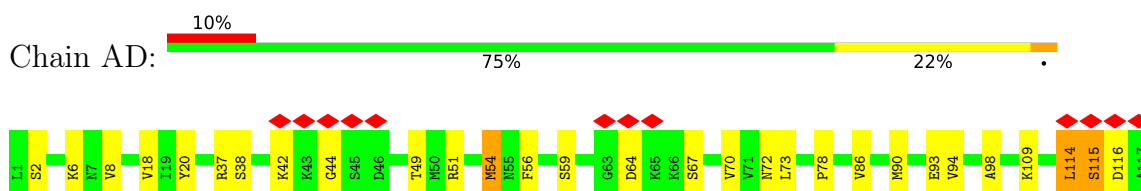
- Molecule 1: Capsid protein



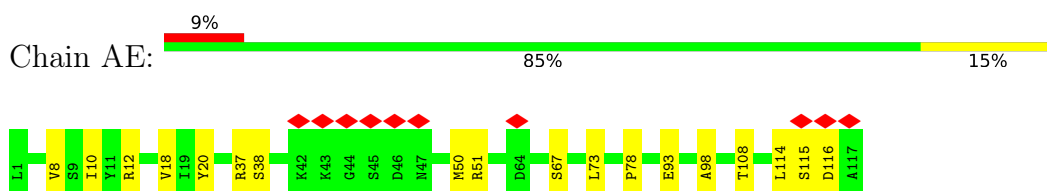
- Molecule 1: Capsid protein



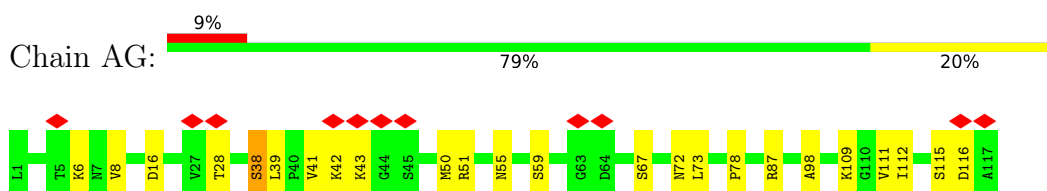
- Molecule 1: Capsid protein



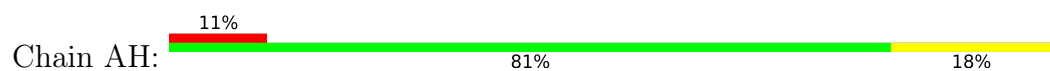
- Molecule 1: Capsid protein



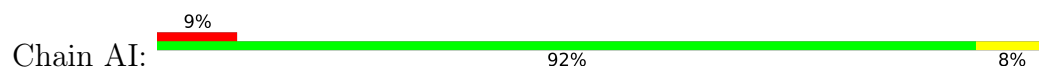
- Molecule 1: Capsid protein



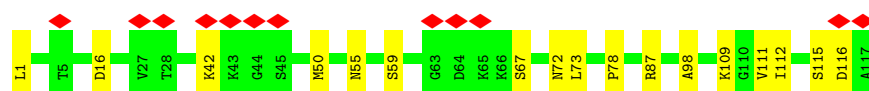
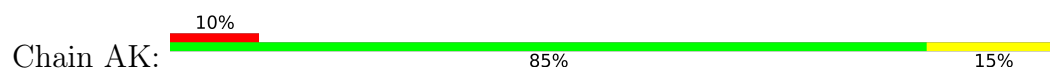
• Molecule 1: Capsid protein



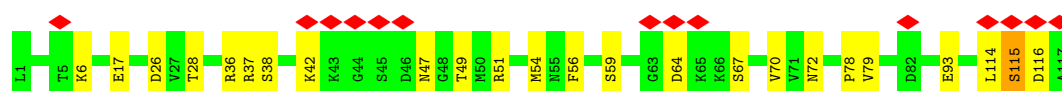
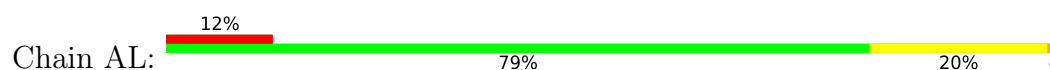
• Molecule 1: Capsid protein



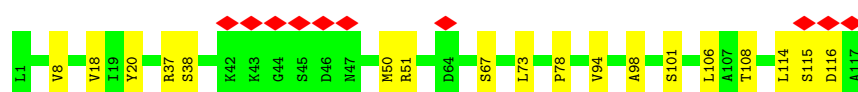
• Molecule 1: Capsid protein



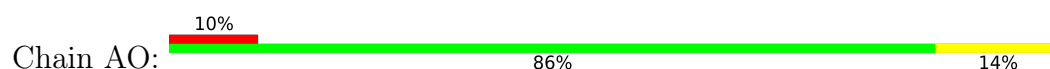
• Molecule 1: Capsid protein



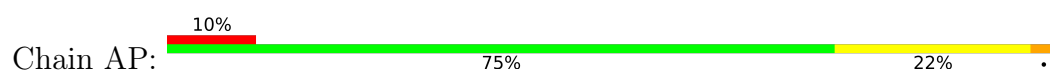
• Molecule 1: Capsid protein

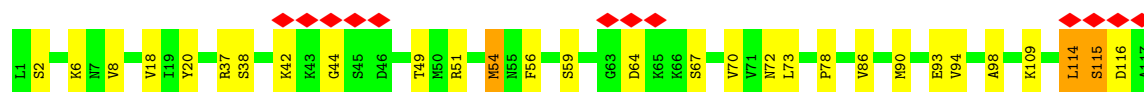


• Molecule 1: Capsid protein

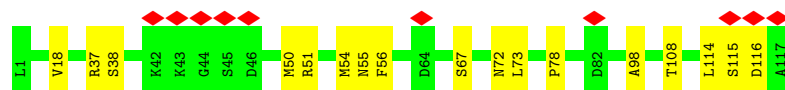
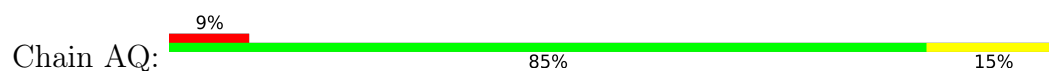


• Molecule 1: Capsid protein

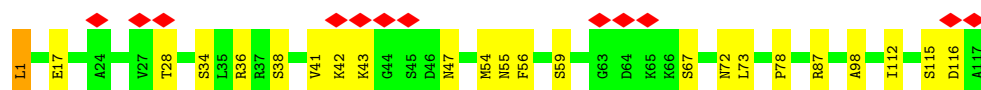
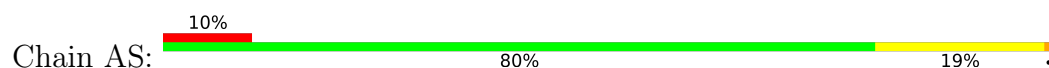




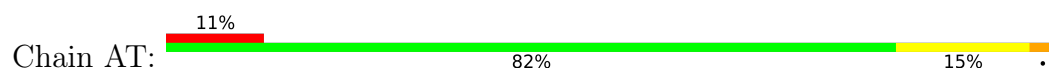
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



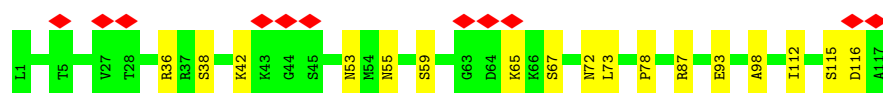
- Molecule 1: Capsid protein



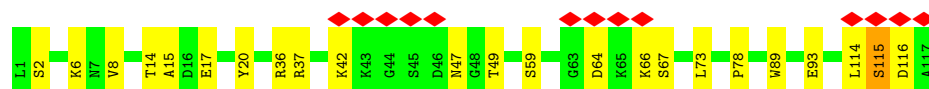
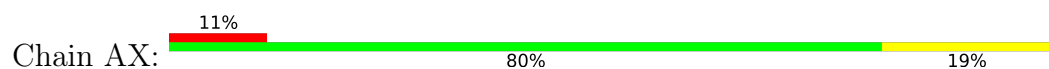
- Molecule 1: Capsid protein



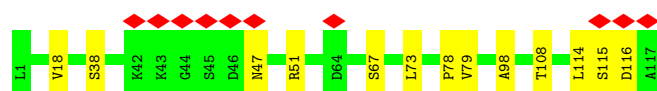
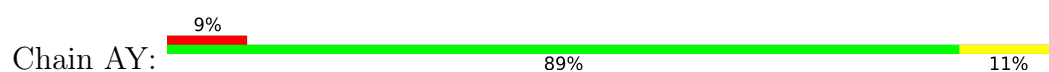
- Molecule 1: Capsid protein



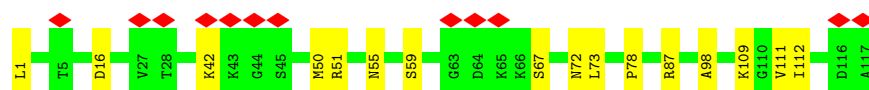
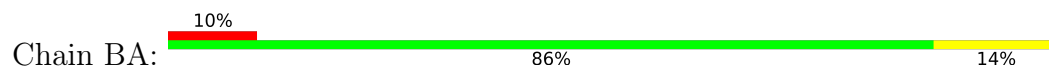
- Molecule 1: Capsid protein



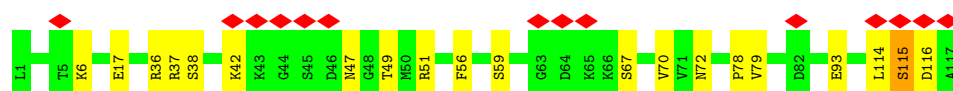
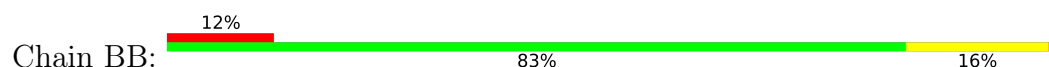
- Molecule 1: Capsid protein



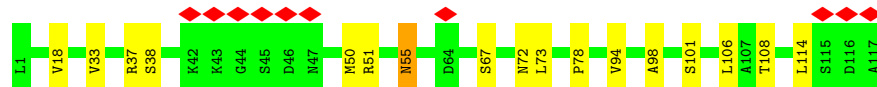
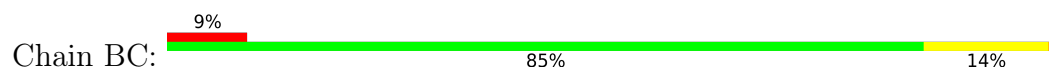
- Molecule 1: Capsid protein



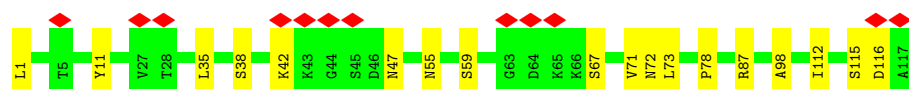
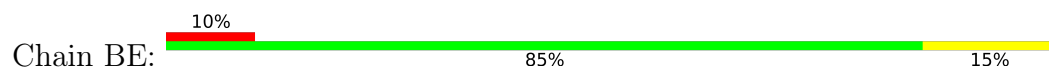
- Molecule 1: Capsid protein



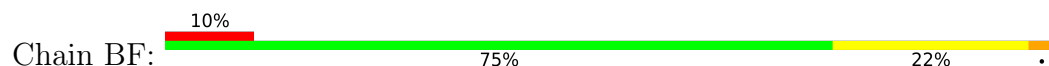
- Molecule 1: Capsid protein



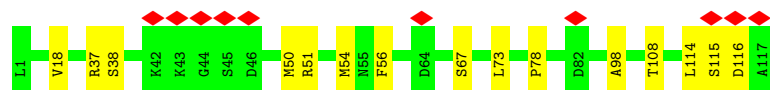
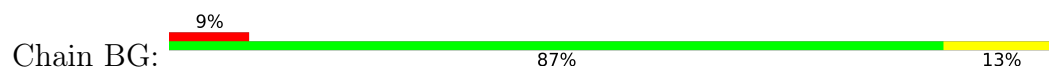
- Molecule 1: Capsid protein



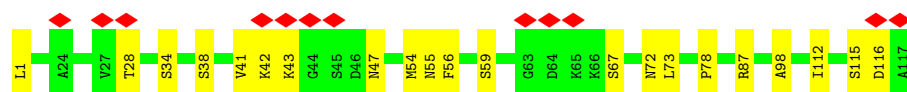
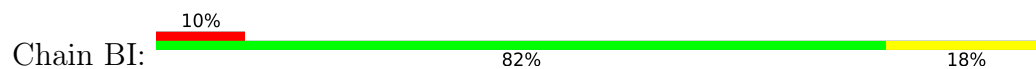
- Molecule 1: Capsid protein



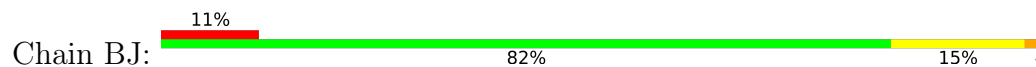
- Molecule 1: Capsid protein



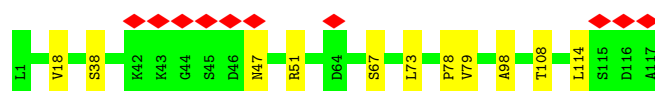
● Molecule 1: Capsid protein



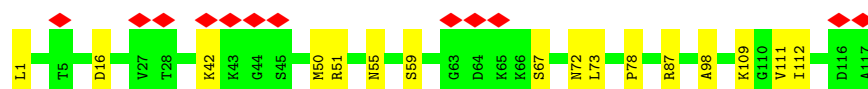
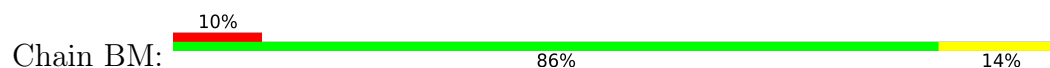
● Molecule 1: Capsid protein



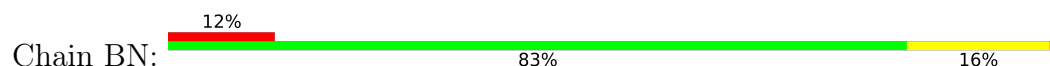
● Molecule 1: Capsid protein



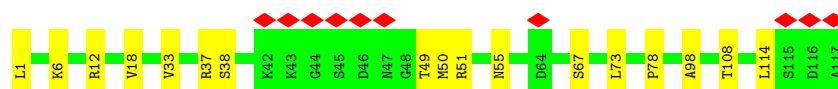
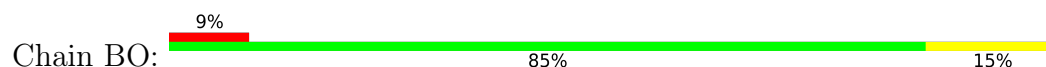
● Molecule 1: Capsid protein



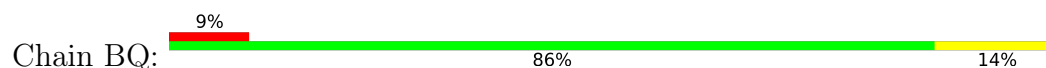
● Molecule 1: Capsid protein

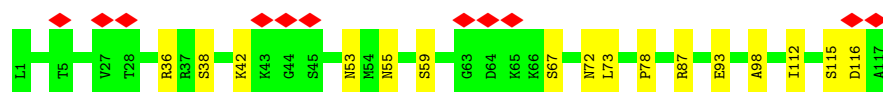


● Molecule 1: Capsid protein

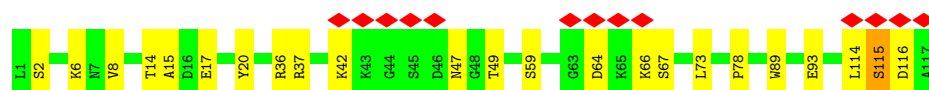
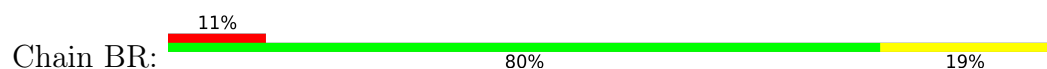


● Molecule 1: Capsid protein

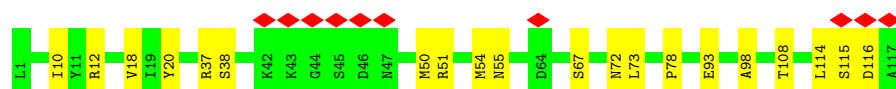
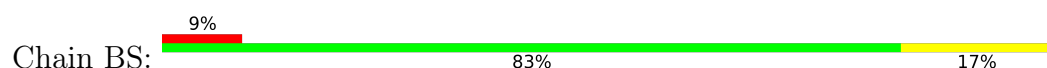




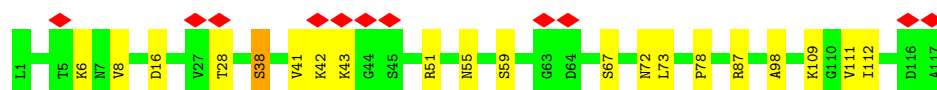
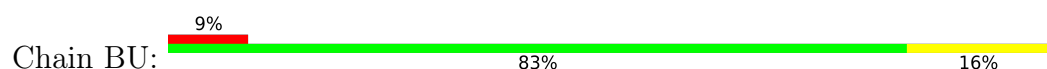
- Molecule 1: Capsid protein



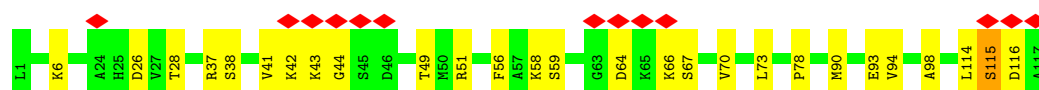
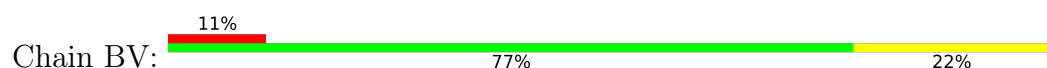
- Molecule 1: Capsid protein



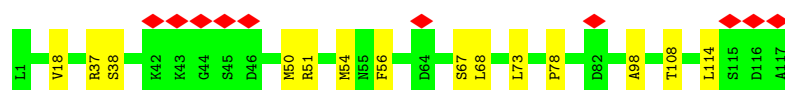
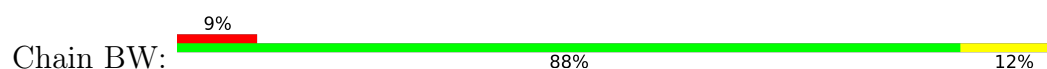
- Molecule 1: Capsid protein



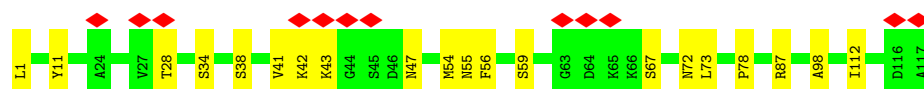
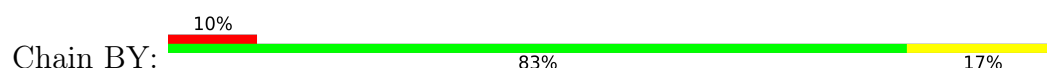
- Molecule 1: Capsid protein



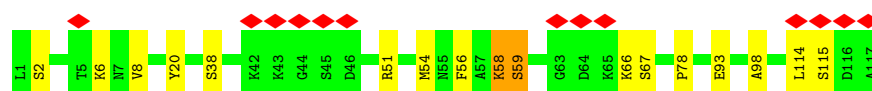
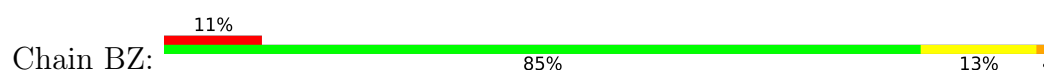
- Molecule 1: Capsid protein



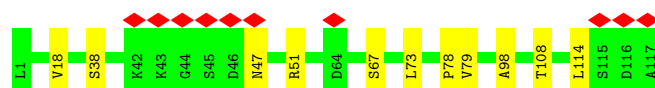
- Molecule 1: Capsid protein



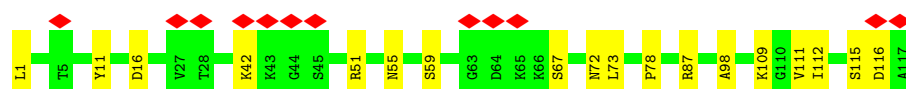
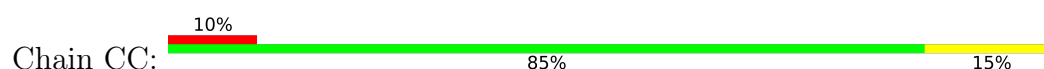
- Molecule 1: Capsid protein



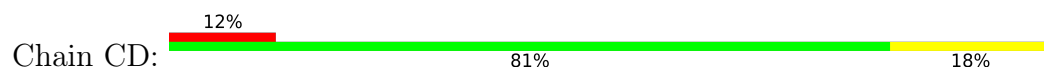
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



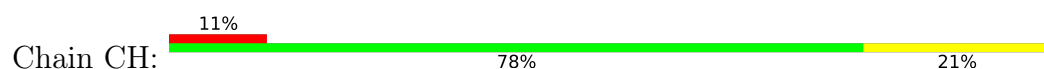
- Molecule 1: Capsid protein



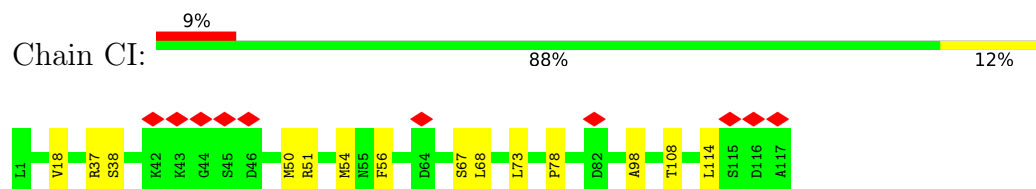
- Molecule 1: Capsid protein



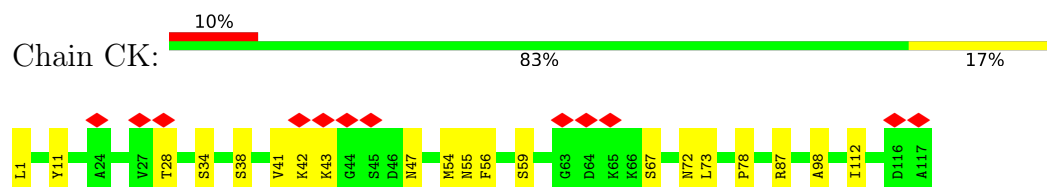
- Molecule 1: Capsid protein



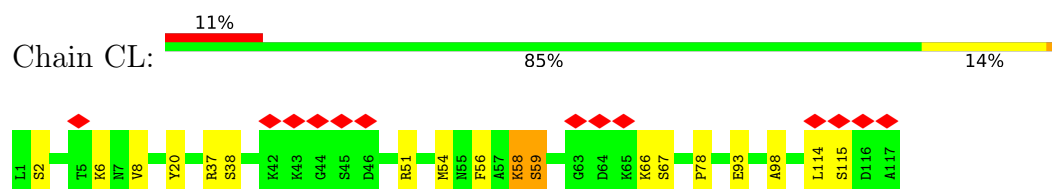
● Molecule 1: Capsid protein



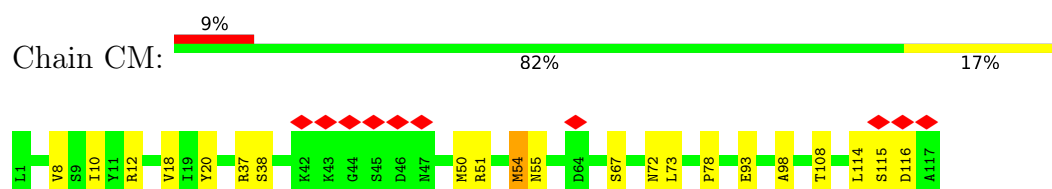
● Molecule 1: Capsid protein



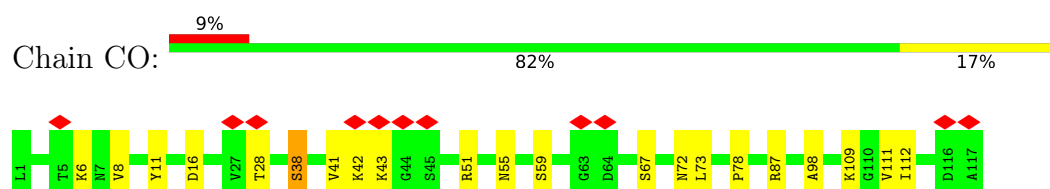
● Molecule 1: Capsid protein



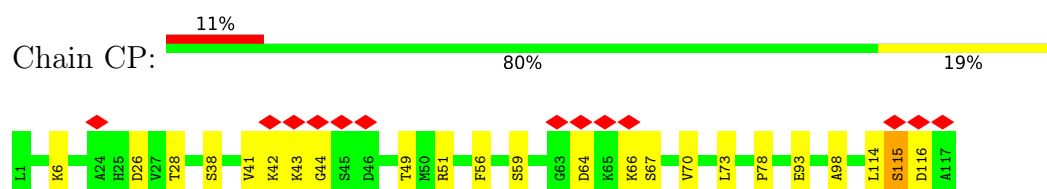
● Molecule 1: Capsid protein



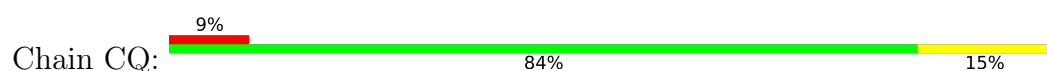
● Molecule 1: Capsid protein



● Molecule 1: Capsid protein

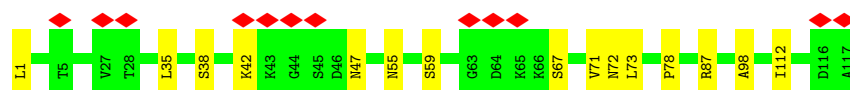
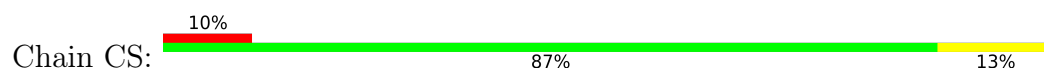


● Molecule 1: Capsid protein

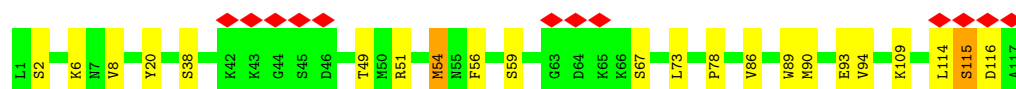
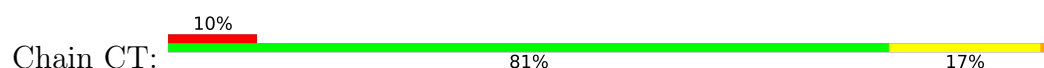




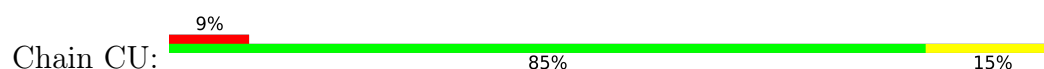
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



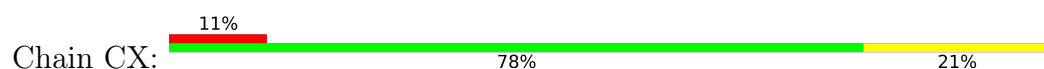
- Molecule 1: Capsid protein



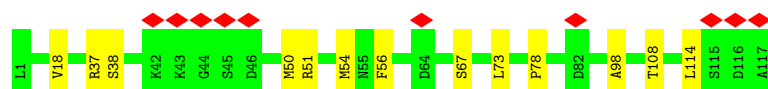
- Molecule 1: Capsid protein



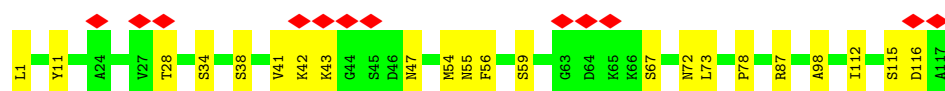
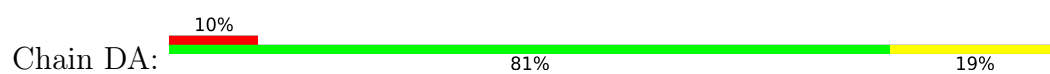
- Molecule 1: Capsid protein



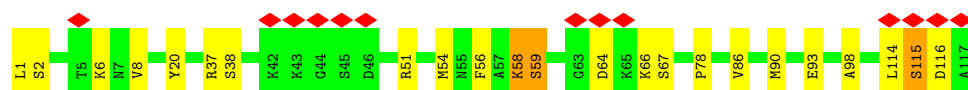
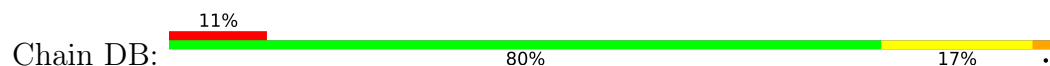
- Molecule 1: Capsid protein



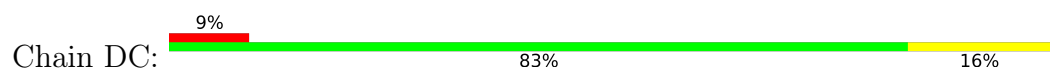
- Molecule 1: Capsid protein



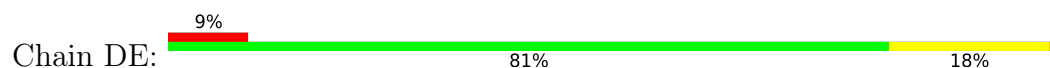
- Molecule 1: Capsid protein



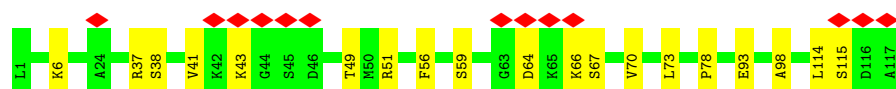
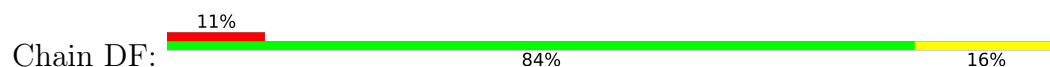
- Molecule 1: Capsid protein



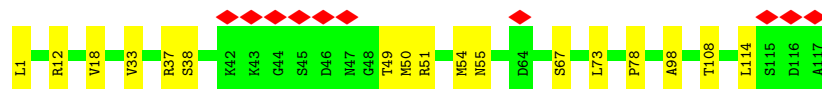
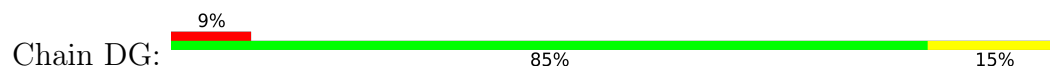
- Molecule 1: Capsid protein



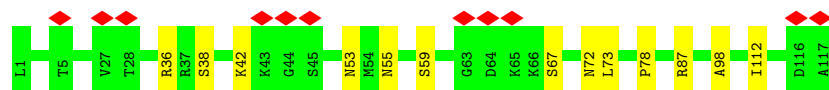
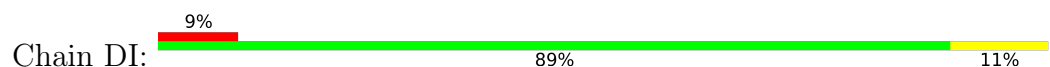
- Molecule 1: Capsid protein



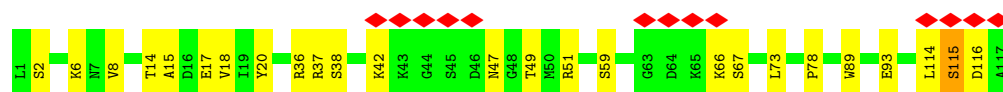
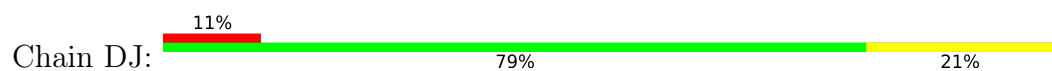
- Molecule 1: Capsid protein



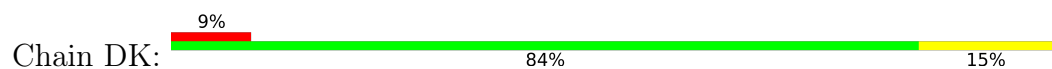
- Molecule 1: Capsid protein



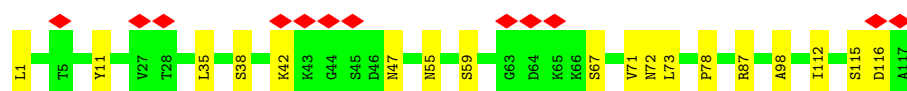
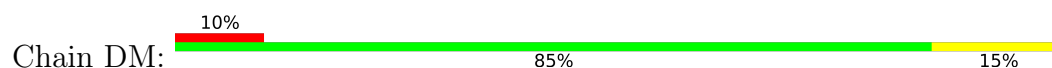
● Molecule 1: Capsid protein



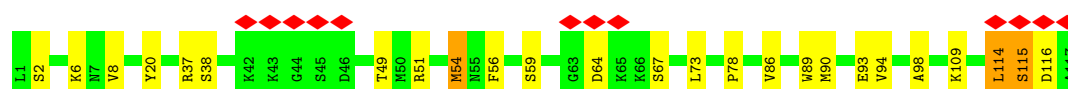
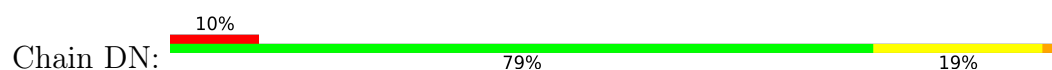
● Molecule 1: Capsid protein



● Molecule 1: Capsid protein



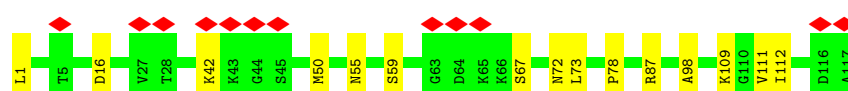
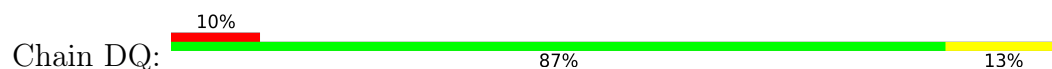
● Molecule 1: Capsid protein



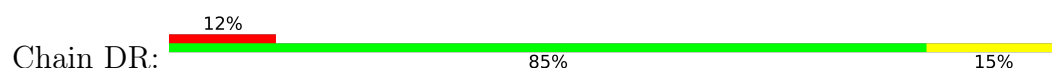
● Molecule 1: Capsid protein

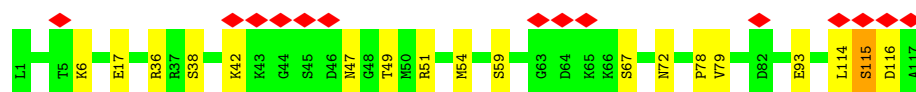


● Molecule 1: Capsid protein

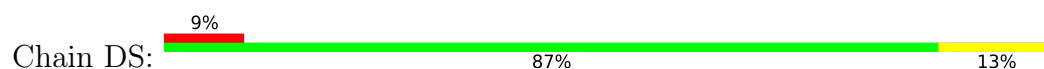


● Molecule 1: Capsid protein

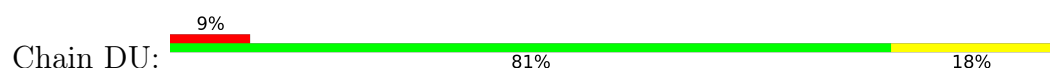




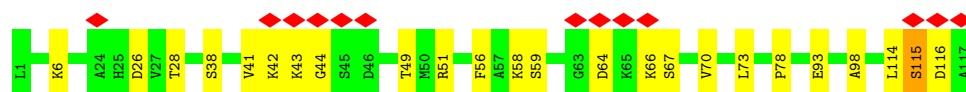
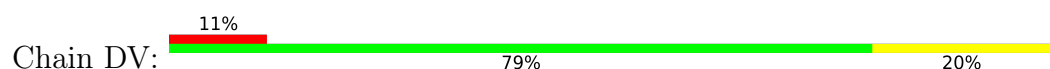
- Molecule 1: Capsid protein



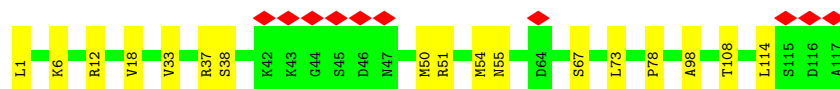
- Molecule 1: Capsid protein



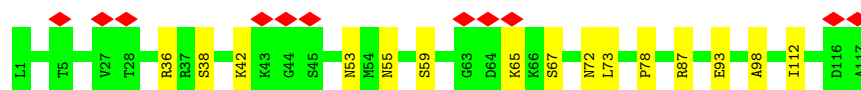
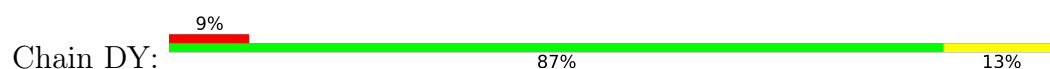
- Molecule 1: Capsid protein



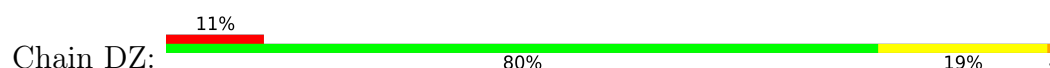
- Molecule 1: Capsid protein



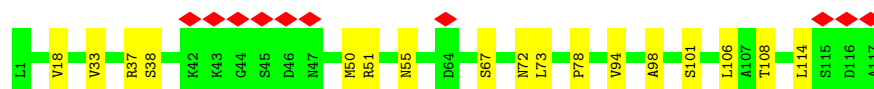
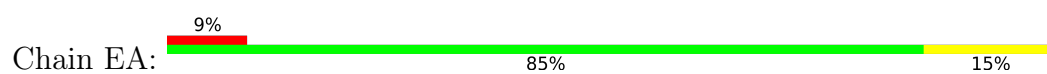
- Molecule 1: Capsid protein



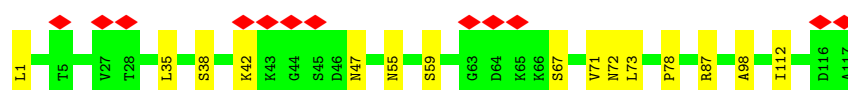
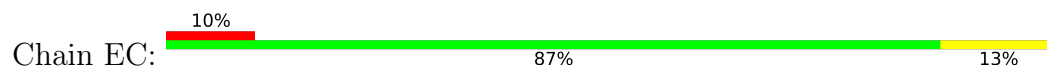
- Molecule 1: Capsid protein



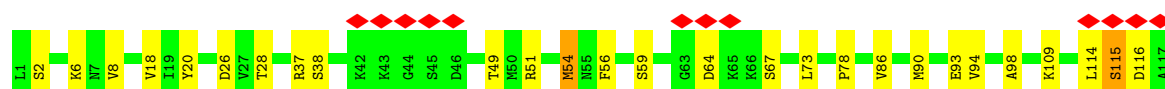
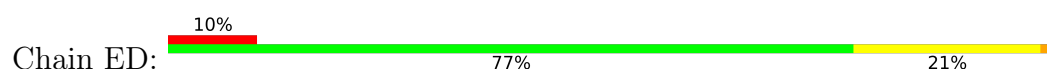
- Molecule 1: Capsid protein



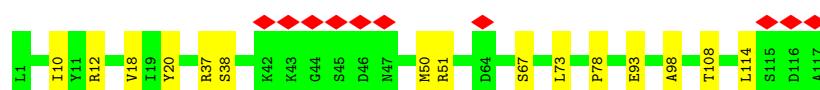
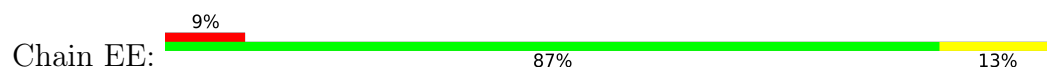
- Molecule 1: Capsid protein



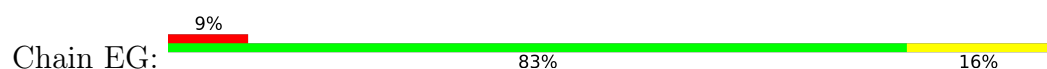
- Molecule 1: Capsid protein



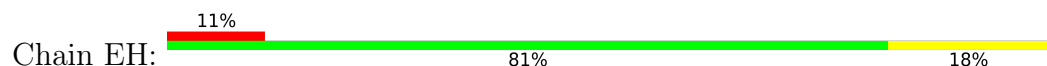
- Molecule 1: Capsid protein



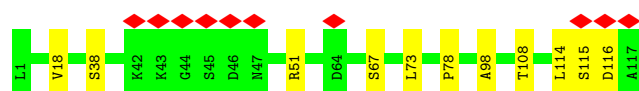
- Molecule 1: Capsid protein



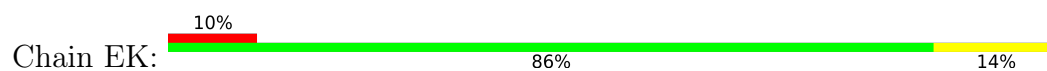
- Molecule 1: Capsid protein



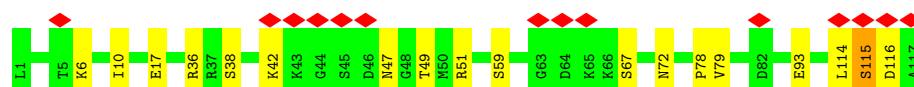
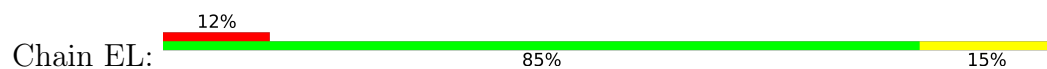
- Molecule 1: Capsid protein



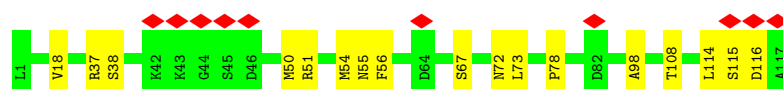
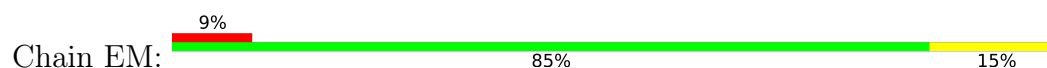
● Molecule 1: Capsid protein



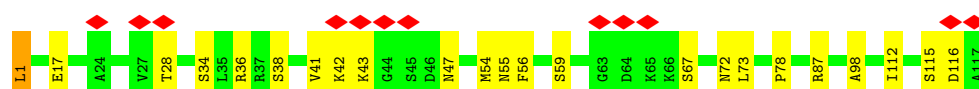
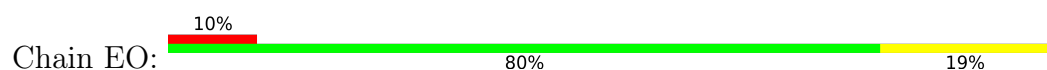
● Molecule 1: Capsid protein



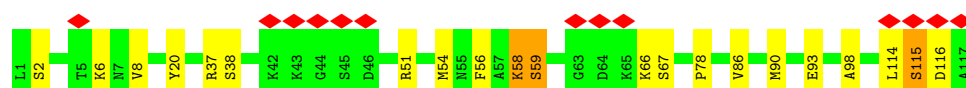
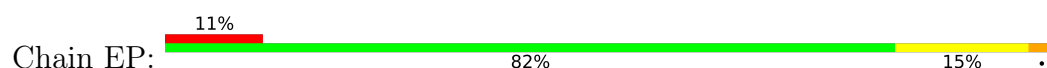
● Molecule 1: Capsid protein



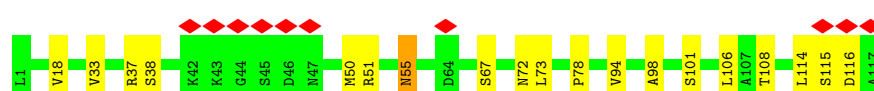
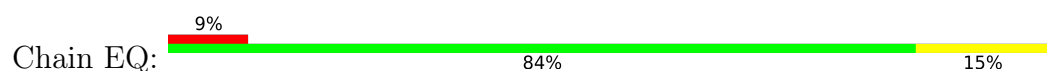
● Molecule 1: Capsid protein



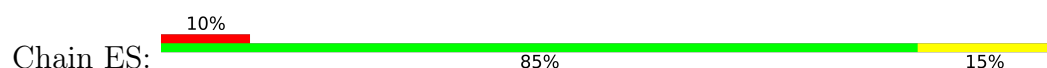
● Molecule 1: Capsid protein



● Molecule 1: Capsid protein

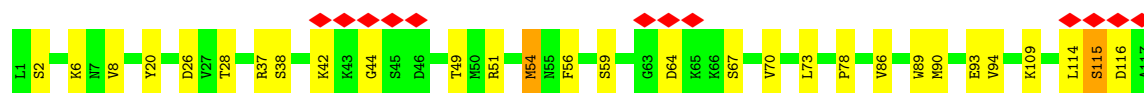
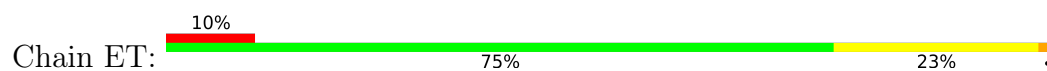


● Molecule 1: Capsid protein

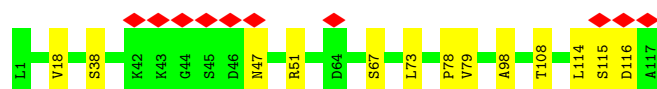




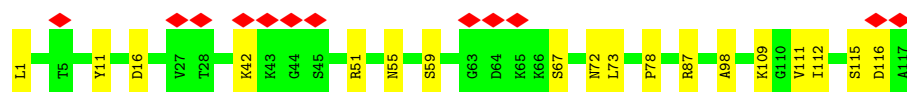
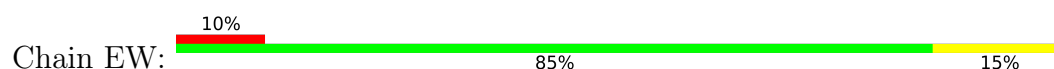
- Molecule 1: Capsid protein



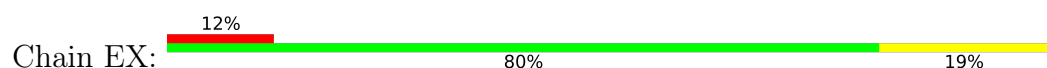
- Molecule 1: Capsid protein



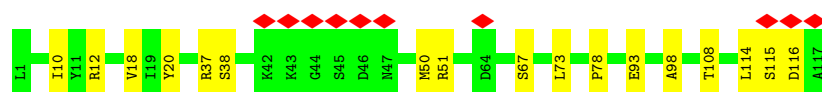
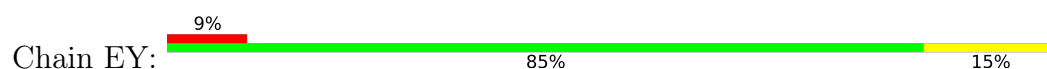
- Molecule 1: Capsid protein



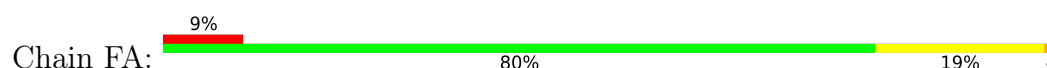
- Molecule 1: Capsid protein



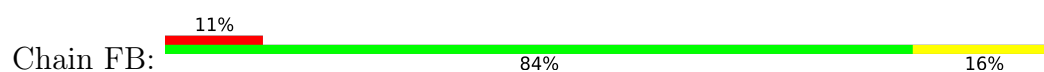
- Molecule 1: Capsid protein



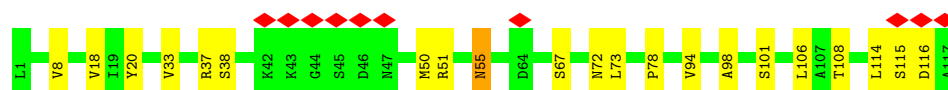
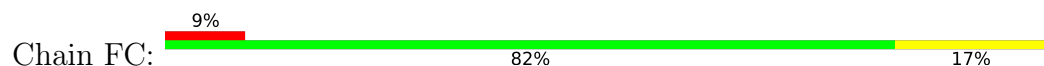
- Molecule 1: Capsid protein



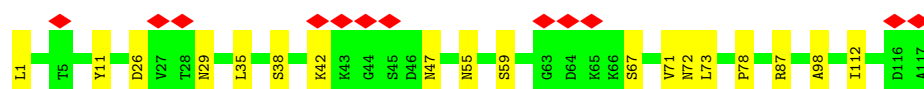
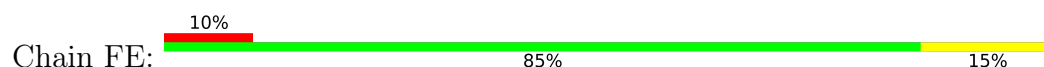
- Molecule 1: Capsid protein



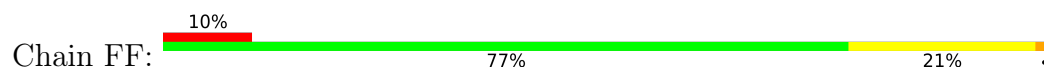
- Molecule 1: Capsid protein



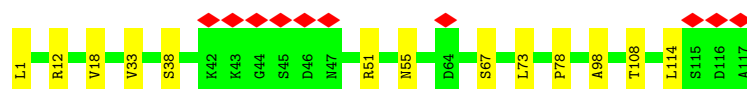
- Molecule 1: Capsid protein



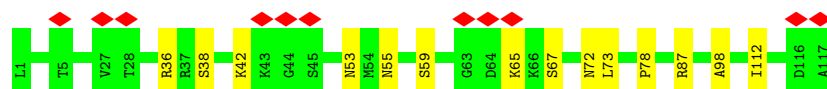
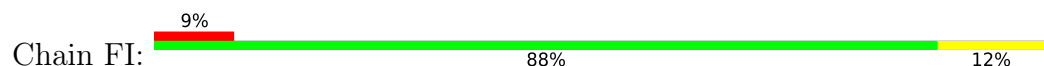
- Molecule 1: Capsid protein



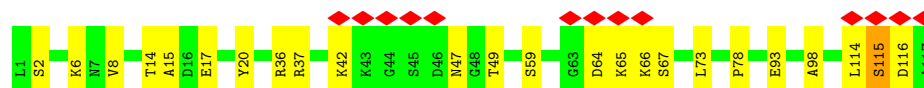
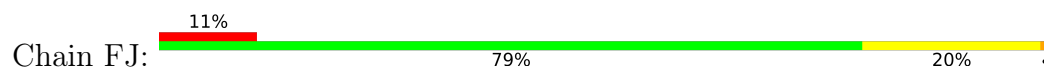
- Molecule 1: Capsid protein



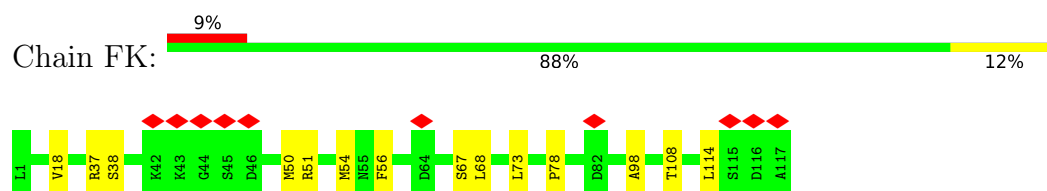
- Molecule 1: Capsid protein



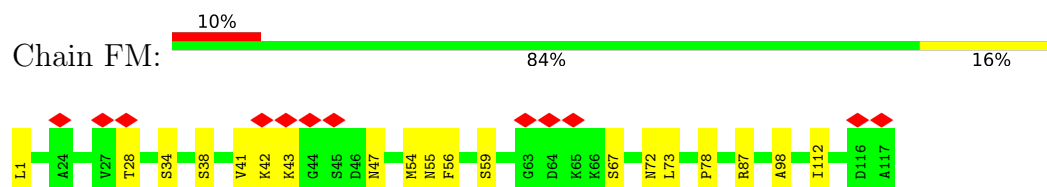
- Molecule 1: Capsid protein



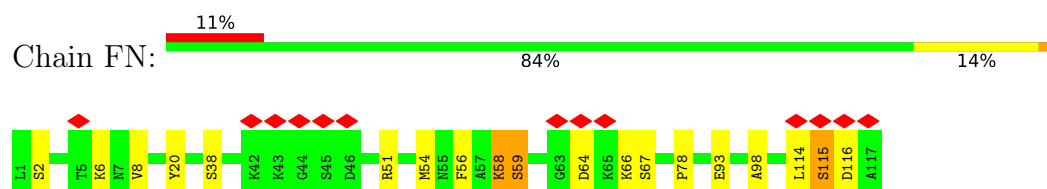
- Molecule 1: Capsid protein



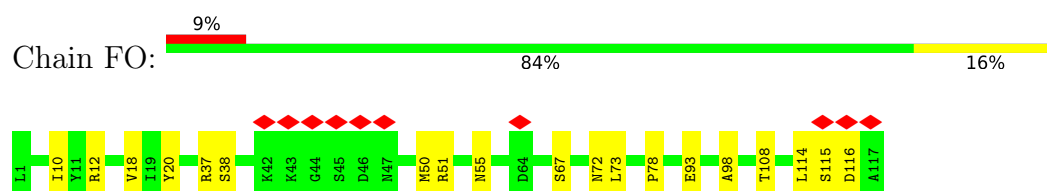
- Molecule 1: Capsid protein



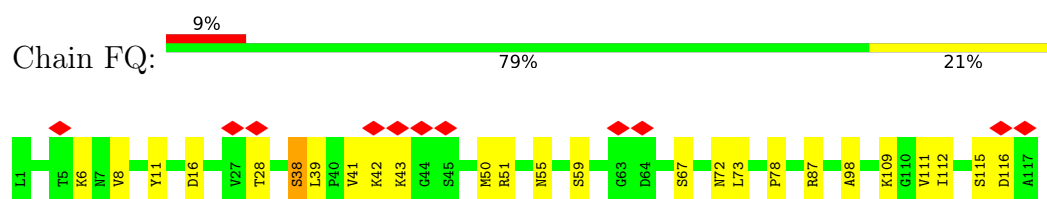
- Molecule 1: Capsid protein



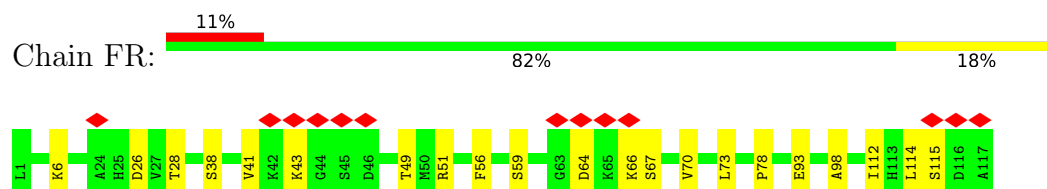
- Molecule 1: Capsid protein



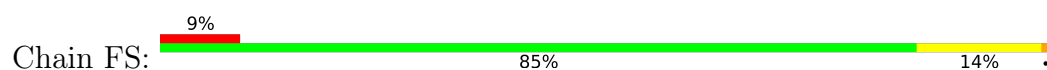
- Molecule 1: Capsid protein

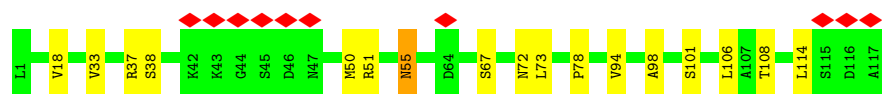


- Molecule 1: Capsid protein

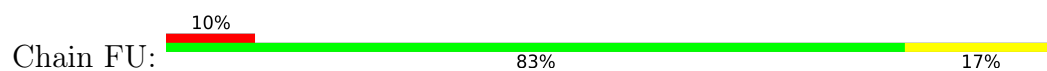


- Molecule 1: Capsid protein

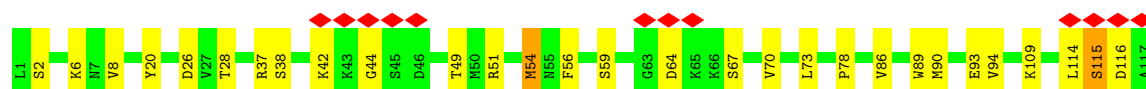




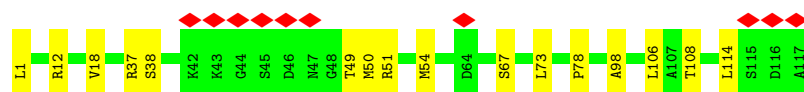
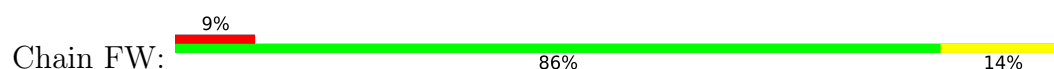
- Molecule 1: Capsid protein



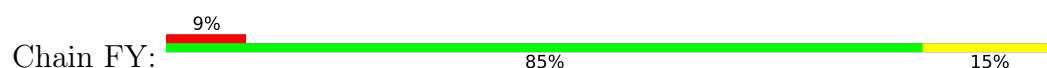
- Molecule 1: Capsid protein



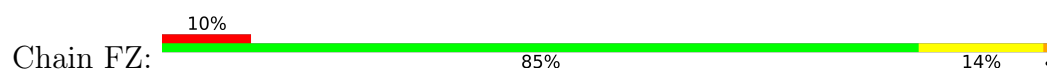
- Molecule 1: Capsid protein



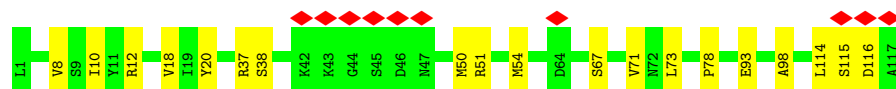
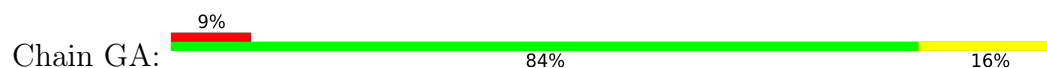
- Molecule 1: Capsid protein



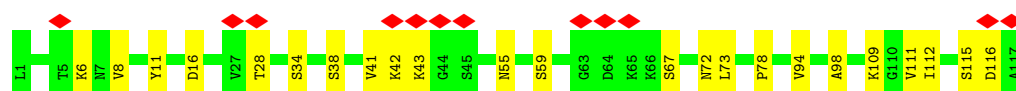
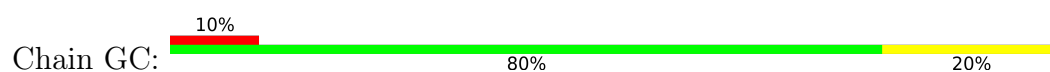
- Molecule 1: Capsid protein



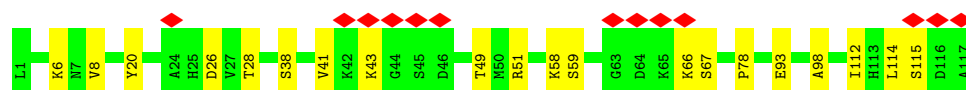
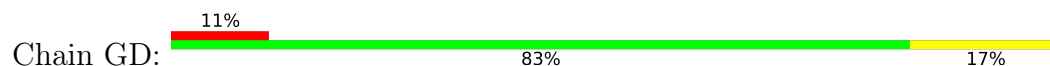
- Molecule 1: Capsid protein



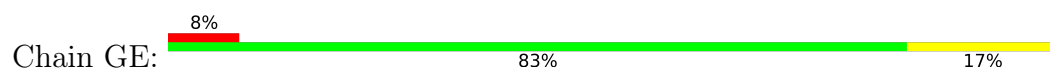
- Molecule 1: Capsid protein



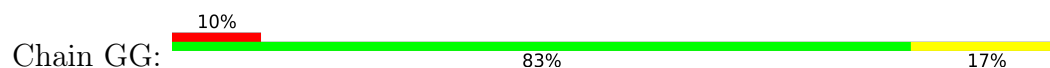
- Molecule 1: Capsid protein



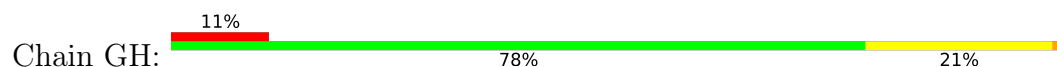
- Molecule 1: Capsid protein



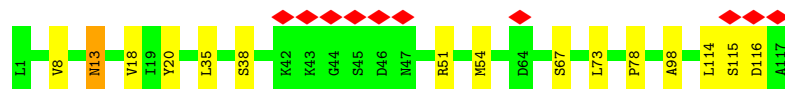
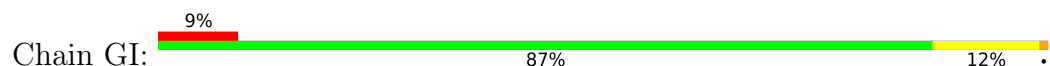
- Molecule 1: Capsid protein



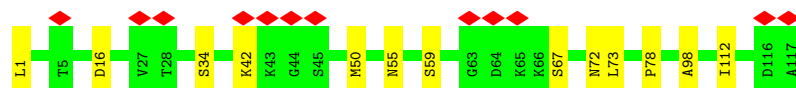
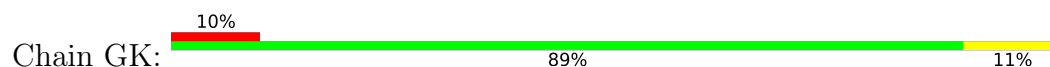
- Molecule 1: Capsid protein



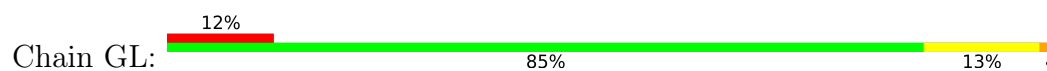
- Molecule 1: Capsid protein



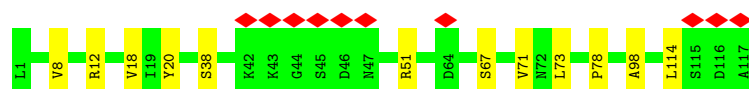
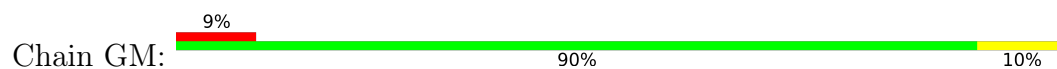
- Molecule 1: Capsid protein



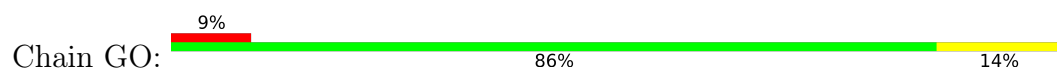
• Molecule 1: Capsid protein



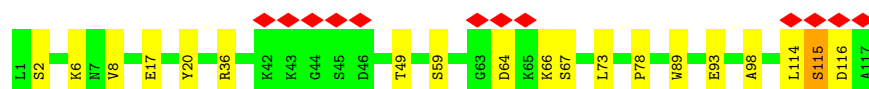
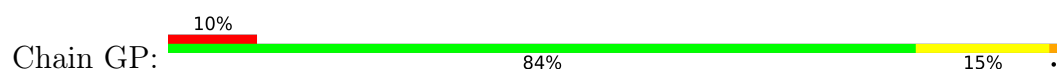
• Molecule 1: Capsid protein



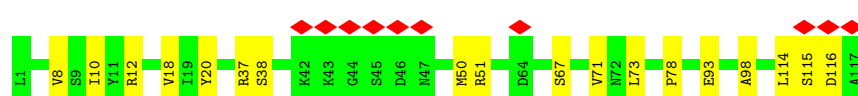
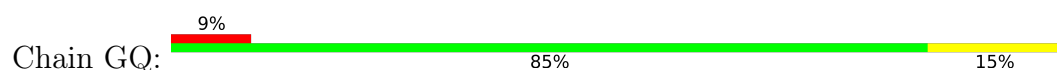
• Molecule 1: Capsid protein



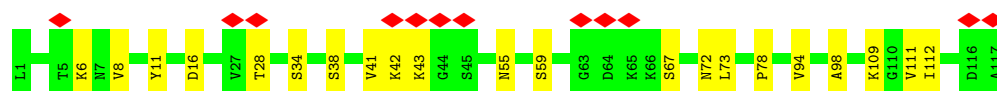
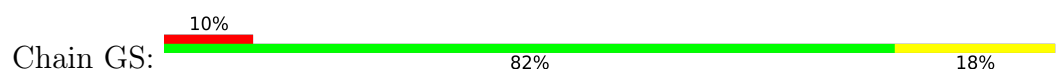
• Molecule 1: Capsid protein



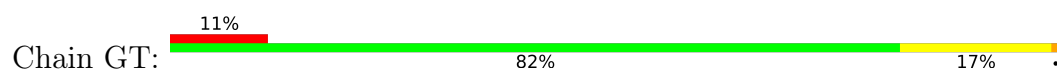
• Molecule 1: Capsid protein

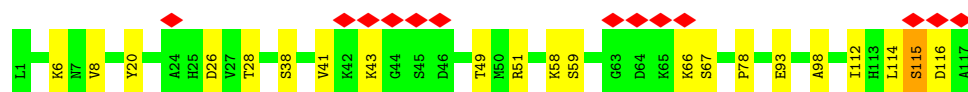


• Molecule 1: Capsid protein

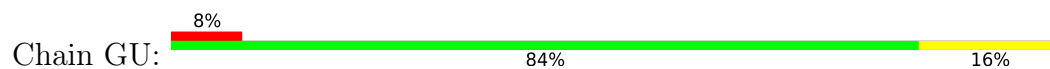


• Molecule 1: Capsid protein

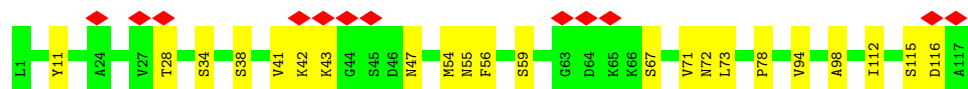
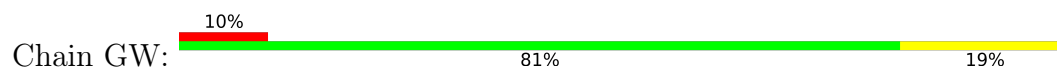




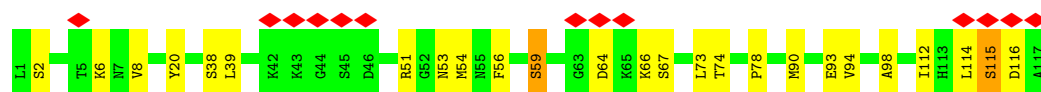
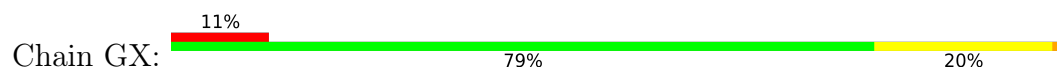
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



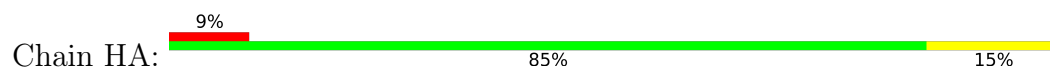
- Molecule 1: Capsid protein



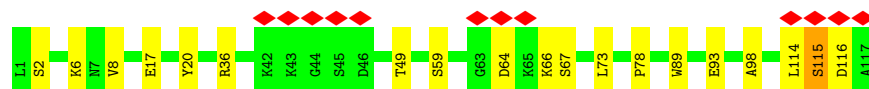
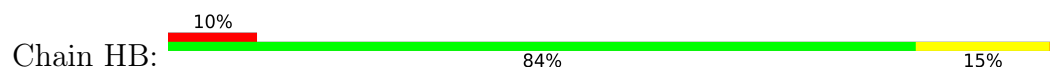
- Molecule 1: Capsid protein



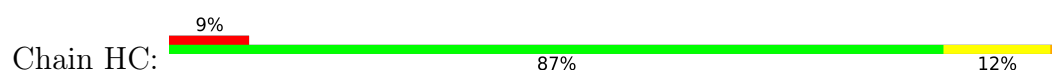
- Molecule 1: Capsid protein



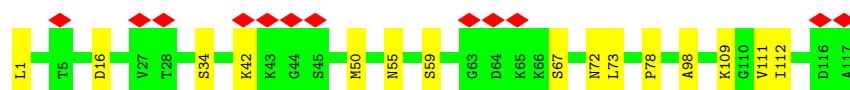
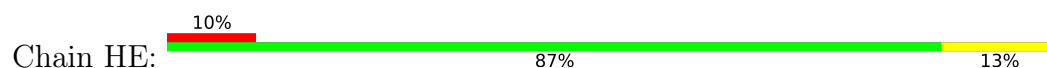
- Molecule 1: Capsid protein



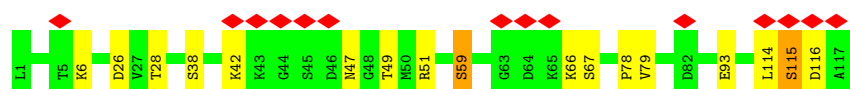
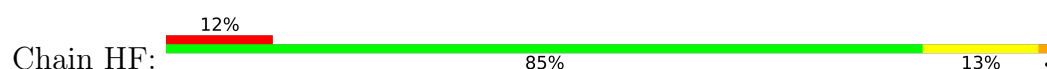
- Molecule 1: Capsid protein



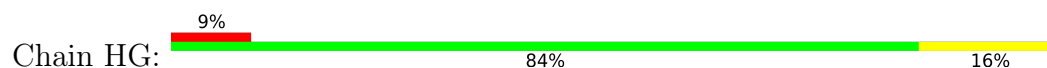
• Molecule 1: Capsid protein



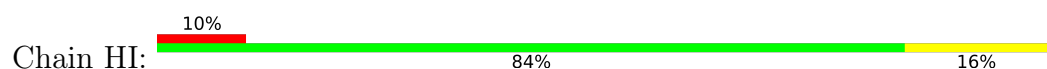
• Molecule 1: Capsid protein



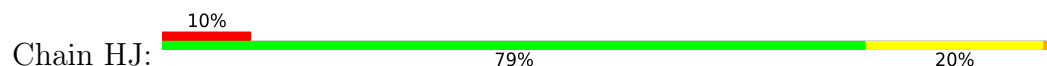
• Molecule 1: Capsid protein



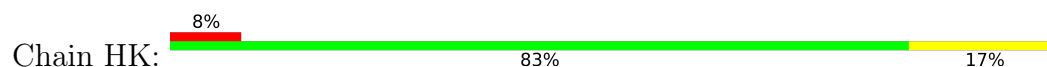
• Molecule 1: Capsid protein



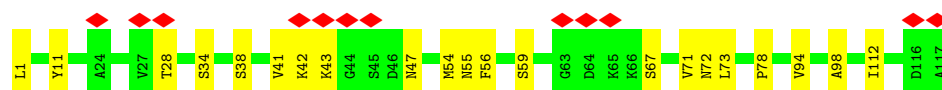
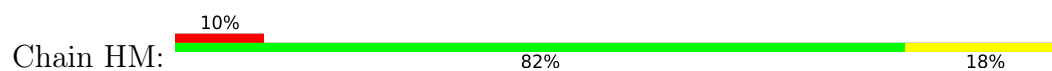
• Molecule 1: Capsid protein



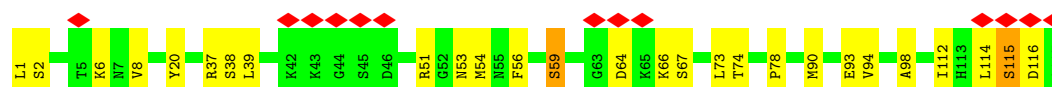
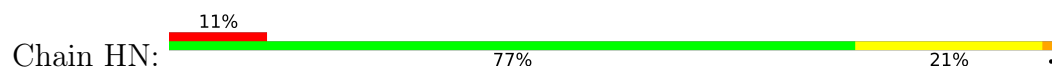
• Molecule 1: Capsid protein



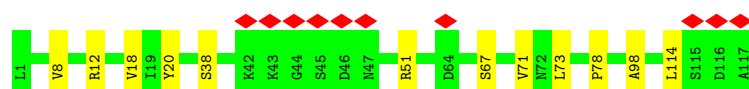
• Molecule 1: Capsid protein



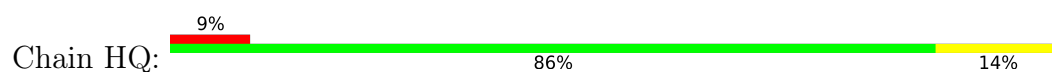
• Molecule 1: Capsid protein



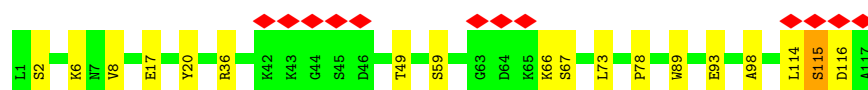
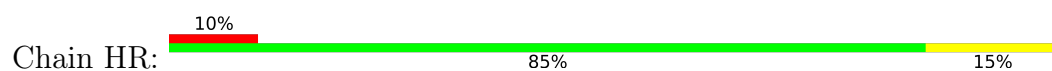
• Molecule 1: Capsid protein



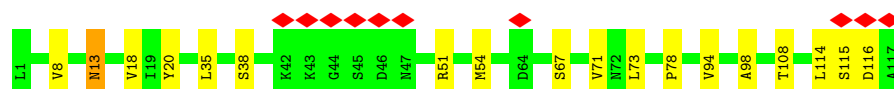
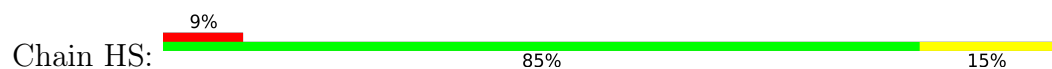
• Molecule 1: Capsid protein



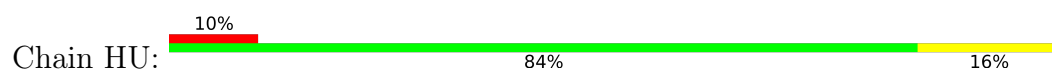
• Molecule 1: Capsid protein

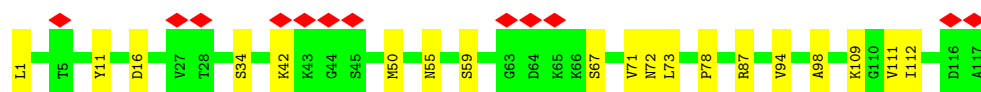


• Molecule 1: Capsid protein

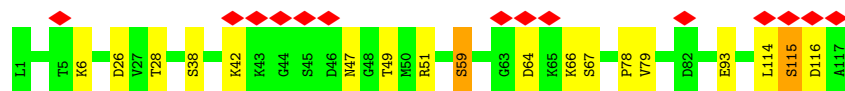
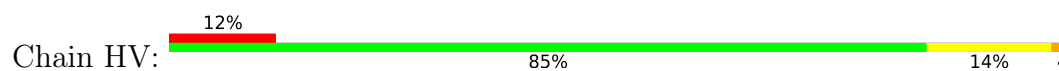


• Molecule 1: Capsid protein

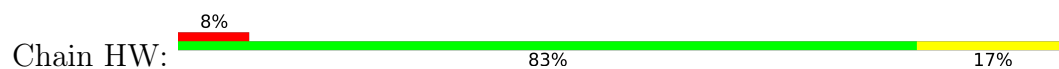




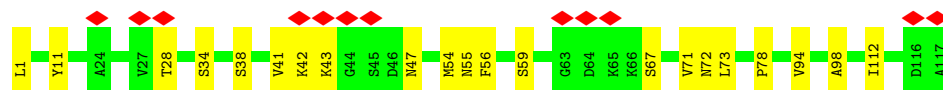
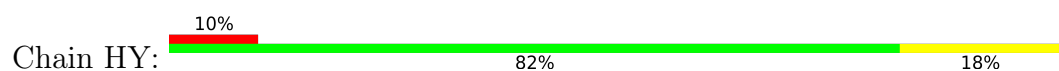
- Molecule 1: Capsid protein



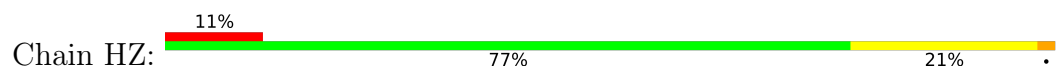
- Molecule 1: Capsid protein



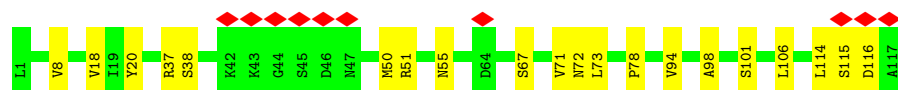
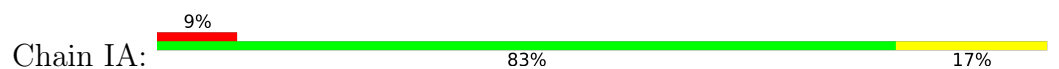
- Molecule 1: Capsid protein



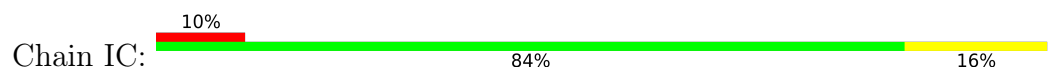
- Molecule 1: Capsid protein



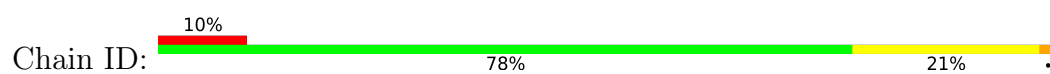
- Molecule 1: Capsid protein



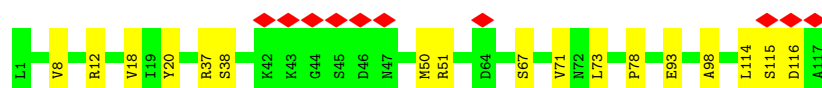
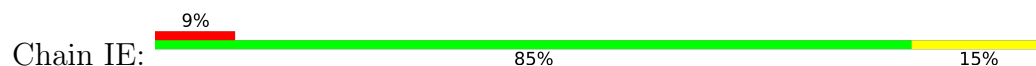
- Molecule 1: Capsid protein



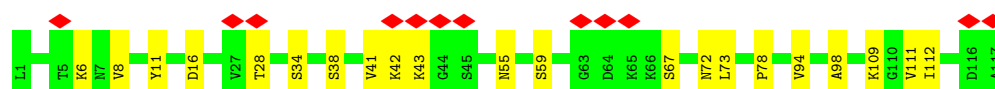
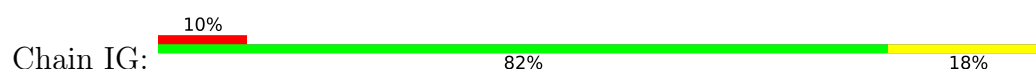
- Molecule 1: Capsid protein



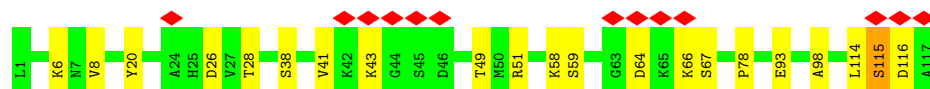
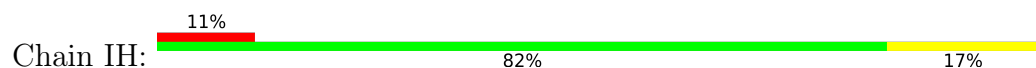
- Molecule 1: Capsid protein



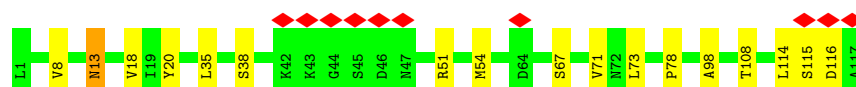
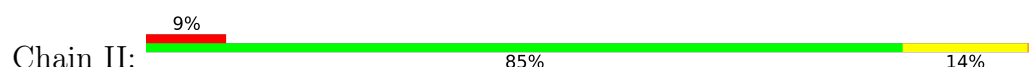
- Molecule 1: Capsid protein



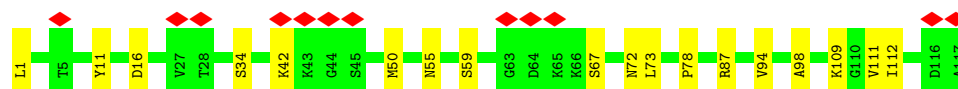
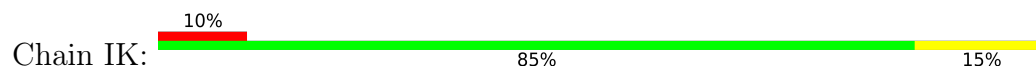
- Molecule 1: Capsid protein



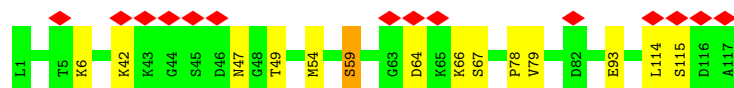
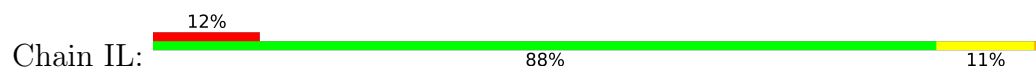
- Molecule 1: Capsid protein



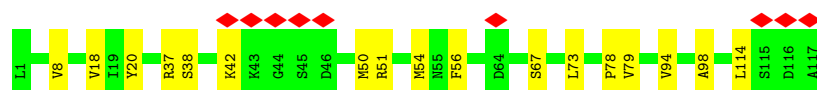
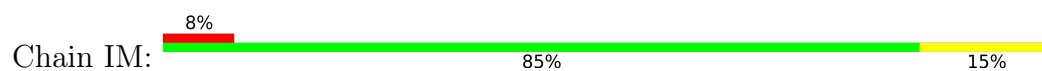
- Molecule 1: Capsid protein



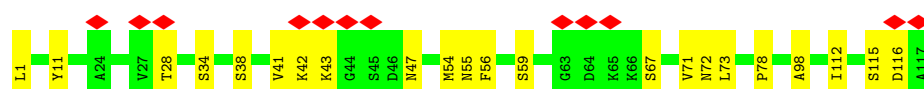
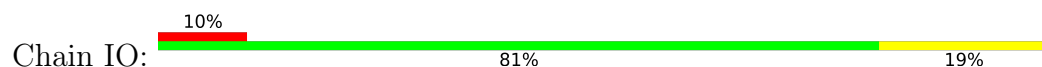
- Molecule 1: Capsid protein



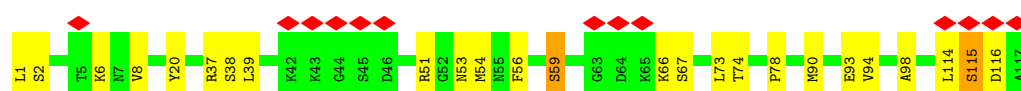
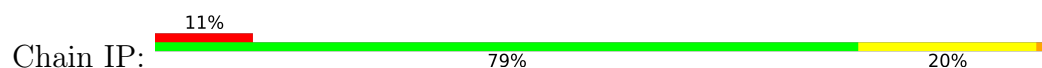
• Molecule 1: Capsid protein



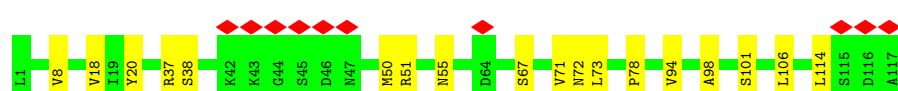
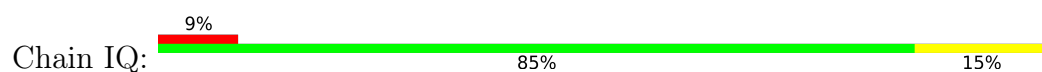
• Molecule 1: Capsid protein



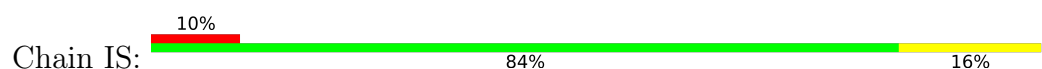
• Molecule 1: Capsid protein



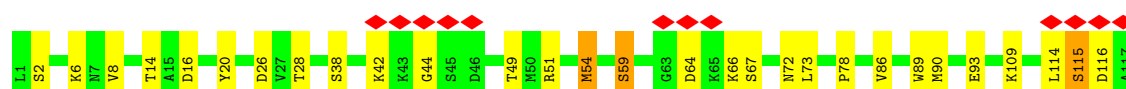
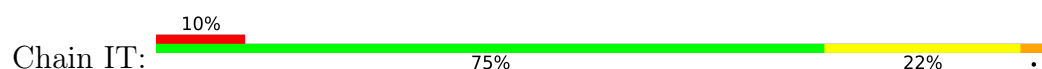
• Molecule 1: Capsid protein



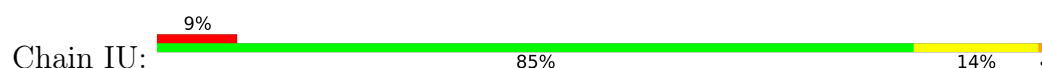
• Molecule 1: Capsid protein

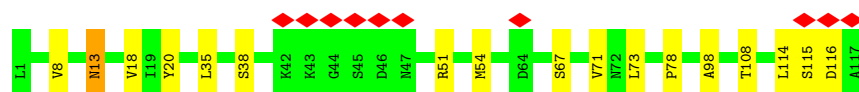


• Molecule 1: Capsid protein

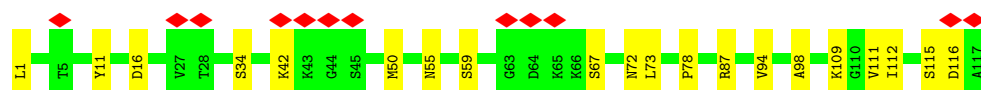
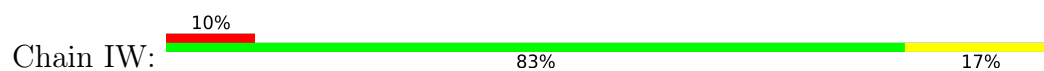


• Molecule 1: Capsid protein

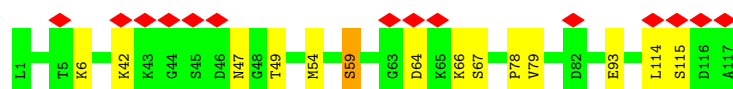




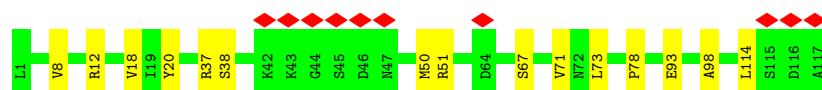
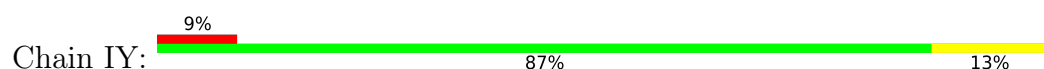
- Molecule 1: Capsid protein



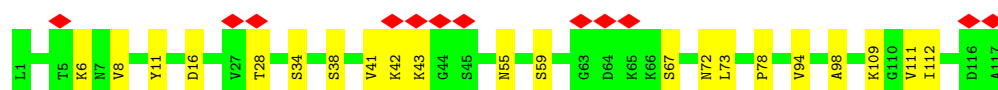
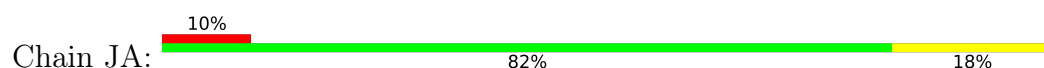
- Molecule 1: Capsid protein



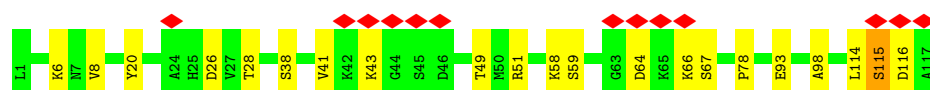
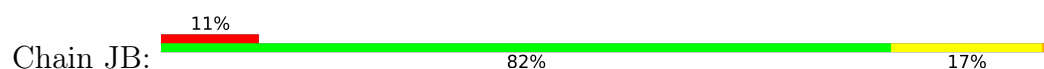
- Molecule 1: Capsid protein



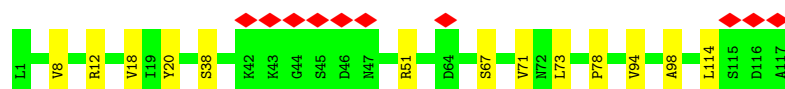
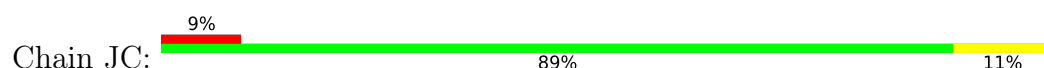
- Molecule 1: Capsid protein



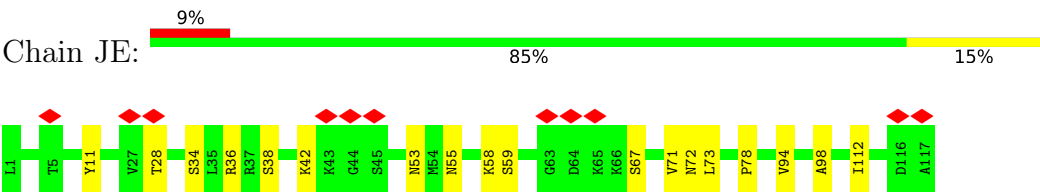
- Molecule 1: Capsid protein



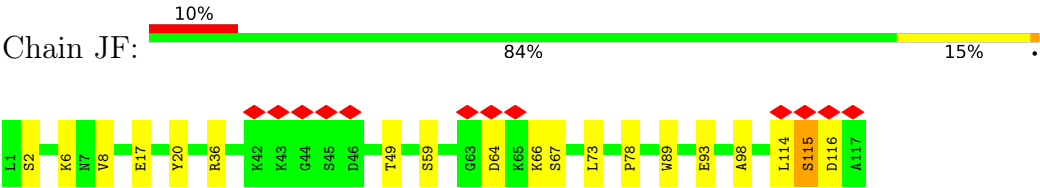
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



• Molecule 1: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	50209	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	400.896, 400.896, 400.896	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.783, 0.783, 0.783	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.14	0/883	0.35	0/1201
1	AC	0.13	0/883	0.32	0/1201
1	AD	0.13	0/883	0.34	0/1201
1	AE	0.14	0/883	0.34	0/1201
1	AG	0.13	0/883	0.31	0/1201
1	AH	0.13	0/883	0.34	0/1201
1	AI	0.14	0/883	0.35	0/1201
1	AK	0.13	0/883	0.31	0/1201
1	AL	0.14	0/883	0.35	0/1201
1	AM	0.14	0/883	0.35	0/1201
1	AO	0.13	0/883	0.32	0/1201
1	AP	0.13	0/883	0.34	0/1201
1	AQ	0.13	0/883	0.34	0/1201
1	AS	0.14	0/883	0.32	0/1201
1	AT	0.13	0/883	0.32	0/1201
1	AU	0.13	0/883	0.35	0/1201
1	AW	0.14	0/883	0.32	0/1201
1	AX	0.13	0/883	0.34	0/1201
1	AY	0.14	0/883	0.35	0/1201
1	BA	0.13	0/883	0.30	0/1201
1	BB	0.14	0/883	0.36	0/1201
1	BC	0.14	0/883	0.35	0/1201
1	BE	0.13	0/883	0.32	0/1201
1	BF	0.13	0/883	0.34	0/1201
1	BG	0.13	0/883	0.34	0/1201
1	BI	0.13	0/883	0.32	0/1201
1	BJ	0.13	0/883	0.32	0/1201
1	BK	0.14	0/883	0.35	0/1201
1	BM	0.13	0/883	0.30	0/1201
1	BN	0.14	0/883	0.35	0/1201
1	BO	0.13	0/883	0.35	0/1201
1	BQ	0.14	0/883	0.32	0/1201
1	BR	0.13	0/883	0.34	0/1201
1	BS	0.14	0/883	0.34	0/1201

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BU	0.14	0/883	0.31	0/1201
1	BV	0.13	0/883	0.34	0/1201
1	BW	0.13	0/883	0.34	0/1201
1	BY	0.14	0/883	0.32	0/1201
1	BZ	0.13	0/883	0.32	0/1201
1	CA	0.14	0/883	0.35	0/1201
1	CC	0.14	0/883	0.30	0/1201
1	CD	0.14	0/883	0.35	0/1201
1	CE	0.13	0/883	0.35	0/1201
1	CG	0.14	0/883	0.32	0/1201
1	CH	0.13	0/883	0.34	0/1201
1	CI	0.13	0/883	0.34	0/1201
1	CK	0.14	0/883	0.32	0/1201
1	CL	0.13	0/883	0.32	0/1201
1	CM	0.14	0/883	0.34	0/1201
1	CO	0.13	0/883	0.31	0/1201
1	CP	0.13	0/883	0.34	0/1201
1	CQ	0.13	0/883	0.35	0/1201
1	CS	0.13	0/883	0.32	0/1201
1	CT	0.13	0/883	0.34	0/1201
1	CU	0.13	0/883	0.35	0/1201
1	CW	0.14	0/883	0.32	0/1201
1	CX	0.13	0/883	0.34	0/1201
1	CY	0.13	0/883	0.34	0/1201
1	DA	0.13	0/883	0.32	0/1201
1	DB	0.13	0/883	0.32	0/1201
1	DC	0.14	0/883	0.34	0/1201
1	DE	0.13	0/883	0.31	0/1201
1	DF	0.13	0/883	0.34	0/1201
1	DG	0.13	0/883	0.35	0/1201
1	DI	0.14	0/883	0.32	0/1201
1	DJ	0.13	0/883	0.34	0/1201
1	DK	0.14	0/883	0.35	0/1201
1	DM	0.13	0/883	0.32	0/1201
1	DN	0.13	0/883	0.34	0/1201
1	DO	0.14	0/883	0.35	0/1201
1	DQ	0.13	0/883	0.31	0/1201
1	DR	0.14	0/883	0.35	0/1201
1	DS	0.14	0/883	0.34	0/1201
1	DU	0.13	0/883	0.31	0/1201
1	DV	0.13	0/883	0.34	0/1201
1	DW	0.13	0/883	0.35	0/1201
1	DY	0.14	0/883	0.32	0/1201

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DZ	0.13	0/883	0.34	0/1201
1	EA	0.14	0/883	0.35	0/1201
1	EC	0.13	0/883	0.32	0/1201
1	ED	0.13	0/883	0.34	0/1201
1	EE	0.14	0/883	0.34	0/1201
1	EG	0.14	0/883	0.31	0/1201
1	EH	0.13	0/883	0.34	0/1201
1	EI	0.14	0/883	0.35	0/1201
1	EK	0.14	0/883	0.31	0/1201
1	EL	0.14	0/883	0.35	0/1201
1	EM	0.13	0/883	0.34	0/1201
1	EO	0.14	0/883	0.32	0/1201
1	EP	0.13	0/883	0.32	0/1201
1	EQ	0.13	0/883	0.35	0/1201
1	ES	0.13	0/883	0.32	0/1201
1	ET	0.13	0/883	0.34	0/1201
1	EU	0.14	0/883	0.35	0/1201
1	EW	0.14	0/883	0.31	0/1201
1	EX	0.14	0/883	0.35	0/1201
1	EY	0.14	0/883	0.34	0/1201
1	FA	0.13	0/883	0.31	0/1201
1	FB	0.13	0/883	0.34	0/1201
1	FC	0.13	0/883	0.35	0/1201
1	FE	0.13	0/883	0.32	0/1201
1	FF	0.13	0/883	0.34	0/1201
1	FG	0.13	0/883	0.35	0/1201
1	FI	0.14	0/883	0.32	0/1201
1	FJ	0.13	0/883	0.34	0/1201
1	FK	0.13	0/883	0.34	0/1201
1	FM	0.13	0/883	0.32	0/1201
1	FN	0.13	0/883	0.32	0/1201
1	FO	0.14	0/883	0.34	0/1201
1	FQ	0.13	0/883	0.31	0/1201
1	FR	0.13	0/883	0.34	0/1201
1	FS	0.14	0/883	0.35	0/1201
1	FU	0.13	0/883	0.32	0/1201
1	FV	0.13	0/883	0.34	0/1201
1	FW	0.13	0/883	0.35	0/1201
1	FY	0.13	0/883	0.30	0/1201
1	FZ	0.12	0/883	0.32	0/1201
1	GA	0.13	0/883	0.32	0/1201
1	GC	0.13	0/883	0.29	0/1201
1	GD	0.13	0/883	0.32	0/1201

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GE	0.12	0/883	0.31	0/1201
1	GG	0.13	0/883	0.30	0/1201
1	GH	0.12	0/883	0.30	0/1201
1	GI	0.13	0/883	0.33	0/1201
1	GK	0.13	0/883	0.28	0/1201
1	GL	0.13	0/883	0.34	0/1201
1	GM	0.13	0/883	0.32	0/1201
1	GO	0.13	0/883	0.30	0/1201
1	GP	0.12	0/883	0.32	0/1201
1	GQ	0.13	0/883	0.32	0/1201
1	GS	0.13	0/883	0.29	0/1201
1	GT	0.12	0/883	0.32	0/1201
1	GU	0.12	0/883	0.31	0/1201
1	GW	0.13	0/883	0.30	0/1201
1	GX	0.12	0/883	0.30	0/1201
1	GY	0.13	0/883	0.32	0/1201
1	HA	0.13	0/883	0.30	0/1201
1	HB	0.12	0/883	0.32	0/1201
1	HC	0.13	0/883	0.33	0/1201
1	HE	0.13	0/883	0.28	0/1201
1	HF	0.13	0/883	0.34	0/1201
1	HG	0.12	0/883	0.32	0/1201
1	HI	0.13	0/883	0.30	0/1201
1	HJ	0.13	0/883	0.32	0/1201
1	HK	0.12	0/883	0.31	0/1201
1	HM	0.13	0/883	0.30	0/1201
1	HN	0.12	0/883	0.30	0/1201
1	HO	0.13	0/883	0.32	0/1201
1	HQ	0.13	0/883	0.30	0/1201
1	HR	0.12	0/883	0.32	0/1201
1	HS	0.13	0/883	0.33	0/1201
1	HU	0.13	0/883	0.29	0/1201
1	HV	0.13	0/883	0.34	0/1201
1	HW	0.12	0/883	0.31	0/1201
1	HY	0.13	0/883	0.30	0/1201
1	HZ	0.12	0/883	0.30	0/1201
1	IA	0.12	0/883	0.32	0/1201
1	IC	0.13	0/883	0.31	0/1201
1	ID	0.13	0/883	0.32	0/1201
1	IE	0.13	0/883	0.32	0/1201
1	IG	0.13	0/883	0.29	0/1201
1	IH	0.13	0/883	0.32	0/1201
1	II	0.13	0/883	0.33	0/1201

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	IK	0.13	0/883	0.28	0/1201
1	IL	0.13	0/883	0.34	0/1201
1	IM	0.12	0/883	0.31	0/1201
1	IO	0.13	0/883	0.30	0/1201
1	IP	0.12	0/883	0.30	0/1201
1	IQ	0.12	0/883	0.32	0/1201
1	IS	0.13	0/883	0.30	0/1201
1	IT	0.13	0/883	0.32	0/1201
1	IU	0.13	0/883	0.33	0/1201
1	IW	0.13	0/883	0.29	0/1201
1	IX	0.13	0/883	0.34	0/1201
1	IY	0.13	0/883	0.32	0/1201
1	JA	0.13	0/883	0.29	0/1201
1	JB	0.13	0/883	0.32	0/1201
1	JC	0.13	0/883	0.32	0/1201
1	JE	0.13	0/883	0.30	0/1201
1	JF	0.12	0/883	0.32	0/1201
All	All	0.13	0/158940	0.33	0/216180

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	AA	869	0	880	14	0
1	AC	869	0	880	13	0
1	AD	869	0	880	19	0
1	AE	869	0	880	14	0
1	AG	869	0	880	15	0
1	AH	869	0	880	15	0
1	AI	869	0	880	8	0
1	AK	869	0	880	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AL	869	0	880	15	0
1	AM	869	0	880	13	0
1	AO	869	0	880	13	0
1	AP	869	0	880	19	0
1	AQ	869	0	880	12	0
1	AS	869	0	880	16	0
1	AT	869	0	880	13	0
1	AU	869	0	880	11	0
1	AW	869	0	880	12	0
1	AX	869	0	880	14	0
1	AY	869	0	880	10	0
1	BA	869	0	880	11	0
1	BB	869	0	880	11	0
1	BC	869	0	880	13	0
1	BE	869	0	880	13	0
1	BF	869	0	880	18	0
1	BG	869	0	880	11	0
1	BI	869	0	880	14	0
1	BJ	869	0	880	14	0
1	BK	869	0	880	9	0
1	BM	869	0	880	11	0
1	BN	869	0	880	11	0
1	BO	869	0	880	12	0
1	BQ	869	0	880	12	0
1	BR	869	0	880	14	0
1	BS	869	0	880	16	0
1	BU	869	0	880	13	0
1	BV	869	0	880	17	0
1	BW	869	0	880	11	0
1	BY	869	0	880	14	0
1	BZ	869	0	880	10	0
1	CA	869	0	880	9	0
1	CC	869	0	880	12	0
1	CD	869	0	880	13	0
1	CE	869	0	880	12	0
1	CG	869	0	880	12	0
1	CH	869	0	880	16	0
1	CI	869	0	880	11	0
1	CK	869	0	880	14	0
1	CL	869	0	880	11	0
1	CM	869	0	880	17	0
1	CO	869	0	880	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CP	869	0	880	14	0
1	CQ	869	0	880	14	0
1	CS	869	0	880	12	0
1	CT	869	0	880	12	0
1	CU	869	0	880	12	0
1	CW	869	0	880	11	0
1	CX	869	0	880	15	0
1	CY	869	0	880	10	0
1	DA	869	0	880	16	0
1	DB	869	0	880	15	0
1	DC	869	0	880	15	0
1	DE	869	0	880	14	0
1	DF	869	0	880	12	0
1	DG	869	0	880	12	0
1	DI	869	0	880	10	0
1	DJ	869	0	880	15	0
1	DK	869	0	880	14	0
1	DM	869	0	880	14	0
1	DN	869	0	880	16	0
1	DO	869	0	880	9	0
1	DQ	869	0	880	12	0
1	DR	869	0	880	11	0
1	DS	869	0	880	12	0
1	DU	869	0	880	14	0
1	DV	869	0	880	15	0
1	DW	869	0	880	13	0
1	DY	869	0	880	11	0
1	DZ	869	0	880	14	0
1	EA	869	0	880	13	0
1	EC	869	0	880	12	0
1	ED	869	0	880	17	0
1	EE	869	0	880	12	0
1	EG	869	0	880	13	0
1	EH	869	0	880	14	0
1	EI	869	0	880	9	0
1	EK	869	0	880	12	0
1	EL	869	0	880	10	0
1	EM	869	0	880	12	0
1	EO	869	0	880	16	0
1	EP	869	0	880	13	0
1	EQ	869	0	880	14	0
1	ES	869	0	880	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ET	869	0	880	17	0
1	EU	869	0	880	10	0
1	EW	869	0	880	12	0
1	EX	869	0	880	13	0
1	EY	869	0	880	13	0
1	FA	869	0	880	15	0
1	FB	869	0	880	12	0
1	FC	869	0	880	15	0
1	FE	869	0	880	14	0
1	FF	869	0	880	16	0
1	FG	869	0	880	10	0
1	FI	869	0	880	10	0
1	FJ	869	0	880	14	0
1	FK	869	0	880	11	0
1	FM	869	0	880	14	0
1	FN	869	0	880	12	0
1	FO	869	0	880	14	0
1	FQ	869	0	880	16	0
1	FR	869	0	880	13	0
1	FS	869	0	880	13	0
1	FU	869	0	880	14	0
1	FV	869	0	880	17	0
1	FW	869	0	880	12	0
1	FY	869	0	880	13	0
1	FZ	869	0	880	10	0
1	GA	869	0	880	14	0
1	GC	869	0	880	15	0
1	GD	869	0	880	12	0
1	GE	869	0	880	14	0
1	GG	869	0	880	16	0
1	GH	869	0	880	17	0
1	GI	869	0	880	11	0
1	GK	869	0	880	10	0
1	GL	869	0	880	11	0
1	GM	869	0	880	10	0
1	GO	869	0	880	11	0
1	GP	869	0	880	12	0
1	GQ	869	0	880	14	0
1	GS	869	0	880	14	0
1	GT	869	0	880	13	0
1	GU	869	0	880	13	0
1	GW	869	0	880	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GX	869	0	880	16	0
1	GY	869	0	880	10	0
1	HA	869	0	880	12	0
1	HB	869	0	880	12	0
1	HC	869	0	880	11	0
1	HE	869	0	880	11	0
1	HF	869	0	880	11	0
1	HG	869	0	880	14	0
1	HI	869	0	880	15	0
1	HJ	869	0	880	13	0
1	HK	869	0	880	14	0
1	HM	869	0	880	17	0
1	HN	869	0	880	17	0
1	HO	869	0	880	10	0
1	HQ	869	0	880	11	0
1	HR	869	0	880	11	0
1	HS	869	0	880	14	0
1	HU	869	0	880	15	0
1	HV	869	0	880	12	0
1	HW	869	0	880	14	0
1	HY	869	0	880	17	0
1	HZ	869	0	880	17	0
1	IA	869	0	880	14	0
1	IC	869	0	880	15	0
1	ID	869	0	880	13	0
1	IE	869	0	880	13	0
1	IG	869	0	880	14	0
1	IH	869	0	880	13	0
1	II	869	0	880	13	0
1	IK	869	0	880	14	0
1	IL	869	0	880	10	0
1	IM	869	0	880	12	0
1	IO	869	0	880	17	0
1	IP	869	0	880	16	0
1	IQ	869	0	880	13	0
1	IS	869	0	880	15	0
1	IT	869	0	880	16	0
1	IU	869	0	880	13	0
1	IW	869	0	880	15	0
1	IX	869	0	880	10	0
1	IY	869	0	880	12	0
1	JA	869	0	880	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JB	869	0	880	13	0
1	JC	869	0	880	11	0
1	JE	869	0	880	13	0
1	JF	869	0	880	12	0
All	All	156420	0	158400	1657	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 5.

All (1657) 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:DJ:59:SER:HB3	1:DJ:66:LYS:HE2	1.58	0.85
1:CX:59:SER:HB3	1:CX:66:LYS:HE2	1.59	0.84
1:DZ:59:SER:HB3	1:DZ:66:LYS:HE2	1.59	0.84
1:AX:59:SER:HB3	1:AX:66:LYS:HE2	1.59	0.83
1:FJ:59:SER:HB3	1:FJ:66:LYS:HE2	1.59	0.83
1:BR:59:SER:HB3	1:BR:66:LYS:HE2	1.58	0.83
1:CH:59:SER:HB3	1:CH:66:LYS:HE2	1.59	0.82
1:BV:93:GLU:OE2	1:JF:6:LYS:NZ	2.18	0.76
1:CP:93:GLU:OE1	1:FJ:6:LYS:NZ	2.18	0.76
1:IQ:38:SER:HB2	1:IQ:51:ARG:HB2	1.68	0.76
1:GA:38:SER:HB2	1:GA:51:ARG:HB2	1.68	0.76
1:CX:6:LYS:NZ	1:FR:93:GLU:OE1	2.18	0.75
1:DJ:6:LYS:NZ	1:GD:93:GLU:OE2	2.18	0.75
1:IE:38:SER:HB2	1:IE:51:ARG:HB2	1.68	0.75
1:AH:93:GLU:OE2	1:HR:6:LYS:NZ	2.18	0.75
1:IY:38:SER:HB2	1:IY:51:ARG:HB2	1.68	0.75
1:GQ:38:SER:HB2	1:GQ:51:ARG:HB2	1.68	0.75
1:AX:6:LYS:NZ	1:IH:93:GLU:OE2	2.18	0.75
1:BR:6:LYS:NZ	1:JB:93:GLU:OE2	2.18	0.75
1:DF:93:GLU:OE2	1:FZ:6:LYS:NZ	2.18	0.75
1:DZ:6:LYS:NZ	1:GT:93:GLU:OE2	2.18	0.75
1:FS:38:SER:HB2	1:FS:51:ARG:HB2	1.69	0.75
1:EH:93:GLU:OE2	1:HB:6:LYS:NZ	2.18	0.74
1:BC:38:SER:HB2	1:BC:51:ARG:HB2	1.69	0.74
1:DK:38:SER:HB2	1:DK:51:ARG:HB2	1.69	0.74
1:DV:93:GLU:OE2	1:GP:6:LYS:NZ	2.18	0.74
1:CQ:38:SER:HB2	1:CQ:51:ARG:HB2	1.69	0.74
1:EQ:38:SER:HB2	1:EQ:51:ARG:HB2	1.69	0.74
1:FC:38:SER:HB2	1:FC:51:ARG:HB2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HG:38:SER:HB2	1:HG:51:ARG:HB2	1.68	0.74
1:JC:38:SER:HB2	1:JC:51:ARG:HB2	1.70	0.74
1:EA:38:SER:HB2	1:EA:51:ARG:HB2	1.69	0.74
1:IA:38:SER:HB2	1:IA:51:ARG:HB2	1.68	0.74
1:BS:38:SER:HB2	1:BS:51:ARG:HB2	1.70	0.74
1:CH:6:LYS:NZ	1:FB:93:GLU:OE1	2.18	0.74
1:CM:38:SER:HB2	1:CM:51:ARG:HB2	1.70	0.74
1:GI:38:SER:HB2	1:GI:51:ARG:HB2	1.70	0.74
1:HC:38:SER:HB2	1:HC:51:ARG:HB2	1.70	0.74
1:HO:38:SER:HB2	1:HO:51:ARG:HB2	1.70	0.73
1:IU:38:SER:HB2	1:IU:51:ARG:HB2	1.70	0.73
1:GM:38:SER:HB2	1:GM:51:ARG:HB2	1.70	0.73
1:GY:38:SER:HB2	1:GY:51:ARG:HB2	1.70	0.73
1:HS:38:SER:HB2	1:HS:51:ARG:HB2	1.70	0.73
1:II:38:SER:HB2	1:II:51:ARG:HB2	1.70	0.73
1:AM:38:SER:HB2	1:AM:51:ARG:HB2	1.69	0.73
1:EY:38:SER:HB2	1:EY:51:ARG:HB2	1.70	0.73
1:DC:38:SER:HB2	1:DC:51:ARG:HB2	1.70	0.73
1:AA:38:SER:HB2	1:AA:51:ARG:HB2	1.69	0.72
1:BJ:59:SER:HB3	1:BJ:66:LYS:HE2	1.71	0.72
1:CY:38:SER:HB2	1:CY:51:ARG:HB2	1.71	0.72
1:DG:38:SER:HB2	1:DG:51:ARG:HB2	1.71	0.72
1:HK:38:SER:HB2	1:HK:51:ARG:HB2	1.71	0.72
1:CU:38:SER:HB2	1:CU:51:ARG:HB2	1.71	0.72
1:FC:55:ASN:ND2	1:FC:72:ASN:OD1	2.21	0.72
1:HW:38:SER:HB2	1:HW:51:ARG:HB2	1.71	0.72
1:CQ:55:ASN:ND2	1:CQ:72:ASN:OD1	2.23	0.72
1:EQ:55:ASN:ND2	1:EQ:72:ASN:OD1	2.21	0.72
1:AE:38:SER:HB2	1:AE:51:ARG:HB2	1.70	0.72
1:FO:38:SER:HB2	1:FO:51:ARG:HB2	1.70	0.72
1:DW:38:SER:HB2	1:DW:51:ARG:HB2	1.71	0.72
1:CE:38:SER:HB2	1:CE:51:ARG:HB2	1.71	0.72
1:AQ:38:SER:HB2	1:AQ:51:ARG:HB2	1.71	0.72
1:DB:59:SER:HB3	1:DB:66:LYS:HE2	1.72	0.72
1:BZ:59:SER:HB3	1:BZ:66:LYS:HE2	1.72	0.72
1:CL:59:SER:HB3	1:CL:66:LYS:HE2	1.72	0.72
1:EM:38:SER:HB2	1:EM:51:ARG:HB2	1.71	0.72
1:EP:6:LYS:NZ	1:HJ:93:GLU:OE1	2.23	0.72
1:FW:38:SER:HB2	1:FW:51:ARG:HB2	1.72	0.72
1:HR:59:SER:HB3	1:HR:66:LYS:HE2	1.72	0.72
1:JF:59:SER:HB3	1:JF:66:LYS:HE2	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:38:SER:HB2	1:AU:51:ARG:HB2	1.71	0.71
1:BO:38:SER:HB2	1:BO:51:ARG:HB2	1.71	0.71
1:FF:86:VAL:HG12	1:FF:90:MET:HE2	1.72	0.71
1:ET:86:VAL:HG12	1:ET:90:MET:HE2	1.73	0.71
1:FG:38:SER:HB2	1:FG:51:ARG:HB2	1.71	0.71
1:GU:38:SER:HB2	1:GU:51:ARG:HB2	1.71	0.71
1:AT:59:SER:HB3	1:AT:66:LYS:HE2	1.71	0.71
1:BG:38:SER:HB2	1:BG:51:ARG:HB2	1.71	0.71
1:EP:59:SER:HB3	1:EP:66:LYS:HE2	1.71	0.71
1:IM:38:SER:HB2	1:IM:51:ARG:HB2	1.71	0.71
1:CI:38:SER:HB2	1:CI:51:ARG:HB2	1.71	0.71
1:DS:38:SER:HB2	1:DS:51:ARG:HB2	1.70	0.71
1:EE:38:SER:HB2	1:EE:51:ARG:HB2	1.70	0.71
1:BW:38:SER:HB2	1:BW:51:ARG:HB2	1.71	0.71
1:FZ:59:SER:HB3	1:FZ:66:LYS:HE2	1.72	0.71
1:GE:38:SER:HB2	1:GE:51:ARG:HB2	1.71	0.71
1:AP:86:VAL:HG12	1:AP:90:MET:HE2	1.73	0.70
1:BI:55:ASN:ND2	1:BI:72:ASN:OD1	2.23	0.70
1:FK:38:SER:HB2	1:FK:51:ARG:HB2	1.72	0.70
1:AD:86:VAL:HG12	1:AD:90:MET:HE2	1.73	0.70
1:FN:59:SER:HB3	1:FN:66:LYS:HE2	1.72	0.70
1:ED:86:VAL:HG12	1:ED:90:MET:HE2	1.73	0.70
1:FV:86:VAL:HG12	1:FV:90:MET:HE2	1.73	0.70
1:GP:59:SER:HB3	1:GP:66:LYS:HE2	1.72	0.69
1:BJ:6:LYS:NZ	1:IT:93:GLU:OE1	2.23	0.69
1:HB:59:SER:HB3	1:HB:66:LYS:HE2	1.72	0.69
1:CT:86:VAL:HG12	1:CT:90:MET:HE2	1.73	0.69
1:CL:6:LYS:NZ	1:FF:93:GLU:OE1	2.24	0.69
1:BZ:6:LYS:NZ	1:ET:93:GLU:OE1	2.24	0.69
1:HJ:86:VAL:HG12	1:HJ:90:MET:HE2	1.75	0.69
1:IT:86:VAL:HG12	1:IT:90:MET:HE2	1.75	0.69
1:BF:86:VAL:HG12	1:BF:90:MET:HE2	1.73	0.69
1:ID:86:VAL:HG12	1:ID:90:MET:HE2	1.75	0.69
1:AI:38:SER:HB2	1:AI:51:ARG:HB2	1.76	0.68
1:DN:86:VAL:HG12	1:DN:90:MET:HE2	1.73	0.68
1:DO:38:SER:HB2	1:DO:51:ARG:HB2	1.76	0.68
1:EI:38:SER:HB2	1:EI:51:ARG:HB2	1.76	0.68
1:FJ:17:GLU:HB2	1:FJ:36:ARG:HG3	1.76	0.68
1:BF:93:GLU:OE1	1:IP:6:LYS:NZ	2.24	0.68
1:AX:17:GLU:HB2	1:AX:36:ARG:HG3	1.76	0.67
1:CA:38:SER:HB2	1:CA:51:ARG:HB2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EL:93:GLU:OE1	1:HF:6:LYS:NZ	2.25	0.67
1:BR:17:GLU:HB2	1:BR:36:ARG:HG3	1.76	0.67
1:DB:6:LYS:NZ	1:FV:93:GLU:OE1	2.24	0.67
1:CH:17:GLU:HB2	1:CH:36:ARG:HG3	1.76	0.67
1:DR:93:GLU:OE1	1:GL:6:LYS:NZ	2.25	0.67
1:ED:93:GLU:OE1	1:GX:6:LYS:NZ	2.24	0.67
1:EU:38:SER:HB2	1:EU:51:ARG:HB2	1.76	0.67
1:CL:93:GLU:OE1	1:FF:6:LYS:NZ	2.27	0.67
1:BZ:93:GLU:OE1	1:ET:6:LYS:NZ	2.27	0.67
1:DZ:17:GLU:HB2	1:DZ:36:ARG:HG3	1.76	0.67
1:EP:93:GLU:OE1	1:HJ:6:LYS:NZ	2.27	0.67
1:AT:6:LYS:NZ	1:ID:93:GLU:OE1	2.23	0.67
1:AT:93:GLU:OE1	1:ID:6:LYS:NZ	2.27	0.67
1:BB:93:GLU:OE1	1:IL:6:LYS:NZ	2.25	0.67
1:BN:93:GLU:OE1	1:IX:6:LYS:NZ	2.25	0.67
1:BJ:93:GLU:OE1	1:IT:6:LYS:NZ	2.27	0.67
1:CT:6:LYS:NZ	1:FN:93:GLU:OE1	2.27	0.66
1:AY:38:SER:HB2	1:AY:51:ARG:HB2	1.76	0.66
1:DB:93:GLU:OE1	1:FV:6:LYS:NZ	2.27	0.66
1:BK:38:SER:HB2	1:BK:51:ARG:HB2	1.76	0.66
1:DJ:17:GLU:HB2	1:DJ:36:ARG:HG3	1.76	0.66
1:CX:17:GLU:HB2	1:CX:36:ARG:HG3	1.76	0.66
1:DN:6:LYS:NZ	1:GH:93:GLU:OE1	2.29	0.66
1:ED:6:LYS:NZ	1:GX:93:GLU:OE1	2.29	0.66
1:AD:6:LYS:NZ	1:HN:93:GLU:OE1	2.28	0.65
1:AP:6:LYS:NZ	1:HZ:93:GLU:OE1	2.29	0.65
1:BE:55:ASN:ND2	1:BE:72:ASN:OD1	2.30	0.65
1:BF:6:LYS:NZ	1:IP:93:GLU:OE1	2.28	0.65
1:AD:93:GLU:OE1	1:HN:6:LYS:NZ	2.24	0.65
1:AP:93:GLU:OE1	1:HZ:6:LYS:NZ	2.24	0.65
1:FU:55:ASN:ND2	1:FU:72:ASN:OD1	2.31	0.64
1:AM:67:SER:HB3	1:AO:78:PRO:HG2	1.80	0.64
1:DC:55:ASN:ND2	1:DC:72:ASN:OD1	2.31	0.64
1:EQ:67:SER:HB3	1:ES:78:PRO:HG2	1.80	0.64
1:FC:67:SER:HB3	1:FE:78:PRO:HG2	1.80	0.64
1:FO:55:ASN:ND2	1:FO:72:ASN:OD1	2.31	0.64
1:AA:67:SER:HB3	1:AC:78:PRO:HG2	1.80	0.64
1:GS:55:ASN:ND2	1:GS:72:ASN:OD1	2.31	0.64
1:AE:67:SER:HB3	1:AG:78:PRO:HG2	1.80	0.64
1:BC:67:SER:HB3	1:BE:78:PRO:HG2	1.80	0.64
1:CT:78:PRO:HG2	1:FN:67:SER:HB3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:67:SER:HB3	1:EC:78:PRO:HG2	1.80	0.64
1:FS:67:SER:HB3	1:FU:78:PRO:HG2	1.80	0.64
1:CD:6:LYS:NZ	1:EX:93:GLU:OE1	2.24	0.63
1:DB:67:SER:HB3	1:FV:78:PRO:HG2	1.80	0.63
1:CD:93:GLU:OE1	1:EX:6:LYS:NZ	2.24	0.63
1:DK:67:SER:HB3	1:DM:78:PRO:HG2	1.80	0.63
1:CQ:67:SER:HB3	1:CS:78:PRO:HG2	1.80	0.63
1:BS:67:SER:HB3	1:BU:78:PRO:HG2	1.80	0.63
1:CM:67:SER:HB3	1:CO:78:PRO:HG2	1.80	0.63
1:DS:78:PRO:HG2	1:DU:67:SER:HB3	1.81	0.63
1:EE:78:PRO:HG2	1:EG:67:SER:HB3	1.81	0.63
1:FO:78:PRO:HG2	1:FQ:67:SER:HB3	1.81	0.63
1:DC:67:SER:HB3	1:DE:78:PRO:HG2	1.80	0.62
1:EY:67:SER:HB3	1:FA:78:PRO:HG2	1.80	0.62
1:AQ:78:PRO:HG2	1:AS:67:SER:HB3	1.81	0.62
1:CT:93:GLU:OE1	1:FN:6:LYS:NZ	2.24	0.62
1:ED:78:PRO:HG2	1:GX:67:SER:HB3	1.81	0.62
1:EM:78:PRO:HG2	1:EO:67:SER:HB3	1.81	0.62
1:EY:78:PRO:HG2	1:FA:67:SER:HB3	1.81	0.62
1:FK:78:PRO:HG2	1:FM:67:SER:HB3	1.81	0.62
1:AL:17:GLU:HB2	1:AL:36:ARG:HG3	1.82	0.62
1:BF:78:PRO:HG2	1:IP:67:SER:HB3	1.81	0.62
1:DC:78:PRO:HG2	1:DE:67:SER:HB3	1.81	0.62
1:DN:78:PRO:HG2	1:GH:67:SER:HB3	1.81	0.62
1:BG:78:PRO:HG2	1:BI:67:SER:HB3	1.81	0.62
1:DE:38:SER:HB3	1:DE:51:ARG:HG3	1.81	0.62
1:EE:67:SER:HB3	1:EG:78:PRO:HG2	1.80	0.62
1:FA:38:SER:HB3	1:FA:51:ARG:HG3	1.81	0.62
1:AE:78:PRO:HG2	1:AG:67:SER:HB3	1.81	0.62
1:BS:78:PRO:HG2	1:BU:67:SER:HB3	1.81	0.62
1:BZ:67:SER:HB3	1:ET:78:PRO:HG2	1.80	0.62
1:DN:93:GLU:OE1	1:GH:6:LYS:NZ	2.24	0.62
1:AL:93:GLU:OE1	1:HV:6:LYS:NZ	2.25	0.62
1:CM:78:PRO:HG2	1:CO:67:SER:HB3	1.81	0.62
1:CY:78:PRO:HG2	1:DA:67:SER:HB3	1.81	0.62
1:DS:67:SER:HB3	1:DU:78:PRO:HG2	1.80	0.62
1:CE:78:PRO:HG2	1:CG:67:SER:HB3	1.82	0.62
1:FG:78:PRO:HG2	1:FI:67:SER:HB3	1.82	0.62
1:AG:38:SER:HB3	1:AG:51:ARG:HG3	1.81	0.62
1:CL:67:SER:HB3	1:FF:78:PRO:HG2	1.80	0.62
1:CY:67:SER:HB3	1:DA:78:PRO:HG2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BN:17:GLU:HB2	1:BN:36:ARG:HG3	1.82	0.61
1:BG:67:SER:HB3	1:BI:78:PRO:HG2	1.82	0.61
1:DU:38:SER:HB3	1:DU:51:ARG:HG3	1.81	0.61
1:EG:38:SER:HB3	1:EG:51:ARG:HG3	1.81	0.61
1:BB:17:GLU:HB2	1:BB:36:ARG:HG3	1.82	0.61
1:AA:78:PRO:HG2	1:AC:67:SER:HB3	1.82	0.61
1:FO:67:SER:HB3	1:FQ:78:PRO:HG2	1.80	0.61
1:AM:78:PRO:HG2	1:AO:67:SER:HB3	1.82	0.61
1:EA:78:PRO:HG2	1:EC:67:SER:HB3	1.82	0.61
1:AI:78:PRO:HG2	1:AK:67:SER:HB3	1.83	0.61
1:BU:38:SER:HB3	1:BU:51:ARG:HG3	1.81	0.61
1:BZ:38:SER:HB3	1:BZ:51:ARG:HG3	1.83	0.61
1:CU:78:PRO:HG2	1:CW:67:SER:HB3	1.82	0.61
1:EQ:78:PRO:HG2	1:ES:67:SER:HB3	1.83	0.61
1:FC:78:PRO:HG2	1:FE:67:SER:HB3	1.83	0.61
1:BJ:38:SER:HB3	1:BJ:51:ARG:HG3	1.83	0.61
1:DG:78:PRO:HG2	1:DI:67:SER:HB3	1.82	0.61
1:EH:78:PRO:HG2	1:HB:67:SER:HB3	1.83	0.61
1:AE:12:ARG:NH1	1:HU:16:ASP:OD1	2.34	0.61
1:AP:78:PRO:HG2	1:HZ:67:SER:HB3	1.81	0.61
1:CH:67:SER:HB3	1:FB:78:PRO:HG2	1.83	0.61
1:CL:38:SER:HB3	1:CL:51:ARG:HG3	1.83	0.61
1:CO:38:SER:HB3	1:CO:51:ARG:HG3	1.81	0.61
1:FN:38:SER:HB3	1:FN:51:ARG:HG3	1.83	0.61
1:FQ:38:SER:HB3	1:FQ:51:ARG:HG3	1.81	0.61
1:AD:78:PRO:HG2	1:HN:67:SER:HB3	1.81	0.61
1:BB:6:LYS:NZ	1:IL:93:GLU:OE1	2.30	0.61
1:DF:78:PRO:HG2	1:FZ:67:SER:HB3	1.83	0.61
1:DV:78:PRO:HG2	1:GP:67:SER:HB3	1.83	0.61
1:DW:78:PRO:HG2	1:DY:67:SER:HB3	1.82	0.60
1:AU:78:PRO:HG2	1:AW:67:SER:HB3	1.82	0.60
1:BW:78:PRO:HG2	1:BY:67:SER:HB3	1.81	0.60
1:CI:78:PRO:HG2	1:CK:67:SER:HB3	1.81	0.60
1:BN:6:LYS:NZ	1:IX:93:GLU:OE1	2.30	0.60
1:BO:78:PRO:HG2	1:BQ:67:SER:HB3	1.82	0.60
1:CC:16:ASP:OD1	1:EY:12:ARG:NH1	2.33	0.60
1:CH:78:PRO:HG2	1:FB:67:SER:HB3	1.84	0.60
1:CD:17:GLU:HB2	1:CD:36:ARG:HG3	1.82	0.60
1:DC:12:ARG:NH1	1:EW:16:ASP:OD1	2.33	0.60
1:AL:6:LYS:NZ	1:HV:93:GLU:OE1	2.30	0.60
1:CI:67:SER:HB3	1:CK:78:PRO:HG2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DO:78:PRO:HG2	1:DQ:67:SER:HB3	1.83	0.60
1:EX:17:GLU:HB2	1:EX:36:ARG:HG3	1.82	0.60
1:BM:16:ASP:OD1	1:FO:12:ARG:NH1	2.33	0.60
1:CM:12:ARG:NH1	1:DQ:16:ASP:OD1	2.33	0.60
1:EE:12:ARG:NH1	1:IK:16:ASP:OD1	2.34	0.60
1:EI:78:PRO:HG2	1:EK:67:SER:HB3	1.83	0.60
1:EL:17:GLU:HB2	1:EL:36:ARG:HG3	1.82	0.60
1:FK:67:SER:HB3	1:FM:78:PRO:HG2	1.82	0.60
1:GK:16:ASP:OD1	1:IY:12:ARG:NH1	2.34	0.60
1:BF:38:SER:HB3	1:BF:51:ARG:HG3	1.84	0.60
1:BS:12:ARG:NH1	1:EK:16:ASP:OD1	2.33	0.60
1:BW:67:SER:HB3	1:BY:78:PRO:HG2	1.82	0.60
1:CA:78:PRO:HG2	1:CC:67:SER:HB3	1.83	0.60
1:DS:12:ARG:NH1	1:IW:16:ASP:OD1	2.34	0.60
1:ED:38:SER:HB3	1:ED:51:ARG:HG3	1.83	0.60
1:EU:78:PRO:HG2	1:EW:67:SER:HB3	1.83	0.60
1:FV:38:SER:HB3	1:FV:51:ARG:HG3	1.84	0.60
1:GL:42:LYS:HD3	1:GL:47:ASN:HA	1.84	0.60
1:HF:42:LYS:HD3	1:HF:47:ASN:HA	1.84	0.60
1:AH:78:PRO:HG2	1:HR:67:SER:HB3	1.83	0.60
1:BK:78:PRO:HG2	1:BM:67:SER:HB3	1.83	0.60
1:DN:38:SER:HB3	1:DN:51:ARG:HG3	1.84	0.60
1:DR:17:GLU:HB2	1:DR:36:ARG:HG3	1.82	0.60
1:FS:78:PRO:HG2	1:FU:67:SER:HB3	1.82	0.60
1:HE:16:ASP:OD1	1:IE:12:ARG:NH1	2.34	0.60
1:IX:42:LYS:HD3	1:IX:47:ASN:HA	1.84	0.60
1:AI:67:SER:HB3	1:AK:78:PRO:HG2	1.84	0.60
1:AY:78:PRO:HG2	1:BA:67:SER:HB3	1.83	0.60
1:BC:78:PRO:HG2	1:BE:67:SER:HB3	1.82	0.60
1:CL:78:PRO:HG2	1:FF:67:SER:HB3	1.84	0.60
1:IC:55:ASN:ND2	1:IC:72:ASN:OD1	2.34	0.60
1:IL:42:LYS:HD3	1:IL:47:ASN:HA	1.84	0.60
1:AK:16:ASP:OD1	1:GQ:12:ARG:NH1	2.34	0.59
1:AT:38:SER:HB3	1:AT:51:ARG:HG3	1.83	0.59
1:BZ:78:PRO:HG2	1:ET:67:SER:HB3	1.84	0.59
1:CQ:78:PRO:HG2	1:CS:67:SER:HB3	1.82	0.59
1:CX:67:SER:HB3	1:FR:78:PRO:HG2	1.83	0.59
1:EP:38:SER:HB3	1:EP:51:ARG:HG3	1.83	0.59
1:CT:38:SER:HB3	1:CT:51:ARG:HG3	1.84	0.59
1:CX:78:PRO:HG2	1:FR:67:SER:HB3	1.84	0.59
1:DK:78:PRO:HG2	1:DM:67:SER:HB3	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JF:17:GLU:HB2	1:JF:36:ARG:HG3	1.84	0.59
1:AQ:67:SER:HB3	1:AS:78:PRO:HG2	1.82	0.59
1:CA:67:SER:HB3	1:CC:78:PRO:HG2	1.84	0.59
1:DA:55:ASN:ND2	1:DA:72:ASN:OD1	2.35	0.59
1:EU:67:SER:HB3	1:EW:78:PRO:HG2	1.84	0.59
1:IQ:67:SER:HB3	1:IS:78:PRO:HG2	1.85	0.59
1:AD:38:SER:HB3	1:AD:51:ARG:HG3	1.84	0.59
1:EM:67:SER:HB3	1:EO:78:PRO:HG2	1.82	0.59
1:FZ:17:GLU:HB2	1:FZ:36:ARG:HG3	1.84	0.59
1:HV:42:LYS:HD3	1:HV:47:ASN:HA	1.84	0.59
1:AP:38:SER:HB3	1:AP:51:ARG:HG3	1.84	0.59
1:AU:67:SER:HB3	1:AW:78:PRO:HG2	1.85	0.59
1:AX:78:PRO:HG2	1:IH:67:SER:HB3	1.84	0.59
1:BO:67:SER:HB3	1:BQ:78:PRO:HG2	1.85	0.59
1:DB:38:SER:HB3	1:DB:51:ARG:HG3	1.83	0.59
1:BA:16:ASP:OD1	1:GA:12:ARG:NH1	2.34	0.59
1:BR:78:PRO:HG2	1:JB:67:SER:HB3	1.84	0.59
1:CK:55:ASN:ND2	1:CK:72:ASN:OD1	2.35	0.59
1:DJ:78:PRO:HG2	1:GD:67:SER:HB3	1.84	0.59
1:DR:42:LYS:HD3	1:DR:47:ASN:HA	1.85	0.59
1:EL:42:LYS:HD3	1:EL:47:ASN:HA	1.85	0.59
1:FW:78:PRO:HG2	1:FY:67:SER:HB3	1.85	0.59
1:IE:67:SER:HB3	1:IG:78:PRO:HG2	1.85	0.59
1:IY:67:SER:HB3	1:JA:78:PRO:HG2	1.85	0.59
1:CP:67:SER:HB3	1:FJ:78:PRO:HG2	1.84	0.59
1:CT:67:SER:HB3	1:FN:78:PRO:HG2	1.84	0.59
1:DO:67:SER:HB3	1:DQ:78:PRO:HG2	1.84	0.59
1:EI:67:SER:HB3	1:EK:78:PRO:HG2	1.84	0.59
1:GQ:67:SER:HB3	1:GS:78:PRO:HG2	1.85	0.59
1:BV:78:PRO:HG2	1:JF:67:SER:HB3	1.83	0.59
1:CP:78:PRO:HG2	1:FJ:67:SER:HB3	1.83	0.59
1:DW:67:SER:HB3	1:DY:78:PRO:HG2	1.85	0.59
1:EL:6:LYS:NZ	1:HF:93:GLU:OE1	2.30	0.59
1:GP:17:GLU:HB2	1:GP:36:ARG:HG3	1.84	0.59
1:GQ:78:PRO:HG2	1:GS:67:SER:HB3	1.84	0.59
1:HB:17:GLU:HB2	1:HB:36:ARG:HG3	1.84	0.59
1:DR:6:LYS:NZ	1:GL:93:GLU:OE1	2.30	0.59
1:FF:38:SER:HB3	1:FF:51:ARG:HG3	1.84	0.59
1:GA:78:PRO:HG2	1:GC:67:SER:HB3	1.84	0.59
1:BN:78:PRO:HG2	1:IX:67:SER:HB3	1.85	0.58
1:CD:42:LYS:HD3	1:CD:47:ASN:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EX:42:LYS:HD3	1:EX:47:ASN:HA	1.85	0.58
1:BB:78:PRO:HG2	1:IL:67:SER:HB3	1.86	0.58
1:CD:67:SER:HB3	1:EX:78:PRO:HG2	1.84	0.58
1:CD:78:PRO:HG2	1:EX:67:SER:HB3	1.84	0.58
1:ET:38:SER:HB3	1:ET:51:ARG:HG3	1.84	0.58
1:AY:67:SER:HB3	1:BA:78:PRO:HG2	1.84	0.58
1:AL:42:LYS:HD3	1:AL:47:ASN:HA	1.85	0.58
1:AS:55:ASN:ND2	1:AS:72:ASN:OD1	2.36	0.58
1:DB:78:PRO:HG2	1:FV:67:SER:HB3	1.84	0.58
1:DZ:78:PRO:HG2	1:GT:67:SER:HB3	1.84	0.58
1:EO:55:ASN:ND2	1:EO:72:ASN:OD1	2.36	0.58
1:FM:55:ASN:ND2	1:FM:72:ASN:OD1	2.36	0.58
1:HR:17:GLU:HB2	1:HR:36:ARG:HG3	1.85	0.58
1:BK:67:SER:HB3	1:BM:78:PRO:HG2	1.84	0.58
1:AH:59:SER:HB3	1:AH:66:LYS:HE3	1.86	0.58
1:EL:78:PRO:HG2	1:HF:67:SER:HB3	1.85	0.58
1:EP:78:PRO:HG2	1:HJ:67:SER:HB3	1.84	0.58
1:AL:78:PRO:HG2	1:HV:67:SER:HB3	1.86	0.58
1:BJ:78:PRO:HG2	1:IT:67:SER:HB3	1.84	0.58
1:BV:59:SER:HB3	1:BV:66:LYS:HE3	1.86	0.58
1:CP:59:SER:HB3	1:CP:66:LYS:HE3	1.86	0.58
1:CU:67:SER:HB3	1:CW:78:PRO:HG2	1.85	0.58
1:DG:67:SER:HB3	1:DI:78:PRO:HG2	1.85	0.58
1:DR:78:PRO:HG2	1:GL:67:SER:HB3	1.86	0.58
1:IE:78:PRO:HG2	1:IG:67:SER:HB3	1.84	0.58
1:IY:78:PRO:HG2	1:JA:67:SER:HB3	1.84	0.58
1:AT:78:PRO:HG2	1:ID:67:SER:HB3	1.84	0.58
1:FG:67:SER:HB3	1:FI:78:PRO:HG2	1.85	0.58
1:HG:67:SER:HB3	1:HI:78:PRO:HG2	1.85	0.58
1:IA:67:SER:HB3	1:IC:78:PRO:HG2	1.85	0.58
1:FR:59:SER:HB3	1:FR:66:LYS:HE3	1.86	0.58
1:CE:67:SER:HB3	1:CG:78:PRO:HG2	1.85	0.57
1:DF:59:SER:HB3	1:DF:66:LYS:HE3	1.86	0.57
1:FB:59:SER:HB3	1:FB:66:LYS:HE3	1.86	0.57
1:BJ:67:SER:HB3	1:IT:78:PRO:HG2	1.85	0.57
1:FY:55:ASN:ND2	1:FY:72:ASN:OD1	2.37	0.57
1:GA:67:SER:HB3	1:GC:78:PRO:HG2	1.85	0.57
1:CI:98:ALA:HB1	1:CK:73:LEU:HD22	1.87	0.57
1:GI:78:PRO:HG2	1:GK:67:SER:HB3	1.87	0.57
1:GO:55:ASN:ND2	1:GO:72:ASN:OD1	2.37	0.57
1:HA:55:ASN:ND2	1:HA:72:ASN:OD1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:78:PRO:HG2	1:HE:67:SER:HB3	1.87	0.57
1:JE:55:ASN:ND2	1:JE:72:ASN:OD1	2.37	0.57
1:HQ:55:ASN:ND2	1:HQ:72:ASN:OD1	2.37	0.57
1:BN:42:LYS:HD3	1:BN:47:ASN:HA	1.85	0.57
1:BB:42:LYS:HD3	1:BB:47:ASN:HA	1.85	0.57
1:GE:78:PRO:HG2	1:GG:67:SER:HB3	1.87	0.57
1:BW:98:ALA:HB1	1:BY:73:LEU:HD22	1.87	0.57
1:CY:98:ALA:HB1	1:DA:73:LEU:HD22	1.87	0.57
1:HS:78:PRO:HG2	1:HU:67:SER:HB3	1.87	0.57
1:AT:67:SER:HB3	1:ID:78:PRO:HG2	1.85	0.56
1:DR:38:SER:HB3	1:DR:51:ARG:HG3	1.87	0.56
1:EL:38:SER:HB3	1:EL:51:ARG:HG3	1.87	0.56
1:AQ:98:ALA:HB1	1:AS:73:LEU:HD22	1.87	0.56
1:AX:93:GLU:OE1	1:IH:6:LYS:NZ	2.29	0.56
1:CD:38:SER:HB3	1:CD:51:ARG:HG3	1.87	0.56
1:CW:55:ASN:ND2	1:CW:72:ASN:OD1	2.38	0.56
1:CX:98:ALA:HB1	1:FR:73:LEU:HD12	1.87	0.56
1:EM:98:ALA:HB1	1:EO:73:LEU:HD22	1.87	0.56
1:EP:67:SER:HB3	1:HJ:78:PRO:HG2	1.85	0.56
1:DY:55:ASN:ND2	1:DY:72:ASN:OD1	2.39	0.56
1:EX:38:SER:HB3	1:EX:51:ARG:HG3	1.87	0.56
1:GU:78:PRO:HG2	1:GW:67:SER:HB3	1.87	0.56
1:IS:55:ASN:ND2	1:IS:72:ASN:OD1	2.38	0.56
1:CH:98:ALA:HB1	1:FB:73:LEU:HD12	1.88	0.56
1:CP:64:ASP:OD1	1:CP:64:ASP:N	2.37	0.56
1:CU:12:ARG:NH1	1:FA:16:ASP:OD1	2.39	0.56
1:DE:16:ASP:OD1	1:DG:12:ARG:NH1	2.39	0.56
1:FI:55:ASN:ND2	1:FI:72:ASN:OD1	2.39	0.56
1:GW:34:SER:HB2	1:GW:55:ASN:HB3	1.88	0.56
1:HW:78:PRO:HG2	1:HY:67:SER:HB3	1.87	0.56
1:BR:93:GLU:OE1	1:JB:6:LYS:NZ	2.29	0.56
1:BV:64:ASP:OD1	1:BV:64:ASP:N	2.37	0.56
1:DF:73:LEU:HD12	1:FZ:98:ALA:HB1	1.88	0.56
1:DW:12:ARG:NH1	1:JA:16:ASP:OD1	2.39	0.56
1:FK:98:ALA:HB1	1:FM:73:LEU:HD22	1.87	0.56
1:FW:67:SER:HB3	1:FY:78:PRO:HG2	1.87	0.56
1:HK:78:PRO:HG2	1:HM:67:SER:HB3	1.87	0.56
1:CG:55:ASN:ND2	1:CG:72:ASN:OD1	2.39	0.56
1:IA:55:ASN:OD1	1:IA:72:ASN:ND2	2.39	0.56
1:AX:73:LEU:HD12	1:IH:98:ALA:HB1	1.88	0.56
1:BR:73:LEU:HD12	1:JB:98:ALA:HB1	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CP:73:LEU:HD12	1:FJ:98:ALA:HB1	1.87	0.56
1:DV:6:LYS:NZ	1:GP:93:GLU:OE1	2.30	0.56
1:DV:59:SER:HB3	1:DV:66:LYS:HE3	1.86	0.56
1:EH:59:SER:HB3	1:EH:66:LYS:HE3	1.86	0.56
1:HG:55:ASN:OD1	1:HG:72:ASN:ND2	2.39	0.56
1:IQ:98:ALA:HB1	1:IS:73:LEU:HD22	1.88	0.56
1:AH:73:LEU:HD12	1:HR:98:ALA:HB1	1.88	0.56
1:EH:6:LYS:NZ	1:HB:93:GLU:OE1	2.30	0.56
1:II:78:PRO:HG2	1:IK:67:SER:HB3	1.87	0.56
1:CP:6:LYS:NZ	1:FJ:93:GLU:OE1	2.29	0.55
1:DE:109:LYS:HB2	1:DE:111:VAL:HG23	1.88	0.55
1:FA:109:LYS:HB2	1:FA:111:VAL:HG23	1.88	0.55
1:IU:78:PRO:HG2	1:IW:67:SER:HB3	1.87	0.55
1:AU:12:ARG:NH1	1:DU:16:ASP:OD1	2.39	0.55
1:BB:38:SER:HB3	1:BB:51:ARG:HG3	1.87	0.55
1:BO:12:ARG:NH1	1:EG:16:ASP:OD1	2.39	0.55
1:DI:55:ASN:ND2	1:DI:72:ASN:OD1	2.39	0.55
1:DJ:67:SER:HB3	1:GD:78:PRO:HG2	1.88	0.55
1:DZ:73:LEU:HD12	1:GT:98:ALA:HB1	1.88	0.55
1:AA:98:ALA:HB1	1:AC:73:LEU:HD22	1.87	0.55
1:AW:55:ASN:ND2	1:AW:72:ASN:OD1	2.39	0.55
1:BC:98:ALA:HB1	1:BE:73:LEU:HD22	1.87	0.55
1:DK:98:ALA:HB1	1:DM:73:LEU:HD22	1.87	0.55
1:FQ:109:LYS:HB2	1:FQ:111:VAL:HG23	1.88	0.55
1:BN:38:SER:HB3	1:BN:51:ARG:HG3	1.87	0.55
1:BQ:55:ASN:ND2	1:BQ:72:ASN:OD1	2.39	0.55
1:CH:73:LEU:HD12	1:FB:98:ALA:HB1	1.88	0.55
1:CP:98:ALA:HB1	1:FJ:73:LEU:HD12	1.88	0.55
1:FG:12:ARG:NH1	1:FQ:16:ASP:OD1	2.39	0.55
1:FS:98:ALA:HB1	1:FU:73:LEU:HD22	1.87	0.55
1:BK:18:VAL:HG23	1:BM:112:ILE:HD12	1.89	0.55
1:BV:6:LYS:NZ	1:JF:93:GLU:OE1	2.30	0.55
1:HO:78:PRO:HG2	1:HQ:67:SER:HB3	1.88	0.55
1:HS:18:VAL:HG23	1:HU:112:ILE:HD12	1.89	0.55
1:AY:18:VAL:HG23	1:BA:112:ILE:HD12	1.89	0.55
1:BR:67:SER:HB3	1:JB:78:PRO:HG2	1.88	0.55
1:BV:67:SER:HB3	1:JF:78:PRO:HG2	1.89	0.55
1:CE:12:ARG:NH1	1:CO:16:ASP:OD1	2.39	0.55
1:CH:93:GLU:OE1	1:FB:6:LYS:NZ	2.29	0.55
1:DM:55:ASN:ND2	1:DM:72:ASN:OD1	2.40	0.55
1:EG:109:LYS:HB2	1:EG:111:VAL:HG23	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GE:98:ALA:HB1	1:GG:73:LEU:HD22	1.89	0.55
1:AL:38:SER:HB3	1:AL:51:ARG:HG3	1.87	0.55
1:AM:98:ALA:HB1	1:AO:73:LEU:HD22	1.88	0.55
1:AX:67:SER:HB3	1:IH:78:PRO:HG2	1.88	0.55
1:BG:98:ALA:HB1	1:BI:73:LEU:HD22	1.87	0.55
1:BV:73:LEU:HD12	1:JF:98:ALA:HB1	1.88	0.55
1:DU:109:LYS:HB2	1:DU:111:VAL:HG23	1.89	0.55
1:EA:98:ALA:HB1	1:EC:73:LEU:HD22	1.88	0.55
1:BU:16:ASP:OD1	1:FW:12:ARG:NH1	2.39	0.55
1:CS:55:ASN:ND2	1:CS:72:ASN:OD1	2.40	0.55
1:GM:78:PRO:HG2	1:GO:67:SER:HB3	1.88	0.55
1:IA:98:ALA:HB1	1:IC:73:LEU:HD22	1.88	0.55
1:JC:78:PRO:HG2	1:JE:67:SER:HB3	1.88	0.55
1:CQ:98:ALA:HB1	1:CS:73:LEU:HD22	1.88	0.55
1:GG:34:SER:HB2	1:GG:55:ASN:HB3	1.88	0.55
1:HS:67:SER:HB3	1:HU:78:PRO:HG2	1.89	0.55
1:HW:98:ALA:HB1	1:HY:73:LEU:HD22	1.89	0.55
1:IM:78:PRO:HG2	1:IO:67:SER:HB3	1.87	0.55
1:AI:18:VAL:HG23	1:AK:112:ILE:HD12	1.89	0.55
1:DJ:73:LEU:HD12	1:GD:98:ALA:HB1	1.88	0.55
1:DZ:67:SER:HB3	1:GT:78:PRO:HG2	1.88	0.55
1:GY:78:PRO:HG2	1:HA:67:SER:HB3	1.88	0.55
1:HK:98:ALA:HB1	1:HM:73:LEU:HD22	1.90	0.54
1:HQ:34:SER:HB2	1:HQ:55:ASN:HB3	1.90	0.54
1:IQ:55:ASN:OD1	1:IQ:72:ASN:ND2	2.39	0.54
1:DF:67:SER:HB3	1:FZ:78:PRO:HG2	1.89	0.54
1:GM:18:VAL:HG23	1:GO:112:ILE:HD12	1.90	0.54
1:HG:98:ALA:HB1	1:HI:73:LEU:HD22	1.89	0.54
1:AO:55:ASN:ND2	1:AO:72:ASN:OD1	2.40	0.54
1:BS:98:ALA:HB1	1:BU:73:LEU:HD22	1.90	0.54
1:DF:6:LYS:NZ	1:FZ:93:GLU:OE1	2.30	0.54
1:EY:98:ALA:HB1	1:FA:73:LEU:HD22	1.90	0.54
1:FC:98:ALA:HB1	1:FE:73:LEU:HD22	1.88	0.54
1:GI:67:SER:HB3	1:GK:78:PRO:HG2	1.89	0.54
1:GS:16:ASP:OD1	1:GY:12:ARG:NH1	2.41	0.54
1:GY:18:VAL:HG23	1:HA:112:ILE:HD12	1.90	0.54
1:HC:67:SER:HB3	1:HE:78:PRO:HG2	1.89	0.54
1:AC:55:ASN:ND2	1:AC:72:ASN:OD1	2.40	0.54
1:CM:98:ALA:HB1	1:CO:73:LEU:HD22	1.90	0.54
1:FY:34:SER:HB2	1:FY:55:ASN:HB3	1.89	0.54
1:IE:98:ALA:HB1	1:IG:73:LEU:HD22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IU:98:ALA:HB1	1:IW:73:LEU:HD22	1.90	0.54
1:EQ:98:ALA:HB1	1:ES:73:LEU:HD22	1.88	0.54
1:GH:59:SER:HB3	1:GH:66:LYS:HE2	1.90	0.54
1:II:98:ALA:HB1	1:IK:73:LEU:HD22	1.90	0.54
1:IO:55:ASN:OD1	1:IO:72:ASN:ND2	2.38	0.54
1:IY:98:ALA:HB1	1:JA:73:LEU:HD22	1.90	0.54
1:JA:55:ASN:ND2	1:JA:72:ASN:OD1	2.41	0.54
1:BU:109:LYS:HB2	1:BU:111:VAL:HG23	1.88	0.54
1:CI:37:ARG:HB2	1:CI:50:MET:HE1	1.90	0.54
1:CO:109:LYS:HB2	1:CO:111:VAL:HG23	1.89	0.54
1:DJ:93:GLU:OE1	1:GD:6:LYS:NZ	2.29	0.54
1:EC:55:ASN:ND2	1:EC:72:ASN:OD1	2.40	0.54
1:EU:18:VAL:HG23	1:EW:112:ILE:HD12	1.89	0.54
1:GC:16:ASP:OD1	1:JC:12:ARG:NH1	2.40	0.54
1:GQ:98:ALA:HB1	1:GS:73:LEU:HD22	1.90	0.54
1:HO:12:ARG:NH1	1:IG:16:ASP:OD1	2.41	0.54
1:HS:98:ALA:HB1	1:HU:73:LEU:HD22	1.89	0.54
1:HW:67:SER:HB3	1:HY:78:PRO:HG2	1.90	0.54
1:IO:34:SER:HB2	1:IO:55:ASN:HB3	1.90	0.54
1:BW:37:ARG:HB2	1:BW:50:MET:HE1	1.90	0.54
1:CA:18:VAL:HG23	1:CC:112:ILE:HD12	1.89	0.54
1:CX:93:GLU:OE1	1:FR:6:LYS:NZ	2.29	0.54
1:DV:67:SER:HB3	1:GP:78:PRO:HG2	1.89	0.54
1:DV:73:LEU:HD12	1:GP:98:ALA:HB1	1.88	0.54
1:EH:67:SER:HB3	1:HB:78:PRO:HG2	1.89	0.54
1:EH:73:LEU:HD12	1:HB:98:ALA:HB1	1.88	0.54
1:HG:78:PRO:HG2	1:HI:67:SER:HB3	1.90	0.54
1:IG:55:ASN:ND2	1:IG:72:ASN:OD1	2.41	0.54
1:AE:98:ALA:HB1	1:AG:73:LEU:HD22	1.90	0.54
1:AG:16:ASP:OD1	1:GM:12:ARG:NH1	2.41	0.54
1:DC:98:ALA:HB1	1:DE:73:LEU:HD22	1.90	0.54
1:FE:55:ASN:ND2	1:FE:72:ASN:OD1	2.40	0.54
1:IA:78:PRO:HG2	1:IC:67:SER:HB3	1.90	0.54
1:BM:55:ASN:OD1	1:BM:72:ASN:ND2	2.41	0.54
1:CY:37:ARG:HB2	1:CY:50:MET:HE1	1.90	0.54
1:DG:18:VAL:HG23	1:DI:112:ILE:HD12	1.90	0.54
1:GI:18:VAL:HG23	1:GK:112:ILE:HD12	1.89	0.54
1:HI:55:ASN:OD1	1:HI:72:ASN:ND2	2.39	0.54
1:HK:67:SER:HB3	1:HM:78:PRO:HG2	1.90	0.54
1:II:67:SER:HB3	1:IK:78:PRO:HG2	1.89	0.54
1:IU:18:VAL:HG23	1:IW:112:ILE:HD12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:109:LYS:HB2	1:AG:111:VAL:HG23	1.89	0.54
1:AY:98:ALA:HB1	1:BA:73:LEU:HD22	1.90	0.54
1:BO:18:VAL:HG23	1:BQ:112:ILE:HD12	1.90	0.54
1:CE:18:VAL:HG23	1:CG:112:ILE:HD12	1.90	0.54
1:ET:64:ASP:OD1	1:ET:64:ASP:N	2.38	0.54
1:FW:18:VAL:HG23	1:FY:112:ILE:HD12	1.90	0.54
1:GD:59:SER:HB3	1:GD:66:LYS:HE3	1.90	0.54
1:GU:67:SER:HB3	1:GW:78:PRO:HG2	1.90	0.54
1:HC:18:VAL:HG23	1:HE:112:ILE:HD12	1.89	0.54
1:II:18:VAL:HG23	1:IK:112:ILE:HD12	1.89	0.54
1:IU:67:SER:HB3	1:IW:78:PRO:HG2	1.89	0.54
1:AU:18:VAL:HG23	1:AW:112:ILE:HD12	1.90	0.53
1:BK:98:ALA:HB1	1:BM:73:LEU:HD22	1.90	0.53
1:CU:18:VAL:HG23	1:CW:112:ILE:HD12	1.90	0.53
1:CX:73:LEU:HD12	1:FR:98:ALA:HB1	1.88	0.53
1:EI:98:ALA:HB1	1:EK:73:LEU:HD22	1.90	0.53
1:ES:55:ASN:ND2	1:ES:72:ASN:OD1	2.40	0.53
1:BY:55:ASN:ND2	1:BY:72:ASN:OD1	2.39	0.53
1:DO:98:ALA:HB1	1:DQ:73:LEU:HD22	1.90	0.53
1:DS:98:ALA:HB1	1:DU:73:LEU:HD22	1.90	0.53
1:ED:98:ALA:HB1	1:GX:73:LEU:HD12	1.90	0.53
1:BG:37:ARG:HB2	1:BG:50:MET:HE1	1.90	0.53
1:FF:64:ASP:OD1	1:FF:64:ASP:N	2.38	0.53
1:DN:98:ALA:HB1	1:GH:73:LEU:HD12	1.90	0.53
1:EE:98:ALA:HB1	1:EG:73:LEU:HD22	1.90	0.53
1:EW:55:ASN:OD1	1:EW:72:ASN:ND2	2.41	0.53
1:FG:18:VAL:HG23	1:FI:112:ILE:HD12	1.90	0.53
1:IM:98:ALA:HB1	1:IO:73:LEU:HD22	1.89	0.53
1:JE:34:SER:HB2	1:JE:55:ASN:HB3	1.90	0.53
1:CC:55:ASN:OD1	1:CC:72:ASN:ND2	2.41	0.53
1:GC:55:ASN:ND2	1:GC:72:ASN:OD1	2.41	0.53
1:GT:59:SER:HB3	1:GT:66:LYS:HE3	1.90	0.53
1:HO:18:VAL:HG23	1:HQ:112:ILE:HD12	1.90	0.53
1:EU:98:ALA:HB1	1:EW:73:LEU:HD22	1.90	0.53
1:GA:98:ALA:HB1	1:GC:73:LEU:HD22	1.90	0.53
1:GO:34:SER:HB2	1:GO:55:ASN:HB3	1.90	0.53
1:GX:53:ASN:OD1	1:GX:74:THR:OG1	2.26	0.53
1:HA:34:SER:HB2	1:HA:55:ASN:HB3	1.90	0.53
1:HC:98:ALA:HB1	1:HE:73:LEU:HD22	1.89	0.53
1:JC:18:VAL:HG23	1:JE:112:ILE:HD12	1.90	0.53
1:GI:98:ALA:HB1	1:GK:73:LEU:HD22	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GX:59:SER:HB3	1:GX:66:LYS:HE2	1.90	0.53
1:AH:67:SER:HB3	1:HR:78:PRO:HG2	1.89	0.53
1:CA:98:ALA:HB1	1:CC:73:LEU:HD22	1.90	0.53
1:DZ:93:GLU:OE1	1:GT:6:LYS:NZ	2.29	0.53
1:AL:67:SER:HB3	1:HV:78:PRO:HG2	1.91	0.53
1:BB:67:SER:HB3	1:IL:78:PRO:HG2	1.91	0.53
1:BN:67:SER:HB3	1:IX:78:PRO:HG2	1.91	0.53
1:ED:67:SER:HB3	1:GX:78:PRO:HG2	1.91	0.53
1:EI:18:VAL:HG23	1:EK:112:ILE:HD12	1.89	0.53
1:HY:34:SER:HB2	1:HY:55:ASN:HB3	1.90	0.53
1:DO:18:VAL:HG23	1:DQ:112:ILE:HD12	1.89	0.53
1:GE:67:SER:HB3	1:GG:78:PRO:HG2	1.90	0.53
1:HN:59:SER:HB3	1:HN:66:LYS:HE2	1.90	0.53
1:HY:55:ASN:OD1	1:HY:72:ASN:ND2	2.38	0.53
1:AD:67:SER:HB3	1:HN:78:PRO:HG2	1.91	0.52
1:AG:55:ASN:ND2	1:AG:72:ASN:OD1	2.43	0.52
1:AI:98:ALA:HB1	1:AK:73:LEU:HD22	1.90	0.52
1:HZ:59:SER:HB3	1:HZ:66:LYS:HE2	1.90	0.52
1:AP:67:SER:HB3	1:HZ:78:PRO:HG2	1.91	0.52
1:FW:98:ALA:HB1	1:FY:73:LEU:HD22	1.92	0.52
1:HG:37:ARG:HB2	1:HG:50:MET:HE1	1.92	0.52
1:HM:34:SER:HB2	1:HM:55:ASN:HB3	1.90	0.52
1:IA:37:ARG:HB2	1:IA:50:MET:HE1	1.92	0.52
1:IH:59:SER:HB3	1:IH:66:LYS:HE3	1.90	0.52
1:IQ:78:PRO:HG2	1:IS:67:SER:HB3	1.90	0.52
1:AD:98:ALA:HB1	1:HN:73:LEU:HD12	1.90	0.52
1:AP:98:ALA:HB1	1:HZ:73:LEU:HD12	1.90	0.52
1:CE:98:ALA:HB1	1:CG:73:LEU:HD22	1.92	0.52
1:GC:34:SER:HB2	1:GC:55:ASN:HB3	1.91	0.52
1:HU:34:SER:HB2	1:HU:55:ASN:HB3	1.91	0.52
1:IP:59:SER:HB3	1:IP:66:LYS:HE2	1.90	0.52
1:JB:59:SER:HB3	1:JB:66:LYS:HE3	1.90	0.52
1:BF:98:ALA:HB1	1:IP:73:LEU:HD12	1.90	0.52
1:GU:98:ALA:HB1	1:GW:73:LEU:HD22	1.89	0.52
1:HM:55:ASN:OD1	1:HM:72:ASN:ND2	2.38	0.52
1:IM:67:SER:HB3	1:IO:78:PRO:HG2	1.90	0.52
1:CU:98:ALA:HB1	1:CW:73:LEU:HD22	1.92	0.52
1:DG:98:ALA:HB1	1:DI:73:LEU:HD22	1.92	0.52
1:EK:55:ASN:OD1	1:EK:72:ASN:ND2	2.41	0.52
1:EL:67:SER:HB3	1:HF:78:PRO:HG2	1.91	0.52
1:AH:6:LYS:NZ	1:HR:93:GLU:OE1	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IP:53:ASN:OD1	1:IP:74:THR:OG1	2.26	0.52
1:AL:64:ASP:OD1	1:AL:64:ASP:N	2.38	0.52
1:DQ:55:ASN:OD1	1:DQ:72:ASN:ND2	2.41	0.52
1:DR:67:SER:HB3	1:GL:78:PRO:HG2	1.91	0.52
1:FK:37:ARG:HB2	1:FK:50:MET:HE1	1.90	0.52
1:IG:34:SER:HB2	1:IG:55:ASN:HB3	1.91	0.52
1:IT:64:ASP:OD1	1:IT:64:ASP:N	2.38	0.52
1:JA:34:SER:HB2	1:JA:55:ASN:HB3	1.91	0.52
1:JB:64:ASP:OD1	1:JB:64:ASP:N	2.38	0.52
1:IQ:37:ARG:HB2	1:IQ:50:MET:HE1	1.92	0.52
1:JC:98:ALA:HB1	1:JE:73:LEU:HD22	1.92	0.52
1:BF:67:SER:HB3	1:IP:78:PRO:HG2	1.91	0.52
1:CM:55:ASN:ND2	1:CM:72:ASN:OD1	2.43	0.52
1:DW:18:VAL:HG23	1:DY:112:ILE:HD12	1.90	0.52
1:EH:64:ASP:OD1	1:EH:64:ASP:N	2.37	0.52
1:FO:98:ALA:HB1	1:FQ:73:LEU:HD22	1.90	0.52
1:IH:64:ASP:OD1	1:IH:64:ASP:N	2.38	0.52
1:AQ:37:ARG:HB2	1:AQ:50:MET:HE1	1.90	0.52
1:BS:55:ASN:ND2	1:BS:72:ASN:OD1	2.43	0.52
1:DW:98:ALA:HB1	1:DY:73:LEU:HD22	1.92	0.52
1:GM:67:SER:HB3	1:GO:78:PRO:HG2	1.92	0.52
1:GY:67:SER:HB3	1:HA:78:PRO:HG2	1.92	0.51
1:DV:64:ASP:OD1	1:DV:64:ASP:N	2.37	0.51
1:HE:34:SER:HB2	1:HE:55:ASN:HB3	1.91	0.51
1:IK:55:ASN:OD1	1:IK:72:ASN:ND2	2.40	0.51
1:IW:55:ASN:OD1	1:IW:72:ASN:ND2	2.40	0.51
1:AK:55:ASN:OD1	1:AK:72:ASN:ND2	2.41	0.51
1:AU:98:ALA:HB1	1:AW:73:LEU:HD22	1.92	0.51
1:BO:98:ALA:HB1	1:BQ:73:LEU:HD22	1.92	0.51
1:BY:42:LYS:HE2	1:BY:47:ASN:HA	1.93	0.51
1:CQ:37:ARG:HB2	1:CQ:50:MET:HE1	1.93	0.51
1:DK:37:ARG:HB2	1:DK:50:MET:HE1	1.93	0.51
1:DN:67:SER:HB3	1:GH:78:PRO:HG2	1.91	0.51
1:GK:34:SER:HB2	1:GK:55:ASN:HB3	1.91	0.51
1:HM:41:VAL:HG12	1:HM:43:LYS:HG3	1.93	0.51
1:HY:41:VAL:HG12	1:HY:43:LYS:HG3	1.93	0.51
1:JC:67:SER:HB3	1:JE:78:PRO:HG2	1.92	0.51
1:CK:42:LYS:HE2	1:CK:47:ASN:HA	1.93	0.51
1:EM:37:ARG:HB2	1:EM:50:MET:HE1	1.90	0.51
1:FQ:55:ASN:ND2	1:FQ:72:ASN:OD1	2.43	0.51
1:FS:37:ARG:HB2	1:FS:50:MET:HE1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HO:98:ALA:HB1	1:HQ:73:LEU:HD22	1.92	0.51
1:DA:42:LYS:HE2	1:DA:47:ASN:HA	1.93	0.51
1:EA:37:ARG:HB2	1:EA:50:MET:HE1	1.93	0.51
1:ET:42:LYS:NZ	1:ET:44:GLY:O	2.36	0.51
1:GM:98:ALA:HB1	1:GO:73:LEU:HD22	1.92	0.51
1:GY:98:ALA:HB1	1:HA:73:LEU:HD22	1.92	0.51
1:HO:67:SER:HB3	1:HQ:78:PRO:HG2	1.92	0.51
1:BC:37:ARG:HB2	1:BC:50:MET:HE1	1.93	0.51
1:DS:93:GLU:OE2	1:DU:6:LYS:HD3	2.11	0.51
1:EY:93:GLU:OE2	1:FA:6:LYS:HD3	2.11	0.51
1:DC:93:GLU:OE2	1:DE:6:LYS:HD3	2.11	0.51
1:EE:93:GLU:OE2	1:EG:6:LYS:HD3	2.11	0.51
1:IO:42:LYS:HE2	1:IO:47:ASN:HA	1.93	0.51
1:AS:42:LYS:HE2	1:AS:47:ASN:HA	1.93	0.51
1:AD:73:LEU:HD22	1:HN:98:ALA:HB1	1.93	0.51
1:AP:73:LEU:HD22	1:HZ:98:ALA:HB1	1.93	0.51
1:AY:108:THR:HG21	1:BA:87:ARG:HG3	1.93	0.51
1:BK:108:THR:HG21	1:BM:87:ARG:HG3	1.93	0.51
1:CO:55:ASN:ND2	1:CO:72:ASN:OD1	2.43	0.51
1:EO:42:LYS:HE2	1:EO:47:ASN:HA	1.93	0.51
1:HN:64:ASP:OD1	1:HN:64:ASP:N	2.38	0.51
1:DB:54:MET:HG2	1:DB:56:PHE:CE1	2.46	0.50
1:FG:98:ALA:HB1	1:FI:73:LEU:HD22	1.92	0.50
1:GC:109:LYS:HB2	1:GC:111:VAL:HG23	1.93	0.50
1:AA:37:ARG:HB2	1:AA:50:MET:HE1	1.93	0.50
1:BS:93:GLU:OE2	1:BU:6:LYS:HD3	2.11	0.50
1:CM:93:GLU:OE2	1:CO:6:LYS:HD3	2.11	0.50
1:DN:64:ASP:OD1	1:DN:64:ASP:N	2.38	0.50
1:BI:42:LYS:HE2	1:BI:47:ASN:HA	1.93	0.50
1:BU:55:ASN:ND2	1:BU:72:ASN:OD1	2.44	0.50
1:CK:41:VAL:HG12	1:CK:43:LYS:HG3	1.93	0.50
1:CU:108:THR:HG21	1:CW:87:ARG:HG3	1.94	0.50
1:DE:55:ASN:ND2	1:DE:72:ASN:OD1	2.43	0.50
1:DG:108:THR:HG21	1:DI:87:ARG:HG3	1.94	0.50
1:ED:73:LEU:HD22	1:GX:98:ALA:HB1	1.94	0.50
1:FM:42:LYS:HE2	1:FM:47:ASN:HA	1.93	0.50
1:AS:41:VAL:HG12	1:AS:43:LYS:HG3	1.93	0.50
1:BY:41:VAL:HG12	1:BY:43:LYS:HG3	1.93	0.50
1:EO:41:VAL:HG12	1:EO:43:LYS:HG3	1.93	0.50
1:GG:42:LYS:HE2	1:GG:47:ASN:HA	1.93	0.50
1:HZ:64:ASP:OD1	1:HZ:64:ASP:N	2.38	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:106:LEU:HD22	1:IC:35:LEU:HD22	1.94	0.50
1:IE:93:GLU:OE2	1:IG:6:LYS:HD3	2.12	0.50
1:IP:54:MET:HG2	1:IP:56:PHE:CE1	2.47	0.50
1:IY:93:GLU:OE2	1:JA:6:LYS:HD3	2.12	0.50
1:AM:37:ARG:HB2	1:AM:50:MET:HE1	1.93	0.50
1:FA:55:ASN:ND2	1:FA:72:ASN:OD1	2.43	0.50
1:FO:93:GLU:OE2	1:FQ:6:LYS:HD3	2.11	0.50
1:HG:106:LEU:HD22	1:HI:35:LEU:HD22	1.94	0.50
1:IO:41:VAL:HG12	1:IO:43:LYS:HG3	1.93	0.50
1:AT:54:MET:HG2	1:AT:56:PHE:CE1	2.46	0.50
1:BJ:54:MET:HG2	1:BJ:56:PHE:CE1	2.46	0.50
1:EP:54:MET:HG2	1:EP:56:PHE:CE1	2.46	0.50
1:HZ:54:MET:HG2	1:HZ:56:PHE:CE1	2.47	0.50
1:JA:109:LYS:HB2	1:JA:111:VAL:HG23	1.93	0.50
1:CT:89:TRP:CD1	1:FN:58:LYS:HD2	2.47	0.50
1:DU:55:ASN:ND2	1:DU:72:ASN:OD1	2.43	0.50
1:FC:37:ARG:HB2	1:FC:50:MET:HE1	1.93	0.50
1:FC:106:LEU:HD22	1:FE:35:LEU:HD22	1.93	0.50
1:GH:53:ASN:OD1	1:GH:74:THR:OG1	2.26	0.50
1:GW:41:VAL:HG12	1:GW:43:LYS:HG3	1.93	0.50
1:HN:54:MET:HG2	1:HN:56:PHE:CE1	2.47	0.50
1:IG:109:LYS:HB2	1:IG:111:VAL:HG23	1.93	0.50
1:DS:73:LEU:HD22	1:DU:98:ALA:HB1	1.94	0.50
1:EQ:37:ARG:HB2	1:EQ:50:MET:HE1	1.93	0.50
1:EY:73:LEU:HD22	1:FA:98:ALA:HB1	1.94	0.50
1:FG:108:THR:HG21	1:FI:87:ARG:HG3	1.94	0.50
1:GW:42:LYS:HE2	1:GW:47:ASN:HA	1.93	0.50
1:HM:42:LYS:HE2	1:HM:47:ASN:HA	1.93	0.50
1:HN:53:ASN:OD1	1:HN:74:THR:OG1	2.26	0.50
1:HY:42:LYS:HE2	1:HY:47:ASN:HA	1.93	0.50
1:HZ:53:ASN:OD1	1:HZ:74:THR:OG1	2.26	0.50
1:CL:58:LYS:HD2	1:FF:89:TRP:CD1	2.47	0.50
1:DA:41:VAL:HG12	1:DA:43:LYS:HG3	1.93	0.50
1:DB:58:LYS:HD2	1:FV:89:TRP:CD1	2.47	0.50
1:EE:73:LEU:HD22	1:EG:98:ALA:HB1	1.94	0.50
1:EG:55:ASN:ND2	1:EG:72:ASN:OD1	2.43	0.50
1:FN:54:MET:HG2	1:FN:56:PHE:CE1	2.46	0.50
1:AP:64:ASP:OD1	1:AP:64:ASP:N	2.38	0.49
1:BZ:58:LYS:HD2	1:ET:89:TRP:CD1	2.47	0.49
1:CL:54:MET:HG2	1:CL:56:PHE:CE1	2.46	0.49
1:GG:41:VAL:HG12	1:GG:43:LYS:HG3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:106:LEU:HD22	1:AO:35:LEU:HD22	1.94	0.49
1:GA:93:GLU:OE2	1:GC:6:LYS:HD3	2.12	0.49
1:AH:64:ASP:OD1	1:AH:64:ASP:N	2.37	0.49
1:BI:41:VAL:HG12	1:BI:43:LYS:HG3	1.93	0.49
1:BO:108:THR:HG21	1:BQ:87:ARG:HG3	1.94	0.49
1:BZ:54:MET:HG2	1:BZ:56:PHE:CE1	2.46	0.49
1:CO:11:TYR:O	1:FJ:37:ARG:NH2	2.40	0.49
1:DC:73:LEU:HD22	1:DE:98:ALA:HB1	1.94	0.49
1:GX:54:MET:HG2	1:GX:56:PHE:CE1	2.47	0.49
1:AA:106:LEU:HD22	1:AC:35:LEU:HD22	1.94	0.49
1:AT:58:LYS:HD2	1:ID:89:TRP:CD1	2.47	0.49
1:AU:108:THR:HG21	1:AW:87:ARG:HG3	1.94	0.49
1:DJ:37:ARG:NH2	1:GC:11:TYR:O	2.38	0.49
1:EA:106:LEU:HD22	1:EC:35:LEU:HD22	1.94	0.49
1:EU:108:THR:HG21	1:EW:87:ARG:HG3	1.93	0.49
1:FF:54:MET:HG2	1:FF:56:PHE:CE1	2.47	0.49
1:FO:18:VAL:HG23	1:FQ:112:ILE:HD12	1.94	0.49
1:AD:64:ASP:OD1	1:AD:64:ASP:N	2.38	0.49
1:AE:18:VAL:HG23	1:AG:112:ILE:HD12	1.95	0.49
1:BC:106:LEU:HD22	1:BE:35:LEU:HD22	1.93	0.49
1:CA:108:THR:HG21	1:CC:87:ARG:HG3	1.93	0.49
1:EP:58:LYS:HD2	1:HJ:89:TRP:CD1	2.47	0.49
1:ET:54:MET:HG2	1:ET:56:PHE:CE1	2.47	0.49
1:FM:41:VAL:HG12	1:FM:43:LYS:HG3	1.93	0.49
1:GH:54:MET:HG2	1:GH:56:PHE:CE1	2.47	0.49
1:AT:98:ALA:HB1	1:ID:73:LEU:HD22	1.95	0.49
1:DW:108:THR:HG21	1:DY:87:ARG:HG3	1.94	0.49
1:EP:98:ALA:HB1	1:HJ:73:LEU:HD22	1.95	0.49
1:GQ:93:GLU:OE2	1:GS:6:LYS:HD3	2.12	0.49
1:GU:37:ARG:HB2	1:GU:50:MET:HE1	1.95	0.49
1:HR:8:VAL:HB	1:HR:20:TYR:HB3	1.95	0.49
1:AP:54:MET:HG2	1:AP:56:PHE:CE1	2.48	0.49
1:CT:54:MET:HG2	1:CT:56:PHE:CE1	2.47	0.49
1:DO:108:THR:HG21	1:DQ:87:ARG:HG3	1.93	0.49
1:AD:54:MET:HG2	1:AD:56:PHE:CE1	2.48	0.49
1:AI:108:THR:HG21	1:AK:87:ARG:HG3	1.93	0.49
1:CE:108:THR:HG21	1:CG:87:ARG:HG3	1.94	0.49
1:CI:108:THR:HG21	1:CK:87:ARG:HG3	1.95	0.49
1:FV:54:MET:HG2	1:FV:56:PHE:CE1	2.47	0.49
1:GS:109:LYS:HB2	1:GS:111:VAL:HG23	1.93	0.49
1:IC:34:SER:HB2	1:IC:55:ASN:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IS:34:SER:HB2	1:IS:55:ASN:HB3	1.95	0.49
1:JF:8:VAL:HB	1:JF:20:TYR:HB3	1.95	0.49
1:AE:93:GLU:OE2	1:AG:6:LYS:HD3	2.11	0.49
1:BS:73:LEU:HD22	1:BU:98:ALA:HB1	1.94	0.49
1:EI:108:THR:HG21	1:EK:87:ARG:HG3	1.93	0.49
1:IQ:106:LEU:HD22	1:IS:35:LEU:HD22	1.94	0.49
1:BF:73:LEU:HD22	1:IP:98:ALA:HB1	1.93	0.49
1:BW:108:THR:HG21	1:BY:87:ARG:HG3	1.95	0.49
1:DN:73:LEU:HD22	1:GH:98:ALA:HB1	1.93	0.49
1:FK:108:THR:HG21	1:FM:87:ARG:HG3	1.95	0.49
1:FW:108:THR:HG21	1:FY:87:ARG:HG3	1.94	0.49
1:GT:26:ASP:OD2	1:GT:28:THR:N	2.43	0.49
1:BF:54:MET:HG2	1:BF:56:PHE:CE1	2.48	0.48
1:BG:108:THR:HG21	1:BI:87:ARG:HG3	1.95	0.48
1:BJ:58:LYS:HD2	1:IT:89:TRP:CD1	2.47	0.48
1:CM:73:LEU:HD22	1:CO:98:ALA:HB1	1.94	0.48
1:DN:54:MET:HG2	1:DN:56:PHE:CE1	2.48	0.48
1:HG:94:VAL:HG11	1:HI:71:VAL:HG11	1.95	0.48
1:ED:54:MET:HG2	1:ED:56:PHE:CE1	2.48	0.48
1:FN:64:ASP:OD1	1:FN:64:ASP:N	2.38	0.48
1:FR:64:ASP:OD1	1:FR:64:ASP:N	2.37	0.48
1:IQ:94:VAL:HG11	1:IS:71:VAL:HG11	1.95	0.48
1:JB:26:ASP:OD2	1:JB:28:THR:N	2.43	0.48
1:AE:73:LEU:HD22	1:AG:98:ALA:HB1	1.94	0.48
1:DK:106:LEU:HD22	1:DM:35:LEU:HD22	1.94	0.48
1:IA:94:VAL:HG11	1:IC:71:VAL:HG11	1.95	0.48
1:IE:73:LEU:HD22	1:IG:98:ALA:HB1	1.94	0.48
1:JF:64:ASP:OD1	1:JF:64:ASP:N	2.38	0.48
1:AI:73:LEU:HD22	1:AK:98:ALA:HB1	1.96	0.48
1:CA:73:LEU:HD13	1:CC:73:LEU:HD13	1.96	0.48
1:EQ:106:LEU:HD22	1:ES:35:LEU:HD22	1.95	0.48
1:IH:26:ASP:OD2	1:IH:28:THR:N	2.43	0.48
1:IW:34:SER:HB2	1:IW:55:ASN:HB3	1.95	0.48
1:EU:73:LEU:HD13	1:EW:73:LEU:HD13	1.96	0.48
1:HW:54:MET:HE2	1:HW:56:PHE:CZ	2.48	0.48
1:IK:34:SER:HB2	1:IK:55:ASN:HB3	1.95	0.48
1:IY:73:LEU:HD22	1:JA:98:ALA:HB1	1.94	0.48
1:AQ:73:LEU:HD22	1:AS:98:ALA:HB1	1.96	0.48
1:BZ:98:ALA:HB1	1:ET:73:LEU:HD22	1.96	0.48
1:DK:73:LEU:HD22	1:DM:98:ALA:HB1	1.96	0.48
1:DO:73:LEU:HD22	1:DQ:98:ALA:HB1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EI:73:LEU:HD22	1:EK:98:ALA:HB1	1.95	0.48
1:GE:37:ARG:HB2	1:GE:50:MET:HE1	1.95	0.48
1:BJ:98:ALA:HB1	1:IT:73:LEU:HD22	1.95	0.48
1:CL:98:ALA:HB1	1:FF:73:LEU:HD22	1.96	0.48
1:DC:18:VAL:HG23	1:DE:112:ILE:HD12	1.94	0.48
1:EE:18:VAL:HG23	1:EG:112:ILE:HD12	1.95	0.48
1:EM:73:LEU:HD22	1:EO:98:ALA:HB1	1.96	0.48
1:GI:13:ASN:C	1:GI:13:ASN:ND2	2.72	0.48
1:GT:38:SER:HB3	1:GT:51:ARG:HG3	1.96	0.48
1:AA:73:LEU:HD22	1:AC:98:ALA:HB1	1.96	0.48
1:AI:73:LEU:HD13	1:AK:73:LEU:HD13	1.95	0.48
1:DS:18:VAL:HG23	1:DU:112:ILE:HD12	1.95	0.48
1:FO:73:LEU:HD22	1:FQ:98:ALA:HB1	1.94	0.48
1:GA:37:ARG:HB2	1:GA:50:MET:HE1	1.96	0.48
1:GQ:73:LEU:HD22	1:GS:98:ALA:HB1	1.94	0.48
1:HC:13:ASN:C	1:HC:13:ASN:ND2	2.72	0.48
1:II:73:LEU:HD22	1:IK:98:ALA:HB1	1.96	0.48
1:IY:18:VAL:HG23	1:JA:112:ILE:HD12	1.96	0.48
1:AL:115:SER:HA	1:AL:116:ASP:HA	1.68	0.48
1:AX:64:ASP:OD1	1:AX:64:ASP:N	2.38	0.48
1:BR:64:ASP:OD1	1:BR:64:ASP:N	2.38	0.48
1:BS:18:VAL:HG23	1:BU:112:ILE:HD12	1.94	0.48
1:CY:108:THR:HG21	1:DA:87:ARG:HG3	1.95	0.48
1:FS:106:LEU:HD22	1:FU:35:LEU:HD22	1.95	0.48
1:GP:8:VAL:HB	1:GP:20:TYR:HB3	1.95	0.48
1:IE:18:VAL:HG23	1:IG:112:ILE:HD12	1.96	0.48
1:IM:73:LEU:HD22	1:IO:98:ALA:HB1	1.95	0.48
1:IU:73:LEU:HD22	1:IW:98:ALA:HB1	1.96	0.48
1:AM:73:LEU:HD22	1:AO:98:ALA:HB1	1.96	0.48
1:EY:18:VAL:HG23	1:FA:112:ILE:HD12	1.95	0.48
1:FS:73:LEU:HD22	1:FU:98:ALA:HB1	1.96	0.48
1:FZ:8:VAL:HB	1:FZ:20:TYR:HB3	1.95	0.48
1:GE:73:LEU:HD22	1:GG:98:ALA:HB1	1.96	0.48
1:HB:8:VAL:HB	1:HB:20:TYR:HB3	1.95	0.48
1:HW:73:LEU:HD22	1:HY:98:ALA:HB1	1.95	0.48
1:AY:73:LEU:HD22	1:BA:98:ALA:HB1	1.95	0.47
1:BC:73:LEU:HD22	1:BE:98:ALA:HB1	1.96	0.47
1:BK:73:LEU:HD22	1:BM:98:ALA:HB1	1.95	0.47
1:BR:37:ARG:NH2	1:JA:11:TYR:O	2.38	0.47
1:CM:18:VAL:HG23	1:CO:112:ILE:HD12	1.95	0.47
1:GA:18:VAL:HG23	1:GC:112:ILE:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:73:LEU:HD22	1:GC:98:ALA:HB1	1.94	0.47
1:GI:73:LEU:HD22	1:GK:98:ALA:HB1	1.96	0.47
1:HS:73:LEU:HD22	1:HU:98:ALA:HB1	1.96	0.47
1:AX:37:ARG:NH2	1:IG:11:TYR:O	2.38	0.47
1:CE:73:LEU:HD13	1:CG:73:LEU:HD13	1.96	0.47
1:CI:73:LEU:HD22	1:CK:98:ALA:HB1	1.96	0.47
1:CQ:73:LEU:HD22	1:CS:98:ALA:HB1	1.97	0.47
1:EM:108:THR:HG21	1:EO:87:ARG:HG3	1.95	0.47
1:GQ:18:VAL:HG23	1:GS:112:ILE:HD12	1.96	0.47
1:GS:34:SER:HB2	1:GS:55:ASN:HB3	1.95	0.47
1:HC:73:LEU:HD22	1:HE:98:ALA:HB1	1.96	0.47
1:HW:37:ARG:HB2	1:HW:50:MET:HE1	1.95	0.47
1:IL:64:ASP:OD1	1:IL:64:ASP:N	2.39	0.47
1:IM:37:ARG:HB2	1:IM:50:MET:HE1	1.95	0.47
1:AQ:108:THR:HG21	1:AS:87:ARG:HG3	1.95	0.47
1:BW:73:LEU:HD22	1:BY:98:ALA:HB1	1.97	0.47
1:CH:37:ARG:NH2	1:FA:11:TYR:O	2.40	0.47
1:DB:98:ALA:HB1	1:FV:73:LEU:HD22	1.96	0.47
1:HK:37:ARG:HB2	1:HK:50:MET:HE1	1.95	0.47
1:AQ:18:VAL:HG23	1:AS:112:ILE:HD12	1.97	0.47
1:AU:73:LEU:HD13	1:AW:73:LEU:HD13	1.96	0.47
1:CY:73:LEU:HD22	1:DA:98:ALA:HB1	1.96	0.47
1:BG:18:VAL:HG23	1:BI:112:ILE:HD12	1.97	0.47
1:BO:73:LEU:HD13	1:BQ:73:LEU:HD13	1.96	0.47
1:EM:18:VAL:HG23	1:EO:112:ILE:HD12	1.97	0.47
1:EU:73:LEU:HD22	1:EW:98:ALA:HB1	1.95	0.47
1:HB:115:SER:HA	1:HB:116:ASP:HA	1.71	0.47
1:IM:54:MET:HE2	1:IM:56:PHE:CZ	2.48	0.47
1:AH:98:ALA:HB1	1:HR:73:LEU:HD12	1.97	0.47
1:CA:73:LEU:HD22	1:CC:98:ALA:HB1	1.95	0.47
1:IH:38:SER:HB3	1:IH:51:ARG:HG3	1.96	0.47
1:IT:8:VAL:HB	1:IT:20:TYR:HB3	1.97	0.47
1:IX:64:ASP:OD1	1:IX:64:ASP:N	2.39	0.47
1:JB:38:SER:HB3	1:JB:51:ARG:HG3	1.96	0.47
1:BJ:115:SER:HA	1:BJ:116:ASP:HA	1.71	0.47
1:CL:37:ARG:NH2	1:FE:11:TYR:O	2.41	0.47
1:DB:64:ASP:OD1	1:DB:64:ASP:N	2.38	0.47
1:EH:98:ALA:HB1	1:HB:73:LEU:HD12	1.96	0.47
1:FG:73:LEU:HD22	1:FI:98:ALA:HB1	1.97	0.47
1:FK:73:LEU:HD22	1:FM:98:ALA:HB1	1.96	0.47
1:GD:38:SER:HB3	1:GD:51:ARG:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GI:73:LEU:HD13	1:GK:73:LEU:HD13	1.97	0.47
1:GP:115:SER:HA	1:GP:116:ASP:HA	1.71	0.47
1:HC:73:LEU:HD13	1:HE:73:LEU:HD13	1.97	0.47
1:HK:73:LEU:HD22	1:HM:98:ALA:HB1	1.96	0.47
1:HS:13:ASN:C	1:HS:13:ASN:ND2	2.73	0.47
1:HV:115:SER:HA	1:HV:116:ASP:HA	1.66	0.47
1:ID:8:VAL:HB	1:ID:20:TYR:HB3	1.97	0.47
1:II:13:ASN:C	1:II:13:ASN:ND2	2.72	0.47
1:CH:115:SER:HA	1:CH:116:ASP:HA	1.71	0.47
1:DF:64:ASP:OD1	1:DF:64:ASP:N	2.37	0.47
1:DS:37:ARG:HB2	1:DS:50:MET:HE1	1.97	0.47
1:DZ:37:ARG:NH2	1:GS:11:TYR:O	2.38	0.47
1:EE:37:ARG:HB2	1:EE:50:MET:HE1	1.97	0.47
1:HG:73:LEU:HD22	1:HI:98:ALA:HB1	1.97	0.47
1:HJ:8:VAL:HB	1:HJ:20:TYR:HB3	1.97	0.47
1:HS:73:LEU:HD13	1:HU:73:LEU:HD13	1.97	0.47
1:IA:73:LEU:HD22	1:IC:98:ALA:HB1	1.97	0.47
1:AM:108:THR:HG21	1:AO:87:ARG:HG3	1.97	0.47
1:BA:55:ASN:OD1	1:BA:72:ASN:ND2	2.41	0.47
1:BF:115:SER:HA	1:BF:116:ASP:HA	1.72	0.47
1:GE:54:MET:HE2	1:GE:56:PHE:CZ	2.50	0.47
1:IY:37:ARG:HB2	1:IY:50:MET:HE1	1.96	0.47
1:AA:108:THR:HG21	1:AC:87:ARG:HG3	1.97	0.47
1:AE:37:ARG:HB2	1:AE:50:MET:HE1	1.97	0.47
1:AE:73:LEU:HD13	1:AG:73:LEU:HD13	1.97	0.47
1:DG:73:LEU:HD13	1:DI:73:LEU:HD13	1.96	0.47
1:DW:73:LEU:HD22	1:DY:98:ALA:HB1	1.97	0.47
1:EA:73:LEU:HD13	1:EC:73:LEU:HD13	1.97	0.47
1:EA:108:THR:HG21	1:EC:87:ARG:HG3	1.97	0.47
1:EQ:108:THR:HG21	1:ES:87:ARG:HG3	1.97	0.47
1:FG:73:LEU:HD13	1:FI:73:LEU:HD13	1.96	0.47
1:FO:73:LEU:HD13	1:FQ:73:LEU:HD13	1.97	0.47
1:FW:73:LEU:HD13	1:FY:73:LEU:HD13	1.97	0.47
1:GU:73:LEU:HD22	1:GW:98:ALA:HB1	1.96	0.47
1:ID:115:SER:HA	1:ID:116:ASP:HA	1.72	0.47
1:AY:73:LEU:HD13	1:BA:73:LEU:HD13	1.96	0.46
1:BK:73:LEU:HD13	1:BM:73:LEU:HD13	1.96	0.46
1:BV:115:SER:HA	1:BV:116:ASP:HA	1.72	0.46
1:CP:115:SER:HA	1:CP:116:ASP:HA	1.72	0.46
1:CQ:106:LEU:HD22	1:CS:35:LEU:HD22	1.95	0.46
1:CU:73:LEU:HD13	1:CW:73:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:115:SER:HA	1:DB:116:ASP:HA	1.71	0.46
1:FC:108:THR:HG21	1:FE:87:ARG:HG3	1.97	0.46
1:GQ:37:ARG:HB2	1:GQ:50:MET:HE1	1.96	0.46
1:GY:73:LEU:HD13	1:HA:73:LEU:HD13	1.97	0.46
1:IE:37:ARG:HB2	1:IE:50:MET:HE1	1.96	0.46
1:IP:115:SER:HA	1:IP:116:ASP:HA	1.71	0.46
1:IU:13:ASN:C	1:IU:13:ASN:ND2	2.73	0.46
1:IU:73:LEU:HD13	1:IW:73:LEU:HD13	1.96	0.46
1:CQ:73:LEU:HD13	1:CS:73:LEU:HD13	1.97	0.46
1:DV:98:ALA:HB1	1:GP:73:LEU:HD12	1.97	0.46
1:FB:64:ASP:OD1	1:FB:64:ASP:N	2.37	0.46
1:FO:37:ARG:HB2	1:FO:50:MET:HE1	1.97	0.46
1:GM:73:LEU:HD13	1:GO:73:LEU:HD13	1.97	0.46
1:HO:73:LEU:HD22	1:HQ:98:ALA:HB1	1.97	0.46
1:II:73:LEU:HD13	1:IK:73:LEU:HD13	1.96	0.46
1:BE:42:LYS:HE2	1:BE:47:ASN:HA	1.97	0.46
1:BS:37:ARG:HB2	1:BS:50:MET:HE1	1.97	0.46
1:BS:73:LEU:HD13	1:BU:73:LEU:HD13	1.97	0.46
1:CM:37:ARG:HB2	1:CM:50:MET:HE1	1.97	0.46
1:CM:73:LEU:HD13	1:CO:73:LEU:HD13	1.97	0.46
1:DO:73:LEU:HD13	1:DQ:73:LEU:HD13	1.96	0.46
1:EA:73:LEU:HD22	1:EC:98:ALA:HB1	1.97	0.46
1:EI:73:LEU:HD13	1:EK:73:LEU:HD13	1.96	0.46
1:EQ:73:LEU:HD13	1:ES:73:LEU:HD13	1.97	0.46
1:FK:18:VAL:HG23	1:FM:112:ILE:HD12	1.97	0.46
1:FO:108:THR:HG21	1:FQ:87:ARG:HG3	1.98	0.46
1:FZ:115:SER:HA	1:FZ:116:ASP:HA	1.71	0.46
1:EA:94:VAL:HG11	1:EC:71:VAL:HG11	1.98	0.46
1:FC:73:LEU:HD13	1:FE:73:LEU:HD13	1.97	0.46
1:FU:42:LYS:HE2	1:FU:47:ASN:HA	1.97	0.46
1:GT:115:SER:HA	1:GT:116:ASP:HA	1.72	0.46
1:JC:73:LEU:HD22	1:JE:98:ALA:HB1	1.97	0.46
1:BC:94:VAL:HG11	1:BE:71:VAL:HG11	1.98	0.46
1:DG:73:LEU:HD22	1:DI:98:ALA:HB1	1.97	0.46
1:DW:73:LEU:HD13	1:DY:73:LEU:HD13	1.96	0.46
1:FS:94:VAL:HG11	1:FU:71:VAL:HG11	1.98	0.46
1:ID:59:SER:HB3	1:ID:66:LYS:HE2	1.97	0.46
1:BW:18:VAL:HG23	1:BY:112:ILE:HD12	1.97	0.46
1:CQ:108:THR:HG21	1:CS:87:ARG:HG3	1.97	0.46
1:CY:18:VAL:HG23	1:DA:112:ILE:HD12	1.97	0.46
1:FC:73:LEU:HD22	1:FE:98:ALA:HB1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FV:115:SER:HA	1:FV:116:ASP:HA	1.72	0.46
1:IT:59:SER:HB3	1:IT:66:LYS:HE2	1.97	0.46
1:BG:73:LEU:HD13	1:BI:73:LEU:HD13	1.98	0.46
1:BG:73:LEU:HD22	1:BI:98:ALA:HB1	1.97	0.46
1:BV:98:ALA:HB1	1:JF:73:LEU:HD12	1.97	0.46
1:CE:73:LEU:HD22	1:CG:98:ALA:HB1	1.97	0.46
1:DK:94:VAL:HG11	1:DM:71:VAL:HG11	1.98	0.46
1:DK:108:THR:HG21	1:DM:87:ARG:HG3	1.97	0.46
1:DN:115:SER:HA	1:DN:116:ASP:HA	1.72	0.46
1:EC:42:LYS:HE2	1:EC:47:ASN:HA	1.98	0.46
1:EM:73:LEU:HD13	1:EO:73:LEU:HD13	1.98	0.46
1:ES:42:LYS:HE2	1:ES:47:ASN:HA	1.97	0.46
1:GA:73:LEU:HD13	1:GC:73:LEU:HD13	1.98	0.46
1:HJ:59:SER:HB3	1:HJ:66:LYS:HE2	1.97	0.46
1:HJ:115:SER:HA	1:HJ:116:ASP:HA	1.72	0.46
1:AQ:73:LEU:HD13	1:AS:73:LEU:HD13	1.98	0.46
1:BF:42:LYS:NZ	1:BF:44:GLY:O	2.36	0.46
1:BR:42:LYS:HD3	1:BR:47:ASN:HA	1.98	0.46
1:CT:73:LEU:HD22	1:FN:98:ALA:HB1	1.96	0.46
1:CU:73:LEU:HD22	1:CW:98:ALA:HB1	1.97	0.46
1:DF:98:ALA:HB1	1:FZ:73:LEU:HD12	1.97	0.46
1:DZ:42:LYS:HD3	1:DZ:47:ASN:HA	1.98	0.46
1:EQ:73:LEU:HD22	1:ES:98:ALA:HB1	1.97	0.46
1:IE:73:LEU:HD13	1:IG:73:LEU:HD13	1.98	0.46
1:IQ:73:LEU:HD22	1:IS:98:ALA:HB1	1.97	0.46
1:IY:73:LEU:HD13	1:JA:73:LEU:HD13	1.98	0.46
1:AX:42:LYS:HD3	1:AX:47:ASN:HA	1.98	0.46
1:BB:115:SER:HA	1:BB:116:ASP:HA	1.68	0.46
1:CI:18:VAL:HG23	1:CK:112:ILE:HD12	1.97	0.46
1:FE:42:LYS:HE2	1:FE:47:ASN:HA	1.97	0.46
1:GK:50:MET:HE2	1:GK:50:MET:HB2	1.91	0.46
1:HK:54:MET:HE2	1:HK:56:PHE:CZ	2.51	0.46
1:BO:73:LEU:HD22	1:BQ:98:ALA:HB1	1.97	0.46
1:CP:26:ASP:OD2	1:CP:28:THR:N	2.48	0.46
1:DC:73:LEU:HD13	1:DE:73:LEU:HD13	1.97	0.46
1:DS:108:THR:HG21	1:DU:87:ARG:HG3	1.98	0.46
1:GM:73:LEU:HD22	1:GO:98:ALA:HB1	1.97	0.46
1:HG:73:LEU:HD13	1:HI:73:LEU:HD13	1.98	0.46
1:AH:115:SER:HA	1:AH:116:ASP:HA	1.72	0.45
1:AU:73:LEU:HD22	1:AW:98:ALA:HB1	1.97	0.45
1:CQ:94:VAL:HG11	1:CS:71:VAL:HG11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DS:73:LEU:HD13	1:DU:73:LEU:HD13	1.97	0.45
1:FV:42:LYS:NZ	1:FV:44:GLY:O	2.36	0.45
1:GQ:73:LEU:HD13	1:GS:73:LEU:HD13	1.98	0.45
1:GY:73:LEU:HD22	1:HA:98:ALA:HB1	1.97	0.45
1:CH:64:ASP:OD1	1:CH:64:ASP:N	2.38	0.45
1:CX:37:ARG:NH2	1:FQ:11:TYR:O	2.40	0.45
1:EA:18:VAL:HG23	1:EC:112:ILE:HD12	1.98	0.45
1:EE:108:THR:HG21	1:EG:87:ARG:HG3	1.98	0.45
1:EP:37:ARG:NH2	1:HI:11:TYR:O	2.39	0.45
1:GX:115:SER:HA	1:GX:116:ASP:HA	1.71	0.45
1:HE:50:MET:HE2	1:HE:50:MET:HB2	1.91	0.45
1:HO:73:LEU:HD13	1:HQ:73:LEU:HD13	1.97	0.45
1:CH:8:VAL:HB	1:CH:20:TYR:HB3	1.99	0.45
1:CQ:18:VAL:HG23	1:CS:112:ILE:HD12	1.98	0.45
1:EE:73:LEU:HD13	1:EG:73:LEU:HD13	1.97	0.45
1:AE:108:THR:HG21	1:AG:87:ARG:HG3	1.98	0.45
1:AM:73:LEU:HD13	1:AO:73:LEU:HD13	1.97	0.45
1:AO:42:LYS:HE2	1:AO:47:ASN:HA	1.98	0.45
1:FJ:42:LYS:HD3	1:FJ:47:ASN:HA	1.98	0.45
1:FS:18:VAL:HG23	1:FU:112:ILE:HD12	1.98	0.45
1:GL:59:SER:HB3	1:GL:66:LYS:HD3	1.98	0.45
1:GX:38:SER:HB3	1:GX:51:ARG:HG3	1.99	0.45
1:HJ:38:SER:HB3	1:HJ:51:ARG:HB2	1.98	0.45
1:HN:38:SER:HB3	1:HN:51:ARG:HG3	1.99	0.45
1:IA:73:LEU:HD13	1:IC:73:LEU:HD13	1.98	0.45
1:IL:59:SER:HB3	1:IL:66:LYS:HD3	1.98	0.45
1:IS:42:LYS:HE2	1:IS:47:ASN:HA	1.99	0.45
1:AA:94:VAL:HG11	1:AC:71:VAL:HG11	1.98	0.45
1:AC:42:LYS:HE2	1:AC:47:ASN:HA	1.97	0.45
1:AM:94:VAL:HG11	1:AO:71:VAL:HG11	1.98	0.45
1:BS:108:THR:HG21	1:BU:87:ARG:HG3	1.98	0.45
1:CD:115:SER:HA	1:CD:116:ASP:HA	1.67	0.45
1:CH:42:LYS:HD3	1:CH:47:ASN:HA	1.98	0.45
1:CM:108:THR:HG21	1:CO:87:ARG:HG3	1.98	0.45
1:EY:73:LEU:HD13	1:FA:73:LEU:HD13	1.97	0.45
1:FJ:8:VAL:HB	1:FJ:20:TYR:HB3	1.99	0.45
1:FR:26:ASP:OD1	1:FR:28:THR:N	2.49	0.45
1:GU:73:LEU:HD13	1:GW:73:LEU:HD13	1.99	0.45
1:HU:50:MET:HE2	1:HU:50:MET:HB2	1.90	0.45
1:HZ:38:SER:HB3	1:HZ:51:ARG:HG3	1.99	0.45
1:IQ:73:LEU:HD13	1:IS:73:LEU:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IT:38:SER:HB3	1:IT:51:ARG:HB2	1.99	0.45
1:AM:18:VAL:HG23	1:AO:112:ILE:HD12	1.98	0.45
1:AT:37:ARG:NH2	1:IC:11:TYR:O	2.40	0.45
1:DC:37:ARG:HB2	1:DC:50:MET:HE1	1.97	0.45
1:ED:37:ARG:NH2	1:GW:11:TYR:O	2.39	0.45
1:FS:73:LEU:HD13	1:FU:73:LEU:HD13	1.98	0.45
1:GH:38:SER:HB3	1:GH:51:ARG:HG3	1.99	0.45
1:GU:54:MET:HE2	1:GU:56:PHE:CZ	2.51	0.45
1:HF:59:SER:HB3	1:HF:66:LYS:HD3	1.99	0.45
1:HI:34:SER:HB2	1:HI:55:ASN:HB3	1.97	0.45
1:JC:73:LEU:HD13	1:JE:73:LEU:HD13	1.97	0.45
1:AH:38:SER:HB3	1:AH:51:ARG:HG3	1.99	0.45
1:BC:73:LEU:HD13	1:BE:73:LEU:HD13	1.98	0.45
1:BN:115:SER:HA	1:BN:116:ASP:HA	1.68	0.45
1:BW:73:LEU:HD13	1:BY:73:LEU:HD13	1.98	0.45
1:EY:37:ARG:HB2	1:EY:50:MET:HE1	1.97	0.45
1:HV:42:LYS:HB2	1:HV:42:LYS:HE2	1.72	0.45
1:IL:42:LYS:HB2	1:IL:42:LYS:HE2	1.72	0.45
1:IX:59:SER:HB3	1:IX:66:LYS:HD3	1.99	0.45
1:AA:18:VAL:HG23	1:AC:112:ILE:HD12	1.98	0.45
1:AL:42:LYS:HB2	1:AL:42:LYS:HE2	1.72	0.45
1:AL:54:MET:HE3	1:AL:54:MET:HB2	1.84	0.45
1:BC:18:VAL:HG23	1:BE:112:ILE:HD12	1.98	0.45
1:BV:38:SER:HB3	1:BV:51:ARG:HG3	1.99	0.45
1:CT:115:SER:HA	1:CT:116:ASP:HA	1.72	0.45
1:DC:115:SER:HA	1:DC:116:ASP:HA	1.80	0.45
1:DJ:8:VAL:HB	1:DJ:20:TYR:HB3	1.99	0.45
1:DK:18:VAL:HG23	1:DM:112:ILE:HD12	1.98	0.45
1:EQ:18:VAL:HG23	1:ES:112:ILE:HD12	1.98	0.45
1:FC:94:VAL:HG11	1:FE:71:VAL:HG11	1.98	0.45
1:FW:73:LEU:HD22	1:FY:98:ALA:HB1	1.98	0.45
1:CP:38:SER:HB3	1:CP:51:ARG:HG3	1.99	0.45
1:CS:42:LYS:HE2	1:CS:47:ASN:HA	1.97	0.45
1:CX:8:VAL:HB	1:CX:20:TYR:HB3	1.99	0.45
1:CX:42:LYS:HD3	1:CX:47:ASN:HA	1.98	0.45
1:FS:108:THR:HG21	1:FU:87:ARG:HG3	1.97	0.45
1:ID:38:SER:HB3	1:ID:51:ARG:HB2	1.99	0.45
1:IL:54:MET:HE3	1:IL:54:MET:HB2	1.78	0.45
1:AT:115:SER:HA	1:AT:116:ASP:HA	1.71	0.45
1:BC:108:THR:HG21	1:BE:87:ARG:HG3	1.97	0.45
1:DJ:42:LYS:HD3	1:DJ:47:ASN:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DN:37:ARG:NH2	1:GG:11:TYR:O	2.39	0.45
1:EX:115:SER:HA	1:EX:116:ASP:HA	1.67	0.45
1:GE:42:LYS:HE3	1:GE:79:VAL:HG11	1.99	0.45
1:GU:18:VAL:HG23	1:GW:112:ILE:HD12	1.99	0.45
1:CI:73:LEU:HD13	1:CK:73:LEU:HD13	1.99	0.44
1:EA:55:ASN:OD1	1:EA:72:ASN:OD1	2.35	0.44
1:HS:35:LEU:HD21	1:HS:54:MET:HE3	1.99	0.44
1:CX:115:SER:HA	1:CX:116:ASP:HA	1.71	0.44
1:DM:42:LYS:HE2	1:DM:47:ASN:HA	1.97	0.44
1:DZ:8:VAL:HB	1:DZ:20:TYR:HB3	1.99	0.44
1:EQ:94:VAL:HG11	1:ES:71:VAL:HG11	1.98	0.44
1:EY:108:THR:HG21	1:FA:87:ARG:HG3	1.98	0.44
1:FC:18:VAL:HG23	1:FE:112:ILE:HD12	1.98	0.44
1:FK:73:LEU:HD13	1:FM:73:LEU:HD13	1.98	0.44
1:GD:26:ASP:OD2	1:GD:28:THR:N	2.43	0.44
1:HI:42:LYS:HE2	1:HI:47:ASN:HA	1.99	0.44
1:BJ:37:ARG:NH2	1:IS:11:TYR:O	2.40	0.44
1:DK:73:LEU:HD13	1:DM:73:LEU:HD13	1.99	0.44
1:DV:115:SER:HA	1:DV:116:ASP:HA	1.72	0.44
1:EH:115:SER:HA	1:EH:116:ASP:HA	1.72	0.44
1:GE:18:VAL:HG23	1:GG:112:ILE:HD12	1.99	0.44
1:GL:26:ASP:OD1	1:GL:28:THR:N	2.49	0.44
1:HV:59:SER:HB3	1:HV:66:LYS:HD3	1.99	0.44
1:IC:42:LYS:HE2	1:IC:47:ASN:HA	1.99	0.44
1:IM:42:LYS:HE3	1:IM:79:VAL:HG11	1.99	0.44
1:AK:50:MET:HE2	1:AK:50:MET:HB2	1.89	0.44
1:BY:11:TYR:O	1:ET:37:ARG:NH2	2.42	0.44
1:CK:11:TYR:O	1:FF:37:ARG:NH2	2.42	0.44
1:DC:108:THR:HG21	1:DE:87:ARG:HG3	1.98	0.44
1:EP:115:SER:HA	1:EP:116:ASP:HA	1.71	0.44
1:EY:115:SER:HA	1:EY:116:ASP:HA	1.80	0.44
1:GL:115:SER:HA	1:GL:116:ASP:HA	1.66	0.44
1:HY:43:LYS:HB2	1:HY:43:LYS:HE2	1.90	0.44
1:IT:26:ASP:OD2	1:IT:28:THR:N	2.50	0.44
1:IX:42:LYS:HB2	1:IX:42:LYS:HE2	1.72	0.44
1:BR:8:VAL:HB	1:BR:20:TYR:HB3	1.99	0.44
1:BV:26:ASP:OD1	1:BV:28:THR:N	2.49	0.44
1:DU:115:SER:HA	1:DU:116:ASP:HA	1.83	0.44
1:GU:94:VAL:HG11	1:GW:71:VAL:HG11	2.00	0.44
1:HF:26:ASP:OD1	1:HF:28:THR:N	2.49	0.44
1:HK:18:VAL:HG23	1:HM:112:ILE:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:8:VAL:HB	1:AX:20:TYR:HB3	1.99	0.44
1:CY:73:LEU:HD13	1:DA:73:LEU:HD13	1.99	0.44
1:DF:37:ARG:NH2	1:FY:11:TYR:O	2.45	0.44
1:DF:38:SER:HB3	1:DF:51:ARG:HG3	1.99	0.44
1:DJ:115:SER:HA	1:DJ:116:ASP:HA	1.72	0.44
1:DQ:50:MET:HE2	1:DQ:50:MET:HB2	1.89	0.44
1:GH:8:VAL:HB	1:GH:20:TYR:HB3	2.00	0.44
1:GU:42:LYS:HE3	1:GU:79:VAL:HG11	2.00	0.44
1:HK:73:LEU:HD13	1:HM:73:LEU:HD13	1.98	0.44
1:HW:18:VAL:HG23	1:HY:112:ILE:HD12	1.99	0.44
1:IX:54:MET:HE3	1:IX:54:MET:HB2	1.78	0.44
1:FB:38:SER:HB3	1:FB:51:ARG:HG3	1.99	0.44
1:GI:115:SER:HA	1:GI:116:ASP:HA	1.85	0.44
1:HN:8:VAL:HB	1:HN:20:TYR:HB3	2.00	0.44
1:IP:38:SER:HB3	1:IP:51:ARG:HG3	1.99	0.44
1:JB:115:SER:HA	1:JB:116:ASP:HA	1.72	0.44
1:FQ:115:SER:HA	1:FQ:116:ASP:HA	1.83	0.44
1:HM:43:LYS:HB2	1:HM:43:LYS:HE2	1.90	0.44
1:HW:73:LEU:HD13	1:HY:73:LEU:HD13	1.99	0.44
1:IH:115:SER:HA	1:IH:116:ASP:HA	1.72	0.44
1:AK:115:SER:HA	1:AK:116:ASP:HA	1.82	0.44
1:DA:43:LYS:HB2	1:DA:43:LYS:HE2	1.90	0.44
1:HC:115:SER:HA	1:HC:116:ASP:HA	1.85	0.44
1:HF:115:SER:HA	1:HF:116:ASP:HA	1.67	0.44
1:HZ:8:VAL:HB	1:HZ:20:TYR:HB3	2.00	0.44
1:II:35:LEU:HD21	1:II:54:MET:HE3	1.99	0.44
1:IU:35:LEU:HD21	1:IU:54:MET:HE3	1.99	0.44
1:AA:73:LEU:HD13	1:AC:73:LEU:HD13	1.99	0.43
1:AP:54:MET:HE2	1:AP:54:MET:HB2	1.81	0.43
1:DA:34:SER:HB2	1:DA:55:ASN:HB3	2.00	0.43
1:GW:54:MET:HE2	1:GW:56:PHE:CZ	2.53	0.43
1:HC:35:LEU:HD21	1:HC:54:MET:HE3	1.99	0.43
1:IW:115:SER:HA	1:IW:116:ASP:HA	1.82	0.43
1:DC:54:MET:HE2	1:DC:54:MET:HB2	1.89	0.43
1:DV:38:SER:HB3	1:DV:51:ARG:HG3	1.99	0.43
1:EK:50:MET:HE2	1:EK:50:MET:HB2	1.89	0.43
1:GE:73:LEU:HD13	1:GG:73:LEU:HD13	1.99	0.43
1:GI:35:LEU:HD21	1:GI:54:MET:HE3	1.99	0.43
1:GW:115:SER:HA	1:GW:116:ASP:HA	1.85	0.43
1:HK:8:VAL:HB	1:HK:20:TYR:HB3	2.00	0.43
1:HN:115:SER:HA	1:HN:116:ASP:HA	1.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IM:18:VAL:HG23	1:IO:112:ILE:HD12	1.99	0.43
1:IM:73:LEU:HD13	1:IO:73:LEU:HD13	1.99	0.43
1:IP:90:MET:HA	1:IP:94:VAL:HB	2.00	0.43
1:AO:11:TYR:O	1:HZ:37:ARG:NH2	2.40	0.43
1:DO:115:SER:HA	1:DO:116:ASP:HA	1.85	0.43
1:ED:115:SER:HA	1:ED:116:ASP:HA	1.72	0.43
1:EH:38:SER:HB3	1:EH:51:ARG:HG3	1.99	0.43
1:EI:115:SER:HA	1:EI:116:ASP:HA	1.85	0.43
1:HK:42:LYS:HE3	1:HK:79:VAL:HG11	1.99	0.43
1:HN:90:MET:HA	1:HN:94:VAL:HB	2.00	0.43
1:HW:8:VAL:HB	1:HW:20:TYR:HB3	2.00	0.43
1:HZ:90:MET:HA	1:HZ:94:VAL:HB	2.00	0.43
1:IO:43:LYS:HB2	1:IO:43:LYS:HE2	1.90	0.43
1:AC:11:TYR:O	1:HN:37:ARG:NH2	2.41	0.43
1:AS:34:SER:HB2	1:AS:55:ASN:HB3	2.00	0.43
1:BE:11:TYR:O	1:IP:37:ARG:NH2	2.40	0.43
1:BS:115:SER:HA	1:BS:116:ASP:HA	1.80	0.43
1:CK:34:SER:HB2	1:CK:55:ASN:HB3	2.00	0.43
1:EO:34:SER:HB2	1:EO:55:ASN:HB3	2.00	0.43
1:FN:115:SER:HA	1:FN:116:ASP:HA	1.71	0.43
1:FS:55:ASN:ND2	1:FS:72:ASN:OD1	2.52	0.43
1:GE:94:VAL:HG11	1:GG:71:VAL:HG11	2.00	0.43
1:GE:115:SER:HA	1:GE:116:ASP:HA	1.83	0.43
1:HQ:36:ARG:HH21	1:HQ:53:ASN:HD22	1.67	0.43
1:HW:42:LYS:HE3	1:HW:79:VAL:HG11	1.99	0.43
1:AQ:55:ASN:ND2	1:AQ:72:ASN:OD1	2.51	0.43
1:BC:55:ASN:ND2	1:BC:72:ASN:OD1	2.52	0.43
1:DK:55:ASN:ND2	1:DK:72:ASN:OD1	2.52	0.43
1:FJ:64:ASP:OD1	1:FJ:64:ASP:N	2.38	0.43
1:FK:54:MET:HE2	1:FK:56:PHE:CZ	2.54	0.43
1:GE:8:VAL:HB	1:GE:20:TYR:HB3	2.00	0.43
1:IP:8:VAL:HB	1:IP:20:TYR:HB3	2.00	0.43
1:AP:42:LYS:NZ	1:AP:44:GLY:O	2.36	0.43
1:BF:37:ARG:NH2	1:IO:11:TYR:O	2.39	0.43
1:DY:36:ARG:HH21	1:DY:53:ASN:HD22	1.67	0.43
1:FR:38:SER:HB3	1:FR:51:ARG:HG3	1.99	0.43
1:IT:115:SER:HA	1:IT:116:ASP:HA	1.72	0.43
1:AD:54:MET:HE2	1:AD:54:MET:HB2	1.81	0.43
1:CW:36:ARG:HH21	1:CW:53:ASN:HD22	1.66	0.43
1:DW:6:LYS:NZ	1:DY:93:GLU:OE2	2.43	0.43
1:EM:55:ASN:ND2	1:EM:72:ASN:OD1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EW:115:SER:HA	1:EW:116:ASP:HA	1.82	0.43
1:EX:26:ASP:OD1	1:EX:28:THR:N	2.49	0.43
1:FY:36:ARG:HH21	1:FY:53:ASN:HD22	1.66	0.43
1:GH:90:MET:HA	1:GH:94:VAL:HB	2.00	0.43
1:GU:8:VAL:HB	1:GU:20:TYR:HB3	2.00	0.43
1:HK:94:VAL:HG11	1:HM:71:VAL:HG11	2.00	0.43
1:AD:42:LYS:NZ	1:AD:44:GLY:O	2.36	0.43
1:AW:36:ARG:HH21	1:AW:53:ASN:HD22	1.67	0.43
1:AW:115:SER:HA	1:AW:116:ASP:HA	1.86	0.43
1:CD:26:ASP:OD1	1:CD:28:THR:N	2.49	0.43
1:DM:115:SER:HA	1:DM:116:ASP:HA	1.85	0.43
1:EX:47:ASN:HB3	1:EX:79:VAL:HB	2.01	0.43
1:FV:8:VAL:HB	1:FV:20:TYR:HB3	2.01	0.43
1:GX:90:MET:HA	1:GX:94:VAL:HB	2.00	0.43
1:HW:94:VAL:HG11	1:HY:71:VAL:HG11	2.00	0.43
1:HY:54:MET:HE2	1:HY:56:PHE:CZ	2.54	0.43
1:IO:54:MET:HE2	1:IO:56:PHE:CZ	2.54	0.43
1:AE:115:SER:HA	1:AE:116:ASP:HA	1.80	0.43
1:BF:8:VAL:HB	1:BF:20:TYR:HB3	2.01	0.43
1:BQ:36:ARG:HH21	1:BQ:53:ASN:HD22	1.67	0.43
1:CD:47:ASN:HB3	1:CD:79:VAL:HB	2.01	0.43
1:CY:54:MET:HE2	1:CY:56:PHE:CZ	2.54	0.43
1:DM:11:TYR:O	1:GH:37:ARG:NH2	2.40	0.43
1:ED:26:ASP:OD2	1:ED:28:THR:N	2.51	0.43
1:FO:115:SER:HA	1:FO:116:ASP:HA	1.80	0.43
1:GG:54:MET:HE2	1:GG:56:PHE:CZ	2.53	0.43
1:HV:26:ASP:OD1	1:HV:28:THR:N	2.48	0.43
1:HZ:115:SER:HA	1:HZ:116:ASP:HA	1.71	0.43
1:AD:8:VAL:HB	1:AD:20:TYR:HB3	2.01	0.43
1:AL:47:ASN:HB3	1:AL:79:VAL:HB	2.01	0.43
1:AP:8:VAL:HB	1:AP:20:TYR:HB3	2.01	0.43
1:AP:37:ARG:NH2	1:HY:11:TYR:O	2.39	0.43
1:CM:115:SER:HA	1:CM:116:ASP:HA	1.80	0.43
1:EO:42:LYS:HD3	1:EO:42:LYS:C	2.44	0.43
1:ET:8:VAL:HB	1:ET:20:TYR:HB3	2.01	0.43
1:FF:8:VAL:HB	1:FF:20:TYR:HB3	2.01	0.43
1:GH:115:SER:HA	1:GH:116:ASP:HA	1.71	0.43
1:GX:8:VAL:HB	1:GX:20:TYR:HB3	2.00	0.43
1:HM:54:MET:HE2	1:HM:56:PHE:CZ	2.54	0.43
1:HR:115:SER:HA	1:HR:116:ASP:HA	1.71	0.43
1:HS:8:VAL:HB	1:HS:20:TYR:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HV:64:ASP:OD1	1:HV:64:ASP:N	2.39	0.43
1:AS:42:LYS:HD3	1:AS:42:LYS:C	2.44	0.42
1:DA:11:TYR:O	1:FV:37:ARG:NH2	2.42	0.42
1:ED:8:VAL:HB	1:ED:20:TYR:HB3	2.01	0.42
1:FI:36:ARG:HH21	1:FI:53:ASN:HD22	1.67	0.42
1:HW:115:SER:HA	1:HW:116:ASP:HA	1.83	0.42
1:IM:94:VAL:HG11	1:IO:71:VAL:HG11	2.00	0.42
1:IQ:18:VAL:HG23	1:IS:112:ILE:HD12	2.01	0.42
1:IT:42:LYS:NZ	1:IT:44:GLY:O	2.37	0.42
1:JE:36:ARG:HH21	1:JE:53:ASN:HD22	1.67	0.42
1:AD:37:ARG:NH2	1:HM:11:TYR:O	2.39	0.42
1:AQ:54:MET:HE2	1:AQ:56:PHE:CZ	2.54	0.42
1:CK:54:MET:HE2	1:CK:56:PHE:CZ	2.54	0.42
1:DV:56:PHE:O	1:DV:70:VAL:HA	2.19	0.42
1:DZ:115:SER:HA	1:DZ:116:ASP:HA	1.72	0.42
1:EH:56:PHE:O	1:EH:70:VAL:HA	2.19	0.42
1:EM:54:MET:HE2	1:EM:56:PHE:CZ	2.54	0.42
1:FK:68:LEU:HD12	1:FK:68:LEU:HA	1.91	0.42
1:GA:115:SER:HA	1:GA:116:ASP:HA	1.80	0.42
1:HY:1:LEU:HD12	1:HY:1:LEU:HA	1.88	0.42
1:IQ:71:VAL:HG11	1:IS:94:VAL:HG11	2.01	0.42
1:IT:14:THR:HG22	1:IT:16:ASP:H	1.84	0.42
1:AS:115:SER:HA	1:AS:116:ASP:HA	1.85	0.42
1:BN:37:ARG:NH2	1:IW:11:TYR:O	2.37	0.42
1:BQ:115:SER:HA	1:BQ:116:ASP:HA	1.86	0.42
1:CC:115:SER:HA	1:CC:116:ASP:HA	1.82	0.42
1:FF:115:SER:HA	1:FF:116:ASP:HA	1.72	0.42
1:GL:47:ASN:HB3	1:GL:79:VAL:HB	2.01	0.42
1:HE:55:ASN:OD1	1:HE:72:ASN:ND2	2.51	0.42
1:HF:47:ASN:HB3	1:HF:79:VAL:HB	2.01	0.42
1:HM:1:LEU:HD12	1:HM:1:LEU:HA	1.88	0.42
1:AA:55:ASN:ND2	1:AA:72:ASN:OD1	2.52	0.42
1:AL:26:ASP:OD1	1:AL:28:THR:N	2.49	0.42
1:AY:115:SER:HA	1:AY:116:ASP:HA	1.85	0.42
1:GA:8:VAL:HB	1:GA:20:TYR:HB3	2.02	0.42
1:HA:42:LYS:HD2	1:HA:42:LYS:N	2.35	0.42
1:HA:115:SER:HA	1:HA:116:ASP:HA	1.86	0.42
1:HK:115:SER:HA	1:HK:116:ASP:HA	1.83	0.42
1:HY:42:LYS:HD3	1:HY:42:LYS:C	2.44	0.42
1:ID:26:ASP:OD2	1:ID:28:THR:N	2.50	0.42
1:IK:50:MET:HE2	1:IK:50:MET:HB2	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IL:47:ASN:HB3	1:IL:79:VAL:HB	2.01	0.42
1:AS:54:MET:HE2	1:AS:56:PHE:CZ	2.55	0.42
1:BJ:8:VAL:HB	1:BJ:20:TYR:HB3	2.02	0.42
1:CG:36:ARG:HH21	1:CG:53:ASN:HD22	1.67	0.42
1:DR:42:LYS:HB2	1:DR:42:LYS:HE2	1.72	0.42
1:EO:54:MET:HE2	1:EO:56:PHE:CZ	2.55	0.42
1:GA:71:VAL:HG11	1:GC:94:VAL:HG11	2.02	0.42
1:GK:55:ASN:OD1	1:GK:72:ASN:ND2	2.51	0.42
1:GO:42:LYS:HD2	1:GO:42:LYS:N	2.35	0.42
1:GQ:115:SER:HA	1:GQ:116:ASP:HA	1.80	0.42
1:HM:42:LYS:HD3	1:HM:42:LYS:C	2.44	0.42
1:HS:115:SER:HA	1:HS:116:ASP:HA	1.85	0.42
1:IT:54:MET:HE2	1:IT:54:MET:HB2	1.84	0.42
1:BI:42:LYS:HD3	1:BI:42:LYS:C	2.44	0.42
1:BO:6:LYS:NZ	1:BQ:93:GLU:OE2	2.43	0.42
1:BV:56:PHE:O	1:BV:70:VAL:HA	2.19	0.42
1:EX:42:LYS:HB2	1:EX:42:LYS:HE2	1.72	0.42
1:GW:42:LYS:HD3	1:GW:42:LYS:C	2.44	0.42
1:IA:18:VAL:HG23	1:IC:112:ILE:HD12	2.01	0.42
1:IX:47:ASN:HB3	1:IX:79:VAL:HB	2.01	0.42
1:AP:115:SER:HA	1:AP:116:ASP:HA	1.72	0.42
1:AU:6:LYS:NZ	1:AW:93:GLU:OE2	2.43	0.42
1:BB:37:ARG:NH2	1:IK:11:TYR:O	2.37	0.42
1:CH:42:LYS:HB2	1:CH:42:LYS:HE2	1.90	0.42
1:CM:54:MET:HE2	1:CM:54:MET:HB2	1.89	0.42
1:CP:56:PHE:O	1:CP:70:VAL:HA	2.19	0.42
1:DW:37:ARG:HB2	1:DW:50:MET:HE1	2.02	0.42
1:FM:34:SER:HB2	1:FM:55:ASN:HB3	2.00	0.42
1:FR:56:PHE:O	1:FR:70:VAL:HA	2.19	0.42
1:GX:64:ASP:OD1	1:GX:64:ASP:N	2.38	0.42
1:HJ:26:ASP:OD2	1:HJ:28:THR:N	2.50	0.42
1:HU:55:ASN:OD1	1:HU:72:ASN:ND2	2.49	0.42
1:JE:42:LYS:N	1:JE:42:LYS:HD2	2.35	0.42
1:BR:115:SER:HA	1:BR:116:ASP:HA	1.72	0.42
1:CD:42:LYS:HB2	1:CD:42:LYS:HE2	1.72	0.42
1:EM:115:SER:HA	1:EM:116:ASP:HA	1.87	0.42
1:FB:56:PHE:O	1:FB:70:VAL:HA	2.19	0.42
1:FI:42:LYS:HD2	1:FI:42:LYS:N	2.35	0.42
1:FO:10:ILE:HG12	1:FO:20:TYR:CE2	2.55	0.42
1:GG:42:LYS:HD3	1:GG:42:LYS:C	2.44	0.42
1:HC:8:VAL:HB	1:HC:20:TYR:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HF:42:LYS:HB2	1:HF:42:LYS:HE2	1.72	0.42
1:HG:18:VAL:HG23	1:HI:112:ILE:HD12	2.01	0.42
1:BM:109:LYS:HB2	1:BM:111:VAL:HG23	2.02	0.42
1:BY:54:MET:HE2	1:BY:56:PHE:CZ	2.55	0.42
1:CH:14:THR:HG22	1:CH:15:ALA:N	2.35	0.42
1:DZ:89:TRP:CD1	1:GT:58:LYS:HD3	2.55	0.42
1:EL:42:LYS:HE2	1:EL:42:LYS:HB2	1.72	0.42
1:EO:115:SER:HA	1:EO:116:ASP:HA	1.85	0.42
1:FJ:14:THR:HG22	1:FJ:15:ALA:N	2.35	0.42
1:FW:106:LEU:HD22	1:FY:35:LEU:HG	2.01	0.42
1:GQ:8:VAL:HB	1:GQ:20:TYR:HB3	2.02	0.42
1:IE:71:VAL:HG11	1:IG:94:VAL:HG11	2.02	0.42
1:IM:8:VAL:HB	1:IM:20:TYR:HB3	2.00	0.42
1:IU:115:SER:HA	1:IU:116:ASP:HA	1.85	0.42
1:IW:50:MET:HE2	1:IW:50:MET:HB2	1.91	0.42
1:IY:71:VAL:HG11	1:JA:94:VAL:HG11	2.02	0.42
1:AK:109:LYS:HB2	1:AK:111:VAL:HG23	2.02	0.42
1:AM:115:SER:HA	1:AM:116:ASP:HA	1.84	0.42
1:AS:1:LEU:HD12	1:AS:1:LEU:HA	1.91	0.42
1:BA:109:LYS:HB2	1:BA:111:VAL:HG23	2.02	0.42
1:BS:10:ILE:HG12	1:BS:20:TYR:CE2	2.55	0.42
1:BY:42:LYS:C	1:BY:42:LYS:HD3	2.44	0.42
1:CC:11:TYR:O	1:EX:37:ARG:NH2	2.40	0.42
1:CK:42:LYS:C	1:CK:42:LYS:HD3	2.44	0.42
1:CM:10:ILE:HG12	1:CM:20:TYR:CE2	2.55	0.42
1:DA:42:LYS:C	1:DA:42:LYS:HD3	2.44	0.42
1:DJ:89:TRP:CD1	1:GD:58:LYS:HD3	2.55	0.42
1:DV:41:VAL:HG12	1:DV:43:LYS:HG3	2.02	0.42
1:ET:115:SER:HA	1:ET:116:ASP:HA	1.72	0.42
1:FM:42:LYS:HD3	1:FM:42:LYS:C	2.44	0.42
1:GL:42:LYS:HB2	1:GL:42:LYS:HE2	1.72	0.42
1:HV:47:ASN:HB3	1:HV:79:VAL:HB	2.01	0.42
1:IC:115:SER:HA	1:IC:116:ASP:HA	1.85	0.42
1:IO:42:LYS:HD3	1:IO:42:LYS:C	2.44	0.42
1:AA:115:SER:HA	1:AA:116:ASP:HA	1.85	0.41
1:AX:89:TRP:CD1	1:IH:58:LYS:HD3	2.55	0.41
1:BR:14:THR:HG22	1:BR:15:ALA:N	2.35	0.41
1:BR:89:TRP:CD1	1:JB:58:LYS:HD3	2.55	0.41
1:BV:41:VAL:HG12	1:BV:43:LYS:HG3	2.02	0.41
1:BW:54:MET:HE2	1:BW:56:PHE:CZ	2.54	0.41
1:CU:37:ARG:HB2	1:CU:50:MET:HE1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:54:MET:HE2	1:DA:56:PHE:CZ	2.55	0.41
1:DE:6:LYS:HG2	1:DE:8:VAL:HG13	2.02	0.41
1:DG:37:ARG:HB2	1:DG:50:MET:HE1	2.02	0.41
1:DI:36:ARG:HH21	1:DI:53:ASN:HD22	1.67	0.41
1:DS:10:ILE:HG12	1:DS:20:TYR:CE2	2.55	0.41
1:ED:54:MET:HE2	1:ED:54:MET:HB2	1.82	0.41
1:ED:64:ASP:OD1	1:ED:64:ASP:N	2.38	0.41
1:FB:41:VAL:HG12	1:FB:43:LYS:HG3	2.02	0.41
1:FW:54:MET:HE2	1:FW:54:MET:HB2	1.92	0.41
1:GI:8:VAL:HB	1:GI:20:TYR:HB3	2.02	0.41
1:GX:54:MET:HE3	1:GX:54:MET:HB2	1.86	0.41
1:HO:8:VAL:HB	1:HO:20:TYR:HB3	2.02	0.41
1:IG:6:LYS:HG2	1:IG:8:VAL:HG13	2.02	0.41
1:JA:6:LYS:HG2	1:JA:8:VAL:HG13	2.02	0.41
1:AA:33:VAL:HA	1:AA:55:ASN:O	2.20	0.41
1:BF:64:ASP:OD1	1:BF:64:ASP:N	2.38	0.41
1:BG:54:MET:HE2	1:BG:56:PHE:CZ	2.54	0.41
1:BJ:54:MET:HE3	1:BJ:54:MET:HB2	1.84	0.41
1:CP:41:VAL:HG12	1:CP:43:LYS:HG3	2.02	0.41
1:CT:8:VAL:HB	1:CT:20:TYR:HB3	2.01	0.41
1:DF:41:VAL:HG12	1:DF:43:LYS:HG3	2.02	0.41
1:DF:56:PHE:O	1:DF:70:VAL:HA	2.19	0.41
1:DW:54:MET:HE2	1:DW:54:MET:HB2	1.92	0.41
1:EH:41:VAL:HG12	1:EH:43:LYS:HG3	2.02	0.41
1:EL:47:ASN:HB3	1:EL:79:VAL:HB	2.01	0.41
1:FA:6:LYS:HG2	1:FA:8:VAL:HG13	2.02	0.41
1:GG:43:LYS:HB2	1:GG:43:LYS:HE2	1.90	0.41
1:GG:55:ASN:OD1	1:GG:72:ASN:ND2	2.50	0.41
1:HA:36:ARG:HH21	1:HA:53:ASN:HD22	1.67	0.41
1:HG:71:VAL:HG11	1:HI:94:VAL:HG11	2.01	0.41
1:II:115:SER:HA	1:II:116:ASP:HA	1.85	0.41
1:IU:8:VAL:HB	1:IU:20:TYR:HB3	2.01	0.41
1:AQ:115:SER:HA	1:AQ:116:ASP:HA	1.87	0.41
1:AX:14:THR:HG22	1:AX:15:ALA:N	2.35	0.41
1:BF:90:MET:HA	1:BF:94:VAL:HB	2.02	0.41
1:BI:54:MET:HE2	1:BI:56:PHE:CZ	2.55	0.41
1:BQ:42:LYS:HD2	1:BQ:42:LYS:N	2.35	0.41
1:BS:54:MET:HE2	1:BS:54:MET:HB2	1.89	0.41
1:CD:37:ARG:NH2	1:EW:11:TYR:O	2.40	0.41
1:DR:47:ASN:HB3	1:DR:79:VAL:HB	2.01	0.41
1:DZ:14:THR:HG22	1:DZ:15:ALA:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ED:90:MET:HA	1:ED:94:VAL:HB	2.02	0.41
1:EE:10:ILE:HG12	1:EE:20:TYR:CE2	2.55	0.41
1:EO:1:LEU:HD12	1:EO:1:LEU:HA	1.91	0.41
1:HQ:42:LYS:HD2	1:HQ:42:LYS:N	2.35	0.41
1:IA:71:VAL:HG11	1:IC:94:VAL:HG11	2.01	0.41
1:JC:8:VAL:HB	1:JC:20:TYR:HB3	2.02	0.41
1:AD:115:SER:HA	1:AD:116:ASP:HA	1.72	0.41
1:AH:41:VAL:HG12	1:AH:43:LYS:HG3	2.02	0.41
1:AH:56:PHE:O	1:AH:70:VAL:HA	2.19	0.41
1:BB:47:ASN:HB3	1:BB:79:VAL:HB	2.01	0.41
1:BM:50:MET:HE2	1:BM:50:MET:HB2	1.89	0.41
1:BN:47:ASN:HB3	1:BN:79:VAL:HB	2.01	0.41
1:CL:8:VAL:HB	1:CL:20:TYR:HB3	2.02	0.41
1:GO:36:ARG:HH21	1:GO:53:ASN:HD22	1.67	0.41
1:GT:8:VAL:HB	1:GT:20:TYR:HB3	2.02	0.41
1:II:8:VAL:HB	1:II:20:TYR:HB3	2.02	0.41
1:IS:54:MET:HE2	1:IS:56:PHE:CZ	2.56	0.41
1:AD:90:MET:HA	1:AD:94:VAL:HB	2.02	0.41
1:AG:39:LEU:HD23	1:AG:50:MET:HE1	2.03	0.41
1:AP:90:MET:HA	1:AP:94:VAL:HB	2.03	0.41
1:AW:42:LYS:N	1:AW:42:LYS:HD2	2.35	0.41
1:AX:115:SER:HA	1:AX:116:ASP:HA	1.72	0.41
1:BZ:8:VAL:HB	1:BZ:20:TYR:HB3	2.03	0.41
1:CE:37:ARG:HB2	1:CE:50:MET:HE1	2.02	0.41
1:CI:54:MET:HE2	1:CI:56:PHE:CZ	2.54	0.41
1:DY:42:LYS:HD2	1:DY:42:LYS:N	2.35	0.41
1:GC:6:LYS:HG2	1:GC:8:VAL:HG13	2.02	0.41
1:GW:55:ASN:OD1	1:GW:72:ASN:ND2	2.50	0.41
1:HI:115:SER:HA	1:HI:116:ASP:HA	1.85	0.41
1:ID:14:THR:HG22	1:ID:16:ASP:H	1.84	0.41
1:IQ:8:VAL:HB	1:IQ:20:TYR:HB3	2.01	0.41
1:AE:10:ILE:HG12	1:AE:20:TYR:CE2	2.55	0.41
1:AH:26:ASP:OD1	1:AH:28:THR:N	2.49	0.41
1:AH:58:LYS:HD3	1:HR:89:TRP:CD1	2.56	0.41
1:AL:37:ARG:NH2	1:HU:11:TYR:O	2.37	0.41
1:AU:37:ARG:HB2	1:AU:50:MET:HE1	2.02	0.41
1:BA:50:MET:HE2	1:BA:50:MET:HB2	1.89	0.41
1:BV:58:LYS:HD3	1:JF:89:TRP:CD1	2.56	0.41
1:CE:54:MET:HE2	1:CE:54:MET:HB2	1.92	0.41
1:DC:10:ILE:HG12	1:DC:20:TYR:CE2	2.55	0.41
1:DK:33:VAL:HA	1:DK:55:ASN:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DN:8:VAL:HB	1:DN:20:TYR:HB3	2.01	0.41
1:EY:10:ILE:HG12	1:EY:20:TYR:CE2	2.55	0.41
1:FM:54:MET:HE2	1:FM:56:PHE:CZ	2.55	0.41
1:FQ:6:LYS:HG2	1:FQ:8:VAL:HG13	2.02	0.41
1:FQ:39:LEU:HD23	1:FQ:50:MET:HE1	2.03	0.41
1:FR:41:VAL:HG12	1:FR:43:LYS:HG3	2.02	0.41
1:FW:37:ARG:HB2	1:FW:50:MET:HE1	2.02	0.41
1:IE:8:VAL:HB	1:IE:20:TYR:HB3	2.02	0.41
1:IH:8:VAL:HB	1:IH:20:TYR:HB3	2.02	0.41
1:AT:8:VAL:HB	1:AT:20:TYR:HB3	2.02	0.41
1:BF:114:LEU:HD23	1:IP:1:LEU:HD22	2.03	0.41
1:BO:37:ARG:HB2	1:BO:50:MET:HE1	2.02	0.41
1:BV:37:ARG:NH2	1:JE:11:TYR:O	2.46	0.41
1:CW:42:LYS:HD2	1:CW:42:LYS:N	2.35	0.41
1:CX:38:SER:HB3	1:CX:51:ARG:HB2	2.03	0.41
1:DI:42:LYS:HD2	1:DI:42:LYS:N	2.35	0.41
1:DV:58:LYS:HD3	1:GP:89:TRP:CD1	2.56	0.41
1:DW:33:VAL:HA	1:DW:55:ASN:O	2.21	0.41
1:EP:8:VAL:HB	1:EP:20:TYR:HB3	2.02	0.41
1:FM:43:LYS:HB2	1:FM:43:LYS:HE2	1.90	0.41
1:FU:115:SER:HA	1:FU:116:ASP:HA	1.85	0.41
1:FV:90:MET:HA	1:FV:94:VAL:HB	2.03	0.41
1:GQ:71:VAL:HG11	1:GS:94:VAL:HG11	2.02	0.41
1:GT:41:VAL:HG12	1:GT:43:LYS:HG3	2.02	0.41
1:HJ:14:THR:HG22	1:HJ:16:ASP:H	1.85	0.41
1:IY:8:VAL:HB	1:IY:20:TYR:HB3	2.02	0.41
1:JB:8:VAL:HB	1:JB:20:TYR:HB3	2.02	0.41
1:AS:17:GLU:HB2	1:AS:36:ARG:HG3	2.03	0.41
1:BI:34:SER:HB2	1:BI:55:ASN:HB3	2.03	0.41
1:BJ:86:VAL:O	1:BJ:90:MET:HG3	2.21	0.41
1:CI:68:LEU:HD12	1:CI:68:LEU:HA	1.91	0.41
1:CU:33:VAL:HA	1:CU:55:ASN:O	2.21	0.41
1:DG:33:VAL:HA	1:DG:55:ASN:O	2.21	0.41
1:EH:58:LYS:HD3	1:HB:89:TRP:CD1	2.56	0.41
1:GD:41:VAL:HG12	1:GD:43:LYS:HG3	2.02	0.41
1:HS:71:VAL:HG11	1:HU:94:VAL:HG11	2.03	0.41
1:HU:109:LYS:HB2	1:HU:111:VAL:HG23	2.03	0.41
1:II:71:VAL:HG11	1:IK:94:VAL:HG11	2.03	0.41
1:IU:71:VAL:HG11	1:IW:94:VAL:HG11	2.03	0.41
1:AD:18:VAL:HG23	1:HN:112:ILE:HD12	2.03	0.41
1:AD:56:PHE:O	1:AD:70:VAL:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:56:PHE:O	1:AL:70:VAL:HA	2.21	0.41
1:AO:42:LYS:C	1:AO:42:LYS:HD3	2.46	0.41
1:AP:18:VAL:HG23	1:HZ:112:ILE:HD12	2.03	0.41
1:AP:56:PHE:O	1:AP:70:VAL:HA	2.21	0.41
1:BF:56:PHE:O	1:BF:70:VAL:HA	2.21	0.41
1:CE:6:LYS:NZ	1:CG:93:GLU:OE2	2.43	0.41
1:CU:54:MET:HE2	1:CU:54:MET:HB2	1.92	0.41
1:DJ:14:THR:HG22	1:DJ:15:ALA:N	2.35	0.41
1:DJ:18:VAL:HG23	1:GD:112:ILE:HD12	2.03	0.41
1:DJ:38:SER:HB3	1:DJ:51:ARG:HB2	2.03	0.41
1:DN:114:LEU:HD23	1:GH:1:LEU:HD22	2.03	0.41
1:DQ:109:LYS:HB2	1:DQ:111:VAL:HG23	2.02	0.41
1:DR:115:SER:HA	1:DR:116:ASP:HA	1.68	0.41
1:EC:42:LYS:HD3	1:EC:42:LYS:C	2.46	0.41
1:EH:26:ASP:OD2	1:EH:28:THR:N	2.48	0.41
1:EK:109:LYS:HB2	1:EK:111:VAL:HG23	2.02	0.41
1:EO:17:GLU:HB2	1:EO:36:ARG:HG3	2.03	0.41
1:EP:86:VAL:O	1:EP:90:MET:HG3	2.21	0.41
1:ES:42:LYS:HD3	1:ES:42:LYS:C	2.46	0.41
1:EW:109:LYS:HB2	1:EW:111:VAL:HG23	2.02	0.41
1:FE:42:LYS:HD3	1:FE:42:LYS:C	2.46	0.41
1:FU:26:ASP:OD2	1:FU:29:ASN:HB2	2.21	0.41
1:GD:8:VAL:HB	1:GD:20:TYR:HB3	2.02	0.41
1:GL:38:SER:HB3	1:GL:51:ARG:HG3	2.03	0.41
1:GY:71:VAL:HG11	1:HA:94:VAL:HG11	2.03	0.41
1:HF:38:SER:HB3	1:HF:51:ARG:HG3	2.03	0.41
1:HG:8:VAL:HB	1:HG:20:TYR:HB3	2.02	0.41
1:IA:8:VAL:HB	1:IA:20:TYR:HB3	2.02	0.41
1:IH:41:VAL:HG12	1:IH:43:LYS:HG3	2.02	0.41
1:IO:115:SER:HA	1:IO:116:ASP:HA	1.85	0.41
1:AC:42:LYS:C	1:AC:42:LYS:HD3	2.46	0.41
1:AE:8:VAL:HB	1:AE:20:TYR:HB3	2.03	0.41
1:AH:66:LYS:HE3	1:AH:66:LYS:HB3	1.94	0.41
1:AP:114:LEU:HD23	1:HZ:1:LEU:HD22	2.03	0.41
1:AT:86:VAL:O	1:AT:90:MET:HG3	2.21	0.41
1:CD:56:PHE:O	1:CD:70:VAL:HA	2.21	0.41
1:CP:42:LYS:NZ	1:CP:44:GLY:O	2.50	0.41
1:CX:14:THR:HG22	1:CX:15:ALA:N	2.35	0.41
1:DB:86:VAL:O	1:DB:90:MET:HG3	2.21	0.41
1:DE:39:LEU:HD23	1:DE:50:MET:HE1	2.03	0.41
1:DV:26:ASP:OD2	1:DV:28:THR:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EQ:33:VAL:HA	1:EQ:55:ASN:O	2.21	0.41
1:ES:26:ASP:OD2	1:ES:29:ASN:HB2	2.21	0.41
1:ET:26:ASP:OD2	1:ET:28:THR:N	2.51	0.41
1:FC:115:SER:HA	1:FC:116:ASP:HA	1.85	0.41
1:FJ:115:SER:HA	1:FJ:116:ASP:HA	1.71	0.41
1:FV:26:ASP:OD2	1:FV:28:THR:N	2.51	0.41
1:FV:56:PHE:O	1:FV:70:VAL:HA	2.21	0.41
1:GM:8:VAL:HB	1:GM:20:TYR:HB3	2.02	0.41
1:GP:64:ASP:OD1	1:GP:64:ASP:N	2.38	0.41
1:GS:6:LYS:HG2	1:GS:8:VAL:HG13	2.02	0.41
1:GU:71:VAL:HG11	1:GW:94:VAL:HG11	2.03	0.41
1:GY:8:VAL:HB	1:GY:20:TYR:HB3	2.02	0.41
1:HI:42:LYS:HD3	1:HI:42:LYS:C	2.46	0.41
1:HO:71:VAL:HG11	1:HQ:94:VAL:HG11	2.03	0.41
1:HS:108:THR:HG21	1:HU:87:ARG:HG3	2.02	0.41
1:IE:115:SER:HA	1:IE:116:ASP:HA	1.80	0.41
1:IK:109:LYS:HB2	1:IK:111:VAL:HG23	2.03	0.41
1:IS:42:LYS:HD3	1:IS:42:LYS:C	2.46	0.41
1:JB:41:VAL:HG12	1:JB:43:LYS:HG3	2.02	0.41
1:AD:114:LEU:HD23	1:HN:1:LEU:HD22	2.03	0.40
1:AG:6:LYS:HG2	1:AG:8:VAL:HG13	2.02	0.40
1:AY:47:ASN:HB2	1:AY:79:VAL:HB	2.04	0.40
1:BB:56:PHE:O	1:BB:70:VAL:HA	2.21	0.40
1:BF:26:ASP:OD2	1:BF:28:THR:N	2.51	0.40
1:BG:115:SER:HA	1:BG:116:ASP:HA	1.87	0.40
1:BK:47:ASN:HB2	1:BK:79:VAL:HB	2.04	0.40
1:BN:56:PHE:O	1:BN:70:VAL:HA	2.21	0.40
1:BU:6:LYS:HG2	1:BU:8:VAL:HG13	2.02	0.40
1:CA:47:ASN:HB2	1:CA:79:VAL:HB	2.04	0.40
1:CC:109:LYS:HB2	1:CC:111:VAL:HG23	2.02	0.40
1:DB:8:VAL:HB	1:DB:20:TYR:HB3	2.03	0.40
1:DG:54:MET:HE2	1:DG:54:MET:HB2	1.92	0.40
1:DN:90:MET:HA	1:DN:94:VAL:HB	2.02	0.40
1:ED:18:VAL:HG23	1:GX:112:ILE:HD12	2.03	0.40
1:EG:6:LYS:HG2	1:EG:8:VAL:HG13	2.02	0.40
1:EU:47:ASN:HB2	1:EU:79:VAL:HB	2.04	0.40
1:EX:56:PHE:O	1:EX:70:VAL:HA	2.21	0.40
1:FA:39:LEU:HD23	1:FA:50:MET:HE1	2.03	0.40
1:FC:33:VAL:HA	1:FC:55:ASN:O	2.21	0.40
1:FE:26:ASP:OD2	1:FE:29:ASN:HB2	2.21	0.40
1:FF:26:ASP:OD2	1:FF:28:THR:N	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FV:64:ASP:OD1	1:FV:64:ASP:N	2.38	0.40
1:GH:1:LEU:HD23	1:GH:1:LEU:HA	1.93	0.40
1:GM:71:VAL:HG11	1:GO:94:VAL:HG11	2.03	0.40
1:IC:42:LYS:HD3	1:IC:42:LYS:C	2.46	0.40
1:IP:1:LEU:HD23	1:IP:1:LEU:HA	1.93	0.40
1:IW:109:LYS:HB2	1:IW:111:VAL:HG23	2.03	0.40
1:JC:71:VAL:HG11	1:JE:94:VAL:HG11	2.03	0.40
1:BC:33:VAL:HA	1:BC:55:ASN:O	2.21	0.40
1:BE:115:SER:HA	1:BE:116:ASP:HA	1.85	0.40
1:BI:115:SER:HA	1:BI:116:ASP:HA	1.85	0.40
1:BV:42:LYS:NZ	1:BV:44:GLY:O	2.50	0.40
1:BV:90:MET:HA	1:BV:94:VAL:HB	2.04	0.40
1:CO:6:LYS:HG2	1:CO:8:VAL:HG13	2.02	0.40
1:CW:66:LYS:HZ2	1:CW:66:LYS:HG2	1.75	0.40
1:CX:18:VAL:HG23	1:FR:112:ILE:HD12	2.04	0.40
1:DN:89:TRP:CD1	1:GH:58:LYS:HD3	2.56	0.40
1:DV:42:LYS:NZ	1:DV:44:GLY:O	2.50	0.40
1:EL:115:SER:HA	1:EL:116:ASP:HA	1.68	0.40
1:EQ:115:SER:HA	1:EQ:116:ASP:HA	1.83	0.40
1:FF:42:LYS:NZ	1:FF:44:GLY:O	2.36	0.40
1:FS:33:VAL:HA	1:FS:55:ASN:O	2.21	0.40
1:GA:54:MET:HE2	1:GA:54:MET:HB2	1.84	0.40
1:GC:115:SER:HA	1:GC:116:ASP:HA	1.83	0.40
1:GE:71:VAL:HG11	1:GG:94:VAL:HG11	2.03	0.40
1:IA:115:SER:HA	1:IA:116:ASP:HA	1.83	0.40
1:II:108:THR:HG21	1:IK:87:ARG:HG3	2.02	0.40
1:AM:8:VAL:HB	1:AM:20:TYR:HB3	2.03	0.40
1:BS:12:ARG:HH12	1:EK:16:ASP:CG	2.29	0.40
1:CQ:8:VAL:HB	1:CQ:20:TYR:HB3	2.03	0.40
1:DB:1:LEU:HD23	1:DB:1:LEU:HA	1.93	0.40
1:DK:8:VAL:HB	1:DK:20:TYR:HB3	2.04	0.40
1:DU:6:LYS:HG2	1:DU:8:VAL:HG13	2.02	0.40
1:EA:33:VAL:HA	1:EA:55:ASN:O	2.22	0.40
1:EU:115:SER:HA	1:EU:116:ASP:HA	1.85	0.40
1:FN:8:VAL:HB	1:FN:20:TYR:HB3	2.03	0.40
1:HG:54:MET:HE3	1:HG:54:MET:HB2	1.94	0.40
1:HW:71:VAL:HG11	1:HY:94:VAL:HG11	2.03	0.40
1:IU:108:THR:HG21	1:IW:87:ARG:HG3	2.02	0.40
1:AG:115:SER:HA	1:AG:116:ASP:HA	1.83	0.40
1:AK:16:ASP:CG	1:GQ:12:ARG:HH12	2.29	0.40
1:BO:33:VAL:HA	1:BO:55:ASN:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:68:LEU:HD12	1:BW:68:LEU:HA	1.91	0.40
1:BY:34:SER:HB2	1:BY:55:ASN:HB3	2.03	0.40
1:CM:12:ARG:HH12	1:DQ:16:ASP:CG	2.29	0.40
1:DB:37:ARG:NH2	1:FU:11:TYR:O	2.41	0.40
1:DM:42:LYS:HD3	1:DM:42:LYS:C	2.46	0.40
1:DZ:18:VAL:HG23	1:GT:112:ILE:HD12	2.03	0.40
1:FF:54:MET:HB2	1:FF:54:MET:HE2	1.81	0.40
1:FG:33:VAL:HA	1:FG:55:ASN:O	2.21	0.40
1:FY:42:LYS:HD2	1:FY:42:LYS:N	2.35	0.40
1:HB:64:ASP:OD1	1:HB:64:ASP:N	2.38	0.40
1:HS:94:VAL:HG11	1:HU:71:VAL:HG11	2.04	0.40
1:HV:38:SER:HB3	1:HV:51:ARG:HG3	2.03	0.40
1:IO:1:LEU:HD12	1:IO:1:LEU:HA	1.88	0.40
1:JC:94:VAL:HG11	1:JE:71:VAL:HG11	2.04	0.40
1:CG:11:TYR:O	1:FB:37:ARG:NH2	2.48	0.40
1:CG:34:SER:HB2	1:CG:55:ASN:HB3	2.04	0.40
1:CH:38:SER:HB3	1:CH:51:ARG:HB2	2.03	0.40
1:CM:8:VAL:HB	1:CM:20:TYR:HB3	2.03	0.40
1:CQ:33:VAL:HA	1:CQ:55:ASN:O	2.22	0.40
1:CS:42:LYS:HD3	1:CS:42:LYS:C	2.46	0.40
1:CT:90:MET:HA	1:CT:94:VAL:HB	2.03	0.40
1:DA:115:SER:HA	1:DA:116:ASP:HA	1.85	0.40
1:DR:54:MET:HE3	1:DR:54:MET:HB2	1.84	0.40
1:ET:56:PHE:O	1:ET:70:VAL:HA	2.21	0.40
1:ET:90:MET:HA	1:ET:94:VAL:HB	2.03	0.40
1:FC:8:VAL:HB	1:FC:20:TYR:HB3	2.03	0.40
1:HE:109:LYS:HB2	1:HE:111:VAL:HG23	2.03	0.40
1:HK:71:VAL:HG11	1:HM:94:VAL:HG11	2.03	0.40
1:JF:115:SER:HA	1:JF:116:ASP:HA	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	AC	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	AD	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	AE	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	AG	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	AH	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	AI	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	AK	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	AL	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	AM	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	AO	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	AP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	AQ	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	AS	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	AT	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	AU	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	AW	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	AX	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	AY	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	BA	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	BB	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	BC	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	BE	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	BF	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	BG	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	BI	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	BJ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	BK	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	BM	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	BN	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	BO	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	BQ	115/117 (98%)	113 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BR	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	BS	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	BU	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	BV	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	BW	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	BY	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	BZ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	CA	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	CC	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	CD	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	CE	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	CG	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	CH	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	CI	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	CK	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	CL	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	CM	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	CO	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	CP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	CQ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	CS	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	CT	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	CU	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	CW	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	CX	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	CY	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	DA	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	DB	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	DC	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	DE	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	DF	115/117 (98%)	110 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DG	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	DI	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	DJ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	DK	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	DM	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	DN	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	DO	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	DQ	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	DR	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	DS	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	DU	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	DV	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	DW	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	DY	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	DZ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	EA	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	EC	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	ED	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	EE	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	EG	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	EH	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	EI	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	EK	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	EL	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	EM	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	EO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	EP	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	EQ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	ES	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	ET	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	EU	115/117 (98%)	113 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EW	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	EX	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	EY	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	FA	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	FB	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	FC	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	FE	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	FF	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	FG	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	FI	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	FJ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	FK	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	FM	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	FN	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	FO	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	FQ	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	FR	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	FS	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	FU	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	FV	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	FW	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	FY	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	FZ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GA	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GC	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	GD	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	GE	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	GG	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	GH	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GI	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	GK	115/117 (98%)	114 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GL	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GM	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	GO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	GP	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GQ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GS	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	GT	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	GU	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	GW	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	GX	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GY	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	HA	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	HB	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	HC	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	HE	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	HF	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	HG	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	HI	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	HJ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	HK	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	HM	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	HN	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	HO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	HQ	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	HR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	HS	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	HU	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	HV	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	HW	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	HY	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	HZ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IA	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	IC	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	ID	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	IE	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	IG	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	IH	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	II	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	IK	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	IL	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	IM	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	IO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	IP	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	IQ	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	IS	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	IT	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	IU	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	IW	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	IX	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	IY	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	JA	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	JB	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	JC	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	JE	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	JF	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
All	All	20700/21060 (98%)	20147 (97%)	553 (3%)	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	AA	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	AC	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	AD	98/98 (100%)	90 (92%)	8 (8%)	10	32
1	AE	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	AG	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	AH	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	AI	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	AK	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	AL	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	AM	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	AO	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	AP	98/98 (100%)	90 (92%)	8 (8%)	10	32
1	AQ	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	AS	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	AT	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	AU	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	AW	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	AX	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	AY	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	BA	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	BB	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	BC	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	BE	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	BF	98/98 (100%)	91 (93%)	7 (7%)	13	40
1	BG	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	BI	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	BJ	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	BK	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	BM	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	BN	98/98 (100%)	93 (95%)	5 (5%)	21	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BO	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	BQ	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	BR	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	BS	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	BU	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	BV	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	BW	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	BY	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	BZ	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	CA	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	CC	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	CD	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	CE	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	CG	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	CH	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	CI	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	CK	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	CL	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	CM	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	CO	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	CP	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	CQ	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	CS	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	CT	98/98 (100%)	91 (93%)	7 (7%)	13	40
1	CU	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	CW	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	CX	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	CY	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	DA	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	DB	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	DC	98/98 (100%)	96 (98%)	2 (2%)	48	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	DE	98/98 (100%)	92 (94%)	6 (6%)	17	46	
1	DF	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	DG	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	DI	98/98 (100%)	96 (98%)	2 (2%)	48	78	
1	DJ	98/98 (100%)	94 (96%)	4 (4%)	27	61	
1	DK	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	DM	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	DN	98/98 (100%)	91 (93%)	7 (7%)	13	40	
1	DO	98/98 (100%)	97 (99%)	1 (1%)	68	89	
1	DQ	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	DR	98/98 (100%)	93 (95%)	5 (5%)	21	53	
1	DS	98/98 (100%)	97 (99%)	1 (1%)	68	89	
1	DU	98/98 (100%)	92 (94%)	6 (6%)	17	46	
1	DV	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	DW	98/98 (100%)	96 (98%)	2 (2%)	48	78	
1	DY	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	DZ	98/98 (100%)	94 (96%)	4 (4%)	27	61	
1	EA	98/98 (100%)	96 (98%)	2 (2%)	48	78	
1	EC	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	ED	98/98 (100%)	91 (93%)	7 (7%)	13	40	
1	EE	98/98 (100%)	97 (99%)	1 (1%)	68	89	
1	EG	98/98 (100%)	92 (94%)	6 (6%)	17	46	
1	EH	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	EI	98/98 (100%)	97 (99%)	1 (1%)	68	89	
1	EK	98/98 (100%)	94 (96%)	4 (4%)	27	61	
1	EL	98/98 (100%)	92 (94%)	6 (6%)	17	46	
1	EM	98/98 (100%)	97 (99%)	1 (1%)	68	89	
1	EO	98/98 (100%)	94 (96%)	4 (4%)	27	61	
1	EP	98/98 (100%)	93 (95%)	5 (5%)	21	53	
1	EQ	98/98 (100%)	95 (97%)	3 (3%)	35	69	
1	ES	98/98 (100%)	95 (97%)	3 (3%)	35	69	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ET	98/98 (100%)	91 (93%)	7 (7%)	13	40
1	EU	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	EW	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	EX	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	EY	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	FA	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	FB	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FC	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FE	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FF	98/98 (100%)	91 (93%)	7 (7%)	13	40
1	FG	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	FI	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FJ	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	FK	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	FM	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	FN	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	FO	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	FQ	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	FR	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FS	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FU	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FV	98/98 (100%)	91 (93%)	7 (7%)	13	40
1	FW	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	FY	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	FZ	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	GA	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	GC	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	GD	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	GE	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	GG	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	GH	98/98 (100%)	93 (95%)	5 (5%)	21	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GI	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	GK	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	GL	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	GM	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	GO	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	GP	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	GQ	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	GS	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	GT	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	GU	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	GW	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	GX	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	GY	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	HA	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	HB	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	HC	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	HE	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	HF	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	HG	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	HI	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	HJ	98/98 (100%)	91 (93%)	7 (7%)	13	40
1	HK	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	HM	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	HN	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	HO	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	HQ	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	HR	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	HS	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	HU	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	HV	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	HW	98/98 (100%)	97 (99%)	1 (1%)	68	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HY	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	HZ	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	IA	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	IC	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	ID	98/98 (100%)	90 (92%)	8 (8%)	10	32
1	IE	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	IG	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	IH	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	II	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	IK	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	IL	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	IM	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	IO	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	IP	98/98 (100%)	93 (95%)	5 (5%)	21	53
1	IQ	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	IS	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	IT	98/98 (100%)	90 (92%)	8 (8%)	10	32
1	IU	98/98 (100%)	96 (98%)	2 (2%)	48	78
1	IW	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	IX	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	IY	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	JA	98/98 (100%)	92 (94%)	6 (6%)	17	46
1	JB	98/98 (100%)	95 (97%)	3 (3%)	35	69
1	JC	98/98 (100%)	97 (99%)	1 (1%)	68	89
1	JE	98/98 (100%)	94 (96%)	4 (4%)	27	61
1	JF	98/98 (100%)	94 (96%)	4 (4%)	27	61
All	All	17640/17640 (100%)	17017 (96%)	623 (4%)	32	66

All (623) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	55	ASN
1	AA	101	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	114	LEU
1	AC	1	LEU
1	AC	38	SER
1	AC	59	SER
1	AD	2	SER
1	AD	49	THR
1	AD	54	MET
1	AD	59	SER
1	AD	72	ASN
1	AD	109	LYS
1	AD	114	LEU
1	AD	115	SER
1	AE	114	LEU
1	AG	28	THR
1	AG	38	SER
1	AG	41	VAL
1	AG	42	LYS
1	AG	43	LYS
1	AG	59	SER
1	AH	49	THR
1	AH	114	LEU
1	AH	115	SER
1	AI	114	LEU
1	AK	1	LEU
1	AK	42	LYS
1	AK	59	SER
1	AL	49	THR
1	AL	59	SER
1	AL	72	ASN
1	AL	114	LEU
1	AL	115	SER
1	AM	101	SER
1	AM	114	LEU
1	AO	1	LEU
1	AO	38	SER
1	AO	59	SER
1	AP	2	SER
1	AP	49	THR
1	AP	54	MET
1	AP	59	SER
1	AP	72	ASN
1	AP	109	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AP	114	LEU
1	AP	115	SER
1	AQ	114	LEU
1	AS	1	LEU
1	AS	28	THR
1	AS	38	SER
1	AS	59	SER
1	AT	2	SER
1	AT	58	LYS
1	AT	59	SER
1	AT	114	LEU
1	AT	115	SER
1	AU	1	LEU
1	AU	114	LEU
1	AW	38	SER
1	AW	59	SER
1	AW	65	LYS
1	AX	2	SER
1	AX	49	THR
1	AX	114	LEU
1	AX	115	SER
1	AY	114	LEU
1	BA	1	LEU
1	BA	42	LYS
1	BA	51	ARG
1	BA	59	SER
1	BB	49	THR
1	BB	59	SER
1	BB	72	ASN
1	BB	114	LEU
1	BB	115	SER
1	BC	55	ASN
1	BC	101	SER
1	BC	114	LEU
1	BE	1	LEU
1	BE	38	SER
1	BE	59	SER
1	BF	2	SER
1	BF	49	THR
1	BF	54	MET
1	BF	59	SER
1	BF	109	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BF	114	LEU
1	BF	115	SER
1	BG	114	LEU
1	BI	1	LEU
1	BI	28	THR
1	BI	38	SER
1	BI	59	SER
1	BJ	2	SER
1	BJ	58	LYS
1	BJ	59	SER
1	BJ	114	LEU
1	BJ	115	SER
1	BK	114	LEU
1	BM	1	LEU
1	BM	42	LYS
1	BM	51	ARG
1	BM	59	SER
1	BN	49	THR
1	BN	59	SER
1	BN	72	ASN
1	BN	114	LEU
1	BN	115	SER
1	BO	1	LEU
1	BO	49	THR
1	BO	114	LEU
1	BQ	38	SER
1	BQ	59	SER
1	BR	2	SER
1	BR	49	THR
1	BR	114	LEU
1	BR	115	SER
1	BS	114	LEU
1	BU	28	THR
1	BU	38	SER
1	BU	41	VAL
1	BU	42	LYS
1	BU	43	LYS
1	BU	59	SER
1	BV	49	THR
1	BV	114	LEU
1	BV	115	SER
1	BW	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BY	1	LEU
1	BY	28	THR
1	BY	38	SER
1	BY	59	SER
1	BZ	2	SER
1	BZ	58	LYS
1	BZ	59	SER
1	BZ	114	LEU
1	BZ	115	SER
1	CA	114	LEU
1	CC	1	LEU
1	CC	42	LYS
1	CC	51	ARG
1	CC	59	SER
1	CD	49	THR
1	CD	59	SER
1	CD	72	ASN
1	CD	114	LEU
1	CD	115	SER
1	CE	1	LEU
1	CE	114	LEU
1	CG	38	SER
1	CG	59	SER
1	CH	2	SER
1	CH	49	THR
1	CH	65	LYS
1	CH	114	LEU
1	CH	115	SER
1	CI	114	LEU
1	CK	1	LEU
1	CK	28	THR
1	CK	38	SER
1	CK	59	SER
1	CL	2	SER
1	CL	58	LYS
1	CL	59	SER
1	CL	114	LEU
1	CL	115	SER
1	CM	54	MET
1	CM	114	LEU
1	CO	28	THR
1	CO	38	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CO	41	VAL
1	CO	42	LYS
1	CO	43	LYS
1	CO	59	SER
1	CP	49	THR
1	CP	114	LEU
1	CP	115	SER
1	CQ	55	ASN
1	CQ	101	SER
1	CQ	114	LEU
1	CS	1	LEU
1	CS	38	SER
1	CS	59	SER
1	CT	2	SER
1	CT	49	THR
1	CT	54	MET
1	CT	59	SER
1	CT	109	LYS
1	CT	114	LEU
1	CT	115	SER
1	CU	1	LEU
1	CU	49	THR
1	CU	114	LEU
1	CW	38	SER
1	CW	58	LYS
1	CW	59	SER
1	CX	2	SER
1	CX	49	THR
1	CX	65	LYS
1	CX	114	LEU
1	CX	115	SER
1	CY	114	LEU
1	DA	1	LEU
1	DA	28	THR
1	DA	38	SER
1	DA	59	SER
1	DB	2	SER
1	DB	58	LYS
1	DB	59	SER
1	DB	114	LEU
1	DB	115	SER
1	DC	54	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DC	114	LEU
1	DE	28	THR
1	DE	38	SER
1	DE	41	VAL
1	DE	42	LYS
1	DE	43	LYS
1	DE	59	SER
1	DF	49	THR
1	DF	114	LEU
1	DF	115	SER
1	DG	1	LEU
1	DG	49	THR
1	DG	114	LEU
1	DI	38	SER
1	DI	59	SER
1	DJ	2	SER
1	DJ	49	THR
1	DJ	114	LEU
1	DJ	115	SER
1	DK	55	ASN
1	DK	101	SER
1	DK	114	LEU
1	DM	1	LEU
1	DM	38	SER
1	DM	59	SER
1	DN	2	SER
1	DN	49	THR
1	DN	54	MET
1	DN	59	SER
1	DN	109	LYS
1	DN	114	LEU
1	DN	115	SER
1	DO	114	LEU
1	DQ	1	LEU
1	DQ	42	LYS
1	DQ	59	SER
1	DR	49	THR
1	DR	59	SER
1	DR	72	ASN
1	DR	114	LEU
1	DR	115	SER
1	DS	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DU	28	THR
1	DU	38	SER
1	DU	41	VAL
1	DU	42	LYS
1	DU	43	LYS
1	DU	59	SER
1	DV	49	THR
1	DV	114	LEU
1	DV	115	SER
1	DW	1	LEU
1	DW	114	LEU
1	DY	38	SER
1	DY	59	SER
1	DY	65	LYS
1	DZ	2	SER
1	DZ	49	THR
1	DZ	114	LEU
1	DZ	115	SER
1	EA	101	SER
1	EA	114	LEU
1	EC	1	LEU
1	EC	38	SER
1	EC	59	SER
1	ED	2	SER
1	ED	49	THR
1	ED	54	MET
1	ED	59	SER
1	ED	109	LYS
1	ED	114	LEU
1	ED	115	SER
1	EE	114	LEU
1	EG	28	THR
1	EG	38	SER
1	EG	41	VAL
1	EG	42	LYS
1	EG	43	LYS
1	EG	59	SER
1	EH	49	THR
1	EH	114	LEU
1	EH	115	SER
1	EI	114	LEU
1	EK	1	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EK	42	LYS
1	EK	51	ARG
1	EK	59	SER
1	EL	10	ILE
1	EL	49	THR
1	EL	59	SER
1	EL	72	ASN
1	EL	114	LEU
1	EL	115	SER
1	EM	114	LEU
1	EO	1	LEU
1	EO	28	THR
1	EO	38	SER
1	EO	59	SER
1	EP	2	SER
1	EP	58	LYS
1	EP	59	SER
1	EP	114	LEU
1	EP	115	SER
1	EQ	55	ASN
1	EQ	101	SER
1	EQ	114	LEU
1	ES	1	LEU
1	ES	38	SER
1	ES	59	SER
1	ET	2	SER
1	ET	49	THR
1	ET	54	MET
1	ET	59	SER
1	ET	109	LYS
1	ET	114	LEU
1	ET	115	SER
1	EU	114	LEU
1	EW	1	LEU
1	EW	42	LYS
1	EW	51	ARG
1	EW	59	SER
1	EX	10	ILE
1	EX	49	THR
1	EX	59	SER
1	EX	72	ASN
1	EX	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EX	115	SER
1	EY	114	LEU
1	FA	28	THR
1	FA	38	SER
1	FA	41	VAL
1	FA	42	LYS
1	FA	43	LYS
1	FA	59	SER
1	FB	49	THR
1	FB	114	LEU
1	FB	115	SER
1	FC	55	ASN
1	FC	101	SER
1	FC	114	LEU
1	FE	1	LEU
1	FE	38	SER
1	FE	59	SER
1	FF	2	SER
1	FF	49	THR
1	FF	54	MET
1	FF	59	SER
1	FF	109	LYS
1	FF	114	LEU
1	FF	115	SER
1	FG	1	LEU
1	FG	114	LEU
1	FI	38	SER
1	FI	59	SER
1	FI	65	LYS
1	FJ	2	SER
1	FJ	49	THR
1	FJ	65	LYS
1	FJ	114	LEU
1	FJ	115	SER
1	FK	114	LEU
1	FM	1	LEU
1	FM	28	THR
1	FM	38	SER
1	FM	59	SER
1	FN	2	SER
1	FN	58	LYS
1	FN	59	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	FN	114	LEU
1	FN	115	SER
1	FO	114	LEU
1	FQ	28	THR
1	FQ	38	SER
1	FQ	41	VAL
1	FQ	42	LYS
1	FQ	43	LYS
1	FQ	59	SER
1	FR	49	THR
1	FR	114	LEU
1	FR	115	SER
1	FS	55	ASN
1	FS	101	SER
1	FS	114	LEU
1	FU	1	LEU
1	FU	38	SER
1	FU	59	SER
1	FV	2	SER
1	FV	49	THR
1	FV	54	MET
1	FV	59	SER
1	FV	109	LYS
1	FV	114	LEU
1	FV	115	SER
1	FW	1	LEU
1	FW	49	THR
1	FW	114	LEU
1	FY	28	THR
1	FY	38	SER
1	FY	58	LYS
1	FY	59	SER
1	FZ	2	SER
1	FZ	49	THR
1	FZ	114	LEU
1	FZ	115	SER
1	GA	10	ILE
1	GA	114	LEU
1	GC	28	THR
1	GC	38	SER
1	GC	41	VAL
1	GC	42	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	GC	43	LYS
1	GC	59	SER
1	GD	49	THR
1	GD	114	LEU
1	GD	115	SER
1	GE	114	LEU
1	GG	28	THR
1	GG	38	SER
1	GG	59	SER
1	GH	2	SER
1	GH	39	LEU
1	GH	59	SER
1	GH	114	LEU
1	GH	115	SER
1	GI	13	ASN
1	GI	114	LEU
1	GK	1	LEU
1	GK	42	LYS
1	GK	59	SER
1	GL	49	THR
1	GL	59	SER
1	GL	114	LEU
1	GL	115	SER
1	GM	114	LEU
1	GO	28	THR
1	GO	38	SER
1	GO	58	LYS
1	GO	59	SER
1	GP	2	SER
1	GP	49	THR
1	GP	114	LEU
1	GP	115	SER
1	GQ	10	ILE
1	GQ	114	LEU
1	GS	28	THR
1	GS	38	SER
1	GS	41	VAL
1	GS	42	LYS
1	GS	43	LYS
1	GS	59	SER
1	GT	49	THR
1	GT	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	GT	115	SER
1	GU	10	ILE
1	GU	114	LEU
1	GW	28	THR
1	GW	38	SER
1	GW	59	SER
1	GX	2	SER
1	GX	39	LEU
1	GX	59	SER
1	GX	114	LEU
1	GX	115	SER
1	GY	114	LEU
1	HA	28	THR
1	HA	38	SER
1	HA	58	LYS
1	HA	59	SER
1	HB	2	SER
1	HB	49	THR
1	HB	114	LEU
1	HB	115	SER
1	HC	13	ASN
1	HC	114	LEU
1	HE	1	LEU
1	HE	42	LYS
1	HE	59	SER
1	HF	49	THR
1	HF	59	SER
1	HF	114	LEU
1	HF	115	SER
1	HG	101	SER
1	HG	114	LEU
1	HI	1	LEU
1	HI	38	SER
1	HI	59	SER
1	HJ	2	SER
1	HJ	49	THR
1	HJ	59	SER
1	HJ	72	ASN
1	HJ	109	LYS
1	HJ	114	LEU
1	HJ	115	SER
1	HK	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	HM	28	THR
1	HM	38	SER
1	HM	59	SER
1	HN	2	SER
1	HN	39	LEU
1	HN	59	SER
1	HN	114	LEU
1	HN	115	SER
1	HO	114	LEU
1	HQ	28	THR
1	HQ	38	SER
1	HQ	58	LYS
1	HQ	59	SER
1	HR	2	SER
1	HR	49	THR
1	HR	114	LEU
1	HR	115	SER
1	HS	13	ASN
1	HS	114	LEU
1	HU	1	LEU
1	HU	42	LYS
1	HU	59	SER
1	HV	49	THR
1	HV	59	SER
1	HV	114	LEU
1	HV	115	SER
1	HW	114	LEU
1	HY	28	THR
1	HY	38	SER
1	HY	59	SER
1	HZ	2	SER
1	HZ	39	LEU
1	HZ	59	SER
1	HZ	114	LEU
1	HZ	115	SER
1	IA	101	SER
1	IA	114	LEU
1	IC	1	LEU
1	IC	38	SER
1	IC	59	SER
1	ID	2	SER
1	ID	49	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	ID	54	MET
1	ID	59	SER
1	ID	72	ASN
1	ID	109	LYS
1	ID	114	LEU
1	ID	115	SER
1	IE	114	LEU
1	IG	28	THR
1	IG	38	SER
1	IG	41	VAL
1	IG	42	LYS
1	IG	43	LYS
1	IG	59	SER
1	IH	49	THR
1	IH	114	LEU
1	IH	115	SER
1	II	13	ASN
1	II	114	LEU
1	IK	1	LEU
1	IK	42	LYS
1	IK	59	SER
1	IL	49	THR
1	IL	59	SER
1	IL	114	LEU
1	IL	115	SER
1	IM	114	LEU
1	IO	28	THR
1	IO	38	SER
1	IO	59	SER
1	IP	2	SER
1	IP	39	LEU
1	IP	59	SER
1	IP	114	LEU
1	IP	115	SER
1	IQ	101	SER
1	IQ	114	LEU
1	IS	1	LEU
1	IS	38	SER
1	IS	59	SER
1	IT	2	SER
1	IT	49	THR
1	IT	54	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	IT	59	SER
1	IT	72	ASN
1	IT	109	LYS
1	IT	114	LEU
1	IT	115	SER
1	IU	13	ASN
1	IU	114	LEU
1	IW	1	LEU
1	IW	42	LYS
1	IW	59	SER
1	IX	49	THR
1	IX	59	SER
1	IX	114	LEU
1	IX	115	SER
1	IY	114	LEU
1	JA	28	THR
1	JA	38	SER
1	JA	41	VAL
1	JA	42	LYS
1	JA	43	LYS
1	JA	59	SER
1	JB	49	THR
1	JB	114	LEU
1	JB	115	SER
1	JC	114	LEU
1	JE	28	THR
1	JE	38	SER
1	JE	58	LYS
1	JE	59	SER
1	JF	2	SER
1	JF	49	THR
1	JF	114	LEU
1	JF	115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (252) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	53	ASN
1	AA	76	HIS
1	AC	53	ASN
1	AC	55	ASN
1	AC	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AE	53	ASN
1	AE	55	ASN
1	AI	13	ASN
1	AI	53	ASN
1	AI	55	ASN
1	AK	55	ASN
1	AK	72	ASN
1	AK	76	HIS
1	AM	53	ASN
1	AM	55	ASN
1	AO	53	ASN
1	AO	55	ASN
1	AO	72	ASN
1	AQ	53	ASN
1	AQ	55	ASN
1	AS	53	ASN
1	AS	55	ASN
1	AS	72	ASN
1	AT	7	ASN
1	AU	53	ASN
1	AW	55	ASN
1	AW	72	ASN
1	AX	55	ASN
1	AY	53	ASN
1	AY	55	ASN
1	BA	55	ASN
1	BA	72	ASN
1	BA	76	HIS
1	BC	53	ASN
1	BC	55	ASN
1	BE	7	ASN
1	BE	53	ASN
1	BF	72	ASN
1	BG	53	ASN
1	BI	53	ASN
1	BI	55	ASN
1	BI	72	ASN
1	BJ	72	ASN
1	BK	53	ASN
1	BK	55	ASN
1	BM	55	ASN
1	BM	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BM	76	HIS
1	BO	53	ASN
1	BQ	55	ASN
1	BQ	72	ASN
1	BR	55	ASN
1	BS	53	ASN
1	BW	53	ASN
1	BY	53	ASN
1	BY	55	ASN
1	BY	72	ASN
1	BZ	72	ASN
1	CA	53	ASN
1	CA	55	ASN
1	CC	55	ASN
1	CC	72	ASN
1	CC	76	HIS
1	CE	53	ASN
1	CG	55	ASN
1	CG	72	ASN
1	CH	55	ASN
1	CI	53	ASN
1	CK	53	ASN
1	CK	55	ASN
1	CK	72	ASN
1	CL	72	ASN
1	CM	53	ASN
1	CQ	53	ASN
1	CQ	55	ASN
1	CQ	72	ASN
1	CS	53	ASN
1	CS	55	ASN
1	CS	72	ASN
1	CU	53	ASN
1	CW	55	ASN
1	CW	72	ASN
1	CX	55	ASN
1	CY	53	ASN
1	DA	53	ASN
1	DA	55	ASN
1	DA	72	ASN
1	DB	72	ASN
1	DC	53	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DC	55	ASN
1	DE	53	ASN
1	DE	55	ASN
1	DE	72	ASN
1	DG	53	ASN
1	DI	55	ASN
1	DI	72	ASN
1	DJ	55	ASN
1	DK	53	ASN
1	DK	55	ASN
1	DM	53	ASN
1	DM	55	ASN
1	DM	72	ASN
1	DN	72	ASN
1	DO	13	ASN
1	DO	53	ASN
1	DO	55	ASN
1	DQ	55	ASN
1	DQ	72	ASN
1	DQ	76	HIS
1	DS	53	ASN
1	DS	55	ASN
1	DY	55	ASN
1	DY	72	ASN
1	DZ	55	ASN
1	EA	53	ASN
1	EA	55	ASN
1	EA	76	HIS
1	EC	53	ASN
1	EC	55	ASN
1	EC	72	ASN
1	ED	53	ASN
1	ED	72	ASN
1	EE	53	ASN
1	EE	55	ASN
1	EI	13	ASN
1	EI	53	ASN
1	EI	55	ASN
1	EK	55	ASN
1	EK	72	ASN
1	EK	76	HIS
1	EM	53	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EM	55	ASN
1	EO	53	ASN
1	EO	55	ASN
1	EO	72	ASN
1	EP	7	ASN
1	EQ	53	ASN
1	EQ	55	ASN
1	EQ	72	ASN
1	ES	53	ASN
1	ES	55	ASN
1	ES	72	ASN
1	EU	53	ASN
1	EU	55	ASN
1	EW	55	ASN
1	EW	72	ASN
1	EW	76	HIS
1	EY	53	ASN
1	EY	55	ASN
1	FA	53	ASN
1	FA	55	ASN
1	FA	72	ASN
1	FC	53	ASN
1	FC	55	ASN
1	FC	72	ASN
1	FE	53	ASN
1	FE	55	ASN
1	FE	72	ASN
1	FG	53	ASN
1	FI	55	ASN
1	FI	72	ASN
1	FJ	55	ASN
1	FK	53	ASN
1	FK	55	ASN
1	FM	53	ASN
1	FM	55	ASN
1	FM	72	ASN
1	FO	53	ASN
1	FO	55	ASN
1	FO	72	ASN
1	FS	53	ASN
1	FS	55	ASN
1	FU	53	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	FW	53	ASN
1	FY	55	ASN
1	FY	72	ASN
1	FZ	55	ASN
1	GA	53	ASN
1	GC	55	ASN
1	GC	72	ASN
1	GC	76	HIS
1	GE	53	ASN
1	GI	53	ASN
1	GK	72	ASN
1	GK	76	HIS
1	GL	53	ASN
1	GM	53	ASN
1	GO	55	ASN
1	GO	72	ASN
1	GP	55	ASN
1	GQ	53	ASN
1	GQ	55	ASN
1	GS	53	ASN
1	GS	55	ASN
1	GS	72	ASN
1	GS	76	HIS
1	GU	53	ASN
1	GW	53	ASN
1	GW	55	ASN
1	GW	72	ASN
1	GY	53	ASN
1	HA	55	ASN
1	HA	72	ASN
1	HB	55	ASN
1	HC	53	ASN
1	HE	76	HIS
1	HF	53	ASN
1	HG	72	ASN
1	HG	76	HIS
1	HI	76	HIS
1	HJ	72	ASN
1	HK	53	ASN
1	HO	53	ASN
1	HQ	55	ASN
1	HQ	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	HR	55	ASN
1	HS	53	ASN
1	HU	76	HIS
1	HV	53	ASN
1	HW	53	ASN
1	IA	72	ASN
1	IA	76	HIS
1	IC	55	ASN
1	IC	72	ASN
1	IC	76	HIS
1	ID	72	ASN
1	IE	53	ASN
1	IG	55	ASN
1	IG	72	ASN
1	IG	76	HIS
1	II	7	ASN
1	II	53	ASN
1	IK	76	HIS
1	IL	53	ASN
1	IM	53	ASN
1	IQ	76	HIS
1	IS	55	ASN
1	IS	72	ASN
1	IS	76	HIS
1	IT	72	ASN
1	IU	7	ASN
1	IU	53	ASN
1	IW	76	HIS
1	IX	53	ASN
1	IY	53	ASN
1	JA	55	ASN
1	JA	72	ASN
1	JA	76	HIS
1	JC	53	ASN
1	JE	55	ASN
1	JE	72	ASN
1	JF	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

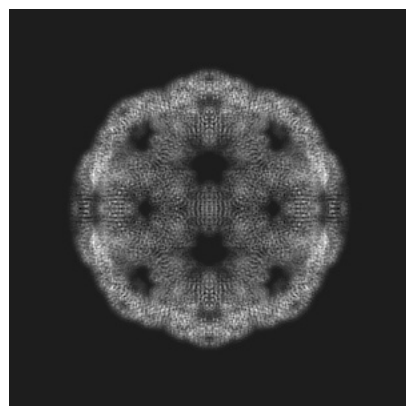
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52007. These allow visual inspection of the internal detail of the map and identification of artifacts.

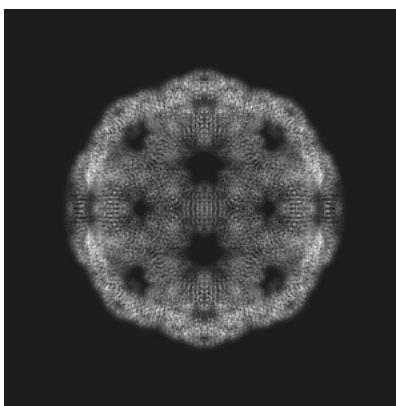
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

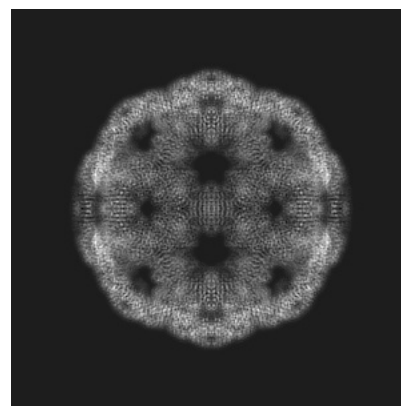
6.1.1 Primary map



X

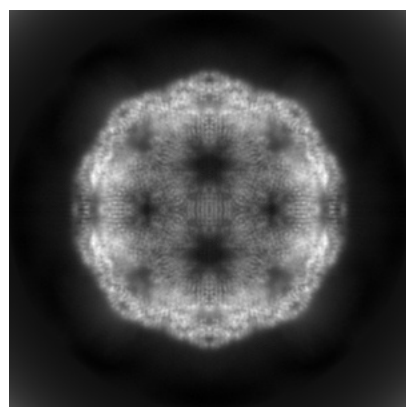


Y

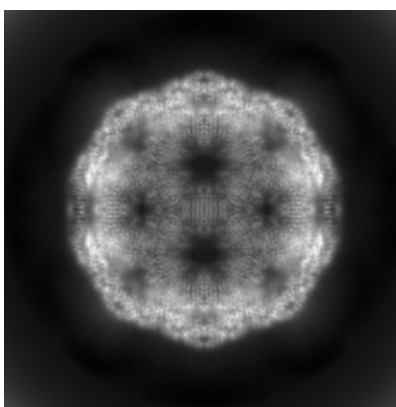


Z

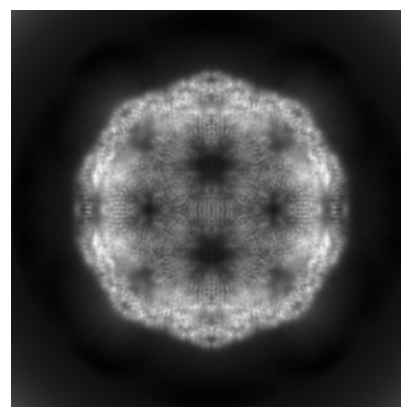
6.1.2 Raw map



X



Y

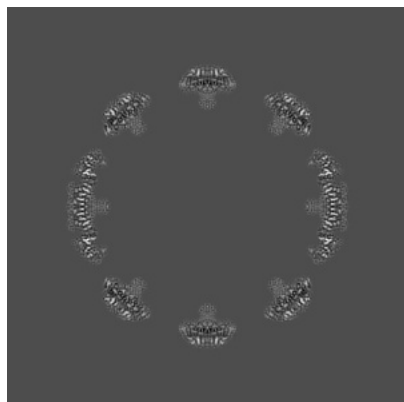


Z

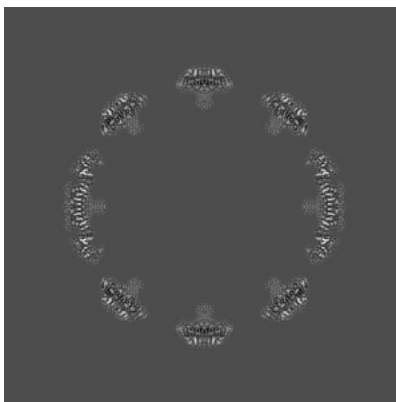
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

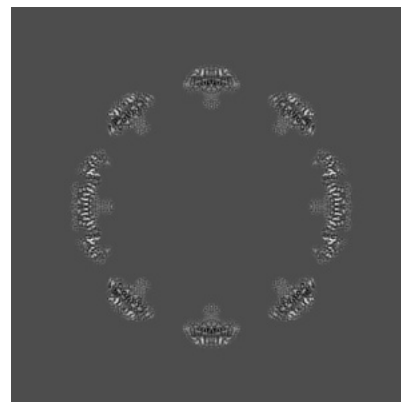
6.2.1 Primary map



X Index: 256

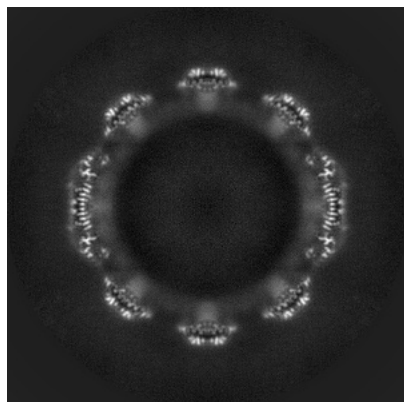


Y Index: 256

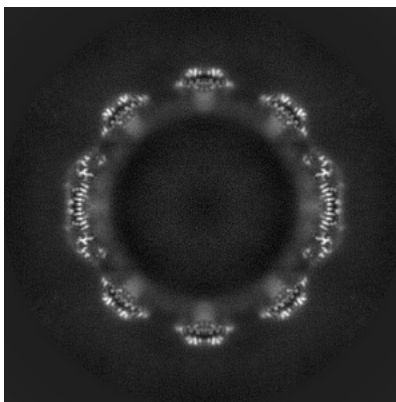


Z Index: 256

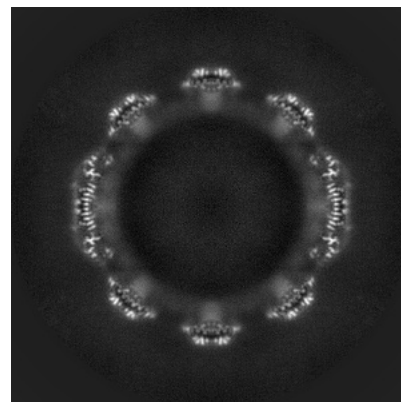
6.2.2 Raw map



X Index: 256



Y Index: 256

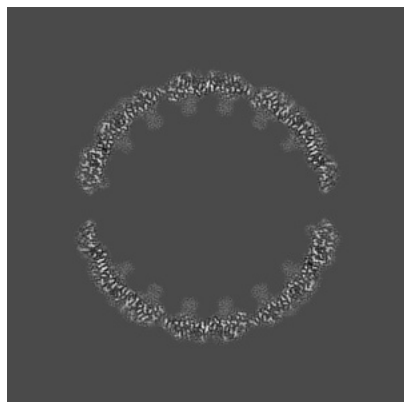


Z Index: 256

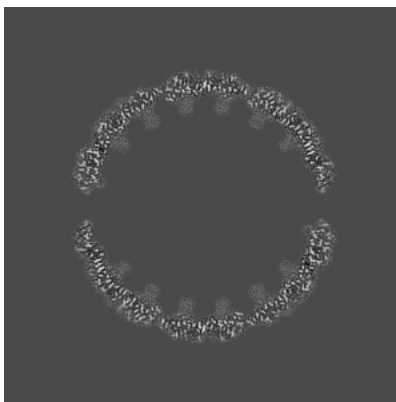
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

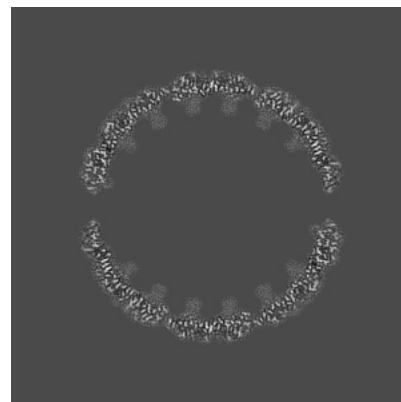
6.3.1 Primary map



X Index: 213

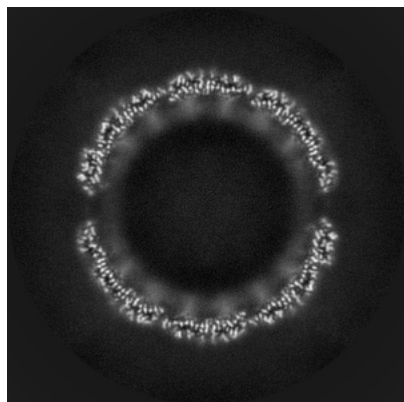


Y Index: 213

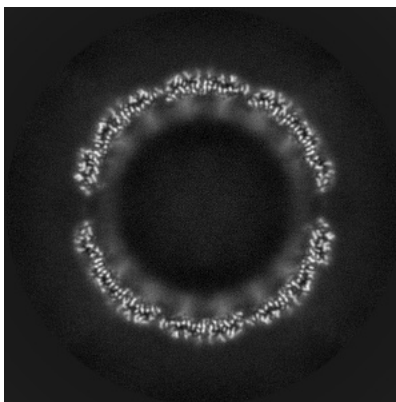


Z Index: 213

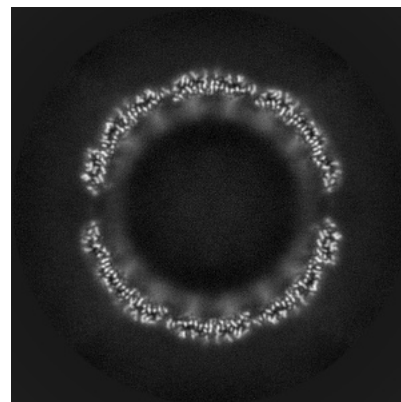
6.3.2 Raw map



X Index: 214



Y Index: 214

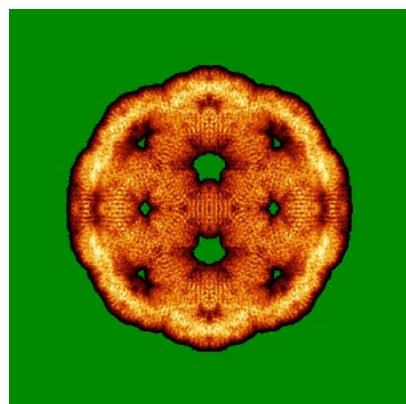


Z Index: 214

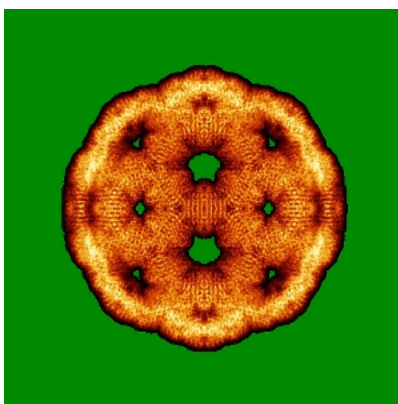
The images above show the largest variance slices of the map in three orthogonal directions.

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

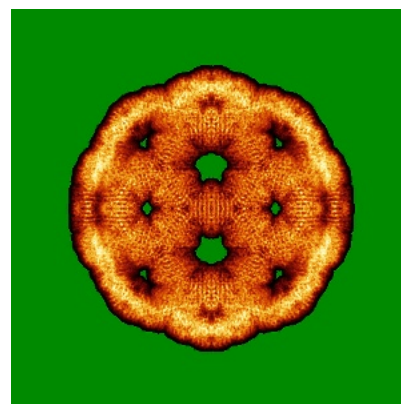
6.4.1 Primary map



X

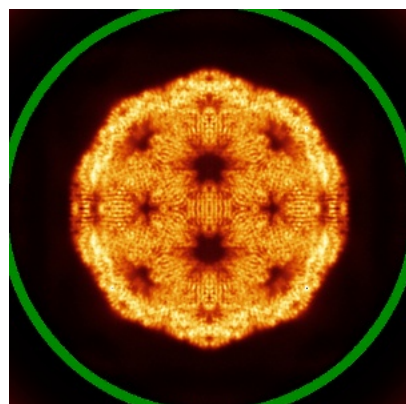


Y

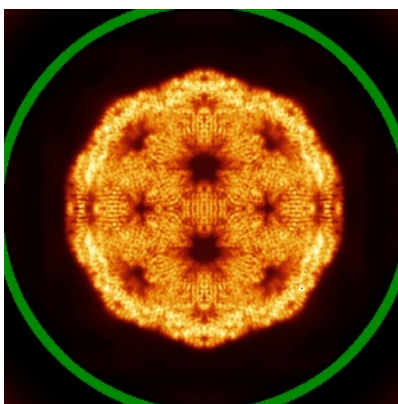


Z

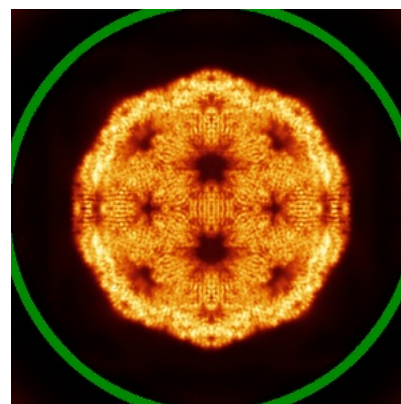
6.4.2 Raw map



X



Y

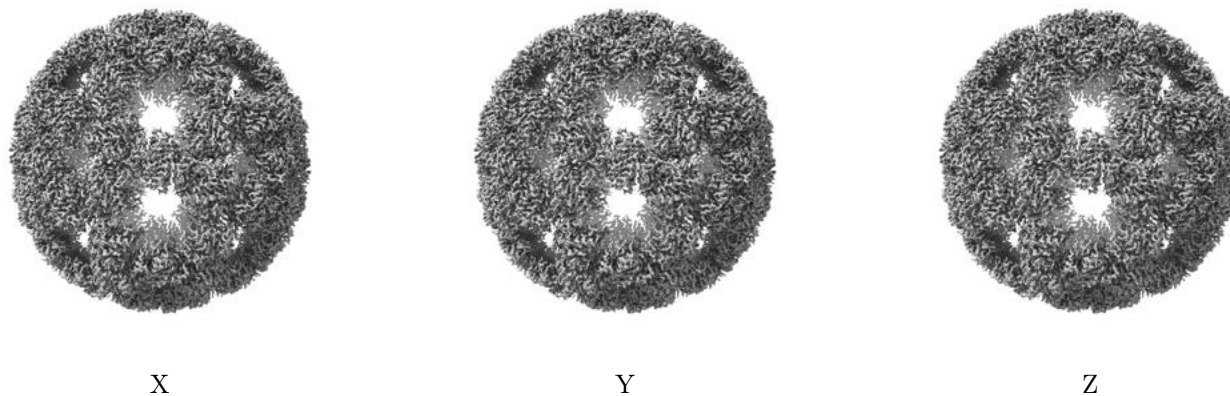


Z

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.

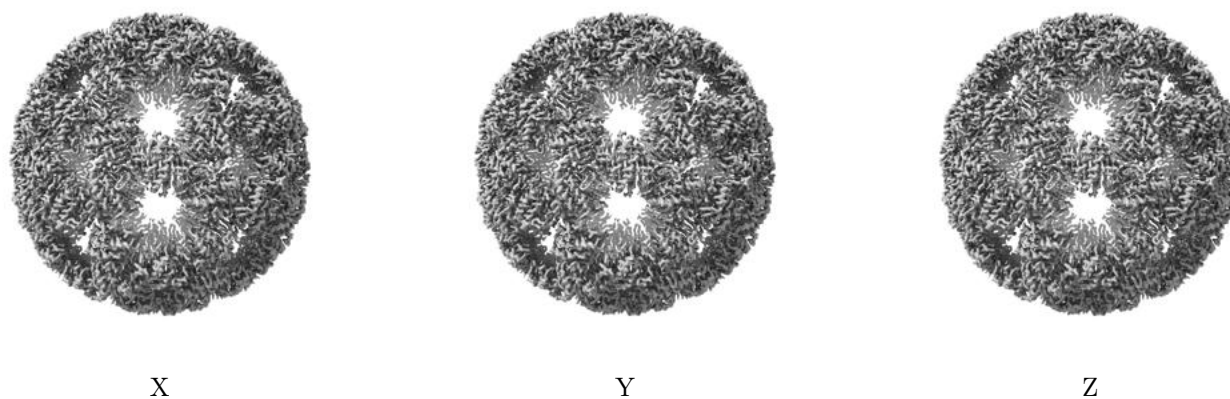
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

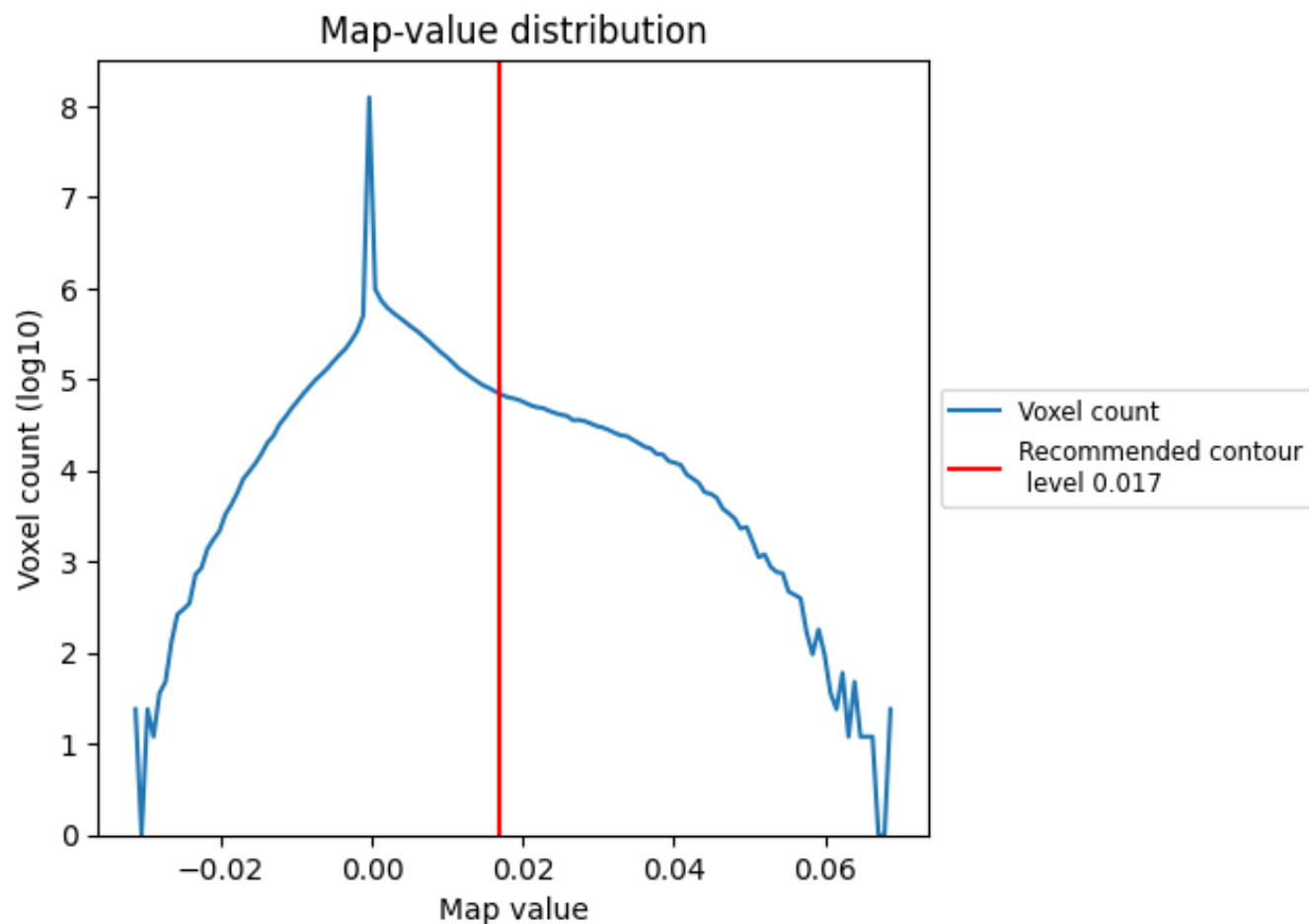
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

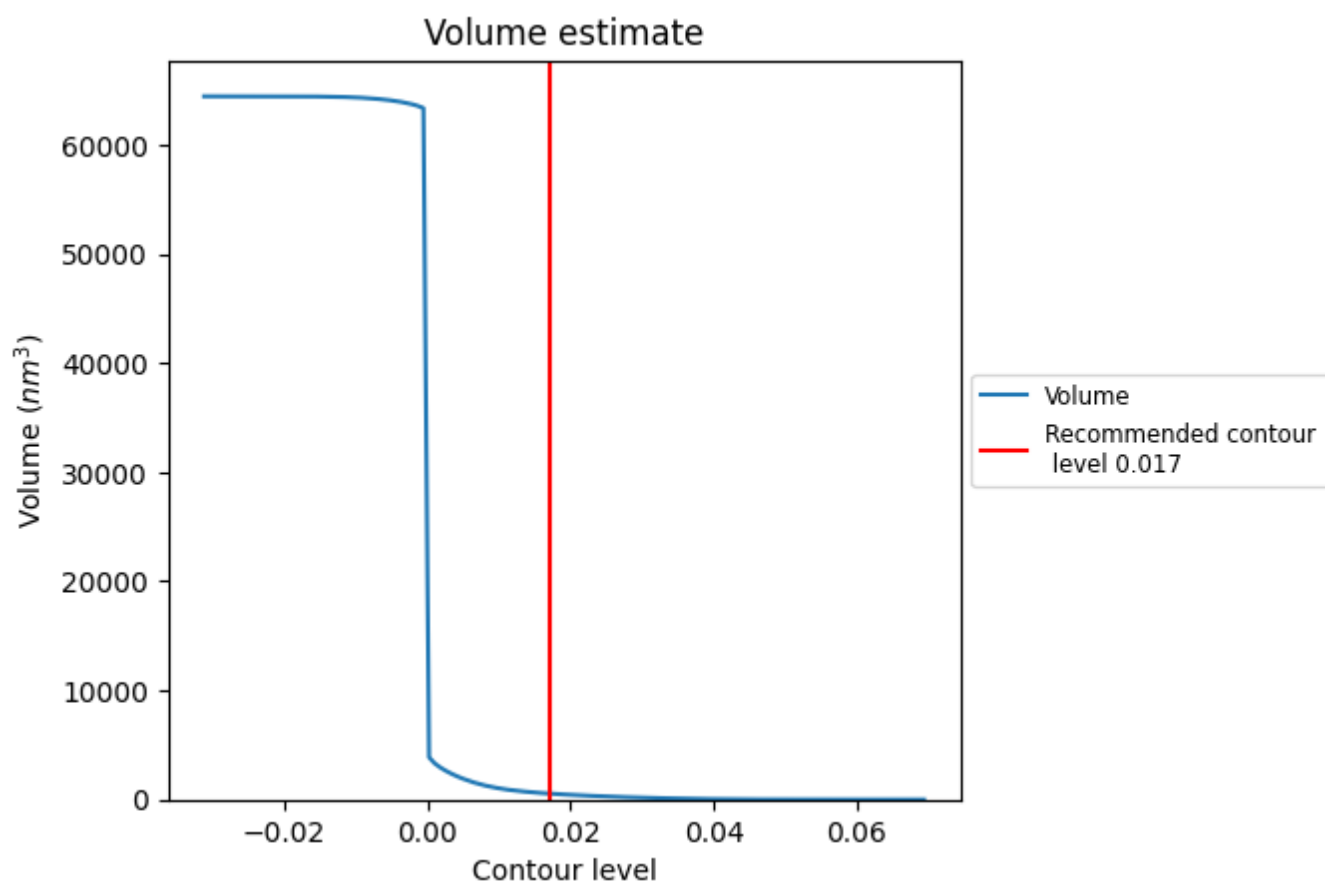
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

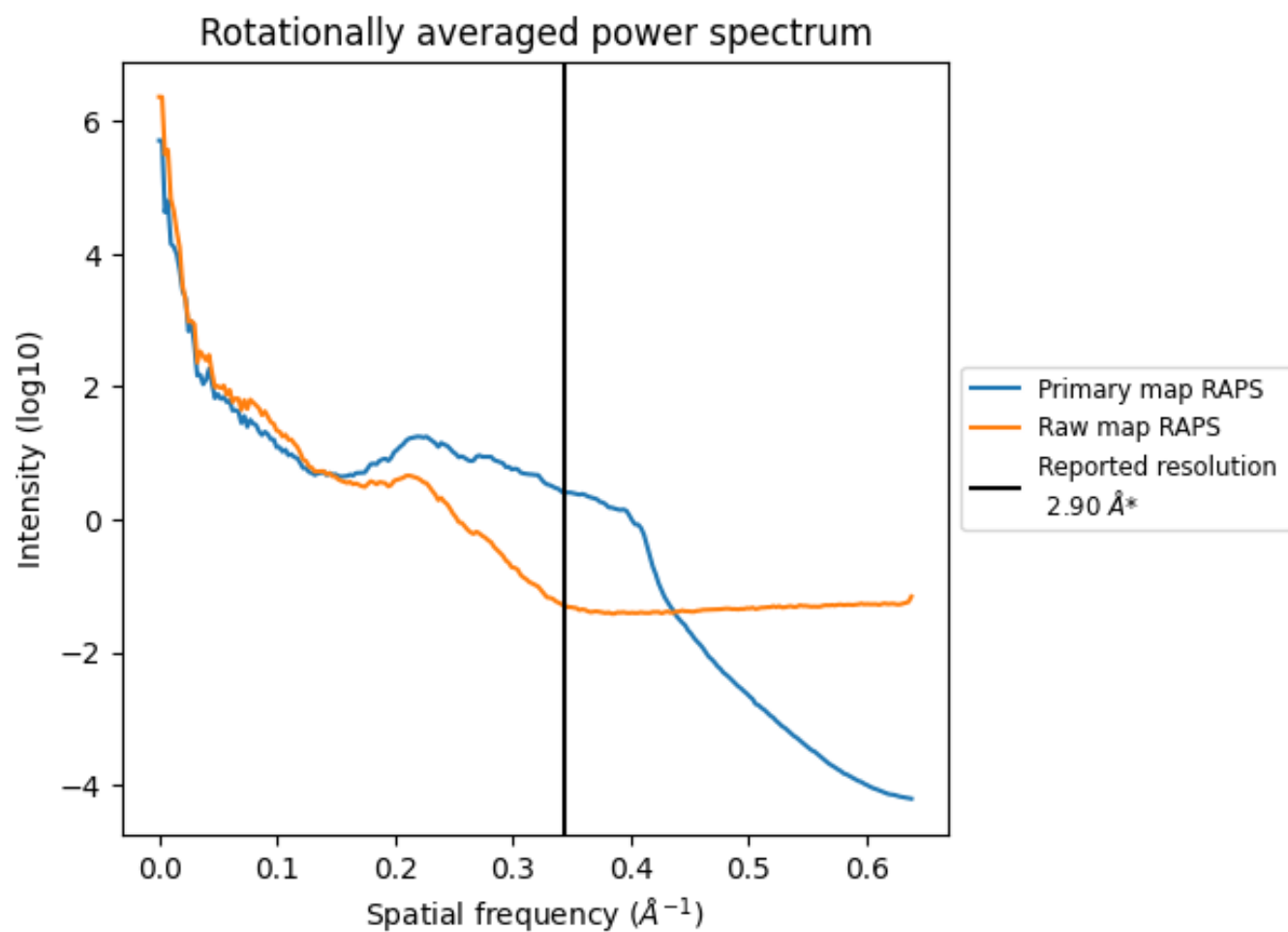
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 550 nm³; this corresponds to an approximate mass of 497 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](#)

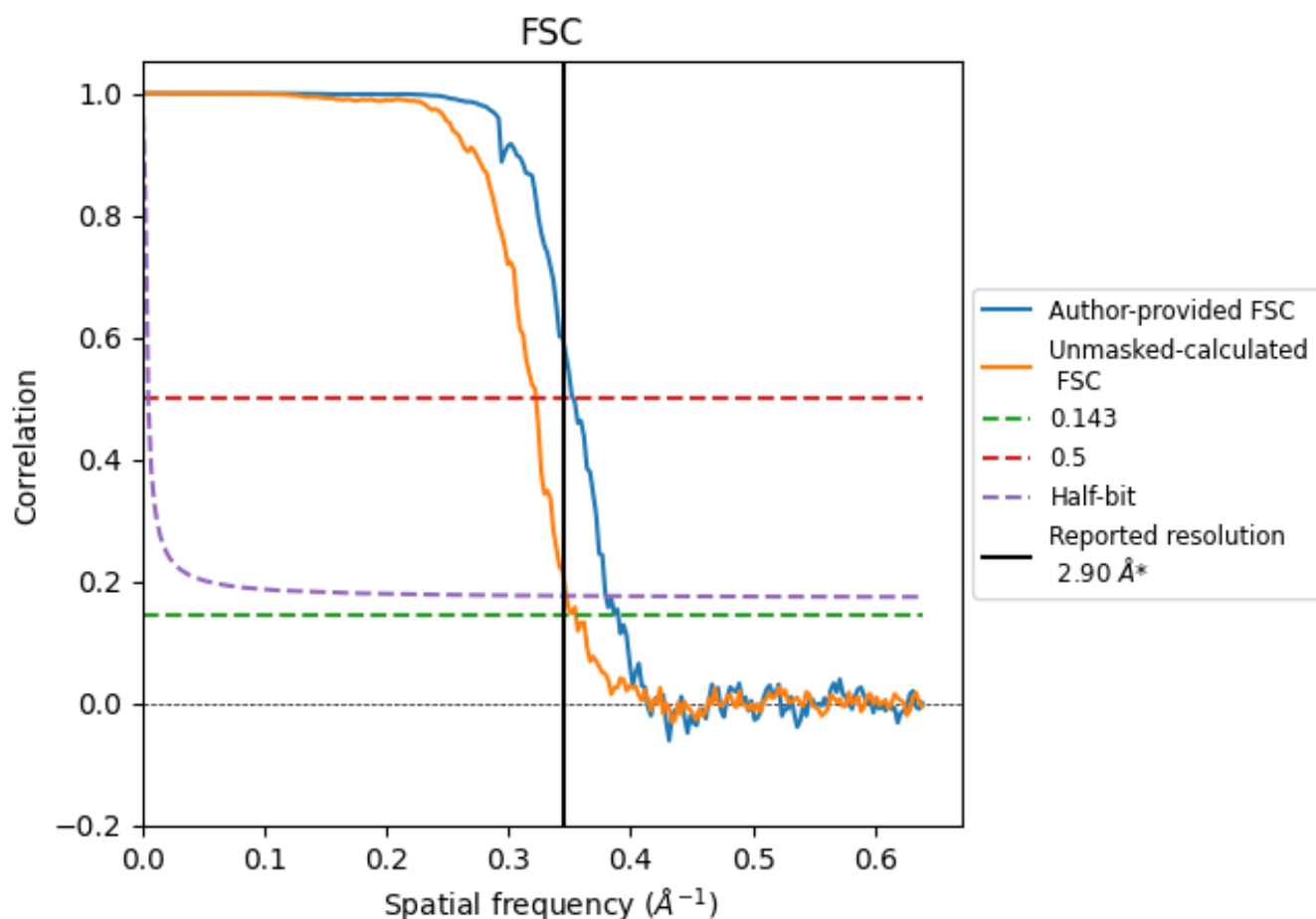


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

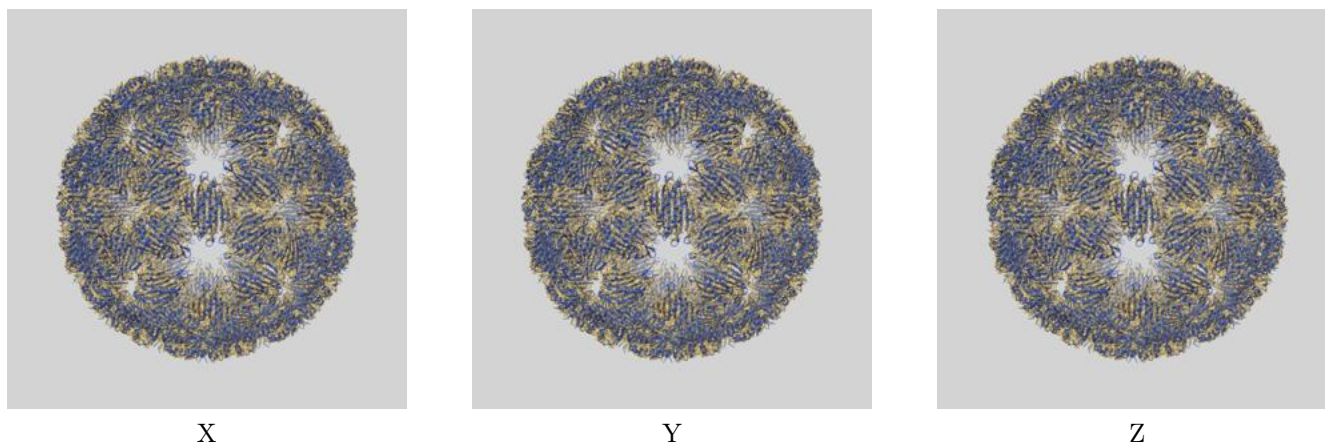
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.57	2.83	2.63
Unmasked-calculated*	2.82	3.10	2.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.57 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

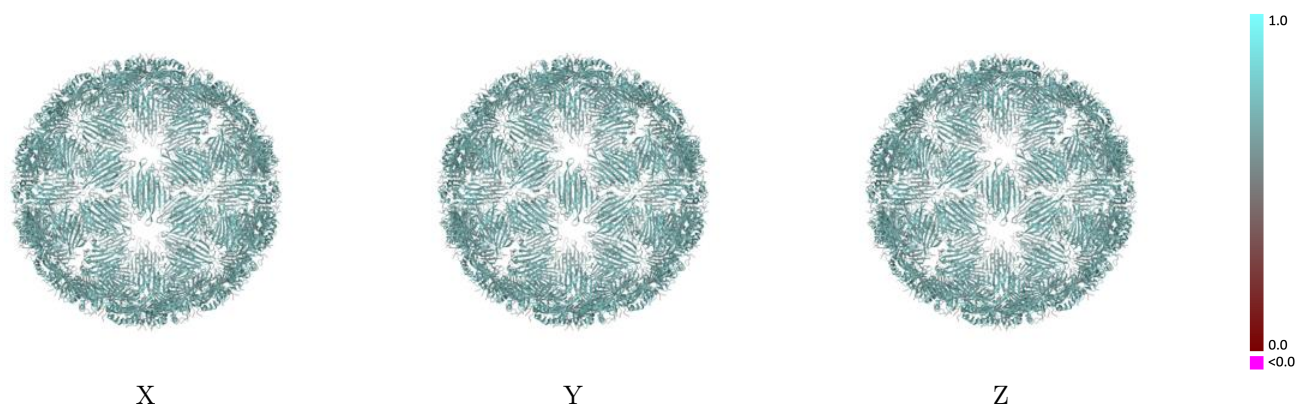
This section contains information regarding the fit between EMDB map EMD-52007 and PDB model 9HAU. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



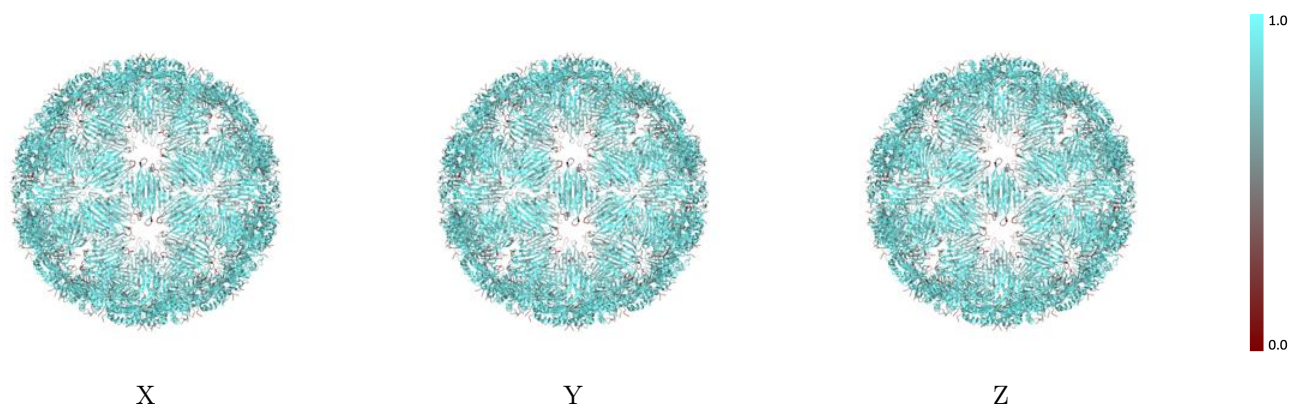
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



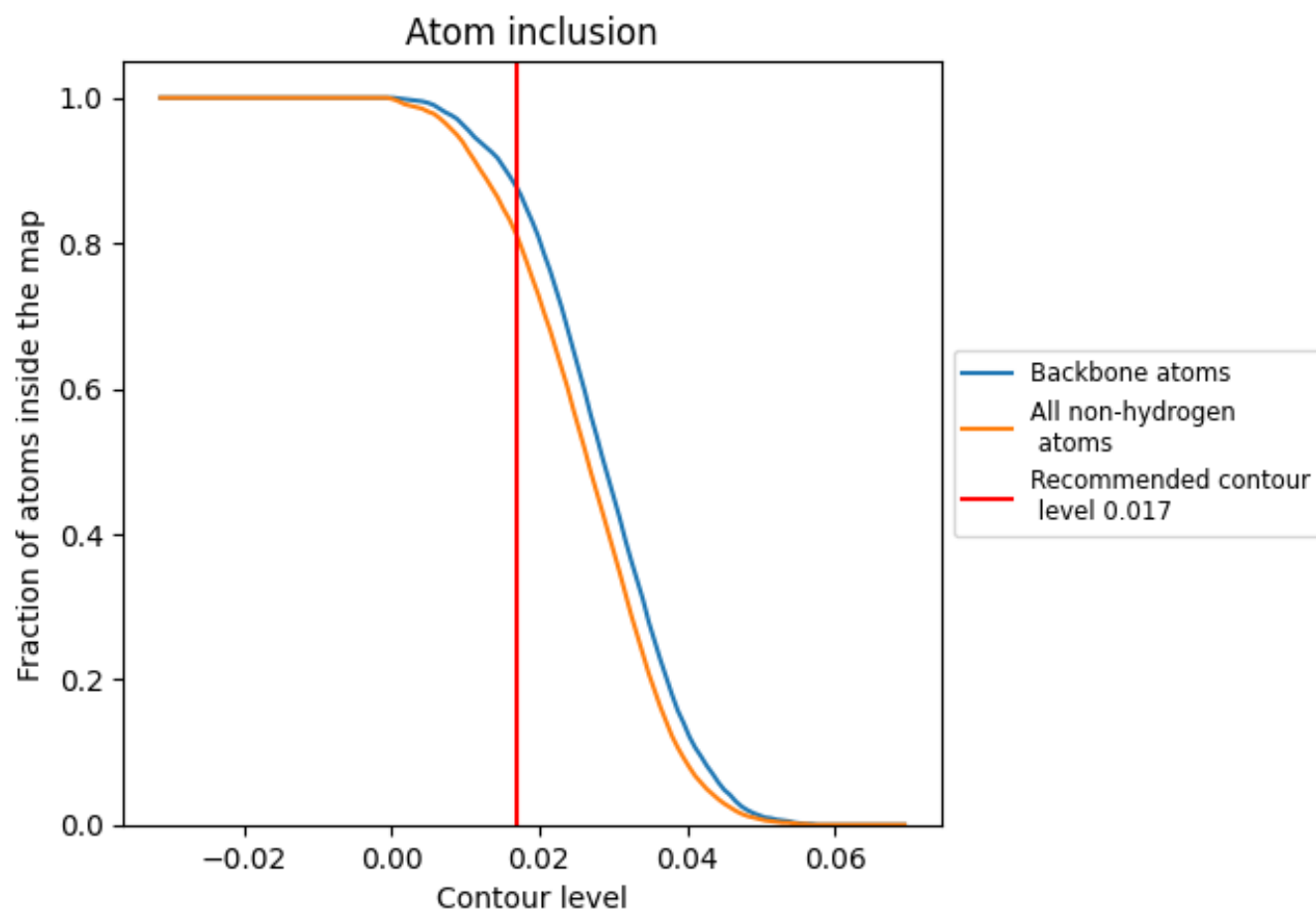
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8100	 0.6620
AA	 0.8410	 0.6670
AC	 0.8270	 0.6660
AD	 0.7590	 0.6570
AE	 0.8390	 0.6660
AG	 0.8220	 0.6650
AH	 0.7640	 0.6540
AI	 0.8360	 0.6670
AK	 0.8210	 0.6640
AL	 0.7510	 0.6530
AM	 0.8390	 0.6670
AO	 0.8270	 0.6670
AP	 0.7590	 0.6580
AQ	 0.8420	 0.6680
AS	 0.8270	 0.6660
AT	 0.7710	 0.6500
AU	 0.8390	 0.6680
AW	 0.8290	 0.6650
AX	 0.7550	 0.6540
AY	 0.8360	 0.6670
BA	 0.8210	 0.6640
BB	 0.7510	 0.6550
BC	 0.8410	 0.6670
BE	 0.8270	 0.6670
BF	 0.7590	 0.6540
BG	 0.8400	 0.6690
BI	 0.8270	 0.6680
BJ	 0.7710	 0.6530
BK	 0.8360	 0.6660
BM	 0.8210	 0.6630
BN	 0.7510	 0.6550
BO	 0.8390	 0.6670
BQ	 0.8290	 0.6650
BR	 0.7530	 0.6540
BS	 0.8390	 0.6630



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BU	 0.8220	 0.6620
BV	 0.7640	 0.6540
BW	 0.8400	 0.6700
BY	 0.8270	 0.6650
BZ	 0.7700	 0.6550
CA	 0.8360	 0.6670
CC	 0.8210	 0.6650
CD	 0.7510	 0.6530
CE	 0.8390	 0.6650
CG	 0.8290	 0.6620
CH	 0.7550	 0.6540
CI	 0.8400	 0.6690
CK	 0.8270	 0.6650
CL	 0.7700	 0.6570
CM	 0.8390	 0.6630
CO	 0.8220	 0.6610
CP	 0.7620	 0.6550
CQ	 0.8410	 0.6680
CS	 0.8280	 0.6680
CT	 0.7590	 0.6560
CU	 0.8390	 0.6680
CW	 0.8290	 0.6640
CX	 0.7550	 0.6520
CY	 0.8400	 0.6660
DA	 0.8270	 0.6650
DB	 0.7700	 0.6540
DC	 0.8400	 0.6660
DE	 0.8220	 0.6640
DF	 0.7640	 0.6560
DG	 0.8390	 0.6680
DI	 0.8290	 0.6640
DJ	 0.7550	 0.6540
DK	 0.8410	 0.6680
DM	 0.8270	 0.6680
DN	 0.7590	 0.6560
DO	 0.8360	 0.6640
DQ	 0.8210	 0.6620
DR	 0.7510	 0.6500
DS	 0.8390	 0.6640
DU	 0.8220	 0.6630
DV	 0.7630	 0.6550
DW	 0.8390	 0.6670

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DY	 0.8290	 0.6650
DZ	 0.7550	 0.6560
EA	 0.8410	 0.6660
EC	 0.8270	 0.6680
ED	 0.7590	 0.6540
EE	 0.8390	 0.6640
EG	 0.8220	 0.6620
EH	 0.7620	 0.6550
EI	 0.8360	 0.6650
EK	 0.8210	 0.6630
EL	 0.7510	 0.6490
EM	 0.8420	 0.6700
EO	 0.8270	 0.6670
EP	 0.7710	 0.6530
EQ	 0.8410	 0.6670
ES	 0.8280	 0.6670
ET	 0.7590	 0.6570
EU	 0.8360	 0.6660
EW	 0.8210	 0.6640
EX	 0.7510	 0.6520
EY	 0.8390	 0.6670
FA	 0.8220	 0.6640
FB	 0.7630	 0.6540
FC	 0.8410	 0.6670
FE	 0.8270	 0.6680
FF	 0.7590	 0.6580
FG	 0.8390	 0.6670
FI	 0.8290	 0.6620
FJ	 0.7550	 0.6520
FK	 0.8410	 0.6690
FM	 0.8270	 0.6670
FN	 0.7700	 0.6520
FO	 0.8400	 0.6640
FQ	 0.8220	 0.6620
FR	 0.7630	 0.6560
FS	 0.8410	 0.6680
FU	 0.8280	 0.6680
FV	 0.7600	 0.6550
FW	 0.8390	 0.6670
FY	 0.8290	 0.6650
FZ	 0.7660	 0.6570
GA	 0.8410	 0.6630

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GC	 0.8200	 0.6640
GD	 0.7630	 0.6590
GE	 0.8450	 0.6700
GG	 0.8350	 0.6670
GH	 0.7780	 0.6550
GI	 0.8360	 0.6660
GK	 0.8240	 0.6640
GL	 0.7530	 0.6530
GM	 0.8450	 0.6700
GO	 0.8310	 0.6650
GP	 0.7660	 0.6540
GQ	 0.8410	 0.6660
GS	 0.8210	 0.6660
GT	 0.7630	 0.6570
GU	 0.8460	 0.6660
GW	 0.8350	 0.6670
GX	 0.7790	 0.6550
GY	 0.8450	 0.6670
HA	 0.8310	 0.6650
HB	 0.7660	 0.6570
HC	 0.8360	 0.6650
HE	 0.8240	 0.6610
HF	 0.7530	 0.6550
HG	 0.8440	 0.6730
HI	 0.8330	 0.6690
HJ	 0.7690	 0.6570
HK	 0.8460	 0.6700
HM	 0.8340	 0.6680
HN	 0.7780	 0.6550
HO	 0.8450	 0.6660
HQ	 0.8310	 0.6630
HR	 0.7670	 0.6570
HS	 0.8360	 0.6680
HU	 0.8240	 0.6650
HV	 0.7530	 0.6540
HW	 0.8450	 0.6700
HY	 0.8350	 0.6680
HZ	 0.7780	 0.6560
IA	 0.8440	 0.6710
IC	 0.8330	 0.6690
ID	 0.7690	 0.6560
IE	 0.8410	 0.6640

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
IG	 0.8200	 0.6620
IH	 0.7630	 0.6550
II	 0.8360	 0.6650
IK	 0.8220	 0.6640
IL	 0.7530	 0.6560
IM	 0.8450	 0.6680
IO	 0.8340	 0.6690
IP	 0.7780	 0.6560
IQ	 0.8440	 0.6670
IS	 0.8330	 0.6660
IT	 0.7690	 0.6570
IU	 0.8360	 0.6630
IW	 0.8220	 0.6650
IX	 0.7530	 0.6560
IY	 0.8410	 0.6640
JA	 0.8200	 0.6620
JB	 0.7630	 0.6540
JC	 0.8450	 0.6680
JE	 0.8310	 0.6640
JF	 0.7670	 0.6550