



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 10:47 PM UTC

PDB ID : 8RVE / pdb_00008rve
EMDB ID : EMD-16844
Title : Vimentin intermediate filament
Authors : Eibauer, M.; Medalia, O.
Deposited on : 2024-02-01
Resolution : 7.20 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

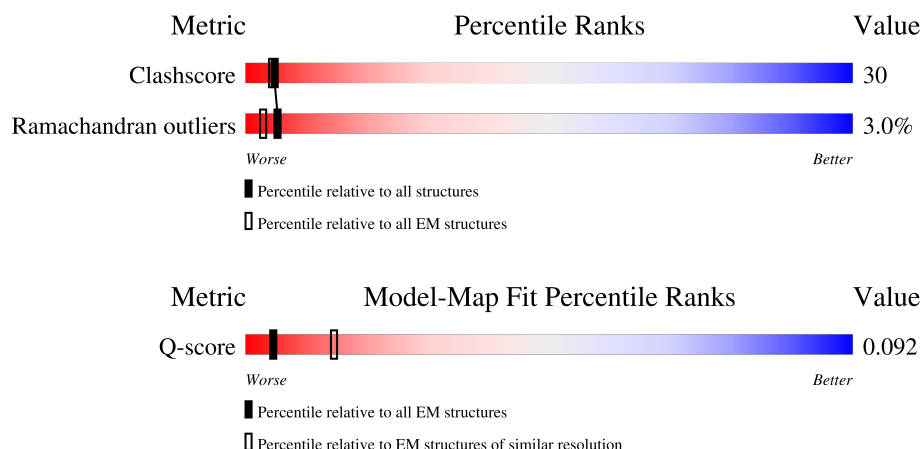
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	444 (6.70 - 7.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	466	
1	1	466	
1	2	466	
1	3	466	
1	4	466	

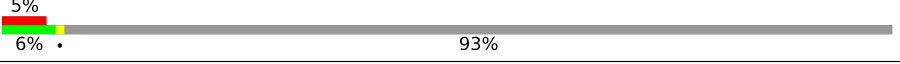
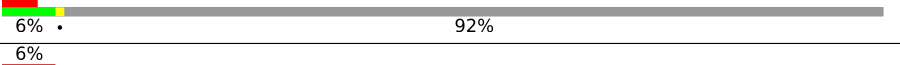
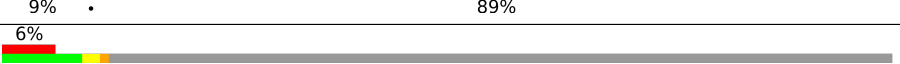
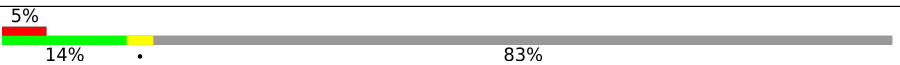
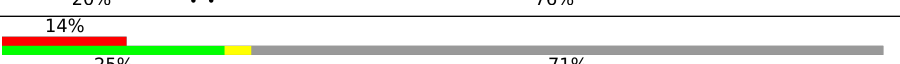
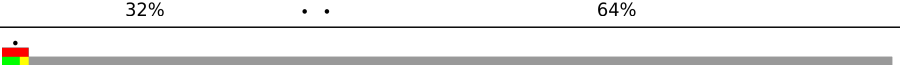
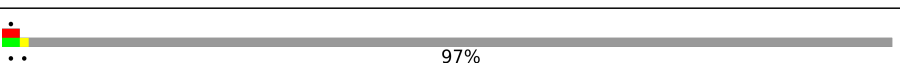
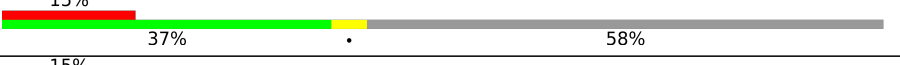
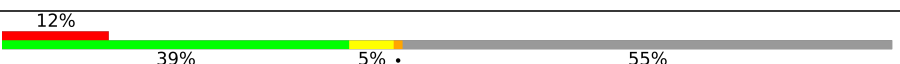
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	5	466	
1	6	466	
1	7	466	
1	8	466	
1	9	466	
1	A	466	
1	AA	466	
1	AB	466	
1	AC	466	
1	AD	466	
1	AE	466	
1	AF	466	
1	AG	466	
1	AH	466	
1	AI	466	
1	AJ	466	
1	AK	466	
1	AL	466	
1	AM	466	
1	AN	466	
1	AO	466	
1	AP	466	
1	B	466	
1	C	466	
1	D	466	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	466	
1	F	466	
1	G	466	
1	H	466	
1	I	466	
1	J	466	
1	K	466	
1	L	466	
1	M	466	
1	N	466	
1	O	466	
1	P	466	
1	Q	466	
1	R	466	
1	S	466	
1	T	466	
1	U	466	
1	V	466	
1	W	466	
1	X	466	
1	Y	466	
1	Z	466	
1	a	466	
1	b	466	
1	c	466	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	d	466	
1	e	466	
1	f	466	
1	g	466	
1	h	466	
1	i	466	
1	j	466	
1	k	466	
1	l	466	
1	m	466	
1	n	466	
1	o	466	
1	p	466	
1	q	466	
1	r	466	
1	s	466	
1	t	466	
1	u	466	
1	v	466	
1	w	466	
1	x	466	
1	y	466	
1	z	466	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 54788 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 Vimentin.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	253	Total	C	N	O	0	0
			1012	506	253	253		
1	1	273	Total	C	N	O	0	0
			1092	546	273	273		
1	2	266	Total	C	N	O	0	0
			1064	532	266	266		
1	3	191	Total	C	N	O	0	0
			764	382	191	191		
1	4	195	Total	C	N	O	0	0
			780	390	195	195		
1	5	267	Total	C	N	O	0	0
			1068	534	267	267		
1	6	263	Total	C	N	O	0	0
			1052	526	263	263		
1	7	142	Total	C	N	O	0	0
			568	284	142	142		
1	8	147	Total	C	N	O	0	0
			588	294	147	147		
1	9	252	Total	C	N	O	0	0
			1008	504	252	252		
1	A	281	Total	C	N	O	0	0
			1124	562	281	281		
1	AA	95	Total	C	N	O	0	0
			380	190	95	95		
1	AB	100	Total	C	N	O	0	0
			400	200	100	100		
1	AC	223	Total	C	N	O	0	0
			892	446	223	223		
1	AD	222	Total	C	N	O	0	0
			888	444	222	222		
1	AE	49	Total	C	N	O	0	0
			196	98	49	49		
1	AF	54	Total	C	N	O	0	0
			216	108	54	54		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AG	199	Total	C	N	O	0	0
			796	398	199	199		
1	AH	199	Total	C	N	O	0	0
			796	398	199	199		
1	AI	167	Total	C	N	O	0	0
			668	334	167	167		
1	AJ	170	Total	C	N	O	0	0
			680	340	170	170		
1	AK	136	Total	C	N	O	0	0
			544	272	136	136		
1	AL	141	Total	C	N	O	0	0
			564	282	141	141		
1	AM	81	Total	C	N	O	0	0
			324	162	81	81		
1	AN	85	Total	C	N	O	0	0
			340	170	85	85		
1	AO	34	Total	C	N	O	0	0
			136	68	34	34		
1	AP	39	Total	C	N	O	0	0
			156	78	39	39		
1	B	269	Total	C	N	O	0	0
			1076	538	269	269		
1	C	281	Total	C	N	O	0	0
			1124	562	281	281		
1	D	278	Total	C	N	O	0	0
			1112	556	278	278		
1	E	33	Total	C	N	O	0	0
			132	66	33	33		
1	F	35	Total	C	N	O	0	0
			140	70	35	35		
1	G	52	Total	C	N	O	0	0
			208	104	52	52		
1	H	54	Total	C	N	O	0	0
			216	108	54	54		
1	I	79	Total	C	N	O	0	0
			316	158	79	79		
1	J	83	Total	C	N	O	0	0
			332	166	83	83		
1	K	107	Total	C	N	O	0	0
			428	214	107	107		
1	L	113	Total	C	N	O	0	0
			452	226	113	113		

Continued on next page...

Continued from previous page...

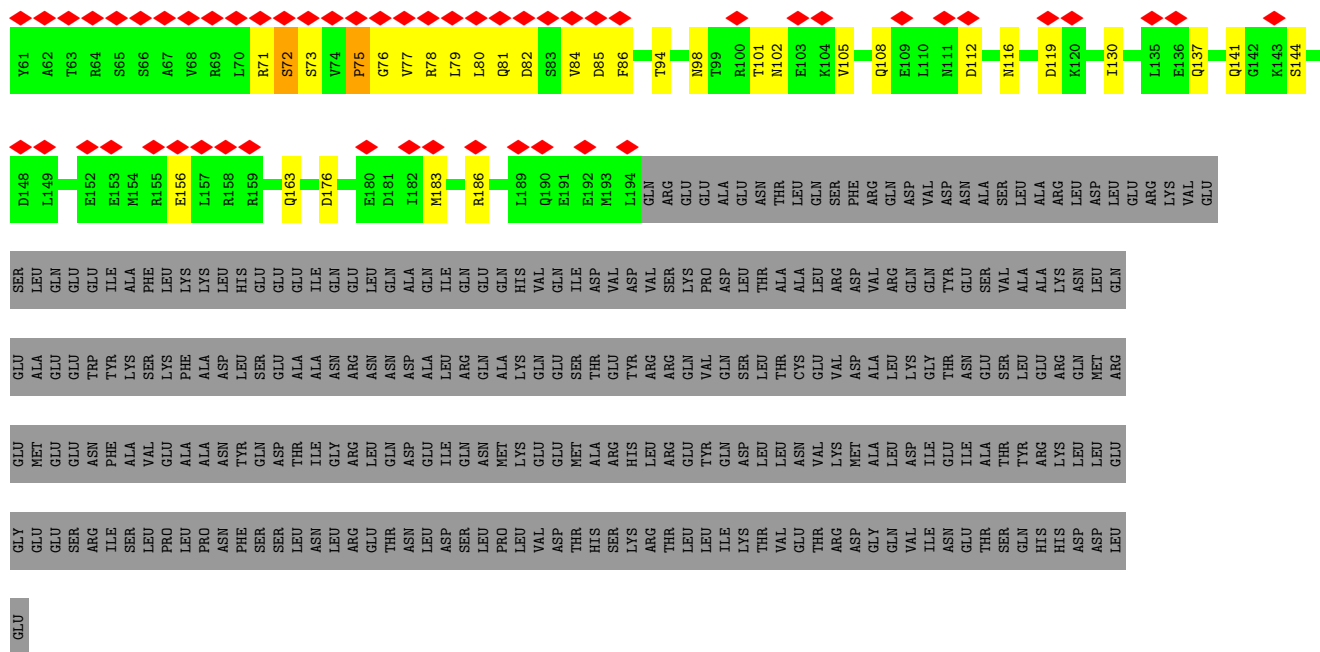
Mol	Chain	Residues	Atoms				AltConf	Trace
1	M	136	Total 544	C 272	N 136	O 136	0	0
1	N	142	Total 568	C 284	N 142	O 142	0	0
1	O	165	Total 660	C 330	N 165	O 165	0	0
1	P	170	Total 680	C 340	N 170	O 170	0	0
1	Q	14	Total 56	C 28	N 14	O 14	0	0
1	R	14	Total 56	C 28	N 14	O 14	0	0
1	S	194	Total 776	C 388	N 194	O 194	0	0
1	T	199	Total 796	C 398	N 199	O 199	0	0
1	U	53	Total 212	C 106	N 53	O 53	0	0
1	V	57	Total 228	C 114	N 57	O 57	0	0
1	W	194	Total 776	C 388	N 194	O 194	0	0
1	X	194	Total 776	C 388	N 194	O 194	0	0
1	Y	99	Total 396	C 198	N 99	O 99	0	0
1	Z	102	Total 408	C 204	N 102	O 102	0	0
1	a	209	Total 836	C 418	N 209	O 209	0	0
1	b	205	Total 820	C 410	N 205	O 205	0	0
1	c	148	Total 592	C 296	N 148	O 148	0	0
1	d	150	Total 600	C 300	N 150	O 150	0	0
1	e	214	Total 856	C 428	N 214	O 214	0	0
1	f	209	Total 836	C 418	N 209	O 209	0	0
1	g	194	Total 776	C 388	N 194	O 194	0	0

Continued on next page...

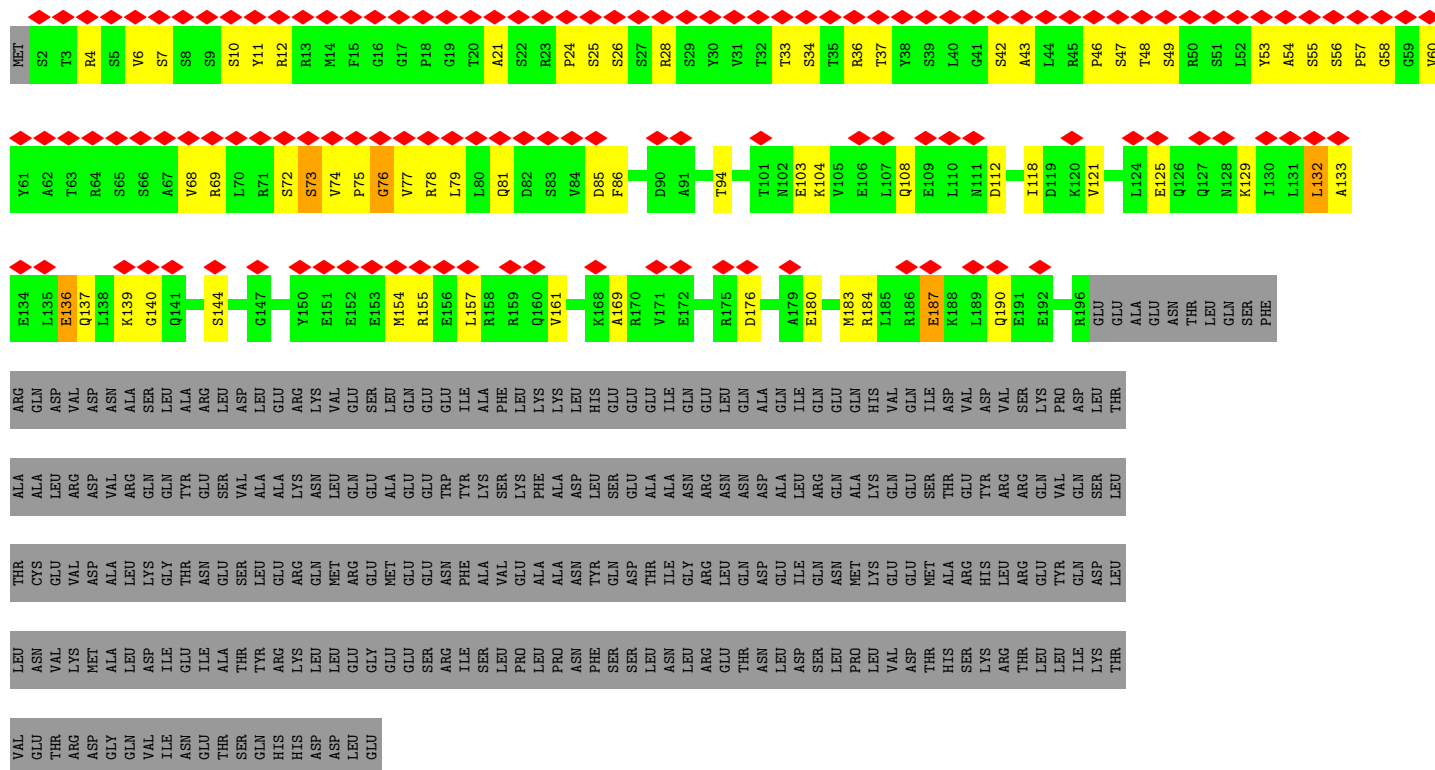
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	h	193	Total	C	N	O	0	0
			772	386	193	193		
1	i	246	Total	C	N	O	0	0
			984	492	246	246		
1	j	237	Total	C	N	O	0	0
			948	474	237	237		
1	k	224	Total	C	N	O	0	0
			896	448	224	224		
1	l	225	Total	C	N	O	0	0
			900	450	225	225		
1	m	265	Total	C	N	O	0	0
			1060	530	265	265		
1	n	253	Total	C	N	O	0	0
			1012	506	253	253		
1	o	254	Total	C	N	O	0	0
			1016	508	254	254		
1	p	253	Total	C	N	O	0	0
			1012	506	253	253		
1	q	283	Total	C	N	O	0	0
			1132	566	283	283		
1	r	278	Total	C	N	O	0	0
			1112	556	278	278		
1	s	277	Total	C	N	O	0	0
			1108	554	277	277		
1	t	266	Total	C	N	O	0	0
			1064	532	266	266		
1	u	258	Total	C	N	O	0	0
			1032	516	258	258		
1	v	254	Total	C	N	O	0	0
			1016	508	254	254		
1	w	259	Total	C	N	O	0	0
			1036	518	259	259		
1	x	250	Total	C	N	O	0	0
			1000	500	250	250		
1	y	224	Total	C	N	O	0	0
			896	448	224	224		
1	z	228	Total	C	N	O	0	0
			912	456	228	228		



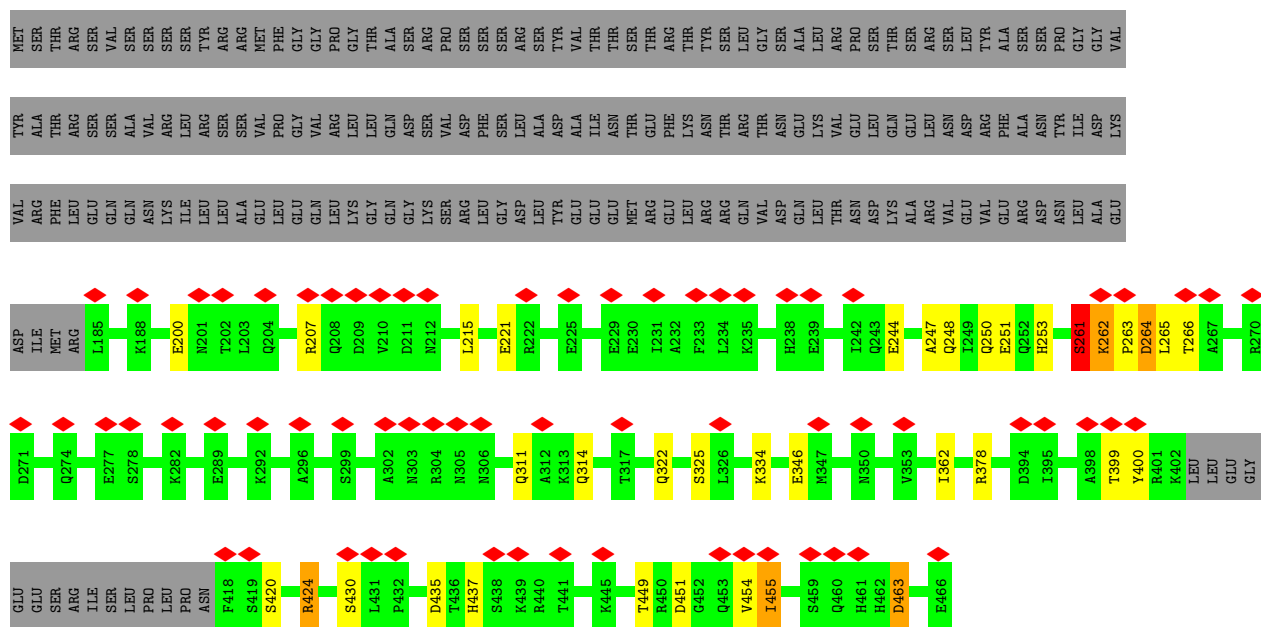


- Molecule 1: Vimentin

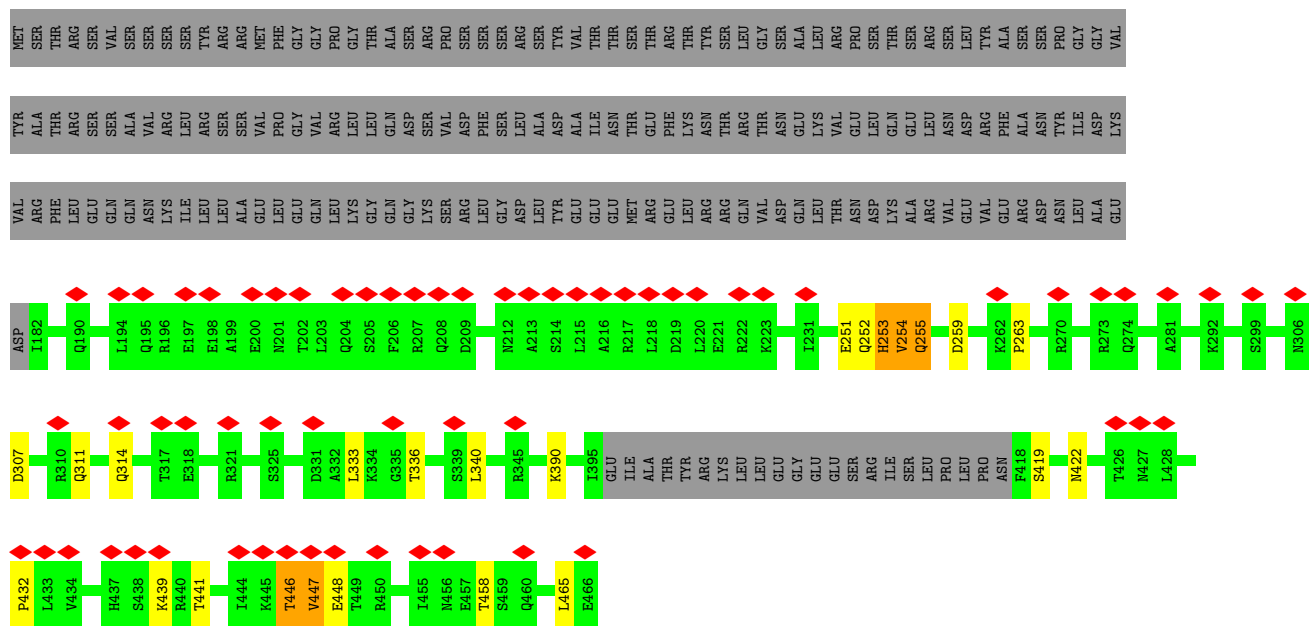


- Molecule 1: Vimentin

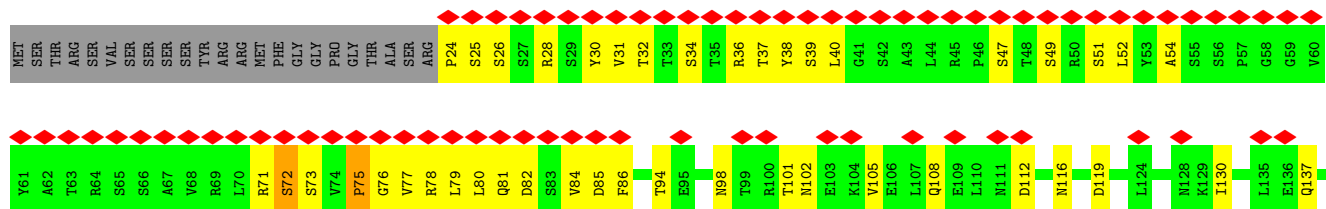


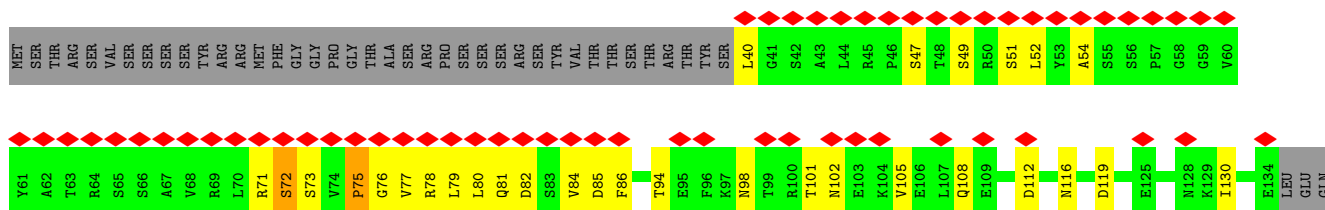


• Molecule 1: Vimentin



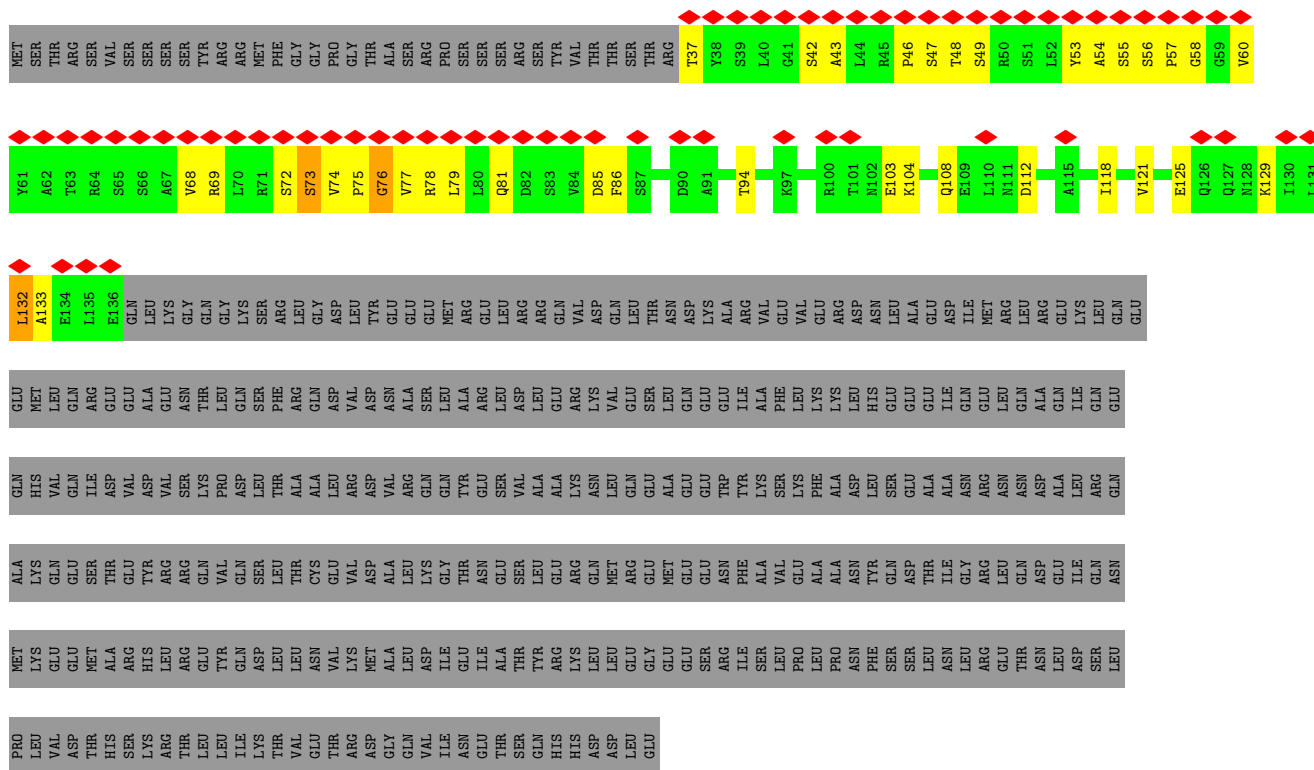
• Molecule 1: Vimentin



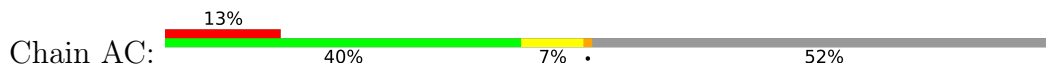


SER	ARG	GLU	VAL
LYS	HIS	TYR	ASP
ARG	LEU	ARG	VAL
THR	ARG	SER	LYS
LEU	GLN	GLY	ASN
LEU	TYR	VAL	PRO
ILE	GLN	GLN	ASP
THR	ASP	SER	LEU
THR	LEU	THR	THR
VAL	LEU	THR	ALA
GLU	ASN	CYS	ALA
THR	VAL	GLU	LEU
ARG	LYS	VAL	ARG
ASP	MET	ASP	ASP
GLY	ALA	ALA	VAL
GLN	LEU	GLN	ARG
VAL	ASP	LYS	GLN
ILE	ILE	GLY	GLN
ASN	GLU	THR	TYR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

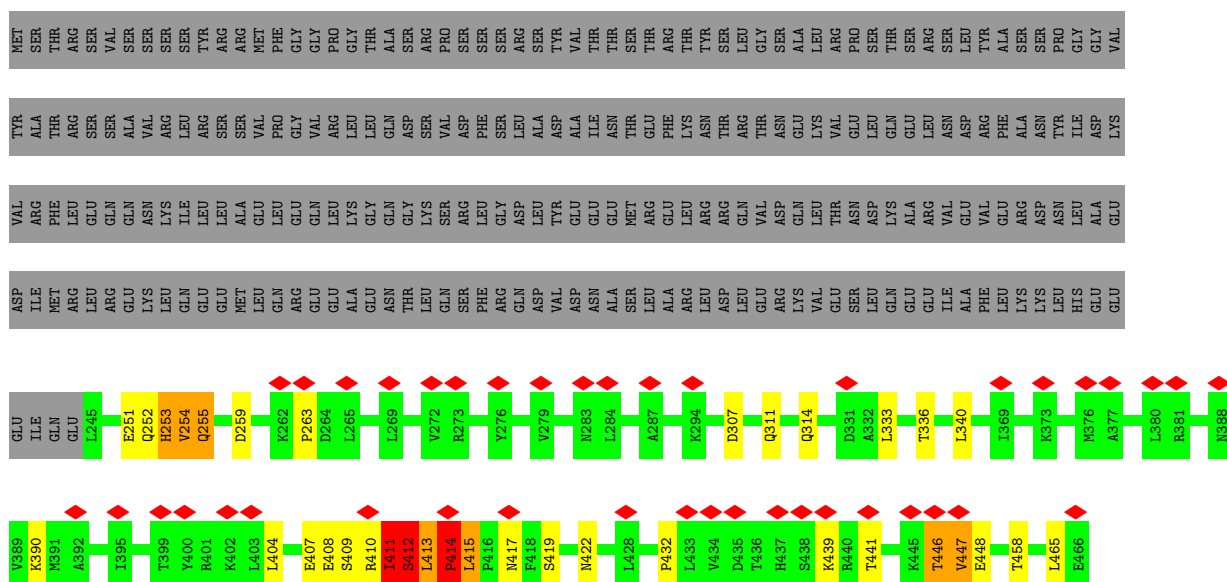
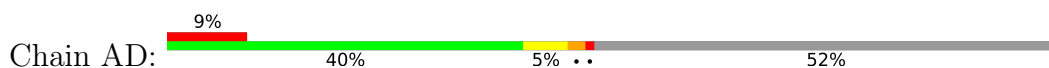
- Molecule 1: Vimentin



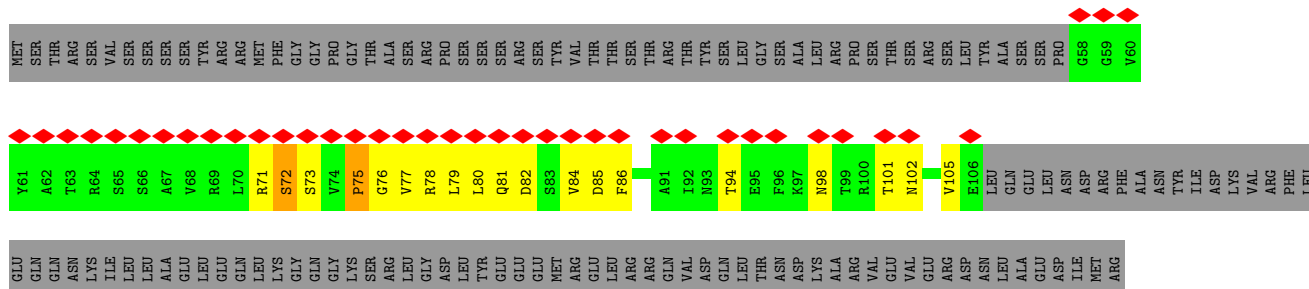
- Molecule 1: Vimentin

[illegible]

- Molecule 1: Vimentin



- Molecule 1: Vimentin

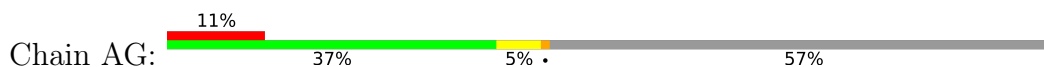


[illegible]

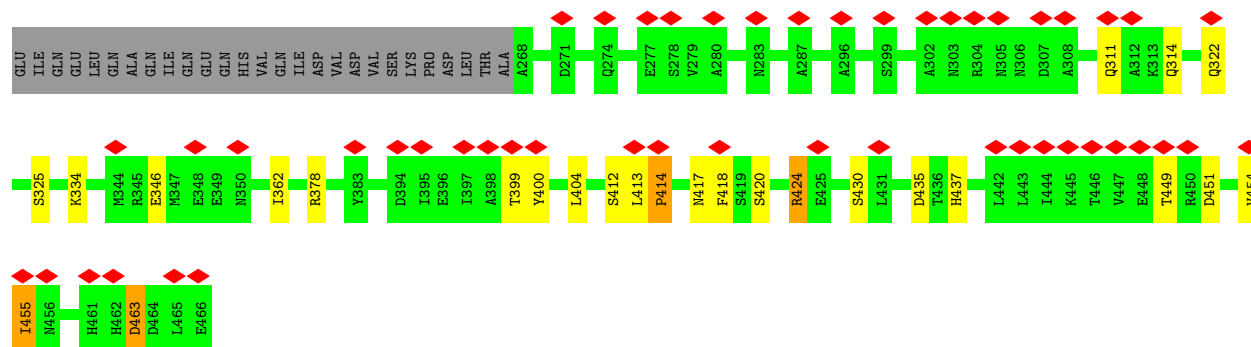
- Molecule 1: Vimentin

[illegible]

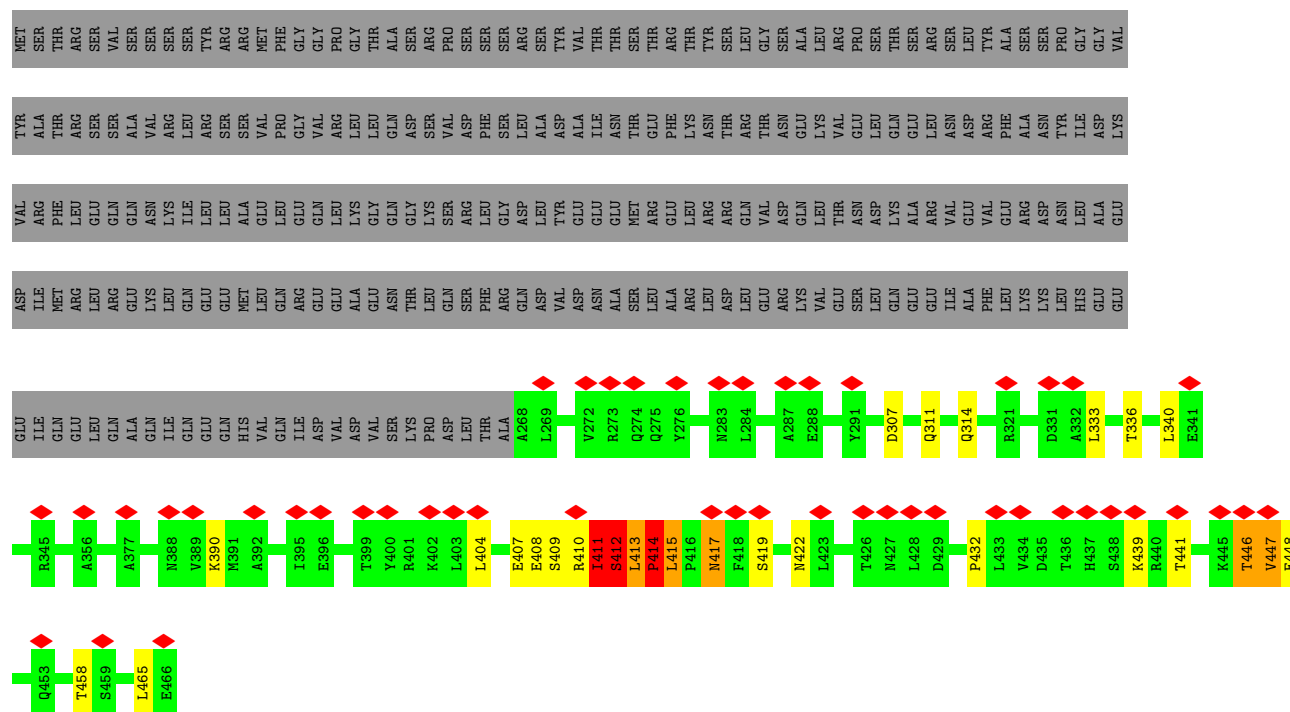
- Molecule 1: Vimentin



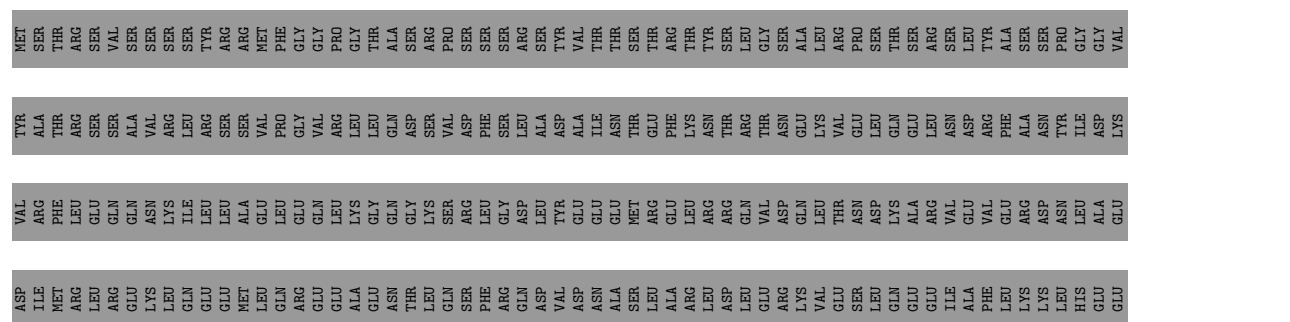
ASP	ILE	ASP	VAL	THR	TYR	MET
ILE	MET	PHE	ARG	THR	ALA	SER
ARG	ARG	LEU	GLU	SER	ARG	SER
ARG	ARG	GLN	GLN	SER	VAL	SER
GLU	GLU	GLN	GLN	ALA	ALA	SER
LYS	ASN	ASN	ASN	VAL	VAL	SER
LEU	LEU	LYS	LYS	ARG	ARG	SER
GLN	GLN	ILE	ILE	LEU	LEU	SER
GLU	GLU	LEU	LEU	ARG	ARG	TYR
GLU	GLU	LEU	LEU	SER	ARG	ARG
MET	MET	ALA	ALA	SER	SER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

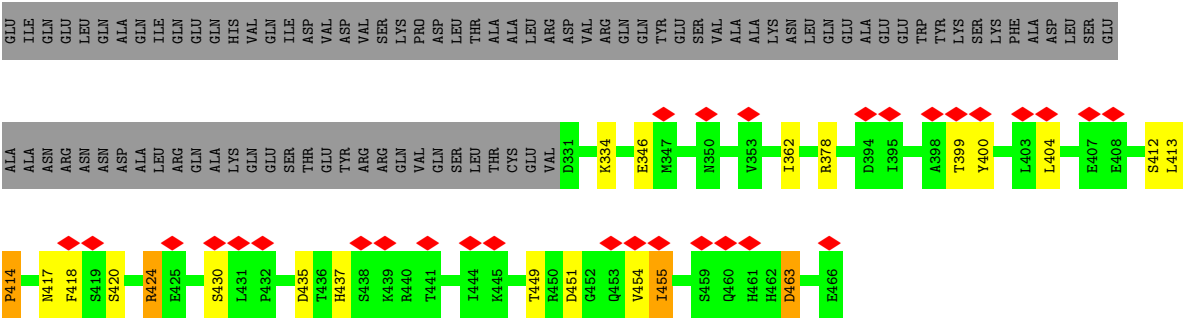


• Molecule 1: Vimentin

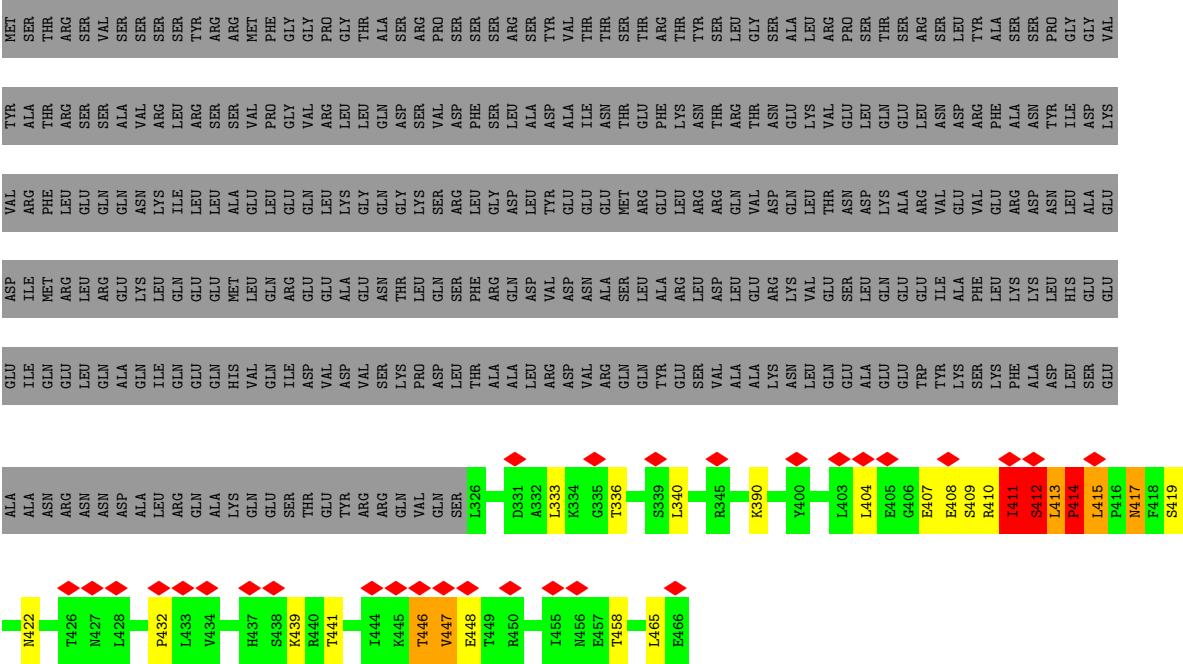


• Molecule 1: Vimentin

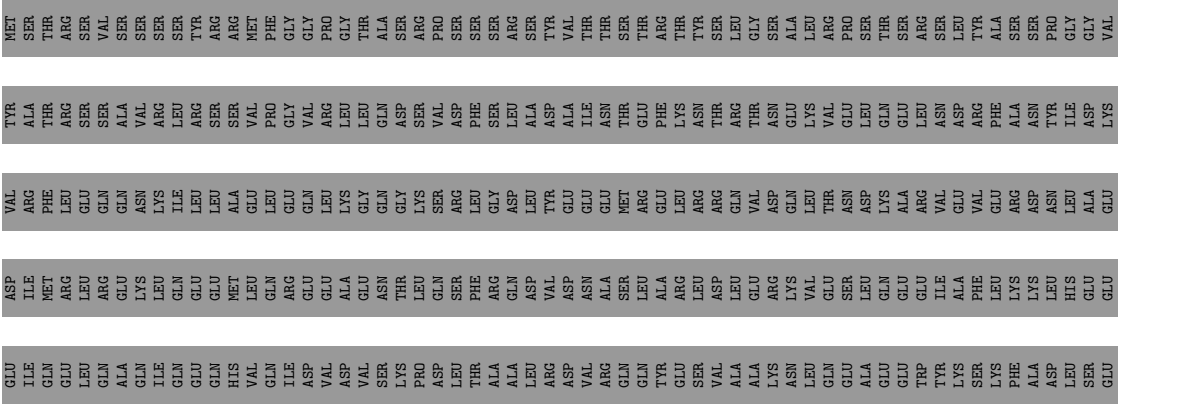




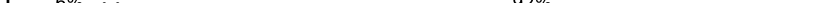
• Molecule 1: Vimentin

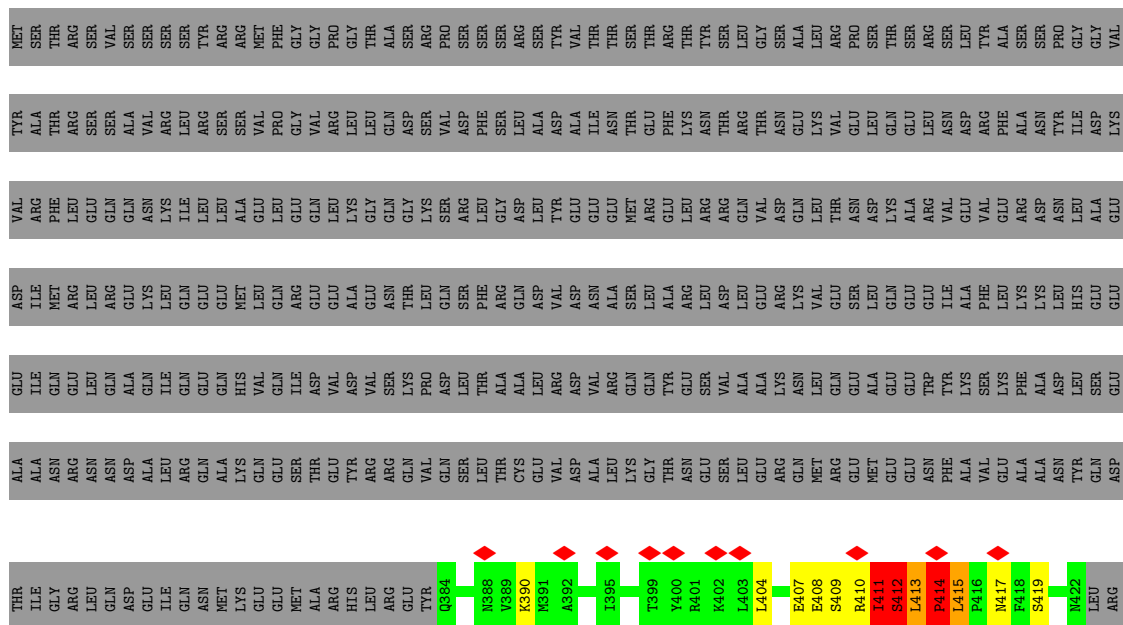


• Molecule 1: Vimentin

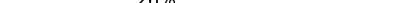


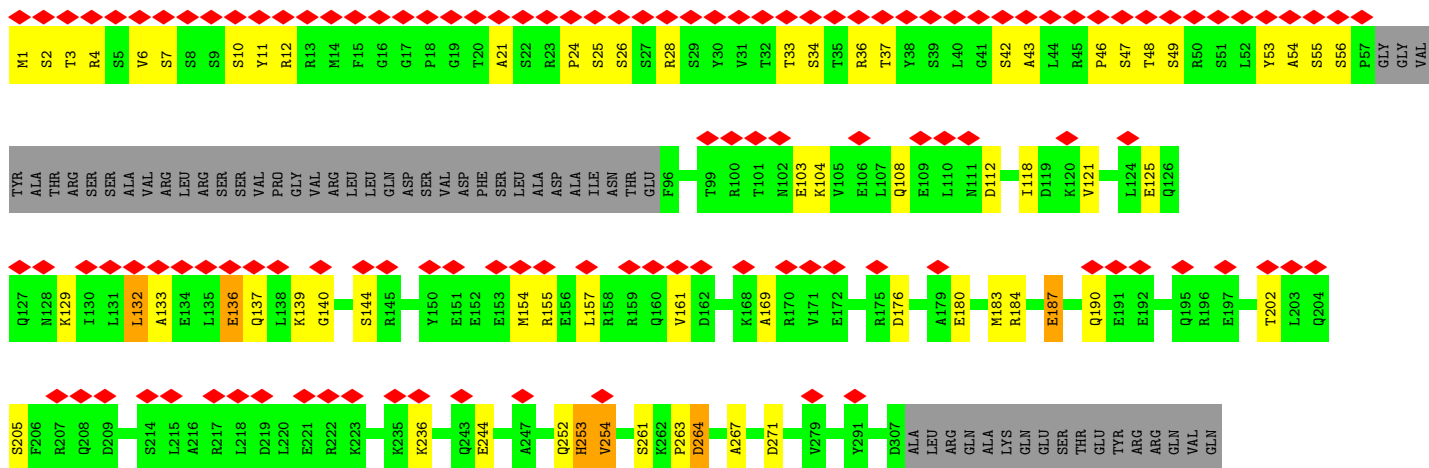
- Molecule 1: Vimentin

Chain AP:  6% 92%



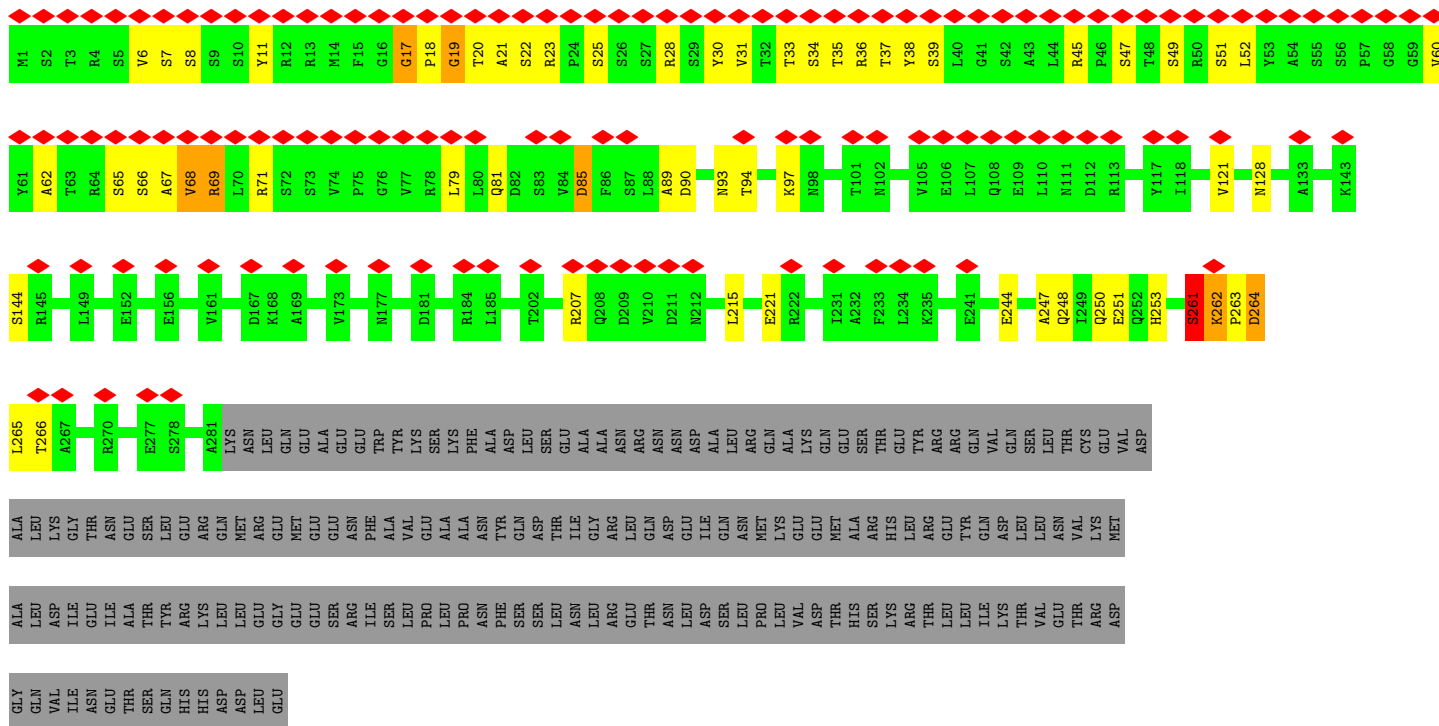
- Molecule 1: Vimentin

Chain B:  26% 44% 13% 1%

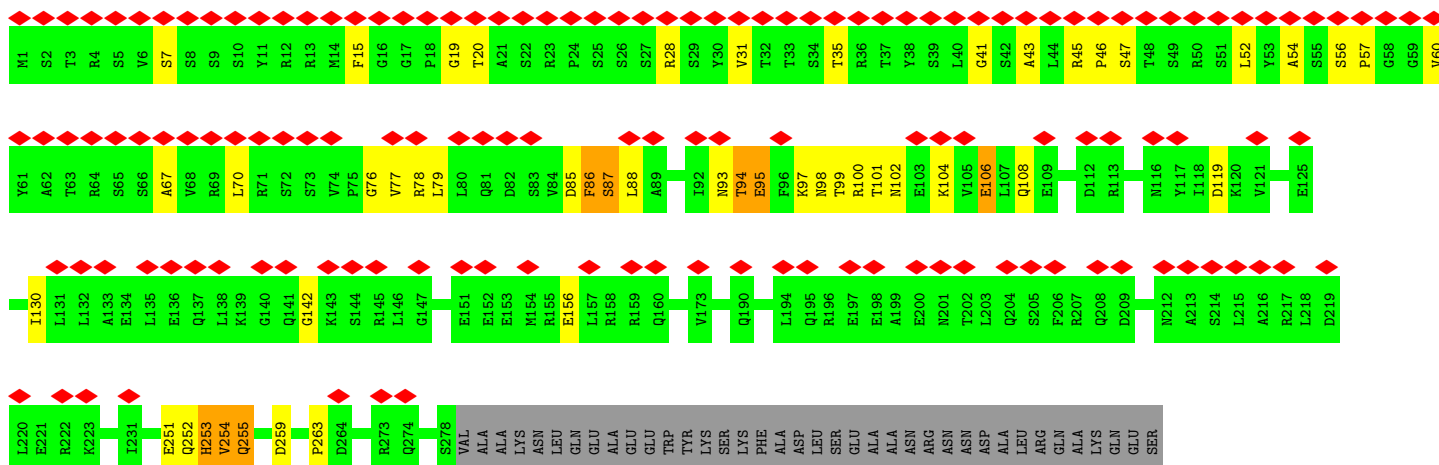


[illegible]

- Molecule 1: Vimentin



- Molecule 1: Vimentin



HIS SER LYS ARG THR LEU ILE LYS THR VAL GLU THR ARG ASP GLY GLN VAL ILE ASN GLU THR SER GLN HIS HIS ASP ASP LEU GLU

- Molecule 1: Vimentin

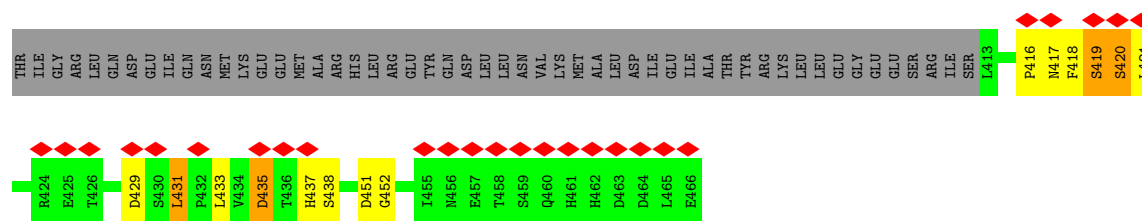


THR	ALA	GLU	ASP	VAL	TYR	MET
ILE	ILE	ILE	ILE	ARG	ALA	SER
GLY	ASN	GLN	MET	PHE	THR	THR
ARG	ARG	GLU	ARG	LEU	ARG	ARG
LEU	ASN	LEU	LEU	GLU	SER	SER
GLN	ASN	GLN	ARG	GLN	SER	VAL
ASP	ASP	ALA	GLU	GLN	ALA	SER
GLU	ALA	GLN	LYS	ASN	VAL	SER
ILE	ILE	ILE	LEU	LYS	ARG	SER
GLN	ARG	GLN	GLN	ILE	LEU	SER
ASN	GLN	GLU	GLU	LEU	ARG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

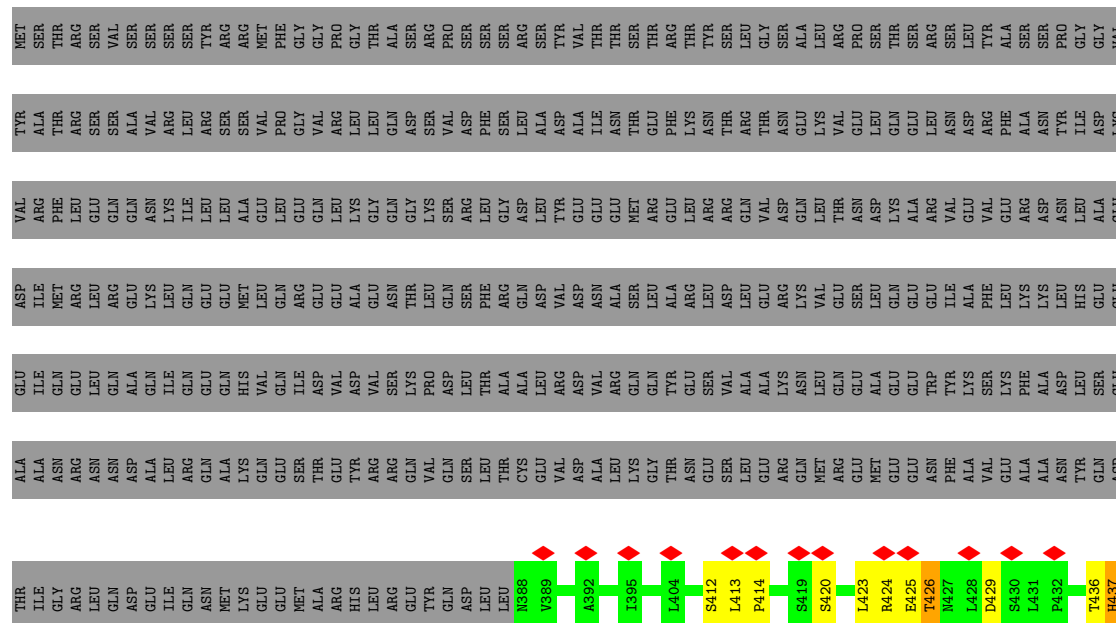
LEU	ASN	ARG	GLU	THR	ASN	ASP	SER	PRO	LEU	V434	D435	T436	H437	S438	K439	R440	K445	T446	V447	E448	T449	R450	D451	K452	Q453	V454	I455	V456	A457	T458	S459	Q460	H461	H462	D463	D464	L465	T466
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 1: Vimentin

[illegible]



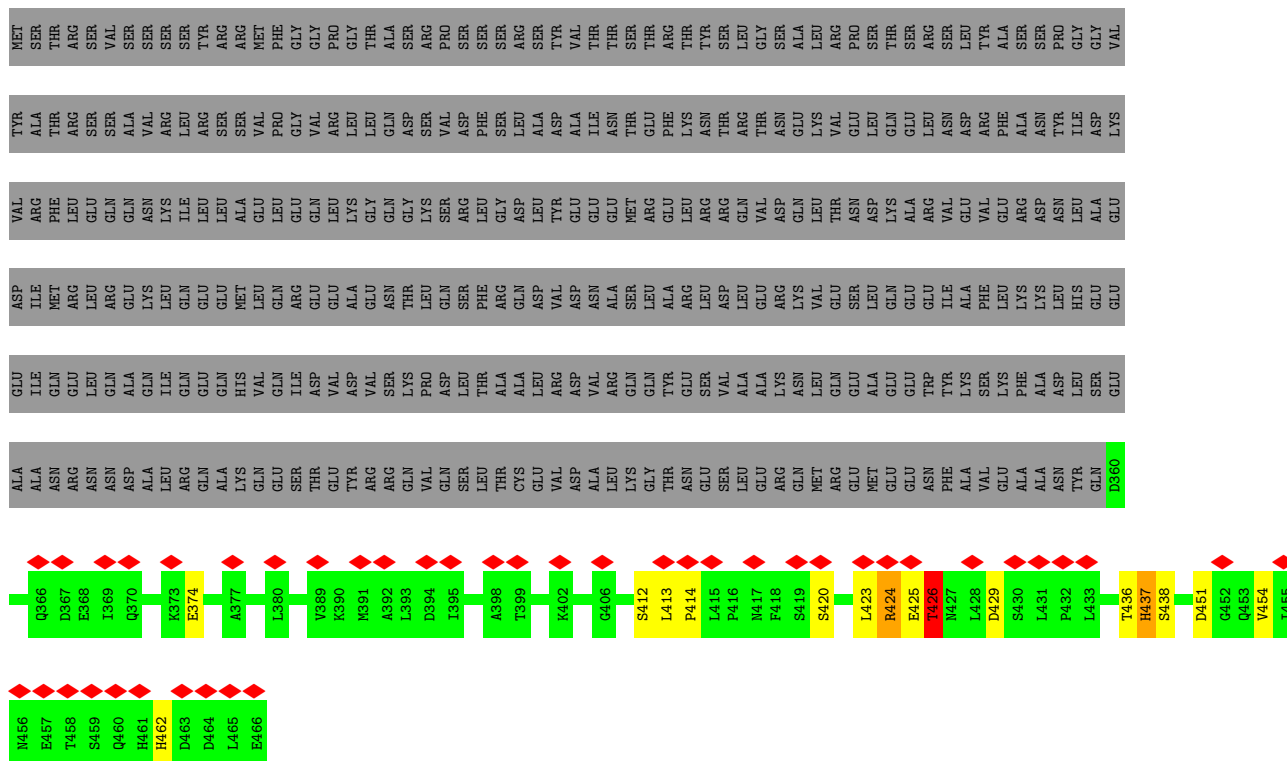
• Molecule 1: Vimentin



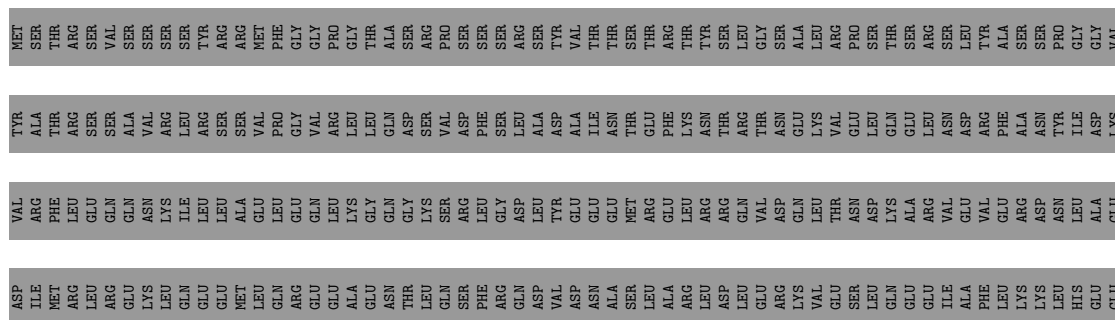
• Molecule 1: Vimentin



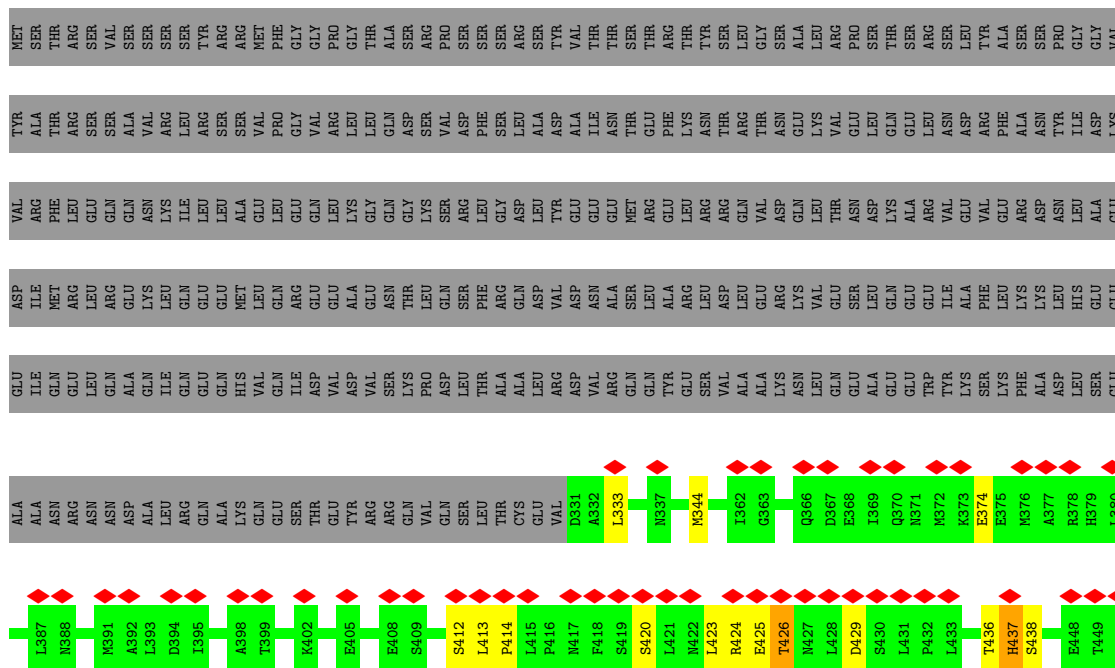
- Molecule 1: Vimentin



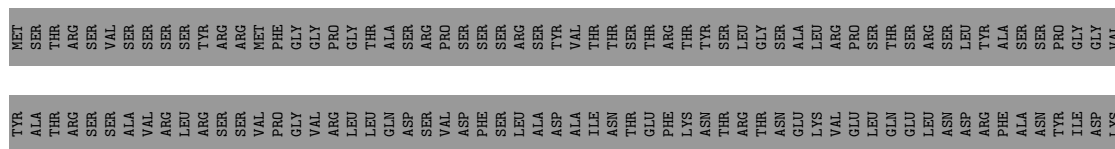
- Molecule 1: Vimentin

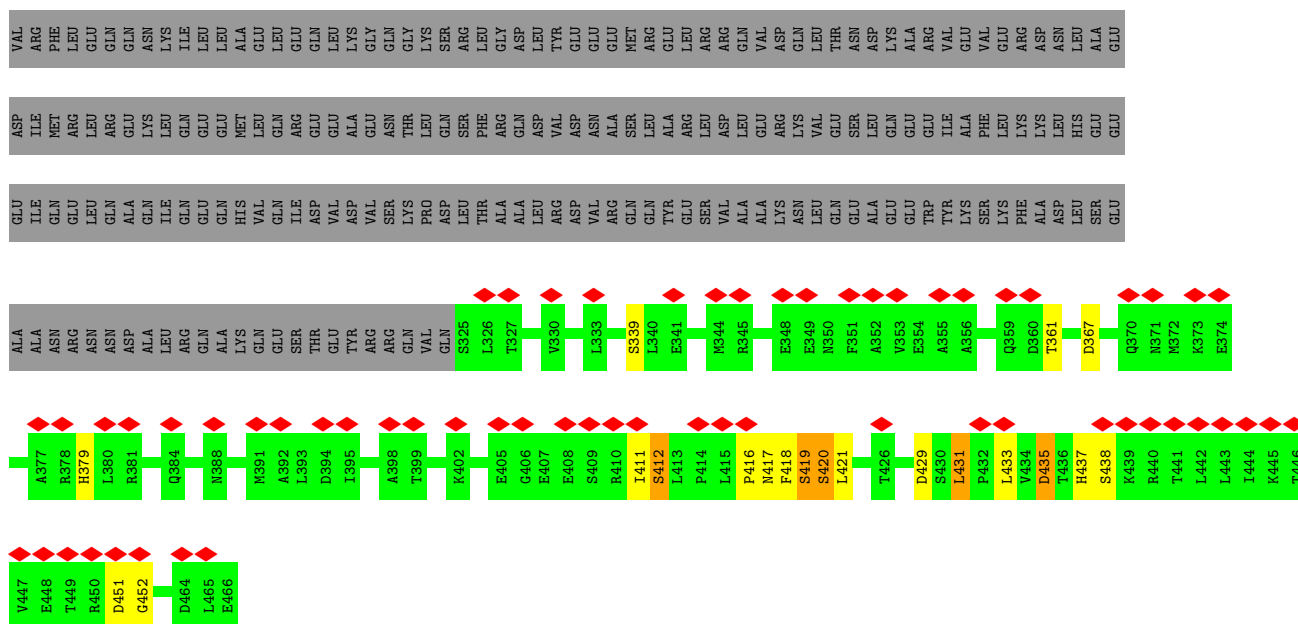


- Molecule 1: Vimentin

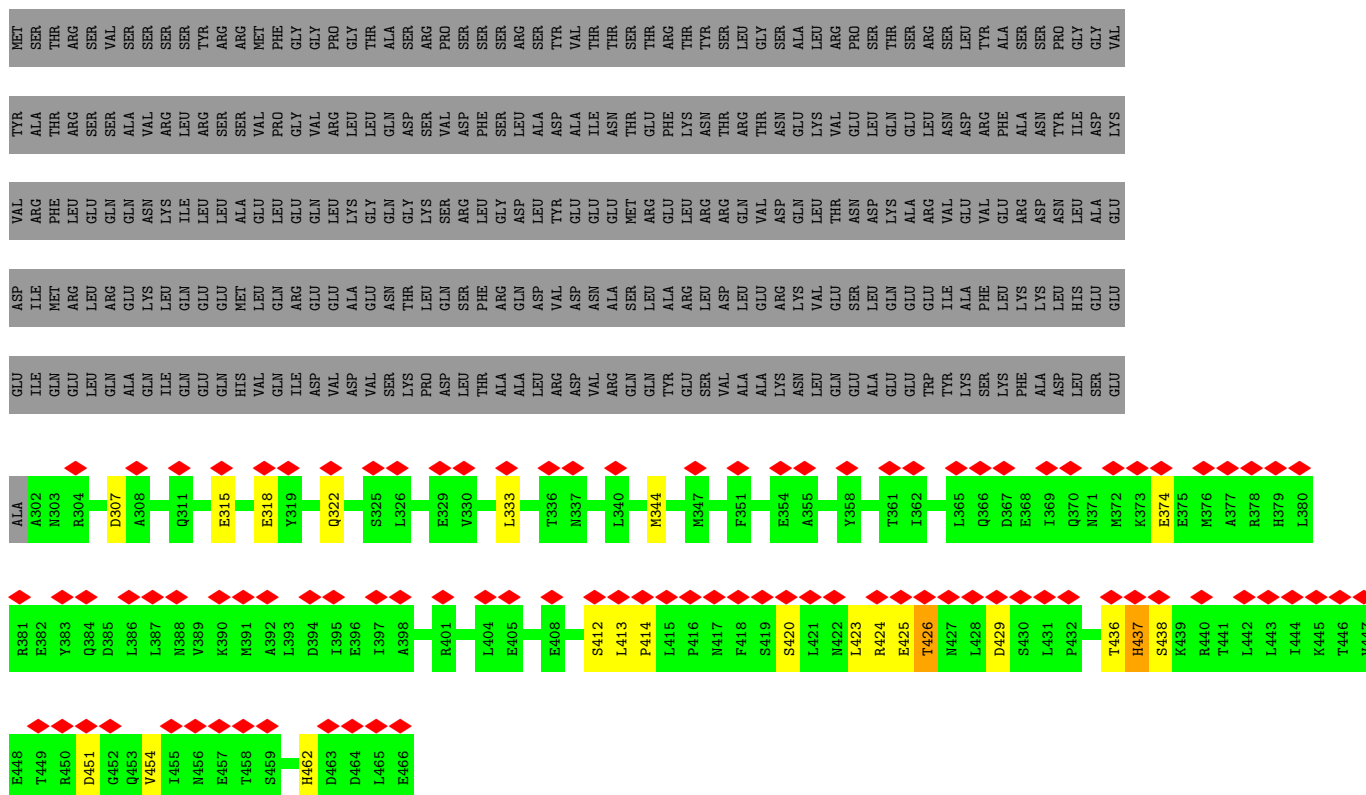


- Molecule 1: Vimentin





- Molecule 1: Vimentin



- Molecule 1: Vimentin



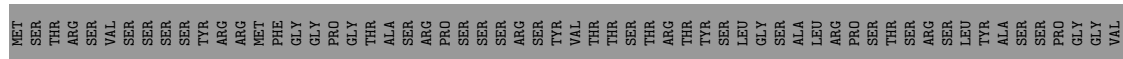
[illegible]

Chain S: 15% 37% 58%

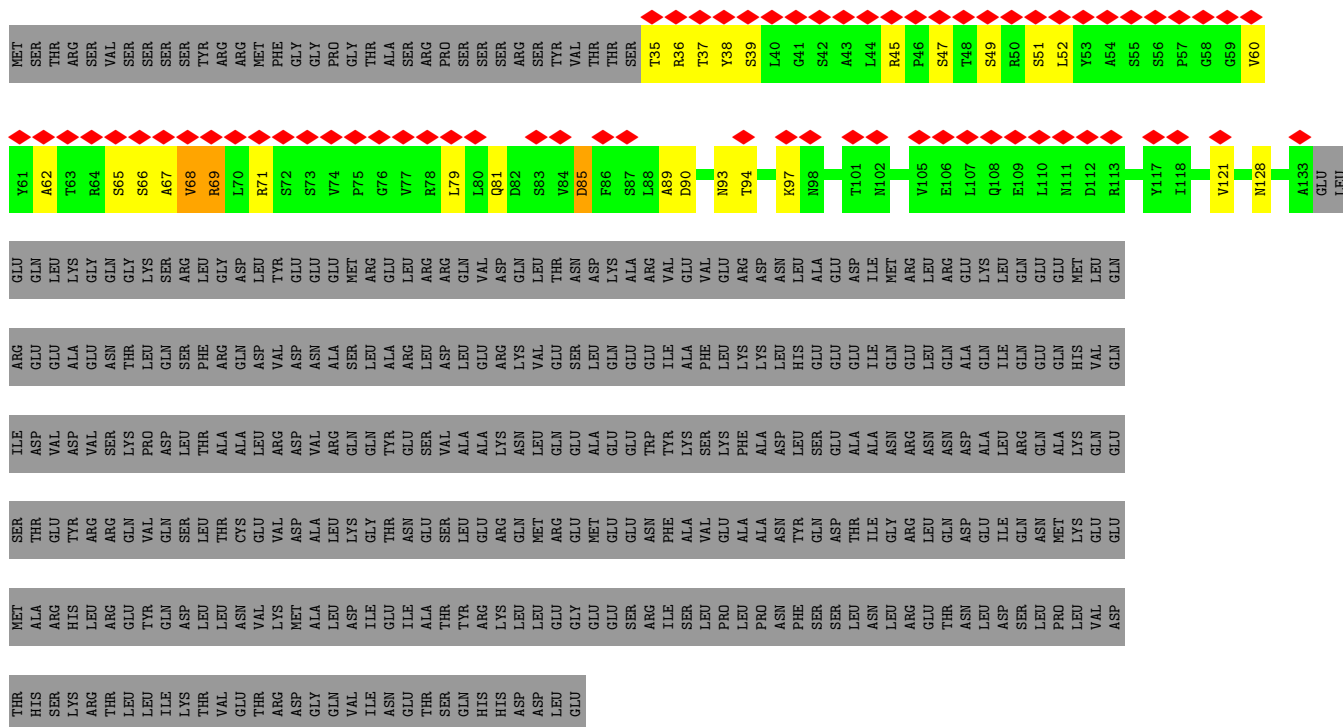
[illegible]

Chain T: 15% 38% 57%

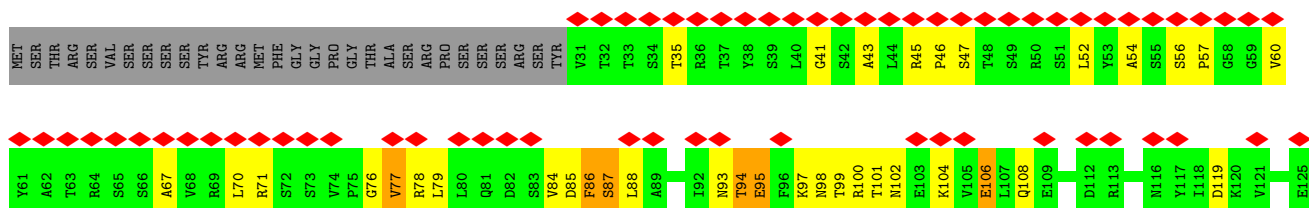


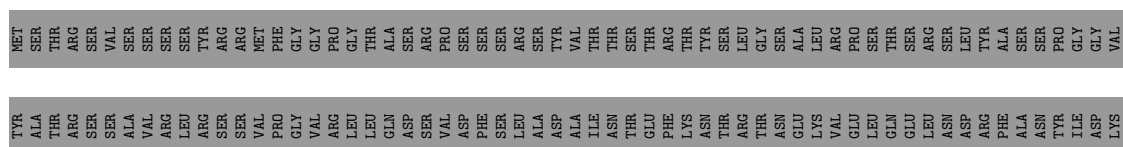


- Molecule 1: Vimentin

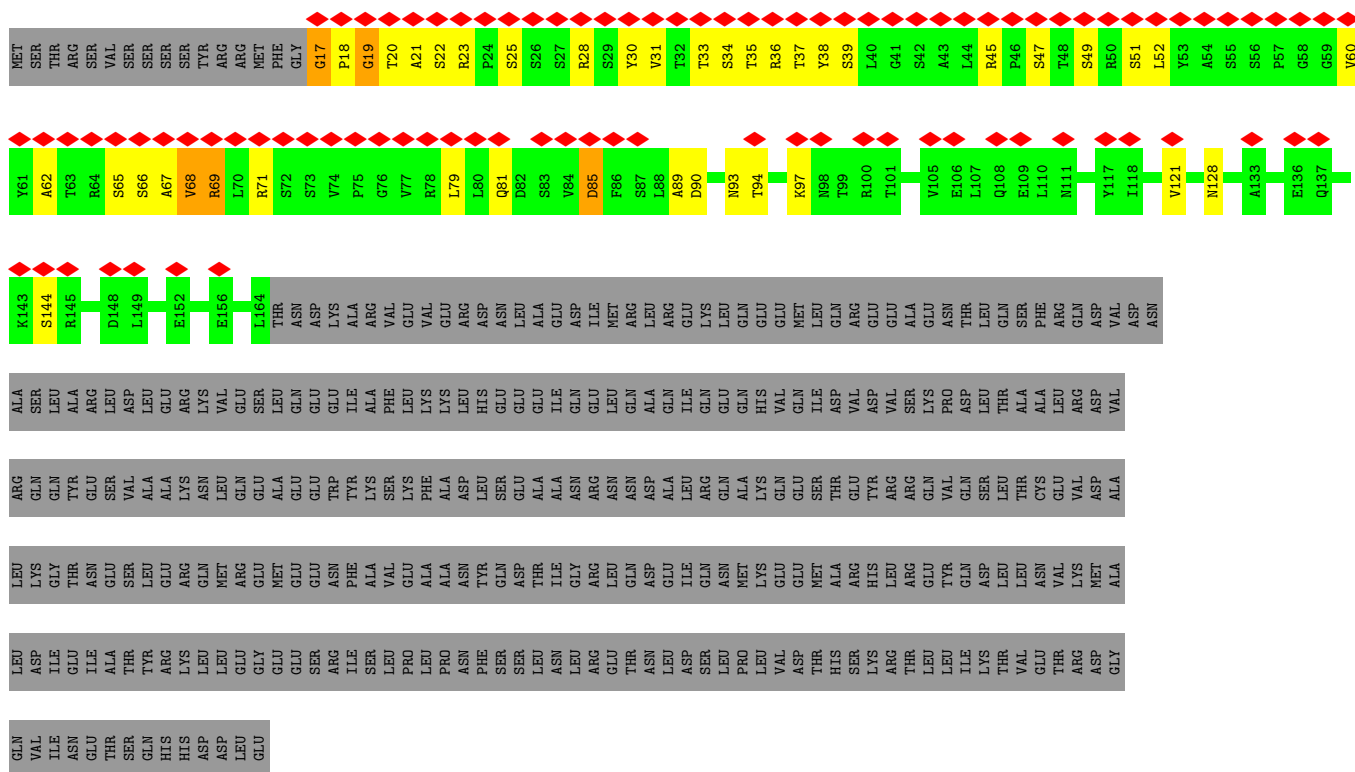


- Molecule 1: Vimentin





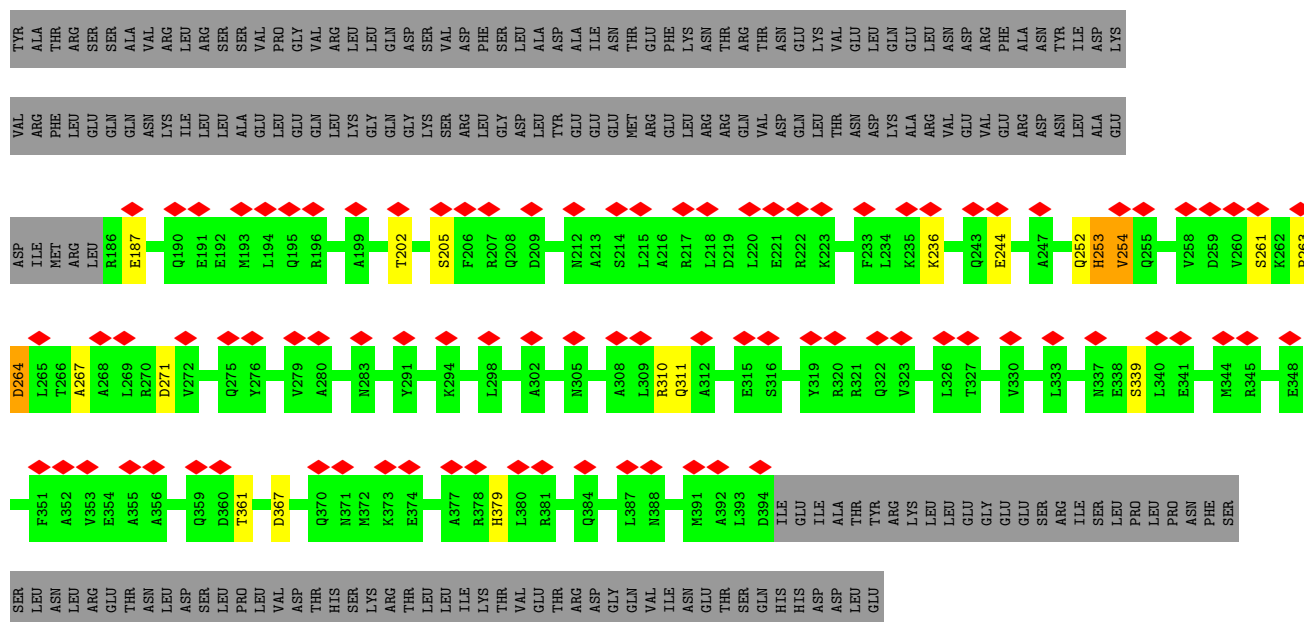
- Molecule 1: Vimentin



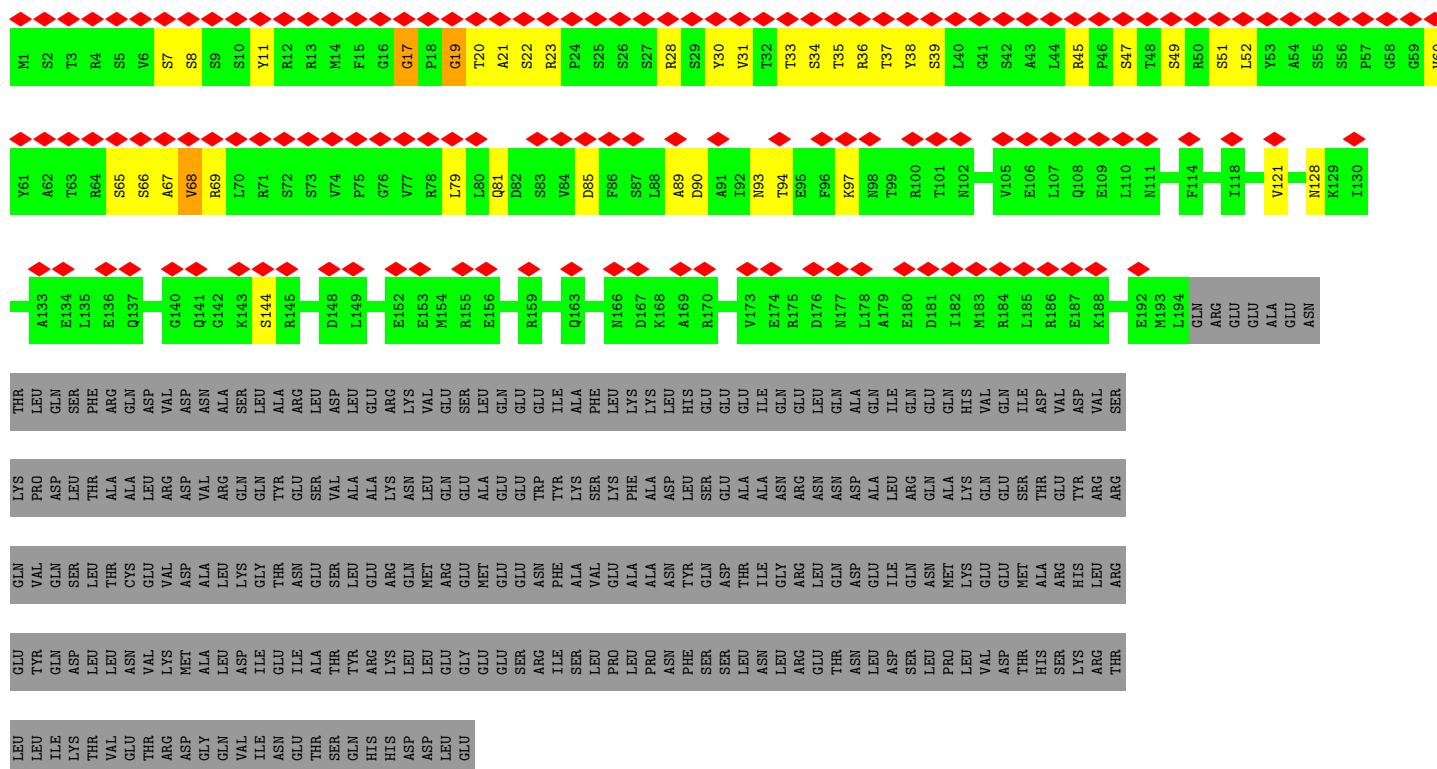
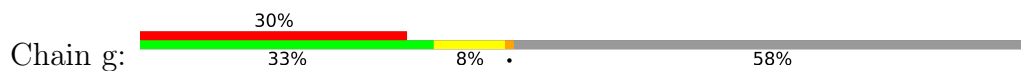
- Molecule 1: Vimentin





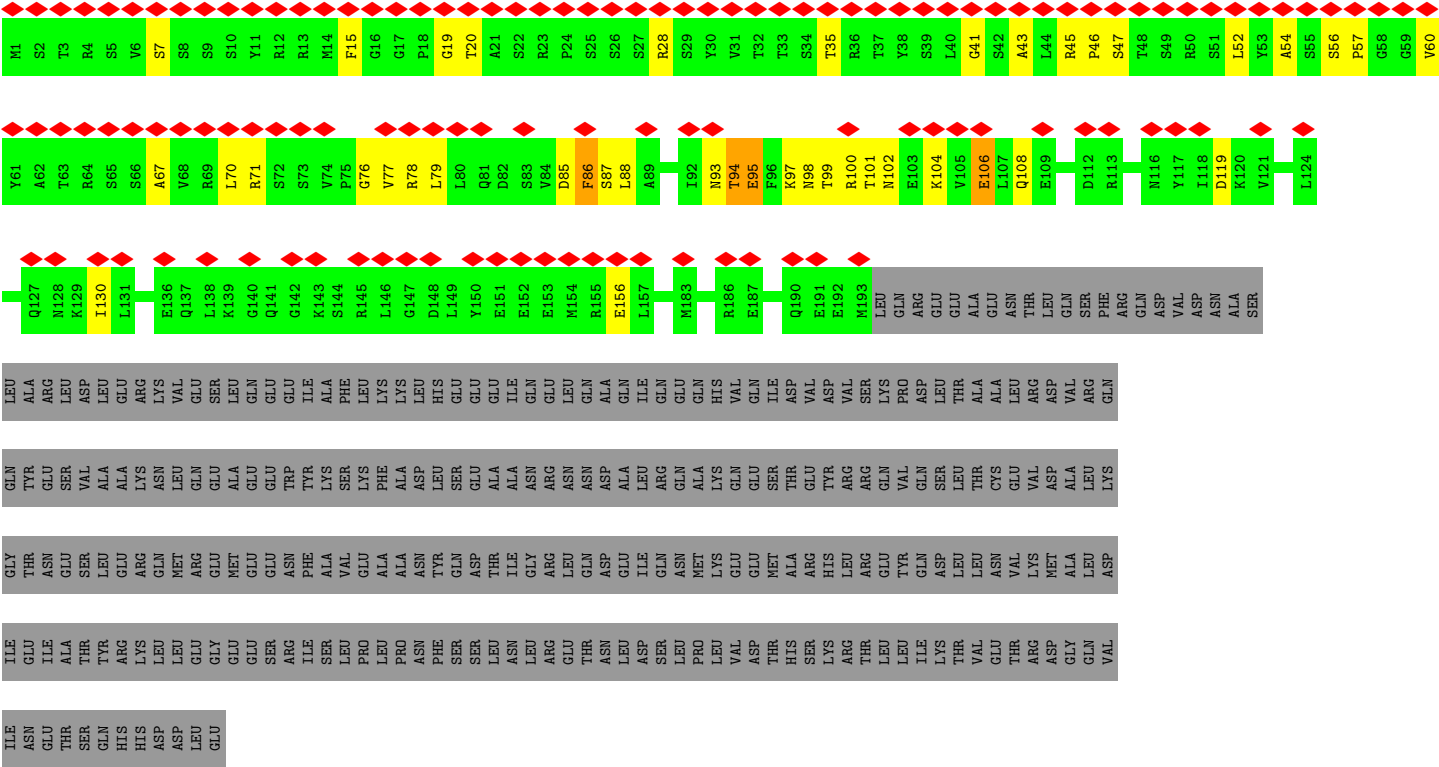


• Molecule 1: Vimentin

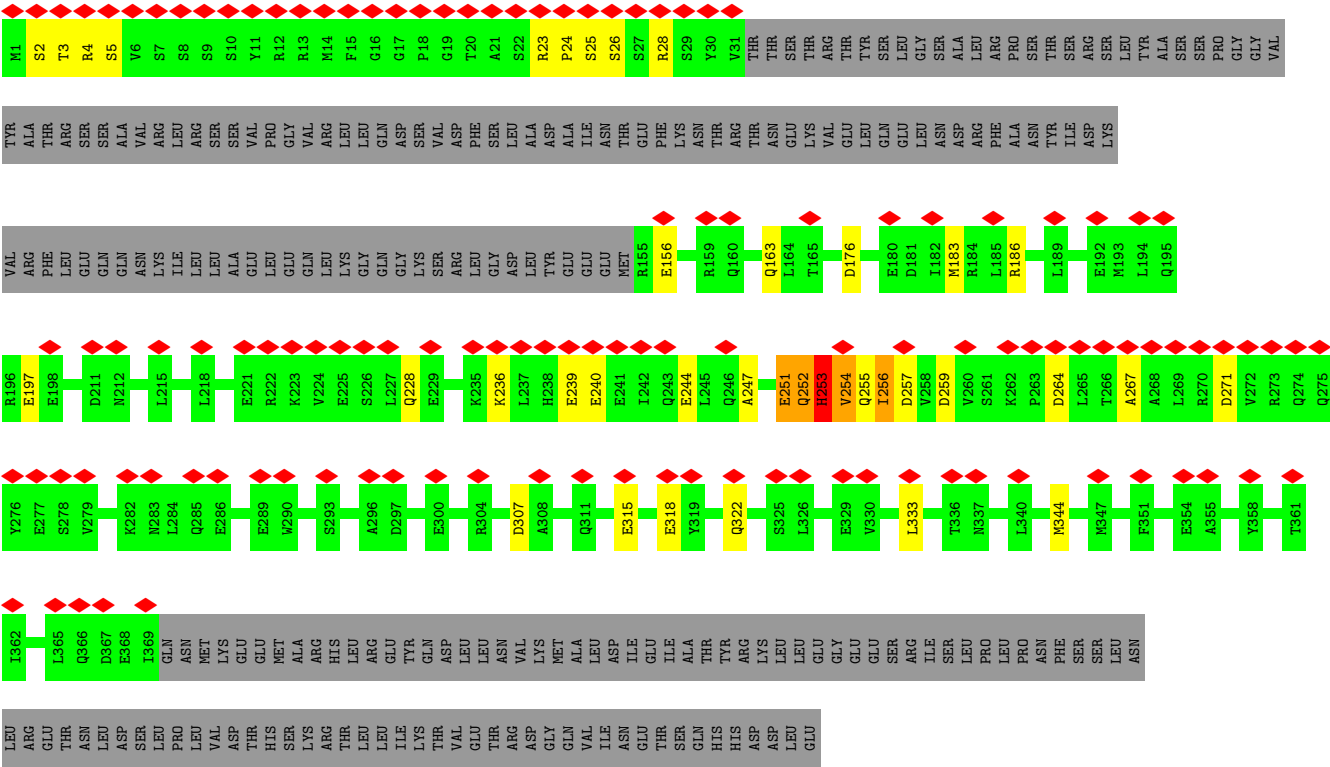


• Molecule 1: Vimentin



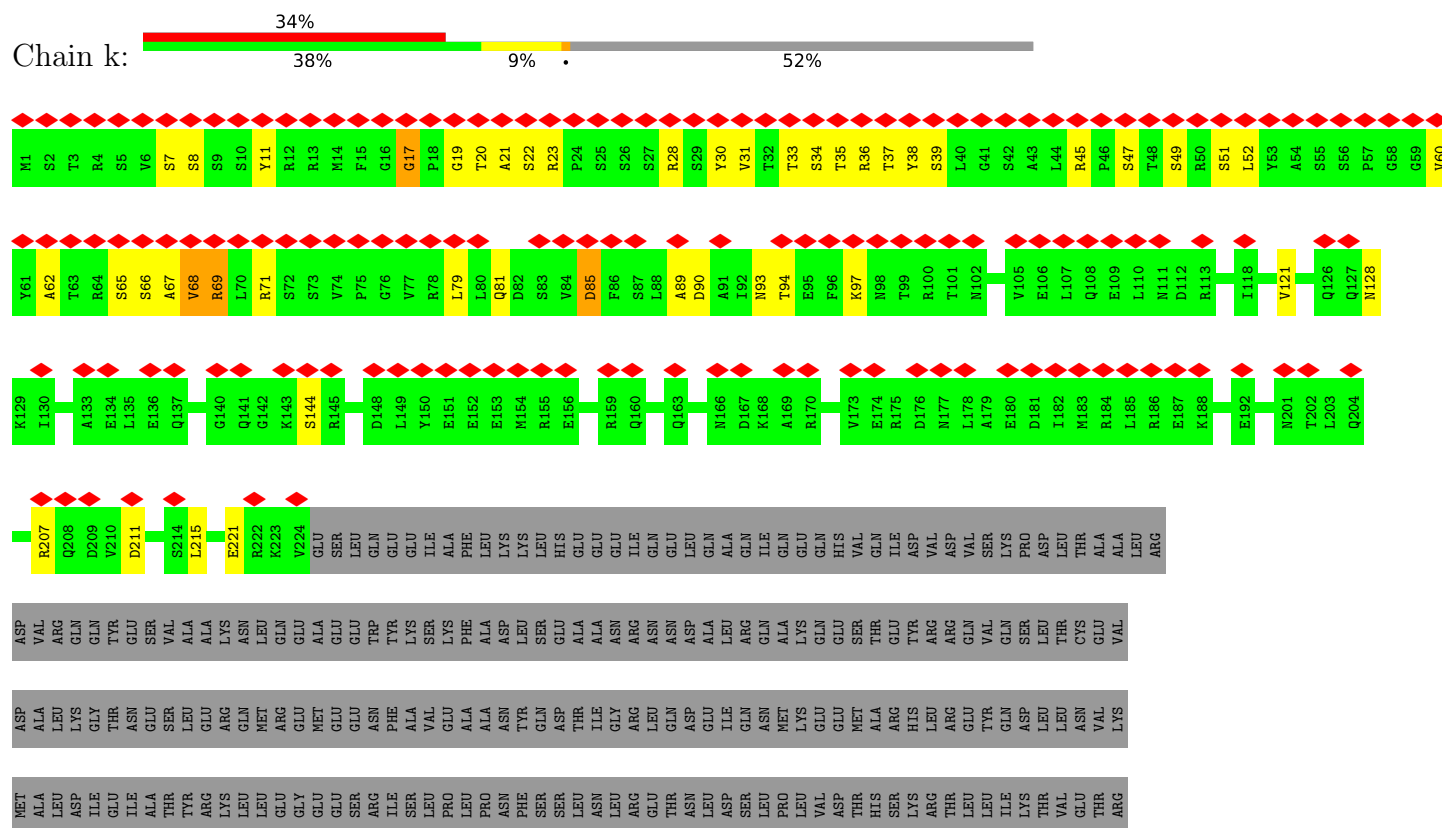


• Molecule 1: Vimentin



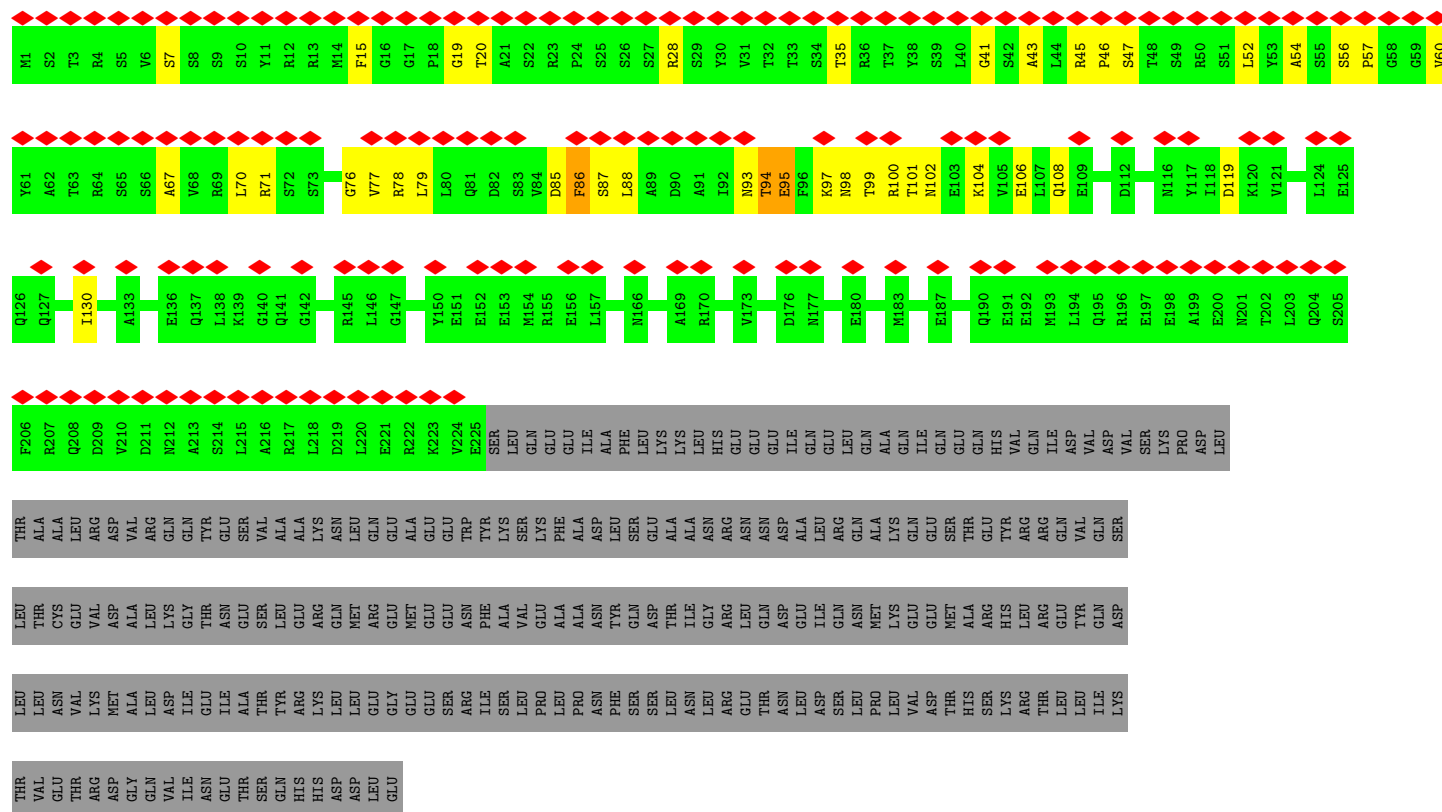
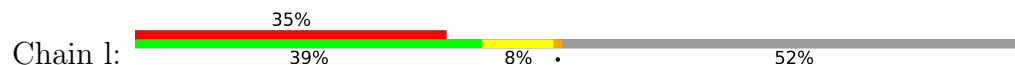
• Molecule 1: Vimentin

- Molecule 1: Vimentin

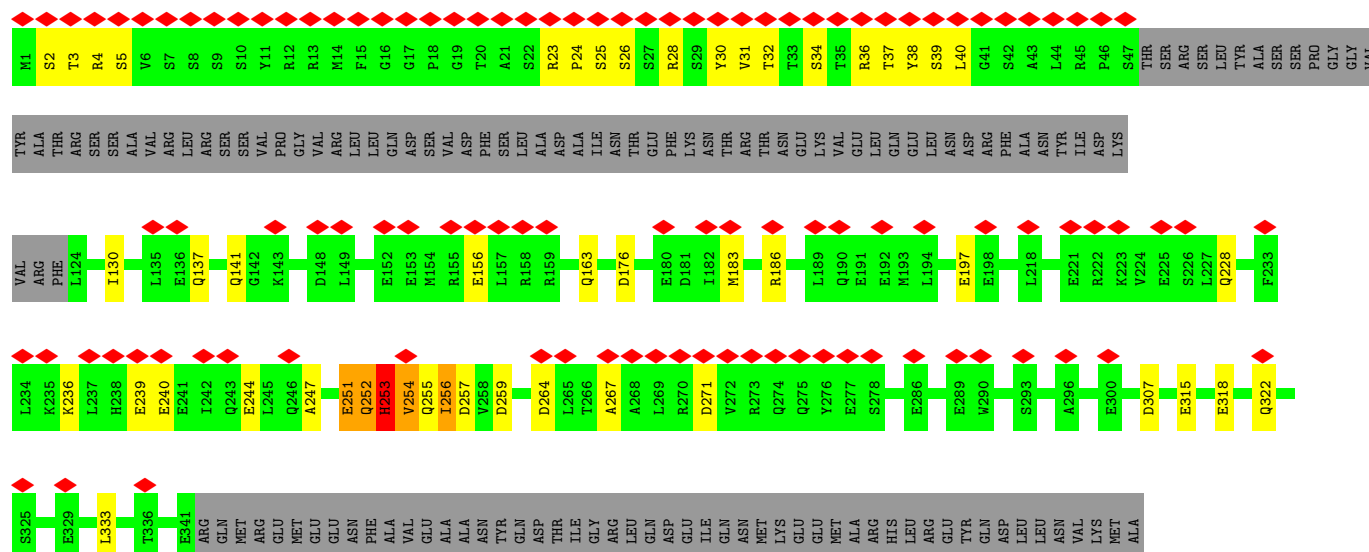


ASP
GLY
GLN
VAL
ILE
ASN
GLU
THR
SER
GLN
HIS
HIS
ASP
ASP
LEU
GLU

• Molecule 1: Vimentin



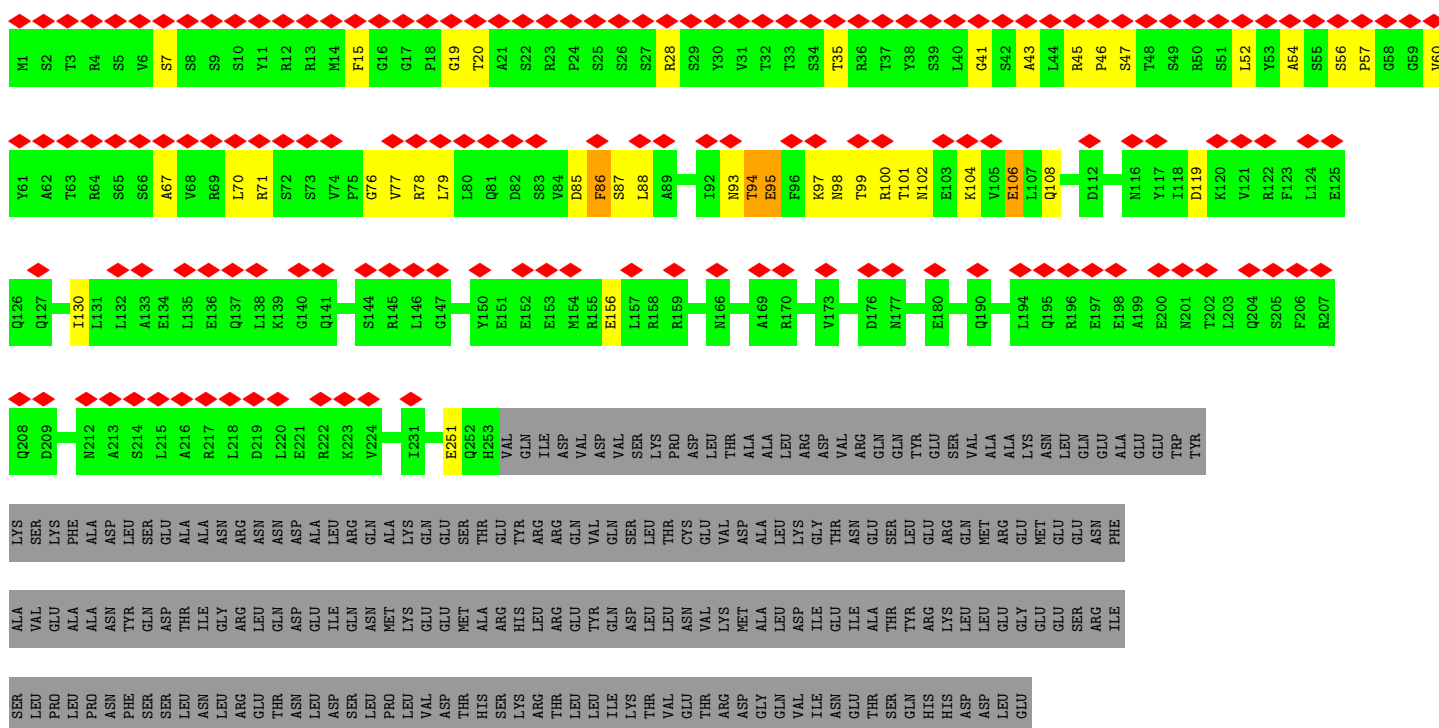
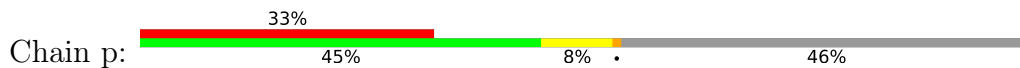
• Molecule 1: Vimentin



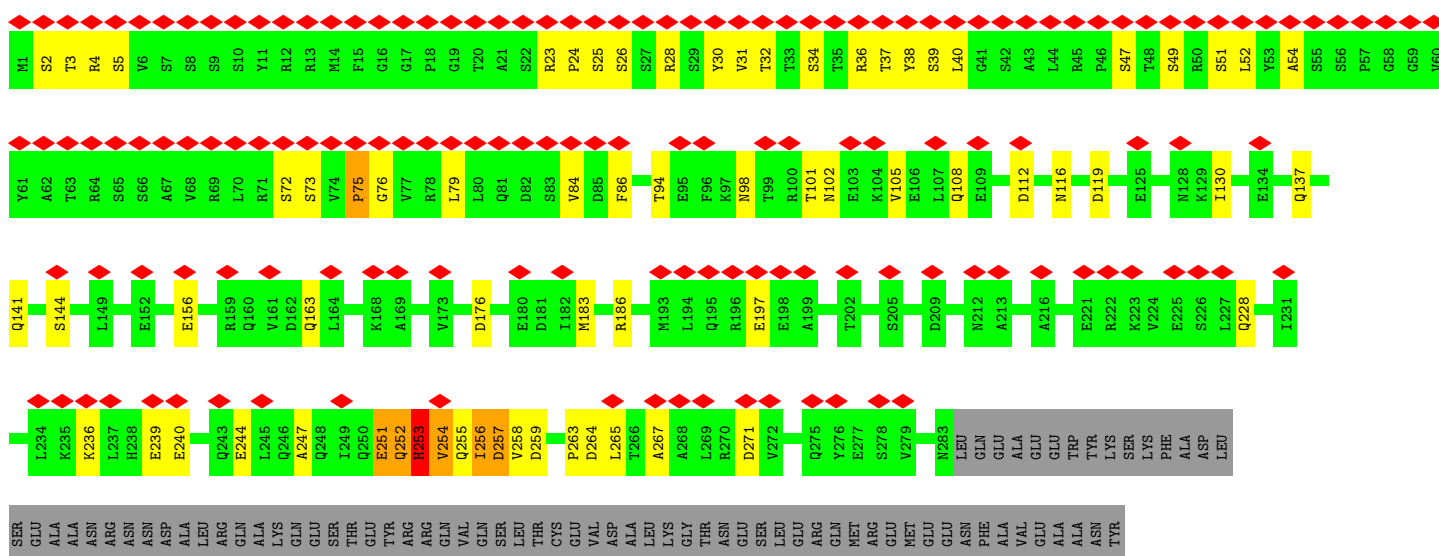
ASN PHE ALA VAL LEU PRO LEU LEU ALA ASN TYR ASP GLN SER THR LEU ASN TLE GLY ARG LEU THR GLN ASP ASN GLU TLE ASP GLN SER THR LEU MET MET LYS LEU VAL ASP GLU MET THR HIS SER ARG LYS HIS LEU ARG THR LEU TYR LYS ASP LEU LEU VAL THR VAL ASN THR VAL ASP MET MET LYS ALA LEU ASP ASP ILE ILE ASN GLU ILE ILE THR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

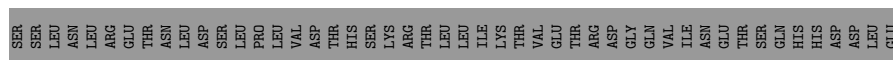
ARG ILE SER LEU PRO LEU LEU PRO ASN PHE SER SER THR LEU ASN LEU ARG LEU THR GLN ASP ASN GLU TLE ASP GLN SER THR LEU MET MET LYS LEU VAL ASP GLU MET THR HIS SER ARG LYS HIS LEU ARG THR LEU TYR LYS ASP LEU LEU VAL THR VAL ASN THR VAL ASP MET MET LYS ALA LEU ASP ASP ILE ILE ASN GLU ILE ILE THR ALA THR THR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

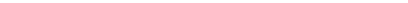
• Molecule 1: Vimentin

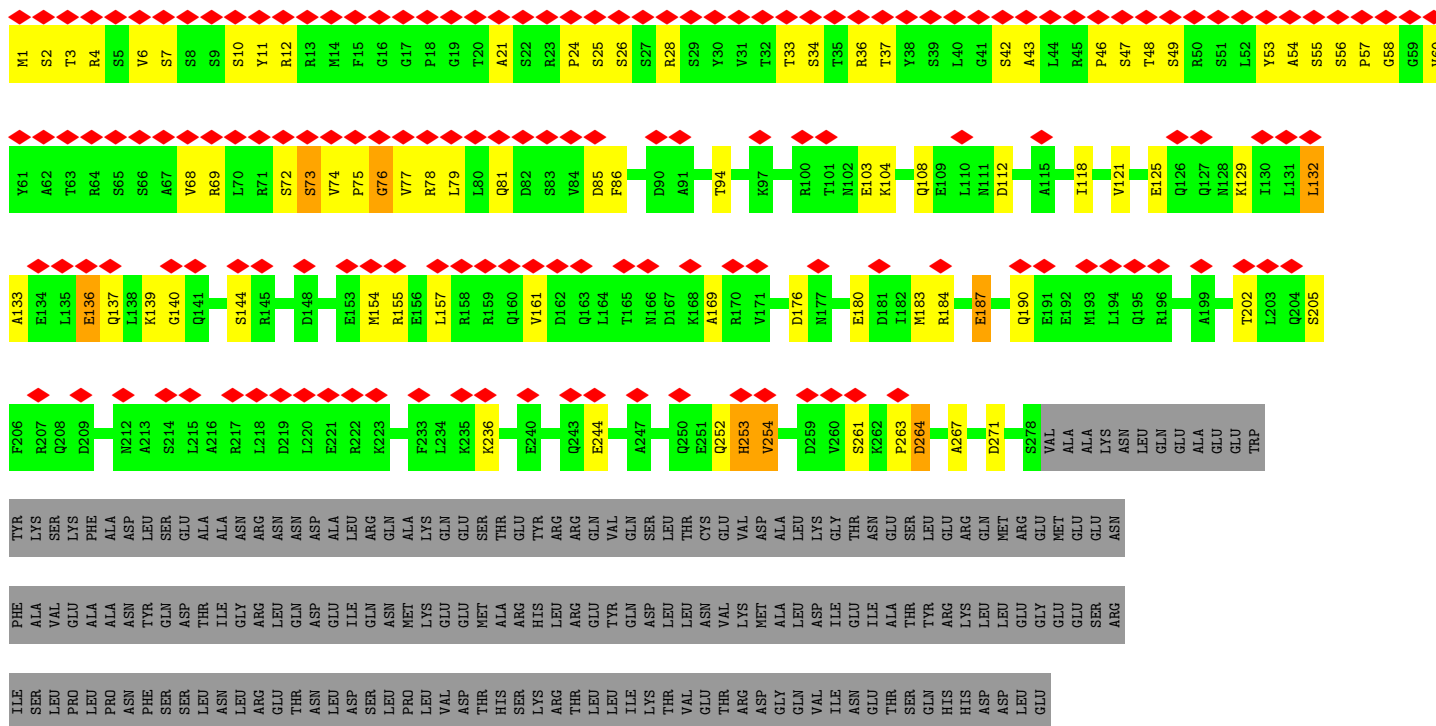


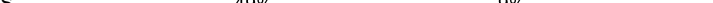
• Molecule 1: Vimentin

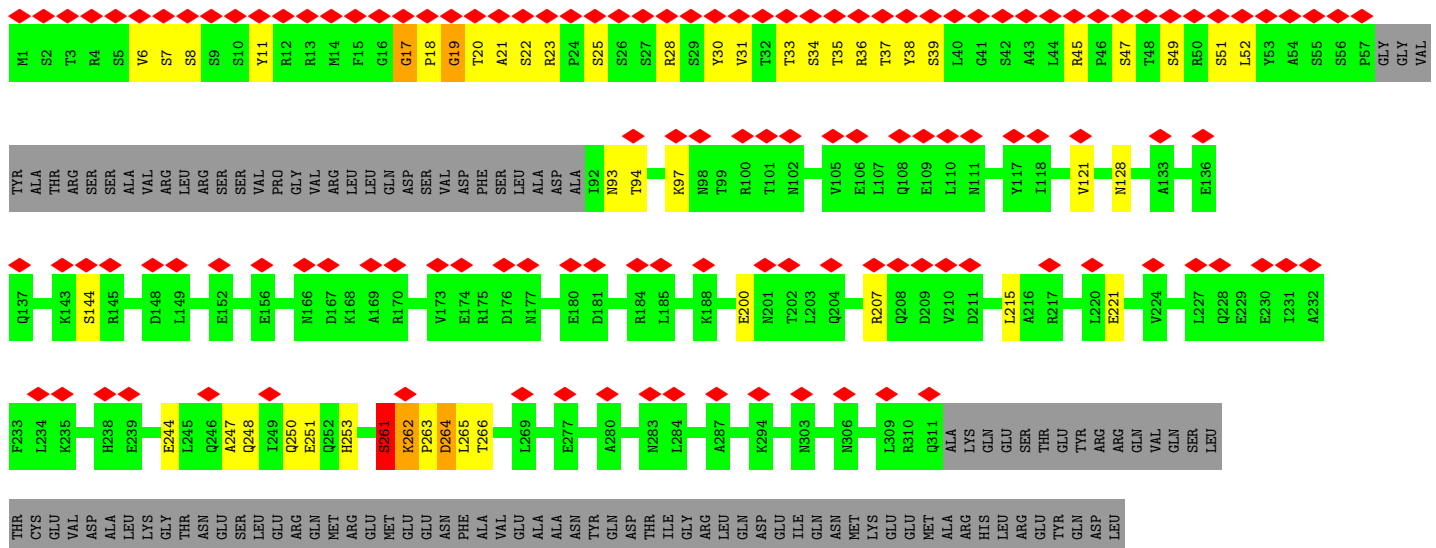


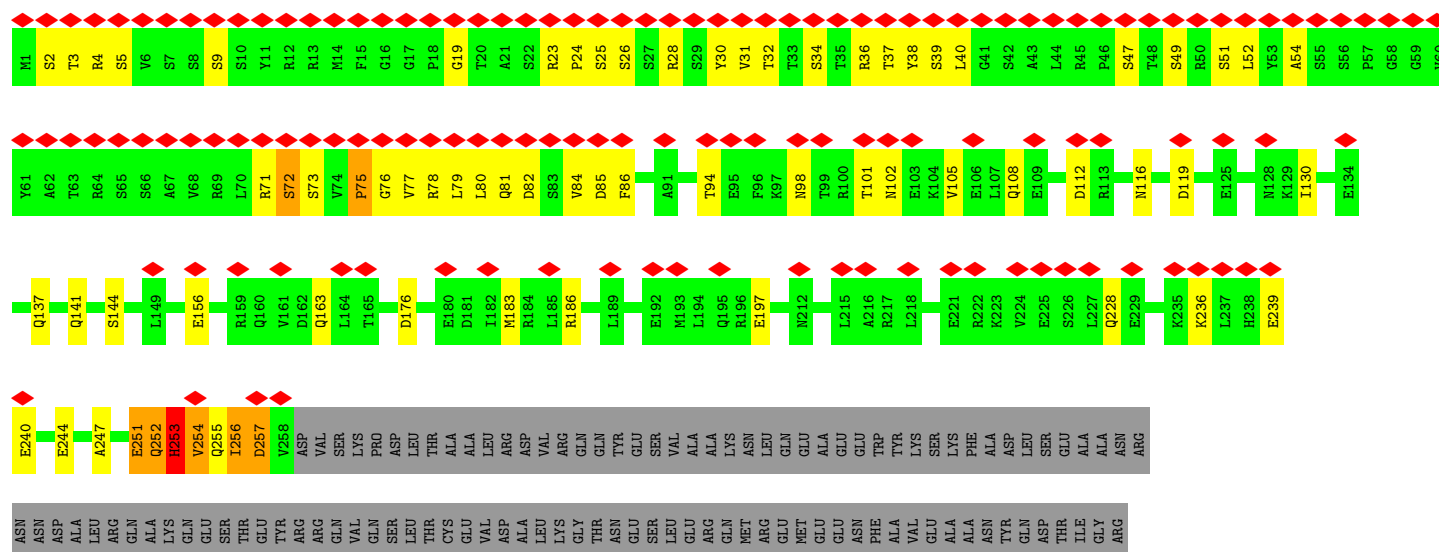


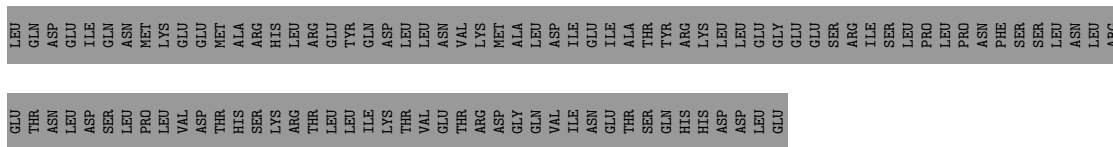
Chain r: 



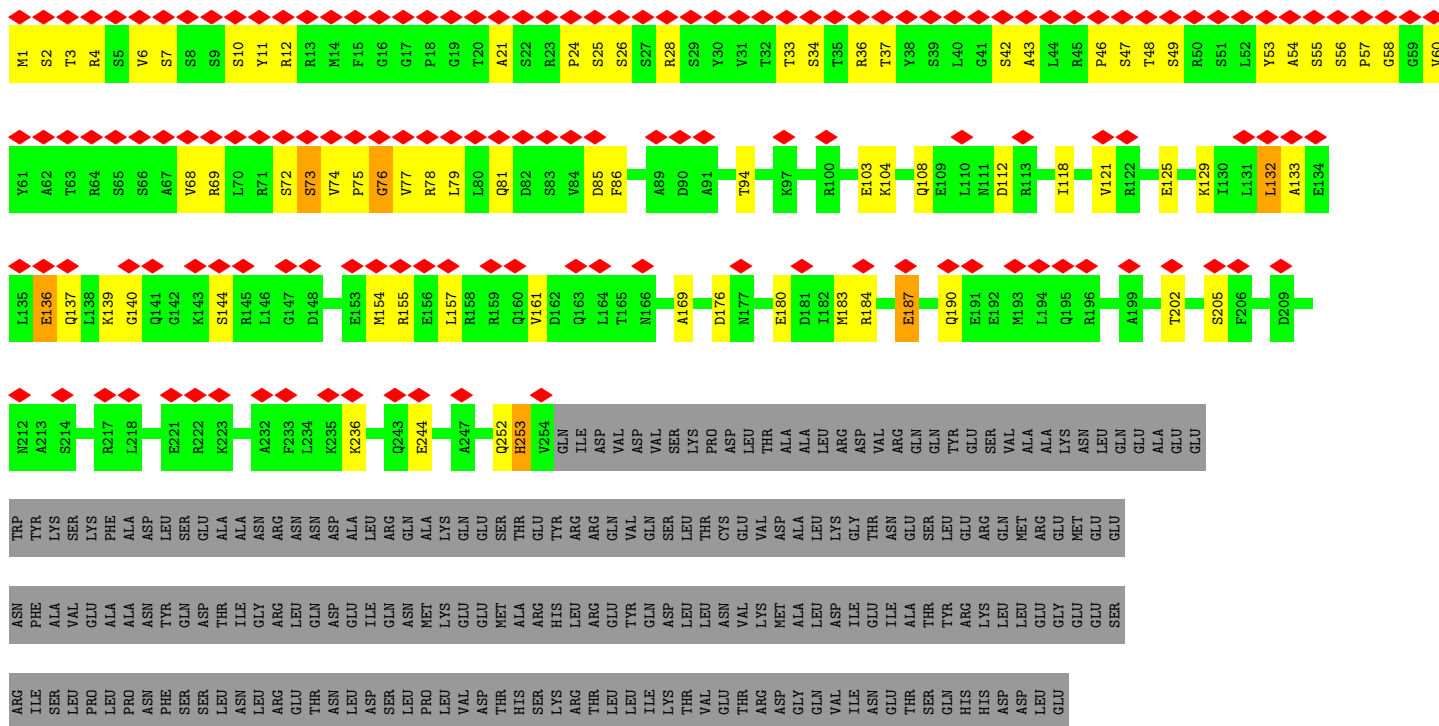
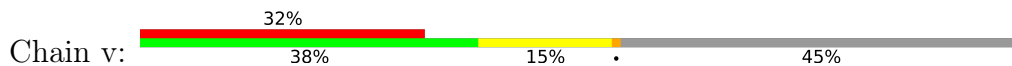
Chain s:  28% 49% 9% 14%



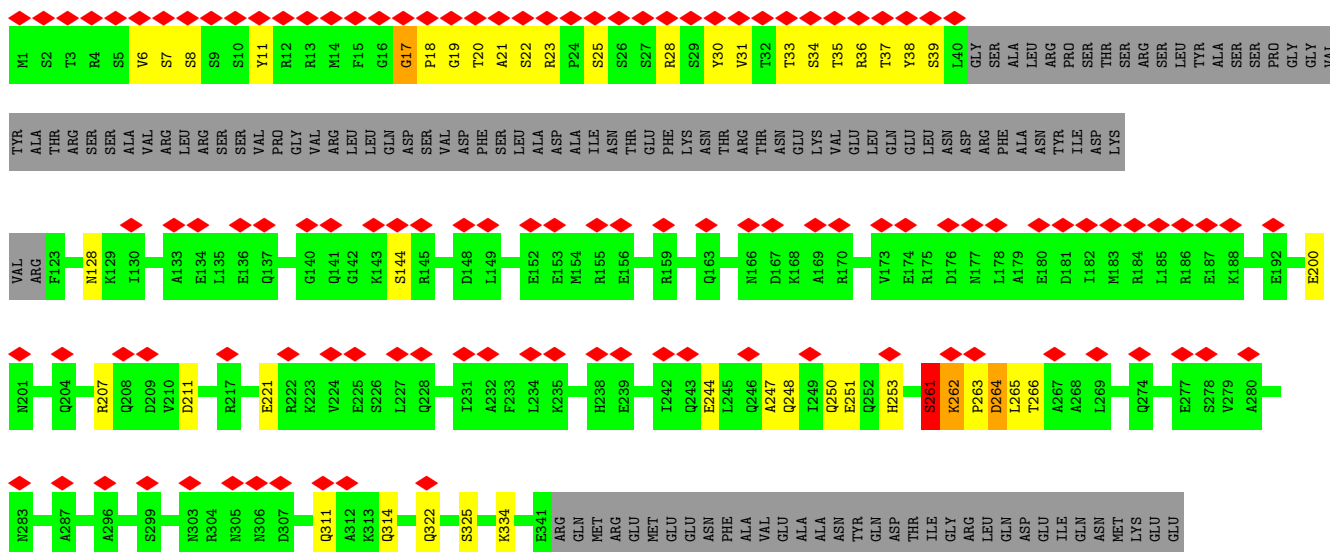




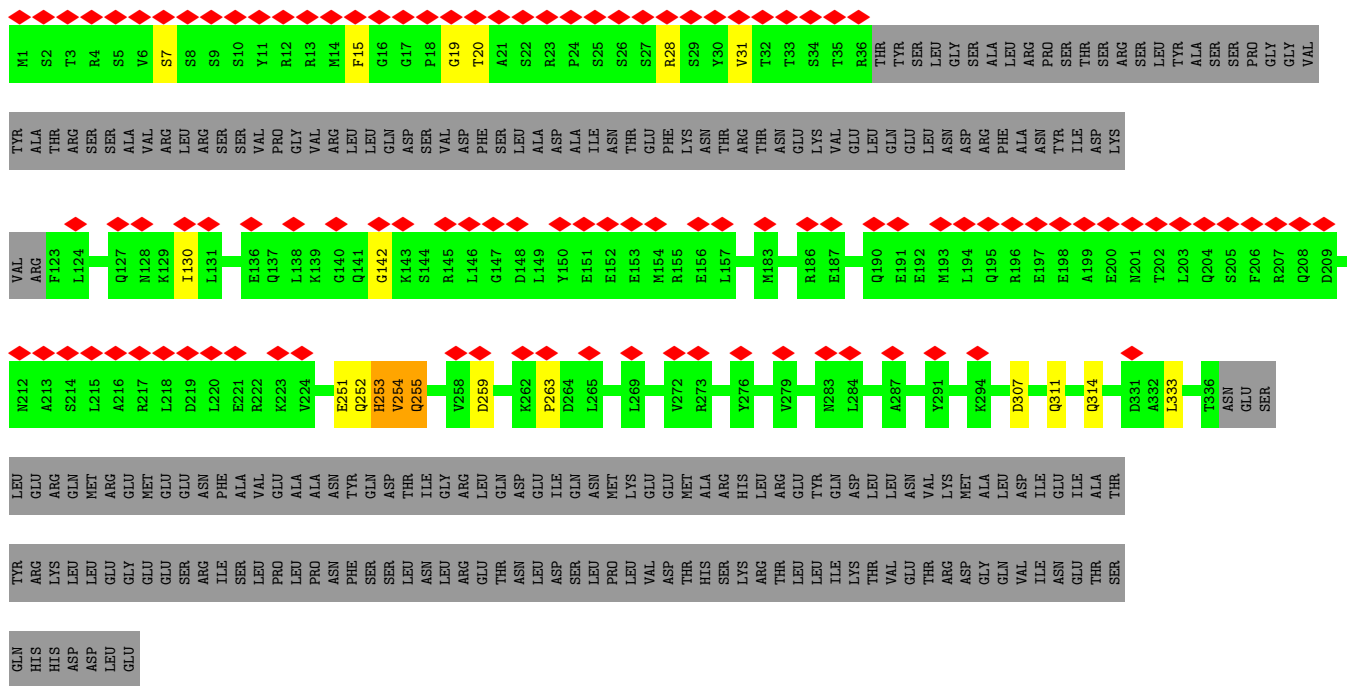
- Molecule 1: Vimentin



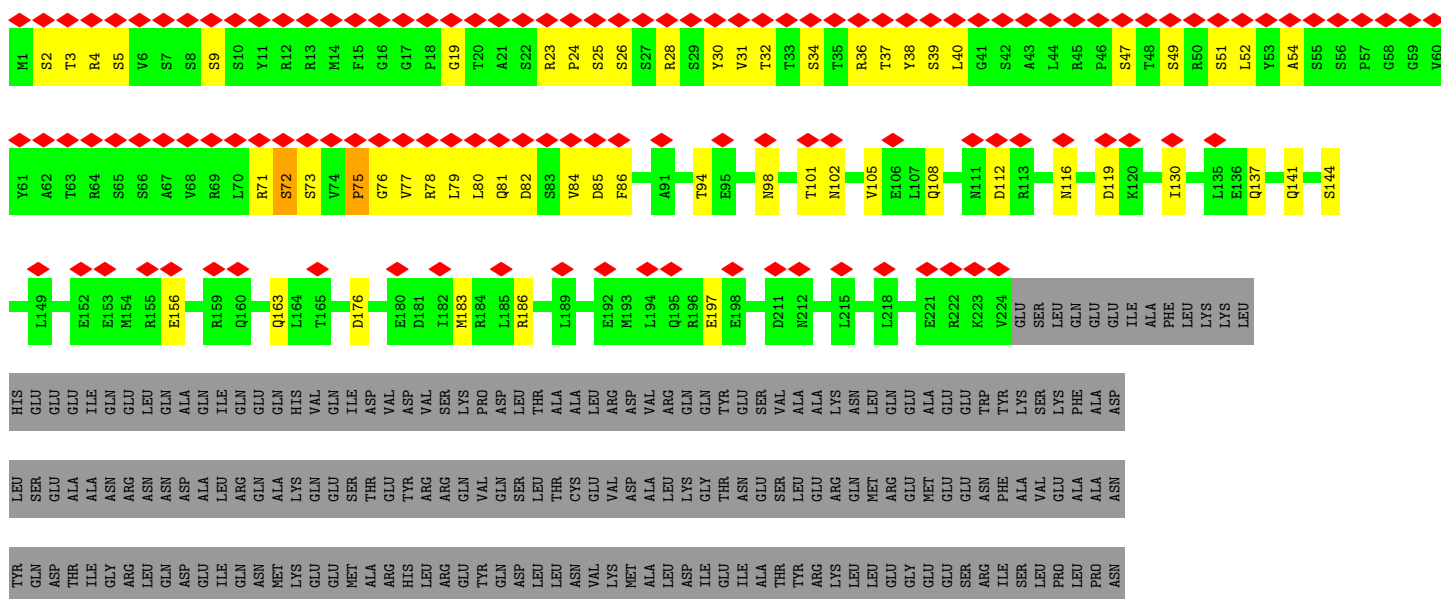
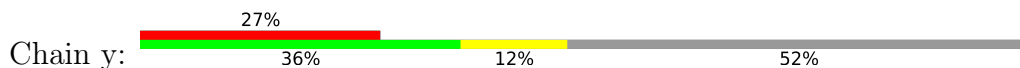
- Molecule 1: Vimentin



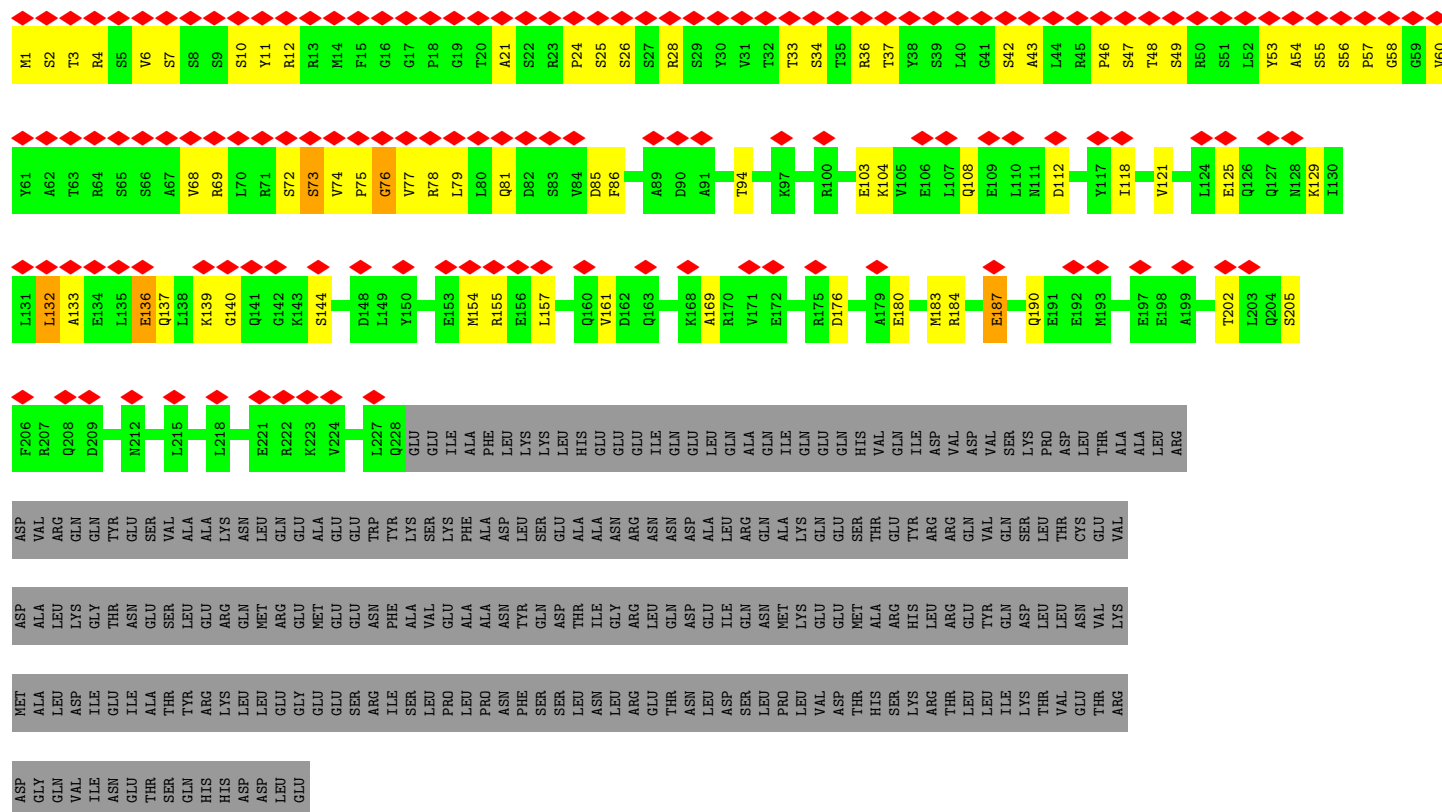
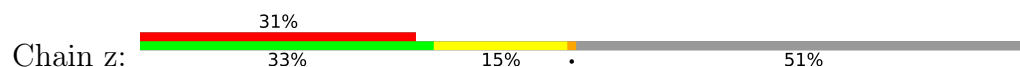
- Molecule 1: Vimentin



- Molecule 1: Vimentin



- Molecule 1: Vimentin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=73.7308°, rise=42.461 Å, axial sym=C1	Depositor
Number of segments used	236920	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	62	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	380.798, 380.798, 380.798	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0021, 1.0021, 1.0021	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	0	1.08	6/1011 (0.6%)	1.88	21/1262 (1.7%)
1	1	1.13	1/1088 (0.1%)	2.65	14/1353 (1.0%)
1	2	0.89	0/1061	1.75	10/1321 (0.8%)
1	3	0.93	0/763	1.68	5/952 (0.5%)
1	4	0.89	0/779	1.66	3/972 (0.3%)
1	5	1.14	1/1065 (0.1%)	2.72	17/1326 (1.3%)
1	6	0.87	0/1050	1.75	10/1309 (0.8%)
1	7	0.92	0/567	1.68	5/707 (0.7%)
1	8	0.88	0/587	1.64	3/732 (0.4%)
1	9	1.18	1/1006 (0.1%)	2.79	19/1254 (1.5%)
1	A	1.00	3/1122 (0.3%)	1.84	14/1399 (1.0%)
1	AA	0.94	0/379	1.71	3/472 (0.6%)
1	AB	0.90	0/399	1.66	3/497 (0.6%)
1	AC	1.22	1/890 (0.1%)	2.90	19/1109 (1.7%)
1	AD	1.11	6/887 (0.7%)	1.93	21/1107 (1.9%)
1	AE	0.94	0/195	1.70	3/242 (1.2%)
1	AF	0.91	0/215	1.70	3/267 (1.1%)
1	AG	0.89	0/795	1.84	14/992 (1.4%)
1	AH	1.12	6/795 (0.8%)	1.85	16/992 (1.6%)
1	AI	0.89	0/667	1.84	14/832 (1.7%)
1	AJ	1.16	6/679 (0.9%)	1.86	16/847 (1.9%)
1	AK	0.90	0/543	1.84	12/677 (1.8%)
1	AL	1.22	6/563 (1.1%)	1.91	16/702 (2.3%)
1	AM	0.96	0/323	2.01	9/402 (2.2%)
1	AN	1.35	6/339 (1.8%)	2.03	11/422 (2.6%)
1	AO	1.12	0/135	2.00	2/167 (1.2%)
1	AP	1.83	6/155 (3.9%)	2.50	11/192 (5.7%)
1	B	0.95	1/1074 (0.1%)	1.71	7/1339 (0.5%)
1	C	1.14	1/1122 (0.1%)	2.60	9/1399 (0.6%)
1	D	0.87	0/1111	1.70	7/1387 (0.5%)
1	E	0.82	0/131	1.68	5/162 (3.1%)
1	F	0.86	0/139	1.67	2/172 (1.2%)
1	G	0.86	0/207	1.75	6/257 (2.3%)
1	H	0.94	0/215	1.62	2/267 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.89	0/315	1.72	6/392 (1.5%)
1	J	0.96	0/331	1.65	3/412 (0.7%)
1	K	0.87	0/427	1.69	6/532 (1.1%)
1	L	0.92	0/451	1.63	3/562 (0.5%)
1	M	0.86	0/543	1.70	6/677 (0.9%)
1	N	0.90	0/567	1.63	3/707 (0.4%)
1	O	0.85	0/659	1.70	6/822 (0.7%)
1	P	0.88	0/679	1.65	5/847 (0.6%)
1	Q	0.87	0/55	1.43	0/67
1	R	0.70	0/55	1.09	0/67
1	S	0.85	0/775	1.69	6/967 (0.6%)
1	T	0.87	0/795	1.63	5/992 (0.5%)
1	U	0.89	0/211	1.65	2/262 (0.8%)
1	V	0.88	0/227	1.60	2/282 (0.7%)
1	W	1.02	3/775 (0.4%)	1.92	12/967 (1.2%)
1	X	1.01	1/775 (0.1%)	1.78	12/967 (1.2%)
1	Y	0.86	0/395	1.63	2/492 (0.4%)
1	Z	0.86	0/407	1.55	2/507 (0.4%)
1	a	1.00	3/835 (0.4%)	1.90	10/1042 (1.0%)
1	b	0.97	1/819 (0.1%)	1.74	10/1022 (1.0%)
1	c	0.85	0/591	1.63	4/737 (0.5%)
1	d	0.86	0/599	1.56	2/747 (0.3%)
1	e	0.99	3/855 (0.4%)	1.86	10/1067 (0.9%)
1	f	0.94	1/835 (0.1%)	1.75	9/1042 (0.9%)
1	g	0.86	0/775	1.60	4/967 (0.4%)
1	h	0.87	0/771	1.62	2/962 (0.2%)
1	i	1.00	3/982 (0.3%)	1.86	10/1224 (0.8%)
1	j	0.94	1/946 (0.1%)	1.78	9/1179 (0.8%)
1	k	0.85	0/895	1.60	4/1117 (0.4%)
1	l	0.85	0/899	1.60	2/1122 (0.2%)
1	m	0.99	3/1058 (0.3%)	1.83	12/1319 (0.9%)
1	n	0.95	1/1010 (0.1%)	1.74	9/1259 (0.7%)
1	o	0.85	0/1015	1.62	4/1267 (0.3%)
1	p	0.86	0/1011	1.60	2/1262 (0.2%)
1	q	1.02	3/1131 (0.3%)	1.84	15/1412 (1.1%)
1	r	0.96	1/1111 (0.1%)	1.74	10/1387 (0.7%)
1	s	1.13	1/1105 (0.1%)	2.60	7/1376 (0.5%)
1	t	0.85	0/1062	1.71	5/1324 (0.4%)
1	u	1.01	3/1031 (0.3%)	1.81	14/1287 (1.1%)
1	v	0.94	1/1015 (0.1%)	1.71	5/1267 (0.4%)
1	w	1.15	1/1033 (0.1%)	2.68	9/1286 (0.7%)
1	x	0.85	0/998	1.72	5/1244 (0.4%)
1	y	0.93	0/895	1.68	5/1117 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	z	0.87	0/911	1.67	3/1137 (0.3%)
All	All	0.98	81/54687 (0.1%)	1.90	594/68182 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	23
1	1	0	20
1	2	0	16
1	3	0	19
1	4	0	21
1	5	0	22
1	6	0	17
1	7	0	17
1	8	0	16
1	9	0	24
1	A	0	33
1	AA	0	16
1	AB	0	11
1	AC	0	23
1	AD	0	23
1	AE	0	9
1	AF	0	7
1	AG	0	18
1	AH	0	21
1	AI	0	18
1	AJ	0	21
1	AK	0	15
1	AL	0	18
1	AM	0	10
1	AN	0	11
1	AO	0	6
1	AP	0	8
1	B	0	24
1	C	0	15
1	D	0	16
1	E	0	3
1	G	0	11
1	H	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	12
1	J	0	7
1	K	0	13
1	L	0	10
1	M	0	15
1	N	0	11
1	O	0	19
1	P	0	13
1	Q	0	1
1	S	0	19
1	T	0	13
1	U	0	1
1	V	0	6
1	W	0	30
1	X	0	18
1	Y	0	3
1	Z	0	9
1	a	0	25
1	b	0	16
1	c	0	5
1	d	0	10
1	e	0	25
1	f	0	16
1	g	0	7
1	h	0	13
1	i	0	26
1	j	0	18
1	k	0	11
1	l	0	11
1	m	0	26
1	n	0	23
1	o	0	11
1	p	0	13
1	q	0	36
1	r	0	31
1	s	0	14
1	t	0	12
1	u	0	33
1	v	0	27
1	w	0	17
1	x	0	11
1	y	0	20

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	z	0	23
All	All	0	1217

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	261	SER	C-N	-24.30	0.83	1.33
1	5	261	SER	C-N	-24.30	0.83	1.33
1	s	261	SER	C-N	-24.30	0.83	1.33
1	9	261	SER	C-N	-24.29	0.83	1.33
1	AC	261	SER	C-N	-24.29	0.83	1.33
1	C	261	SER	C-N	-24.29	0.83	1.33
1	w	261	SER	C-N	-24.29	0.83	1.33
1	f	253	HIS	CA-C	9.84	1.57	1.52
1	X	253	HIS	CA-C	9.83	1.57	1.52
1	j	253	HIS	CA-C	9.80	1.57	1.52
1	r	253	HIS	CA-C	9.80	1.57	1.52
1	b	253	HIS	CA-C	9.79	1.57	1.52
1	B	253	HIS	CA-C	9.79	1.57	1.52
1	v	253	HIS	CA-C	9.78	1.57	1.52
1	n	253	HIS	CA-C	9.75	1.57	1.52
1	AH	413	LEU	CA-C	9.20	1.64	1.52
1	AP	413	LEU	CA-C	9.19	1.64	1.52
1	AD	413	LEU	CA-C	9.18	1.64	1.52
1	AL	413	LEU	CA-C	9.18	1.64	1.52
1	0	413	LEU	CA-C	9.17	1.64	1.52
1	AN	413	LEU	CA-C	9.17	1.64	1.52
1	AJ	413	LEU	CA-C	9.15	1.64	1.52
1	AL	413	LEU	N-CA	7.22	1.56	1.46
1	AD	413	LEU	N-CA	7.20	1.56	1.46
1	AP	413	LEU	N-CA	7.20	1.56	1.46
1	AH	413	LEU	N-CA	7.19	1.56	1.46
1	AJ	413	LEU	N-CA	7.19	1.56	1.46
1	0	413	LEU	N-CA	7.18	1.56	1.46
1	AN	413	LEU	N-CA	7.17	1.56	1.46
1	AH	417	ASN	CA-C	6.82	1.55	1.52
1	AN	417	ASN	CA-C	6.76	1.55	1.52
1	AL	417	ASN	CA-C	6.74	1.55	1.52
1	AP	417	ASN	CA-C	6.74	1.55	1.52
1	AD	417	ASN	CA-C	6.70	1.55	1.52
1	AJ	417	ASN	CA-C	6.69	1.55	1.52
1	0	417	ASN	CA-C	6.64	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	252	GLN	CA-C	6.44	1.61	1.52
1	q	252	GLN	CA-C	6.43	1.61	1.52
1	A	252	GLN	CA-C	6.41	1.61	1.52
1	a	252	GLN	CA-C	6.41	1.61	1.52
1	i	252	GLN	CA-C	6.41	1.61	1.52
1	u	252	GLN	CA-C	6.41	1.61	1.52
1	W	252	GLN	CA-C	6.41	1.61	1.52
1	e	252	GLN	CA-C	6.40	1.61	1.52
1	AN	412	SER	CA-C	5.96	1.60	1.52
1	AH	412	SER	CA-C	5.94	1.60	1.52
1	AP	412	SER	CA-C	5.92	1.60	1.52
1	AJ	412	SER	CA-C	5.91	1.60	1.52
1	0	412	SER	CA-C	5.89	1.60	1.52
1	AD	412	SER	CA-C	5.88	1.60	1.52
1	AL	412	SER	CA-C	5.87	1.60	1.52
1	AP	414	PRO	CA-C	5.72	1.60	1.52
1	AJ	414	PRO	CA-C	5.72	1.60	1.52
1	0	414	PRO	CA-C	5.71	1.60	1.52
1	AN	414	PRO	CA-C	5.71	1.60	1.52
1	AD	414	PRO	CA-C	5.70	1.60	1.52
1	AL	414	PRO	CA-C	5.70	1.60	1.52
1	AH	414	PRO	CA-C	5.69	1.60	1.52
1	AP	411	ILE	CA-C	5.50	1.59	1.52
1	AL	411	ILE	CA-C	5.47	1.59	1.52
1	AJ	411	ILE	CA-C	5.46	1.59	1.52
1	0	411	ILE	CA-C	5.46	1.59	1.52
1	AH	411	ILE	CA-C	5.46	1.59	1.52
1	AN	411	ILE	CA-C	5.45	1.59	1.52
1	AD	411	ILE	CA-C	5.45	1.59	1.52
1	u	254	VAL	N-CA	-5.32	1.39	1.46
1	q	254	VAL	N-CA	-5.31	1.39	1.46
1	i	254	VAL	N-CA	-5.30	1.39	1.46
1	e	254	VAL	N-CA	-5.29	1.39	1.46
1	m	254	VAL	N-CA	-5.28	1.39	1.46
1	A	254	VAL	N-CA	-5.28	1.39	1.46
1	a	254	VAL	N-CA	-5.27	1.39	1.46
1	W	254	VAL	N-CA	-5.26	1.39	1.46
1	m	257	ASP	CA-C	5.03	1.59	1.52
1	a	257	ASP	CA-C	5.03	1.59	1.52
1	W	257	ASP	CA-C	5.03	1.59	1.52
1	A	257	ASP	CA-C	5.03	1.59	1.52
1	q	257	ASP	CA-C	5.03	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	u	257	ASP	CA-C	5.02	1.59	1.52
1	e	257	ASP	CA-C	5.01	1.59	1.52
1	i	257	ASP	CA-C	5.01	1.59	1.52

All (594) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	261	SER	O-C-N	-73.73	37.32	122.84
1	5	261	SER	O-C-N	-73.72	37.33	122.84
1	w	261	SER	O-C-N	-73.71	37.34	122.84
1	9	261	SER	O-C-N	-73.71	37.34	122.84
1	s	261	SER	O-C-N	-73.70	37.35	122.84
1	C	261	SER	O-C-N	-73.70	37.35	122.84
1	AC	261	SER	O-C-N	-73.69	37.35	122.84
1	f	254	VAL	N-CA-C	9.90	121.42	108.35
1	n	254	VAL	N-CA-C	9.89	121.41	108.35
1	X	254	VAL	N-CA-C	9.88	121.39	108.35
1	B	254	VAL	N-CA-C	9.88	121.39	108.35
1	j	254	VAL	N-CA-C	9.88	121.39	108.35
1	1	261	SER	CA-C-N	-9.86	97.73	121.80
1	1	261	SER	C-N-CA	-9.86	97.73	121.80
1	b	254	VAL	N-CA-C	9.86	121.37	108.35
1	5	261	SER	CA-C-N	-9.86	97.74	121.80
1	5	261	SER	C-N-CA	-9.86	97.74	121.80
1	r	254	VAL	N-CA-C	9.86	121.36	108.35
1	9	261	SER	CA-C-N	-9.86	97.75	121.80
1	9	261	SER	C-N-CA	-9.86	97.75	121.80
1	s	261	SER	CA-C-N	-9.86	97.75	121.80
1	s	261	SER	C-N-CA	-9.86	97.75	121.80
1	C	261	SER	CA-C-N	-9.85	97.77	121.80
1	C	261	SER	C-N-CA	-9.85	97.77	121.80
1	w	261	SER	CA-C-N	-9.85	97.78	121.80
1	w	261	SER	C-N-CA	-9.85	97.78	121.80
1	AC	261	SER	CA-C-N	-9.84	97.80	121.80
1	AC	261	SER	C-N-CA	-9.84	97.80	121.80
1	x	253	HIS	CA-C-N	9.75	139.25	121.70
1	x	253	HIS	C-N-CA	9.75	139.25	121.70
1	2	253	HIS	CA-C-N	9.74	139.24	121.70
1	2	253	HIS	C-N-CA	9.74	139.24	121.70
1	t	253	HIS	CA-C-N	9.74	139.23	121.70
1	t	253	HIS	C-N-CA	9.74	139.23	121.70
1	6	253	HIS	CA-C-N	9.74	139.23	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	253	HIS	C-N-CA	9.74	139.23	121.70
1	0	253	HIS	CA-C-N	9.73	139.22	121.70
1	0	253	HIS	C-N-CA	9.73	139.22	121.70
1	D	253	HIS	CA-C-N	9.73	139.22	121.70
1	D	253	HIS	C-N-CA	9.73	139.22	121.70
1	AD	253	HIS	CA-C-N	9.72	139.20	121.70
1	AD	253	HIS	C-N-CA	9.72	139.20	121.70
1	0	410	ARG	CA-C-N	8.78	137.77	121.97
1	0	410	ARG	C-N-CA	8.78	137.77	121.97
1	AP	410	ARG	CA-C-N	8.78	137.77	121.97
1	AP	410	ARG	C-N-CA	8.78	137.77	121.97
1	AH	410	ARG	CA-C-N	8.78	137.77	121.97
1	AH	410	ARG	C-N-CA	8.78	137.77	121.97
1	AJ	410	ARG	CA-C-N	8.78	137.77	121.97
1	AJ	410	ARG	C-N-CA	8.78	137.77	121.97
1	AL	410	ARG	CA-C-N	8.77	137.76	121.97
1	AL	410	ARG	C-N-CA	8.77	137.76	121.97
1	AN	410	ARG	CA-C-N	8.76	137.74	121.97
1	AN	410	ARG	C-N-CA	8.76	137.74	121.97
1	AD	410	ARG	CA-C-N	8.76	137.73	121.97
1	AD	410	ARG	C-N-CA	8.76	137.73	121.97
1	X	253	HIS	CA-C-O	-8.70	114.25	119.55
1	f	253	HIS	CA-C-O	-8.69	114.25	119.55
1	b	253	HIS	CA-C-O	-8.65	114.27	119.55
1	r	253	HIS	CA-C-O	-8.63	114.28	119.55
1	B	253	HIS	CA-C-O	-8.62	114.29	119.55
1	j	253	HIS	CA-C-O	-8.62	114.29	119.55
1	v	253	HIS	CA-C-O	-8.62	114.29	119.55
1	n	253	HIS	CA-C-O	-8.60	114.31	119.55
1	i	253	HIS	O-C-N	-8.59	110.46	122.15
1	u	253	HIS	O-C-N	-8.57	110.49	122.15
1	m	253	HIS	O-C-N	-8.56	110.51	122.15
1	q	253	HIS	O-C-N	-8.55	110.53	122.15
1	A	253	HIS	O-C-N	-8.55	110.53	122.15
1	W	253	HIS	O-C-N	-8.55	110.53	122.15
1	e	253	HIS	O-C-N	-8.54	110.54	122.15
1	a	253	HIS	O-C-N	-8.54	110.54	122.15
1	n	253	HIS	N-CA-C	7.94	120.74	108.12
1	B	253	HIS	N-CA-C	7.93	120.72	108.12
1	b	253	HIS	N-CA-C	7.92	120.72	108.12
1	f	253	HIS	N-CA-C	7.92	120.71	108.12
1	j	253	HIS	N-CA-C	7.92	120.72	108.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	253	HIS	N-CA-C	7.91	120.70	108.12
1	r	253	HIS	N-CA-C	7.91	120.70	108.12
1	v	253	HIS	N-CA-C	7.91	120.70	108.12
1	AK	424	ARG	CA-C-N	7.79	135.72	121.70
1	AK	424	ARG	C-N-CA	7.79	135.72	121.70
1	5	424	ARG	CA-C-N	7.78	135.70	121.70
1	5	424	ARG	C-N-CA	7.78	135.70	121.70
1	9	424	ARG	CA-C-N	7.78	135.69	121.70
1	9	424	ARG	C-N-CA	7.78	135.69	121.70
1	AM	424	ARG	CA-C-N	7.77	135.69	121.70
1	AM	424	ARG	C-N-CA	7.77	135.69	121.70
1	AG	424	ARG	CA-C-N	7.76	135.67	121.70
1	AG	424	ARG	C-N-CA	7.76	135.67	121.70
1	AC	424	ARG	CA-C-N	7.76	135.67	121.70
1	AC	424	ARG	C-N-CA	7.76	135.67	121.70
1	AI	424	ARG	CA-C-N	7.76	135.67	121.70
1	AI	424	ARG	C-N-CA	7.76	135.67	121.70
1	M	426	THR	CA-C-O	-7.49	112.90	121.66
1	O	426	THR	CA-C-O	-7.49	112.90	121.66
1	S	426	THR	CA-C-O	-7.48	112.91	121.66
1	I	426	THR	CA-C-O	-7.47	112.92	121.66
1	W	426	THR	CA-C-O	-7.47	112.92	121.66
1	G	426	THR	CA-C-O	-7.46	112.93	121.66
1	K	426	THR	CA-C-O	-7.46	112.93	121.66
1	d	86	PHE	CA-C-N	7.18	135.25	121.54
1	d	86	PHE	C-N-CA	7.18	135.25	121.54
1	Z	86	PHE	CA-C-N	7.18	135.25	121.54
1	Z	86	PHE	C-N-CA	7.18	135.25	121.54
1	p	86	PHE	CA-C-N	7.16	135.22	121.54
1	p	86	PHE	C-N-CA	7.16	135.22	121.54
1	D	86	PHE	CA-C-N	7.16	135.21	121.54
1	D	86	PHE	C-N-CA	7.16	135.21	121.54
1	l	86	PHE	CA-C-N	7.16	135.21	121.54
1	l	86	PHE	C-N-CA	7.16	135.21	121.54
1	AD	253	HIS	O-C-N	-7.15	112.92	122.22
1	h	86	PHE	CA-C-N	7.15	135.19	121.54
1	h	86	PHE	C-N-CA	7.15	135.19	121.54
1	D	253	HIS	O-C-N	-7.15	112.93	122.22
1	t	253	HIS	O-C-N	-7.14	112.94	122.22
1	V	86	PHE	CA-C-N	7.14	135.18	121.54
1	V	86	PHE	C-N-CA	7.14	135.18	121.54
1	2	253	HIS	O-C-N	-7.14	112.94	122.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	253	HIS	O-C-N	-7.14	112.94	122.22
1	x	253	HIS	O-C-N	-7.13	112.95	122.22
1	0	253	HIS	O-C-N	-7.13	112.95	122.22
1	e	251	GLU	N-CA-C	7.02	121.67	113.18
1	W	251	GLU	N-CA-C	7.01	121.67	113.18
1	u	251	GLU	N-CA-C	7.00	121.66	113.18
1	a	251	GLU	N-CA-C	7.00	121.65	113.18
1	q	251	GLU	N-CA-C	7.00	121.64	113.18
1	i	251	GLU	N-CA-C	6.99	121.64	113.18
1	A	251	GLU	N-CA-C	6.98	121.63	113.18
1	m	251	GLU	N-CA-C	6.98	121.63	113.18
1	q	256	ILE	CA-C-N	6.88	134.67	121.54
1	q	256	ILE	C-N-CA	6.88	134.67	121.54
1	m	256	ILE	CA-C-N	6.87	134.65	121.54
1	m	256	ILE	C-N-CA	6.87	134.65	121.54
1	i	256	ILE	CA-C-N	6.86	134.65	121.54
1	i	256	ILE	C-N-CA	6.86	134.65	121.54
1	A	256	ILE	CA-C-N	6.86	134.65	121.54
1	A	256	ILE	C-N-CA	6.86	134.65	121.54
1	e	256	ILE	CA-C-N	6.86	134.64	121.54
1	e	256	ILE	C-N-CA	6.86	134.64	121.54
1	a	256	ILE	CA-C-N	6.86	134.64	121.54
1	a	256	ILE	C-N-CA	6.86	134.64	121.54
1	W	256	ILE	CA-C-N	6.86	134.64	121.54
1	W	256	ILE	C-N-CA	6.86	134.64	121.54
1	u	256	ILE	CA-C-N	6.86	134.64	121.54
1	u	256	ILE	C-N-CA	6.86	134.64	121.54
1	AG	454	VAL	CA-C-N	6.81	133.96	121.70
1	AG	454	VAL	C-N-CA	6.81	133.96	121.70
1	AK	454	VAL	CA-C-N	6.80	133.94	121.70
1	AK	454	VAL	C-N-CA	6.80	133.94	121.70
1	5	454	VAL	CA-C-N	6.79	133.92	121.70
1	5	454	VAL	C-N-CA	6.79	133.92	121.70
1	1	454	VAL	CA-C-N	6.79	133.92	121.70
1	1	454	VAL	C-N-CA	6.79	133.92	121.70
1	9	454	VAL	CA-C-N	6.77	133.89	121.70
1	9	454	VAL	C-N-CA	6.77	133.89	121.70
1	AC	454	VAL	CA-C-N	6.77	133.88	121.70
1	AC	454	VAL	C-N-CA	6.77	133.88	121.70
1	AI	454	VAL	CA-C-N	6.77	133.88	121.70
1	AI	454	VAL	C-N-CA	6.77	133.88	121.70
1	G	436	THR	CA-C-N	6.73	133.81	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	436	THR	C-N-CA	6.73	133.81	121.70
1	I	436	THR	CA-C-N	6.73	133.81	121.70
1	I	436	THR	C-N-CA	6.73	133.81	121.70
1	W	436	THR	CA-C-N	6.73	133.81	121.70
1	W	436	THR	C-N-CA	6.73	133.81	121.70
1	S	436	THR	CA-C-N	6.72	133.81	121.70
1	S	436	THR	C-N-CA	6.72	133.81	121.70
1	K	436	THR	CA-C-N	6.72	133.80	121.70
1	K	436	THR	C-N-CA	6.72	133.80	121.70
1	M	436	THR	CA-C-N	6.72	133.79	121.70
1	M	436	THR	C-N-CA	6.72	133.79	121.70
1	E	436	THR	CA-C-N	6.72	133.79	121.70
1	E	436	THR	C-N-CA	6.72	133.79	121.70
1	O	436	THR	CA-C-N	6.70	133.77	121.70
1	O	436	THR	C-N-CA	6.70	133.77	121.70
1	AH	412	SER	CA-C-O	-6.54	111.15	120.51
1	AL	412	SER	CA-C-O	-6.53	111.17	120.51
1	AP	412	SER	CA-C-O	-6.53	111.17	120.51
1	AN	412	SER	CA-C-O	-6.53	111.18	120.51
1	H	435	ASP	CA-C-N	6.53	133.45	121.70
1	H	435	ASP	C-N-CA	6.53	133.45	121.70
1	AJ	412	SER	CA-C-O	-6.52	111.18	120.51
1	AM	435	ASP	CA-C-N	6.52	133.43	121.70
1	AM	435	ASP	C-N-CA	6.52	133.43	121.70
1	P	435	ASP	CA-C-N	6.52	133.44	121.70
1	P	435	ASP	C-N-CA	6.52	133.44	121.70
1	0	412	SER	CA-C-O	-6.51	111.19	120.51
1	5	435	ASP	CA-C-N	6.51	133.42	121.70
1	5	435	ASP	C-N-CA	6.51	133.42	121.70
1	O	436	THR	O-C-N	-6.51	113.46	122.19
1	AD	412	SER	CA-C-O	-6.51	111.20	120.51
1	N	435	ASP	CA-C-N	6.51	133.42	121.70
1	N	435	ASP	C-N-CA	6.51	133.42	121.70
1	J	435	ASP	CA-C-N	6.51	133.42	121.70
1	J	435	ASP	C-N-CA	6.51	133.42	121.70
1	v	85	ASP	CA-C-N	6.50	133.41	121.70
1	v	85	ASP	C-N-CA	6.50	133.41	121.70
1	4	85	ASP	CA-C-N	6.50	133.40	121.70
1	4	85	ASP	C-N-CA	6.50	133.40	121.70
1	AG	435	ASP	CA-C-N	6.50	133.40	121.70
1	AG	435	ASP	C-N-CA	6.50	133.40	121.70
1	AK	435	ASP	CA-C-N	6.50	133.40	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AK	435	ASP	C-N-CA	6.50	133.40	121.70
1	F	435	ASP	CA-C-N	6.50	133.40	121.70
1	F	435	ASP	C-N-CA	6.50	133.40	121.70
1	AC	435	ASP	CA-C-N	6.49	133.39	121.70
1	AC	435	ASP	C-N-CA	6.49	133.39	121.70
1	AI	435	ASP	CA-C-N	6.49	133.39	121.70
1	AI	435	ASP	C-N-CA	6.49	133.39	121.70
1	r	85	ASP	CA-C-N	6.49	133.39	121.70
1	r	85	ASP	C-N-CA	6.49	133.39	121.70
1	AB	85	ASP	CA-C-N	6.49	133.38	121.70
1	AB	85	ASP	C-N-CA	6.49	133.38	121.70
1	z	85	ASP	CA-C-N	6.49	133.38	121.70
1	z	85	ASP	C-N-CA	6.49	133.38	121.70
1	9	435	ASP	CA-C-N	6.49	133.38	121.70
1	9	435	ASP	C-N-CA	6.49	133.38	121.70
1	8	85	ASP	CA-C-N	6.49	133.38	121.70
1	8	85	ASP	C-N-CA	6.49	133.38	121.70
1	AF	85	ASP	CA-C-N	6.49	133.38	121.70
1	AF	85	ASP	C-N-CA	6.49	133.38	121.70
1	K	436	THR	O-C-N	-6.49	113.50	122.19
1	L	435	ASP	CA-C-N	6.48	133.37	121.70
1	L	435	ASP	C-N-CA	6.48	133.37	121.70
1	T	435	ASP	CA-C-N	6.48	133.37	121.70
1	T	435	ASP	C-N-CA	6.48	133.37	121.70
1	W	436	THR	O-C-N	-6.48	113.51	122.19
1	X	435	ASP	CA-C-N	6.48	133.36	121.70
1	X	435	ASP	C-N-CA	6.48	133.36	121.70
1	M	436	THR	O-C-N	-6.47	113.52	122.19
1	E	436	THR	O-C-N	-6.46	113.54	122.19
1	G	436	THR	O-C-N	-6.45	113.55	122.19
1	S	436	THR	O-C-N	-6.45	113.55	122.19
1	I	436	THR	O-C-N	-6.44	113.56	122.19
1	0	415	LEU	N-CA-C	6.40	121.03	109.44
1	AD	415	LEU	N-CA-C	6.39	121.01	109.44
1	AP	415	LEU	N-CA-C	6.39	121.01	109.44
1	AH	415	LEU	N-CA-C	6.39	121.00	109.44
1	AN	415	LEU	N-CA-C	6.39	121.01	109.44
1	AL	415	LEU	N-CA-C	6.38	120.98	109.44
1	AH	414	PRO	N-CA-C	6.37	125.60	112.47
1	AJ	415	LEU	N-CA-C	6.37	120.97	109.44
1	1	17	GLY	CA-C-N	6.37	127.80	119.84
1	1	17	GLY	C-N-CA	6.37	127.80	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AD	447	VAL	CA-C-N	6.36	133.16	121.70
1	AD	447	VAL	C-N-CA	6.36	133.16	121.70
1	AP	414	PRO	N-CA-C	6.36	125.57	112.47
1	o	17	GLY	CA-C-N	6.36	127.79	119.84
1	o	17	GLY	C-N-CA	6.36	127.79	119.84
1	0	447	VAL	CA-C-N	6.36	133.14	121.70
1	0	447	VAL	C-N-CA	6.36	133.14	121.70
1	AD	414	PRO	N-CA-C	6.36	125.56	112.47
1	0	414	PRO	N-CA-C	6.35	125.56	112.47
1	AN	414	PRO	N-CA-C	6.35	125.56	112.47
1	c	17	GLY	CA-C-N	6.35	127.78	119.84
1	c	17	GLY	C-N-CA	6.35	127.78	119.84
1	AL	414	PRO	N-CA-C	6.35	125.55	112.47
1	C	17	GLY	CA-C-N	6.35	127.77	119.84
1	C	17	GLY	C-N-CA	6.35	127.77	119.84
1	AJ	414	PRO	N-CA-C	6.34	125.53	112.47
1	AH	447	VAL	CA-C-N	6.34	133.11	121.70
1	AH	447	VAL	C-N-CA	6.34	133.11	121.70
1	k	17	GLY	CA-C-N	6.34	127.76	119.84
1	k	17	GLY	C-N-CA	6.34	127.76	119.84
1	AJ	447	VAL	CA-C-N	6.33	133.10	121.70
1	AJ	447	VAL	C-N-CA	6.33	133.10	121.70
1	2	447	VAL	CA-C-N	6.33	133.10	121.70
1	2	447	VAL	C-N-CA	6.33	133.10	121.70
1	AL	447	VAL	CA-C-N	6.33	133.10	121.70
1	AL	447	VAL	C-N-CA	6.33	133.10	121.70
1	s	17	GLY	CA-C-N	6.33	127.75	119.84
1	s	17	GLY	C-N-CA	6.33	127.75	119.84
1	w	17	GLY	CA-C-N	6.32	127.75	119.84
1	w	17	GLY	C-N-CA	6.32	127.75	119.84
1	6	447	VAL	CA-C-N	6.32	133.07	121.70
1	6	447	VAL	C-N-CA	6.32	133.07	121.70
1	b	264	ASP	CA-C-N	6.31	129.60	120.38
1	b	264	ASP	C-N-CA	6.31	129.60	120.38
1	X	264	ASP	CA-C-N	6.31	129.59	120.38
1	X	264	ASP	C-N-CA	6.31	129.59	120.38
1	f	264	ASP	CA-C-N	6.31	129.59	120.38
1	f	264	ASP	C-N-CA	6.31	129.59	120.38
1	j	264	ASP	CA-C-N	6.31	129.59	120.38
1	j	264	ASP	C-N-CA	6.31	129.59	120.38
1	n	264	ASP	CA-C-N	6.31	129.59	120.38
1	n	264	ASP	C-N-CA	6.31	129.59	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ASP	CA-C-N	6.31	129.59	120.38
1	B	264	ASP	C-N-CA	6.31	129.59	120.38
1	i	239	GLU	CA-C-N	6.30	129.24	120.29
1	i	239	GLU	C-N-CA	6.30	129.24	120.29
1	g	17	GLY	CA-C-N	6.30	127.71	119.84
1	g	17	GLY	C-N-CA	6.30	127.71	119.84
1	q	239	GLU	CA-C-N	6.30	129.23	120.29
1	q	239	GLU	C-N-CA	6.30	129.23	120.29
1	r	264	ASP	CA-C-N	6.29	129.57	120.38
1	r	264	ASP	C-N-CA	6.29	129.57	120.38
1	m	239	GLU	CA-C-N	6.29	129.23	120.29
1	m	239	GLU	C-N-CA	6.29	129.23	120.29
1	u	239	GLU	CA-C-N	6.29	129.22	120.29
1	u	239	GLU	C-N-CA	6.29	129.22	120.29
1	A	239	GLU	CA-C-N	6.29	129.22	120.29
1	A	239	GLU	C-N-CA	6.29	129.22	120.29
1	W	257	ASP	N-CA-C	6.29	124.19	110.80
1	a	257	ASP	N-CA-C	6.29	124.19	110.80
1	e	239	GLU	CA-C-N	6.29	129.22	120.29
1	e	239	GLU	C-N-CA	6.29	129.22	120.29
1	A	257	ASP	N-CA-C	6.28	124.17	110.80
1	a	239	GLU	CA-C-N	6.28	129.20	120.29
1	a	239	GLU	C-N-CA	6.28	129.20	120.29
1	m	257	ASP	N-CA-C	6.27	124.16	110.80
1	u	257	ASP	N-CA-C	6.27	124.16	110.80
1	i	257	ASP	N-CA-C	6.27	124.15	110.80
1	e	257	ASP	N-CA-C	6.26	124.14	110.80
1	q	257	ASP	N-CA-C	6.26	124.14	110.80
1	o	85	ASP	CA-C-N	6.04	132.56	121.70
1	o	85	ASP	C-N-CA	6.04	132.56	121.70
1	Y	85	ASP	CA-C-N	6.03	132.55	121.70
1	Y	85	ASP	C-N-CA	6.03	132.55	121.70
1	C	85	ASP	CA-C-N	6.03	132.54	121.70
1	C	85	ASP	C-N-CA	6.03	132.54	121.70
1	g	85	ASP	CA-C-N	6.02	132.53	121.70
1	g	85	ASP	C-N-CA	6.02	132.53	121.70
1	k	85	ASP	CA-C-N	6.01	132.52	121.70
1	k	85	ASP	C-N-CA	6.01	132.52	121.70
1	U	85	ASP	CA-C-N	6.01	132.52	121.70
1	U	85	ASP	C-N-CA	6.01	132.52	121.70
1	c	85	ASP	CA-C-N	6.01	132.52	121.70
1	c	85	ASP	C-N-CA	6.01	132.52	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AI	454	VAL	O-C-N	-5.93	115.16	122.57
1	AC	454	VAL	O-C-N	-5.93	115.16	122.57
1	9	454	VAL	O-C-N	-5.91	115.18	122.57
1	1	454	VAL	O-C-N	-5.89	115.20	122.57
1	P	412	SER	O-C-N	-5.89	116.44	123.27
1	J	412	SER	O-C-N	-5.88	116.45	123.27
1	5	454	VAL	O-C-N	-5.88	115.22	122.57
1	AK	454	VAL	O-C-N	-5.87	115.23	122.57
1	L	412	SER	O-C-N	-5.87	116.46	123.27
1	AG	454	VAL	O-C-N	-5.87	115.23	122.57
1	T	412	SER	O-C-N	-5.87	116.46	123.27
1	b	412	SER	O-C-N	-5.86	116.47	123.27
1	0	413	LEU	O-C-N	-5.85	114.59	121.32
1	AD	413	LEU	O-C-N	-5.85	114.59	121.32
1	AN	413	LEU	O-C-N	-5.85	114.60	121.32
1	N	412	SER	O-C-N	-5.84	116.49	123.27
1	AJ	413	LEU	O-C-N	-5.83	114.61	121.32
1	X	412	SER	O-C-N	-5.83	116.50	123.27
1	AP	413	LEU	O-C-N	-5.83	114.62	121.32
1	AL	413	LEU	O-C-N	-5.83	114.62	121.32
1	AH	413	LEU	O-C-N	-5.82	114.62	121.32
1	7	137	GLN	CA-C-N	5.70	128.71	120.79
1	7	137	GLN	C-N-CA	5.70	128.71	120.79
1	q	137	GLN	CA-C-N	5.69	128.70	120.79
1	q	137	GLN	C-N-CA	5.69	128.70	120.79
1	u	137	GLN	CA-C-N	5.69	128.71	120.79
1	u	137	GLN	C-N-CA	5.69	128.71	120.79
1	A	137	GLN	CA-C-N	5.69	128.70	120.79
1	A	137	GLN	C-N-CA	5.69	128.70	120.79
1	m	137	GLN	CA-C-N	5.69	128.70	120.79
1	m	137	GLN	C-N-CA	5.69	128.70	120.79
1	y	137	GLN	CA-C-N	5.69	128.69	120.79
1	y	137	GLN	C-N-CA	5.69	128.69	120.79
1	3	137	GLN	CA-C-N	5.68	128.69	120.79
1	3	137	GLN	C-N-CA	5.68	128.69	120.79
1	AI	314	GLN	CA-C-N	5.67	128.19	120.54
1	AI	314	GLN	C-N-CA	5.67	128.19	120.54
1	AC	314	GLN	CA-C-N	5.66	128.18	120.54
1	AC	314	GLN	C-N-CA	5.66	128.18	120.54
1	w	314	GLN	CA-C-N	5.66	128.18	120.54
1	w	314	GLN	C-N-CA	5.66	128.18	120.54
1	5	314	GLN	CA-C-N	5.66	128.18	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	314	GLN	C-N-CA	5.66	128.18	120.54
1	1	314	GLN	CA-C-N	5.65	128.17	120.54
1	1	314	GLN	C-N-CA	5.65	128.17	120.54
1	AG	314	GLN	CA-C-N	5.65	128.16	120.54
1	AG	314	GLN	C-N-CA	5.65	128.16	120.54
1	i	252	GLN	CA-C-N	5.65	131.59	121.15
1	i	252	GLN	C-N-CA	5.65	131.59	121.15
1	e	252	GLN	CA-C-N	5.64	131.59	121.15
1	e	252	GLN	C-N-CA	5.64	131.59	121.15
1	u	252	GLN	CA-C-N	5.64	131.59	121.15
1	u	252	GLN	C-N-CA	5.64	131.59	121.15
1	9	314	GLN	CA-C-N	5.64	128.16	120.54
1	9	314	GLN	C-N-CA	5.64	128.16	120.54
1	A	252	GLN	CA-C-N	5.64	131.58	121.15
1	A	252	GLN	C-N-CA	5.64	131.58	121.15
1	q	252	GLN	CA-C-N	5.64	131.58	121.15
1	q	252	GLN	C-N-CA	5.64	131.58	121.15
1	W	252	GLN	CA-C-N	5.63	131.57	121.15
1	W	252	GLN	C-N-CA	5.63	131.57	121.15
1	m	252	GLN	CA-C-N	5.63	131.57	121.15
1	m	252	GLN	C-N-CA	5.63	131.57	121.15
1	a	252	GLN	CA-C-N	5.62	131.56	121.15
1	a	252	GLN	C-N-CA	5.62	131.56	121.15
1	AC	264	ASP	CA-C-N	5.55	132.15	121.54
1	AC	264	ASP	C-N-CA	5.55	132.15	121.54
1	5	264	ASP	CA-C-N	5.55	132.14	121.54
1	5	264	ASP	C-N-CA	5.55	132.14	121.54
1	9	264	ASP	CA-C-N	5.55	132.14	121.54
1	9	264	ASP	C-N-CA	5.55	132.14	121.54
1	C	264	ASP	CA-C-N	5.54	132.13	121.54
1	C	264	ASP	C-N-CA	5.54	132.13	121.54
1	w	264	ASP	CA-C-N	5.54	132.13	121.54
1	w	264	ASP	C-N-CA	5.54	132.13	121.54
1	s	264	ASP	CA-C-N	5.54	132.12	121.54
1	s	264	ASP	C-N-CA	5.54	132.12	121.54
1	1	264	ASP	CA-C-N	5.54	132.11	121.54
1	1	264	ASP	C-N-CA	5.54	132.11	121.54
1	AD	414	PRO	CA-C-N	5.49	130.06	121.17
1	AD	414	PRO	C-N-CA	5.49	130.06	121.17
1	b	310	ARG	CA-C-N	5.48	127.89	120.44
1	b	310	ARG	C-N-CA	5.48	127.89	120.44
1	j	310	ARG	CA-C-N	5.47	127.88	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	310	ARG	C-N-CA	5.47	127.88	120.44
1	n	310	ARG	CA-C-N	5.47	127.88	120.44
1	n	310	ARG	C-N-CA	5.47	127.88	120.44
1	AH	414	PRO	CA-C-N	5.47	130.03	121.17
1	AH	414	PRO	C-N-CA	5.47	130.03	121.17
1	P	310	ARG	CA-C-N	5.47	127.87	120.44
1	P	310	ARG	C-N-CA	5.47	127.87	120.44
1	f	310	ARG	CA-C-N	5.46	127.87	120.44
1	f	310	ARG	C-N-CA	5.46	127.87	120.44
1	T	310	ARG	CA-C-N	5.46	127.87	120.44
1	T	310	ARG	C-N-CA	5.46	127.87	120.44
1	AL	414	PRO	CA-C-N	5.46	130.01	121.17
1	AL	414	PRO	C-N-CA	5.46	130.01	121.17
1	AJ	414	PRO	CA-C-N	5.46	130.01	121.17
1	AJ	414	PRO	C-N-CA	5.46	130.01	121.17
1	AN	414	PRO	CA-C-N	5.46	130.01	121.17
1	AN	414	PRO	C-N-CA	5.46	130.01	121.17
1	X	310	ARG	CA-C-N	5.46	127.86	120.44
1	X	310	ARG	C-N-CA	5.46	127.86	120.44
1	0	414	PRO	CA-C-N	5.46	130.01	121.17
1	0	414	PRO	C-N-CA	5.46	130.01	121.17
1	AP	414	PRO	CA-C-N	5.45	130.00	121.17
1	AP	414	PRO	C-N-CA	5.45	130.00	121.17
1	W	259	ASP	N-CA-C	5.44	117.56	110.43
1	i	259	ASP	N-CA-C	5.43	117.54	110.43
1	A	259	ASP	N-CA-C	5.42	117.54	110.43
1	m	259	ASP	N-CA-C	5.42	117.53	110.43
1	q	259	ASP	N-CA-C	5.42	117.53	110.43
1	e	259	ASP	N-CA-C	5.41	117.52	110.43
1	a	259	ASP	N-CA-C	5.40	117.51	110.43
1	0	412	SER	CA-C-N	5.40	134.97	121.80
1	0	412	SER	C-N-CA	5.40	134.97	121.80
1	AD	412	SER	CA-C-N	5.40	134.97	121.80
1	AD	412	SER	C-N-CA	5.40	134.97	121.80
1	AJ	412	SER	CA-C-N	5.39	134.96	121.80
1	AJ	412	SER	C-N-CA	5.39	134.96	121.80
1	AN	412	SER	CA-C-N	5.39	134.96	121.80
1	AN	412	SER	C-N-CA	5.39	134.96	121.80
1	AP	412	SER	CA-C-N	5.39	134.95	121.80
1	AP	412	SER	C-N-CA	5.39	134.95	121.80
1	AL	412	SER	CA-C-N	5.39	134.95	121.80
1	AL	412	SER	C-N-CA	5.39	134.95	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AH	412	SER	CA-C-N	5.38	134.94	121.80
1	AH	412	SER	C-N-CA	5.38	134.94	121.80
1	AB	74	VAL	CA-C-O	-5.37	117.15	119.94
1	AL	465	LEU	CA-C-N	5.36	131.35	121.70
1	AL	465	LEU	C-N-CA	5.36	131.35	121.70
1	0	465	LEU	CA-C-N	5.36	131.35	121.70
1	0	465	LEU	C-N-CA	5.36	131.35	121.70
1	4	74	VAL	CA-C-O	-5.36	117.16	119.94
1	6	465	LEU	CA-C-N	5.36	131.34	121.70
1	6	465	LEU	C-N-CA	5.36	131.34	121.70
1	AD	465	LEU	CA-C-N	5.36	131.34	121.70
1	AD	465	LEU	C-N-CA	5.36	131.34	121.70
1	AH	465	LEU	CA-C-N	5.36	131.34	121.70
1	AH	465	LEU	C-N-CA	5.36	131.34	121.70
1	AJ	465	LEU	CA-C-N	5.35	131.32	121.70
1	AJ	465	LEU	C-N-CA	5.35	131.32	121.70
1	2	465	LEU	CA-C-N	5.34	131.32	121.70
1	2	465	LEU	C-N-CA	5.34	131.32	121.70
1	AF	74	VAL	CA-C-O	-5.34	117.17	119.94
1	AD	254	VAL	CA-C-N	5.33	131.71	121.54
1	AD	254	VAL	C-N-CA	5.33	131.71	121.54
1	2	254	VAL	CA-C-N	5.31	131.69	121.54
1	2	254	VAL	C-N-CA	5.31	131.69	121.54
1	6	254	VAL	CA-C-N	5.31	131.68	121.54
1	6	254	VAL	C-N-CA	5.31	131.68	121.54
1	0	254	VAL	CA-C-N	5.30	131.67	121.54
1	0	254	VAL	C-N-CA	5.30	131.67	121.54
1	D	254	VAL	CA-C-N	5.30	131.66	121.54
1	D	254	VAL	C-N-CA	5.30	131.66	121.54
1	t	254	VAL	CA-C-N	5.30	131.66	121.54
1	t	254	VAL	C-N-CA	5.30	131.66	121.54
1	v	74	VAL	CA-C-O	-5.29	117.19	119.94
1	x	254	VAL	CA-C-N	5.29	131.64	121.54
1	x	254	VAL	C-N-CA	5.29	131.64	121.54
1	9	362	ILE	CA-C-N	5.29	125.81	119.94
1	9	362	ILE	C-N-CA	5.29	125.81	119.94
1	2	447	VAL	O-C-N	-5.28	115.97	122.57
1	1	362	ILE	CA-C-N	5.28	125.80	119.94
1	1	362	ILE	C-N-CA	5.28	125.80	119.94
1	AC	362	ILE	CA-C-N	5.28	125.80	119.94
1	AC	362	ILE	C-N-CA	5.28	125.80	119.94
1	AM	362	ILE	CA-C-N	5.28	125.80	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AM	362	ILE	C-N-CA	5.28	125.80	119.94
1	AI	362	ILE	CA-C-N	5.27	125.79	119.94
1	AI	362	ILE	C-N-CA	5.27	125.79	119.94
1	r	74	VAL	CA-C-O	-5.27	117.20	119.94
1	AK	362	ILE	CA-C-N	5.27	125.79	119.94
1	AK	362	ILE	C-N-CA	5.27	125.79	119.94
1	5	362	ILE	CA-C-N	5.27	125.79	119.94
1	5	362	ILE	C-N-CA	5.27	125.79	119.94
1	AH	447	VAL	O-C-N	-5.27	115.98	122.57
1	6	447	VAL	O-C-N	-5.26	115.99	122.57
1	AG	362	ILE	CA-C-N	5.26	125.78	119.94
1	AG	362	ILE	C-N-CA	5.26	125.78	119.94
1	AL	447	VAL	O-C-N	-5.25	116.00	122.57
1	AJ	447	VAL	O-C-N	-5.25	116.01	122.57
1	AO	417	ASN	CA-C-N	5.24	131.54	121.54
1	AO	417	ASN	C-N-CA	5.24	131.54	121.54
1	AM	417	ASN	CA-C-N	5.23	131.54	121.54
1	AM	417	ASN	C-N-CA	5.23	131.54	121.54
1	8	74	VAL	CA-C-O	-5.23	117.22	119.94
1	0	447	VAL	O-C-N	-5.23	116.03	122.57
1	AK	417	ASN	CA-C-N	5.23	131.53	121.54
1	AK	417	ASN	C-N-CA	5.23	131.53	121.54
1	AD	447	VAL	O-C-N	-5.23	116.04	122.57
1	3	86	PHE	N-CA-C	5.22	119.13	112.34
1	AE	86	PHE	N-CA-C	5.22	119.13	112.34
1	AG	417	ASN	CA-C-N	5.22	131.51	121.54
1	AG	417	ASN	C-N-CA	5.22	131.51	121.54
1	z	74	VAL	CA-C-O	-5.22	117.23	119.94
1	AC	417	ASN	CA-C-N	5.21	131.50	121.54
1	AC	417	ASN	C-N-CA	5.21	131.50	121.54
1	7	86	PHE	N-CA-C	5.21	119.11	112.34
1	AI	417	ASN	CA-C-N	5.21	131.49	121.54
1	AI	417	ASN	C-N-CA	5.21	131.49	121.54
1	r	263	PRO	CA-C-N	5.21	131.48	121.54
1	r	263	PRO	C-N-CA	5.21	131.48	121.54
1	q	86	PHE	N-CA-C	5.20	119.11	112.34
1	S	451	ASP	CA-C-N	5.20	128.90	123.08
1	S	451	ASP	C-N-CA	5.20	128.90	123.08
1	u	86	PHE	N-CA-C	5.20	119.10	112.34
1	y	86	PHE	N-CA-C	5.20	119.10	112.34
1	j	263	PRO	CA-C-N	5.20	131.47	121.54
1	j	263	PRO	C-N-CA	5.20	131.47	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	263	PRO	CA-C-N	5.20	131.46	121.54
1	n	263	PRO	C-N-CA	5.20	131.46	121.54
1	9	417	ASN	CA-C-N	5.19	131.46	121.54
1	9	417	ASN	C-N-CA	5.19	131.46	121.54
1	B	263	PRO	CA-C-N	5.19	131.46	121.54
1	B	263	PRO	C-N-CA	5.19	131.46	121.54
1	G	451	ASP	CA-C-N	5.19	128.89	123.08
1	G	451	ASP	C-N-CA	5.19	128.89	123.08
1	X	263	PRO	CA-C-N	5.19	131.44	121.54
1	X	263	PRO	C-N-CA	5.19	131.44	121.54
1	O	451	ASP	CA-C-N	5.18	128.88	123.08
1	O	451	ASP	C-N-CA	5.18	128.88	123.08
1	f	263	PRO	CA-C-N	5.18	131.43	121.54
1	f	263	PRO	C-N-CA	5.18	131.43	121.54
1	b	263	PRO	CA-C-N	5.17	131.41	121.54
1	b	263	PRO	C-N-CA	5.17	131.41	121.54
1	AA	86	PHE	N-CA-C	5.17	119.06	112.34
1	K	451	ASP	CA-C-N	5.17	128.87	123.08
1	K	451	ASP	C-N-CA	5.17	128.87	123.08
1	M	451	ASP	CA-C-N	5.16	128.86	123.08
1	M	451	ASP	C-N-CA	5.16	128.86	123.08
1	E	451	ASP	CA-C-N	5.15	128.85	123.08
1	E	451	ASP	C-N-CA	5.15	128.85	123.08
1	y	102	ASN	CA-C-N	5.15	127.18	120.28
1	y	102	ASN	C-N-CA	5.15	127.18	120.28
1	I	451	ASP	CA-C-N	5.15	128.85	123.08
1	I	451	ASP	C-N-CA	5.15	128.85	123.08
1	AE	102	ASN	CA-C-N	5.14	127.17	120.28
1	AE	102	ASN	C-N-CA	5.14	127.17	120.28
1	q	102	ASN	CA-C-N	5.14	127.17	120.28
1	q	102	ASN	C-N-CA	5.14	127.17	120.28
1	3	102	ASN	CA-C-N	5.13	127.16	120.28
1	3	102	ASN	C-N-CA	5.13	127.16	120.28
1	A	102	ASN	CA-C-N	5.13	127.16	120.28
1	A	102	ASN	C-N-CA	5.13	127.16	120.28
1	u	102	ASN	CA-C-N	5.13	127.16	120.28
1	u	102	ASN	C-N-CA	5.13	127.16	120.28
1	AA	102	ASN	CA-C-N	5.12	127.15	120.28
1	AA	102	ASN	C-N-CA	5.12	127.15	120.28
1	AI	435	ASP	O-C-N	-5.12	116.16	122.82
1	7	102	ASN	CA-C-N	5.12	127.13	120.28
1	7	102	ASN	C-N-CA	5.12	127.13	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AC	435	ASP	O-C-N	-5.11	116.17	122.82
1	9	435	ASP	O-C-N	-5.10	116.19	122.82
1	AJ	413	LEU	CA-C-O	-5.10	113.17	120.16
1	AG	435	ASP	O-C-N	-5.09	116.20	122.82
1	5	435	ASP	O-C-N	-5.09	116.21	122.82
1	AK	435	ASP	O-C-N	-5.08	116.21	122.82
1	AN	413	LEU	CA-C-O	-5.08	113.20	120.16
1	AP	413	LEU	CA-C-O	-5.08	113.20	120.16
1	0	413	LEU	CA-C-O	-5.08	113.20	120.16
1	AH	413	LEU	CA-C-O	-5.08	113.20	120.16
1	AL	413	LEU	CA-C-O	-5.07	113.21	120.16
1	AD	413	LEU	CA-C-O	-5.07	113.22	120.16
1	AM	435	ASP	O-C-N	-5.06	116.25	122.82

There are no chirality outliers.

All (1217) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	253	HIS	Peptide
1	0	255	GLN	Mainchain
1	0	263	PRO	Peptide
1	0	307	ASP	Mainchain
1	0	311	GLN	Mainchain
1	0	314	GLN	Mainchain
1	0	333	LEU	Mainchain
1	0	336	THR	Mainchain
1	0	340	LEU	Mainchain
1	0	407	GLU	Mainchain
1	0	408	GLU	Mainchain
1	0	414	PRO	Peptide,Mainchain
1	0	415	LEU	Peptide,Mainchain
1	0	419	SER	Peptide,Mainchain
1	0	422	ASN	Peptide
1	0	432	PRO	Peptide
1	0	446	THR	Peptide
1	0	448	GLU	Peptide,Mainchain
1	0	458	THR	Mainchain
1	1	19	GLY	Mainchain
1	1	207	ARG	Mainchain
1	1	215	LEU	Mainchain
1	1	221	GLU	Mainchain
1	1	253	HIS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	1	261	SER	Peptide,Mainchain
1	1	262	LYS	Peptide
1	1	264	ASP	Mainchain
1	1	311	GLN	Mainchain
1	1	322	GLN	Mainchain
1	1	325	SER	Mainchain
1	1	334	LYS	Mainchain
1	1	437	HIS	Mainchain
1	1	449	THR	Peptide
1	1	451	ASP	Peptide
1	1	455	ILE	Peptide
1	1	463	ASP	Mainchain
1	1	7	SER	Peptide,Mainchain
1	2	156	GLU	Mainchain
1	2	253	HIS	Peptide
1	2	255	GLN	Mainchain
1	2	263	PRO	Peptide
1	2	307	ASP	Mainchain
1	2	311	GLN	Mainchain
1	2	314	GLN	Mainchain
1	2	333	LEU	Mainchain
1	2	336	THR	Mainchain
1	2	340	LEU	Mainchain
1	2	446	THR	Peptide
1	2	448	GLU	Peptide,Mainchain
1	2	458	THR	Mainchain
1	2	7	SER	Peptide,Mainchain
1	3	101	THR	Mainchain
1	3	105	VAL	Peptide,Mainchain
1	3	108	GLN	Peptide,Mainchain
1	3	112	ASP	Mainchain
1	3	116	ASN	Mainchain
1	3	119	ASP	Peptide,Mainchain
1	3	130	ILE	Mainchain
1	3	163	GLN	Mainchain
1	3	183	MET	Mainchain
1	3	186	ARG	Mainchain
1	3	72	SER	Mainchain
1	3	75	PRO	Peptide
1	3	79	LEU	Mainchain
1	3	84	VAL	Mainchain
1	3	94	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	3	98	ASN	Mainchain
1	4	10	SER	Mainchain
1	4	108	GLN	Mainchain
1	4	112	ASP	Mainchain
1	4	118	ILE	Mainchain
1	4	132	LEU	Mainchain
1	4	136	GLU	Mainchain
1	4	140	GLY	Mainchain
1	4	144	SER	Mainchain
1	4	169	ALA	Mainchain
1	4	176	ASP	Mainchain
1	4	180	GLU	Mainchain
1	4	187	GLU	Mainchain
1	4	36	ARG	Peptide,Mainchain
1	4	68	VAL	Peptide
1	4	73	SER	Peptide
1	4	78	ARG	Peptide
1	4	81	GLN	Peptide,Mainchain
1	4	86	PHE	Mainchain
1	4	94	THR	Mainchain
1	5	207	ARG	Mainchain
1	5	215	LEU	Mainchain
1	5	221	GLU	Mainchain
1	5	253	HIS	Mainchain
1	5	261	SER	Peptide,Mainchain
1	5	262	LYS	Peptide
1	5	264	ASP	Mainchain
1	5	311	GLN	Mainchain
1	5	322	GLN	Mainchain
1	5	325	SER	Mainchain
1	5	334	LYS	Mainchain
1	5	378	ARG	Mainchain
1	5	399	THR	Mainchain
1	5	400	TYR	Mainchain
1	5	424	ARG	Mainchain
1	5	430	SER	Peptide
1	5	437	HIS	Mainchain
1	5	449	THR	Peptide
1	5	451	ASP	Peptide
1	5	455	ILE	Peptide
1	5	463	ASP	Mainchain
1	6	253	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	6	255	GLN	Mainchain
1	6	263	PRO	Peptide
1	6	307	ASP	Mainchain
1	6	311	GLN	Mainchain
1	6	314	GLN	Mainchain
1	6	333	LEU	Mainchain
1	6	336	THR	Mainchain
1	6	340	LEU	Mainchain
1	6	419	SER	Peptide,Mainchain
1	6	422	ASN	Peptide
1	6	432	PRO	Peptide
1	6	446	THR	Peptide
1	6	448	GLU	Peptide,Mainchain
1	6	458	THR	Mainchain
1	7	101	THR	Mainchain
1	7	105	VAL	Peptide,Mainchain
1	7	108	GLN	Peptide,Mainchain
1	7	112	ASP	Mainchain
1	7	116	ASN	Mainchain
1	7	119	ASP	Peptide,Mainchain
1	7	130	ILE	Mainchain
1	7	163	GLN	Mainchain
1	7	72	SER	Mainchain
1	7	75	PRO	Peptide
1	7	79	LEU	Mainchain
1	7	84	VAL	Mainchain
1	7	94	THR	Mainchain
1	7	98	ASN	Mainchain
1	8	108	GLN	Mainchain
1	8	112	ASP	Mainchain
1	8	118	ILE	Mainchain
1	8	132	LEU	Mainchain
1	8	136	GLU	Mainchain
1	8	140	GLY	Mainchain
1	8	144	SER	Mainchain
1	8	36	ARG	Peptide,Mainchain
1	8	68	VAL	Peptide
1	8	73	SER	Peptide
1	8	78	ARG	Peptide
1	8	81	GLN	Peptide,Mainchain
1	8	86	PHE	Mainchain
1	8	94	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	9	221	GLU	Mainchain
1	9	253	HIS	Mainchain
1	9	261	SER	Peptide,Mainchain
1	9	262	LYS	Peptide
1	9	264	ASP	Mainchain
1	9	311	GLN	Mainchain
1	9	322	GLN	Mainchain
1	9	325	SER	Mainchain
1	9	334	LYS	Mainchain
1	9	378	ARG	Mainchain
1	9	399	THR	Mainchain
1	9	400	TYR	Mainchain
1	9	404	LEU	Mainchain
1	9	412	SER	Peptide,Mainchain
1	9	414	PRO	Mainchain
1	9	424	ARG	Mainchain
1	9	430	SER	Peptide
1	9	437	HIS	Mainchain
1	9	449	THR	Peptide
1	9	451	ASP	Peptide
1	9	455	ILE	Peptide
1	9	463	ASP	Mainchain
1	A	101	THR	Mainchain
1	A	105	VAL	Peptide,Mainchain
1	A	108	GLN	Peptide,Mainchain
1	A	112	ASP	Mainchain
1	A	116	ASN	Mainchain
1	A	119	ASP	Peptide,Mainchain
1	A	130	ILE	Mainchain
1	A	163	GLN	Mainchain
1	A	183	MET	Mainchain
1	A	186	ARG	Mainchain
1	A	197	GLU	Mainchain
1	A	228	GLN	Peptide
1	A	236	LYS	Mainchain
1	A	240	GLU	Mainchain
1	A	244	GLU	Mainchain
1	A	247	ALA	Mainchain
1	A	251	GLU	Mainchain
1	A	253	HIS	Peptide,Mainchain
1	A	254	VAL	Mainchain
1	A	255	GLN	Peptide,Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	256	ILE	Peptide,Mainchain
1	A	264	ASP	Peptide
1	A	267	ALA	Mainchain
1	A	271	ASP	Mainchain
1	A	307	ASP	Mainchain
1	A	94	THR	Mainchain
1	A	98	ASN	Mainchain
1	AA	101	THR	Mainchain
1	AA	105	VAL	Peptide,Mainchain
1	AA	108	GLN	Peptide,Mainchain
1	AA	112	ASP	Mainchain
1	AA	116	ASN	Mainchain
1	AA	119	ASP	Peptide,Mainchain
1	AA	130	ILE	Mainchain
1	AA	72	SER	Mainchain
1	AA	75	PRO	Peptide
1	AA	79	LEU	Mainchain
1	AA	84	VAL	Mainchain
1	AA	94	THR	Mainchain
1	AA	98	ASN	Mainchain
1	AB	108	GLN	Mainchain
1	AB	112	ASP	Mainchain
1	AB	118	ILE	Mainchain
1	AB	132	LEU	Mainchain
1	AB	68	VAL	Peptide
1	AB	73	SER	Peptide
1	AB	78	ARG	Peptide
1	AB	81	GLN	Peptide,Mainchain
1	AB	86	PHE	Mainchain
1	AB	94	THR	Mainchain
1	AC	253	HIS	Mainchain
1	AC	261	SER	Peptide,Mainchain
1	AC	262	LYS	Peptide
1	AC	264	ASP	Mainchain
1	AC	311	GLN	Mainchain
1	AC	322	GLN	Mainchain
1	AC	325	SER	Mainchain
1	AC	334	LYS	Mainchain
1	AC	378	ARG	Mainchain
1	AC	399	THR	Mainchain
1	AC	400	TYR	Mainchain
1	AC	404	LEU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	AC	412	SER	Peptide,Mainchain
1	AC	414	PRO	Mainchain
1	AC	424	ARG	Mainchain
1	AC	430	SER	Peptide
1	AC	437	HIS	Mainchain
1	AC	449	THR	Peptide
1	AC	451	ASP	Peptide
1	AC	455	ILE	Peptide
1	AC	463	ASP	Mainchain
1	AD	253	HIS	Peptide
1	AD	255	GLN	Mainchain
1	AD	263	PRO	Peptide
1	AD	307	ASP	Mainchain
1	AD	311	GLN	Mainchain
1	AD	314	GLN	Mainchain
1	AD	333	LEU	Mainchain
1	AD	336	THR	Mainchain
1	AD	340	LEU	Mainchain
1	AD	407	GLU	Mainchain
1	AD	408	GLU	Mainchain
1	AD	414	PRO	Peptide,Mainchain
1	AD	415	LEU	Peptide,Mainchain
1	AD	419	SER	Peptide,Mainchain
1	AD	422	ASN	Peptide
1	AD	432	PRO	Peptide
1	AD	446	THR	Peptide
1	AD	448	GLU	Peptide,Mainchain
1	AD	458	THR	Mainchain
1	AE	101	THR	Mainchain
1	AE	105	VAL	Peptide,Mainchain
1	AE	72	SER	Mainchain
1	AE	75	PRO	Peptide
1	AE	79	LEU	Mainchain
1	AE	84	VAL	Mainchain
1	AE	94	THR	Mainchain
1	AE	98	ASN	Mainchain
1	AF	68	VAL	Peptide
1	AF	73	SER	Peptide
1	AF	78	ARG	Peptide
1	AF	81	GLN	Peptide,Mainchain
1	AF	86	PHE	Mainchain
1	AF	94	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	AG	311	GLN	Mainchain
1	AG	322	GLN	Mainchain
1	AG	325	SER	Mainchain
1	AG	334	LYS	Mainchain
1	AG	378	ARG	Mainchain
1	AG	399	THR	Mainchain
1	AG	400	TYR	Mainchain
1	AG	404	LEU	Mainchain
1	AG	412	SER	Peptide,Mainchain
1	AG	414	PRO	Mainchain
1	AG	424	ARG	Mainchain
1	AG	430	SER	Peptide
1	AG	437	HIS	Mainchain
1	AG	449	THR	Peptide
1	AG	451	ASP	Peptide
1	AG	455	ILE	Peptide
1	AG	463	ASP	Mainchain
1	AH	307	ASP	Mainchain
1	AH	311	GLN	Mainchain
1	AH	314	GLN	Mainchain
1	AH	333	LEU	Mainchain
1	AH	336	THR	Mainchain
1	AH	340	LEU	Mainchain
1	AH	407	GLU	Mainchain
1	AH	408	GLU	Mainchain
1	AH	414	PRO	Peptide,Mainchain
1	AH	415	LEU	Peptide,Mainchain
1	AH	417	ASN	Mainchain
1	AH	419	SER	Peptide,Mainchain
1	AH	422	ASN	Peptide
1	AH	432	PRO	Peptide
1	AH	446	THR	Peptide
1	AH	448	GLU	Peptide,Mainchain
1	AH	458	THR	Mainchain
1	AI	311	GLN	Mainchain
1	AI	322	GLN	Mainchain
1	AI	325	SER	Mainchain
1	AI	334	LYS	Mainchain
1	AI	378	ARG	Mainchain
1	AI	399	THR	Mainchain
1	AI	400	TYR	Mainchain
1	AI	404	LEU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	AI	412	SER	Peptide,Mainchain
1	AI	414	PRO	Mainchain
1	AI	424	ARG	Mainchain
1	AI	430	SER	Peptide
1	AI	437	HIS	Mainchain
1	AI	449	THR	Peptide
1	AI	451	ASP	Peptide
1	AI	455	ILE	Peptide
1	AI	463	ASP	Mainchain
1	AJ	307	ASP	Mainchain
1	AJ	311	GLN	Mainchain
1	AJ	314	GLN	Mainchain
1	AJ	333	LEU	Mainchain
1	AJ	336	THR	Mainchain
1	AJ	340	LEU	Mainchain
1	AJ	407	GLU	Mainchain
1	AJ	408	GLU	Mainchain
1	AJ	414	PRO	Peptide,Mainchain
1	AJ	415	LEU	Peptide,Mainchain
1	AJ	417	ASN	Mainchain
1	AJ	419	SER	Peptide,Mainchain
1	AJ	422	ASN	Peptide
1	AJ	432	PRO	Peptide
1	AJ	446	THR	Peptide
1	AJ	448	GLU	Peptide,Mainchain
1	AJ	458	THR	Mainchain
1	AK	334	LYS	Mainchain
1	AK	378	ARG	Mainchain
1	AK	399	THR	Mainchain
1	AK	400	TYR	Mainchain
1	AK	404	LEU	Mainchain
1	AK	412	SER	Peptide,Mainchain
1	AK	414	PRO	Mainchain
1	AK	424	ARG	Mainchain
1	AK	430	SER	Peptide
1	AK	437	HIS	Mainchain
1	AK	449	THR	Peptide
1	AK	451	ASP	Peptide
1	AK	455	ILE	Peptide
1	AK	463	ASP	Mainchain
1	AL	333	LEU	Mainchain
1	AL	336	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	AL	340	LEU	Mainchain
1	AL	407	GLU	Mainchain
1	AL	408	GLU	Mainchain
1	AL	414	PRO	Peptide,Mainchain
1	AL	415	LEU	Peptide,Mainchain
1	AL	417	ASN	Mainchain
1	AL	419	SER	Peptide,Mainchain
1	AL	422	ASN	Peptide
1	AL	432	PRO	Peptide
1	AL	446	THR	Peptide
1	AL	448	GLU	Peptide,Mainchain
1	AL	458	THR	Mainchain
1	AM	378	ARG	Mainchain
1	AM	399	THR	Mainchain
1	AM	400	TYR	Mainchain
1	AM	404	LEU	Mainchain
1	AM	412	SER	Peptide,Mainchain
1	AM	414	PRO	Mainchain
1	AM	424	ARG	Mainchain
1	AM	430	SER	Peptide
1	AM	437	HIS	Mainchain
1	AN	407	GLU	Mainchain
1	AN	408	GLU	Mainchain
1	AN	414	PRO	Peptide,Mainchain
1	AN	415	LEU	Peptide,Mainchain
1	AN	417	ASN	Mainchain
1	AN	419	SER	Peptide,Mainchain
1	AN	422	ASN	Peptide
1	AN	432	PRO	Peptide
1	AO	399	THR	Mainchain
1	AO	400	TYR	Mainchain
1	AO	404	LEU	Mainchain
1	AO	412	SER	Peptide,Mainchain
1	AO	414	PRO	Mainchain
1	AP	407	GLU	Mainchain
1	AP	408	GLU	Mainchain
1	AP	414	PRO	Peptide,Mainchain
1	AP	415	LEU	Peptide,Mainchain
1	AP	419	SER	Peptide,Mainchain
1	B	10	SER	Mainchain
1	B	108	GLN	Mainchain
1	B	112	ASP	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	118	ILE	Mainchain
1	B	132	LEU	Mainchain
1	B	136	GLU	Mainchain
1	B	140	GLY	Mainchain
1	B	144	SER	Mainchain
1	B	169	ALA	Mainchain
1	B	176	ASP	Mainchain
1	B	180	GLU	Mainchain
1	B	187	GLU	Mainchain
1	B	202	THR	Mainchain
1	B	205	SER	Mainchain
1	B	236	LYS	Mainchain
1	B	244	GLU	Mainchain
1	B	252	GLN	Peptide
1	B	253	HIS	Mainchain
1	B	254	VAL	Peptide,Mainchain
1	B	267	ALA	Mainchain
1	B	271	ASP	Mainchain
1	B	36	ARG	Peptide,Mainchain
1	C	121	VAL	Mainchain
1	C	128	ASN	Mainchain
1	C	144	SER	Mainchain
1	C	19	GLY	Mainchain
1	C	207	ARG	Mainchain
1	C	215	LEU	Mainchain
1	C	221	GLU	Mainchain
1	C	253	HIS	Mainchain
1	C	261	SER	Peptide,Mainchain
1	C	262	LYS	Peptide
1	C	264	ASP	Mainchain
1	C	68	VAL	Peptide
1	C	7	SER	Peptide,Mainchain
1	D	106	GLU	Mainchain
1	D	119	ASP	Mainchain
1	D	130	ILE	Mainchain
1	D	156	GLU	Mainchain
1	D	253	HIS	Peptide
1	D	255	GLN	Mainchain
1	D	263	PRO	Peptide
1	D	28	ARG	Mainchain
1	D	7	SER	Peptide,Mainchain
1	D	78	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	86	PHE	Peptide
1	D	88	LEU	Mainchain
1	D	94	THR	Mainchain
1	D	95	GLU	Mainchain
1	D	98	ASN	Mainchain
1	E	437	HIS	Peptide
1	E	438	SER	Mainchain
1	E	462	HIS	Mainchain
1	G	420	SER	Peptide
1	G	423	LEU	Peptide,Mainchain
1	G	424	ARG	Peptide
1	G	425	GLU	Peptide
1	G	426	THR	Peptide,Mainchain
1	G	429	ASP	Peptide
1	G	437	HIS	Peptide
1	G	438	SER	Mainchain
1	G	462	HIS	Mainchain
1	H	417	ASN	Peptide
1	H	419	SER	Peptide,Mainchain
1	H	421	LEU	Peptide
1	H	429	ASP	Peptide
1	I	412	SER	Peptide
1	I	420	SER	Peptide
1	I	423	LEU	Peptide,Mainchain
1	I	424	ARG	Peptide
1	I	425	GLU	Peptide
1	I	426	THR	Peptide,Mainchain
1	I	429	ASP	Peptide
1	I	437	HIS	Peptide
1	I	438	SER	Mainchain
1	I	462	HIS	Mainchain
1	J	412	SER	Peptide,Mainchain
1	J	417	ASN	Peptide
1	J	419	SER	Peptide,Mainchain
1	J	421	LEU	Peptide
1	J	429	ASP	Peptide
1	K	374	GLU	Mainchain
1	K	412	SER	Peptide
1	K	420	SER	Peptide
1	K	423	LEU	Peptide,Mainchain
1	K	424	ARG	Peptide
1	K	425	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	K	426	THR	Peptide,Mainchain
1	K	429	ASP	Peptide
1	K	437	HIS	Peptide
1	K	438	SER	Mainchain
1	K	462	HIS	Mainchain
1	L	361	THR	Mainchain
1	L	367	ASP	Mainchain
1	L	379	HIS	Mainchain
1	L	412	SER	Peptide,Mainchain
1	L	417	ASN	Peptide
1	L	419	SER	Peptide,Mainchain
1	L	421	LEU	Peptide
1	L	429	ASP	Peptide
1	M	333	LEU	Mainchain
1	M	344	MET	Mainchain
1	M	374	GLU	Mainchain
1	M	412	SER	Peptide
1	M	420	SER	Peptide
1	M	423	LEU	Peptide,Mainchain
1	M	424	ARG	Peptide
1	M	425	GLU	Peptide
1	M	426	THR	Peptide,Mainchain
1	M	429	ASP	Peptide
1	M	437	HIS	Peptide
1	M	438	SER	Mainchain
1	M	462	HIS	Mainchain
1	N	339	SER	Mainchain
1	N	361	THR	Mainchain
1	N	367	ASP	Mainchain
1	N	379	HIS	Mainchain
1	N	412	SER	Peptide,Mainchain
1	N	417	ASN	Peptide
1	N	419	SER	Peptide,Mainchain
1	N	421	LEU	Peptide
1	N	429	ASP	Peptide
1	O	307	ASP	Mainchain
1	O	315	GLU	Mainchain
1	O	318	GLU	Mainchain
1	O	322	GLN	Mainchain
1	O	333	LEU	Mainchain
1	O	344	MET	Mainchain
1	O	374	GLU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	O	412	SER	Peptide
1	O	420	SER	Peptide
1	O	423	LEU	Peptide,Mainchain
1	O	424	ARG	Peptide
1	O	425	GLU	Peptide
1	O	426	THR	Peptide,Mainchain
1	O	429	ASP	Peptide
1	O	437	HIS	Peptide
1	O	438	SER	Mainchain
1	O	462	HIS	Mainchain
1	P	311	GLN	Mainchain
1	P	325	SER	Mainchain
1	P	339	SER	Mainchain
1	P	361	THR	Mainchain
1	P	367	ASP	Mainchain
1	P	379	HIS	Mainchain
1	P	412	SER	Peptide,Mainchain
1	P	417	ASN	Peptide
1	P	419	SER	Peptide,Mainchain
1	P	421	LEU	Peptide
1	P	429	ASP	Peptide
1	Q	68	VAL	Peptide
1	S	307	ASP	Mainchain
1	S	315	GLU	Mainchain
1	S	318	GLU	Mainchain
1	S	322	GLN	Mainchain
1	S	333	LEU	Mainchain
1	S	344	MET	Mainchain
1	S	374	GLU	Mainchain
1	S	412	SER	Peptide
1	S	420	SER	Peptide
1	S	423	LEU	Peptide,Mainchain
1	S	424	ARG	Peptide
1	S	425	GLU	Peptide
1	S	426	THR	Peptide,Mainchain
1	S	429	ASP	Peptide
1	S	437	HIS	Peptide
1	S	438	SER	Mainchain
1	S	462	HIS	Mainchain
1	T	271	ASP	Mainchain
1	T	311	GLN	Mainchain
1	T	339	SER	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	T	361	THR	Mainchain
1	T	367	ASP	Mainchain
1	T	379	HIS	Mainchain
1	T	412	SER	Peptide,Mainchain
1	T	417	ASN	Peptide
1	T	419	SER	Peptide,Mainchain
1	T	421	LEU	Peptide
1	T	429	ASP	Peptide
1	U	68	VAL	Peptide
1	V	78	ARG	Peptide
1	V	86	PHE	Peptide
1	V	88	LEU	Mainchain
1	V	94	THR	Mainchain
1	V	95	GLU	Mainchain
1	V	98	ASN	Mainchain
1	W	247	ALA	Mainchain
1	W	251	GLU	Mainchain
1	W	253	HIS	Peptide,Mainchain
1	W	254	VAL	Mainchain
1	W	255	GLN	Peptide,Mainchain
1	W	256	ILE	Peptide,Mainchain
1	W	264	ASP	Peptide
1	W	267	ALA	Mainchain
1	W	271	ASP	Mainchain
1	W	307	ASP	Mainchain
1	W	315	GLU	Mainchain
1	W	318	GLU	Mainchain
1	W	322	GLN	Mainchain
1	W	333	LEU	Mainchain
1	W	344	MET	Mainchain
1	W	374	GLU	Mainchain
1	W	412	SER	Peptide
1	W	420	SER	Peptide
1	W	423	LEU	Peptide,Mainchain
1	W	424	ARG	Peptide
1	W	425	GLU	Peptide
1	W	426	THR	Peptide,Mainchain
1	W	429	ASP	Peptide
1	W	437	HIS	Peptide
1	W	438	SER	Mainchain
1	X	252	GLN	Peptide
1	X	253	HIS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	X	254	VAL	Peptide,Mainchain
1	X	267	ALA	Mainchain
1	X	271	ASP	Mainchain
1	X	311	GLN	Mainchain
1	X	339	SER	Mainchain
1	X	361	THR	Mainchain
1	X	367	ASP	Mainchain
1	X	379	HIS	Mainchain
1	X	412	SER	Peptide,Mainchain
1	X	417	ASN	Peptide
1	X	419	SER	Peptide,Mainchain
1	X	421	LEU	Peptide
1	X	429	ASP	Peptide
1	Y	121	VAL	Mainchain
1	Y	128	ASN	Mainchain
1	Y	68	VAL	Peptide
1	Z	106	GLU	Mainchain
1	Z	119	ASP	Mainchain
1	Z	130	ILE	Mainchain
1	Z	78	ARG	Peptide
1	Z	86	PHE	Peptide
1	Z	88	LEU	Mainchain
1	Z	94	THR	Mainchain
1	Z	95	GLU	Mainchain
1	Z	98	ASN	Mainchain
1	a	228	GLN	Peptide
1	a	236	LYS	Mainchain
1	a	240	GLU	Mainchain
1	a	244	GLU	Mainchain
1	a	247	ALA	Mainchain
1	a	251	GLU	Mainchain
1	a	253	HIS	Peptide,Mainchain
1	a	254	VAL	Mainchain
1	a	255	GLN	Peptide,Mainchain
1	a	256	ILE	Peptide,Mainchain
1	a	264	ASP	Peptide
1	a	267	ALA	Mainchain
1	a	271	ASP	Mainchain
1	a	307	ASP	Mainchain
1	a	315	GLU	Mainchain
1	a	318	GLU	Mainchain
1	a	322	GLN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	a	333	LEU	Mainchain
1	a	344	MET	Mainchain
1	a	374	GLU	Mainchain
1	a	412	SER	Peptide
1	a	420	SER	Peptide
1	b	236	LYS	Mainchain
1	b	244	GLU	Mainchain
1	b	252	GLN	Peptide
1	b	253	HIS	Mainchain
1	b	254	VAL	Peptide,Mainchain
1	b	267	ALA	Mainchain
1	b	271	ASP	Mainchain
1	b	311	GLN	Mainchain
1	b	339	SER	Mainchain
1	b	361	THR	Mainchain
1	b	367	ASP	Mainchain
1	b	379	HIS	Mainchain
1	b	412	SER	Peptide,Mainchain
1	b	417	ASN	Peptide
1	c	121	VAL	Mainchain
1	c	128	ASN	Mainchain
1	c	144	SER	Mainchain
1	c	19	GLY	Mainchain
1	c	68	VAL	Peptide
1	d	119	ASP	Mainchain
1	d	130	ILE	Mainchain
1	d	156	GLU	Mainchain
1	d	28	ARG	Mainchain
1	d	78	ARG	Peptide
1	d	86	PHE	Peptide
1	d	88	LEU	Mainchain
1	d	94	THR	Mainchain
1	d	95	GLU	Mainchain
1	d	98	ASN	Mainchain
1	e	186	ARG	Mainchain
1	e	197	GLU	Mainchain
1	e	228	GLN	Peptide
1	e	236	LYS	Mainchain
1	e	240	GLU	Mainchain
1	e	244	GLU	Mainchain
1	e	247	ALA	Mainchain
1	e	251	GLU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	e	253	HIS	Peptide,Mainchain
1	e	254	VAL	Mainchain
1	e	255	GLN	Peptide,Mainchain
1	e	256	ILE	Peptide,Mainchain
1	e	264	ASP	Peptide
1	e	267	ALA	Mainchain
1	e	271	ASP	Mainchain
1	e	307	ASP	Mainchain
1	e	315	GLU	Mainchain
1	e	318	GLU	Mainchain
1	e	322	GLN	Mainchain
1	e	333	LEU	Mainchain
1	e	344	MET	Mainchain
1	e	374	GLU	Mainchain
1	f	187	GLU	Mainchain
1	f	202	THR	Mainchain
1	f	205	SER	Mainchain
1	f	236	LYS	Mainchain
1	f	244	GLU	Mainchain
1	f	252	GLN	Peptide
1	f	253	HIS	Mainchain
1	f	254	VAL	Peptide,Mainchain
1	f	267	ALA	Mainchain
1	f	271	ASP	Mainchain
1	f	311	GLN	Mainchain
1	f	339	SER	Mainchain
1	f	361	THR	Mainchain
1	f	367	ASP	Mainchain
1	f	379	HIS	Mainchain
1	g	121	VAL	Mainchain
1	g	128	ASN	Mainchain
1	g	144	SER	Mainchain
1	g	19	GLY	Mainchain
1	g	68	VAL	Peptide
1	g	7	SER	Peptide,Mainchain
1	h	106	GLU	Mainchain
1	h	119	ASP	Mainchain
1	h	130	ILE	Mainchain
1	h	156	GLU	Mainchain
1	h	28	ARG	Mainchain
1	h	7	SER	Peptide,Mainchain
1	h	78	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	h	86	PHE	Peptide
1	h	88	LEU	Mainchain
1	h	94	THR	Mainchain
1	h	95	GLU	Mainchain
1	h	98	ASN	Mainchain
1	i	163	GLN	Mainchain
1	i	183	MET	Mainchain
1	i	186	ARG	Mainchain
1	i	197	GLU	Mainchain
1	i	228	GLN	Peptide
1	i	236	LYS	Mainchain
1	i	240	GLU	Mainchain
1	i	244	GLU	Mainchain
1	i	247	ALA	Mainchain
1	i	251	GLU	Mainchain
1	i	253	HIS	Peptide,Mainchain
1	i	254	VAL	Mainchain
1	i	255	GLN	Peptide,Mainchain
1	i	256	ILE	Peptide,Mainchain
1	i	264	ASP	Peptide
1	i	267	ALA	Mainchain
1	i	271	ASP	Mainchain
1	i	307	ASP	Mainchain
1	i	315	GLU	Mainchain
1	i	318	GLU	Mainchain
1	i	322	GLN	Mainchain
1	i	333	LEU	Mainchain
1	i	344	MET	Mainchain
1	j	10	SER	Mainchain
1	j	169	ALA	Mainchain
1	j	176	ASP	Mainchain
1	j	180	GLU	Mainchain
1	j	187	GLU	Mainchain
1	j	202	THR	Mainchain
1	j	205	SER	Mainchain
1	j	236	LYS	Mainchain
1	j	244	GLU	Mainchain
1	j	252	GLN	Peptide
1	j	253	HIS	Mainchain
1	j	254	VAL	Peptide,Mainchain
1	j	267	ALA	Mainchain
1	j	271	ASP	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	j	311	GLN	Mainchain
1	j	339	SER	Mainchain
1	j	361	THR	Mainchain
1	k	121	VAL	Mainchain
1	k	128	ASN	Mainchain
1	k	144	SER	Mainchain
1	k	19	GLY	Mainchain
1	k	207	ARG	Mainchain
1	k	211	ASP	Mainchain
1	k	215	LEU	Mainchain
1	k	221	GLU	Mainchain
1	k	68	VAL	Peptide
1	k	7	SER	Peptide,Mainchain
1	l	119	ASP	Mainchain
1	l	130	ILE	Mainchain
1	l	28	ARG	Mainchain
1	l	7	SER	Peptide,Mainchain
1	l	78	ARG	Peptide
1	l	86	PHE	Peptide
1	l	88	LEU	Mainchain
1	l	94	THR	Mainchain
1	l	95	GLU	Mainchain
1	l	98	ASN	Mainchain
1	m	130	ILE	Mainchain
1	m	163	GLN	Mainchain
1	m	183	MET	Mainchain
1	m	186	ARG	Mainchain
1	m	197	GLU	Mainchain
1	m	228	GLN	Peptide
1	m	236	LYS	Mainchain
1	m	240	GLU	Mainchain
1	m	244	GLU	Mainchain
1	m	247	ALA	Mainchain
1	m	251	GLU	Mainchain
1	m	253	HIS	Peptide,Mainchain
1	m	254	VAL	Mainchain
1	m	255	GLN	Peptide,Mainchain
1	m	256	ILE	Peptide,Mainchain
1	m	264	ASP	Peptide
1	m	267	ALA	Mainchain
1	m	271	ASP	Mainchain
1	m	307	ASP	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	m	315	GLU	Mainchain
1	m	318	GLU	Mainchain
1	m	322	GLN	Mainchain
1	m	333	LEU	Mainchain
1	n	10	SER	Mainchain
1	n	132	LEU	Mainchain
1	n	136	GLU	Mainchain
1	n	140	GLY	Mainchain
1	n	144	SER	Mainchain
1	n	169	ALA	Mainchain
1	n	176	ASP	Mainchain
1	n	180	GLU	Mainchain
1	n	187	GLU	Mainchain
1	n	202	THR	Mainchain
1	n	205	SER	Mainchain
1	n	236	LYS	Mainchain
1	n	244	GLU	Mainchain
1	n	252	GLN	Peptide
1	n	253	HIS	Mainchain
1	n	254	VAL	Peptide,Mainchain
1	n	267	ALA	Mainchain
1	n	271	ASP	Mainchain
1	n	311	GLN	Mainchain
1	n	325	SER	Mainchain
1	n	36	ARG	Peptide,Mainchain
1	o	121	VAL	Mainchain
1	o	128	ASN	Mainchain
1	o	144	SER	Mainchain
1	o	19	GLY	Mainchain
1	o	207	ARG	Mainchain
1	o	215	LEU	Mainchain
1	o	221	GLU	Mainchain
1	o	253	HIS	Mainchain
1	o	68	VAL	Peptide
1	o	7	SER	Peptide,Mainchain
1	p	106	GLU	Mainchain
1	p	119	ASP	Mainchain
1	p	130	ILE	Mainchain
1	p	156	GLU	Mainchain
1	p	28	ARG	Mainchain
1	p	7	SER	Peptide,Mainchain
1	p	78	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	p	86	PHE	Peptide
1	p	88	LEU	Mainchain
1	p	94	THR	Mainchain
1	p	95	GLU	Mainchain
1	p	98	ASN	Mainchain
1	q	101	THR	Mainchain
1	q	105	VAL	Peptide,Mainchain
1	q	108	GLN	Peptide,Mainchain
1	q	112	ASP	Mainchain
1	q	116	ASN	Mainchain
1	q	119	ASP	Peptide,Mainchain
1	q	130	ILE	Mainchain
1	q	163	GLN	Mainchain
1	q	183	MET	Mainchain
1	q	186	ARG	Mainchain
1	q	197	GLU	Mainchain
1	q	228	GLN	Peptide
1	q	236	LYS	Mainchain
1	q	240	GLU	Mainchain
1	q	244	GLU	Mainchain
1	q	247	ALA	Mainchain
1	q	251	GLU	Mainchain
1	q	253	HIS	Peptide,Mainchain
1	q	254	VAL	Mainchain
1	q	255	GLN	Peptide,Mainchain
1	q	256	ILE	Peptide,Mainchain
1	q	264	ASP	Peptide
1	q	267	ALA	Mainchain
1	q	271	ASP	Mainchain
1	q	72	SER	Mainchain
1	q	75	PRO	Peptide
1	q	79	LEU	Mainchain
1	q	84	VAL	Mainchain
1	q	94	THR	Mainchain
1	q	98	ASN	Mainchain
1	r	10	SER	Mainchain
1	r	108	GLN	Mainchain
1	r	112	ASP	Mainchain
1	r	118	ILE	Mainchain
1	r	132	LEU	Mainchain
1	r	136	GLU	Mainchain
1	r	140	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	r	144	SER	Mainchain
1	r	169	ALA	Mainchain
1	r	176	ASP	Mainchain
1	r	180	GLU	Mainchain
1	r	187	GLU	Mainchain
1	r	202	THR	Mainchain
1	r	205	SER	Mainchain
1	r	236	LYS	Mainchain
1	r	244	GLU	Mainchain
1	r	252	GLN	Peptide
1	r	253	HIS	Mainchain
1	r	254	VAL	Peptide,Mainchain
1	r	267	ALA	Mainchain
1	r	271	ASP	Mainchain
1	r	36	ARG	Peptide,Mainchain
1	r	68	VAL	Peptide
1	r	73	SER	Peptide
1	r	78	ARG	Peptide
1	r	81	GLN	Peptide,Mainchain
1	r	86	PHE	Mainchain
1	r	94	THR	Mainchain
1	s	121	VAL	Mainchain
1	s	128	ASN	Mainchain
1	s	144	SER	Mainchain
1	s	19	GLY	Mainchain
1	s	207	ARG	Mainchain
1	s	215	LEU	Mainchain
1	s	221	GLU	Mainchain
1	s	253	HIS	Mainchain
1	s	261	SER	Peptide,Mainchain
1	s	262	LYS	Peptide
1	s	264	ASP	Mainchain
1	s	7	SER	Peptide,Mainchain
1	t	106	GLU	Mainchain
1	t	119	ASP	Mainchain
1	t	130	ILE	Mainchain
1	t	253	HIS	Peptide
1	t	255	GLN	Mainchain
1	t	263	PRO	Peptide
1	t	28	ARG	Mainchain
1	t	7	SER	Peptide,Mainchain
1	t	94	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	t	95	GLU	Mainchain
1	t	98	ASN	Mainchain
1	u	101	THR	Mainchain
1	u	105	VAL	Peptide,Mainchain
1	u	108	GLN	Peptide,Mainchain
1	u	112	ASP	Mainchain
1	u	116	ASN	Mainchain
1	u	119	ASP	Peptide,Mainchain
1	u	130	ILE	Mainchain
1	u	163	GLN	Mainchain
1	u	183	MET	Mainchain
1	u	186	ARG	Mainchain
1	u	197	GLU	Mainchain
1	u	228	GLN	Peptide
1	u	236	LYS	Mainchain
1	u	240	GLU	Mainchain
1	u	244	GLU	Mainchain
1	u	247	ALA	Mainchain
1	u	251	GLU	Mainchain
1	u	253	HIS	Peptide,Mainchain
1	u	254	VAL	Mainchain
1	u	255	GLN	Peptide,Mainchain
1	u	256	ILE	Peptide,Mainchain
1	u	72	SER	Mainchain
1	u	75	PRO	Peptide
1	u	79	LEU	Mainchain
1	u	84	VAL	Mainchain
1	u	94	THR	Mainchain
1	u	98	ASN	Mainchain
1	v	10	SER	Mainchain
1	v	108	GLN	Mainchain
1	v	112	ASP	Mainchain
1	v	118	ILE	Mainchain
1	v	132	LEU	Mainchain
1	v	136	GLU	Mainchain
1	v	140	GLY	Mainchain
1	v	144	SER	Mainchain
1	v	169	ALA	Mainchain
1	v	176	ASP	Mainchain
1	v	180	GLU	Mainchain
1	v	187	GLU	Mainchain
1	v	202	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	v	205	SER	Mainchain
1	v	236	LYS	Mainchain
1	v	244	GLU	Mainchain
1	v	252	GLN	Peptide
1	v	253	HIS	Mainchain
1	v	36	ARG	Peptide,Mainchain
1	v	68	VAL	Peptide
1	v	73	SER	Peptide
1	v	78	ARG	Peptide
1	v	81	GLN	Peptide,Mainchain
1	v	86	PHE	Mainchain
1	v	94	THR	Mainchain
1	w	128	ASN	Mainchain
1	w	144	SER	Mainchain
1	w	19	GLY	Mainchain
1	w	207	ARG	Mainchain
1	w	211	ASP	Mainchain
1	w	221	GLU	Mainchain
1	w	253	HIS	Mainchain
1	w	261	SER	Peptide,Mainchain
1	w	262	LYS	Peptide
1	w	264	ASP	Mainchain
1	w	311	GLN	Mainchain
1	w	322	GLN	Mainchain
1	w	325	SER	Mainchain
1	w	334	LYS	Mainchain
1	w	7	SER	Peptide,Mainchain
1	x	130	ILE	Mainchain
1	x	253	HIS	Peptide
1	x	255	GLN	Mainchain
1	x	263	PRO	Peptide
1	x	28	ARG	Mainchain
1	x	307	ASP	Mainchain
1	x	311	GLN	Mainchain
1	x	314	GLN	Mainchain
1	x	333	LEU	Mainchain
1	x	7	SER	Peptide,Mainchain
1	y	101	THR	Mainchain
1	y	105	VAL	Peptide,Mainchain
1	y	108	GLN	Peptide,Mainchain
1	y	112	ASP	Mainchain
1	y	116	ASN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	y	119	ASP	Peptide,Mainchain
1	y	130	ILE	Mainchain
1	y	163	GLN	Mainchain
1	y	183	MET	Mainchain
1	y	186	ARG	Mainchain
1	y	197	GLU	Mainchain
1	y	72	SER	Mainchain
1	y	75	PRO	Peptide
1	y	79	LEU	Mainchain
1	y	84	VAL	Mainchain
1	y	94	THR	Mainchain
1	y	98	ASN	Mainchain
1	z	10	SER	Mainchain
1	z	108	GLN	Mainchain
1	z	112	ASP	Mainchain
1	z	118	ILE	Mainchain
1	z	132	LEU	Mainchain
1	z	136	GLU	Mainchain
1	z	140	GLY	Mainchain
1	z	144	SER	Mainchain
1	z	169	ALA	Mainchain
1	z	176	ASP	Mainchain
1	z	180	GLU	Mainchain
1	z	187	GLU	Mainchain
1	z	202	THR	Mainchain
1	z	205	SER	Mainchain
1	z	36	ARG	Peptide,Mainchain
1	z	68	VAL	Peptide
1	z	73	SER	Peptide
1	z	78	ARG	Peptide
1	z	81	GLN	Peptide,Mainchain
1	z	86	PHE	Mainchain
1	z	94	THR	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1012	0	256	6	0
1	1	1092	0	279	37	0
1	2	1064	0	276	1	0
1	3	764	0	202	90	0
1	4	780	0	201	143	0
1	5	1068	0	267	27	0
1	6	1052	0	265	2	0
1	7	568	0	149	88	0
1	8	588	0	149	126	0
1	9	1008	0	253	26	0
1	A	1124	0	291	79	0
1	AA	380	0	99	54	0
1	AB	400	0	102	94	0
1	AC	892	0	224	26	0
1	AD	888	0	225	6	0
1	AE	196	0	53	35	0
1	AF	216	0	56	50	0
1	AG	796	0	203	4	0
1	AH	796	0	203	5	0
1	AI	668	0	171	4	0
1	AJ	680	0	174	5	0
1	AK	544	0	140	4	0
1	AL	564	0	145	5	0
1	AM	324	0	81	0	0
1	AN	340	0	85	5	0
1	AO	136	0	33	0	0
1	AP	156	0	38	5	0
1	B	1076	0	271	134	0
1	C	1124	0	282	145	0
1	D	1112	0	289	97	0
1	E	132	0	34	3	0
1	F	140	0	36	6	0
1	G	208	0	51	3	0
1	H	216	0	51	26	0
1	I	316	0	79	3	0
1	J	332	0	82	29	0
1	K	428	0	109	4	0
1	L	452	0	114	29	0
1	M	544	0	140	3	0
1	N	568	0	145	29	0
1	O	660	0	169	3	0
1	P	680	0	173	28	0
1	Q	56	0	13	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	56	0	11	9	0
1	S	776	0	198	3	0
1	T	796	0	202	29	0
1	U	212	0	49	55	0
1	V	228	0	55	68	0
1	W	776	0	195	11	0
1	X	776	0	194	24	0
1	Y	396	0	92	81	0
1	Z	408	0	101	92	0
1	a	836	0	211	11	0
1	b	820	0	206	21	0
1	c	592	0	148	112	0
1	d	600	0	159	100	0
1	e	856	0	216	12	0
1	f	836	0	211	1	0
1	g	776	0	198	124	0
1	h	772	0	205	100	0
1	i	984	0	251	39	0
1	j	948	0	242	45	0
1	k	896	0	228	120	0
1	l	900	0	237	100	0
1	m	1060	0	274	63	0
1	n	1012	0	260	87	0
1	o	1016	0	258	134	0
1	p	1012	0	265	101	0
1	q	1132	0	295	89	0
1	r	1112	0	285	159	0
1	s	1108	0	279	112	0
1	t	1064	0	276	63	0
1	u	1032	0	271	118	0
1	v	1016	0	262	160	0
1	w	1036	0	266	77	0
1	x	1000	0	262	9	0
1	y	896	0	237	101	0
1	z	912	0	236	158	0
All	All	54788	0	13993	2073	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 30.

All (2073) 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)
1:4:125:GLU:CA	1:p:104:LYS:C	1.76	1.59
1:8:125:GLU:CA	1:D:104:LYS:C	1.76	1.59
1:B:125:GLU:CA	1:Z:104:LYS:C	1.76	1.58
1:AB:125:GLU:CA	1:t:104:LYS:C	1.76	1.56
1:d:104:LYS:C	1:r:125:GLU:CA	1.76	1.56
1:l:104:LYS:C	1:z:125:GLU:CA	1.76	1.56
1:AC:261:SER:C	1:AC:262:LYS:CA	1.79	1.55
1:s:261:SER:C	1:s:262:LYS:CA	1.79	1.53
1:9:261:SER:C	1:9:262:LYS:CA	1.79	1.53
1:C:94:THR:CA	1:X:419:SER:N	1.71	1.53
1:h:104:LYS:C	1:v:125:GLU:CA	1.76	1.53
1:T:419:SER:N	1:o:94:THR:CA	1.71	1.52
1:C:261:SER:C	1:C:262:LYS:CA	1.79	1.52
1:H:419:SER:N	1:U:94:THR:CA	1.71	1.52
1:L:419:SER:N	1:c:94:THR:CA	1.71	1.51
1:J:419:SER:N	1:Y:94:THR:CA	1.71	1.50
1:w:261:SER:C	1:w:262:LYS:CA	1.79	1.50
1:P:419:SER:N	1:k:94:THR:CA	1.71	1.50
1:N:419:SER:N	1:g:94:THR:CA	1.71	1.49
1:k:38:TYR:H	1:z:55:SER:N	1.00	1.49
1:1:261:SER:C	1:1:262:LYS:CA	1.79	1.49
1:5:261:SER:C	1:5:262:LYS:CA	1.79	1.49
1:L:451:ASP:CA	1:r:190:GLN:CA	1.90	1.49
1:c:66:SER:CA	1:r:26:SER:CA	1.91	1.49
1:P:451:ASP:CA	1:z:190:GLN:CA	1.90	1.49
1:g:66:SER:CA	1:v:26:SER:CA	1.91	1.48
1:b:419:SER:N	1:s:94:THR:CA	1.71	1.48
1:H:451:ASP:CA	1:n:190:GLN:CA	1.90	1.48
1:k:66:SER:CA	1:z:26:SER:CA	1.91	1.48
1:B:190:GLN:CA	1:J:451:ASP:CA	1.91	1.48
1:4:55:SER:H	1:o:38:TYR:N	1.12	1.48
1:F:451:ASP:CA	1:j:190:GLN:CA	1.90	1.47
1:AF:55:SER:N	1:w:38:TYR:H	1.00	1.47
1:N:451:ASP:CA	1:v:190:GLN:CA	1.90	1.47
1:8:26:SER:CA	1:C:66:SER:CA	1.91	1.46
1:B:55:SER:H	1:Y:38:TYR:N	1.12	1.46
1:C:94:THR:CA	1:X:419:SER:CA	1.93	1.46
1:J:419:SER:CA	1:Y:94:THR:CA	1.93	1.46
1:L:419:SER:CA	1:c:94:THR:CA	1.93	1.46
1:b:419:SER:CA	1:s:94:THR:CA	1.93	1.46
1:4:190:GLN:CA	1:T:451:ASP:CA	1.90	1.46
1:B:26:SER:CA	1:Y:66:SER:CA	1.91	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:55:SER:N	1:o:38:TYR:H	1.00	1.45
1:4:137:GLN:N	1:p:93:ASN:CA	1.80	1.45
1:B:55:SER:N	1:Y:38:TYR:H	1.00	1.45
1:g:38:TYR:N	1:v:55:SER:H	1.12	1.45
1:n:1:MET:CA	1:y:72:SER:H	1.29	1.45
1:4:26:SER:CA	1:o:66:SER:CA	1.91	1.44
1:AB:55:SER:H	1:s:38:TYR:N	1.12	1.44
1:AE:72:SER:H	1:z:1:MET:CA	1.29	1.44
1:B:137:GLN:N	1:Z:93:ASN:CA	1.80	1.44
1:d:93:ASN:CA	1:r:137:GLN:N	1.80	1.44
1:8:137:GLN:N	1:D:93:ASN:CA	1.80	1.44
1:P:419:SER:CA	1:k:94:THR:CA	1.93	1.44
1:U:66:SER:CA	1:n:26:SER:CA	1.91	1.44
1:V:93:ASN:CA	1:n:137:GLN:N	1.80	1.44
1:3:81:GLN:H	1:A:4:ARG:N	1.16	1.44
1:7:72:SER:H	1:r:1:MET:CA	1.29	1.44
1:T:419:SER:CA	1:o:94:THR:CA	1.93	1.44
1:AA:72:SER:H	1:v:1:MET:CA	1.29	1.43
1:H:419:SER:CA	1:U:94:THR:CA	1.93	1.43
1:N:419:SER:CA	1:g:94:THR:CA	1.93	1.43
1:7:36:ARG:CA	1:D:57:PRO:O	1.67	1.43
1:AB:55:SER:N	1:s:38:TYR:H	1.00	1.43
1:l:93:ASN:CA	1:z:137:GLN:N	1.80	1.43
1:k:38:TYR:N	1:z:55:SER:H	1.12	1.42
1:k:66:SER:C	1:z:26:SER:CA	1.79	1.42
1:3:36:ARG:CA	1:p:57:PRO:O	1.67	1.42
1:V:57:PRO:O	1:m:36:ARG:CA	1.67	1.42
1:3:72:SER:H	1:B:1:MET:CA	1.29	1.41
1:8:55:SER:H	1:C:38:TYR:N	1.12	1.41
1:AF:55:SER:H	1:w:38:TYR:N	1.12	1.41
1:h:93:ASN:CA	1:v:137:GLN:N	1.80	1.41
1:U:66:SER:C	1:n:26:SER:CA	1.79	1.41
1:A:36:ARG:CA	1:Z:57:PRO:O	1.67	1.41
1:7:81:GLN:H	1:q:4:ARG:N	1.16	1.41
1:8:55:SER:N	1:C:38:TYR:H	1.00	1.41
1:AE:81:GLN:H	1:y:4:ARG:N	1.16	1.41
1:g:38:TYR:H	1:v:55:SER:N	1.00	1.41
1:j:1:MET:CA	1:u:72:SER:H	1.29	1.41
1:c:38:TYR:H	1:r:55:SER:N	1.00	1.41
1:4:125:GLU:CA	1:p:104:LYS:CA	2.00	1.40
1:c:38:TYR:N	1:r:55:SER:H	1.12	1.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:57:PRO:O	1:q:36:ARG:CA	1.67	1.40
1:h:57:PRO:O	1:u:36:ARG:CA	1.67	1.40
1:B:125:GLU:CA	1:Z:104:LYS:CA	2.00	1.39
1:4:26:SER:CA	1:o:66:SER:C	1.79	1.39
1:8:125:GLU:CA	1:D:104:LYS:CA	2.00	1.39
1:l:57:PRO:O	1:y:36:ARG:CA	1.67	1.39
1:AA:81:GLN:H	1:u:4:ARG:N	1.16	1.39
1:i:4:ARG:N	1:u:81:GLN:H	1.16	1.38
1:l:104:LYS:CA	1:z:125:GLU:CA	2.00	1.38
1:h:104:LYS:CA	1:v:125:GLU:CA	2.00	1.38
1:m:4:ARG:N	1:y:81:GLN:H	1.16	1.38
1:AB:125:GLU:CA	1:t:104:LYS:CA	2.00	1.38
1:P:418:PHE:CA	1:k:93:ASN:O	1.72	1.38
1:4:133:ALA:N	1:p:97:LYS:CA	1.87	1.38
1:V:97:LYS:CA	1:n:133:ALA:N	1.87	1.37
1:d:104:LYS:CA	1:r:125:GLU:CA	2.00	1.37
1:P:419:SER:CA	1:k:94:THR:N	1.88	1.37
1:l:97:LYS:CA	1:z:133:ALA:N	1.87	1.37
1:4:103:GLU:N	1:m:253:HIS:CA	1.88	1.37
1:C:93:ASN:O	1:X:418:PHE:CA	1.72	1.37
1:T:419:SER:CA	1:o:94:THR:N	1.88	1.37
1:H:419:SER:CA	1:U:94:THR:N	1.88	1.37
1:L:418:PHE:CA	1:c:93:ASN:O	1.72	1.36
1:AB:133:ALA:N	1:t:97:LYS:CA	1.87	1.36
1:i:253:HIS:CA	1:z:103:GLU:N	1.88	1.36
1:H:418:PHE:CA	1:U:93:ASN:O	1.72	1.36
1:B:48:THR:C	1:Y:45:ARG:O	1.69	1.36
1:d:97:LYS:CA	1:r:133:ALA:N	1.87	1.36
1:B:133:ALA:N	1:Z:97:LYS:CA	1.87	1.36
1:N:419:SER:CA	1:g:94:THR:N	1.88	1.36
1:N:418:PHE:CA	1:g:93:ASN:O	1.72	1.35
1:g:45:ARG:O	1:v:48:THR:C	1.69	1.35
1:h:97:LYS:CA	1:v:133:ALA:N	1.87	1.35
1:J:418:PHE:CA	1:Y:93:ASN:O	1.72	1.35
1:T:418:PHE:CA	1:o:93:ASN:O	1.72	1.35
1:b:418:PHE:CA	1:s:93:ASN:O	1.72	1.35
1:c:66:SER:C	1:r:26:SER:CA	1.79	1.34
1:8:133:ALA:N	1:D:97:LYS:CA	1.87	1.34
1:C:94:THR:N	1:X:419:SER:CA	1.88	1.34
1:J:419:SER:CA	1:Y:94:THR:N	1.88	1.34
1:k:45:ARG:O	1:z:48:THR:C	1.69	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:48:THR:C	1:o:45:ARG:O	1.69	1.34
1:c:45:ARG:O	1:r:48:THR:C	1.69	1.33
1:m:2:SER:O	1:y:82:ASP:CA	1.76	1.33
1:7:81:GLN:N	1:q:4:ARG:N	1.76	1.33
1:8:48:THR:C	1:C:45:ARG:O	1.69	1.33
1:8:26:SER:CA	1:C:66:SER:C	1.79	1.33
1:AB:103:GLU:N	1:q:253:HIS:CA	1.88	1.33
1:AF:103:GLU:N	1:u:253:HIS:CA	1.88	1.33
1:7:82:ASP:CA	1:q:2:SER:O	1.76	1.33
1:AB:48:THR:C	1:s:45:ARG:O	1.69	1.33
1:L:419:SER:CA	1:c:94:THR:N	1.88	1.32
1:a:253:HIS:CA	1:r:103:GLU:N	1.88	1.32
1:b:419:SER:CA	1:s:94:THR:N	1.88	1.32
1:e:253:HIS:CA	1:v:103:GLU:N	1.88	1.32
1:3:81:GLN:N	1:A:4:ARG:N	1.76	1.32
1:B:103:GLU:N	1:W:253:HIS:CA	1.88	1.32
1:3:82:ASP:CA	1:A:2:SER:O	1.76	1.32
1:AA:82:ASP:CA	1:u:2:SER:O	1.76	1.32
1:AE:82:ASP:CA	1:y:2:SER:O	1.76	1.32
1:g:66:SER:C	1:v:26:SER:CA	1.79	1.31
1:8:103:GLU:N	1:A:253:HIS:CA	1.88	1.31
1:AA:81:GLN:N	1:u:4:ARG:N	1.76	1.31
1:B:26:SER:CA	1:Y:66:SER:C	1.79	1.31
1:i:2:SER:O	1:u:82:ASP:CA	1.76	1.31
1:i:4:ARG:N	1:u:81:GLN:N	1.76	1.31
1:B:104:LYS:N	1:W:252:GLN:O	1.64	1.31
1:m:4:ARG:N	1:y:81:GLN:N	1.76	1.31
1:AF:104:LYS:N	1:u:252:GLN:O	1.64	1.30
1:AE:81:GLN:N	1:y:4:ARG:N	1.76	1.30
1:i:252:GLN:O	1:z:104:LYS:N	1.64	1.30
1:4:104:LYS:N	1:m:252:GLN:O	1.64	1.30
1:AB:132:LEU:C	1:t:97:LYS:CA	2.06	1.29
1:4:132:LEU:C	1:p:97:LYS:CA	2.06	1.29
1:V:97:LYS:CA	1:n:132:LEU:C	2.06	1.29
1:d:97:LYS:CA	1:r:132:LEU:C	2.06	1.29
1:h:97:LYS:CA	1:v:132:LEU:C	2.06	1.29
1:8:104:LYS:N	1:A:252:GLN:O	1.64	1.29
1:8:132:LEU:C	1:D:97:LYS:CA	2.06	1.29
1:B:132:LEU:C	1:Z:97:LYS:CA	2.06	1.29
1:a:252:GLN:O	1:r:104:LYS:N	1.64	1.29
1:4:103:GLU:CA	1:m:253:HIS:C	2.06	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:252:GLN:O	1:v:104:LYS:N	1.64	1.29
1:B:103:GLU:CA	1:W:253:HIS:C	2.06	1.28
1:8:103:GLU:CA	1:A:253:HIS:C	2.06	1.28
1:AB:104:LYS:N	1:q:252:GLN:O	1.64	1.28
1:9:247:ALA:C	1:D:95:GLU:O	1.77	1.28
1:C:247:ALA:C	1:Z:95:GLU:O	1.77	1.28
1:AB:103:GLU:CA	1:q:253:HIS:C	2.06	1.28
1:AF:103:GLU:CA	1:u:253:HIS:C	2.06	1.28
1:l:97:LYS:CA	1:z:132:LEU:C	2.06	1.28
1:e:253:HIS:C	1:v:103:GLU:CA	2.06	1.27
1:a:253:HIS:C	1:r:103:GLU:CA	2.06	1.27
1:d:95:GLU:O	1:s:247:ALA:C	1.77	1.27
1:3:81:GLN:N	1:A:4:ARG:H	1.31	1.27
1:P:418:PHE:H	1:k:97:LYS:N	0.97	1.27
1:i:253:HIS:C	1:z:103:GLU:CA	2.06	1.27
1:1:247:ALA:C	1:l:95:GLU:O	1.77	1.26
1:AC:247:ALA:C	1:t:95:GLU:O	1.77	1.26
1:5:247:ALA:C	1:p:95:GLU:O	1.77	1.26
1:V:95:GLU:O	1:o:247:ALA:C	1.77	1.26
1:h:95:GLU:O	1:w:247:ALA:C	1.77	1.26
1:AE:81:GLN:N	1:y:4:ARG:H	1.31	1.25
1:i:4:ARG:H	1:u:81:GLN:N	1.31	1.25
1:L:418:PHE:H	1:c:97:LYS:N	0.97	1.24
1:m:4:ARG:H	1:y:81:GLN:N	1.31	1.24
1:3:76:GLY:O	1:o:21:ALA:O	1.56	1.24
1:AA:81:GLN:N	1:u:4:ARG:H	1.31	1.23
1:h:104:LYS:O	1:v:125:GLU:CA	1.87	1.23
1:AA:78:ARG:CA	1:v:2:SER:O	1.87	1.23
1:j:2:SER:O	1:u:78:ARG:CA	1.86	1.23
1:b:418:PHE:H	1:s:97:LYS:N	0.97	1.23
1:n:2:SER:O	1:y:78:ARG:CA	1.87	1.23
1:7:76:GLY:O	1:C:21:ALA:O	1.56	1.22
1:7:78:ARG:CA	1:r:2:SER:O	1.86	1.22
1:k:21:ALA:O	1:y:76:GLY:O	1.56	1.22
1:3:78:ARG:CA	1:B:2:SER:O	1.87	1.22
1:4:125:GLU:CA	1:p:104:LYS:O	1.87	1.22
1:N:418:PHE:H	1:g:97:LYS:N	0.97	1.22
1:L:451:ASP:C	1:r:190:GLN:CA	2.13	1.22
1:AE:78:ARG:CA	1:z:2:SER:O	1.87	1.21
1:N:451:ASP:C	1:v:190:GLN:CA	2.13	1.21
1:B:103:GLU:CA	1:W:253:HIS:N	2.04	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:418:PHE:N	1:c:97:LYS:H	1.27	1.21
1:J:418:PHE:H	1:Y:97:LYS:N	0.97	1.21
1:T:418:PHE:H	1:o:97:LYS:N	0.97	1.21
1:j:2:SER:O	1:u:78:ARG:N	1.74	1.21
1:C:97:LYS:N	1:X:418:PHE:H	0.97	1.20
1:l:104:LYS:O	1:z:125:GLU:CA	1.87	1.20
1:4:103:GLU:CA	1:m:253:HIS:N	2.04	1.20
1:8:103:GLU:CA	1:A:253:HIS:N	2.04	1.20
1:AB:125:GLU:CA	1:t:104:LYS:O	1.86	1.20
1:AF:103:GLU:CA	1:u:253:HIS:N	2.04	1.20
1:a:253:HIS:N	1:r:103:GLU:CA	2.04	1.20
1:g:81:GLN:CA	1:v:154:MET:CA	2.20	1.20
1:F:451:ASP:C	1:j:190:GLN:CA	2.13	1.20
1:3:30:TYR:O	1:o:66:SER:O	1.60	1.20
1:4:55:SER:N	1:o:38:TYR:N	1.77	1.20
1:AA:76:GLY:O	1:s:21:ALA:O	1.56	1.20
1:U:66:SER:O	1:m:30:TYR:O	1.60	1.20
1:k:81:GLN:CA	1:z:154:MET:CA	2.20	1.20
1:7:30:TYR:O	1:C:66:SER:O	1.60	1.20
1:7:78:ARG:N	1:r:2:SER:O	1.74	1.20
1:A:30:TYR:O	1:Y:66:SER:O	1.60	1.20
1:H:451:ASP:C	1:n:190:GLN:CA	2.13	1.20
1:c:81:GLN:CA	1:r:154:MET:CA	2.20	1.20
1:g:8:SER:O	1:j:12:ARG:N	1.75	1.20
1:k:66:SER:O	1:y:30:TYR:O	1.60	1.20
1:w:8:SER:O	1:z:12:ARG:N	1.75	1.20
1:7:81:GLN:N	1:q:4:ARG:H	1.31	1.19
1:4:190:GLN:CA	1:T:451:ASP:C	2.13	1.19
1:B:12:ARG:N	1:o:8:SER:O	1.75	1.19
1:d:104:LYS:O	1:r:125:GLU:CA	1.87	1.19
1:n:2:SER:O	1:y:78:ARG:N	1.74	1.19
1:P:451:ASP:C	1:z:190:GLN:CA	2.13	1.19
1:AE:76:GLY:O	1:w:21:ALA:O	1.56	1.19
1:AE:78:ARG:N	1:z:2:SER:O	1.74	1.19
1:e:253:HIS:N	1:v:103:GLU:CA	2.04	1.19
1:i:253:HIS:N	1:z:103:GLU:CA	2.04	1.19
1:C:8:SER:O	1:r:12:ARG:N	1.75	1.19
1:c:21:ALA:O	1:q:76:GLY:O	1.56	1.19
1:g:21:ALA:O	1:u:76:GLY:O	1.56	1.19
1:s:8:SER:O	1:v:12:ARG:N	1.75	1.19
1:AB:103:GLU:CA	1:q:253:HIS:N	2.04	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:154:MET:CA	1:o:81:GLN:CA	2.20	1.18
1:8:125:GLU:CA	1:D:104:LYS:O	1.86	1.18
1:B:190:GLN:CA	1:J:451:ASP:C	2.13	1.18
1:k:38:TYR:N	1:z:55:SER:N	1.77	1.18
1:3:78:ARG:N	1:B:2:SER:O	1.74	1.18
1:B:125:GLU:CA	1:Z:104:LYS:O	1.87	1.18
1:U:81:GLN:CA	1:n:154:MET:CA	2.20	1.18
1:k:8:SER:O	1:n:12:ARG:N	1.75	1.18
1:AA:78:ARG:N	1:v:2:SER:O	1.74	1.18
1:8:154:MET:CA	1:C:81:GLN:CA	2.20	1.18
1:B:154:MET:CA	1:Y:81:GLN:CA	2.20	1.18
1:1:8:SER:O	1:4:12:ARG:N	1.75	1.17
1:4:57:PRO:C	1:o:33:THR:O	1.88	1.17
1:c:66:SER:O	1:q:30:TYR:O	1.60	1.17
1:AE:72:SER:CA	1:z:1:MET:O	1.93	1.17
1:g:66:SER:O	1:u:30:TYR:O	1.60	1.17
1:j:1:MET:O	1:u:72:SER:CA	1.93	1.17
1:AE:72:SER:N	1:z:1:MET:CA	2.08	1.16
1:a:253:HIS:CA	1:r:103:GLU:C	2.18	1.16
1:B:28:ARG:O	1:Y:66:SER:N	1.79	1.16
1:g:33:THR:O	1:v:57:PRO:C	1.88	1.16
1:8:103:GLU:C	1:A:253:HIS:CA	2.18	1.16
1:c:66:SER:N	1:r:28:ARG:O	1.79	1.16
1:i:253:HIS:CA	1:z:103:GLU:C	2.18	1.16
1:j:1:MET:CA	1:u:72:SER:N	2.08	1.16
1:n:1:MET:CA	1:y:72:SER:N	2.08	1.16
1:n:1:MET:O	1:y:72:SER:CA	1.93	1.16
1:7:72:SER:N	1:r:1:MET:CA	2.08	1.16
1:7:72:SER:CA	1:r:1:MET:O	1.93	1.16
1:8:28:ARG:O	1:C:66:SER:N	1.79	1.16
1:AB:55:SER:N	1:s:38:TYR:N	1.77	1.16
1:U:66:SER:N	1:n:28:ARG:O	1.79	1.16
1:4:28:ARG:O	1:o:66:SER:N	1.79	1.16
1:B:55:SER:N	1:Y:38:TYR:N	1.77	1.16
1:g:66:SER:N	1:v:28:ARG:O	1.79	1.16
1:AA:72:SER:CA	1:v:1:MET:O	1.93	1.15
1:B:103:GLU:C	1:W:253:HIS:CA	2.18	1.15
1:c:33:THR:O	1:r:57:PRO:C	1.88	1.15
1:e:253:HIS:CA	1:v:103:GLU:C	2.18	1.15
1:O:411:ILE:CA	1:C:266:THR:CA	2.24	1.15
1:5:266:THR:CA	1:AL:411:ILE:CA	2.24	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:57:PRO:C	1:C:33:THR:O	1.88	1.15
1:AA:72:SER:N	1:v:1:MET:CA	2.08	1.15
1:AB:57:PRO:C	1:s:33:THR:O	1.88	1.15
1:H:418:PHE:H	1:U:97:LYS:N	0.97	1.15
1:3:52:LEU:CA	1:p:43:ALA:CA	2.25	1.15
1:4:103:GLU:C	1:m:253:HIS:CA	2.18	1.15
1:7:52:LEU:CA	1:D:43:ALA:CA	2.25	1.15
1:9:266:THR:CA	1:AN:411:ILE:CA	2.24	1.15
1:A:52:LEU:CA	1:Z:43:ALA:CA	2.25	1.15
1:AB:103:GLU:C	1:q:253:HIS:CA	2.18	1.15
1:AF:54:ALA:CA	1:w:37:THR:C	2.20	1.15
1:AF:57:PRO:C	1:w:33:THR:O	1.88	1.15
1:AH:411:ILE:CA	1:w:266:THR:CA	2.24	1.15
1:k:33:THR:O	1:z:57:PRO:C	1.88	1.15
1:g:37:THR:C	1:v:54:ALA:CA	2.20	1.15
1:3:72:SER:CA	1:B:1:MET:O	1.93	1.15
1:AB:54:ALA:CA	1:s:37:THR:C	2.20	1.15
1:AF:103:GLU:C	1:u:253:HIS:CA	2.18	1.15
1:P:418:PHE:N	1:k:97:LYS:N	1.72	1.15
1:c:37:THR:C	1:r:54:ALA:CA	2.20	1.15
1:k:66:SER:N	1:z:28:ARG:O	1.79	1.15
1:w:11:TYR:O	1:z:6:VAL:C	1.90	1.15
1:1:11:TYR:O	1:4:6:VAL:C	1.90	1.14
1:3:72:SER:N	1:B:1:MET:CA	2.08	1.14
1:AC:266:THR:CA	1:AP:411:ILE:CA	2.24	1.14
1:h:43:ALA:CA	1:u:52:LEU:CA	2.25	1.14
1:h:101:THR:CA	1:v:129:LYS:CA	2.26	1.14
1:B:54:ALA:CA	1:Y:37:THR:C	2.20	1.14
1:l:101:THR:CA	1:z:129:LYS:CA	2.26	1.14
1:1:266:THR:CA	1:AJ:411:ILE:CA	2.24	1.14
1:k:11:TYR:O	1:n:6:VAL:C	1.90	1.14
1:k:37:THR:C	1:z:54:ALA:CA	2.20	1.14
1:8:54:ALA:CA	1:C:37:THR:C	2.20	1.14
1:AD:411:ILE:CA	1:s:266:THR:CA	2.24	1.14
1:AA:52:LEU:CA	1:t:43:ALA:CA	2.25	1.14
1:B:6:VAL:C	1:o:11:TYR:O	1.90	1.13
1:C:11:TYR:O	1:r:6:VAL:O	1.67	1.13
1:d:43:ALA:CA	1:q:52:LEU:CA	2.25	1.13
1:g:11:TYR:O	1:j:6:VAL:C	1.90	1.13
1:k:34:SER:C	1:z:57:PRO:CA	2.20	1.13
1:4:54:ALA:CA	1:o:37:THR:C	2.20	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:11:TYR:O	1:v:6:VAL:C	1.90	1.13
1:B:6:VAL:O	1:o:11:TYR:O	1.67	1.13
1:l:43:ALA:CA	1:y:52:LEU:CA	2.25	1.13
1:1:11:TYR:O	1:4:6:VAL:O	1.67	1.12
1:8:129:LYS:CA	1:D:101:THR:CA	2.26	1.13
1:P:418:PHE:N	1:k:97:LYS:H	1.27	1.12
1:V:101:THR:CA	1:n:129:LYS:CA	2.26	1.13
1:d:101:THR:CA	1:r:129:LYS:CA	2.26	1.12
1:k:11:TYR:O	1:n:6:VAL:O	1.67	1.13
1:AB:57:PRO:CA	1:s:34:SER:C	2.19	1.12
1:C:11:TYR:O	1:r:6:VAL:C	1.90	1.12
1:B:129:LYS:CA	1:Z:101:THR:CA	2.26	1.12
1:4:129:LYS:CA	1:p:101:THR:CA	2.26	1.12
1:AB:129:LYS:CA	1:t:101:THR:CA	2.26	1.12
1:c:34:SER:C	1:r:57:PRO:CA	2.19	1.12
1:J:418:PHE:N	1:Y:97:LYS:N	1.72	1.12
1:d:57:PRO:N	1:q:37:THR:O	1.83	1.12
1:T:418:PHE:N	1:o:97:LYS:N	1.72	1.11
1:s:11:TYR:O	1:v:6:VAL:O	1.67	1.11
1:4:57:PRO:CA	1:o:34:SER:C	2.19	1.11
1:R:76:GLY:O	1:i:156:GLU:O	1.69	1.11
1:g:11:TYR:O	1:j:6:VAL:O	1.67	1.11
1:C:248:GLN:N	1:Z:95:GLU:O	1.82	1.11
1:A:156:GLU:O	1:Z:76:GLY:O	1.69	1.11
1:AF:57:PRO:CA	1:w:34:SER:C	2.19	1.11
1:w:11:TYR:O	1:z:6:VAL:O	1.67	1.11
1:7:156:GLU:O	1:D:76:GLY:O	1.69	1.11
1:H:418:PHE:N	1:U:97:LYS:H	1.27	1.11
1:V:57:PRO:N	1:m:37:THR:O	1.83	1.11
1:V:76:GLY:O	1:m:156:GLU:O	1.69	1.11
1:8:57:PRO:CA	1:C:34:SER:C	2.19	1.10
1:V:95:GLU:O	1:o:248:GLN:N	1.82	1.10
1:d:76:GLY:O	1:q:156:GLU:O	1.69	1.10
1:h:76:GLY:O	1:u:156:GLU:O	1.69	1.10
1:l:76:GLY:O	1:y:156:GLU:O	1.69	1.10
1:7:37:THR:O	1:D:57:PRO:N	1.83	1.10
1:g:34:SER:C	1:v:57:PRO:CA	2.20	1.10
1:h:95:GLU:O	1:w:248:GLN:N	1.82	1.10
1:3:37:THR:O	1:p:57:PRO:N	1.83	1.10
1:3:156:GLU:O	1:p:76:GLY:O	1.69	1.10
1:A:37:THR:O	1:Z:57:PRO:N	1.83	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:57:PRO:N	1:y:37:THR:O	1.83	1.10
1:b:418:PHE:N	1:s:97:LYS:N	1.72	1.10
1:5:248:GLN:N	1:p:95:GLU:O	1.82	1.09
1:9:248:GLN:N	1:D:95:GLU:O	1.82	1.09
1:h:57:PRO:N	1:u:37:THR:O	1.83	1.09
1:l:248:GLN:N	1:l:95:GLU:O	1.82	1.09
1:d:95:GLU:O	1:s:248:GLN:N	1.82	1.09
1:T:418:PHE:N	1:o:97:LYS:H	1.27	1.09
1:Q:79:LEU:CA	1:j:157:LEU:O	2.01	1.09
1:g:79:LEU:CA	1:v:157:LEU:O	2.01	1.09
1:k:79:LEU:CA	1:z:157:LEU:O	2.01	1.09
1:c:79:LEU:CA	1:r:157:LEU:O	2.01	1.09
1:g:38:TYR:N	1:v:55:SER:N	1.77	1.09
1:AC:248:GLN:N	1:t:95:GLU:O	1.82	1.08
1:U:79:LEU:CA	1:n:157:LEU:O	2.01	1.08
1:3:51:SER:O	1:p:43:ALA:CA	1.99	1.08
1:4:157:LEU:O	1:o:79:LEU:CA	2.01	1.08
1:AB:49:SER:O	1:s:45:ARG:CA	2.02	1.08
1:B:49:SER:O	1:Y:45:ARG:CA	2.02	1.08
1:c:47:SER:O	1:r:46:PRO:O	1.72	1.08
1:8:157:LEU:O	1:C:79:LEU:CA	2.01	1.08
1:B:157:LEU:O	1:Y:79:LEU:CA	2.01	1.08
1:c:45:ARG:CA	1:r:49:SER:O	2.02	1.08
1:AF:55:SER:N	1:w:38:TYR:N	1.77	1.07
1:N:418:PHE:N	1:g:97:LYS:H	1.27	1.07
1:l:93:ASN:CA	1:z:137:GLN:H	1.53	1.07
1:4:49:SER:O	1:o:45:ARG:CA	2.02	1.07
1:8:49:SER:O	1:C:45:ARG:CA	2.02	1.07
1:V:101:THR:N	1:n:129:LYS:CA	2.17	1.07
1:l:43:ALA:CA	1:y:51:SER:O	1.99	1.07
1:g:45:ARG:CA	1:v:49:SER:O	2.02	1.07
1:g:47:SER:O	1:v:46:PRO:O	1.72	1.07
1:l:101:THR:N	1:z:129:LYS:CA	2.17	1.07
1:4:129:LYS:CA	1:p:101:THR:N	2.17	1.07
1:V:97:LYS:O	1:n:129:LYS:O	1.73	1.07
1:d:93:ASN:CA	1:r:137:GLN:H	1.53	1.07
1:h:101:THR:N	1:v:129:LYS:CA	2.17	1.07
1:k:45:ARG:CA	1:z:49:SER:O	2.02	1.07
1:l:97:LYS:O	1:z:129:LYS:O	1.73	1.07
1:4:129:LYS:O	1:p:97:LYS:O	1.73	1.06
1:h:97:LYS:O	1:v:129:LYS:O	1.73	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:76:GLY:CA	1:s:20:THR:O	2.03	1.06
1:AF:76:GLY:CA	1:w:20:THR:O	2.03	1.06
1:N:418:PHE:N	1:g:97:LYS:N	1.72	1.06
1:c:38:TYR:N	1:r:55:SER:N	1.77	1.06
1:7:75:PRO:O	1:C:22:SER:CA	1.98	1.06
1:AA:75:PRO:O	1:s:22:SER:CA	1.98	1.06
1:B:137:GLN:H	1:Z:93:ASN:CA	1.53	1.06
1:4:46:PRO:O	1:o:47:SER:O	1.72	1.06
1:8:46:PRO:O	1:C:47:SER:O	1.72	1.06
1:AB:46:PRO:O	1:s:47:SER:O	1.72	1.06
1:AB:129:LYS:CA	1:t:101:THR:N	2.17	1.06
1:B:129:LYS:CA	1:Z:101:THR:N	2.17	1.06
1:g:20:THR:O	1:v:76:GLY:CA	2.03	1.06
1:k:47:SER:O	1:z:46:PRO:O	1.72	1.06
1:B:46:PRO:O	1:Y:47:SER:O	1.72	1.06
1:B:129:LYS:O	1:Z:97:LYS:O	1.73	1.06
1:h:93:ASN:CA	1:v:137:GLN:H	1.53	1.06
1:8:129:LYS:CA	1:D:101:THR:N	2.17	1.05
1:J:418:PHE:N	1:Y:97:LYS:H	1.27	1.05
1:c:20:THR:O	1:r:76:GLY:CA	2.03	1.05
1:d:101:THR:N	1:r:129:LYS:CA	2.17	1.05
1:m:3:THR:C	1:y:81:GLN:H	1.55	1.05
1:B:11:TYR:C	1:o:8:SER:O	2.00	1.05
1:d:97:LYS:O	1:r:129:LYS:O	1.73	1.05
1:g:8:SER:O	1:j:11:TYR:C	2.00	1.05
1:w:8:SER:O	1:z:11:TYR:C	2.00	1.05
1:1:8:SER:O	1:4:11:TYR:C	2.00	1.05
1:3:75:PRO:O	1:o:22:SER:CA	1.98	1.05
1:8:129:LYS:O	1:D:97:LYS:O	1.73	1.05
1:8:76:GLY:CA	1:C:20:THR:O	2.03	1.05
1:AB:129:LYS:O	1:t:97:LYS:O	1.73	1.04
1:3:81:GLN:H	1:A:3:THR:C	1.55	1.04
1:7:51:SER:O	1:D:43:ALA:CA	1.99	1.04
1:b:418:PHE:N	1:s:97:LYS:H	1.27	1.04
1:k:20:THR:O	1:z:76:GLY:CA	2.03	1.04
1:H:418:PHE:C	1:U:93:ASN:O	2.01	1.04
1:P:418:PHE:C	1:k:93:ASN:O	2.01	1.04
1:s:8:SER:O	1:v:11:TYR:C	2.00	1.04
1:C:8:SER:O	1:r:11:TYR:C	2.00	1.04
1:C:97:LYS:H	1:X:418:PHE:N	1.27	1.04
1:T:418:PHE:C	1:o:93:ASN:O	2.01	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:43:ALA:CA	1:u:51:SER:O	1.99	1.04
1:i:3:THR:C	1:u:81:GLN:H	1.55	1.04
1:k:8:SER:O	1:n:11:TYR:C	2.00	1.04
1:k:22:SER:CA	1:y:75:PRO:O	1.98	1.04
1:A:51:SER:O	1:Z:43:ALA:CA	1.99	1.04
1:N:418:PHE:C	1:g:93:ASN:O	2.01	1.03
1:4:76:GLY:CA	1:o:20:THR:O	2.03	1.03
1:J:418:PHE:C	1:Y:93:ASN:O	2.01	1.03
1:V:93:ASN:CA	1:n:137:GLN:H	1.53	1.03
1:AE:75:PRO:O	1:w:22:SER:CA	1.98	1.02
1:b:418:PHE:C	1:s:93:ASN:O	2.01	1.02
1:d:43:ALA:CA	1:q:51:SER:O	1.99	1.02
1:k:38:TYR:N	1:z:54:ALA:CA	2.23	1.02
1:C:93:ASN:O	1:X:418:PHE:C	2.01	1.02
1:C:97:LYS:N	1:X:418:PHE:N	1.72	1.02
1:g:38:TYR:N	1:v:54:ALA:CA	2.23	1.02
1:3:23:ARG:O	1:p:70:LEU:CA	2.06	1.01
1:H:418:PHE:N	1:U:97:LYS:N	1.72	1.01
1:L:418:PHE:C	1:c:93:ASN:O	2.01	1.01
1:V:60:VAL:CA	1:m:34:SER:O	2.08	1.01
1:V:70:LEU:CA	1:m:23:ARG:O	2.06	1.01
1:d:60:VAL:CA	1:q:34:SER:O	2.08	1.01
1:3:34:SER:O	1:p:60:VAL:CA	2.08	1.01
1:A:23:ARG:O	1:Z:70:LEU:CA	2.06	1.01
1:h:60:VAL:CA	1:u:34:SER:O	2.08	1.01
1:7:81:GLN:H	1:q:3:THR:C	1.55	1.00
1:B:54:ALA:CA	1:Y:38:TYR:N	2.23	1.00
1:c:38:TYR:N	1:r:54:ALA:CA	2.23	1.00
1:l:60:VAL:CA	1:y:34:SER:O	2.08	1.00
1:8:54:ALA:CA	1:C:38:TYR:N	2.23	1.00
1:4:54:ALA:CA	1:o:38:TYR:N	2.23	1.00
1:8:55:SER:N	1:C:38:TYR:N	1.77	1.00
1:AA:51:SER:O	1:t:43:ALA:CA	1.99	1.00
1:AB:54:ALA:CA	1:s:38:TYR:N	2.23	1.00
1:B:125:GLU:N	1:Z:104:LYS:O	1.95	1.00
1:7:34:SER:O	1:D:60:VAL:CA	2.08	1.00
1:c:22:SER:CA	1:q:75:PRO:O	1.98	1.00
1:d:70:LEU:CA	1:q:23:ARG:O	2.06	1.00
1:8:125:GLU:N	1:D:104:LYS:O	1.95	1.00
1:d:104:LYS:O	1:r:125:GLU:N	1.95	1.00
1:8:137:GLN:H	1:D:93:ASN:CA	1.53	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:419:SER:N	1:g:94:THR:N	2.02	1.00
1:3:37:THR:C	1:p:57:PRO:N	2.20	0.99
1:H:419:SER:N	1:U:94:THR:N	2.02	0.99
1:P:419:SER:N	1:k:94:THR:N	2.02	0.99
1:d:57:PRO:N	1:q:37:THR:C	2.20	0.99
1:4:125:GLU:N	1:p:104:LYS:O	1.95	0.99
1:A:34:SER:O	1:Z:60:VAL:CA	2.08	0.99
1:T:419:SER:N	1:o:94:THR:N	2.02	0.99
1:AE:81:GLN:N	1:y:3:THR:C	2.03	0.99
1:l:57:PRO:N	1:y:37:THR:C	2.20	0.99
1:V:57:PRO:N	1:m:37:THR:C	2.20	0.99
1:C:94:THR:N	1:X:419:SER:N	2.02	0.99
1:l:70:LEU:CA	1:y:23:ARG:O	2.06	0.99
1:AB:125:GLU:N	1:t:104:LYS:O	1.95	0.99
1:R:70:LEU:CA	1:i:23:ARG:O	2.06	0.99
1:h:57:PRO:N	1:u:37:THR:C	2.20	0.98
1:7:37:THR:C	1:D:57:PRO:N	2.20	0.98
1:L:418:PHE:N	1:c:97:LYS:N	1.72	0.98
1:V:102:ASN:CA	1:o:250:GLN:O	2.12	0.98
1:4:137:GLN:H	1:p:93:ASN:CA	1.53	0.98
1:A:37:THR:C	1:Z:57:PRO:N	2.20	0.98
1:h:104:LYS:O	1:v:125:GLU:N	1.95	0.97
1:C:250:GLN:O	1:Z:102:ASN:CA	2.12	0.97
1:h:87:SER:CA	1:u:141:GLN:CA	2.42	0.97
1:l:104:LYS:O	1:z:125:GLU:N	1.95	0.97
1:h:102:ASN:CA	1:w:250:GLN:O	2.12	0.97
1:8:42:SER:C	1:C:52:LEU:H	1.73	0.97
1:A:141:GLN:CA	1:Z:87:SER:CA	2.42	0.97
1:1:250:GLN:O	1:l:102:ASN:CA	2.12	0.97
1:l:87:SER:CA	1:y:141:GLN:CA	2.42	0.97
1:4:42:SER:C	1:o:52:LEU:H	1.73	0.97
1:d:102:ASN:CA	1:s:250:GLN:O	2.12	0.97
1:h:70:LEU:CA	1:u:23:ARG:O	2.06	0.97
1:7:141:GLN:CA	1:D:87:SER:CA	2.42	0.97
1:AC:250:GLN:O	1:t:102:ASN:CA	2.12	0.97
1:4:57:PRO:CA	1:o:34:SER:O	2.13	0.97
1:AB:42:SER:C	1:s:52:LEU:H	1.73	0.97
1:V:87:SER:CA	1:m:141:GLN:CA	2.42	0.97
1:d:87:SER:CA	1:q:141:GLN:CA	2.42	0.97
1:J:419:SER:N	1:Y:94:THR:N	2.02	0.97
1:3:141:GLN:CA	1:p:87:SER:CA	2.42	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:81:GLN:H	1:u:3:THR:C	1.55	0.96
1:AF:76:GLY:HA3	1:w:20:THR:O	1.09	0.96
1:5:250:GLN:O	1:p:102:ASN:CA	2.12	0.96
1:AF:57:PRO:CA	1:w:34:SER:O	2.13	0.96
1:9:250:GLN:O	1:D:102:ASN:CA	2.12	0.96
1:g:22:SER:CA	1:u:75:PRO:O	1.98	0.96
1:k:34:SER:O	1:z:57:PRO:CA	2.13	0.96
1:k:52:LEU:H	1:z:42:SER:C	1.73	0.96
1:AF:54:ALA:CA	1:w:38:TYR:N	2.23	0.96
1:B:42:SER:C	1:Y:52:LEU:H	1.73	0.96
1:8:57:PRO:CA	1:C:34:SER:O	2.13	0.96
1:4:60:VAL:CA	1:o:31:VAL:O	2.14	0.95
1:c:17:GLY:HA2	1:r:75:PRO:N	1.81	0.95
1:9:261:SER:CA	1:9:262:LYS:N	2.29	0.95
1:AE:81:GLN:H	1:y:3:THR:C	1.55	0.95
1:c:52:LEU:H	1:r:42:SER:C	1.73	0.95
1:g:52:LEU:H	1:v:42:SER:C	1.73	0.95
1:g:34:SER:O	1:v:57:PRO:CA	2.13	0.95
1:AA:81:GLN:N	1:u:3:THR:C	2.03	0.95
1:AC:261:SER:CA	1:AC:262:LYS:N	2.29	0.95
1:g:17:GLY:HA2	1:v:75:PRO:N	1.81	0.95
1:s:261:SER:CA	1:s:262:LYS:N	2.29	0.95
1:C:261:SER:CA	1:C:262:LYS:N	2.29	0.95
1:5:261:SER:CA	1:5:262:LYS:N	2.29	0.95
1:i:3:THR:C	1:u:81:GLN:N	2.03	0.95
1:7:81:GLN:N	1:q:3:THR:C	2.03	0.95
1:g:31:VAL:O	1:v:60:VAL:CA	2.14	0.95
1:4:75:PRO:N	1:o:17:GLY:HA2	1.81	0.95
1:AB:57:PRO:CA	1:s:34:SER:O	2.13	0.95
1:c:31:VAL:O	1:r:60:VAL:CA	2.14	0.95
1:c:34:SER:O	1:r:57:PRO:CA	2.13	0.95
1:8:60:VAL:CA	1:C:31:VAL:O	2.14	0.95
1:AF:75:PRO:N	1:w:17:GLY:HA2	1.81	0.95
1:b:419:SER:N	1:s:94:THR:N	2.02	0.94
1:AB:75:PRO:N	1:s:17:GLY:HA2	1.81	0.94
1:8:75:PRO:N	1:C:17:GLY:HA2	1.81	0.94
1:AB:60:VAL:CA	1:s:31:VAL:O	2.14	0.94
1:AF:60:VAL:CA	1:w:31:VAL:O	2.14	0.94
1:w:261:SER:CA	1:w:262:LYS:N	2.29	0.94
1:1:261:SER:CA	1:1:262:LYS:N	2.29	0.94
1:k:31:VAL:O	1:z:60:VAL:CA	2.14	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:251:GLU:CA	1:AN:390:LYS:CA	2.47	0.93
1:4:137:GLN:CA	1:p:93:ASN:CA	2.46	0.93
1:h:93:ASN:CA	1:v:137:GLN:CA	2.46	0.93
1:k:17:GLY:HA2	1:z:75:PRO:N	1.81	0.93
1:0:390:LYS:CA	1:D:251:GLU:CA	2.47	0.93
1:AP:404:LEU:CA	1:r:261:SER:O	2.17	0.93
1:6:251:GLU:CA	1:AL:390:LYS:CA	2.47	0.93
1:6:390:LYS:CA	1:p:251:GLU:CA	2.47	0.93
1:8:137:GLN:CA	1:D:93:ASN:CA	2.46	0.93
1:AD:390:LYS:CA	1:t:251:GLU:CA	2.47	0.93
1:AD:404:LEU:CA	1:b:261:SER:O	2.17	0.93
1:L:419:SER:N	1:c:94:THR:N	2.02	0.93
1:AD:251:GLU:CA	1:AP:390:LYS:CA	2.47	0.93
1:9:261:SER:C	1:9:262:LYS:N	0.83	0.93
1:AC:261:SER:C	1:AC:262:LYS:N	0.83	0.93
1:C:261:SER:C	1:C:262:LYS:N	0.83	0.93
1:s:261:SER:C	1:s:262:LYS:N	0.83	0.93
1:d:93:ASN:CA	1:r:137:GLN:CA	2.46	0.93
1:5:261:SER:C	1:5:262:LYS:N	0.83	0.93
1:w:261:SER:C	1:w:262:LYS:N	0.83	0.93
1:V:93:ASN:CA	1:n:137:GLN:CA	2.46	0.93
1:2:251:GLU:CA	1:AJ:390:LYS:CA	2.47	0.92
1:1:261:SER:C	1:1:262:LYS:N	0.83	0.92
1:l:93:ASN:CA	1:z:137:GLN:CA	2.46	0.92
1:AH:390:LYS:CA	1:x:251:GLU:CA	2.47	0.92
1:AN:404:LEU:CA	1:B:261:SER:O	2.17	0.92
1:B:137:GLN:CA	1:Z:93:ASN:CA	2.46	0.92
1:0:404:LEU:CA	1:X:261:SER:O	2.17	0.92
1:8:76:GLY:HA3	1:C:20:THR:O	1.09	0.92
1:AH:404:LEU:CA	1:f:261:SER:O	2.17	0.91
1:AJ:404:LEU:CA	1:j:261:SER:O	2.17	0.91
1:AL:404:LEU:CA	1:n:261:SER:O	2.17	0.91
1:d:46:PRO:O	1:r:43:ALA:CA	2.19	0.90
1:AF:103:GLU:C	1:u:252:GLN:O	2.14	0.90
1:8:54:ALA:C	1:C:38:TYR:N	2.30	0.90
1:g:30:TYR:N	1:q:52:LEU:O	2.05	0.90
1:7:52:LEU:O	1:s:30:TYR:N	2.05	0.90
1:8:103:GLU:C	1:A:252:GLN:O	2.14	0.90
1:AB:103:GLU:C	1:q:252:GLN:O	2.14	0.89
1:c:20:THR:O	1:r:76:GLY:HA3	1.09	0.89
1:B:54:ALA:C	1:Y:38:TYR:N	2.30	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:47:SER:C	1:z:46:PRO:O	2.16	0.89
1:B:103:GLU:C	1:W:252:GLN:O	2.14	0.89
1:k:38:TYR:N	1:z:54:ALA:C	2.30	0.89
1:9:248:GLN:N	1:D:95:GLU:C	2.31	0.89
1:AA:52:LEU:O	1:w:30:TYR:N	2.06	0.89
1:AA:82:ASP:CA	1:u:2:SER:C	2.46	0.89
1:e:252:GLN:O	1:v:103:GLU:C	2.14	0.89
1:g:47:SER:C	1:v:46:PRO:O	2.16	0.89
1:AB:54:ALA:C	1:s:38:TYR:N	2.30	0.89
1:a:252:GLN:O	1:r:103:GLU:C	2.15	0.89
1:A:52:LEU:O	1:c:30:TYR:N	2.05	0.89
1:AB:43:ALA:CA	1:t:46:PRO:O	2.19	0.89
1:k:30:TYR:N	1:u:52:LEU:O	2.05	0.89
1:4:103:GLU:C	1:m:252:GLN:O	2.14	0.89
1:V:95:GLU:C	1:o:248:GLN:N	2.31	0.89
1:C:248:GLN:N	1:Z:95:GLU:C	2.31	0.89
1:g:38:TYR:N	1:v:54:ALA:C	2.30	0.89
1:4:54:ALA:C	1:o:38:TYR:N	2.30	0.88
1:m:2:SER:C	1:y:82:ASP:CA	2.46	0.88
1:3:82:ASP:CA	1:A:2:SER:C	2.46	0.88
1:d:95:GLU:C	1:s:248:GLN:N	2.31	0.88
1:i:252:GLN:O	1:z:103:GLU:C	2.15	0.88
1:3:52:LEU:O	1:C:30:TYR:N	2.05	0.88
1:c:38:TYR:N	1:r:54:ALA:C	2.30	0.88
1:7:82:ASP:CA	1:q:2:SER:C	2.46	0.88
1:AB:46:PRO:O	1:s:47:SER:C	2.16	0.88
1:h:46:PRO:O	1:v:43:ALA:CA	2.19	0.88
1:i:2:SER:C	1:u:82:ASP:CA	2.46	0.88
1:5:248:GLN:CA	1:p:95:GLU:CA	2.52	0.88
1:AC:248:GLN:CA	1:t:95:GLU:CA	2.52	0.88
1:AF:54:ALA:C	1:w:38:TYR:N	2.30	0.88
1:5:248:GLN:N	1:p:95:GLU:C	2.31	0.88
1:4:46:PRO:O	1:o:47:SER:C	2.16	0.88
1:B:43:ALA:CA	1:Z:46:PRO:O	2.19	0.88
1:U:66:SER:N	1:n:28:ARG:C	2.32	0.88
1:c:47:SER:C	1:r:46:PRO:O	2.16	0.88
1:d:95:GLU:CA	1:s:248:GLN:CA	2.52	0.88
1:7:32:THR:H	1:C:66:SER:CA	1.87	0.87
1:9:248:GLN:CA	1:D:95:GLU:CA	2.52	0.87
1:g:66:SER:CA	1:u:32:THR:H	1.87	0.87
1:4:43:ALA:CA	1:p:46:PRO:O	2.19	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:95:GLU:CA	1:w:248:GLN:CA	2.52	0.87
1:AE:82:ASP:CA	1:y:2:SER:C	2.46	0.87
1:B:46:PRO:O	1:Y:47:SER:C	2.16	0.87
1:g:66:SER:N	1:v:28:ARG:C	2.32	0.87
1:o:30:TYR:N	1:y:52:LEU:O	2.05	0.87
1:8:46:PRO:O	1:C:47:SER:C	2.16	0.87
1:h:95:GLU:C	1:w:248:GLN:N	2.31	0.87
1:V:95:GLU:CA	1:o:248:GLN:CA	2.52	0.87
1:l:248:GLN:N	1:l:95:GLU:C	2.31	0.87
1:AC:248:GLN:N	1:t:95:GLU:C	2.31	0.87
1:C:248:GLN:CA	1:Z:95:GLU:CA	2.52	0.87
1:k:66:SER:CA	1:y:32:THR:H	1.87	0.87
1:l:248:GLN:CA	1:l:95:GLU:CA	2.52	0.87
1:c:66:SER:CA	1:q:32:THR:H	1.87	0.87
1:3:32:THR:H	1:o:66:SER:CA	1.87	0.86
1:d:52:LEU:H	1:r:37:THR:CA	1.88	0.86
1:4:76:GLY:HA3	1:o:20:THR:O	1.09	0.86
1:h:52:LEU:H	1:v:37:THR:CA	1.88	0.86
1:8:25:SER:H	1:C:68:VAL:C	1.80	0.86
1:A:32:THR:H	1:Y:66:SER:CA	1.87	0.86
1:4:37:THR:CA	1:p:52:LEU:H	1.88	0.86
1:AB:37:THR:CA	1:t:52:LEU:H	1.88	0.86
1:AC:346:GLU:C	1:q:176:ASP:O	2.18	0.86
1:V:52:LEU:H	1:n:37:THR:CA	1.88	0.86
1:l:52:LEU:H	1:z:37:THR:CA	1.88	0.86
1:B:28:ARG:C	1:Y:66:SER:N	2.32	0.86
1:AG:346:GLU:C	1:u:176:ASP:O	2.18	0.86
1:B:37:THR:CA	1:Z:52:LEU:H	1.88	0.86
1:U:66:SER:CA	1:m:32:THR:H	1.87	0.86
1:l:346:GLU:C	1:i:176:ASP:O	2.18	0.86
1:AI:346:GLU:C	1:y:176:ASP:O	2.18	0.86
1:l:46:PRO:O	1:z:43:ALA:CA	2.19	0.85
1:3:176:ASP:O	1:AK:346:GLU:C	2.18	0.85
1:g:20:THR:O	1:v:76:GLY:HA3	1.09	0.85
1:l:346:GLU:CA	1:i:176:ASP:O	2.25	0.85
1:3:72:SER:N	1:B:1:MET:H3	1.75	0.85
1:AA:51:SER:O	1:t:43:ALA:C	2.20	0.85
1:P:411:ILE:CA	1:l:106:GLU:C	2.50	0.85
1:k:66:SER:N	1:z:28:ARG:C	2.32	0.85
1:7:51:SER:O	1:D:43:ALA:C	2.20	0.85
1:7:72:SER:N	1:r:1:MET:N	2.25	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:346:GLU:C	1:A:176:ASP:O	2.18	0.85
1:5:346:GLU:C	1:m:176:ASP:O	2.18	0.85
1:8:37:THR:CA	1:D:52:LEU:H	1.88	0.85
1:8:103:GLU:CA	1:A:253:HIS:CA	0.85	0.85
1:AB:103:GLU:CA	1:q:253:HIS:CA	0.85	0.85
1:AF:103:GLU:CA	1:u:253:HIS:CA	0.85	0.85
1:AI:346:GLU:CA	1:y:176:ASP:O	2.25	0.85
1:4:33:THR:N	1:o:60:VAL:O	2.10	0.85
1:8:33:THR:N	1:C:60:VAL:O	2.10	0.85
1:B:103:GLU:CA	1:W:253:HIS:CA	0.85	0.85
1:d:43:ALA:C	1:q:51:SER:O	2.20	0.85
1:e:253:HIS:CA	1:v:103:GLU:CA	0.85	0.85
1:k:60:VAL:O	1:z:33:THR:N	2.10	0.85
1:5:261:SER:O	1:5:262:LYS:CA	2.06	0.85
1:a:253:HIS:CA	1:r:103:GLU:CA	0.85	0.85
1:i:253:HIS:CA	1:z:103:GLU:CA	0.85	0.85
1:3:51:SER:O	1:p:43:ALA:C	2.20	0.85
1:4:103:GLU:CA	1:m:253:HIS:CA	0.85	0.85
1:J:411:ILE:CA	1:Z:106:GLU:C	2.50	0.85
1:N:411:ILE:CA	1:h:106:GLU:C	2.50	0.85
1:5:346:GLU:CA	1:m:176:ASP:O	2.25	0.84
1:AG:346:GLU:CA	1:u:176:ASP:O	2.25	0.84
1:D:106:GLU:C	1:X:411:ILE:CA	2.50	0.84
1:7:36:ARG:H	1:D:60:VAL:CA	1.90	0.84
1:A:51:SER:O	1:Z:43:ALA:C	2.20	0.84
1:L:411:ILE:CA	1:d:106:GLU:C	2.50	0.84
1:g:60:VAL:O	1:v:33:THR:N	2.10	0.84
1:h:43:ALA:C	1:u:51:SER:O	2.20	0.84
1:L:419:SER:N	1:c:93:ASN:C	2.36	0.84
1:b:411:ILE:CA	1:t:106:GLU:C	2.50	0.84
1:8:28:ARG:C	1:C:66:SER:N	2.32	0.84
1:AC:346:GLU:CA	1:q:176:ASP:O	2.25	0.84
1:B:33:THR:N	1:Y:60:VAL:O	2.10	0.84
1:T:411:ILE:CA	1:p:106:GLU:C	2.50	0.84
1:b:419:SER:N	1:s:93:ASN:C	2.36	0.84
1:3:176:ASP:O	1:AK:346:GLU:CA	2.25	0.84
1:AE:72:SER:N	1:z:1:MET:H3	1.75	0.84
1:h:56:SER:CA	1:u:37:THR:CA	2.55	0.84
1:8:43:ALA:CA	1:D:46:PRO:O	2.19	0.84
1:b:416:PRO:O	1:s:97:LYS:CA	2.25	0.84
1:c:66:SER:N	1:r:28:ARG:C	2.32	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:1:MET:H3	1:u:72:SER:N	1.75	0.84
1:k:20:THR:O	1:z:76:GLY:HA3	1.09	0.84
1:3:72:SER:N	1:B:1:MET:N	2.25	0.84
1:7:37:THR:CA	1:D:56:SER:CA	2.55	0.84
1:AA:72:SER:N	1:v:1:MET:N	2.25	0.84
1:AB:48:THR:O	1:s:45:ARG:O	1.96	0.84
1:AE:72:SER:N	1:z:1:MET:N	2.25	0.84
1:l:43:ALA:C	1:y:51:SER:O	2.20	0.84
1:l:56:SER:CA	1:y:37:THR:CA	2.55	0.84
1:9:346:GLU:CA	1:A:176:ASP:O	2.25	0.84
1:U:60:VAL:O	1:n:33:THR:N	2.10	0.84
1:j:1:MET:N	1:u:72:SER:N	2.25	0.84
1:AB:76:GLY:HA3	1:s:20:THR:O	1.09	0.83
1:d:56:SER:CA	1:q:37:THR:CA	2.55	0.83
1:d:60:VAL:CA	1:q:36:ARG:H	1.90	0.83
1:h:60:VAL:CA	1:u:36:ARG:H	1.90	0.83
1:l:60:VAL:CA	1:y:36:ARG:H	1.90	0.83
1:n:1:MET:N	1:y:72:SER:N	2.25	0.83
1:3:36:ARG:H	1:p:60:VAL:CA	1.90	0.83
1:c:45:ARG:O	1:r:48:THR:O	1.96	0.83
1:c:60:VAL:O	1:r:33:THR:N	2.10	0.83
1:A:37:THR:CA	1:Z:56:SER:CA	2.55	0.83
1:H:419:SER:N	1:U:93:ASN:C	2.36	0.83
1:T:419:SER:N	1:o:93:ASN:C	2.36	0.83
1:V:60:VAL:CA	1:m:36:ARG:H	1.90	0.83
1:P:416:PRO:O	1:k:97:LYS:CA	2.25	0.83
1:C:93:ASN:C	1:X:419:SER:N	2.36	0.83
1:J:419:SER:N	1:Y:93:ASN:C	2.36	0.83
1:N:416:PRO:O	1:g:97:LYS:CA	2.25	0.83
1:N:419:SER:N	1:g:93:ASN:C	2.36	0.83
1:AA:72:SER:N	1:v:1:MET:H3	1.76	0.83
1:T:416:PRO:O	1:o:97:LYS:CA	2.25	0.83
1:1:261:SER:O	1:1:262:LYS:CA	2.06	0.83
1:3:37:THR:CA	1:p:56:SER:CA	2.55	0.83
1:A:36:ARG:H	1:Z:60:VAL:CA	1.90	0.83
1:P:419:SER:N	1:k:93:ASN:C	2.36	0.83
1:k:45:ARG:O	1:z:48:THR:O	1.96	0.83
1:C:97:LYS:CA	1:X:416:PRO:O	2.25	0.83
1:V:56:SER:CA	1:m:37:THR:CA	2.55	0.83
1:AB:77:VAL:N	1:s:21:ALA:O	1.96	0.83
1:L:416:PRO:O	1:c:97:LYS:CA	2.25	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:45:ARG:O	1:v:48:THR:O	1.96	0.83
1:4:48:THR:O	1:o:45:ARG:O	1.96	0.82
1:AF:77:VAL:N	1:w:21:ALA:O	1.96	0.82
1:c:68:VAL:C	1:r:25:SER:H	1.80	0.82
1:l:43:ALA:CA	1:y:51:SER:C	2.53	0.82
1:g:21:ALA:O	1:v:77:VAL:N	1.96	0.82
1:8:48:THR:O	1:C:45:ARG:O	1.96	0.82
1:B:48:THR:O	1:Y:45:ARG:O	1.96	0.82
1:H:416:PRO:O	1:U:97:LYS:CA	2.25	0.82
1:7:72:SER:N	1:r:1:MET:H3	1.77	0.81
1:g:23:ARG:H	1:v:76:GLY:CA	1.93	0.81
1:k:21:ALA:O	1:z:77:VAL:N	1.96	0.81
1:4:28:ARG:C	1:o:66:SER:N	2.32	0.81
1:AA:51:SER:C	1:t:43:ALA:CA	2.53	0.81
1:J:416:PRO:O	1:Y:97:LYS:CA	2.25	0.81
1:N:418:PHE:C	1:g:93:ASN:C	2.48	0.81
1:k:23:ARG:H	1:z:76:GLY:CA	1.94	0.81
1:4:76:GLY:CA	1:o:23:ARG:H	1.93	0.81
1:AB:76:GLY:CA	1:s:23:ARG:H	1.94	0.81
1:AF:75:PRO:CA	1:w:17:GLY:HA2	2.10	0.81
1:H:418:PHE:C	1:U:93:ASN:C	2.48	0.81
1:T:418:PHE:C	1:o:93:ASN:C	2.48	0.81
1:4:57:PRO:O	1:o:33:THR:O	1.99	0.81
1:AB:75:PRO:CA	1:s:17:GLY:HA2	2.10	0.81
1:A:51:SER:C	1:Z:43:ALA:CA	2.53	0.81
1:P:418:PHE:C	1:k:93:ASN:C	2.48	0.81
1:g:17:GLY:HA2	1:v:75:PRO:CA	2.10	0.81
1:4:75:PRO:CA	1:o:17:GLY:HA2	2.10	0.81
1:AF:57:PRO:O	1:w:33:THR:O	1.99	0.81
1:d:43:ALA:CA	1:q:51:SER:C	2.53	0.81
1:h:43:ALA:CA	1:u:51:SER:C	2.53	0.81
1:7:51:SER:C	1:D:43:ALA:CA	2.53	0.81
1:L:418:PHE:C	1:c:93:ASN:C	2.48	0.81
1:3:51:SER:C	1:p:43:ALA:CA	2.53	0.81
1:C:93:ASN:C	1:X:418:PHE:C	2.48	0.81
1:7:81:GLN:H	1:q:4:ARG:H	0.85	0.81
1:AF:76:GLY:CA	1:w:23:ARG:H	1.94	0.81
1:b:418:PHE:C	1:s:93:ASN:C	2.48	0.81
1:8:76:GLY:CA	1:C:23:ARG:H	1.94	0.80
1:J:418:PHE:C	1:Y:93:ASN:C	2.48	0.80
1:c:23:ARG:H	1:r:76:GLY:CA	1.94	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:33:THR:O	1:r:57:PRO:O	1.99	0.80
1:9:261:SER:O	1:9:262:LYS:CA	2.05	0.80
1:g:33:THR:O	1:v:57:PRO:O	1.99	0.80
1:C:261:SER:O	1:C:262:LYS:CA	2.06	0.80
1:c:17:GLY:HA2	1:r:75:PRO:CA	2.10	0.80
1:w:261:SER:O	1:w:262:LYS:CA	2.06	0.80
1:8:57:PRO:O	1:C:33:THR:O	1.99	0.80
1:k:66:SER:CA	1:z:26:SER:C	2.55	0.80
1:8:75:PRO:CA	1:C:17:GLY:HA2	2.10	0.80
1:c:21:ALA:O	1:r:77:VAL:N	1.96	0.80
1:k:33:THR:O	1:z:57:PRO:O	1.99	0.80
1:4:26:SER:C	1:o:66:SER:CA	2.55	0.80
1:8:26:SER:C	1:C:66:SER:CA	2.55	0.80
1:U:68:VAL:C	1:n:25:SER:H	1.80	0.80
1:k:17:GLY:HA2	1:z:75:PRO:CA	2.10	0.80
1:U:66:SER:CA	1:n:26:SER:C	2.55	0.80
1:AB:57:PRO:O	1:s:33:THR:O	1.99	0.80
1:B:26:SER:C	1:Y:66:SER:CA	2.55	0.80
1:c:66:SER:CA	1:r:26:SER:C	2.55	0.79
1:g:66:SER:CA	1:v:26:SER:C	2.55	0.79
1:AA:73:SER:CA	1:t:20:THR:CA	2.61	0.79
1:d:20:THR:CA	1:q:73:SER:CA	2.61	0.79
1:o:28:ARG:O	1:y:54:ALA:CA	2.31	0.79
1:AE:73:SER:CA	1:x:20:THR:CA	2.61	0.79
1:h:20:THR:CA	1:u:73:SER:CA	2.61	0.79
1:3:54:ALA:CA	1:C:28:ARG:O	2.31	0.79
1:7:73:SER:CA	1:D:20:THR:CA	2.61	0.79
1:AB:42:SER:CA	1:s:52:LEU:H	1.96	0.79
1:Q:68:VAL:C	1:j:25:SER:H	1.80	0.79
1:8:42:SER:CA	1:C:52:LEU:H	1.96	0.79
1:A:54:ALA:CA	1:c:28:ARG:O	2.31	0.79
1:B:42:SER:CA	1:Y:52:LEU:H	1.96	0.78
1:k:28:ARG:O	1:u:54:ALA:CA	2.31	0.78
1:l:71:ARG:C	1:y:23:ARG:CA	2.48	0.78
1:k:52:LEU:H	1:z:42:SER:CA	1.96	0.78
1:7:54:ALA:CA	1:s:28:ARG:O	2.31	0.78
1:c:52:LEU:H	1:r:42:SER:CA	1.96	0.78
1:B:104:LYS:CA	1:W:252:GLN:O	2.32	0.78
1:g:28:ARG:O	1:q:54:ALA:CA	2.31	0.78
1:AA:54:ALA:CA	1:w:28:ARG:O	2.31	0.78
1:AF:104:LYS:CA	1:u:252:GLN:O	2.32	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:252:GLN:O	1:r:104:LYS:CA	2.32	0.78
1:d:79:LEU:N	1:r:155:ARG:CA	2.47	0.78
1:AE:73:SER:CA	1:x:20:THR:N	2.47	0.78
1:V:79:LEU:N	1:n:155:ARG:CA	2.47	0.78
1:e:252:GLN:O	1:v:104:LYS:CA	2.32	0.78
1:h:20:THR:N	1:u:73:SER:CA	2.47	0.78
1:l:20:THR:N	1:y:73:SER:CA	2.47	0.78
1:l:20:THR:CA	1:y:73:SER:CA	2.61	0.78
1:l:79:LEU:N	1:z:155:ARG:CA	2.47	0.78
1:4:155:ARG:CA	1:p:79:LEU:N	2.47	0.78
1:AB:104:LYS:CA	1:q:252:GLN:O	2.32	0.78
1:4:104:LYS:CA	1:m:252:GLN:O	2.32	0.78
1:g:52:LEU:H	1:v:42:SER:CA	1.96	0.78
1:3:81:GLN:H	1:A:4:ARG:H	0.85	0.78
1:8:155:ARG:CA	1:D:79:LEU:N	2.47	0.78
1:B:56:SER:CA	1:Y:35:THR:C	2.56	0.78
1:c:35:THR:C	1:r:56:SER:CA	2.56	0.78
1:3:73:SER:CA	1:p:20:THR:CA	2.61	0.77
1:4:42:SER:CA	1:o:52:LEU:H	1.96	0.77
1:B:155:ARG:CA	1:Z:79:LEU:N	2.47	0.77
1:d:20:THR:N	1:q:73:SER:CA	2.47	0.77
1:3:73:SER:CA	1:p:20:THR:N	2.47	0.77
1:7:73:SER:CA	1:D:20:THR:N	2.47	0.77
1:8:56:SER:CA	1:C:35:THR:C	2.57	0.77
1:AA:73:SER:CA	1:t:20:THR:N	2.47	0.77
1:h:79:LEU:N	1:v:155:ARG:CA	2.47	0.77
1:g:68:VAL:C	1:v:25:SER:H	1.80	0.77
1:AC:261:SER:O	1:AC:262:LYS:CA	2.05	0.77
1:4:24:PRO:CA	1:o:69:ARG:N	2.48	0.77
1:AB:56:SER:CA	1:s:35:THR:C	2.56	0.77
1:U:69:ARG:N	1:n:24:PRO:CA	2.48	0.77
1:c:69:ARG:N	1:r:24:PRO:CA	2.48	0.77
1:s:261:SER:O	1:s:262:LYS:CA	2.06	0.77
1:4:77:VAL:N	1:o:21:ALA:O	1.96	0.77
1:8:104:LYS:CA	1:A:252:GLN:O	2.32	0.77
1:i:252:GLN:O	1:z:104:LYS:CA	2.32	0.77
1:k:69:ARG:N	1:z:24:PRO:CA	2.48	0.77
1:V:71:ARG:C	1:m:23:ARG:CA	2.48	0.77
1:AF:56:SER:CA	1:w:35:THR:C	2.56	0.76
1:d:93:ASN:CA	1:r:136:GLU:C	2.59	0.76
1:8:24:PRO:CA	1:C:69:ARG:N	2.48	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:69:ARG:N	1:j:24:PRO:CA	2.48	0.76
1:g:35:THR:C	1:v:56:SER:CA	2.57	0.76
1:4:56:SER:CA	1:o:35:THR:C	2.56	0.76
1:B:24:PRO:CA	1:Y:69:ARG:N	2.48	0.76
1:g:69:ARG:N	1:v:24:PRO:CA	2.48	0.76
1:k:68:VAL:C	1:z:25:SER:H	1.80	0.76
1:l:93:ASN:CA	1:z:136:GLU:C	2.59	0.76
1:AE:81:GLN:H	1:y:4:ARG:H	0.85	0.76
1:d:57:PRO:CA	1:q:37:THR:O	2.34	0.76
1:A:37:THR:O	1:Z:57:PRO:CA	2.33	0.76
1:L:451:ASP:O	1:r:190:GLN:CA	2.34	0.76
1:3:28:ARG:O	1:o:69:ARG:N	2.19	0.75
1:3:37:THR:O	1:p:57:PRO:CA	2.33	0.75
1:A:28:ARG:O	1:Y:69:ARG:N	2.20	0.75
1:C:247:ALA:CA	1:Z:95:GLU:O	2.34	0.75
1:h:102:ASN:H	1:w:251:GLU:CA	1.99	0.75
1:7:24:PRO:O	1:D:70:LEU:O	1.91	0.75
1:k:69:ARG:N	1:y:28:ARG:O	2.20	0.75
1:l:57:PRO:CA	1:y:37:THR:O	2.33	0.75
1:m:4:ARG:H	1:y:81:GLN:H	0.85	0.75
1:k:35:THR:C	1:z:56:SER:CA	2.56	0.75
1:n:1:MET:H3	1:y:72:SER:N	1.81	0.75
1:V:57:PRO:CA	1:m:37:THR:O	2.33	0.75
1:c:69:ARG:N	1:q:28:ARG:O	2.19	0.75
1:5:247:ALA:CA	1:p:95:GLU:O	2.34	0.75
1:V:93:ASN:CA	1:n:136:GLU:C	2.59	0.75
1:h:57:PRO:CA	1:u:37:THR:O	2.33	0.75
1:h:71:ARG:C	1:u:23:ARG:CA	2.48	0.75
1:3:23:ARG:CA	1:p:71:ARG:C	2.49	0.75
1:4:136:GLU:C	1:p:93:ASN:CA	2.59	0.75
1:V:95:GLU:O	1:o:247:ALA:CA	2.34	0.75
1:d:95:GLU:O	1:s:247:ALA:CA	2.34	0.75
1:s:8:SER:C	1:v:12:ARG:N	2.45	0.75
1:9:247:ALA:CA	1:D:95:GLU:O	2.34	0.75
1:Q:69:ARG:N	1:i:28:ARG:O	2.19	0.75
1:7:28:ARG:O	1:C:69:ARG:N	2.19	0.75
1:c:45:ARG:O	1:r:49:SER:N	2.20	0.75
1:8:49:SER:N	1:C:45:ARG:O	2.20	0.75
1:d:102:ASN:H	1:s:251:GLU:CA	1.99	0.75
1:5:251:GLU:CA	1:p:102:ASN:H	1.99	0.74
1:7:37:THR:O	1:D:57:PRO:CA	2.34	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:451:ASP:O	1:v:190:GLN:CA	2.34	0.74
1:g:8:SER:C	1:j:12:ARG:N	2.45	0.74
1:l:247:ALA:CA	1:l:95:GLU:O	2.35	0.74
1:7:26:SER:O	1:D:67:ALA:CA	2.30	0.74
1:9:251:GLU:CA	1:D:102:ASN:H	1.99	0.74
1:C:94:THR:H	1:X:419:SER:CA	2.00	0.74
1:U:69:ARG:N	1:m:28:ARG:O	2.20	0.74
1:g:69:ARG:N	1:u:28:ARG:O	2.19	0.74
1:k:8:SER:C	1:n:12:ARG:N	2.45	0.74
1:4:25:SER:H	1:o:68:VAL:C	1.80	0.74
1:AC:251:GLU:CA	1:t:102:ASN:H	1.99	0.74
1:B:136:GLU:C	1:Z:93:ASN:CA	2.59	0.74
1:B:190:GLN:CA	1:J:451:ASP:O	2.34	0.74
1:C:8:SER:C	1:r:12:ARG:N	2.45	0.74
1:k:45:ARG:O	1:z:49:SER:N	2.20	0.74
1:8:136:GLU:C	1:D:93:ASN:CA	2.59	0.74
1:AC:247:ALA:CA	1:t:95:GLU:O	2.34	0.74
1:P:451:ASP:O	1:z:190:GLN:CA	2.34	0.74
1:l:19:GLY:C	1:y:73:SER:O	2.31	0.74
1:w:8:SER:C	1:z:12:ARG:N	2.45	0.74
1:3:73:SER:O	1:p:19:GLY:C	2.31	0.74
1:C:251:GLU:CA	1:Z:102:ASN:H	1.99	0.74
1:J:419:SER:CA	1:Y:94:THR:H	2.00	0.74
1:7:73:SER:O	1:D:19:GLY:C	2.31	0.74
1:AA:72:SER:H	1:v:1:MET:C	1.96	0.74
1:h:95:GLU:O	1:w:247:ALA:CA	2.35	0.74
1:AE:72:SER:H	1:z:1:MET:C	1.96	0.74
1:h:93:ASN:CA	1:v:136:GLU:C	2.59	0.74
1:AB:49:SER:N	1:s:45:ARG:O	2.20	0.74
1:F:451:ASP:O	1:j:190:GLN:CA	2.34	0.74
1:A:23:ARG:CA	1:Z:71:ARG:C	2.48	0.74
1:T:419:SER:C	1:o:94:THR:CA	2.61	0.74
1:V:102:ASN:H	1:o:251:GLU:CA	1.99	0.74
1:7:72:SER:H	1:r:1:MET:C	1.96	0.74
1:B:12:ARG:N	1:o:8:SER:C	2.45	0.74
1:B:49:SER:N	1:Y:45:ARG:O	2.20	0.74
1:H:451:ASP:O	1:n:190:GLN:CA	2.34	0.74
1:h:19:GLY:C	1:u:73:SER:O	2.31	0.74
1:i:4:ARG:H	1:u:81:GLN:H	0.85	0.74
1:l:8:SER:C	1:4:12:ARG:N	2.45	0.73
1:3:72:SER:H	1:B:1:MET:C	1.96	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:419:SER:C	1:Y:94:THR:CA	2.61	0.73
1:1:251:GLU:CA	1:l:102:ASN:H	1.99	0.73
1:4:190:GLN:CA	1:T:451:ASP:O	2.34	0.73
1:AE:73:SER:O	1:x:19:GLY:C	2.31	0.73
1:n:1:MET:C	1:y:72:SER:H	1.96	0.73
1:H:419:SER:C	1:U:94:THR:CA	2.61	0.73
1:P:419:SER:C	1:k:94:THR:CA	2.61	0.73
1:d:67:ALA:C	1:q:25:SER:O	2.24	0.73
1:g:45:ARG:O	1:v:49:SER:N	2.20	0.73
1:AA:73:SER:O	1:t:19:GLY:C	2.31	0.73
1:j:1:MET:C	1:u:72:SER:H	1.96	0.73
1:4:49:SER:N	1:o:45:ARG:O	2.20	0.73
1:R:70:LEU:O	1:i:24:PRO:O	1.91	0.73
1:C:94:THR:CA	1:X:419:SER:C	2.61	0.73
1:N:419:SER:C	1:g:94:THR:CA	2.61	0.73
1:d:71:ARG:C	1:q:23:ARG:CA	2.48	0.73
1:V:97:LYS:CA	1:n:133:ALA:H	2.01	0.73
1:b:419:SER:C	1:s:94:THR:CA	2.61	0.73
1:AB:133:ALA:CA	1:t:94:THR:O	2.37	0.72
1:C:248:GLN:N	1:Z:95:GLU:CA	2.53	0.72
1:1:248:GLN:N	1:l:95:GLU:CA	2.52	0.72
1:3:26:SER:O	1:p:67:ALA:CA	2.30	0.72
1:d:94:THR:O	1:r:133:ALA:CA	2.37	0.72
1:h:94:THR:O	1:v:133:ALA:CA	2.37	0.72
1:l:94:THR:O	1:z:133:ALA:CA	2.37	0.72
1:4:133:ALA:H	1:p:97:LYS:CA	2.01	0.72
1:B:25:SER:H	1:Y:68:VAL:C	1.80	0.72
1:d:70:LEU:O	1:q:24:PRO:O	1.91	0.72
1:d:19:GLY:C	1:q:73:SER:O	2.31	0.72
1:3:24:PRO:O	1:p:70:LEU:O	1.91	0.72
1:5:248:GLN:N	1:p:95:GLU:CA	2.52	0.72
1:L:419:SER:C	1:c:94:THR:CA	2.61	0.72
1:7:25:SER:O	1:D:67:ALA:C	2.24	0.72
1:AC:248:GLN:N	1:t:95:GLU:CA	2.53	0.72
1:V:94:THR:O	1:n:133:ALA:CA	2.37	0.72
1:d:95:GLU:CA	1:s:248:GLN:N	2.52	0.72
1:h:95:GLU:CA	1:w:248:GLN:N	2.53	0.72
1:l:97:LYS:CA	1:z:133:ALA:H	2.01	0.72
1:N:419:SER:CA	1:g:94:THR:H	2.00	0.72
1:c:66:SER:N	1:q:32:THR:H	1.87	0.72
1:4:133:ALA:CA	1:p:94:THR:O	2.37	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:133:ALA:CA	1:D:94:THR:O	2.37	0.71
1:A:25:SER:O	1:Z:67:ALA:C	2.24	0.71
1:AA:81:GLN:CA	1:u:4:ARG:N	2.38	0.71
1:B:133:ALA:CA	1:Z:94:THR:O	2.37	0.71
1:R:71:ARG:C	1:i:23:ARG:CA	2.48	0.71
1:g:66:SER:N	1:u:32:THR:H	1.87	0.71
1:7:81:GLN:CA	1:q:4:ARG:N	2.38	0.71
1:8:77:VAL:N	1:C:21:ALA:O	1.96	0.71
1:9:248:GLN:N	1:D:95:GLU:CA	2.53	0.71
1:AF:76:GLY:CA	1:w:23:ARG:N	2.54	0.71
1:L:419:SER:CA	1:c:94:THR:H	2.00	0.71
1:k:23:ARG:N	1:z:76:GLY:CA	2.54	0.71
1:V:95:GLU:CA	1:o:248:GLN:N	2.52	0.71
1:3:32:THR:H	1:o:66:SER:N	1.87	0.71
1:4:55:SER:H	1:o:38:TYR:CA	2.04	0.71
1:U:66:SER:N	1:m:32:THR:H	1.87	0.71
1:b:419:SER:CA	1:s:94:THR:H	2.00	0.71
1:l:70:LEU:O	1:y:24:PRO:O	1.91	0.71
1:A:32:THR:H	1:Y:66:SER:N	1.87	0.71
1:c:23:ARG:N	1:r:76:GLY:CA	2.54	0.71
1:7:32:THR:H	1:C:66:SER:N	1.87	0.71
1:AF:55:SER:H	1:w:38:TYR:CA	2.04	0.71
1:4:26:SER:O	1:o:65:SER:C	2.34	0.70
1:c:65:SER:C	1:r:26:SER:O	2.34	0.70
1:g:23:ARG:N	1:v:76:GLY:CA	2.53	0.70
1:k:66:SER:N	1:y:32:THR:H	1.87	0.70
1:AB:76:GLY:CA	1:s:23:ARG:N	2.54	0.70
1:k:66:SER:CA	1:y:32:THR:N	2.55	0.70
1:7:32:THR:N	1:C:66:SER:CA	2.55	0.70
1:7:73:SER:C	1:D:19:GLY:C	2.60	0.70
1:8:26:SER:O	1:C:65:SER:C	2.34	0.70
1:AB:133:ALA:CA	1:t:97:LYS:CA	2.70	0.70
1:B:26:SER:O	1:Y:65:SER:C	2.34	0.70
1:g:38:TYR:CA	1:v:55:SER:H	2.04	0.70
1:h:19:GLY:C	1:u:73:SER:C	2.60	0.70
1:4:76:GLY:CA	1:o:23:ARG:N	2.53	0.70
1:A:32:THR:N	1:Y:66:SER:CA	2.55	0.70
1:AA:73:SER:C	1:t:19:GLY:C	2.60	0.70
1:AB:55:SER:H	1:s:38:TYR:CA	2.04	0.70
1:AE:73:SER:C	1:x:19:GLY:C	2.60	0.70
1:h:97:LYS:CA	1:v:133:ALA:CA	2.69	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:32:THR:N	1:o:66:SER:CA	2.55	0.70
1:c:66:SER:CA	1:q:32:THR:N	2.55	0.70
1:d:19:GLY:C	1:q:73:SER:C	2.60	0.70
1:g:66:SER:CA	1:u:32:THR:N	2.55	0.70
1:U:66:SER:CA	1:m:32:THR:N	2.55	0.70
1:U:65:SER:C	1:n:26:SER:O	2.34	0.70
1:k:65:SER:C	1:z:26:SER:O	2.34	0.70
1:3:73:SER:C	1:p:19:GLY:C	2.60	0.70
1:B:133:ALA:CA	1:Z:97:LYS:CA	2.70	0.70
1:8:76:GLY:CA	1:C:23:ARG:N	2.54	0.69
1:T:419:SER:CA	1:o:94:THR:H	2.00	0.69
1:d:97:LYS:CA	1:r:133:ALA:CA	2.70	0.69
1:H:419:SER:CA	1:U:94:THR:H	2.00	0.69
1:l:19:GLY:C	1:y:73:SER:C	2.60	0.69
1:g:65:SER:C	1:v:26:SER:O	2.34	0.69
1:l:97:LYS:CA	1:z:133:ALA:CA	2.70	0.69
1:4:133:ALA:CA	1:p:97:LYS:CA	2.70	0.69
1:8:133:ALA:CA	1:D:97:LYS:CA	2.69	0.69
1:B:187:GLU:CA	1:J:452:GLY:HA2	2.23	0.69
1:N:452:GLY:HA2	1:v:187:GLU:CA	2.23	0.69
1:P:419:SER:CA	1:k:94:THR:H	2.00	0.69
1:V:60:VAL:H	1:m:36:ARG:CA	2.06	0.69
1:h:67:ALA:C	1:u:25:SER:O	2.24	0.69
1:d:19:GLY:HA3	1:q:73:SER:O	1.92	0.69
1:A:36:ARG:CA	1:Z:60:VAL:H	2.06	0.69
1:P:452:GLY:HA2	1:z:187:GLU:CA	2.23	0.69
1:l:19:GLY:HA3	1:y:73:SER:O	1.92	0.69
1:8:55:SER:H	1:C:38:TYR:CA	2.04	0.68
1:B:133:ALA:H	1:Z:97:LYS:CA	2.01	0.68
1:4:187:GLU:CA	1:T:452:GLY:HA2	2.23	0.68
1:AE:73:SER:O	1:x:19:GLY:HA3	1.92	0.68
1:c:38:TYR:CA	1:r:55:SER:H	2.04	0.68
1:h:19:GLY:HA3	1:u:73:SER:O	1.92	0.68
1:k:38:TYR:CA	1:z:55:SER:H	2.04	0.68
1:l:60:VAL:H	1:y:36:ARG:CA	2.06	0.68
1:R:67:ALA:CA	1:i:26:SER:O	2.29	0.68
1:V:97:LYS:C	1:n:133:ALA:N	2.52	0.68
1:h:60:VAL:H	1:u:36:ARG:CA	2.06	0.68
1:7:73:SER:O	1:D:19:GLY:HA3	1.92	0.68
1:8:133:ALA:H	1:D:97:LYS:CA	2.01	0.68
1:F:452:GLY:HA2	1:j:187:GLU:CA	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:73:SER:O	1:t:19:GLY:HA3	1.92	0.68
1:H:452:GLY:HA2	1:n:187:GLU:CA	2.23	0.68
1:V:97:LYS:CA	1:n:133:ALA:CA	2.70	0.68
1:d:97:LYS:C	1:r:133:ALA:N	2.52	0.68
1:3:36:ARG:CA	1:p:60:VAL:H	2.06	0.68
1:d:60:VAL:H	1:q:36:ARG:CA	2.06	0.68
1:3:25:SER:O	1:p:67:ALA:C	2.24	0.68
1:8:43:ALA:O	1:D:46:PRO:C	2.16	0.68
1:AE:81:GLN:CA	1:y:4:ARG:N	2.38	0.68
1:L:452:GLY:HA2	1:r:187:GLU:CA	2.23	0.68
1:V:67:ALA:CA	1:m:26:SER:O	2.30	0.68
1:h:97:LYS:CA	1:v:133:ALA:H	2.01	0.68
1:h:97:LYS:C	1:v:133:ALA:N	2.52	0.68
1:8:133:ALA:N	1:D:97:LYS:C	2.52	0.68
1:7:36:ARG:CA	1:D:60:VAL:H	2.06	0.68
1:4:133:ALA:N	1:p:97:LYS:C	2.52	0.67
1:B:43:ALA:O	1:Z:46:PRO:C	2.16	0.67
1:i:4:ARG:N	1:u:81:GLN:CA	2.38	0.67
1:l:97:LYS:CA	1:z:132:LEU:CA	2.73	0.67
1:AB:133:ALA:N	1:t:97:LYS:C	2.52	0.67
1:AE:72:SER:CA	1:z:1:MET:C	2.68	0.67
1:B:155:ARG:CA	1:Z:79:LEU:CA	2.73	0.67
1:h:97:LYS:CA	1:v:132:LEU:CA	2.73	0.67
1:j:1:MET:C	1:u:72:SER:CA	2.68	0.67
1:3:73:SER:O	1:p:19:GLY:HA3	1.92	0.67
1:4:155:ARG:CA	1:p:79:LEU:CA	2.73	0.67
1:8:155:ARG:CA	1:D:79:LEU:CA	2.73	0.67
1:B:133:ALA:N	1:Z:97:LYS:C	2.52	0.67
1:h:70:LEU:O	1:u:24:PRO:O	1.91	0.67
1:h:79:LEU:CA	1:v:155:ARG:CA	2.72	0.67
1:l:97:LYS:C	1:z:133:ALA:N	2.52	0.67
1:3:72:SER:CA	1:B:1:MET:C	2.68	0.67
1:A:26:SER:O	1:Z:67:ALA:CA	2.29	0.67
1:3:81:GLN:CA	1:A:4:ARG:N	2.38	0.67
1:V:79:LEU:CA	1:n:155:ARG:CA	2.73	0.67
1:l:79:LEU:CA	1:z:155:ARG:CA	2.72	0.67
1:AA:72:SER:CA	1:v:1:MET:C	2.68	0.67
1:N:451:ASP:O	1:v:190:GLN:C	2.38	0.67
1:8:132:LEU:CA	1:D:97:LYS:CA	2.73	0.66
1:7:36:ARG:N	1:D:60:VAL:CA	2.58	0.66
1:A:24:PRO:O	1:Z:70:LEU:O	1.91	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:CA	1:Z:97:LYS:CA	2.73	0.66
1:l:60:VAL:CA	1:y:36:ARG:N	2.58	0.66
1:l:67:ALA:C	1:y:25:SER:O	2.24	0.66
1:3:36:ARG:N	1:p:60:VAL:CA	2.58	0.66
1:7:72:SER:CA	1:r:1:MET:C	2.68	0.66
1:H:451:ASP:O	1:n:190:GLN:C	2.38	0.66
1:L:451:ASP:O	1:r:190:GLN:C	2.38	0.66
1:P:451:ASP:O	1:z:190:GLN:C	2.38	0.66
1:d:60:VAL:CA	1:q:36:ARG:N	2.58	0.66
1:4:132:LEU:CA	1:p:97:LYS:CA	2.73	0.66
1:V:60:VAL:CA	1:m:36:ARG:N	2.58	0.66
1:V:97:LYS:CA	1:n:132:LEU:CA	2.73	0.66
1:g:89:ALA:O	1:v:139:LYS:O	2.14	0.66
1:k:89:ALA:O	1:z:139:LYS:O	2.14	0.66
1:AB:133:ALA:H	1:t:97:LYS:CA	2.01	0.66
1:d:79:LEU:CA	1:r:155:ARG:CA	2.73	0.66
1:n:1:MET:C	1:y:72:SER:CA	2.68	0.66
1:B:55:SER:H	1:Y:38:TYR:CA	2.04	0.66
1:A:36:ARG:N	1:Z:60:VAL:CA	2.58	0.66
1:c:89:ALA:O	1:r:139:LYS:O	2.14	0.66
1:d:97:LYS:CA	1:r:132:LEU:CA	2.73	0.66
1:AB:132:LEU:CA	1:t:97:LYS:CA	2.73	0.66
1:B:190:GLN:C	1:J:451:ASP:O	2.38	0.66
1:8:139:LYS:O	1:C:89:ALA:O	2.14	0.66
1:AB:43:ALA:O	1:t:46:PRO:C	2.16	0.66
1:4:58:GLY:N	1:o:33:THR:O	2.29	0.65
1:4:139:LYS:O	1:o:89:ALA:O	2.14	0.65
1:B:139:LYS:O	1:Y:89:ALA:O	2.14	0.65
1:d:97:LYS:CA	1:r:133:ALA:H	2.01	0.65
1:h:46:PRO:C	1:v:43:ALA:O	2.16	0.65
1:M:454:VAL:H	1:v:183:MET:CA	2.10	0.65
1:O:454:VAL:H	1:z:183:MET:CA	2.10	0.65
1:U:89:ALA:O	1:n:139:LYS:O	2.14	0.65
1:V:67:ALA:C	1:m:25:SER:O	2.24	0.65
1:k:33:THR:O	1:z:58:GLY:N	2.30	0.65
1:4:183:MET:CA	1:S:454:VAL:H	2.10	0.65
1:4:190:GLN:C	1:T:451:ASP:O	2.38	0.65
1:F:451:ASP:O	1:j:190:GLN:C	2.38	0.65
1:R:67:ALA:C	1:i:25:SER:O	2.24	0.65
1:d:67:ALA:CA	1:q:26:SER:O	2.30	0.65
1:l:67:ALA:CA	1:y:26:SER:O	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:C	1:Y:67:ALA:N	2.41	0.65
1:h:67:ALA:CA	1:u:26:SER:O	2.29	0.65
1:AF:58:GLY:N	1:w:33:THR:O	2.29	0.65
1:K:454:VAL:H	1:r:183:MET:CA	2.10	0.65
1:4:137:GLN:H	1:p:93:ASN:C	2.05	0.65
1:AF:76:GLY:HA2	1:w:23:ARG:N	2.12	0.65
1:B:137:GLN:H	1:Z:93:ASN:C	2.05	0.65
1:B:183:MET:CA	1:I:454:VAL:H	2.10	0.65
1:d:93:ASN:C	1:r:137:GLN:H	2.05	0.65
1:g:23:ARG:N	1:v:76:GLY:HA2	2.12	0.64
1:k:23:ARG:N	1:z:76:GLY:HA2	2.12	0.64
1:s:261:SER:O	1:s:262:LYS:N	0.76	0.64
1:c:23:ARG:N	1:r:76:GLY:HA2	2.12	0.64
1:h:60:VAL:CA	1:u:36:ARG:N	2.58	0.64
1:8:76:GLY:HA2	1:C:23:ARG:N	2.12	0.64
1:8:137:GLN:H	1:D:93:ASN:C	2.05	0.64
1:AB:76:GLY:HA2	1:s:23:ARG:N	2.12	0.64
1:E:454:VAL:H	1:j:183:MET:CA	2.10	0.64
1:V:70:LEU:O	1:m:24:PRO:O	1.91	0.64
1:k:17:GLY:CA	1:z:72:SER:O	2.38	0.64
1:4:76:GLY:HA2	1:o:23:ARG:N	2.12	0.64
1:G:454:VAL:H	1:n:183:MET:CA	2.10	0.64
1:8:58:GLY:N	1:C:33:THR:O	2.29	0.64
1:U:52:LEU:N	1:n:42:SER:C	2.55	0.64
1:V:93:ASN:C	1:n:137:GLN:H	2.05	0.64
1:d:46:PRO:C	1:r:43:ALA:O	2.16	0.64
1:g:33:THR:O	1:v:58:GLY:N	2.29	0.64
1:AB:58:GLY:N	1:s:33:THR:O	2.29	0.64
1:C:261:SER:O	1:C:262:LYS:N	0.76	0.64
1:8:26:SER:C	1:C:67:ALA:N	2.41	0.64
1:U:67:ALA:N	1:n:26:SER:C	2.41	0.63
1:AC:261:SER:O	1:AC:262:LYS:N	0.76	0.63
1:c:33:THR:O	1:r:58:GLY:N	2.29	0.63
1:T:419:SER:CA	1:o:93:ASN:C	2.70	0.63
1:h:93:ASN:C	1:v:137:GLN:H	2.05	0.63
1:l:93:ASN:C	1:z:137:GLN:H	2.05	0.63
1:H:419:SER:CA	1:U:93:ASN:C	2.70	0.63
1:l:8:SER:O	1:4:11:TYR:CA	2.47	0.63
1:9:261:SER:O	1:9:262:LYS:N	0.76	0.63
1:C:93:ASN:C	1:X:419:SER:CA	2.70	0.63
1:i:253:HIS:CA	1:z:103:GLU:H	2.07	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:SER:O	1:r:11:TYR:CA	2.47	0.63
1:k:8:SER:O	1:n:11:TYR:CA	2.47	0.63
1:l:97:LYS:O	1:z:129:LYS:C	2.42	0.63
1:s:8:SER:C	1:v:12:ARG:CA	2.72	0.63
1:C:8:SER:C	1:r:12:ARG:CA	2.72	0.63
1:s:8:SER:O	1:v:11:TYR:CA	2.47	0.62
1:4:26:SER:C	1:o:67:ALA:N	2.41	0.62
1:J:419:SER:CA	1:Y:93:ASN:C	2.70	0.62
1:O:454:VAL:O	1:z:184:ARG:CA	2.47	0.62
1:V:97:LYS:O	1:n:129:LYS:C	2.42	0.62
1:g:8:SER:C	1:j:12:ARG:CA	2.72	0.62
1:4:43:ALA:O	1:p:46:PRO:C	2.16	0.62
1:4:184:ARG:CA	1:S:454:VAL:O	2.47	0.62
1:8:26:SER:O	1:C:66:SER:CA	2.47	0.62
1:G:454:VAL:O	1:n:184:ARG:CA	2.47	0.62
1:K:454:VAL:O	1:r:184:ARG:CA	2.47	0.62
1:m:4:ARG:N	1:y:81:GLN:CA	2.38	0.62
1:7:77:VAL:H	1:r:3:THR:CA	2.12	0.62
1:AE:77:VAL:H	1:z:3:THR:CA	2.12	0.62
1:E:454:VAL:O	1:j:184:ARG:CA	2.47	0.62
1:g:8:SER:O	1:j:11:TYR:CA	2.47	0.62
1:j:3:THR:CA	1:u:77:VAL:H	2.12	0.62
1:k:66:SER:CA	1:z:26:SER:O	2.47	0.62
1:l:97:LYS:C	1:z:129:LYS:O	2.43	0.62
1:B:26:SER:O	1:Y:66:SER:CA	2.47	0.62
1:4:26:SER:O	1:o:66:SER:CA	2.48	0.62
1:7:40:LEU:CA	1:D:52:LEU:O	2.48	0.62
1:8:72:SER:O	1:C:17:GLY:CA	2.38	0.62
1:h:97:LYS:O	1:v:129:LYS:C	2.42	0.62
1:k:47:SER:C	1:z:46:PRO:C	2.68	0.62
1:w:8:SER:O	1:z:11:TYR:CA	2.47	0.62
1:8:129:LYS:C	1:D:97:LYS:O	2.42	0.62
1:B:46:PRO:C	1:Y:47:SER:C	2.68	0.62
1:V:52:LEU:O	1:m:40:LEU:CA	2.48	0.62
1:V:97:LYS:C	1:n:129:LYS:O	2.42	0.62
1:A:40:LEU:CA	1:Z:52:LEU:O	2.48	0.62
1:U:66:SER:CA	1:n:26:SER:O	2.47	0.62
1:h:52:LEU:O	1:u:40:LEU:CA	2.48	0.62
1:k:8:SER:C	1:n:12:ARG:CA	2.72	0.62
1:w:8:SER:C	1:z:12:ARG:CA	2.72	0.62
1:B:12:ARG:CA	1:o:8:SER:C	2.72	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:CA	1:I:454:VAL:O	2.47	0.61
1:M:454:VAL:O	1:v:184:ARG:CA	2.47	0.61
1:l:52:LEU:O	1:y:40:LEU:CA	2.48	0.61
1:1:8:SER:C	1:4:12:ARG:CA	2.72	0.61
1:3:77:VAL:H	1:B:3:THR:CA	2.12	0.61
1:4:46:PRO:C	1:o:47:SER:C	2.68	0.61
1:4:129:LYS:C	1:p:97:LYS:O	2.42	0.61
1:B:11:TYR:CA	1:o:8:SER:O	2.47	0.61
1:d:52:LEU:O	1:q:40:LEU:CA	2.48	0.61
1:g:47:SER:C	1:v:46:PRO:C	2.68	0.61
1:l:43:ALA:CA	1:y:52:LEU:N	2.63	0.61
1:3:72:SER:N	1:B:1:MET:C	2.57	0.61
1:c:66:SER:CA	1:r:26:SER:O	2.47	0.61
1:AB:46:PRO:C	1:s:47:SER:C	2.68	0.61
1:Q:67:ALA:N	1:j:26:SER:C	2.41	0.61
1:3:52:LEU:N	1:p:43:ALA:CA	2.63	0.61
1:AA:40:LEU:CA	1:t:52:LEU:O	2.48	0.61
1:c:47:SER:C	1:r:46:PRO:C	2.68	0.61
1:n:3:THR:CA	1:y:77:VAL:H	2.12	0.61
1:P:419:SER:N	1:k:93:ASN:O	2.32	0.61
1:g:66:SER:CA	1:v:26:SER:O	2.48	0.61
1:h:43:ALA:CA	1:u:52:LEU:N	2.63	0.61
1:8:46:PRO:C	1:C:47:SER:C	2.68	0.61
1:AF:103:GLU:H	1:u:253:HIS:CA	2.07	0.61
1:L:419:SER:N	1:c:93:ASN:O	2.32	0.61
1:N:418:PHE:N	1:g:93:ASN:O	2.33	0.61
1:3:40:LEU:CA	1:p:52:LEU:O	2.48	0.61
1:a:253:HIS:CA	1:r:103:GLU:H	2.07	0.61
1:d:43:ALA:CA	1:q:52:LEU:N	2.63	0.61
1:j:1:MET:C	1:u:72:SER:N	2.57	0.61
1:4:129:LYS:O	1:p:97:LYS:C	2.43	0.61
1:b:418:PHE:N	1:s:93:ASN:O	2.33	0.61
1:AA:52:LEU:N	1:t:43:ALA:CA	2.63	0.61
1:AA:77:VAL:H	1:v:3:THR:CA	2.12	0.61
1:AB:129:LYS:C	1:t:97:LYS:O	2.42	0.61
1:H:418:PHE:N	1:U:93:ASN:O	2.33	0.61
1:J:419:SER:N	1:Y:93:ASN:O	2.32	0.61
1:1:261:SER:O	1:1:262:LYS:N	0.76	0.60
1:A:52:LEU:N	1:Z:43:ALA:CA	2.63	0.60
1:B:129:LYS:C	1:Z:97:LYS:O	2.42	0.60
1:P:418:PHE:N	1:k:93:ASN:O	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:97:LYS:C	1:v:129:LYS:O	2.43	0.60
1:AA:81:GLN:H	1:u:4:ARG:H	0.85	0.60
1:C:93:ASN:O	1:X:418:PHE:N	2.33	0.60
1:T:419:SER:N	1:o:93:ASN:O	2.32	0.60
1:d:19:GLY:CA	1:q:73:SER:O	2.50	0.60
1:w:261:SER:O	1:w:262:LYS:N	0.76	0.60
1:AA:73:SER:O	1:t:19:GLY:CA	2.50	0.60
1:b:419:SER:CA	1:s:93:ASN:C	2.70	0.60
1:7:52:LEU:N	1:D:43:ALA:CA	2.63	0.60
1:k:67:ALA:N	1:z:26:SER:C	2.41	0.60
1:5:261:SER:O	1:5:262:LYS:N	0.76	0.60
1:AB:103:GLU:H	1:q:253:HIS:CA	2.07	0.60
1:d:97:LYS:O	1:r:129:LYS:C	2.42	0.60
1:AE:72:SER:N	1:z:1:MET:C	2.57	0.60
1:L:419:SER:CA	1:c:93:ASN:C	2.70	0.60
1:8:129:LYS:O	1:D:97:LYS:C	2.43	0.60
1:c:68:VAL:C	1:r:25:SER:N	2.58	0.60
1:c:45:ARG:O	1:r:48:THR:CA	2.49	0.60
1:d:97:LYS:C	1:r:129:LYS:O	2.43	0.60
1:H:419:SER:N	1:U:93:ASN:O	2.32	0.59
1:U:52:LEU:N	1:n:42:SER:CA	2.65	0.59
1:e:253:HIS:CA	1:v:103:GLU:H	2.07	0.59
1:3:31:VAL:CA	1:o:66:SER:O	2.50	0.59
1:5:248:GLN:H	1:p:95:GLU:C	2.10	0.59
1:7:31:VAL:CA	1:C:66:SER:O	2.50	0.59
1:8:103:GLU:H	1:A:253:HIS:CA	2.07	0.59
1:A:31:VAL:CA	1:Y:66:SER:O	2.50	0.59
1:AB:48:THR:CA	1:s:45:ARG:O	2.49	0.59
1:V:95:GLU:C	1:o:248:GLN:H	2.11	0.59
1:h:19:GLY:CA	1:u:73:SER:O	2.50	0.59
1:h:45:ARG:O	1:u:49:SER:N	2.34	0.59
1:k:52:LEU:N	1:z:42:SER:CA	2.65	0.59
1:7:73:SER:O	1:D:19:GLY:CA	2.50	0.59
1:g:68:VAL:C	1:v:25:SER:N	2.58	0.59
1:7:49:SER:N	1:D:45:ARG:O	2.34	0.59
1:AE:73:SER:O	1:x:19:GLY:CA	2.49	0.59
1:U:66:SER:O	1:m:31:VAL:CA	2.50	0.59
1:B:42:SER:CA	1:Y:52:LEU:N	2.65	0.59
1:1:263:PRO:O	1:AJ:412:SER:CA	2.51	0.59
1:7:26:SER:C	1:D:67:ALA:C	2.65	0.59
1:8:25:SER:N	1:C:68:VAL:C	2.58	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:42:SER:CA	1:C:52:LEU:N	2.65	0.59
1:A:49:SER:N	1:Z:45:ARG:O	2.34	0.59
1:c:66:SER:O	1:q:31:VAL:CA	2.51	0.59
1:k:66:SER:O	1:y:31:VAL:CA	2.51	0.59
1:AB:72:SER:O	1:s:17:GLY:CA	2.38	0.59
1:AC:263:PRO:O	1:AP:412:SER:CA	2.51	0.59
1:AD:412:SER:CA	1:s:263:PRO:O	2.51	0.59
1:AH:412:SER:CA	1:w:263:PRO:O	2.51	0.59
1:B:103:GLU:H	1:W:253:HIS:CA	2.07	0.59
1:c:33:THR:C	1:r:57:PRO:C	2.70	0.59
1:g:45:ARG:O	1:v:48:THR:CA	2.49	0.59
1:g:66:SER:O	1:u:31:VAL:CA	2.50	0.59
1:k:68:VAL:C	1:z:25:SER:N	2.59	0.59
1:d:45:ARG:O	1:q:49:SER:N	2.34	0.59
1:3:73:SER:O	1:p:19:GLY:CA	2.50	0.58
1:9:263:PRO:O	1:AN:412:SER:CA	2.51	0.58
1:AB:129:LYS:O	1:t:97:LYS:C	2.43	0.58
1:B:48:THR:CA	1:Y:45:ARG:O	2.49	0.58
1:B:129:LYS:O	1:Z:97:LYS:C	2.43	0.58
1:g:52:LEU:N	1:v:42:SER:CA	2.65	0.58
1:l:19:GLY:CA	1:y:73:SER:O	2.50	0.58
1:AA:49:SER:N	1:t:45:ARG:O	2.34	0.58
1:4:72:SER:O	1:o:17:GLY:CA	2.38	0.58
1:AA:77:VAL:N	1:v:3:THR:CA	2.67	0.58
1:U:68:VAL:C	1:n:25:SER:N	2.58	0.58
1:g:52:LEU:N	1:v:42:SER:C	2.55	0.58
1:l:45:ARG:O	1:y:49:SER:N	2.34	0.58
1:5:263:PRO:O	1:AL:412:SER:CA	2.51	0.58
1:7:72:SER:N	1:r:1:MET:C	2.57	0.58
1:T:418:PHE:N	1:o:93:ASN:O	2.33	0.58
1:c:17:GLY:CA	1:r:72:SER:O	2.38	0.58
1:n:3:THR:CA	1:y:77:VAL:N	2.67	0.58
1:4:57:PRO:C	1:o:33:THR:C	2.70	0.58
1:g:67:ALA:N	1:v:26:SER:C	2.41	0.58
1:0:412:SER:CA	1:C:263:PRO:O	2.51	0.58
1:d:95:GLU:C	1:s:248:GLN:H	2.11	0.58
1:8:48:THR:CA	1:C:45:ARG:O	2.49	0.58
1:9:248:GLN:H	1:D:95:GLU:C	2.11	0.58
1:4:42:SER:CA	1:o:52:LEU:N	2.65	0.58
1:3:49:SER:N	1:p:45:ARG:O	2.34	0.57
1:C:248:GLN:H	1:Z:95:GLU:C	2.11	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:71:ARG:O	1:i:23:ARG:CA	2.52	0.57
1:l:71:ARG:O	1:y:23:ARG:CA	2.52	0.57
1:4:48:THR:CA	1:o:45:ARG:O	2.49	0.57
1:AC:248:GLN:H	1:t:95:GLU:C	2.11	0.57
1:AF:76:GLY:H	1:w:20:THR:C	1.99	0.57
1:g:33:THR:C	1:v:57:PRO:C	2.70	0.57
1:9:261:SER:CA	1:9:262:LYS:CA	2.79	0.57
1:k:33:THR:C	1:z:57:PRO:C	2.70	0.57
1:k:45:ARG:O	1:z:48:THR:CA	2.49	0.57
1:3:77:VAL:N	1:B:3:THR:CA	2.67	0.57
1:N:419:SER:CA	1:g:93:ASN:C	2.70	0.57
1:d:57:PRO:C	1:q:36:ARG:CA	2.70	0.57
1:j:3:THR:CA	1:u:77:VAL:N	2.67	0.57
1:n:1:MET:C	1:y:72:SER:N	2.57	0.57
1:AF:54:ALA:CA	1:w:37:THR:CA	2.83	0.57
1:d:71:ARG:O	1:q:23:ARG:CA	2.52	0.57
1:l:46:PRO:C	1:z:43:ALA:O	2.16	0.57
1:8:103:GLU:C	1:A:252:GLN:C	2.73	0.57
1:AB:54:ALA:CA	1:s:37:THR:CA	2.83	0.57
1:g:37:THR:CA	1:v:54:ALA:CA	2.83	0.57
1:8:57:PRO:C	1:C:33:THR:C	2.70	0.57
1:AB:76:GLY:HA3	1:s:23:ARG:H	1.70	0.57
1:AF:57:PRO:C	1:w:33:THR:C	2.70	0.57
1:L:418:PHE:N	1:c:93:ASN:O	2.33	0.57
1:a:252:GLN:C	1:r:103:GLU:C	2.73	0.57
1:c:52:LEU:N	1:r:42:SER:CA	2.65	0.57
1:3:23:ARG:CA	1:p:71:ARG:O	2.52	0.57
1:AB:42:SER:CA	1:s:52:LEU:N	2.65	0.56
1:AB:57:PRO:C	1:s:33:THR:C	2.70	0.56
1:V:71:ARG:O	1:m:23:ARG:CA	2.52	0.56
1:d:57:PRO:N	1:q:37:THR:N	2.52	0.56
1:k:52:LEU:N	1:z:42:SER:C	2.55	0.56
1:B:54:ALA:CA	1:Y:37:THR:CA	2.83	0.56
1:P:419:SER:CA	1:k:93:ASN:C	2.70	0.56
1:3:37:THR:N	1:p:57:PRO:N	2.52	0.56
1:8:57:PRO:N	1:C:34:SER:O	2.39	0.56
1:8:133:ALA:O	1:D:93:ASN:O	2.24	0.56
1:AB:103:GLU:C	1:q:252:GLN:C	2.73	0.56
1:B:103:GLU:C	1:W:252:GLN:C	2.73	0.56
1:c:34:SER:O	1:r:57:PRO:N	2.39	0.56
1:h:93:ASN:O	1:v:133:ALA:O	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:261:SER:CA	1:s:262:LYS:CA	2.79	0.56
1:4:103:GLU:C	1:m:252:GLN:C	2.73	0.56
1:7:77:VAL:N	1:r:3:THR:CA	2.67	0.56
1:g:31:VAL:C	1:v:60:VAL:CA	2.79	0.56
1:AF:60:VAL:CA	1:w:31:VAL:C	2.79	0.56
1:B:133:ALA:O	1:Z:93:ASN:O	2.24	0.56
1:J:418:PHE:N	1:Y:93:ASN:O	2.33	0.56
1:V:93:ASN:O	1:n:133:ALA:O	2.24	0.56
1:4:133:ALA:O	1:p:93:ASN:O	2.24	0.56
1:c:37:THR:CA	1:r:54:ALA:CA	2.83	0.56
1:l:93:ASN:O	1:z:133:ALA:O	2.24	0.56
1:l:94:THR:CA	1:z:133:ALA:O	2.54	0.56
1:A:23:ARG:CA	1:Z:71:ARG:O	2.52	0.56
1:d:93:ASN:O	1:r:133:ALA:O	2.24	0.56
1:h:71:ARG:O	1:u:23:ARG:CA	2.52	0.56
1:h:94:THR:CA	1:v:133:ALA:O	2.54	0.56
1:k:37:THR:CA	1:z:54:ALA:CA	2.83	0.56
1:4:54:ALA:CA	1:o:37:THR:CA	2.83	0.56
1:4:57:PRO:N	1:o:34:SER:O	2.39	0.56
1:8:54:ALA:CA	1:C:37:THR:CA	2.83	0.56
1:e:252:GLN:C	1:v:103:GLU:C	2.73	0.56
1:k:31:VAL:C	1:z:60:VAL:CA	2.79	0.56
1:V:94:THR:CA	1:n:133:ALA:O	2.54	0.56
1:d:67:ALA:C	1:q:26:SER:C	2.65	0.56
1:AF:103:GLU:C	1:u:252:GLN:C	2.73	0.56
1:c:31:VAL:C	1:r:60:VAL:CA	2.79	0.56
1:4:25:SER:N	1:o:68:VAL:C	2.59	0.55
1:4:133:ALA:O	1:p:94:THR:CA	2.54	0.55
1:8:42:SER:C	1:C:52:LEU:N	2.55	0.55
1:AB:60:VAL:CA	1:s:31:VAL:C	2.79	0.55
1:AB:133:ALA:O	1:t:94:THR:CA	2.54	0.55
1:AE:71:ARG:C	1:z:1:MET:H3	2.14	0.55
1:b:419:SER:N	1:s:93:ASN:O	2.32	0.55
1:i:252:GLN:C	1:z:103:GLU:C	2.73	0.55
1:A:37:THR:N	1:Z:57:PRO:N	2.52	0.55
1:AB:42:SER:C	1:s:52:LEU:N	2.55	0.55
1:AE:80:LEU:C	1:y:4:ARG:H	2.10	0.55
1:AF:72:SER:O	1:w:17:GLY:CA	2.38	0.55
1:4:76:GLY:HA3	1:o:23:ARG:H	1.70	0.55
1:7:36:ARG:CA	1:D:57:PRO:C	2.70	0.55
1:B:133:ALA:O	1:Z:94:THR:CA	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:94:THR:CA	1:r:133:ALA:O	2.54	0.55
1:3:80:LEU:C	1:A:4:ARG:H	2.10	0.55
1:A:37:THR:CA	1:Z:57:PRO:N	2.70	0.55
1:AF:73:SER:O	1:x:15:PHE:CA	2.55	0.55
1:h:57:PRO:N	1:u:37:THR:N	2.52	0.55
1:4:60:VAL:CA	1:o:31:VAL:C	2.79	0.55
1:7:37:THR:CA	1:D:57:PRO:N	2.70	0.55
1:8:133:ALA:O	1:D:94:THR:CA	2.54	0.55
1:c:20:THR:C	1:r:76:GLY:H	1.99	0.55
1:h:15:PHE:CA	1:v:73:SER:O	2.55	0.55
1:AF:76:GLY:HA3	1:w:23:ARG:H	1.70	0.55
1:4:42:SER:C	1:o:52:LEU:N	2.55	0.55
1:k:23:ARG:H	1:z:76:GLY:HA3	1.70	0.55
1:AB:73:SER:O	1:t:15:PHE:CA	2.55	0.55
1:c:52:LEU:N	1:r:42:SER:C	2.55	0.55
1:w:261:SER:CA	1:w:262:LYS:CA	2.79	0.55
1:AB:76:GLY:H	1:s:20:THR:C	1.99	0.55
1:1:261:SER:CA	1:1:262:LYS:CA	2.79	0.54
1:C:11:TYR:O	1:r:6:VAL:CA	2.55	0.54
1:h:57:PRO:N	1:u:37:THR:CA	2.70	0.54
1:3:37:THR:CA	1:p:57:PRO:N	2.70	0.54
1:B:42:SER:C	1:Y:52:LEU:N	2.55	0.54
1:c:23:ARG:H	1:r:76:GLY:HA3	1.70	0.54
1:d:15:PHE:CA	1:r:73:SER:O	2.55	0.54
1:l:15:PHE:CA	1:z:73:SER:O	2.55	0.54
1:3:141:GLN:O	1:p:85:ASP:CA	2.56	0.54
1:4:129:LYS:CA	1:p:100:ARG:C	2.81	0.54
1:A:141:GLN:O	1:Z:85:ASP:CA	2.56	0.54
1:h:45:ARG:CA	1:u:49:SER:CA	2.86	0.54
1:l:100:ARG:C	1:z:129:LYS:CA	2.81	0.54
1:7:141:GLN:O	1:D:85:ASP:CA	2.56	0.54
1:V:85:ASP:CA	1:m:141:GLN:O	2.56	0.54
1:d:99:THR:CA	1:s:251:GLU:N	2.71	0.54
1:3:49:SER:CA	1:p:45:ARG:CA	2.86	0.54
1:4:73:SER:O	1:p:15:PHE:CA	2.55	0.54
1:8:60:VAL:CA	1:C:31:VAL:C	2.79	0.54
1:V:100:ARG:C	1:n:129:LYS:CA	2.81	0.54
1:d:19:GLY:C	1:q:73:SER:CA	2.81	0.54
1:h:95:GLU:C	1:w:248:GLN:H	2.11	0.54
1:AC:251:GLU:N	1:t:99:THR:CA	2.71	0.54
1:N:419:SER:N	1:g:93:ASN:O	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:73:SER:O	1:D:15:PHE:CA	2.55	0.54
1:h:99:THR:CA	1:w:251:GLU:N	2.71	0.54
1:k:11:TYR:O	1:n:6:VAL:CA	2.55	0.54
1:k:34:SER:O	1:z:57:PRO:N	2.39	0.54
1:l:57:PRO:N	1:y:37:THR:N	2.52	0.54
1:9:251:GLU:N	1:D:99:THR:CA	2.71	0.54
1:V:57:PRO:N	1:m:37:THR:CA	2.70	0.54
1:d:57:PRO:N	1:q:37:THR:CA	2.70	0.54
1:l:57:PRO:N	1:y:37:THR:CA	2.70	0.54
1:8:129:LYS:CA	1:D:100:ARG:C	2.81	0.54
1:AA:49:SER:CA	1:t:45:ARG:CA	2.86	0.54
1:B:25:SER:N	1:Y:68:VAL:C	2.58	0.54
1:C:251:GLU:N	1:Z:99:THR:CA	2.71	0.54
1:AF:57:PRO:N	1:w:34:SER:O	2.39	0.54
1:B:129:LYS:CA	1:Z:100:ARG:C	2.81	0.54
1:h:85:ASP:CA	1:u:141:GLN:O	2.56	0.54
1:l:67:ALA:C	1:y:26:SER:C	2.65	0.54
1:l:85:ASP:CA	1:y:141:GLN:O	2.56	0.54
1:1:11:TYR:O	1:4:6:VAL:CA	2.55	0.53
1:7:49:SER:CA	1:D:45:ARG:CA	2.86	0.53
1:AB:133:ALA:H	1:t:97:LYS:C	2.16	0.53
1:V:57:PRO:N	1:m:37:THR:N	2.52	0.53
1:l:19:GLY:C	1:y:73:SER:CA	2.81	0.53
1:l:45:ARG:CA	1:y:49:SER:CA	2.86	0.53
1:s:11:TYR:O	1:v:6:VAL:CA	2.55	0.53
1:5:261:SER:CA	1:5:262:LYS:CA	2.79	0.53
1:7:73:SER:CA	1:D:19:GLY:C	2.81	0.53
1:8:76:GLY:HA3	1:C:23:ARG:H	1.70	0.53
1:AA:82:ASP:N	1:u:2:SER:O	2.31	0.53
1:g:11:TYR:O	1:j:6:VAL:CA	2.55	0.53
1:g:17:GLY:CA	1:v:72:SER:O	2.38	0.53
1:1:248:GLN:H	1:l:95:GLU:C	2.11	0.53
1:A:49:SER:CA	1:Z:45:ARG:CA	2.86	0.53
1:AA:72:SER:N	1:v:1:MET:C	2.57	0.53
1:C:261:SER:CA	1:C:262:LYS:CA	2.79	0.53
1:4:133:ALA:H	1:p:97:LYS:C	2.16	0.53
1:7:82:ASP:N	1:q:2:SER:O	2.31	0.53
1:R:67:ALA:C	1:i:26:SER:C	2.65	0.53
1:d:85:ASP:CA	1:q:141:GLN:O	2.56	0.53
1:3:73:SER:CA	1:p:19:GLY:C	2.81	0.53
1:7:37:THR:N	1:D:57:PRO:N	2.52	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:45:ARG:CA	1:q:49:SER:CA	2.86	0.53
1:g:23:ARG:H	1:v:76:GLY:HA3	1.70	0.53
1:V:67:ALA:C	1:m:26:SER:C	2.65	0.53
1:4:103:GLU:H	1:m:253:HIS:CA	2.07	0.53
1:5:251:GLU:N	1:p:99:THR:CA	2.71	0.53
1:8:56:SER:CA	1:C:36:ARG:N	2.72	0.53
1:AA:73:SER:CA	1:t:19:GLY:C	2.81	0.53
1:AE:73:SER:CA	1:x:19:GLY:C	2.81	0.53
1:V:57:PRO:C	1:m:36:ARG:CA	2.70	0.53
1:h:97:LYS:C	1:v:133:ALA:H	2.16	0.53
1:w:11:TYR:O	1:z:6:VAL:CA	2.55	0.53
1:3:32:THR:H	1:o:66:SER:C	2.17	0.52
1:3:71:ARG:C	1:B:1:MET:H3	2.17	0.52
1:AC:261:SER:CA	1:AC:262:LYS:CA	2.79	0.52
1:B:54:ALA:C	1:Y:37:THR:C	2.74	0.52
1:U:66:SER:C	1:m:32:THR:H	2.17	0.52
1:4:42:SER:CA	1:o:52:LEU:CA	2.88	0.52
1:4:76:GLY:H	1:o:20:THR:C	1.99	0.52
1:B:56:SER:CA	1:Y:36:ARG:N	2.72	0.52
1:C:93:ASN:O	1:X:419:SER:N	2.32	0.52
1:U:52:LEU:CA	1:n:42:SER:CA	2.88	0.52
1:V:99:THR:CA	1:o:251:GLU:N	2.71	0.52
1:g:39:SER:O	1:v:53:TYR:CA	2.57	0.52
1:h:19:GLY:C	1:u:73:SER:CA	2.81	0.52
1:k:36:ARG:N	1:z:56:SER:CA	2.72	0.52
1:l:97:LYS:C	1:z:133:ALA:H	2.16	0.52
1:3:26:SER:C	1:p:67:ALA:C	2.65	0.52
1:7:32:THR:H	1:C:66:SER:C	2.17	0.52
1:AB:129:LYS:CA	1:t:100:ARG:C	2.81	0.52
1:s:11:TYR:C	1:v:7:SER:C	2.77	0.52
1:8:53:TYR:CA	1:C:39:SER:O	2.57	0.52
1:C:11:TYR:C	1:r:7:SER:C	2.77	0.52
1:g:52:LEU:CA	1:v:42:SER:CA	2.88	0.52
1:k:52:LEU:CA	1:z:42:SER:CA	2.88	0.52
1:m:4:ARG:H	1:y:80:LEU:C	2.10	0.52
1:o:30:TYR:CA	1:y:52:LEU:O	2.58	0.52
1:1:346:GLU:O	1:i:176:ASP:O	2.28	0.52
1:3:52:LEU:O	1:C:30:TYR:CA	2.58	0.52
1:9:346:GLU:O	1:A:176:ASP:O	2.28	0.52
1:AA:52:LEU:O	1:w:30:TYR:CA	2.58	0.52
1:AB:57:PRO:N	1:s:34:SER:O	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:52:LEU:CA	1:r:42:SER:CA	2.88	0.52
1:l:251:GLU:N	1:l:99:THR:CA	2.71	0.52
1:4:56:SER:CA	1:o:36:ARG:N	2.72	0.52
1:AB:42:SER:CA	1:s:52:LEU:CA	2.88	0.52
1:c:36:ARG:N	1:r:56:SER:CA	2.72	0.52
1:c:66:SER:C	1:q:32:THR:H	2.17	0.52
1:k:30:TYR:CA	1:u:52:LEU:O	2.58	0.52
1:8:42:SER:CA	1:C:52:LEU:CA	2.88	0.52
1:AB:56:SER:CA	1:s:36:ARG:N	2.72	0.52
1:AI:346:GLU:O	1:y:176:ASP:O	2.28	0.52
1:d:100:ARG:C	1:r:129:LYS:CA	2.81	0.52
1:g:34:SER:O	1:v:57:PRO:N	2.39	0.52
1:3:36:ARG:CA	1:p:57:PRO:C	2.70	0.52
1:B:42:SER:CA	1:Y:52:LEU:CA	2.88	0.52
1:k:11:TYR:C	1:n:7:SER:C	2.77	0.52
1:g:30:TYR:CA	1:q:52:LEU:O	2.58	0.52
1:1:11:TYR:C	1:4:7:SER:C	2.77	0.52
1:3:176:ASP:O	1:AK:346:GLU:O	2.28	0.52
1:7:52:LEU:O	1:s:30:TYR:CA	2.58	0.52
1:AF:56:SER:CA	1:w:36:ARG:N	2.72	0.52
1:B:103:GLU:CA	1:W:252:GLN:C	2.82	0.52
1:4:53:TYR:CA	1:o:39:SER:O	2.57	0.51
1:8:26:SER:O	1:C:66:SER:N	2.44	0.51
1:AB:53:TYR:CA	1:s:39:SER:O	2.57	0.51
1:c:39:SER:O	1:r:53:TYR:CA	2.57	0.51
1:g:36:ARG:N	1:v:56:SER:CA	2.72	0.51
1:AC:346:GLU:O	1:q:176:ASP:O	2.28	0.51
1:B:53:TYR:CA	1:Y:39:SER:O	2.57	0.51
1:Q:68:VAL:C	1:j:25:SER:N	2.58	0.51
1:k:66:SER:C	1:y:32:THR:H	2.17	0.51
1:1:244:GLU:O	1:l:95:GLU:C	2.54	0.51
1:4:26:SER:O	1:o:66:SER:N	2.44	0.51
1:5:244:GLU:O	1:p:95:GLU:C	2.54	0.51
1:B:6:VAL:CA	1:o:11:TYR:O	2.55	0.51
1:8:103:GLU:CA	1:A:252:GLN:C	2.82	0.51
1:A:52:LEU:O	1:c:30:TYR:CA	2.58	0.51
1:AF:53:TYR:CA	1:w:39:SER:O	2.57	0.51
1:B:26:SER:O	1:Y:66:SER:N	2.44	0.51
1:g:66:SER:N	1:v:26:SER:O	2.44	0.51
1:7:80:LEU:C	1:q:4:ARG:H	2.10	0.51
1:AE:77:VAL:N	1:z:3:THR:CA	2.67	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:95:GLU:C	1:o:244:GLU:O	2.54	0.51
1:c:66:SER:N	1:r:26:SER:O	2.44	0.51
1:l:57:PRO:C	1:y:36:ARG:CA	2.70	0.51
1:8:161:VAL:CA	1:C:79:LEU:H	2.24	0.51
1:A:32:THR:H	1:Y:66:SER:C	2.17	0.51
1:AB:46:PRO:C	1:s:49:SER:C	2.49	0.51
1:g:79:LEU:H	1:v:161:VAL:CA	2.24	0.51
1:h:95:GLU:C	1:w:244:GLU:O	2.54	0.51
1:k:66:SER:N	1:z:26:SER:O	2.44	0.51
1:Q:79:LEU:H	1:j:161:VAL:CA	2.24	0.51
1:g:66:SER:C	1:u:32:THR:H	2.17	0.51
1:4:161:VAL:CA	1:o:79:LEU:H	2.24	0.51
1:h:100:ARG:C	1:v:129:LYS:CA	2.81	0.51
1:8:76:GLY:H	1:C:20:THR:C	1.99	0.51
1:A:30:TYR:C	1:Y:66:SER:O	2.50	0.51
1:B:7:SER:C	1:o:11:TYR:C	2.77	0.51
1:5:346:GLU:O	1:m:176:ASP:O	2.28	0.51
1:A:36:ARG:CA	1:Z:57:PRO:C	2.70	0.51
1:C:244:GLU:O	1:Z:95:GLU:C	2.54	0.51
1:U:66:SER:N	1:n:26:SER:O	2.44	0.51
1:c:79:LEU:H	1:r:161:VAL:CA	2.24	0.51
1:d:97:LYS:C	1:r:133:ALA:H	2.16	0.51
1:g:11:TYR:C	1:j:7:SER:C	2.77	0.51
1:w:11:TYR:C	1:z:7:SER:C	2.77	0.51
1:9:244:GLU:O	1:D:95:GLU:C	2.54	0.50
1:AC:244:GLU:O	1:t:95:GLU:C	2.54	0.50
1:B:133:ALA:H	1:Z:97:LYS:C	2.16	0.50
1:V:97:LYS:C	1:n:133:ALA:H	2.16	0.50
1:d:108:GLN:N	1:r:121:VAL:O	2.40	0.50
1:k:28:ARG:O	1:u:54:ALA:N	2.45	0.50
1:k:79:LEU:H	1:z:161:VAL:CA	2.24	0.50
1:k:39:SER:O	1:z:53:TYR:CA	2.57	0.50
1:3:54:ALA:N	1:C:28:ARG:O	2.44	0.50
1:8:133:ALA:H	1:D:97:LYS:C	2.16	0.50
1:AF:54:ALA:C	1:w:37:THR:C	2.75	0.50
1:d:95:GLU:C	1:s:244:GLU:O	2.54	0.50
1:i:4:ARG:H	1:u:80:LEU:C	2.10	0.50
1:o:28:ARG:O	1:y:54:ALA:N	2.45	0.50
1:AG:346:GLU:O	1:u:176:ASP:O	2.28	0.50
1:c:67:ALA:N	1:r:26:SER:C	2.41	0.50
1:g:28:ARG:O	1:q:54:ALA:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:N	1:c:28:ARG:O	2.45	0.50
1:B:161:VAL:CA	1:Y:79:LEU:H	2.24	0.50
1:AA:54:ALA:N	1:w:28:ARG:O	2.44	0.50
1:U:79:LEU:H	1:n:161:VAL:CA	2.24	0.50
1:g:60:VAL:O	1:v:33:THR:CA	2.60	0.50
1:h:57:PRO:C	1:u:36:ARG:CA	2.70	0.50
1:k:37:THR:C	1:z:54:ALA:C	2.74	0.50
1:3:141:GLN:C	1:p:87:SER:CA	2.85	0.49
1:7:54:ALA:N	1:s:28:ARG:O	2.45	0.49
1:AB:121:VAL:O	1:t:108:GLN:N	2.40	0.49
1:l:87:SER:CA	1:y:141:GLN:C	2.85	0.49
1:7:30:TYR:C	1:C:66:SER:O	2.50	0.49
1:c:37:THR:C	1:r:54:ALA:C	2.75	0.49
1:k:60:VAL:O	1:z:33:THR:CA	2.60	0.49
1:l:108:GLN:N	1:z:121:VAL:O	2.40	0.49
1:AB:43:ALA:C	1:t:46:PRO:O	2.56	0.49
1:B:43:ALA:C	1:Z:46:PRO:O	2.56	0.49
1:V:87:SER:CA	1:m:141:GLN:C	2.85	0.49
1:i:2:SER:O	1:u:82:ASP:N	2.31	0.49
1:7:141:GLN:C	1:D:87:SER:CA	2.85	0.49
1:AB:72:SER:O	1:s:17:GLY:HA3	2.13	0.49
1:U:60:VAL:O	1:n:33:THR:CA	2.60	0.49
1:d:46:PRO:O	1:r:43:ALA:C	2.56	0.49
1:8:33:THR:CA	1:C:60:VAL:O	2.60	0.49
1:c:60:VAL:O	1:r:33:THR:CA	2.60	0.49
1:d:87:SER:CA	1:q:141:GLN:C	2.85	0.49
1:w:261:SER:C	1:w:262:LYS:C	2.75	0.49
1:4:49:SER:C	1:o:45:ARG:CA	2.84	0.49
1:c:17:GLY:HA3	1:r:72:SER:O	2.13	0.49
1:4:72:SER:O	1:o:17:GLY:HA3	2.13	0.48
1:A:141:GLN:C	1:Z:87:SER:CA	2.85	0.48
1:j:1:MET:H3	1:u:71:ARG:C	2.19	0.48
1:4:33:THR:CA	1:o:60:VAL:O	2.60	0.48
1:8:121:VAL:O	1:D:108:GLN:N	2.40	0.48
1:AH:409:SER:C	1:AH:411:ILE:H	2.21	0.48
1:h:67:ALA:C	1:u:26:SER:C	2.65	0.48
1:B:33:THR:CA	1:Y:60:VAL:O	2.60	0.48
1:i:252:GLN:C	1:z:103:GLU:CA	2.82	0.48
1:U:66:SER:O	1:m:30:TYR:C	2.50	0.48
1:k:66:SER:O	1:y:30:TYR:C	2.50	0.48
1:l:46:PRO:O	1:z:43:ALA:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:80:LEU:C	1:u:4:ARG:H	2.10	0.48
1:AP:409:SER:C	1:AP:411:ILE:H	2.22	0.48
1:g:49:SER:C	1:v:46:PRO:C	2.49	0.48
1:g:81:GLN:C	1:v:154:MET:CA	2.86	0.48
1:h:87:SER:CA	1:u:141:GLN:C	2.85	0.48
1:h:108:GLN:N	1:v:121:VAL:O	2.40	0.48
1:4:121:VAL:O	1:p:108:GLN:N	2.40	0.48
1:AA:54:ALA:CA	1:w:28:ARG:C	2.87	0.48
1:AB:49:SER:C	1:s:45:ARG:CA	2.84	0.48
1:AJ:409:SER:C	1:AJ:411:ILE:H	2.21	0.48
1:c:45:ARG:CA	1:r:49:SER:C	2.84	0.48
1:8:72:SER:O	1:C:17:GLY:HA3	2.13	0.48
1:AB:103:GLU:CA	1:q:252:GLN:C	2.82	0.48
1:g:28:ARG:C	1:q:54:ALA:CA	2.87	0.48
1:g:33:THR:C	1:v:58:GLY:N	2.72	0.48
1:k:33:THR:C	1:z:58:GLY:N	2.72	0.48
1:7:54:ALA:CA	1:s:28:ARG:C	2.87	0.48
1:A:54:ALA:CA	1:c:28:ARG:C	2.87	0.48
1:4:43:ALA:C	1:p:46:PRO:O	2.56	0.47
1:AB:58:GLY:N	1:s:33:THR:C	2.72	0.47
1:g:66:SER:O	1:u:30:TYR:C	2.49	0.47
1:l:41:GLY:CA	1:z:47:SER:O	2.62	0.47
1:0:409:SER:C	1:0:411:ILE:H	2.21	0.47
1:4:58:GLY:N	1:o:33:THR:C	2.72	0.47
1:AD:409:SER:C	1:AD:411:ILE:H	2.22	0.47
1:AF:58:GLY:N	1:w:33:THR:C	2.72	0.47
1:a:252:GLN:C	1:r:103:GLU:CA	2.82	0.47
1:7:78:ARG:CA	1:q:5:SER:CA	2.93	0.47
1:AN:409:SER:C	1:AN:411:ILE:H	2.21	0.47
1:e:252:GLN:C	1:v:103:GLU:CA	2.82	0.47
1:4:42:SER:O	1:o:51:SER:CA	2.63	0.47
1:A:26:SER:C	1:Z:67:ALA:C	2.65	0.47
1:AF:72:SER:O	1:w:17:GLY:HA3	2.13	0.47
1:o:28:ARG:C	1:y:54:ALA:CA	2.87	0.47
1:3:78:ARG:CA	1:A:5:SER:CA	2.93	0.47
1:4:103:GLU:CA	1:m:252:GLN:C	2.82	0.47
1:AA:78:ARG:CA	1:u:5:SER:CA	2.93	0.47
1:AF:55:SER:N	1:w:37:THR:C	2.66	0.47
1:B:47:SER:O	1:Z:41:GLY:CA	2.62	0.47
1:c:23:ARG:H	1:r:76:GLY:N	2.12	0.47
1:c:33:THR:C	1:r:58:GLY:N	2.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:66:SER:O	1:q:30:TYR:C	2.49	0.47
1:g:17:GLY:HA3	1:v:72:SER:O	2.13	0.47
1:g:51:SER:CA	1:v:42:SER:O	2.62	0.47
1:h:41:GLY:CA	1:v:47:SER:O	2.62	0.47
1:k:17:GLY:HA3	1:z:72:SER:O	2.13	0.47
1:4:47:SER:O	1:p:41:GLY:CA	2.62	0.47
1:8:58:GLY:N	1:C:33:THR:C	2.72	0.47
1:AB:42:SER:O	1:s:51:SER:CA	2.63	0.47
1:AF:103:GLU:CA	1:u:252:GLN:C	2.82	0.47
1:AL:409:SER:C	1:AL:411:ILE:H	2.21	0.47
1:B:121:VAL:O	1:Z:108:GLN:N	2.40	0.47
1:c:51:SER:CA	1:r:42:SER:O	2.62	0.47
1:d:41:GLY:CA	1:r:47:SER:O	2.62	0.47
1:k:28:ARG:C	1:u:54:ALA:CA	2.87	0.47
1:4:54:ALA:C	1:o:37:THR:C	2.74	0.47
1:AB:47:SER:O	1:t:41:GLY:CA	2.62	0.47
1:B:42:SER:O	1:Y:51:SER:CA	2.63	0.47
1:K:454:VAL:O	1:r:184:ARG:N	2.48	0.47
1:h:46:PRO:O	1:v:43:ALA:C	2.56	0.47
1:k:20:THR:C	1:z:76:GLY:H	1.99	0.47
1:8:42:SER:O	1:C:51:SER:CA	2.63	0.47
1:8:47:SER:O	1:D:41:GLY:CA	2.62	0.47
1:AB:54:ALA:C	1:s:37:THR:C	2.74	0.47
1:3:54:ALA:CA	1:C:28:ARG:C	2.87	0.46
1:AA:71:ARG:C	1:v:1:MET:H3	2.22	0.46
1:AA:72:SER:N	1:v:1:MET:O	2.45	0.46
1:l:54:ALA:O	1:y:38:TYR:CA	2.63	0.46
1:l:67:ALA:O	1:y:25:SER:O	2.34	0.46
1:7:25:SER:O	1:D:67:ALA:O	2.34	0.46
1:A:25:SER:O	1:Z:67:ALA:O	2.34	0.46
1:H:420:SER:O	1:U:90:ASP:O	2.33	0.46
1:c:81:GLN:C	1:r:154:MET:CA	2.86	0.46
1:AE:78:ARG:CA	1:y:5:SER:CA	2.93	0.46
1:P:420:SER:O	1:k:90:ASP:O	2.33	0.46
1:i:5:SER:CA	1:u:78:ARG:CA	2.93	0.46
1:k:51:SER:CA	1:z:42:SER:O	2.63	0.46
1:8:43:ALA:C	1:D:46:PRO:O	2.56	0.46
1:L:420:SER:O	1:c:90:ASP:O	2.33	0.46
1:R:67:ALA:O	1:i:25:SER:O	2.34	0.46
1:k:45:ARG:CA	1:z:49:SER:C	2.84	0.46
1:8:54:ALA:C	1:C:37:THR:C	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:CA	1:Z:54:ALA:O	2.63	0.46
1:O:454:VAL:O	1:z:184:ARG:N	2.48	0.46
1:T:420:SER:O	1:o:90:ASP:O	2.33	0.46
1:V:54:ALA:O	1:m:38:TYR:CA	2.63	0.46
1:4:76:GLY:N	1:o:23:ARG:H	2.12	0.46
1:4:184:ARG:N	1:S:454:VAL:O	2.48	0.46
1:d:54:ALA:O	1:q:38:TYR:CA	2.63	0.46
1:h:54:ALA:O	1:u:38:TYR:CA	2.63	0.46
1:h:97:LYS:O	1:v:129:LYS:CA	2.64	0.46
1:k:81:GLN:C	1:z:154:MET:CA	2.86	0.46
1:m:5:SER:CA	1:y:78:ARG:CA	2.93	0.46
1:3:30:TYR:C	1:o:66:SER:O	2.49	0.46
1:4:129:LYS:CA	1:p:97:LYS:O	2.64	0.46
1:B:49:SER:C	1:Y:45:ARG:CA	2.84	0.46
1:B:184:ARG:N	1:I:454:VAL:O	2.48	0.46
1:G:454:VAL:O	1:n:184:ARG:N	2.48	0.46
1:3:38:TYR:CA	1:p:54:ALA:O	2.63	0.46
1:V:67:ALA:O	1:m:25:SER:O	2.34	0.46
1:7:38:TYR:CA	1:D:54:ALA:O	2.63	0.46
1:B:129:LYS:CA	1:Z:97:LYS:O	2.64	0.46
1:C:261:SER:C	1:C:262:LYS:C	2.75	0.46
1:J:420:SER:O	1:Y:90:ASP:O	2.33	0.46
1:1:261:SER:C	1:1:262:LYS:C	2.75	0.46
1:5:261:SER:C	1:5:262:LYS:C	2.75	0.46
1:B:157:LEU:C	1:Y:79:LEU:CA	2.86	0.46
1:C:90:ASP:O	1:X:420:SER:O	2.33	0.46
1:l:97:LYS:O	1:z:129:LYS:CA	2.64	0.46
1:AB:55:SER:N	1:s:37:THR:C	2.66	0.45
1:AB:129:LYS:CA	1:t:97:LYS:O	2.64	0.45
1:d:95:GLU:CA	1:s:248:GLN:H	2.29	0.45
1:k:49:SER:C	1:z:46:PRO:C	2.49	0.45
1:7:36:ARG:CA	1:D:60:VAL:N	2.78	0.45
1:8:49:SER:C	1:C:45:ARG:CA	2.84	0.45
1:A:47:SER:O	1:Z:47:SER:O	2.35	0.45
1:M:454:VAL:O	1:v:184:ARG:N	2.48	0.45
1:N:420:SER:O	1:g:90:ASP:O	2.33	0.45
1:AA:47:SER:O	1:t:47:SER:O	2.35	0.45
1:E:454:VAL:O	1:j:184:ARG:N	2.48	0.45
1:V:97:LYS:O	1:n:129:LYS:CA	2.64	0.45
1:X:431:LEU:C	1:X:433:LEU:H	2.24	0.45
1:4:157:LEU:C	1:o:79:LEU:CA	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:248:GLN:H	1:t:95:GLU:CA	2.29	0.45
1:C:248:GLN:H	1:Z:95:GLU:CA	2.29	0.45
1:g:37:THR:C	1:v:55:SER:N	2.66	0.45
1:3:25:SER:O	1:p:67:ALA:O	2.34	0.45
1:U:79:LEU:CA	1:n:157:LEU:C	2.86	0.45
1:d:47:SER:O	1:q:47:SER:O	2.35	0.45
1:d:67:ALA:O	1:q:25:SER:O	2.34	0.45
1:d:97:LYS:O	1:r:129:LYS:CA	2.64	0.45
1:j:1:MET:O	1:u:72:SER:N	2.45	0.45
1:7:28:ARG:C	1:C:69:ARG:N	2.75	0.45
1:7:47:SER:O	1:D:47:SER:O	2.35	0.45
1:8:129:LYS:CA	1:D:97:LYS:O	2.64	0.45
1:8:154:MET:CA	1:C:81:GLN:C	2.86	0.45
1:A:28:ARG:C	1:Y:69:ARG:N	2.75	0.45
1:k:23:ARG:H	1:z:76:GLY:N	2.12	0.45
1:k:69:ARG:N	1:y:28:ARG:C	2.75	0.45
1:3:47:SER:O	1:p:47:SER:O	2.35	0.45
1:A:36:ARG:CA	1:Z:60:VAL:N	2.78	0.45
1:J:431:LEU:C	1:J:433:LEU:H	2.24	0.45
1:B:154:MET:CA	1:Y:81:GLN:C	2.86	0.45
1:Q:69:ARG:N	1:i:28:ARG:C	2.75	0.45
1:h:47:SER:O	1:u:47:SER:O	2.35	0.45
1:8:157:LEU:C	1:C:79:LEU:CA	2.86	0.45
1:9:248:GLN:H	1:D:95:GLU:CA	2.29	0.45
1:g:20:THR:C	1:v:76:GLY:H	1.99	0.44
1:g:45:ARG:CA	1:v:49:SER:C	2.84	0.44
1:9:261:SER:C	1:9:262:LYS:C	2.75	0.44
1:L:431:LEU:C	1:L:433:LEU:H	2.24	0.44
1:g:69:ARG:N	1:u:28:ARG:C	2.75	0.44
1:k:65:SER:O	1:z:26:SER:O	2.35	0.44
1:7:71:ARG:C	1:r:1:MET:H3	2.26	0.44
1:N:431:LEU:C	1:N:433:LEU:H	2.24	0.44
1:U:69:ARG:N	1:m:28:ARG:C	2.75	0.44
1:U:81:GLN:C	1:n:154:MET:CA	2.86	0.44
1:h:60:VAL:N	1:u:36:ARG:CA	2.78	0.44
1:3:36:ARG:CA	1:p:60:VAL:N	2.78	0.44
1:3:176:ASP:C	1:AK:346:GLU:O	2.61	0.44
1:B:26:SER:O	1:Y:65:SER:O	2.35	0.44
1:B:187:GLU:CA	1:J:452:GLY:CA	2.94	0.44
1:H:431:LEU:C	1:H:433:LEU:H	2.24	0.44
1:P:431:LEU:C	1:P:433:LEU:H	2.24	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:346:GLU:O	1:m:176:ASP:C	2.61	0.44
1:B:46:PRO:C	1:Y:49:SER:C	2.49	0.44
1:l:60:VAL:N	1:y:36:ARG:CA	2.78	0.44
1:1:346:GLU:O	1:i:176:ASP:C	2.61	0.44
1:8:26:SER:O	1:C:65:SER:O	2.35	0.44
1:AI:346:GLU:O	1:y:176:ASP:C	2.61	0.44
1:c:69:ARG:N	1:q:28:ARG:C	2.75	0.44
1:3:28:ARG:C	1:o:69:ARG:N	2.75	0.44
1:8:76:GLY:N	1:C:23:ARG:H	2.12	0.44
1:AC:346:GLU:O	1:q:176:ASP:C	2.61	0.44
1:AG:346:GLU:O	1:u:176:ASP:C	2.61	0.44
1:g:65:SER:O	1:v:26:SER:O	2.35	0.44
1:h:67:ALA:O	1:u:25:SER:O	2.34	0.44
1:k:37:THR:C	1:z:55:SER:N	2.66	0.44
1:l:47:SER:O	1:y:47:SER:O	2.35	0.44
1:4:154:MET:CA	1:o:81:GLN:C	2.86	0.44
1:9:346:GLU:O	1:A:176:ASP:C	2.61	0.43
1:T:431:LEU:C	1:T:433:LEU:H	2.24	0.43
1:U:65:SER:O	1:n:26:SER:O	2.35	0.43
1:c:65:SER:O	1:r:26:SER:O	2.35	0.43
1:4:187:GLU:CA	1:T:452:GLY:CA	2.94	0.43
1:AF:76:GLY:N	1:w:23:ARG:H	2.12	0.43
1:C:251:GLU:CA	1:Z:102:ASN:N	2.77	0.43
1:AB:76:GLY:N	1:s:23:ARG:H	2.12	0.43
1:F:452:GLY:CA	1:j:187:GLU:CA	2.94	0.43
1:d:45:ARG:O	1:q:49:SER:CA	2.66	0.43
1:l:45:ARG:O	1:y:49:SER:CA	2.66	0.43
1:AB:47:SER:O	1:t:41:GLY:HA3	2.19	0.43
1:H:452:GLY:CA	1:n:187:GLU:CA	2.94	0.43
1:3:78:ARG:C	1:B:2:SER:O	2.58	0.43
1:AA:49:SER:CA	1:t:45:ARG:O	2.66	0.43
1:V:60:VAL:N	1:m:36:ARG:CA	2.78	0.43
1:d:77:VAL:O	1:r:155:ARG:O	2.37	0.43
1:l:77:VAL:O	1:z:155:ARG:O	2.37	0.43
1:t:95:GLU:C	1:t:97:LYS:H	2.27	0.43
1:3:49:SER:CA	1:p:45:ARG:O	2.66	0.43
1:AE:78:ARG:C	1:z:2:SER:O	2.58	0.43
1:D:95:GLU:C	1:D:97:LYS:H	2.27	0.43
1:d:95:GLU:C	1:d:97:LYS:H	2.27	0.43
1:g:37:THR:C	1:v:54:ALA:C	2.75	0.43
1:4:26:SER:O	1:o:65:SER:O	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:47:SER:O	1:D:41:GLY:HA3	2.19	0.43
1:A:49:SER:CA	1:Z:45:ARG:O	2.66	0.43
1:P:452:GLY:CA	1:z:187:GLU:CA	2.94	0.43
1:V:95:GLU:C	1:V:97:LYS:H	2.27	0.43
1:g:23:ARG:H	1:v:76:GLY:N	2.12	0.43
1:h:41:GLY:HA3	1:v:47:SER:O	2.19	0.43
1:h:45:ARG:O	1:u:49:SER:CA	2.66	0.43
1:c:79:LEU:CA	1:r:157:LEU:C	2.85	0.43
1:d:35:THR:CA	1:v:69:ARG:CA	2.97	0.43
1:d:41:GLY:HA3	1:r:47:SER:O	2.19	0.43
1:h:77:VAL:O	1:v:155:ARG:O	2.37	0.43
1:h:95:GLU:C	1:h:97:LYS:H	2.27	0.43
1:4:155:ARG:O	1:p:77:VAL:O	2.37	0.43
1:7:49:SER:CA	1:D:45:ARG:O	2.66	0.43
1:B:47:SER:O	1:Z:41:GLY:HA3	2.19	0.43
1:L:418:PHE:H	1:c:97:LYS:H	0.43	0.42
1:V:77:VAL:O	1:n:155:ARG:O	2.37	0.42
1:d:60:VAL:N	1:q:36:ARG:CA	2.78	0.42
1:AF:69:ARG:CA	1:t:35:THR:CA	2.97	0.42
1:4:47:SER:O	1:p:41:GLY:HA3	2.19	0.42
1:8:103:GLU:C	1:A:253:HIS:N	2.64	0.42
1:8:155:ARG:O	1:D:77:VAL:O	2.37	0.42
1:B:155:ARG:O	1:Z:77:VAL:O	2.37	0.42
1:L:452:GLY:CA	1:r:187:GLU:CA	2.94	0.42
1:l:95:GLU:C	1:l:97:LYS:H	2.27	0.42
1:p:95:GLU:C	1:p:97:LYS:H	2.27	0.42
1:4:69:ARG:CA	1:l:35:THR:CA	2.97	0.42
1:J:418:PHE:H	1:Y:97:LYS:H	0.43	0.42
1:T:418:PHE:H	1:o:97:LYS:H	0.43	0.42
1:Z:35:THR:CA	1:r:69:ARG:CA	2.97	0.42
1:c:49:SER:C	1:r:46:PRO:C	2.49	0.42
1:8:55:SER:N	1:C:37:THR:C	2.66	0.42
1:N:418:PHE:H	1:g:97:LYS:H	0.43	0.42
1:5:251:GLU:CA	1:p:102:ASN:N	2.77	0.42
1:AA:78:ARG:C	1:v:2:SER:O	2.58	0.42
1:AB:69:ARG:CA	1:D:35:THR:CA	2.97	0.42
1:AB:103:GLU:C	1:q:253:HIS:N	2.64	0.42
1:h:79:LEU:H	1:v:155:ARG:CA	2.32	0.42
1:7:78:ARG:C	1:r:2:SER:O	2.58	0.42
1:N:452:GLY:CA	1:v:187:GLU:CA	2.94	0.42
1:P:418:PHE:H	1:k:97:LYS:H	0.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:418:PHE:H	1:U:97:LYS:H	0.43	0.42
1:l:52:LEU:O	1:y:39:SER:O	2.38	0.42
1:n:2:SER:O	1:y:78:ARG:C	2.58	0.42
1:3:39:SER:O	1:p:52:LEU:O	2.38	0.42
1:Z:95:GLU:C	1:Z:97:LYS:H	2.27	0.42
1:g:66:SER:N	1:u:32:THR:N	2.64	0.42
1:1:248:GLN:H	1:l:95:GLU:CA	2.29	0.42
1:7:39:SER:O	1:D:52:LEU:O	2.38	0.42
1:AA:71:ARG:CA	1:v:1:MET:N	2.83	0.42
1:D:106:GLU:CA	1:X:411:ILE:CA	2.98	0.42
1:P:411:ILE:CA	1:l:106:GLU:CA	2.98	0.42
1:h:35:THR:CA	1:z:69:ARG:CA	2.97	0.42
1:l:41:GLY:HA3	1:z:47:SER:O	2.19	0.42
1:s:261:SER:C	1:s:262:LYS:C	2.75	0.42
1:3:71:ARG:CA	1:B:1:MET:N	2.83	0.41
1:7:32:THR:H	1:C:66:SER:H	1.66	0.41
1:b:418:PHE:H	1:s:97:LYS:H	0.43	0.41
1:k:79:LEU:CA	1:z:157:LEU:C	2.85	0.41
1:n:1:MET:N	1:y:71:ARG:CA	2.83	0.41
1:7:71:ARG:C	1:r:1:MET:N	2.78	0.41
1:J:411:ILE:CA	1:Z:106:GLU:CA	2.98	0.41
1:T:411:ILE:CA	1:p:106:GLU:CA	2.98	0.41
1:8:69:ARG:CA	1:p:35:THR:CA	2.97	0.41
1:j:1:MET:N	1:u:71:ARG:CA	2.83	0.41
1:4:54:ALA:C	1:o:37:THR:CA	2.94	0.41
1:AE:71:ARG:CA	1:z:1:MET:N	2.83	0.41
1:h:52:LEU:O	1:u:39:SER:O	2.38	0.41
1:4:55:SER:N	1:o:37:THR:C	2.66	0.41
1:5:250:GLN:O	1:p:102:ASN:N	2.54	0.41
1:AB:54:ALA:C	1:s:37:THR:CA	2.94	0.41
1:B:24:PRO:CA	1:Y:69:ARG:CA	2.99	0.41
1:C:97:LYS:H	1:X:418:PHE:H	0.43	0.41
1:7:71:ARG:CA	1:r:1:MET:N	2.83	0.41
1:8:24:PRO:CA	1:C:69:ARG:CA	2.99	0.41
1:9:251:GLU:CA	1:D:102:ASN:N	2.77	0.41
1:AC:250:GLN:O	1:t:102:ASN:N	2.54	0.41
1:N:411:ILE:CA	1:h:106:GLU:CA	2.98	0.41
1:Q:69:ARG:CA	1:j:24:PRO:CA	2.99	0.41
1:c:37:THR:CA	1:r:54:ALA:C	2.94	0.41
1:e:253:HIS:N	1:v:103:GLU:C	2.64	0.41
1:k:37:THR:CA	1:z:54:ALA:C	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:54:ALA:O	1:s:28:ARG:N	2.50	0.41
1:8:46:PRO:C	1:C:49:SER:C	2.49	0.41
1:A:39:SER:O	1:Z:52:LEU:O	2.38	0.41
1:Q:68:VAL:CA	1:i:28:ARG:O	2.69	0.41
1:V:52:LEU:O	1:m:39:SER:O	2.38	0.41
1:V:102:ASN:N	1:o:250:GLN:O	2.54	0.41
1:k:69:ARG:CA	1:z:24:PRO:CA	2.99	0.41
1:AC:261:SER:C	1:AC:262:LYS:C	2.75	0.41
1:d:102:ASN:N	1:s:251:GLU:CA	2.77	0.41
1:g:68:VAL:CA	1:u:28:ARG:O	2.69	0.41
1:g:69:ARG:CA	1:v:24:PRO:CA	2.99	0.41
1:j:2:SER:O	1:u:78:ARG:C	2.58	0.41
1:1:17:GLY:C	1:1:19:GLY:HA3	2.46	0.41
1:1:251:GLU:CA	1:l:102:ASN:N	2.77	0.41
1:4:24:PRO:CA	1:o:69:ARG:CA	2.99	0.41
1:4:136:GLU:N	1:p:93:ASN:O	2.54	0.41
1:8:54:ALA:C	1:C:37:THR:CA	2.94	0.41
1:8:136:GLU:N	1:D:93:ASN:O	2.54	0.41
1:AA:71:ARG:C	1:v:1:MET:N	2.78	0.41
1:B:54:ALA:C	1:Y:37:THR:CA	2.94	0.41
1:C:17:GLY:C	1:C:19:GLY:HA3	2.46	0.41
1:C:90:ASP:O	1:X:419:SER:CA	2.69	0.41
1:U:68:VAL:CA	1:m:28:ARG:O	2.69	0.41
1:U:69:ARG:CA	1:n:24:PRO:CA	2.99	0.41
1:g:17:GLY:C	1:g:19:GLY:HA3	2.46	0.41
1:g:28:ARG:N	1:q:54:ALA:O	2.50	0.41
1:h:102:ASN:N	1:w:251:GLU:CA	2.77	0.41
1:k:68:VAL:CA	1:y:28:ARG:O	2.69	0.41
1:n:1:MET:N	1:y:71:ARG:C	2.78	0.41
1:B:136:GLU:N	1:Z:93:ASN:O	2.54	0.41
1:T:419:SER:CA	1:o:90:ASP:O	2.69	0.41
1:V:93:ASN:O	1:n:136:GLU:N	2.54	0.41
1:b:411:ILE:CA	1:t:106:GLU:CA	2.98	0.41
1:d:52:LEU:O	1:q:39:SER:O	2.38	0.41
1:4:46:PRO:C	1:o:49:SER:C	2.49	0.40
1:5:248:GLN:H	1:p:95:GLU:CA	2.29	0.40
1:A:54:ALA:O	1:c:28:ARG:N	2.50	0.40
1:AF:54:ALA:C	1:w:37:THR:CA	2.94	0.40
1:AA:54:ALA:O	1:w:28:ARG:N	2.50	0.40
1:L:411:ILE:CA	1:d:106:GLU:CA	2.98	0.40
1:L:419:SER:CA	1:c:90:ASP:O	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:17:GLY:C	1:c:19:GLY:HA3	2.46	0.40
1:h:102:ASN:N	1:w:250:GLN:O	2.54	0.40
1:j:1:MET:N	1:u:71:ARG:C	2.78	0.40
1:s:17:GLY:C	1:s:19:GLY:HA3	2.46	0.40
1:l:250:GLN:O	1:l:102:ASN:N	2.54	0.40
1:7:28:ARG:O	1:C:68:VAL:CA	2.69	0.40
1:Q:79:LEU:CA	1:j:157:LEU:C	2.85	0.40
1:U:52:LEU:N	1:n:42:SER:O	2.54	0.40
1:g:37:THR:CA	1:v:54:ALA:C	2.94	0.40
1:3:32:THR:H	1:o:66:SER:H	1.66	0.40
1:A:28:ARG:O	1:Y:68:VAL:CA	2.69	0.40
1:J:419:SER:CA	1:Y:90:ASP:O	2.69	0.40
1:N:419:SER:CA	1:g:90:ASP:O	2.69	0.40
1:c:69:ARG:CA	1:r:24:PRO:CA	2.99	0.40
1:h:95:GLU:CA	1:w:248:GLN:H	2.29	0.40
1:B:155:ARG:CA	1:Z:79:LEU:H	2.32	0.40
1:K:424:ARG:C	1:K:426:THR:H	2.30	0.40
1:d:93:ASN:O	1:r:136:GLU:N	2.54	0.40
1:d:102:ASN:N	1:s:250:GLN:O	2.54	0.40
1:g:11:TYR:C	1:j:6:VAL:O	2.55	0.40
1:l:93:ASN:O	1:z:136:GLU:N	2.54	0.40
1:o:17:GLY:C	1:o:19:GLY:HA3	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	251/466 (54%)	220 (88%)	19 (8%)	12 (5%)	2	16
1	1	265/466 (57%)	234 (88%)	25 (9%)	6 (2%)	5	28
1	2	260/466 (56%)	238 (92%)	14 (5%)	8 (3%)	3	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	189/466 (41%)	156 (82%)	29 (15%)	4 (2%)	5	30
1	4	193/466 (41%)	162 (84%)	26 (14%)	5 (3%)	4	25
1	5	261/466 (56%)	228 (87%)	28 (11%)	5 (2%)	6	32
1	6	259/466 (56%)	237 (92%)	14 (5%)	8 (3%)	3	22
1	7	140/466 (30%)	117 (84%)	21 (15%)	2 (1%)	9	40
1	8	106/466 (23%)	91 (86%)	12 (11%)	3 (3%)	4	24
1	9	195/466 (42%)	164 (84%)	28 (14%)	3 (2%)	8	40
1	A	250/466 (54%)	215 (86%)	28 (11%)	7 (3%)	4	24
1	AA	93/466 (20%)	77 (83%)	15 (16%)	1 (1%)	11	46
1	AB	98/466 (21%)	85 (87%)	11 (11%)	2 (2%)	6	31
1	AC	219/466 (47%)	181 (83%)	31 (14%)	7 (3%)	3	21
1	AD	220/466 (47%)	189 (86%)	19 (9%)	12 (6%)	1	14
1	AE	47/466 (10%)	36 (77%)	10 (21%)	1 (2%)	5	30
1	AF	52/466 (11%)	40 (77%)	10 (19%)	2 (4%)	2	19
1	AG	197/466 (42%)	168 (85%)	23 (12%)	6 (3%)	3	22
1	AH	197/466 (42%)	172 (87%)	17 (9%)	8 (4%)	2	18
1	AI	165/466 (35%)	136 (82%)	23 (14%)	6 (4%)	2	20
1	AJ	168/466 (36%)	143 (85%)	17 (10%)	8 (5%)	2	16
1	AK	134/466 (29%)	105 (78%)	23 (17%)	6 (4%)	2	17
1	AL	139/466 (30%)	115 (83%)	16 (12%)	8 (6%)	1	14
1	AM	79/466 (17%)	63 (80%)	12 (15%)	4 (5%)	1	15
1	AN	83/466 (18%)	68 (82%)	11 (13%)	4 (5%)	2	16
1	AO	32/466 (7%)	25 (78%)	3 (9%)	4 (12%)	0	4
1	AP	37/466 (8%)	26 (70%)	7 (19%)	4 (11%)	0	6
1	B	265/466 (57%)	240 (91%)	21 (8%)	4 (2%)	8	40
1	C	225/466 (48%)	185 (82%)	32 (14%)	8 (4%)	2	20
1	D	249/466 (53%)	224 (90%)	18 (7%)	7 (3%)	4	24
1	E	31/466 (7%)	19 (61%)	11 (36%)	1 (3%)	3	21
1	F	33/466 (7%)	26 (79%)	4 (12%)	3 (9%)	0	8
1	G	50/466 (11%)	31 (62%)	18 (36%)	1 (2%)	6	31
1	H	52/466 (11%)	36 (69%)	11 (21%)	5 (10%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	77/466 (16%)	55 (71%)	19 (25%)	3 (4%)	2	19
1	J	81/466 (17%)	65 (80%)	11 (14%)	5 (6%)	1	13
1	K	105/466 (22%)	83 (79%)	19 (18%)	3 (3%)	3	23
1	L	111/466 (24%)	95 (86%)	11 (10%)	5 (4%)	2	17
1	M	134/466 (29%)	112 (84%)	19 (14%)	3 (2%)	5	29
1	N	140/466 (30%)	124 (89%)	11 (8%)	5 (4%)	2	20
1	O	163/466 (35%)	141 (86%)	19 (12%)	3 (2%)	6	34
1	P	168/466 (36%)	152 (90%)	11 (6%)	5 (3%)	3	22
1	Q	12/466 (3%)	6 (50%)	4 (33%)	2 (17%)	0	2
1	R	12/466 (3%)	9 (75%)	2 (17%)	1 (8%)	0	9
1	S	192/466 (41%)	170 (88%)	19 (10%)	3 (2%)	7	38
1	T	197/466 (42%)	181 (92%)	11 (6%)	5 (2%)	4	26
1	U	51/466 (11%)	37 (72%)	10 (20%)	4 (8%)	1	10
1	V	55/466 (12%)	43 (78%)	9 (16%)	3 (6%)	1	14
1	W	192/466 (41%)	172 (90%)	13 (7%)	7 (4%)	2	20
1	X	192/466 (41%)	175 (91%)	11 (6%)	6 (3%)	3	22
1	Y	97/466 (21%)	78 (80%)	15 (16%)	4 (4%)	2	18
1	Z	100/466 (22%)	84 (84%)	13 (13%)	3 (3%)	3	22
1	a	139/466 (30%)	130 (94%)	5 (4%)	4 (3%)	3	23
1	b	19/466 (4%)	17 (90%)	2 (10%)	0	100	100
1	c	146/466 (31%)	119 (82%)	21 (14%)	6 (4%)	2	18
1	d	69/466 (15%)	61 (88%)	5 (7%)	3 (4%)	2	17
1	e	185/466 (40%)	175 (95%)	7 (4%)	3 (2%)	7	38
1	f	95/466 (20%)	89 (94%)	5 (5%)	1 (1%)	11	46
1	j	140/466 (30%)	129 (92%)	9 (6%)	2 (1%)	9	40
1	k	127/466 (27%)	105 (83%)	18 (14%)	4 (3%)	3	22
1	q	159/466 (34%)	148 (93%)	6 (4%)	5 (3%)	3	22
1	r	276/466 (59%)	240 (87%)	30 (11%)	6 (2%)	5	29
1	s	271/466 (58%)	243 (90%)	23 (8%)	5 (2%)	6	34
1	t	262/466 (56%)	240 (92%)	16 (6%)	6 (2%)	5	28
1	u	256/466 (55%)	216 (84%)	35 (14%)	5 (2%)	6	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	252/466 (54%)	219 (87%)	28 (11%)	5 (2%)	6	31
1	w	253/466 (54%)	230 (91%)	18 (7%)	5 (2%)	6	31
1	x	246/466 (53%)	228 (93%)	12 (5%)	6 (2%)	4	27
1	y	222/466 (48%)	186 (84%)	32 (14%)	4 (2%)	6	34
1	z	226/466 (48%)	195 (86%)	26 (12%)	5 (2%)	5	29
All	All	10656/32620 (33%)	9204 (86%)	1132 (11%)	320 (3%)	5	22

All (320) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	413	LEU
1	0	414	PRO
1	1	18	PRO
1	1	265	LEU
1	5	265	LEU
1	9	265	LEU
1	A	263	PRO
1	A	265	LEU
1	AC	265	LEU
1	AC	413	LEU
1	AC	418	PHE
1	AD	413	LEU
1	AD	414	PRO
1	AG	413	LEU
1	AG	418	PHE
1	AH	413	LEU
1	AH	414	PRO
1	AI	413	LEU
1	AI	418	PHE
1	AJ	413	LEU
1	AJ	414	PRO
1	AK	413	LEU
1	AK	418	PHE
1	AL	413	LEU
1	AL	414	PRO
1	AM	413	LEU
1	AM	418	PHE
1	AN	413	LEU
1	AN	414	PRO
1	AO	413	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AO	418	PHE
1	AP	413	LEU
1	AP	414	PRO
1	B	264	ASP
1	C	18	PRO
1	C	265	LEU
1	D	87	SER
1	H	431	LEU
1	I	414	PRO
1	J	431	LEU
1	K	414	PRO
1	L	431	LEU
1	M	414	PRO
1	N	431	LEU
1	O	414	PRO
1	P	431	LEU
1	S	414	PRO
1	T	431	LEU
1	V	87	SER
1	W	263	PRO
1	W	265	LEU
1	W	414	PRO
1	X	264	ASP
1	X	431	LEU
1	Z	87	SER
1	a	263	PRO
1	a	265	LEU
1	c	18	PRO
1	d	87	SER
1	e	263	PRO
1	e	265	LEU
1	f	264	ASP
1	j	264	ASP
1	q	263	PRO
1	q	265	LEU
1	r	264	ASP
1	s	18	PRO
1	s	265	LEU
1	w	18	PRO
1	w	265	LEU
1	0	254	VAL
1	0	259	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	447	VAL
1	1	455	ILE
1	1	463	ASP
1	2	254	VAL
1	2	259	ASP
1	2	447	VAL
1	4	21	ALA
1	4	76	GLY
1	4	79	LEU
1	5	455	ILE
1	5	463	ASP
1	6	254	VAL
1	6	259	ASP
1	6	447	VAL
1	8	76	GLY
1	8	79	LEU
1	9	455	ILE
1	9	463	ASP
1	A	257	ASP
1	AB	76	GLY
1	AB	79	LEU
1	AC	455	ILE
1	AC	463	ASP
1	AD	254	VAL
1	AD	259	ASP
1	AD	447	VAL
1	AF	76	GLY
1	AF	79	LEU
1	AG	455	ILE
1	AG	463	ASP
1	AH	447	VAL
1	AI	455	ILE
1	AI	463	ASP
1	AJ	447	VAL
1	AK	455	ILE
1	AK	463	ASP
1	AL	447	VAL
1	B	21	ALA
1	C	69	ARG
1	C	71	ARG
1	D	254	VAL
1	D	259	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	437	HIS
1	F	438	SER
1	H	437	HIS
1	H	438	SER
1	J	437	HIS
1	J	438	SER
1	L	437	HIS
1	L	438	SER
1	N	437	HIS
1	N	438	SER
1	P	437	HIS
1	P	438	SER
1	Q	69	ARG
1	Q	71	ARG
1	T	437	HIS
1	T	438	SER
1	U	69	ARG
1	U	71	ARG
1	W	257	ASP
1	X	437	HIS
1	X	438	SER
1	Y	69	ARG
1	Y	71	ARG
1	a	257	ASP
1	c	69	ARG
1	c	71	ARG
1	e	257	ASP
1	j	21	ALA
1	k	69	ARG
1	k	71	ARG
1	q	257	ASP
1	r	21	ALA
1	r	76	GLY
1	r	79	LEU
1	t	254	VAL
1	t	259	ASP
1	u	257	ASP
1	v	21	ALA
1	v	76	GLY
1	v	79	LEU
1	x	254	VAL
1	x	259	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	z	21	ALA
1	z	76	GLY
1	z	79	LEU
1	0	252	GLN
1	0	255	GLN
1	0	412	SER
1	0	441	THR
1	2	252	GLN
1	2	255	GLN
1	2	441	THR
1	6	252	GLN
1	6	255	GLN
1	6	441	THR
1	AD	252	GLN
1	AD	255	GLN
1	AD	412	SER
1	AD	441	THR
1	AH	412	SER
1	AH	441	THR
1	AJ	412	SER
1	AJ	441	THR
1	AL	412	SER
1	AL	441	THR
1	AN	412	SER
1	AP	412	SER
1	C	85	ASP
1	D	252	GLN
1	D	255	GLN
1	U	85	ASP
1	Y	85	ASP
1	c	85	ASP
1	k	85	ASP
1	t	252	GLN
1	t	255	GLN
1	x	252	GLN
1	x	255	GLN
1	0	439	LYS
1	1	200	GLU
1	2	439	LYS
1	3	9	SER
1	3	19	GLY
1	3	85	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	200	GLU
1	6	439	LYS
1	7	85	ASP
1	A	9	SER
1	A	19	GLY
1	AA	85	ASP
1	AD	439	LYS
1	AE	85	ASP
1	AH	439	LYS
1	AJ	439	LYS
1	AL	439	LYS
1	C	25	SER
1	C	62	ALA
1	F	435	ASP
1	H	420	SER
1	H	435	ASP
1	J	420	SER
1	J	435	ASP
1	L	420	SER
1	L	435	ASP
1	N	420	SER
1	N	435	ASP
1	P	420	SER
1	P	435	ASP
1	T	420	SER
1	T	435	ASP
1	U	62	ALA
1	X	420	SER
1	X	435	ASP
1	Y	62	ALA
1	c	25	SER
1	c	62	ALA
1	k	62	ALA
1	s	25	SER
1	s	200	GLU
1	u	9	SER
1	u	19	GLY
1	u	85	ASP
1	w	25	SER
1	w	200	GLU
1	y	9	SER
1	y	19	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	y	85	ASP
1	0	411	ILE
1	0	446	THR
1	2	446	THR
1	4	34	SER
1	5	420	SER
1	6	446	THR
1	8	34	SER
1	AC	420	SER
1	AD	411	ILE
1	AD	446	THR
1	AG	420	SER
1	AH	411	ILE
1	AH	446	THR
1	AI	420	SER
1	AJ	411	ILE
1	AJ	446	THR
1	AK	420	SER
1	AL	411	ILE
1	AL	446	THR
1	AM	420	SER
1	AN	411	ILE
1	AO	420	SER
1	AP	411	ILE
1	B	4	ARG
1	B	34	SER
1	E	437	HIS
1	G	437	HIS
1	I	437	HIS
1	K	437	HIS
1	M	437	HIS
1	O	437	HIS
1	S	437	HIS
1	W	437	HIS
1	q	144	SER
1	r	34	SER
1	v	4	ARG
1	v	34	SER
1	z	34	SER
1	3	144	SER
1	4	4	ARG
1	7	144	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	SER
1	AC	414	PRO
1	AG	414	PRO
1	AI	414	PRO
1	AK	414	PRO
1	AM	414	PRO
1	AO	414	PRO
1	I	413	LEU
1	K	413	LEU
1	M	413	LEU
1	O	413	LEU
1	S	413	LEU
1	W	413	LEU
1	r	4	ARG
1	u	144	SER
1	y	144	SER
1	z	4	ARG
1	V	84	VAL
1	d	84	VAL
1	l	6	VAL
1	C	6	VAL
1	D	31	VAL
1	R	77	VAL
1	V	77	VAL
1	Z	77	VAL
1	Z	84	VAL
1	d	77	VAL
1	t	31	VAL
1	w	6	VAL
1	x	31	VAL
1	A	258	VAL
1	D	142	GLY
1	W	258	VAL
1	a	258	VAL
1	q	258	VAL
1	s	6	VAL
1	t	142	GLY
1	x	142	GLY

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	2
1	5	2
1	9	2
1	AC	2
1	C	2
1	s	2
1	w	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	263:PRO	C	264:ASP	N	2.24
1	5	263:PRO	C	264:ASP	N	2.24
1	9	263:PRO	C	264:ASP	N	2.24
1	AC	263:PRO	C	264:ASP	N	2.24
1	C	263:PRO	C	264:ASP	N	2.24

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	s	263:PRO	C	264:ASP	N	2.24
1	w	263:PRO	C	264:ASP	N	2.24
1	1	261:SER	C	262:LYS	N	0.83
1	5	261:SER	C	262:LYS	N	0.83
1	9	261:SER	C	262:LYS	N	0.83
1	AC	261:SER	C	262:LYS	N	0.83
1	C	261:SER	C	262:LYS	N	0.83
1	s	261:SER	C	262:LYS	N	0.83
1	w	261:SER	C	262:LYS	N	0.83

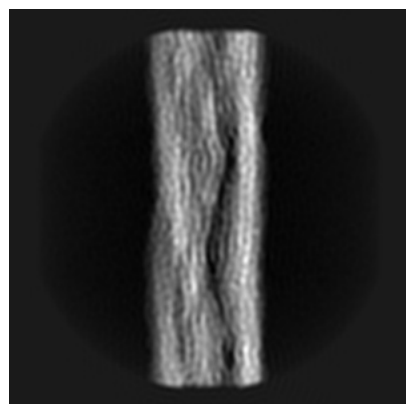
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16844. These allow visual inspection of the internal detail of the map and identification of artifacts.

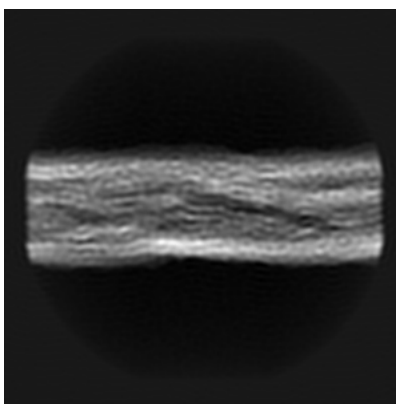
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

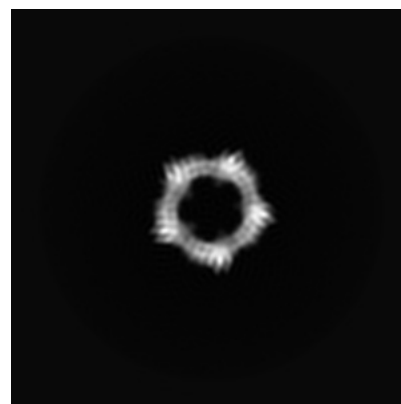
6.1.1 Primary map



X

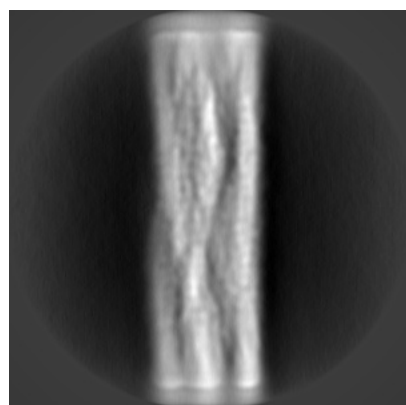


Y

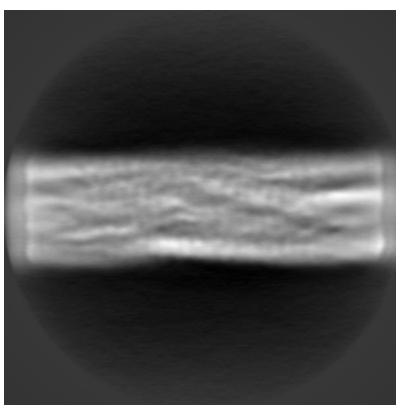


Z

6.1.2 Raw map



X



Y

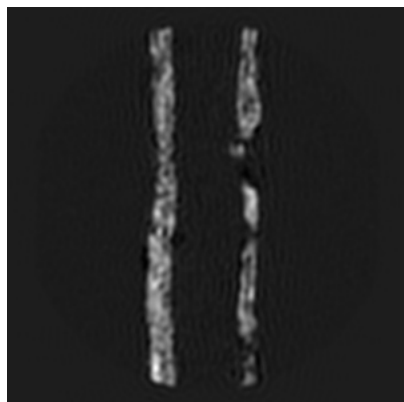


Z

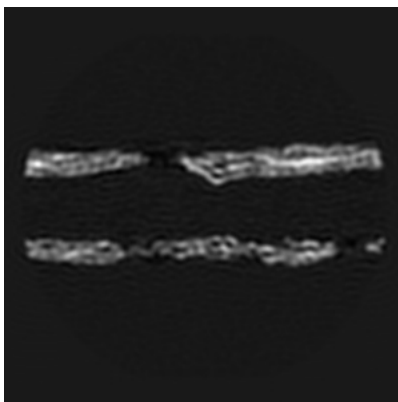
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 190

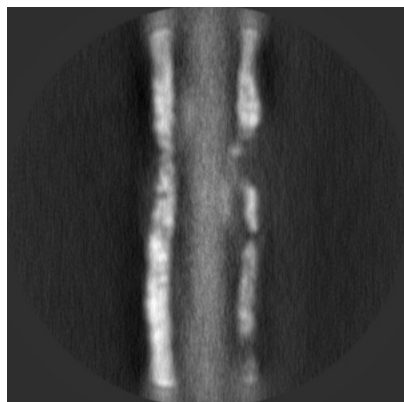


Y Index: 190

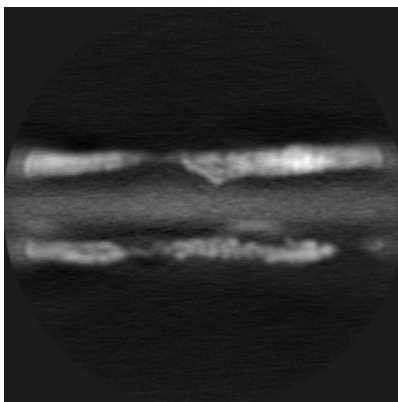


Z Index: 190

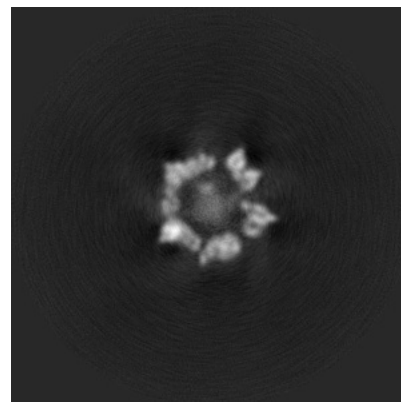
6.2.2 Raw map



X Index: 190



Y Index: 190

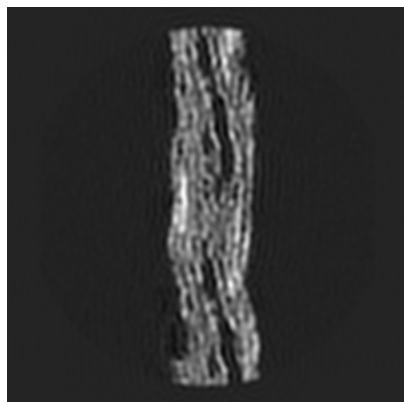


Z Index: 190

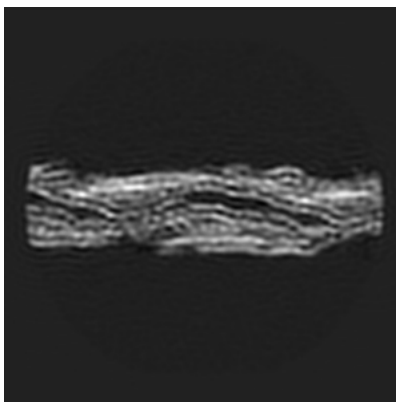
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 155

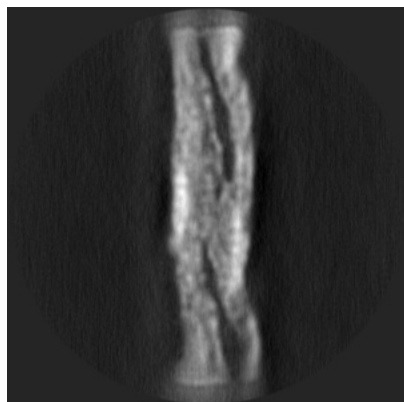


Y Index: 229

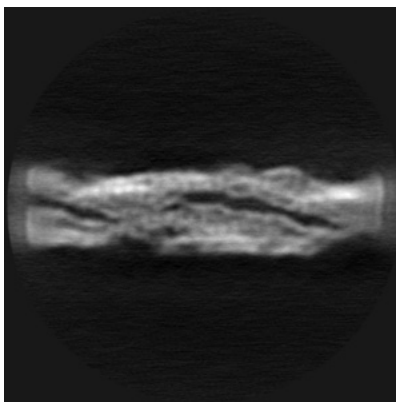


Z Index: 160

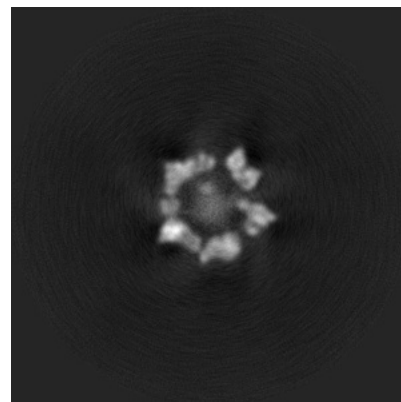
6.3.2 Raw map



X Index: 153



Y Index: 229

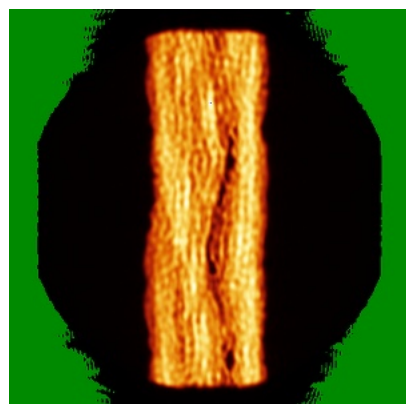


Z Index: 194

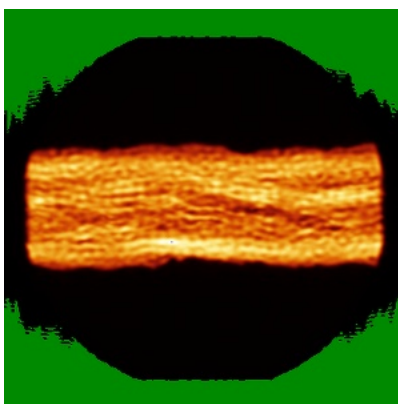
The images above show the largest variance slices of the map in three orthogonal directions.

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

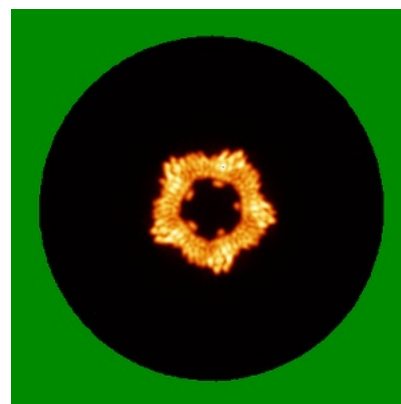
6.4.1 Primary map



X

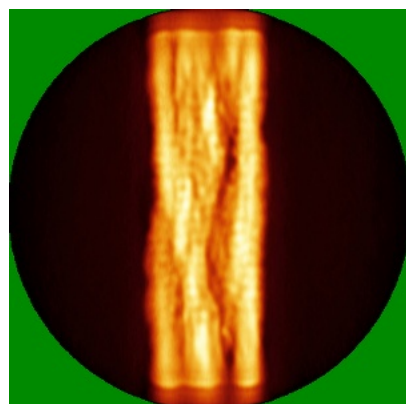


Y

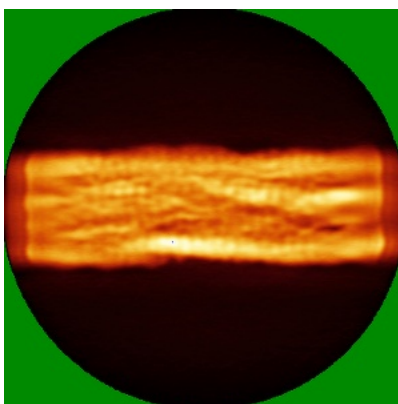


Z

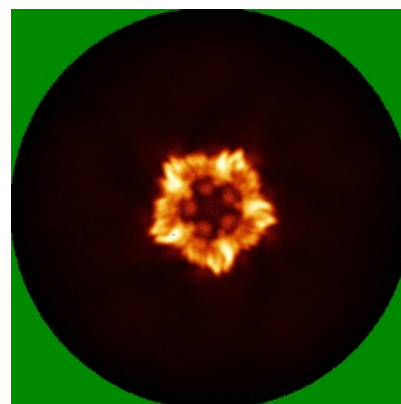
6.4.2 Raw map



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.

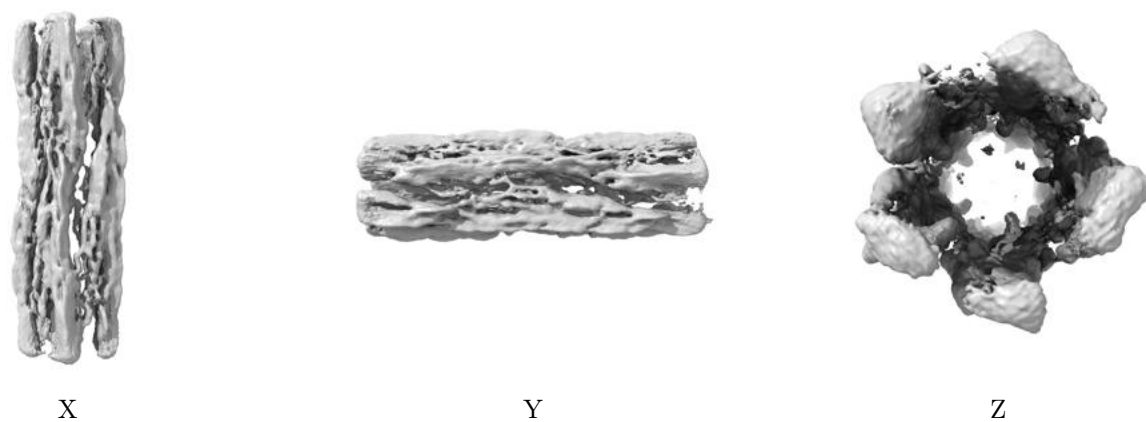
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation [i](#)

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

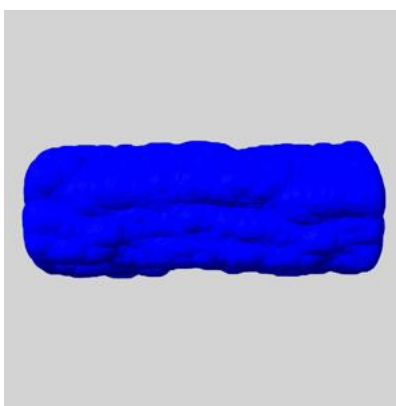
A mask typically either:

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

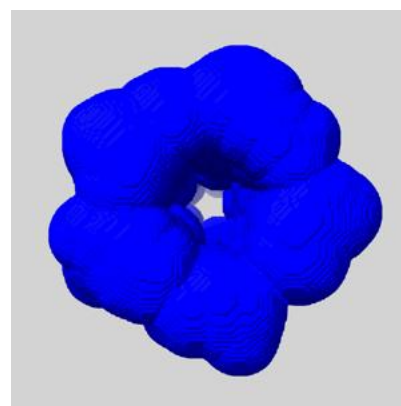
6.6.1 emd_16844_msk_1.map [i](#)



X



Y

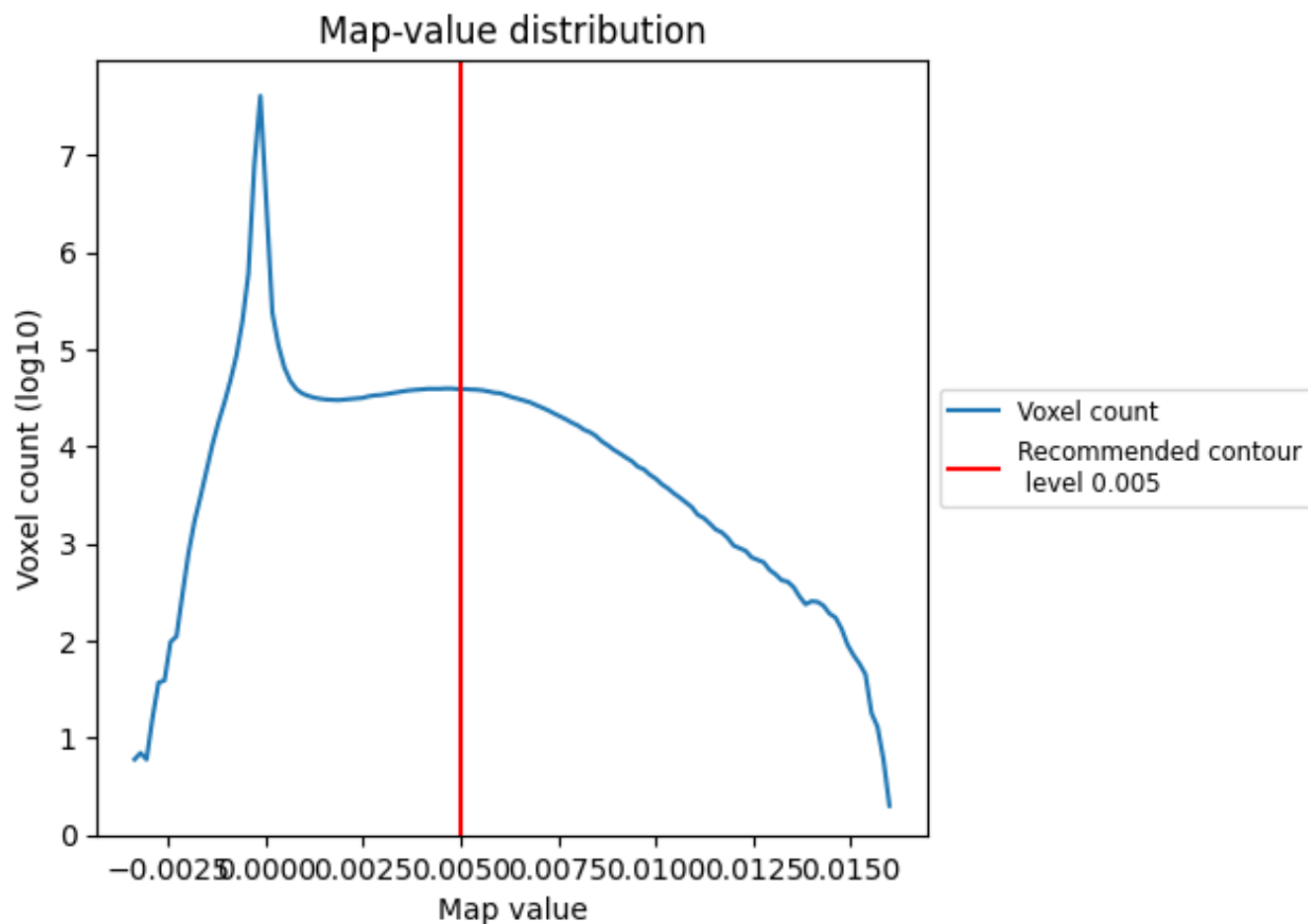


Z

7 Map analysis [i](#)

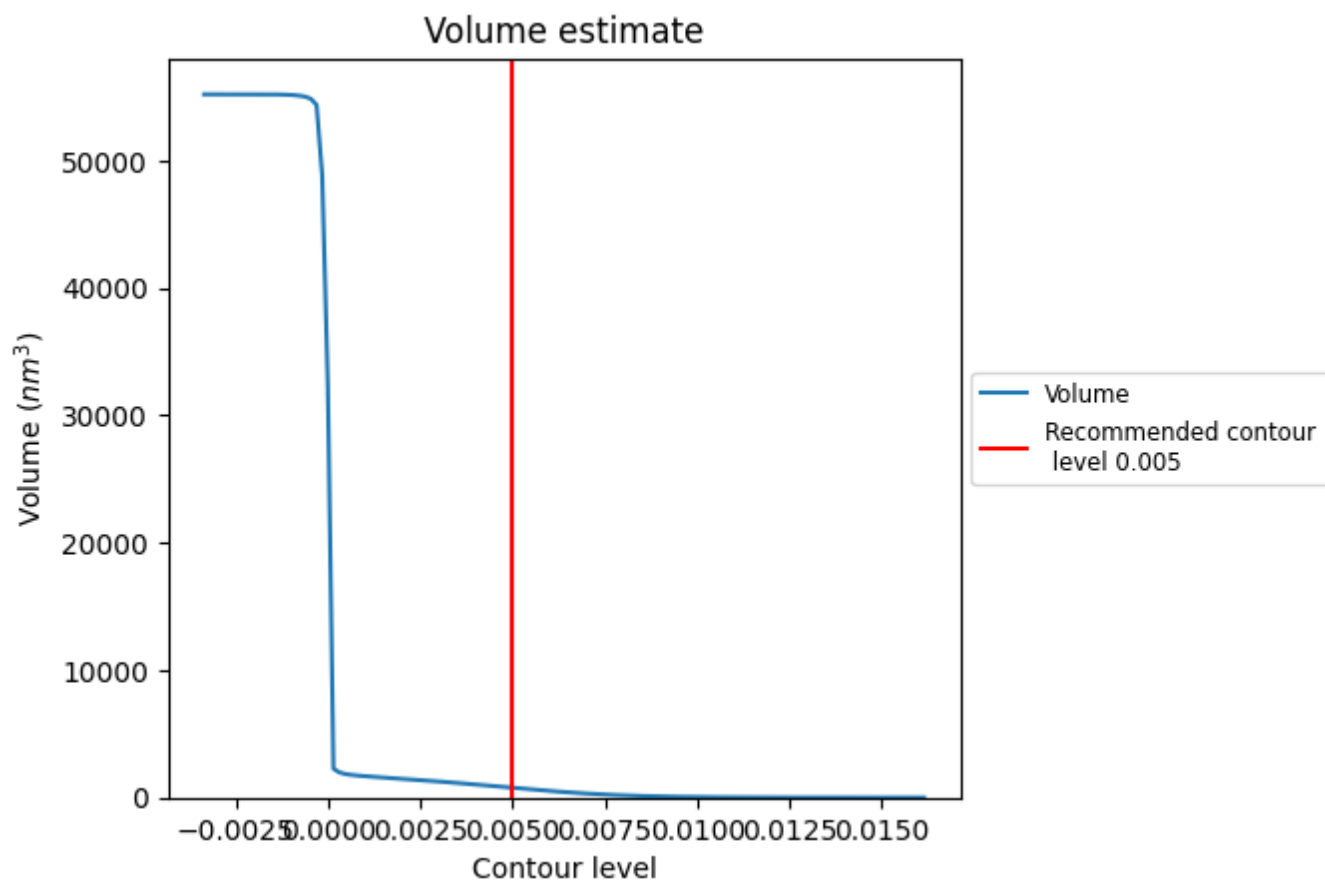
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

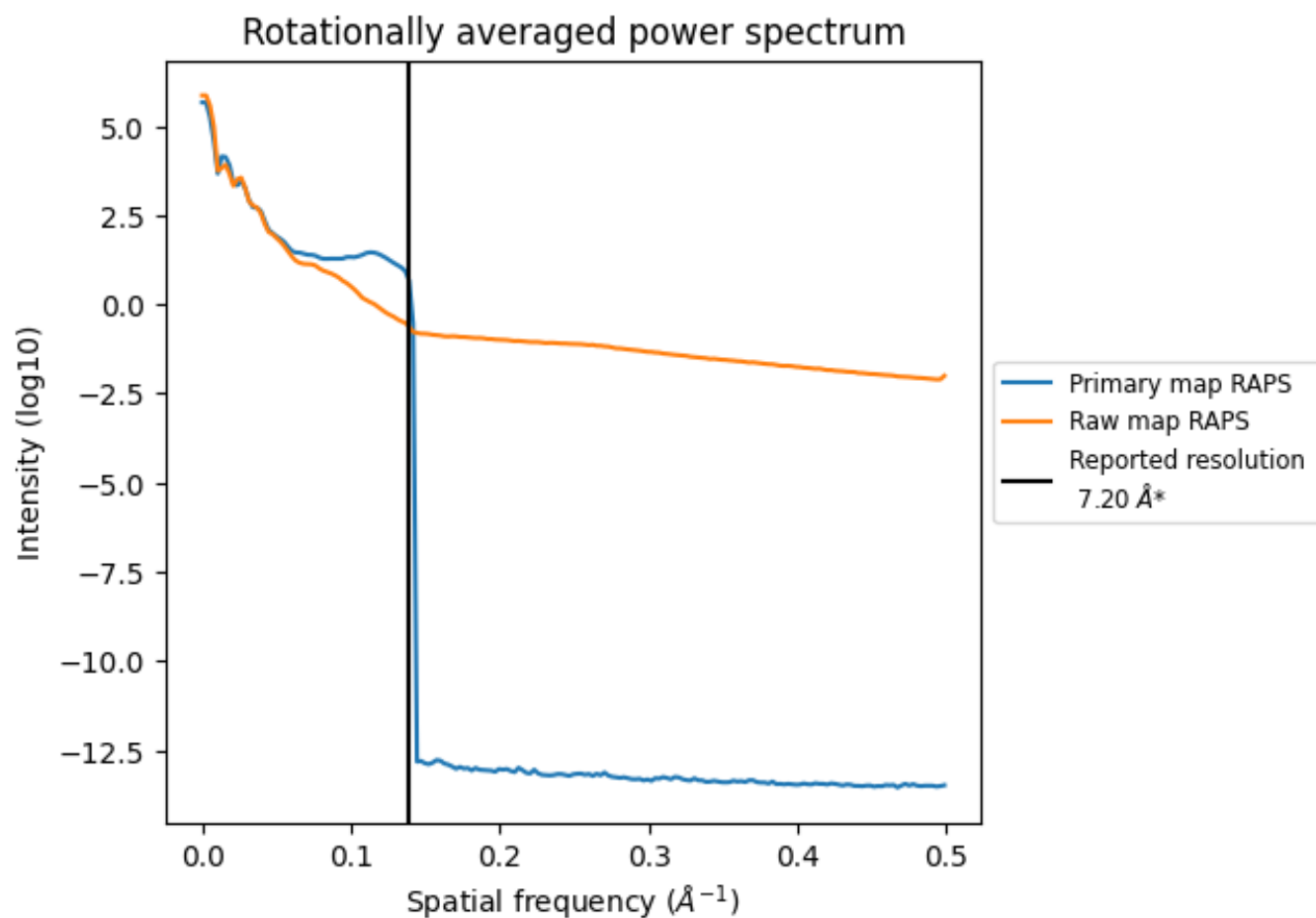
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 768 nm³; this corresponds to an approximate mass of 694 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

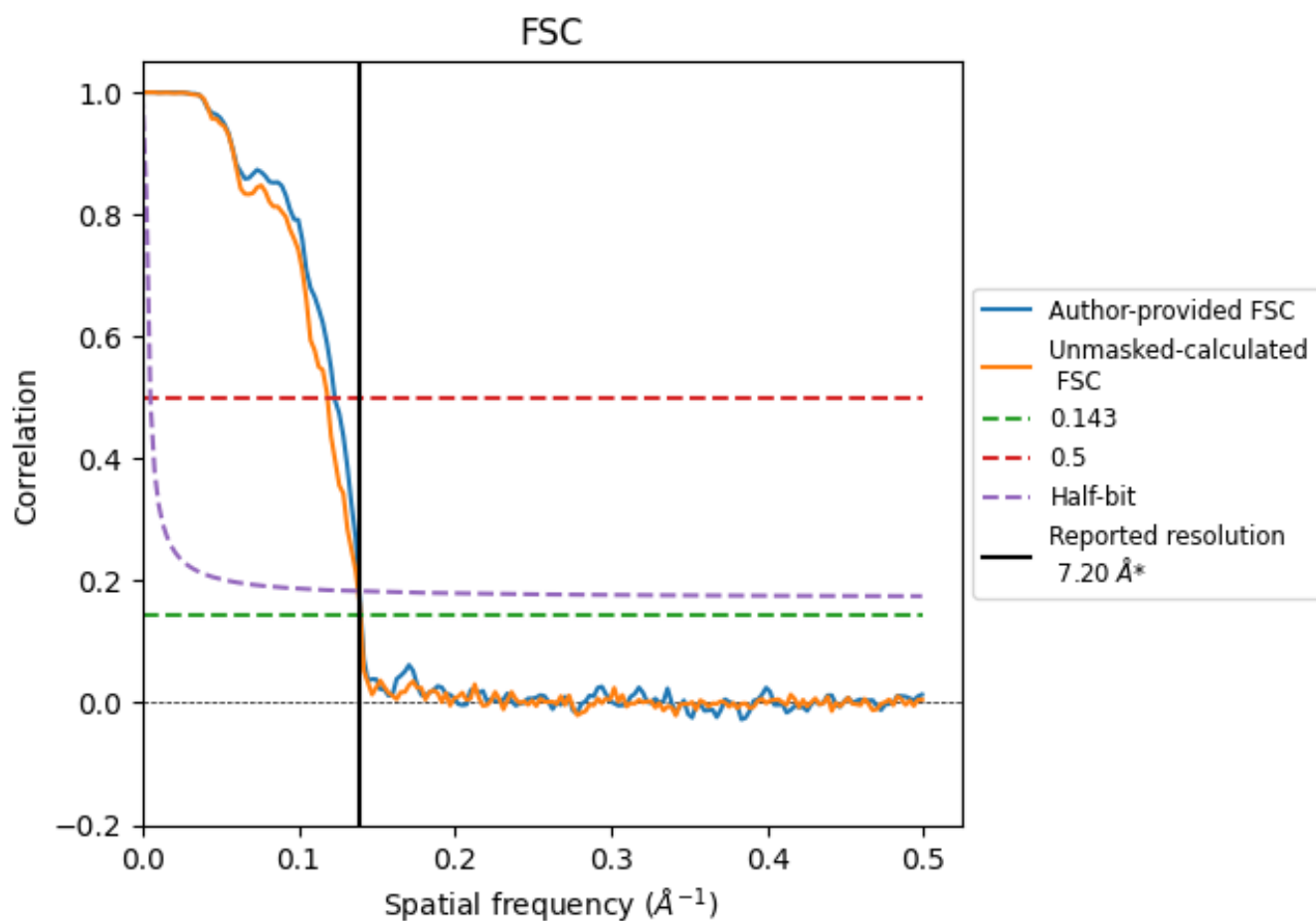


*Reported resolution corresponds to spatial frequency of 0.139 Å⁻¹

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 0.139 Å⁻¹

8.2 Resolution estimates [i](#)

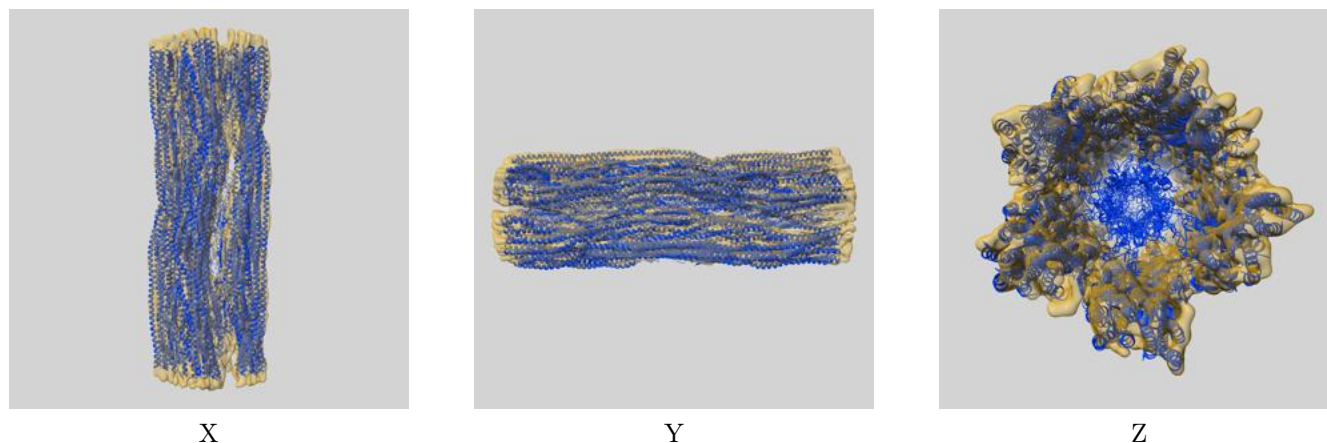
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.15	8.12	7.20
Unmasked-calculated*	7.16	8.44	7.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

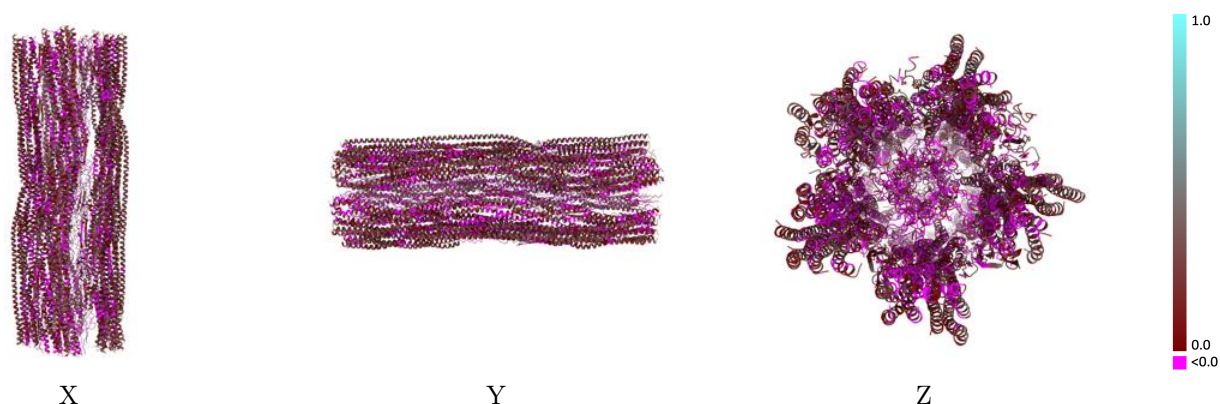
This section contains information regarding the fit between EMDB map EMD-16844 and PDB model 8RVE. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



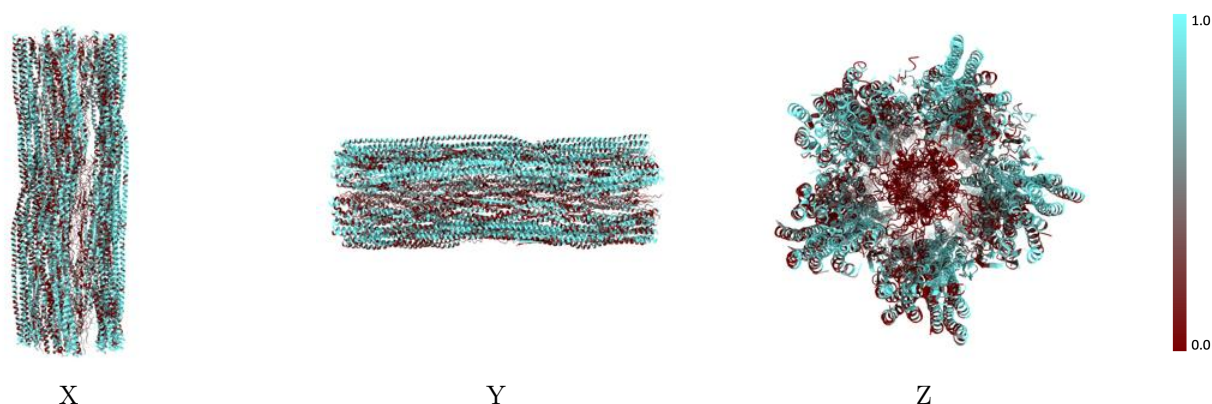
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



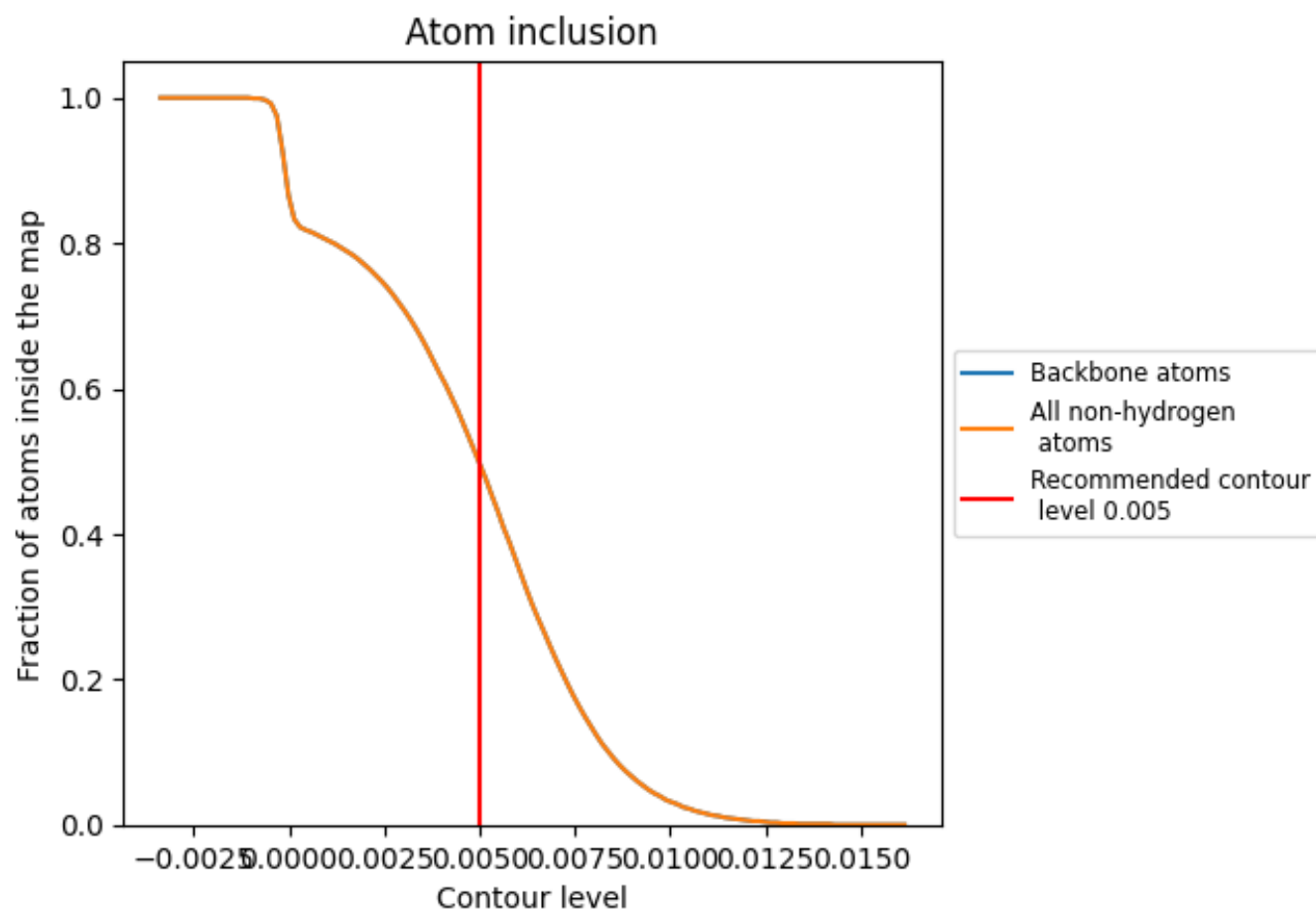
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4970	 0.0920
0	 0.8250	 0.1680
1	 0.5410	 0.0730
2	 0.5630	 0.0820
3	 0.3770	 0.0510
4	 0.2820	 0.0750
5	 0.6830	 0.0840
6	 0.7030	 0.1090
7	 0.3500	 0.0680
8	 0.2760	 0.0540
9	 0.6940	 0.1300
A	 0.5140	 0.0930
AA	 0.3160	 0.0240
AB	 0.3000	 0.0570
AC	 0.6500	 0.0890
AD	 0.7540	 0.1890
AE	 0.2040	 -0.0010
AF	 0.2590	 0.0200
AG	 0.6810	 0.0890
AH	 0.6870	 0.1600
AI	 0.7200	 0.0860
AJ	 0.6650	 0.0950
AK	 0.7100	 0.0940
AL	 0.7310	 0.1290
AM	 0.6940	 0.1020
AN	 0.7940	 0.1600
AO	 0.5510	 0.0780
AP	 0.6150	 0.1930
B	 0.4970	 0.1110
C	 0.4750	 0.1070
D	 0.4510	 0.0870
E	 0.3560	 0.0870
F	 0.4640	 0.0610
G	 0.4180	 0.1060
H	 0.4310	 0.0640



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
I	 0.6490	 0.1830
J	 0.5060	 0.0960
K	 0.5510	 0.1580
L	 0.5350	 0.1280
M	 0.4780	 0.1290
N	 0.4910	 0.1420
O	 0.4090	 0.1240
P	 0.4590	 0.1490
Q	 0.0540	 0.0500
R	 0.1250	 0.0700
S	 0.5750	 0.1620
T	 0.5680	 0.1650
U	 0.1740	 0.0250
V	 0.1670	 -0.0820
W	 0.7650	 0.2040
X	 0.7730	 0.1980
Y	 0.2830	 0.0730
Z	 0.2870	 0.0490
a	 0.6840	 0.1720
b	 0.6110	 0.1650
c	 0.3140	 0.0730
d	 0.2930	 0.0250
e	 0.5310	 0.1250
f	 0.5020	 0.1390
g	 0.2440	 0.0460
h	 0.3120	 -0.0040
i	 0.4550	 0.0750
j	 0.4950	 0.1140
k	 0.2530	 0.0370
l	 0.2490	 0.0010
m	 0.5130	 0.0800
n	 0.4900	 0.1180
o	 0.3540	 0.0750
p	 0.3580	 0.0410
q	 0.4180	 0.0470
r	 0.3760	 0.0690
s	 0.4700	 0.0930
t	 0.4990	 0.0710
u	 0.4290	 0.0280
v	 0.3550	 0.0400
w	 0.4820	 0.0720
x	 0.5250	 0.0540

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
y	 0.4100	 0.0390
z	 0.3190	 0.0280