



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:53 PM UTC

PDB ID : 6Q16 / pdb_00006q16
EMDB ID : EMD-20556
Title : Focussed refinement of InvGN0N1:PrgHK:SpaPQR:PrgIJ from Salmonella SPI-1 injectisome NC-base
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2019-08-02
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

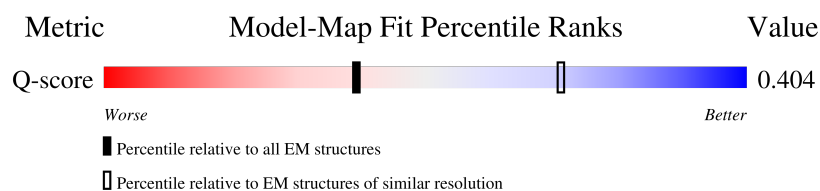
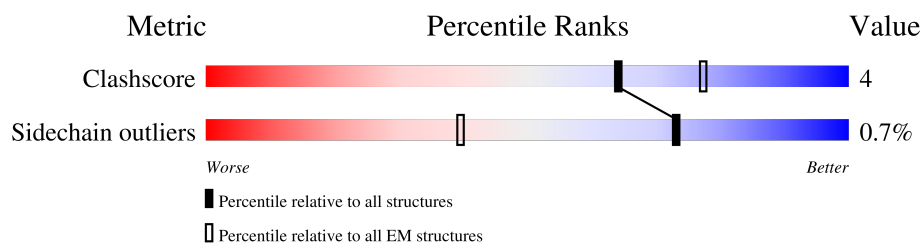
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

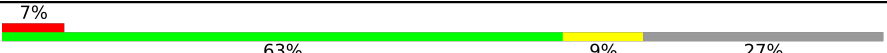
The reported resolution of this entry is 4.10 Å.

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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	AA	252	
1	AB	252	
1	AC	252	
1	AD	252	
1	AE	252	

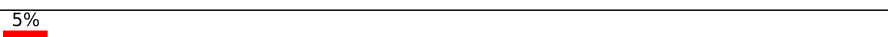
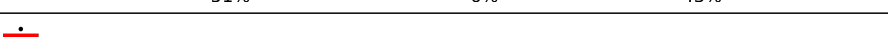
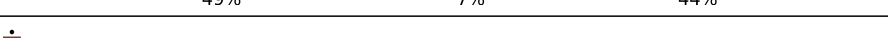
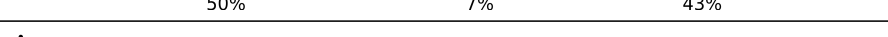
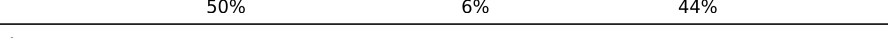
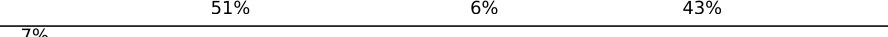
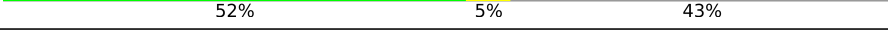
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Mol	Chain	Length	Quality of chain
1	AF	252	
1	AG	252	
1	AH	252	
1	AI	252	
1	AJ	252	
1	AK	252	
1	AL	252	
1	o	252	
1	p	252	
1	q	252	
1	r	252	
1	s	252	
1	t	252	
1	u	252	
1	v	252	
1	w	252	
1	x	252	
1	y	252	
1	z	252	
2	A	562	
2	B	562	
2	C	562	
2	D	562	
2	F	562	
2	G	562	

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Mol	Chain	Length	Quality of chain
2	H	562	
2	I	562	
2	J	562	
2	K	562	
2	L	562	
2	M	562	
2	N	562	
2	O	562	
2	P	562	
2	Q	562	
3	E	392	
3	R	392	
3	S	392	
3	T	392	
3	U	392	
3	V	392	
3	W	392	
3	X	392	
3	Y	392	
3	Z	392	
3	a	392	
3	b	392	
3	c	392	
3	d	392	
3	e	392	

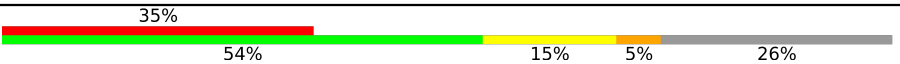
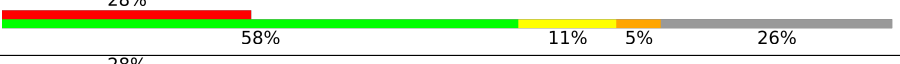
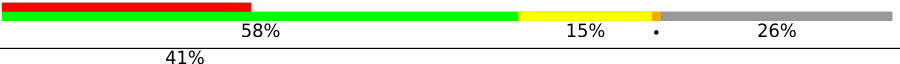
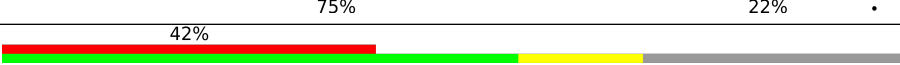
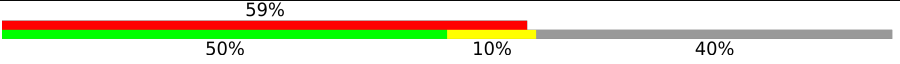
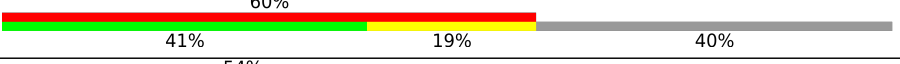
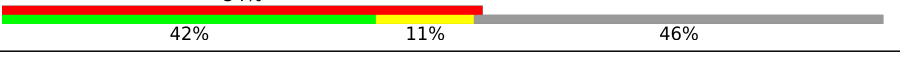
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Mol	Chain	Length	Quality of chain
3	f	392	
3	g	392	
3	h	392	
3	i	392	
3	j	392	
3	k	392	
3	l	392	
3	m	392	
3	n	392	
4	0	224	
4	1	224	
4	2	224	
4	3	224	
4	4	224	
5	5	263	
6	6	86	
6	7	86	
6	8	86	
6	9	86	
7	AM	101	
7	AN	101	
7	AO	101	
7	AP	101	
7	AQ	101	
7	AR	101	

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Mol	Chain	Length	Quality of chain
8	AS	80	
8	AT	80	
8	AU	80	
8	AV	80	
8	AW	80	
8	AX	80	
8	AY	80	
8	AZ	80	
8	BA	80	
8	BB	80	
8	BC	80	
8	BD	80	
8	BE	80	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 118198 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipoprotein PrgK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AB	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AC	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AD	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AE	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AF	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AG	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AH	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AI	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AL	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	o	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	p	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	q	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	r	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	s	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	t	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	u	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	w	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	x	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	y	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	z	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AJ	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AK	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		

- Molecule 2 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	B	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	C	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	D	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		
2	F	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	G	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	H	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	I	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	J	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	K	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	L	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	M	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	O	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	P	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	Q	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		

- Molecule 3 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	R	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	S	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
3	T	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	U	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	V	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
3	W	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	X	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	Y	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
3	Z	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	a	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	b	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
3	c	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	d	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	e	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	g	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	h	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
3	i	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	j	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	k	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
3	l	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
3	m	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
3	n	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		

- Molecule 4 is a protein called Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	199	Total	C	N	O	S	0	0
			1562	1041	231	279	11		
4	1	199	Total	C	N	O	S	0	0
			1569	1047	232	279	11		
4	2	197	Total	C	N	O	S	0	0
			1553	1037	230	275	11		
4	3	204	Total	C	N	O	S	0	0
			1606	1071	238	286	11		
4	4	221	Total	C	N	O	S	1	0
			1758	1163	266	318	11		

- Molecule 5 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	247	Total	C	N	O	S	0	0
			1885	1252	300	320	13		

- Molecule 6 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	53	Total	C	N	O	S	0	0
			405	276	61	67	1		
6	7	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
6	8	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
6	9	84	Total	C	N	O	S	0	0
			647	438	97	109	3		

- Molecule 7 is a protein called Protein PrgJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AM	39	Total	C	N	O	S	0	0
			298	187	49	60	2		
7	AN	78	Total	C	N	O	S	7	0
			644	396	116	130	2		
7	AO	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AP	89	Total	C	N	O	S	0	0
			675	416	115	141	3		
7	AQ	89	Total	C	N	O	S	0	0
			675	416	115	141	3		
7	AR	88	Total	C	N	O	S	0	0
			667	410	114	140	3		

- Molecule 8 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AS	59	Total	C	N	O	0	0
			466	294	80	92		
8	AT	59	Total	C	N	O	0	0
			466	294	80	92		
8	AU	59	Total	C	N	O	0	0
			466	294	80	92		
8	AV	59	Total	C	N	O	0	0
			466	294	80	92		
8	AW	59	Total	C	N	O	0	0
			466	294	80	92		
8	AX	73	Total	C	N	O	0	0
			574	362	95	117		
8	AY	78	Total	C	N	O	0	0
			612	387	101	124		
8	AZ	57	Total	C	N	O	0	0
			460	289	76	95		

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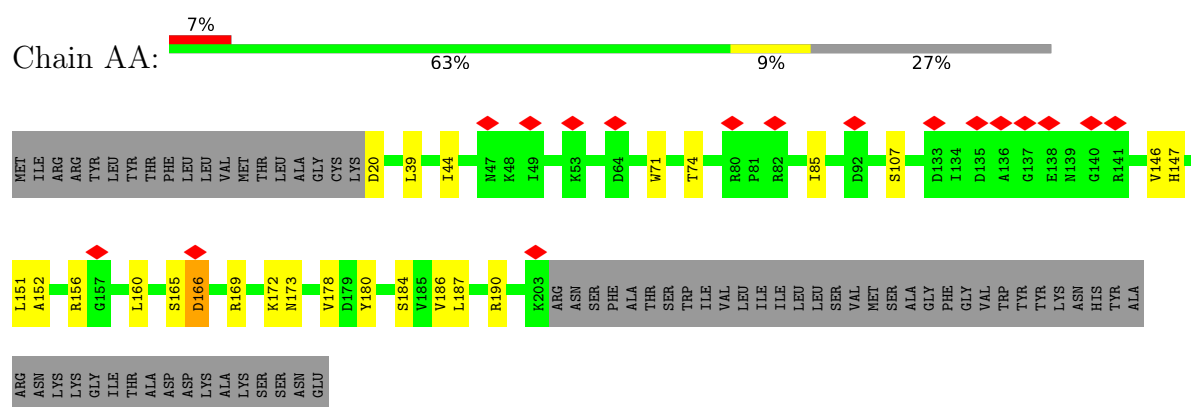
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Mol	Chain	Residues	Atoms				AltConf	Trace
8	BA	54	Total	C	N	O	0	0
			437	275	73	89		
8	BB	48	Total	C	N	O	0	0
			388	247	64	77		
8	BC	48	Total	C	N	O	0	0
			388	247	64	77		
8	BD	48	Total	C	N	O	0	0
			388	247	64	77		
8	BE	43	Total	C	N	O	0	0
			346	219	59	68		

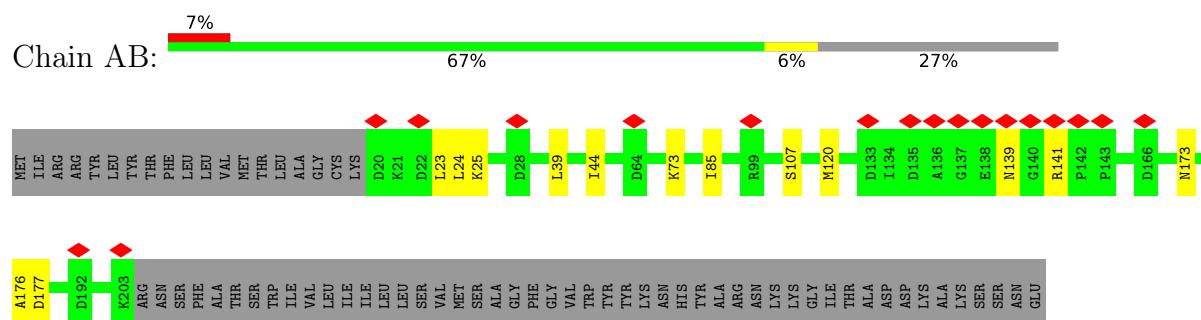
3 Residue-property plots

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

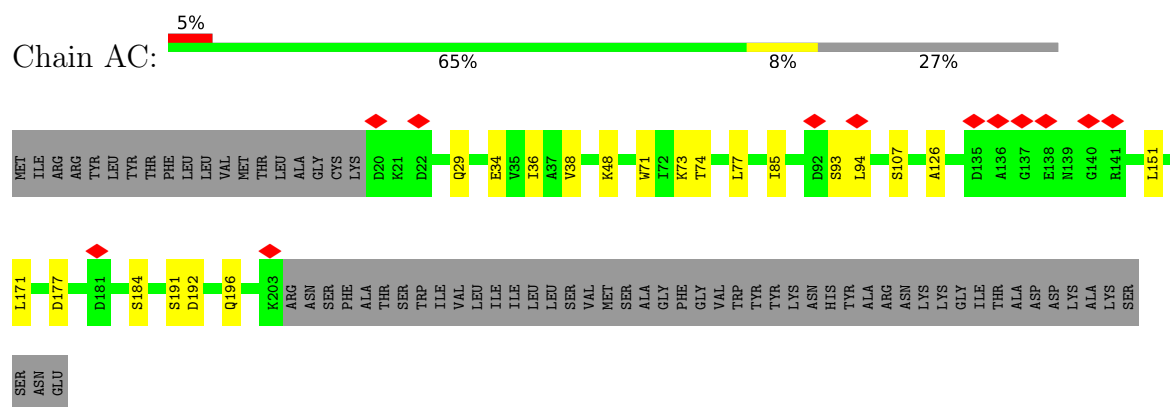
• Molecule 1: Lipoprotein PrgK



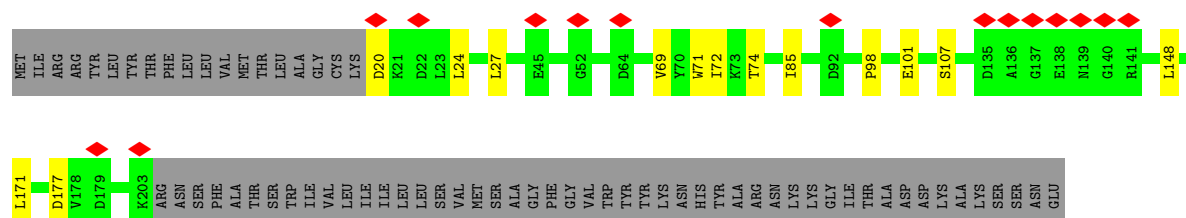
• Molecule 1: Lipoprotein PrgK



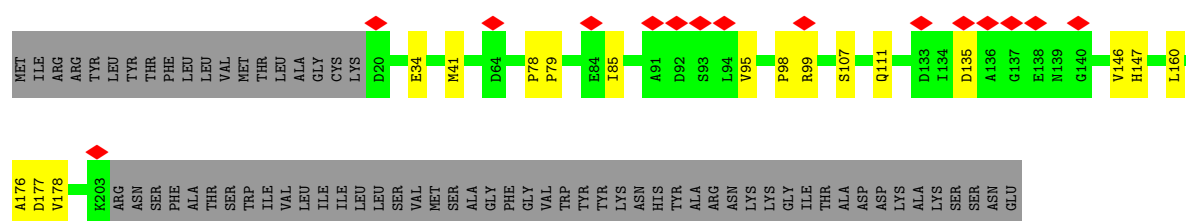
• Molecule 1: Lipoprotein PrgK



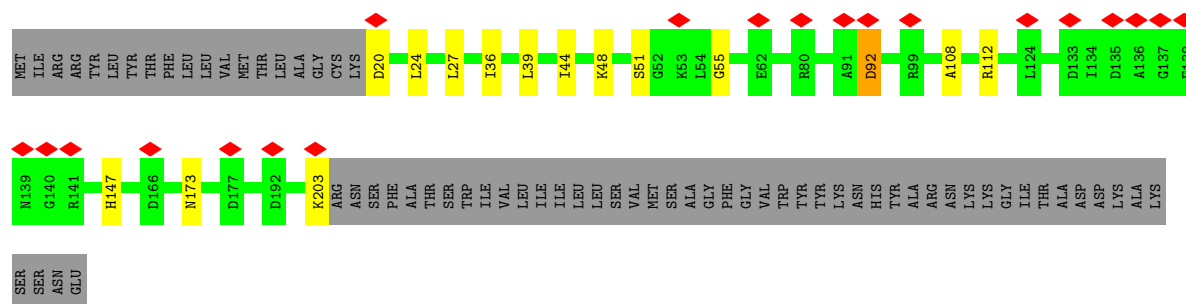
• Molecule 1: Lipoprotein PrgK

Chain AD: 

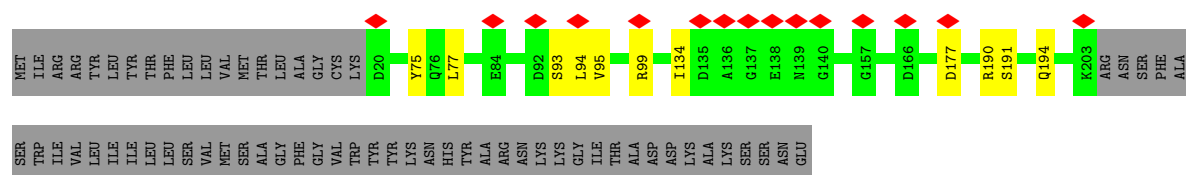
• Molecule 1: Lipoprotein PrgK

Chain AE: 

• Molecule 1: Lipoprotein PrgK

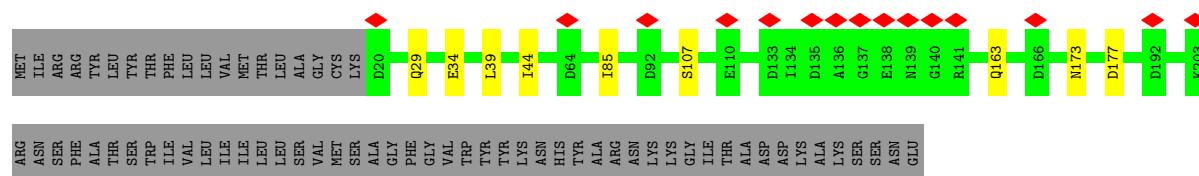
Chain AF: 

• Molecule 1: Lipoprotein PrgK

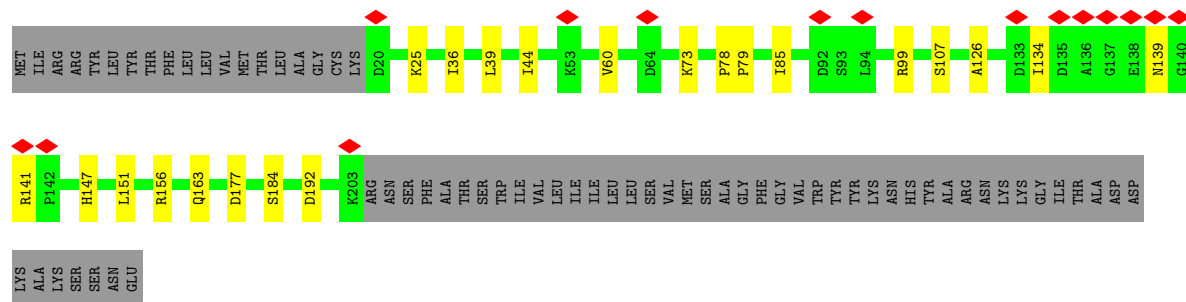
Chain AG: 

• Molecule 1: Lipoprotein PrgK

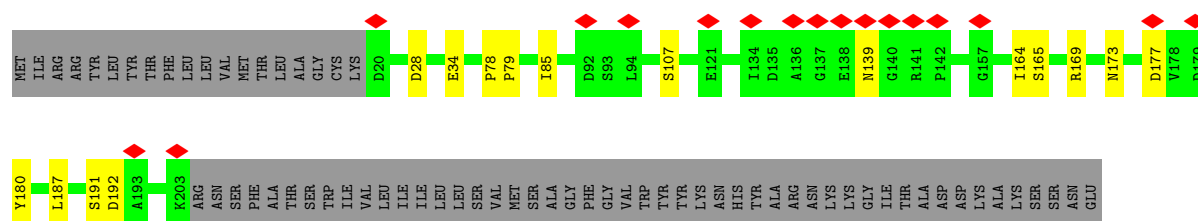
Chain AH: 



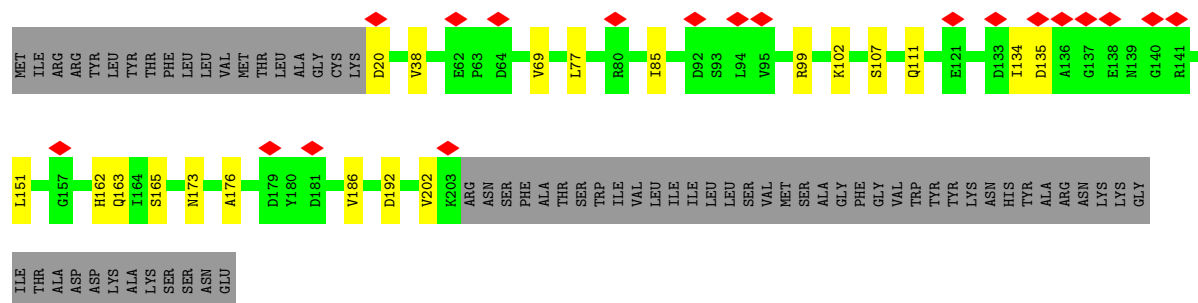
• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK

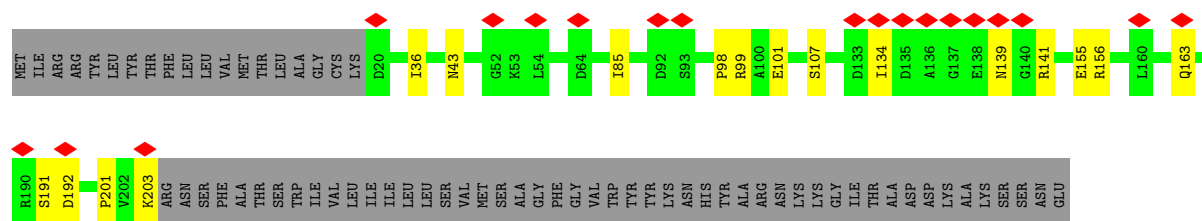


• Molecule 1: Lipoprotein PrgK

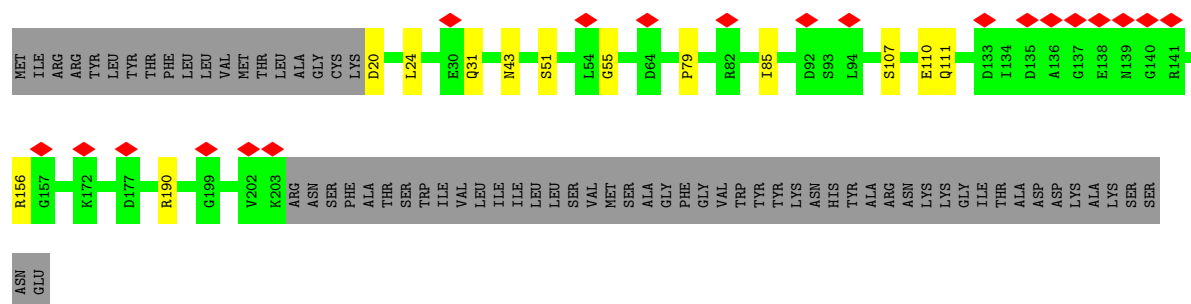


• Molecule 1: Lipoprotein PrgK

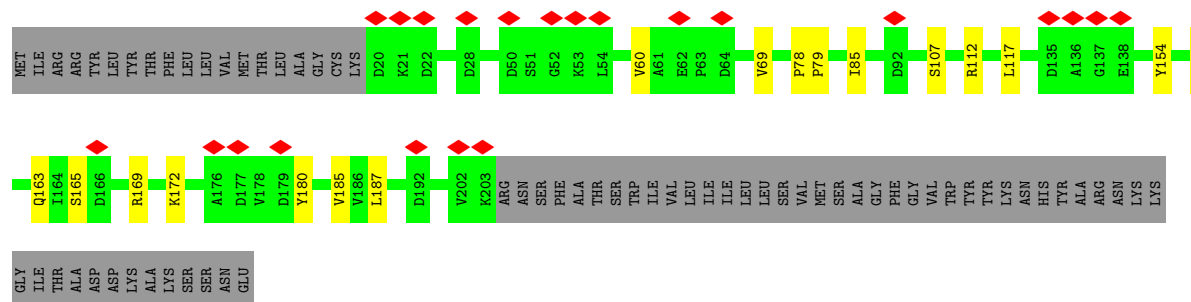




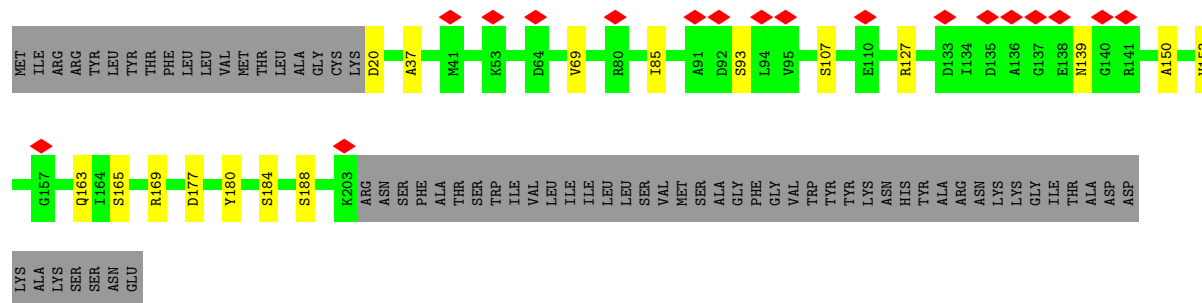
- Molecule 1: Lipoprotein PrgK



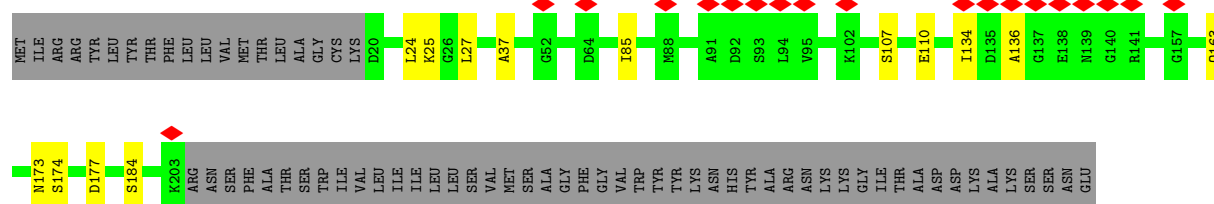
- Molecule 1: Lipoprotein PrgK



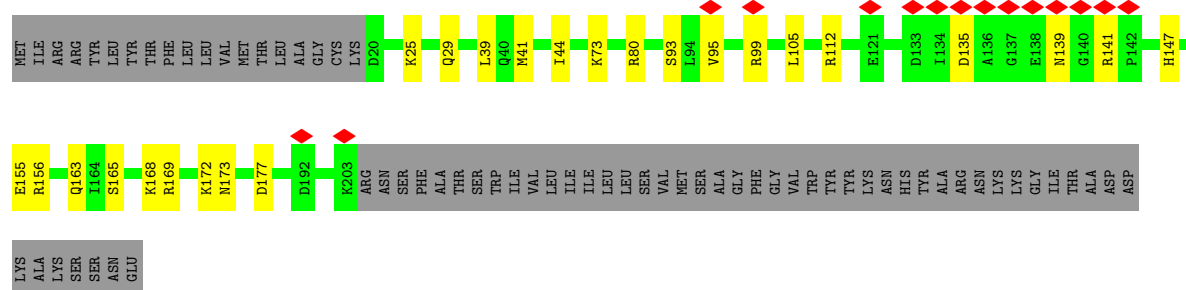
- Molecule 1: Lipoprotein PrgK



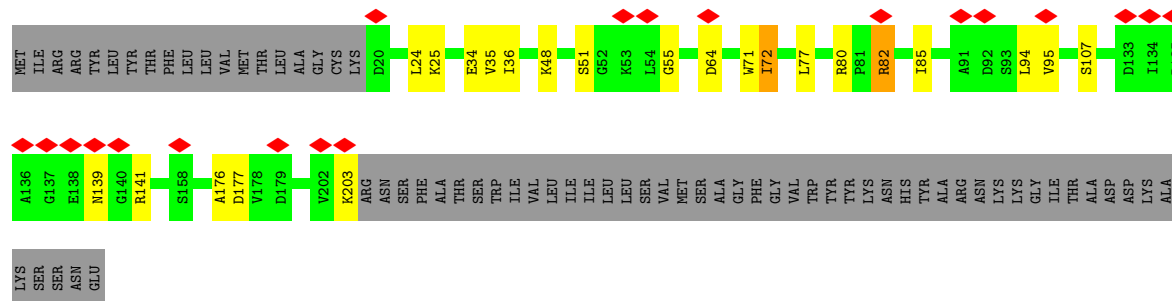
- Molecule 1: Lipoprotein PrgK



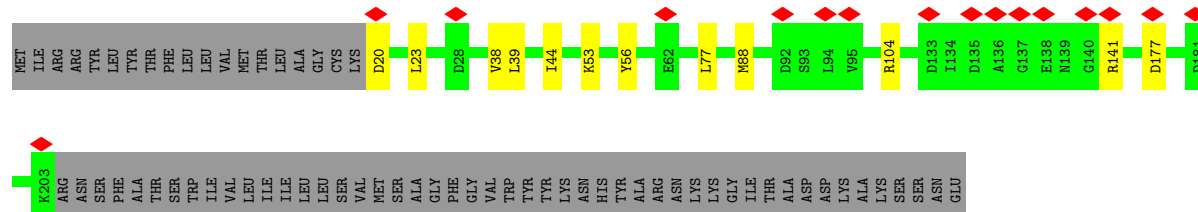
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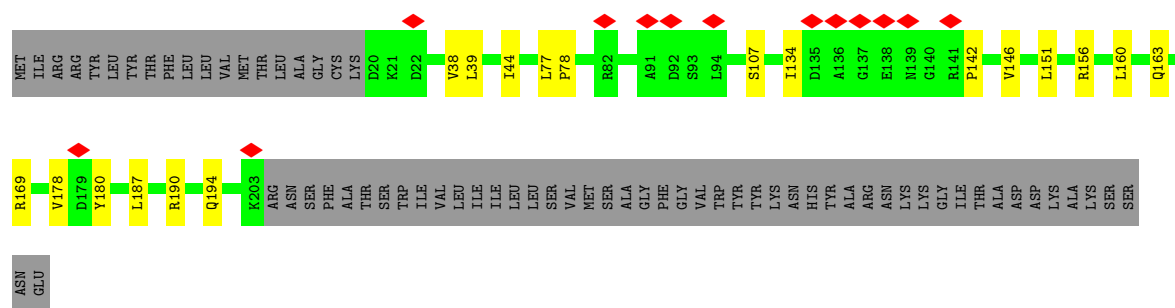
- Molecule 1: Lipoprotein PrgK



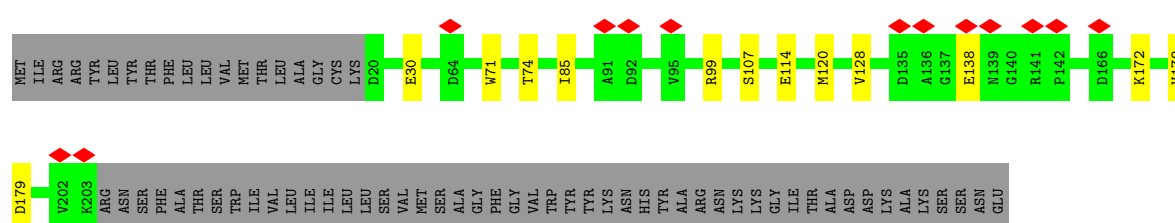
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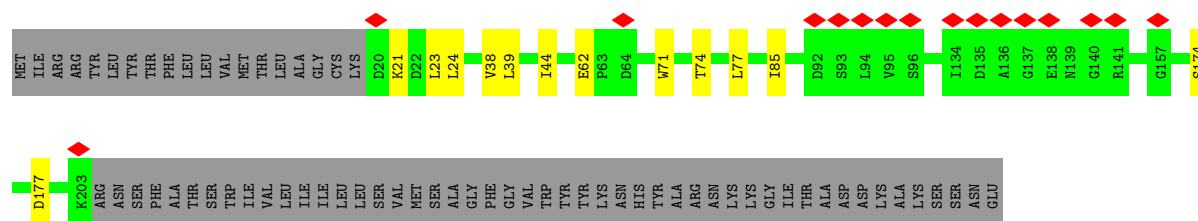
- Molecule 1: Lipoprotein PrgK



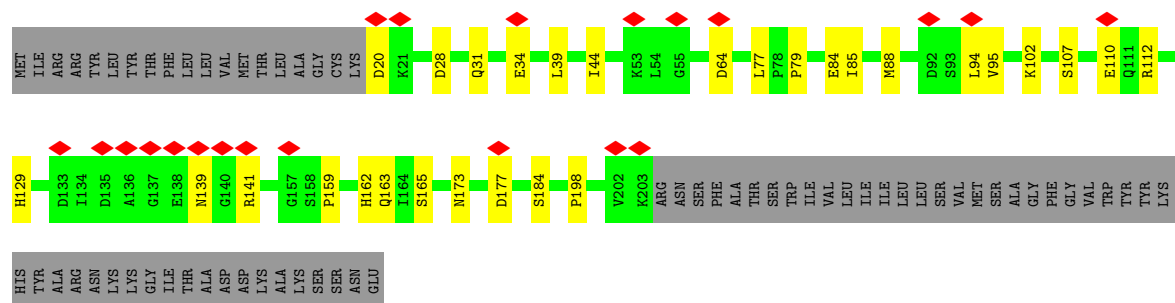
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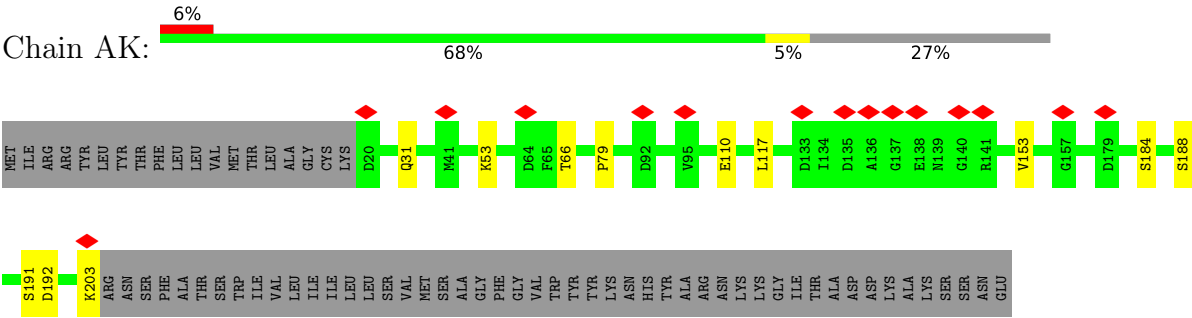
- Molecule 1: Lipoprotein PrgK



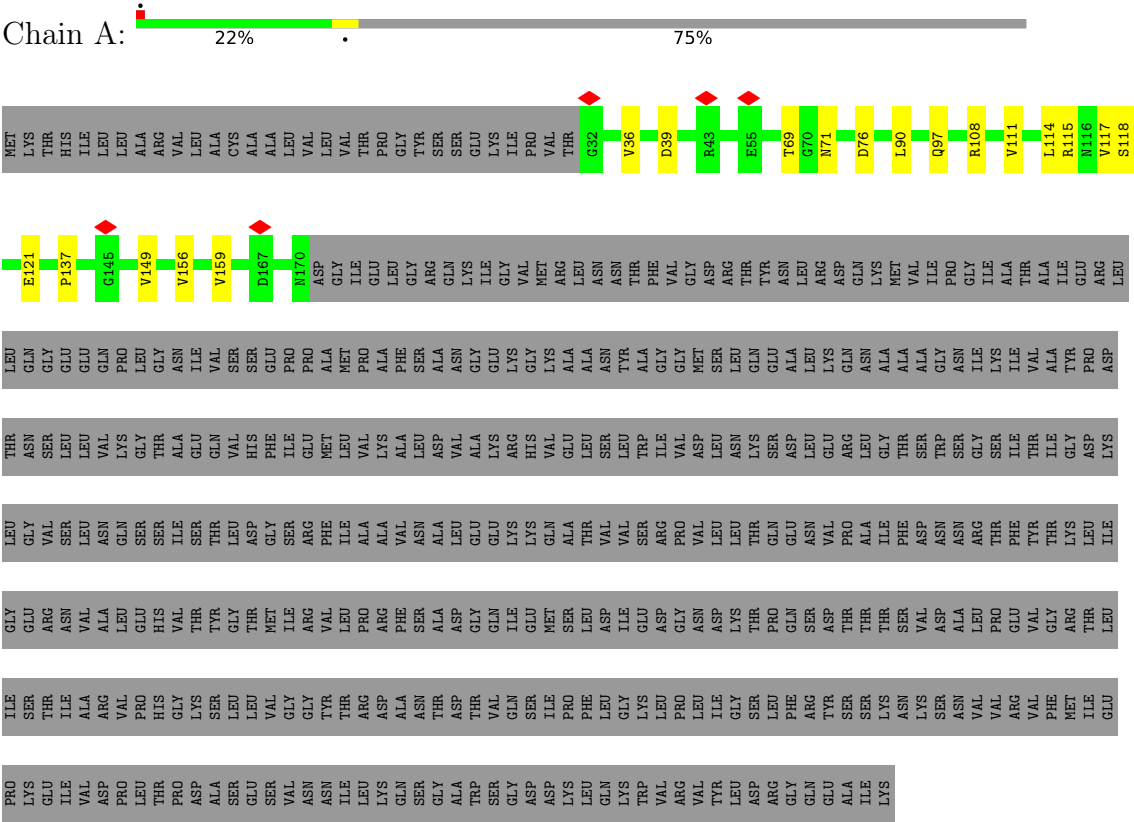
- Molecule 1: Lipoprotein PrgK



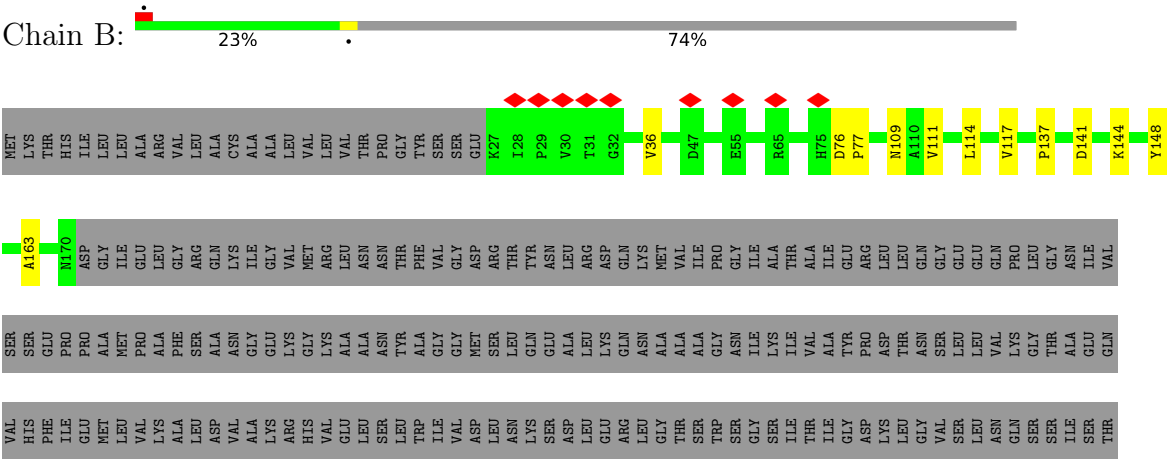
- Molecule 1: Lipoprotein PrgK



● Molecule 2: Protein InvG



● Molecule 2: Protein InvG



[illegible]

- Molecule 2: Protein InvG

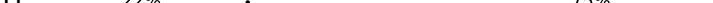
[illegible]

- Molecule 2: Protein InvG

[illegible]

[illegible]

- Molecule 2: Protein InvG

Chain H:  22% . 75%

ASN	ASN	GLY	ARG	ARG	PHE	GLU	PRO	ASP	MET
ASN	ASN	TYR	VAL	VAL	PHE	MET	ALA	GLY	LYS
ILE	ILE	THR	LEU	LEU	ILE	MET	VAL	ILE	THR
LEU	LEU	ARG	PRO	ARG	ALA	VAL	LYS	GLU	HIS
LEU	LEU	ASP	ARG	ARG	VAL	LEU	ALA	GLY	LEU
GLN	GLN	ALA	PHE	PHE	ASN	ALA	PHE	GLY	LEU
SER	SER	ASN	SER	SER	ASN	LEU	SER	ARG	LEU
GLY	GLY	THR	ALA	ALA	ALA	ASP	ALA	GLN	ALA
ALA	ALA	ASP	ASP	ASP	LEU	VAL	ASN	LYS	ARG
TRP	TRP	THR	GLY	GLY	GLU	ALA	GLY	ILE	VAL
SER	SER	VAL	GLN	GLN	GLU	LYS	GLY	GLY	LEU
GLY	GLY	GLN	ILE	ILE	LYS	ARG	LEU	VAL	ALA
ASP	ASP	SER	GLU	GLU	LYS	HIS	GLY	MET	CYS
ASN	ASN	ILE	MET	MET	GLN	VAL	GLY	ARG	ALA
LYS	LYS	PRO	SER	SER	VAL	GLU	ALA	LYS	ALA
LEU	LEU	PHE	LEU	LEU	THR	LEU	LEU	ILE	VAL
GLN	GLN	LEU	ASP	VAL	VAL	SER	ALA	ASN	VAL
LYS	LYS	GLY	ILE	ILE	VAL	LEU	TYR	THR	LEU
TRP	TRP	LYS	GLU	SER	SER	TRP	ALA	PHE	VAL
VAL	VAL	LEU	ASP	ASP	ARG	ILE	GLY	VAL	THR
ARG	ARG	PRO	GLY	PRO	PRO	VAL	GLY	GLY	PRO
VAL	VAL	LEU	ASN	VAL	VAL	ASP	MET	ASP	GLY
TYR	TYR	ILE	ASP	LEU	LEU	SER	SER	ARG	TYR
LEU	LEU	GLY	LYS	LEU	THR	ASN	LEU	THR	SER
ASP	ASP	SER	THR	THR	THR	LYS	GLN	TYR	SER
GLY	GLY	LEU	GLN	GLN	GLN	ASP	GLU	ASN	GLU
GLN	GLN	ARG	SER	SER	GLU	ASP	LEU	ARG	ILE
GLU	GLU	THR	ASP	VAL	ASN	GLU	LYS	ASP	VAL
ALA	ALA	SER	THR	PRO	PRO	ARG	LYS	GLN	VAL
ILE	ILE	SER	THR	THR	ALA	LEU	ASN	LYS	THR
LYS	LYS	LYS	THR	THR	ILE	GLY	ASN	GLY	G32
		ASN	SER	PHE	THR	THR	ALA	VAL	S33
		ASN	VAL	VAL	ASP	SPR	ALA	ILE	G34
		SER	ASP	ASN	ASN	TRP	GLY	PRO	F35
		VAL	ALA	ASN	ASN	SER	ASN	GLY	V36
		VAL	LEU	LEU	ARG	GLY	ILE	ILE	
		VAL	PRO	THR	THR	GLY	LYS	THR	L42
		ARG	GLU	PHE	THR	ILE	VAL	ALA	
		VAL	VAL	TYR	TYR	ILE	VAL	ALA	K64
		PHE	GLY	THR	THR	ILE	VAL	ILE	E55
		MET	ARG	LYS	LYS	GLY	TYR	GLU	P56
		ILE	THR	LEU	ILE	ASP	PRO	ARG	V57
		GLU	ILE	GLY	LYS	THR	THR	LEU	
		PRO	ILE	GLY	GLY	THR	ASN	LEU	K66
		LYS	THR	THR	GLU	VAL	SER	GLY	
		ILE	ILE	THR	ASN	SER	GLY	GLU	I99
		VAL	ALA	VAL	VAL	LEU	LEU	GLU	
		ASP	ARG	ARG	ALA	LEU	VAL	GLU	M107
		PRO	VAL	LEU	LEU	GLN	LYS	PRO	
		LEU	PRO	GLU	THR	SER	GLY	LEU	L138
		THR	HIS	HIS	THR	THR	THR	GLY	R139
		PRO	GLY	VAL	VAL	ILE	ALA	ASN	
		ASP	LYS	THR	THR	GLU	GLY	ILE	R143
		ALA	SER	TYR	THR	GLN	VAL	VAL	
		SER	LEU	GLY	GLY	VAL	VAL	SER	V149
		GLU	LEU	THR	THR	ASP	HIS	SER	S150
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		VAL	GLY	THR	THR	ILE	THR	DEU	

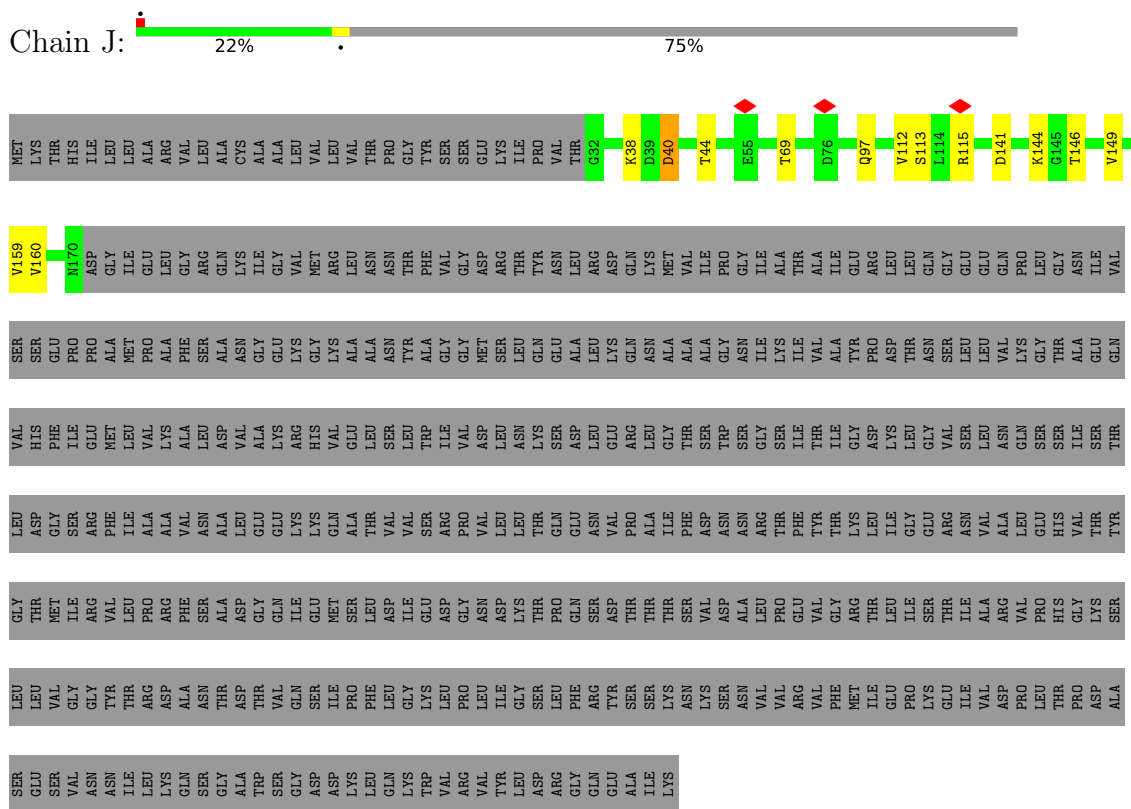
- Molecule 2: Protein InvG

Chain I: 23% 74%

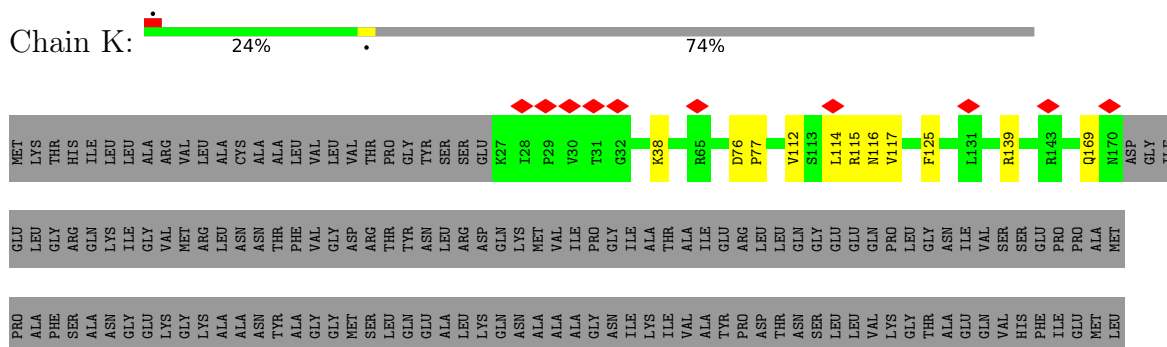
[illegible]

[illegible]

- Molecule 2: Protein InvG



- Molecule 2: Protein InvG



[illegible]

- Molecule 2: Protein InvG

[illegible]

- Molecule 2: Protein InvG



PRO	LEU	GLY	ASN	ILE	VAL	SER	SER	GLU	PRO	PRO	ALA	ALA	MET	PRO	ALA	PHE	GLY	LYS	GLY	LYS	ALA	ALA	GLN	GLY	GLU	GLY	ASN	ALA	ALA	ASN	ASN	TYR	ALA	ALA	GLY	GLY	MET	SER	LEU	GLN	GLU	ALA	LEU	LYS	GLN	ASN	ALA	ALA	GLY	ASN	ILE	ILE	ILE	ILE	VAL	VAL	ALA	ALA	TYR	PRO	ASP	THR	ASN	LEU	GLU	VAL
P152	P153		M158		A163	T164	M165	N170	ASP	GLY	ILE	GLU	GLY	LEU	ARG	GLN	LYS	ILE	GLY	VAL	MET	ARG	LEU	ASN	ASN	THR	PHE	GLY	VAL	GLY	ASP	ARG	THR	TYR	ASN	LEU	ARG	ASP	GLN	LYS	MET	VAL	ILE	ILE	PRO	GLY	ILE	ALA	ALA	THR	ALA	ILE	ALA	ILE	GLU	ARG	LEU	LEU	GLN	GLY	GLU	GLN				
MET	THR	LYS	HIS	ILE	LEU	LEU	ALA	ARG	VAL	LEU	ALA	CYS	ALA	ALA	LEU	LEU	VAL	VAL	THR	PRO	GLY	TYR	SER	SER	GLU	K27	I28	P29	V30	T31	G32		D39	T44	E55	T69	Q97	L114	R115	N120	E121	N124	F125	L126	R139	G140	R143	F147																		

[illegible]

- Molecule 2: Protein InvG

Chain N: 22% 75%

[illegible]

- Molecule 2: Protein InvG

Chain 0: 23% 74%

[illegible]

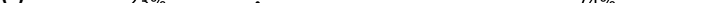
[illegible]

- Molecule 2: Protein InvG

Chain P: 21% 75%

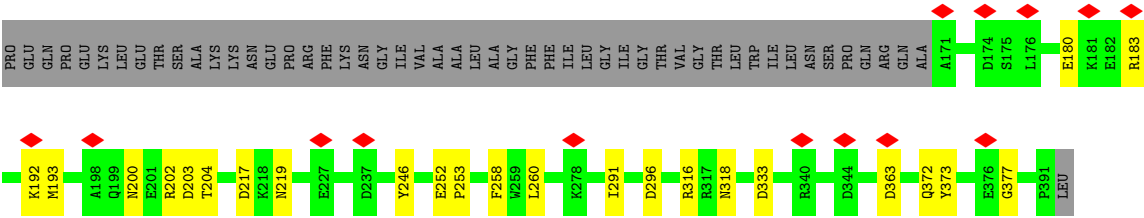
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- Molecule 2: Protein InvG

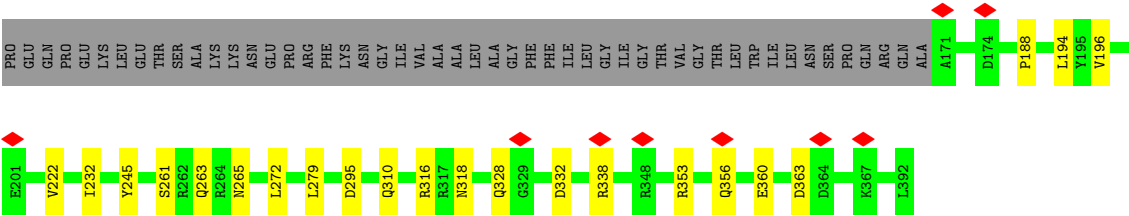
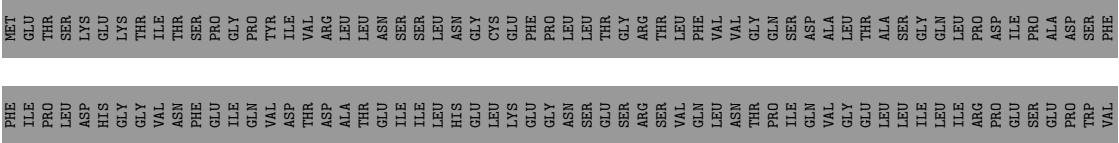
Chain Q:  23% 74%

MET	LYS	THR	HIS	ILE	LEU	LEU	ALA	ARG	VAL	LEU	ALA	CYS	ALA	ALA	LEU	VAL	LEU	THR	PRO	GLY	TYR	SER	SER	GLU	K27	I28	P29	V30	T31	V36	D39	D40	T44	T69	N78	Q87	Q97	S105	R115	D141	K144	V149	M158	V159	M161
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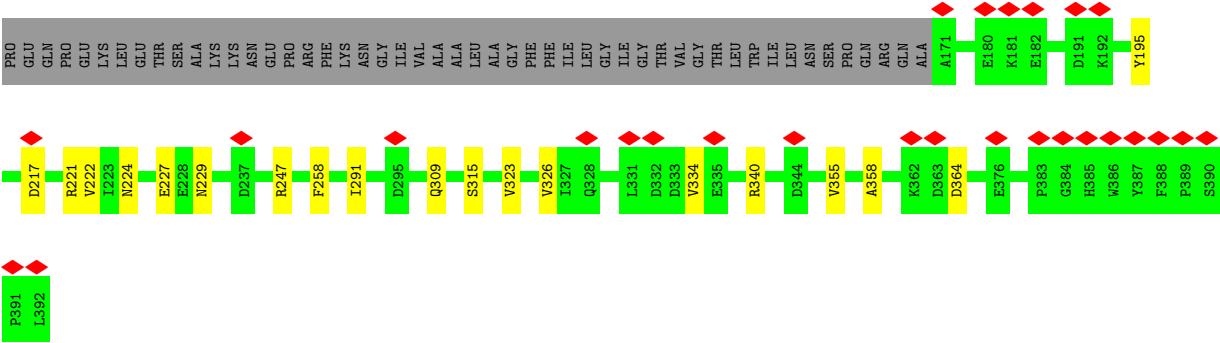
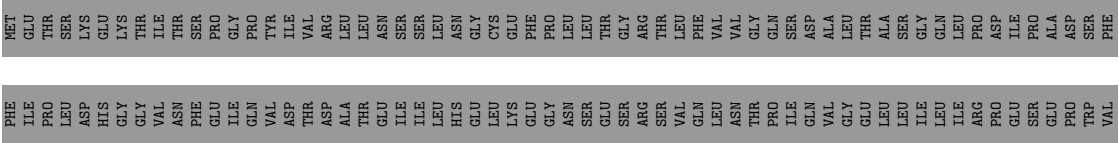




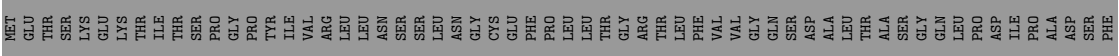
• Molecule 3: Protein PrgH



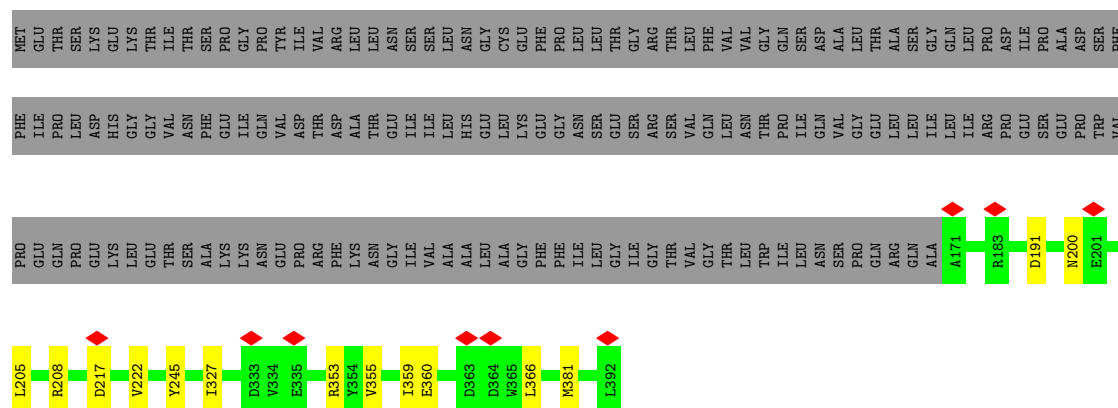
• Molecule 3: Protein PrgH



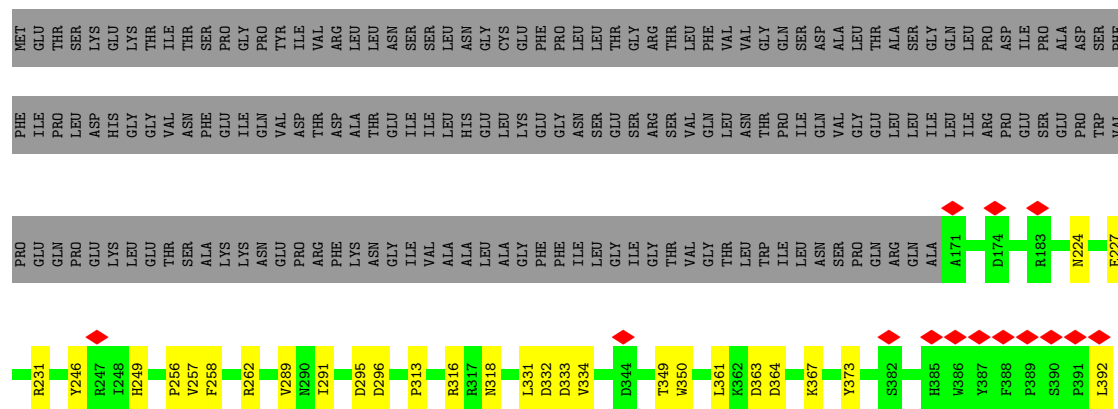
• Molecule 3: Protein PrgH



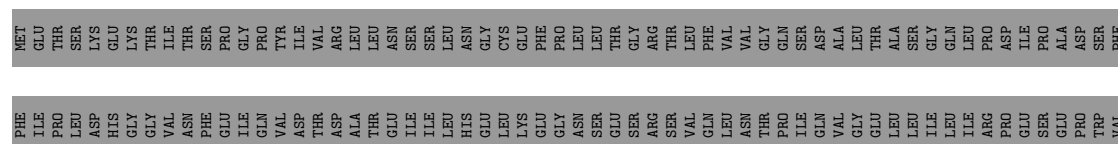
- Molecule 3: Protein PrgH

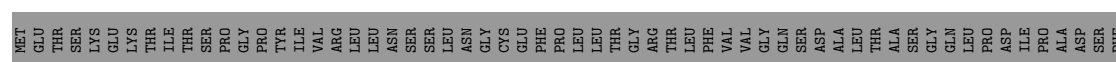


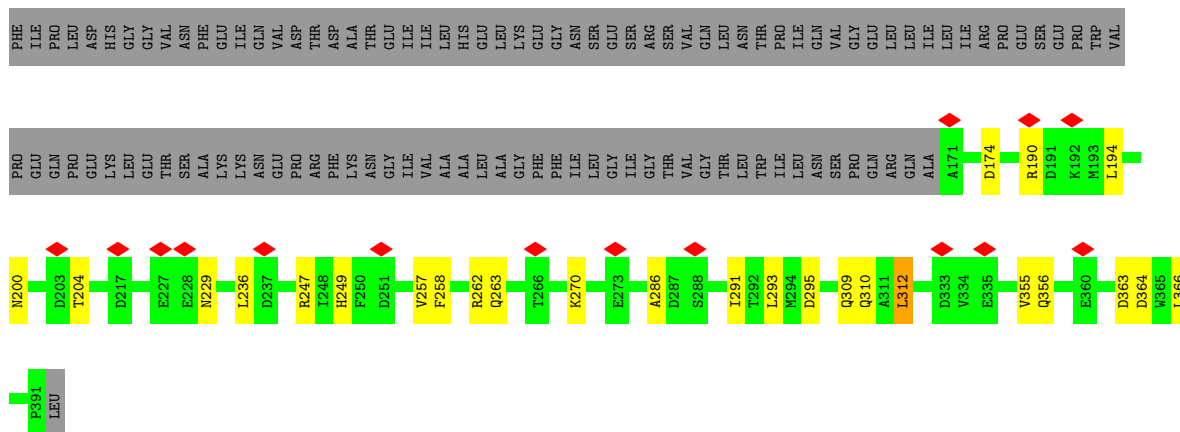
- Molecule 3: Protein PrgH



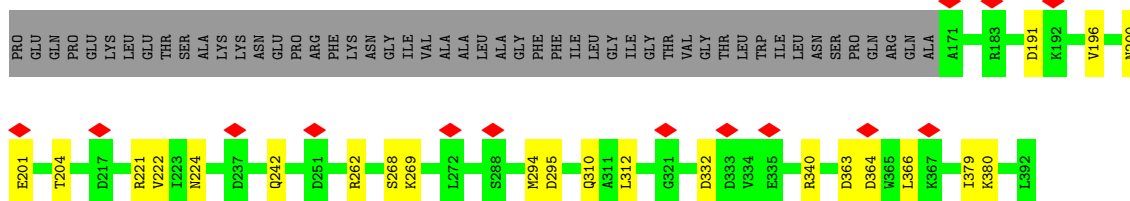
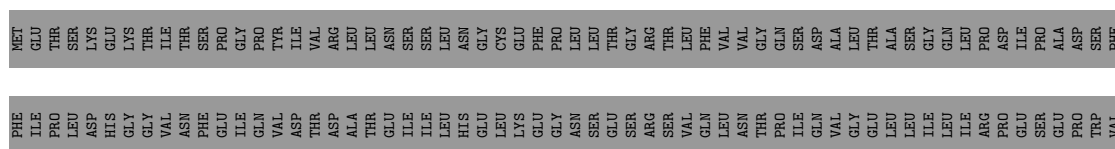
- Molecule 3: Protein PrgH



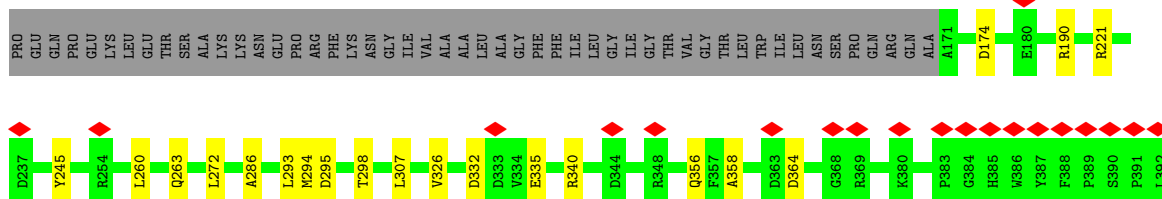




- Molecule 3: Protein PrgH

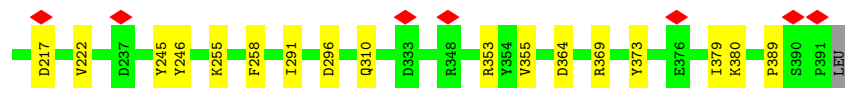


- Molecule 3: Protein PrgH



- Molecule 3: Protein PrgH

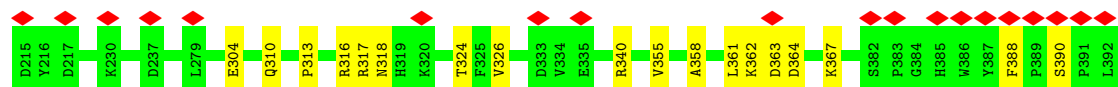




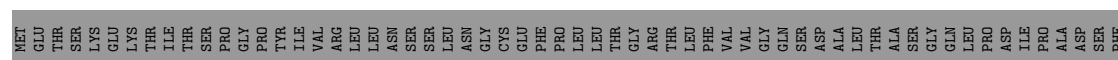
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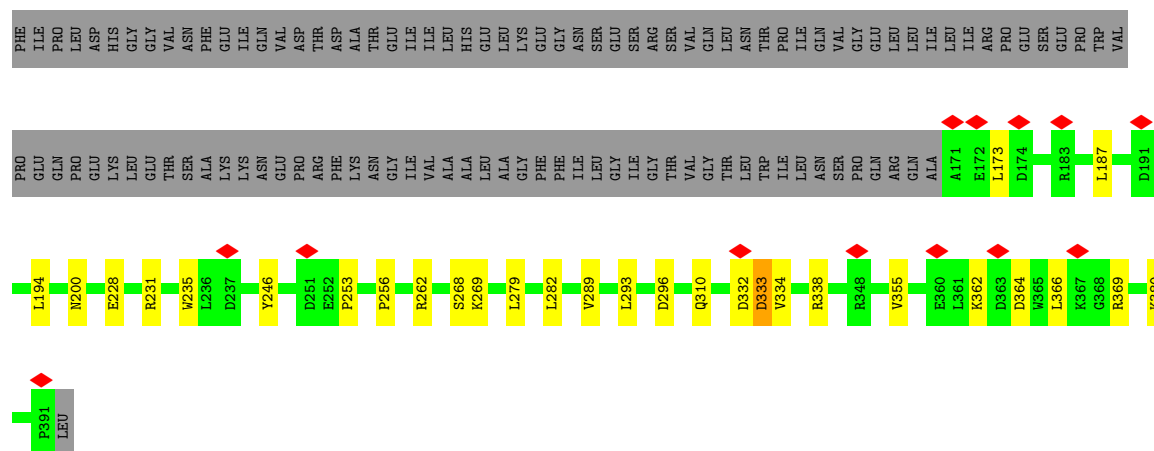


Chain 1: 5% 51% 5% 43%



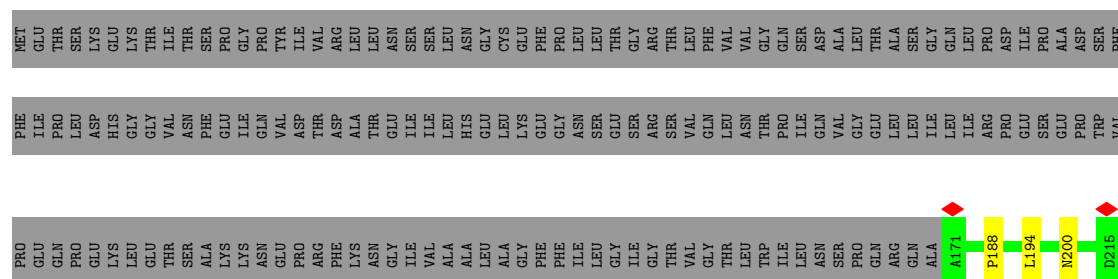
Chain m:





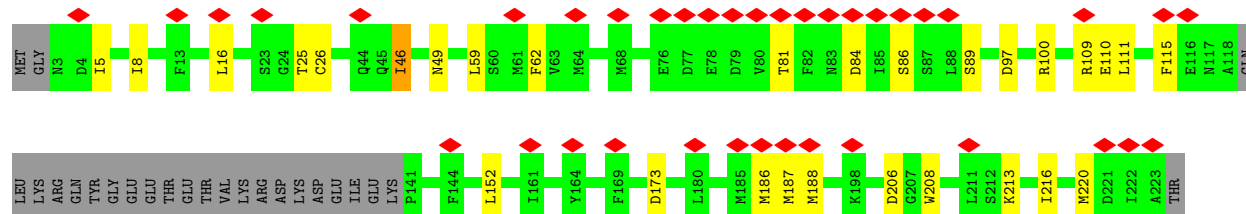
• Molecule 3: Protein PrGH

Chain n: 53% 43%



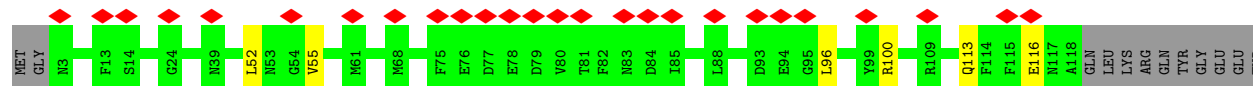
• Molecule 4: Surface presentation of antigens protein SpaP

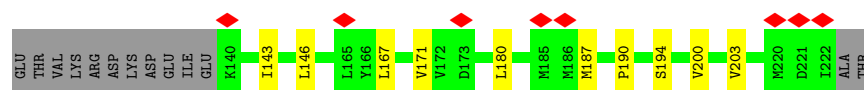
Chain 0: 17% 76% 12% 11%



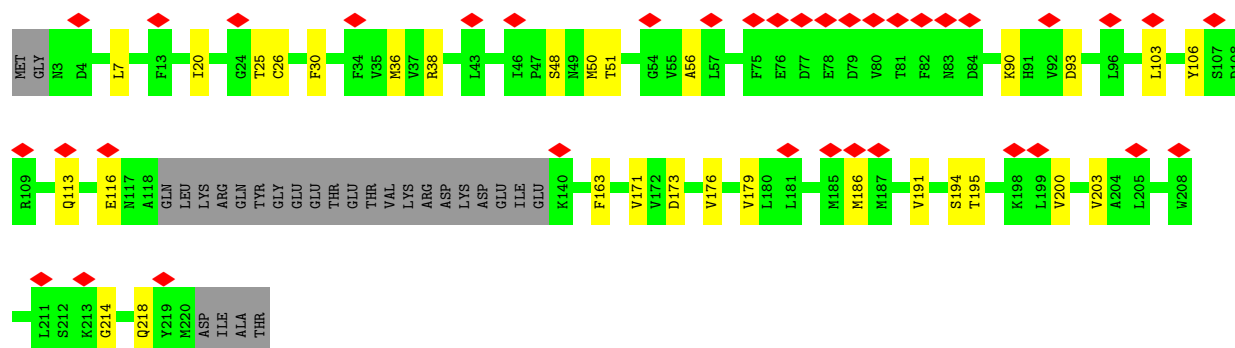
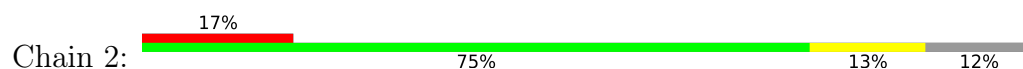
• Molecule 4: Surface presentation of antigens protein SpaP

Chain 1: 15% 82% 7% 11%

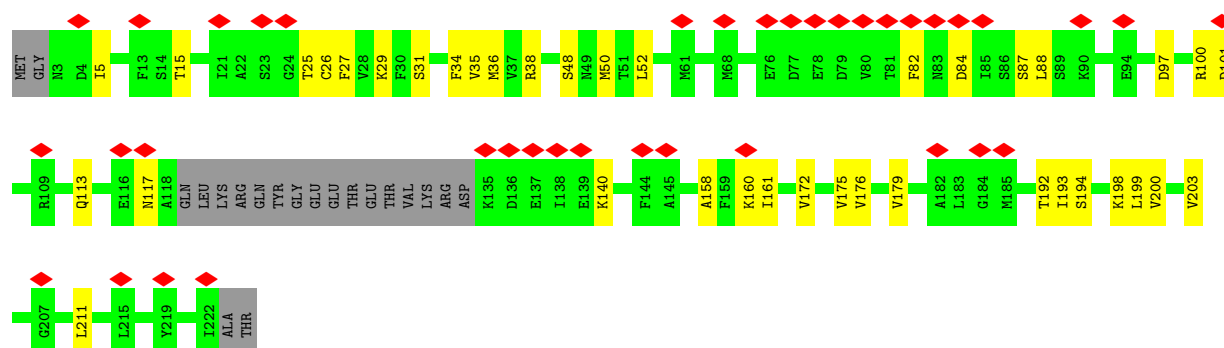
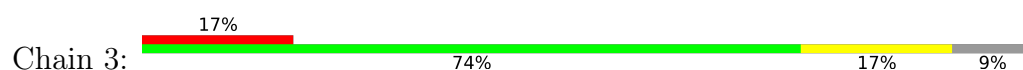




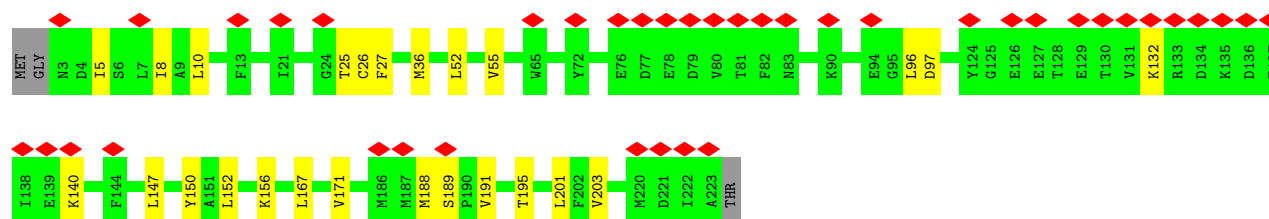
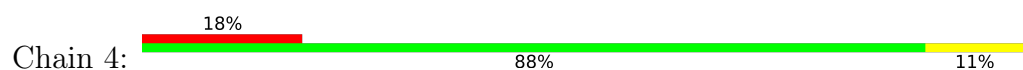
• Molecule 4: Surface presentation of antigens protein SpaP



• Molecule 4: Surface presentation of antigens protein SpaP



• Molecule 4: Surface presentation of antigens protein SpaP

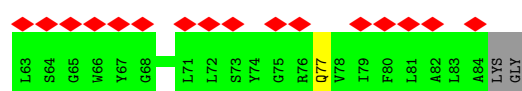
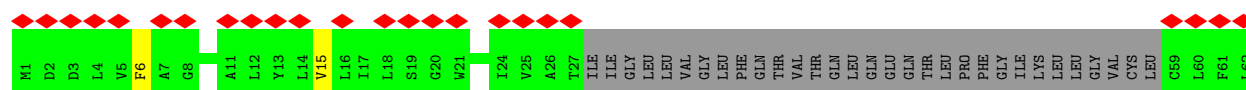


• Molecule 5: Surface presentation of antigens protein SpaR

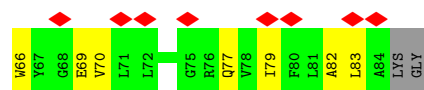




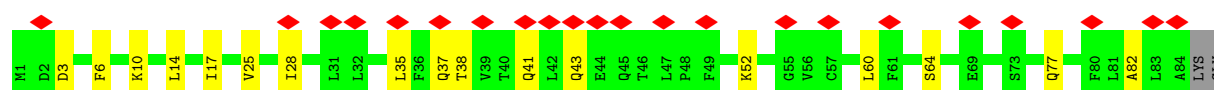
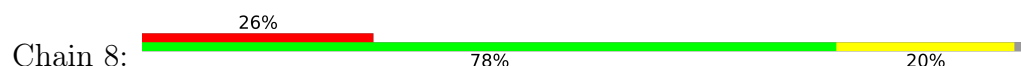
• Molecule 6: Surface presentation of antigens protein SpaQ



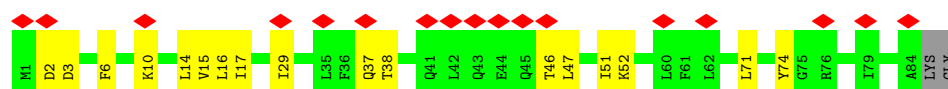
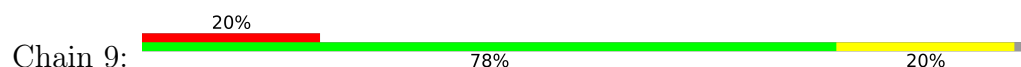
• Molecule 6: Surface presentation of antigens protein SpaQ



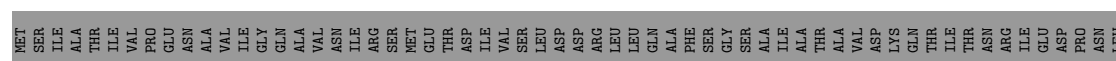
• Molecule 6: Surface presentation of antigens protein SpaQ

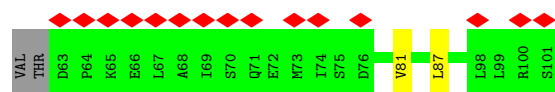


• Molecule 6: Surface presentation of antigens protein SpaQ

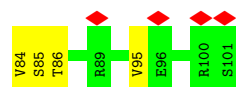
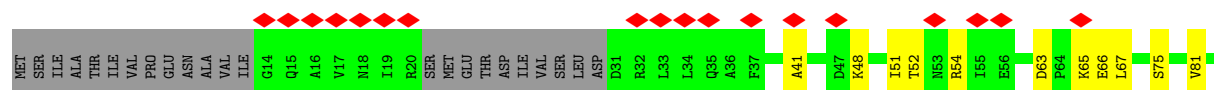


• Molecule 7: Protein PrgJ

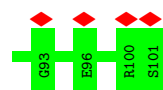
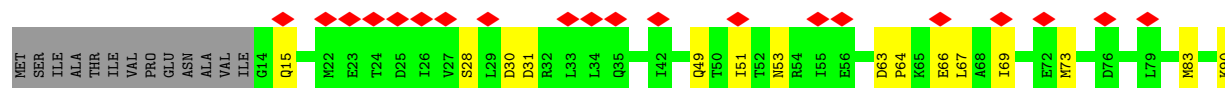
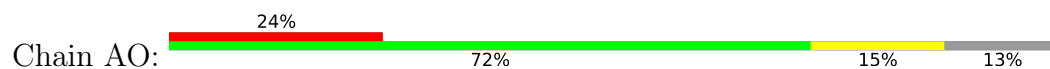




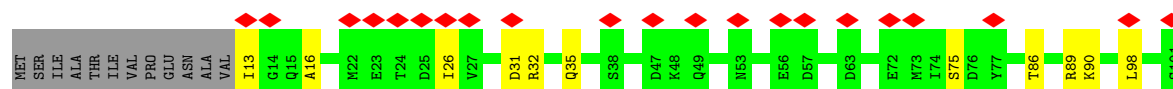
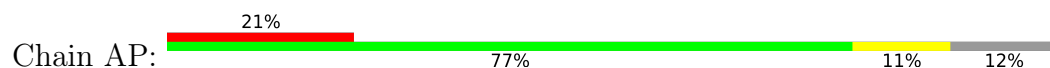
• Molecule 7: Protein PrgJ



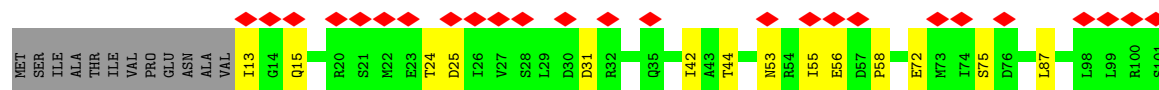
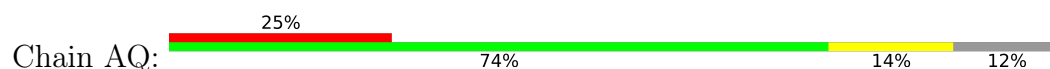
• Molecule 7: Protein PrgJ



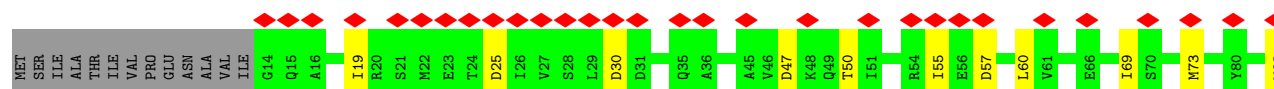
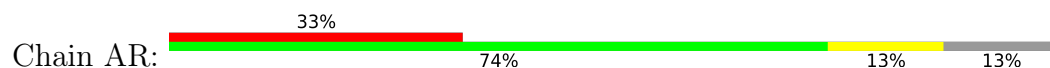
• Molecule 7: Protein PrgJ

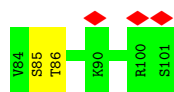


• Molecule 7: Protein PrgJ

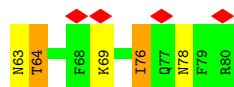
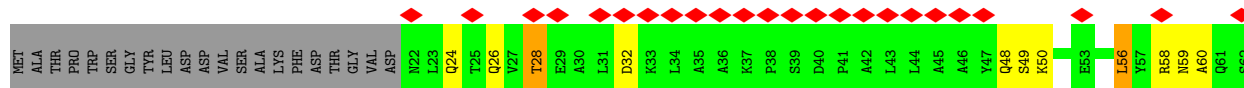


• Molecule 7: Protein PrgJ

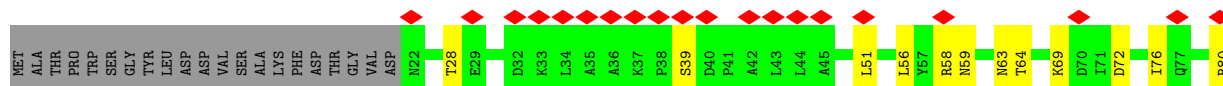




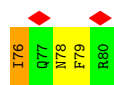
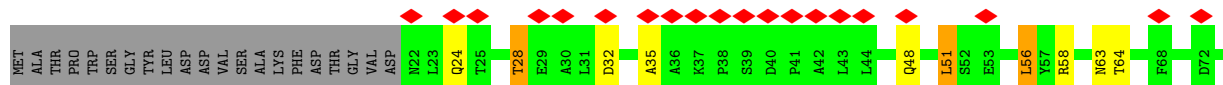
• Molecule 8: Protein PrgI



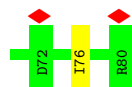
• Molecule 8: Protein PrgI



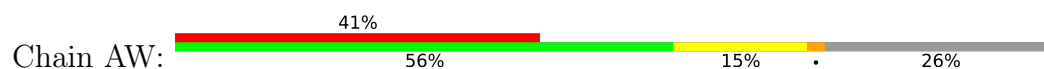
• Molecule 8: Protein PrgI

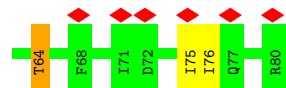
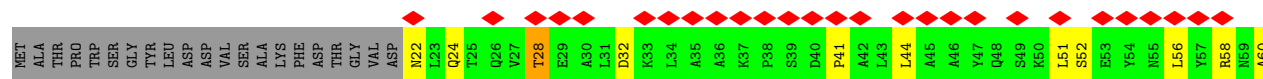


• Molecule 8: Protein PrgI

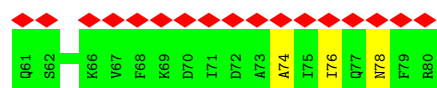
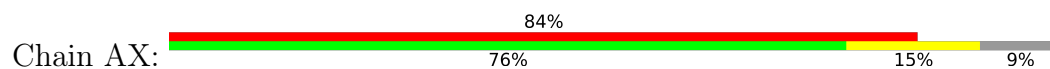


• Molecule 8: Protein PrgI

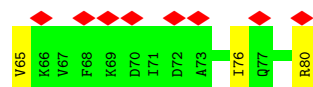
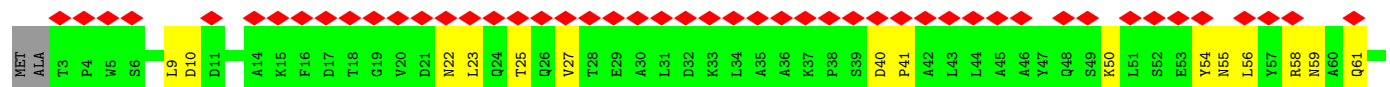
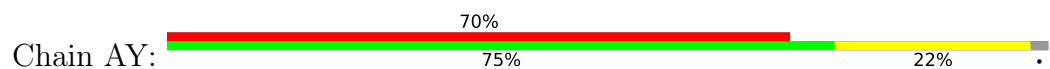




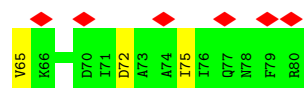
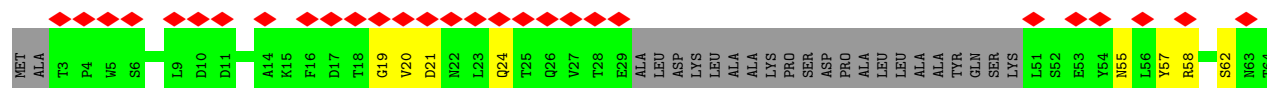
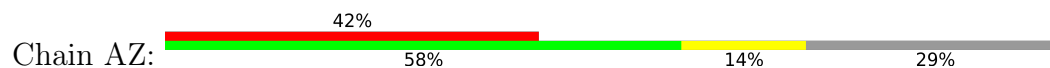
• Molecule 8: Protein PrgI



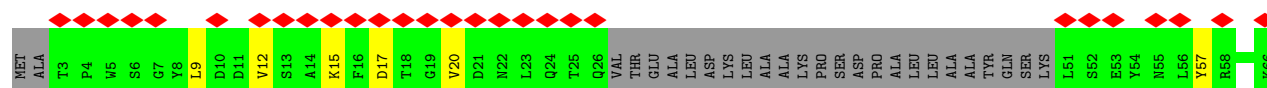
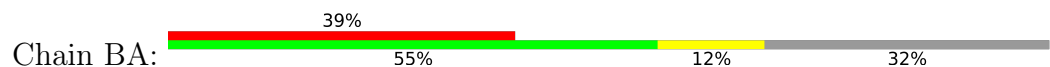
• Molecule 8: Protein PrgI



• Molecule 8: Protein PrgI

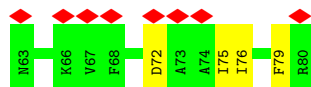
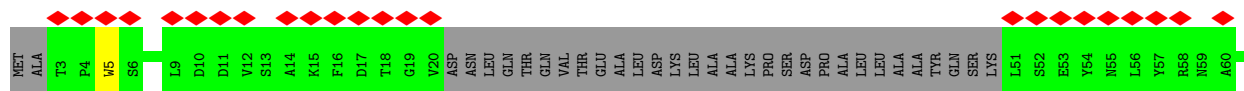
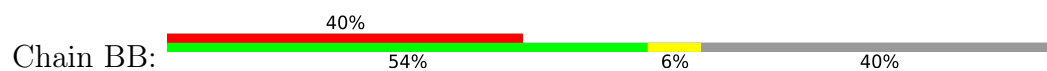


• Molecule 8: Protein PrgI

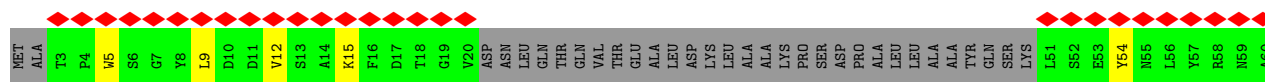




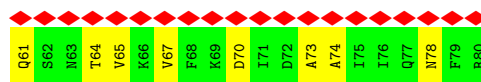
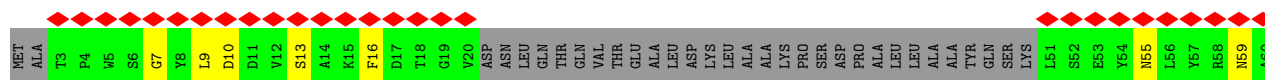
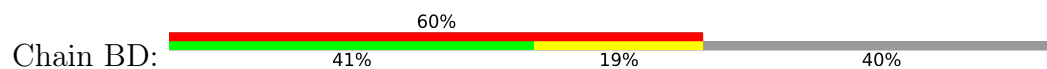
- Molecule 8: Protein PrgI



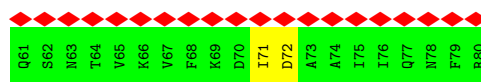
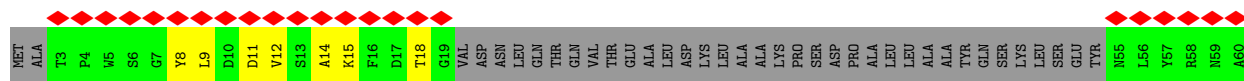
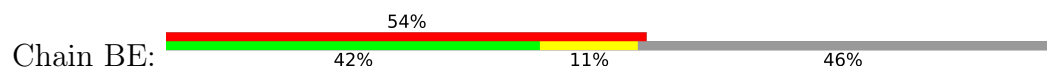
- Molecule 8: Protein PrgI



- Molecule 8: Protein PrgI



- Molecule 8: Protein PrgI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19141	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 ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	427.5, 427.5, 427.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.36	0/1458	0.61	0/1979
1	AB	0.34	0/1458	0.59	0/1979
1	AC	0.37	0/1458	0.61	0/1979
1	AD	0.34	0/1458	0.60	0/1979
1	AE	0.36	0/1458	0.60	0/1979
1	AF	0.34	0/1458	0.59	0/1979
1	AG	0.35	0/1458	0.59	0/1979
1	AH	0.34	0/1458	0.61	0/1979
1	AI	0.36	0/1458	0.62	0/1979
1	AJ	0.37	0/1458	0.66	0/1979
1	AK	0.34	0/1458	0.61	0/1979
1	AL	0.35	0/1458	0.60	0/1979
1	o	0.34	0/1458	0.58	0/1979
1	p	0.33	0/1458	0.59	0/1979
1	q	0.34	0/1458	0.57	0/1979
1	r	0.33	0/1458	0.61	0/1979
1	s	0.33	0/1458	0.61	0/1979
1	t	0.35	0/1458	0.65	0/1979
1	u	0.35	0/1458	0.65	0/1979
1	v	0.42	0/1458	0.65	0/1979
1	w	0.34	0/1458	0.60	0/1979
1	x	0.36	0/1458	0.65	1/1979 (0.1%)
1	y	0.36	0/1458	0.62	0/1979
1	z	0.36	0/1458	0.63	0/1979
2	A	0.33	0/1131	0.64	1/1525 (0.1%)
2	B	0.33	0/1181	0.63	0/1593
2	C	0.33	0/1131	0.62	0/1525
2	D	0.34	0/1170	0.61	0/1579
2	F	0.34	0/1131	0.64	0/1525
2	G	0.34	0/1181	0.66	2/1593 (0.1%)
2	H	0.37	0/1131	0.65	1/1525 (0.1%)
2	I	0.33	0/1181	0.60	0/1593
2	J	0.35	0/1131	0.62	0/1525
2	K	0.35	0/1181	0.65	0/1593

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	L	0.34	0/1131	0.64	0/1525
2	M	0.32	0/1170	0.62	0/1579
2	N	0.35	0/1131	0.63	0/1525
2	O	0.34	0/1181	0.62	0/1593
2	P	0.33	0/1131	0.61	0/1525
2	Q	0.34	0/1181	0.65	0/1593
3	E	0.31	0/1881	0.60	0/2541
3	R	0.32	0/1872	0.64	0/2530
3	S	0.32	0/1876	0.63	0/2536
3	T	0.31	0/1881	0.58	0/2541
3	U	0.31	0/1872	0.62	0/2530
3	V	0.31	0/1876	0.61	0/2536
3	W	0.31	0/1881	0.62	0/2541
3	X	0.31	0/1872	0.62	0/2530
3	Y	0.32	0/1876	0.63	0/2536
3	Z	0.31	0/1881	0.59	0/2541
3	a	0.31	0/1872	0.60	0/2530
3	b	0.31	0/1876	0.62	0/2536
3	c	0.32	0/1881	0.61	0/2541
3	d	0.32	0/1872	0.56	0/2530
3	e	0.32	0/1876	0.62	0/2536
3	f	0.31	0/1881	0.61	0/2541
3	g	0.30	0/1872	0.59	0/2530
3	h	0.33	0/1876	0.66	0/2536
3	i	0.30	0/1881	0.58	0/2541
3	j	0.32	0/1872	0.62	0/2530
3	k	0.33	0/1876	0.64	0/2536
3	l	0.33	0/1881	0.63	0/2541
3	m	0.31	0/1872	0.62	0/2530
3	n	0.32	0/1876	0.62	0/2536
4	0	0.34	0/1598	0.67	0/2172
4	1	0.32	0/1605	0.68	1/2181 (0.0%)
4	2	0.30	0/1589	0.67	0/2159
4	3	0.33	0/1642	0.62	0/2230
4	4	0.34	0/1799	0.65	0/2441
5	5	0.34	0/1935	0.72	0/2647
6	6	0.27	0/414	0.71	0/565
6	7	0.30	0/657	0.70	0/897
6	8	0.32	0/657	0.74	0/897
6	9	0.32	0/660	0.66	0/900
7	AM	0.37	0/300	0.87	0/403
7	AN	0.28	0/646	0.63	0/870
7	AO	0.31	0/671	0.65	0/908

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	AP	0.31	0/679	0.71	0/919
7	AQ	0.28	0/679	0.64	0/919
7	AR	0.29	0/671	0.71	0/908
8	AS	0.31	0/472	0.65	0/638
8	AT	0.29	0/472	0.61	0/638
8	AU	0.32	0/472	0.61	0/638
8	AV	0.33	0/472	0.73	0/638
8	AW	0.30	0/472	0.59	0/638
8	AX	0.27	0/582	0.61	0/788
8	AY	0.32	0/623	0.67	0/846
8	AZ	0.24	0/467	0.51	0/632
8	BA	0.24	0/444	0.50	0/600
8	BB	0.28	0/395	0.67	0/533
8	BC	0.25	0/395	0.56	0/533
8	BD	0.26	0/395	0.58	0/533
8	BE	0.27	0/352	0.69	0/474
All	All	0.33	0/120713	0.63	6/163413 (0.0%)

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
3	b	0	1
6	8	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	134	ILE	N-CA-C	-7.48	106.60	113.71
2	A	90	LEU	CA-CB-CG	5.32	134.93	116.30
4	1	167	LEU	N-CA-C	5.20	121.31	109.81
2	H	143	ARG	CA-CB-CG	5.19	124.47	114.10
2	G	29	PRO	CA-C-N	5.11	131.18	121.97
2	G	29	PRO	C-N-CA	5.11	131.18	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	8	41	GLN	Peptide
3	b	366	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1431	0	1424	17	0
1	AB	1431	0	1424	10	0
1	AC	1431	0	1424	14	0
1	AD	1431	0	1424	9	0
1	AE	1431	0	1424	14	0
1	AF	1431	0	1424	13	0
1	AG	1431	0	1424	7	0
1	AH	1431	0	1424	9	0
1	AI	1431	0	1424	14	0
1	AJ	1431	0	1424	22	0
1	AK	1431	0	1424	9	0
1	AL	1431	0	1424	12	0
1	o	1431	0	1424	18	0
1	p	1431	0	1424	12	0
1	q	1431	0	1424	8	0
1	r	1431	0	1424	12	0
1	s	1431	0	1424	13	0
1	t	1431	0	1424	13	0
1	u	1431	0	1424	20	0
1	v	1431	0	1424	17	0
1	w	1431	0	1424	10	0
1	x	1431	0	1424	12	0
1	y	1431	0	1424	9	0
1	z	1431	0	1424	8	0
2	A	1108	0	1103	11	0
2	B	1154	0	1163	8	0
2	C	1108	0	1103	11	0
2	D	1146	0	1150	9	0
2	F	1108	0	1103	10	0
2	G	1154	0	1163	8	0
2	H	1108	0	1103	6	0
2	I	1154	0	1163	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1108	0	1103	8	0
2	K	1154	0	1163	10	0
2	L	1108	0	1103	13	0
2	M	1146	0	1150	11	0
2	N	1108	0	1103	10	0
2	O	1154	0	1163	10	0
2	P	1108	0	1103	13	0
2	Q	1154	0	1163	11	0
3	E	1836	0	1800	16	0
3	R	1827	0	1789	17	0
3	S	1831	0	1788	17	0
3	T	1836	0	1800	17	0
3	U	1827	0	1789	21	0
3	V	1831	0	1788	12	0
3	W	1836	0	1800	16	0
3	X	1827	0	1789	17	0
3	Y	1831	0	1788	14	0
3	Z	1836	0	1800	11	0
3	a	1827	0	1789	11	0
3	b	1831	0	1788	10	0
3	c	1836	0	1800	19	0
3	d	1827	0	1789	10	0
3	e	1831	0	1788	12	0
3	f	1836	0	1800	17	0
3	g	1827	0	1789	17	0
3	h	1831	0	1788	19	0
3	i	1836	0	1800	17	0
3	j	1827	0	1789	13	0
3	k	1831	0	1788	12	0
3	l	1836	0	1800	15	0
3	m	1827	0	1789	18	0
3	n	1831	0	1788	8	0
4	0	1562	0	1597	22	0
4	1	1569	0	1613	9	0
4	2	1553	0	1598	24	0
4	3	1606	0	1649	22	0
4	4	1758	0	1806	19	0
5	5	1885	0	1931	31	0
6	6	405	0	418	2	0
6	7	644	0	685	11	0
6	8	644	0	685	10	0
6	9	647	0	692	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AM	298	0	307	1	0
7	AN	644	0	654	11	0
7	AO	667	0	672	10	0
7	AP	675	0	683	8	0
7	AQ	675	0	683	10	0
7	AR	667	0	672	9	0
8	AS	466	0	470	14	0
8	AT	466	0	470	5	0
8	AU	466	0	470	10	0
8	AV	466	0	470	7	0
8	AW	466	0	470	9	0
8	AX	574	0	566	8	0
8	AY	612	0	598	11	0
8	AZ	460	0	435	9	0
8	BA	437	0	413	6	0
8	BB	388	0	369	4	0
8	BC	388	0	369	7	0
8	BD	388	0	369	9	0
8	BE	346	0	329	7	0
All	All	118198	0	117437	955	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 4.

All (955) 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:v:139:ASN:HD21	1:v:141:ARG:HE	1.32	0.77
2:Q:39:ASP:H	2:Q:69:THR:HG22	1.55	0.72
3:V:267:MET:HG3	3:V:271:GLU:HG3	1.74	0.69
2:I:169:GLN:HE22	2:J:115:ARG:HA	1.57	0.69
2:A:39:ASP:H	2:A:69:THR:HG22	1.59	0.68
3:U:340:ARG:HH21	1:s:163:GLN:HE21	1.42	0.68
3:V:340:ARG:HH21	1:t:163:GLN:HE21	1.43	0.67
1:t:136:ALA:O	4:0:109:ARG:NH1	2.29	0.66
4:0:46:ILE:HD12	5:5:97:ALA:HB1	1.77	0.65
3:m:173:LEU:HD12	3:m:194:LEU:HD23	1.78	0.65
3:R:316:ARG:HH21	3:R:318:ASN:HD21	1.43	0.65
3:Y:328:GLN:HG2	3:Y:360:GLU:HB3	1.77	0.65
1:AI:85:ILE:HB	1:AI:107:SER:HB2	1.79	0.64
8:AW:52:SER:HB2	8:BC:69:LYS:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AP:31:ASP:O	7:AP:35:GLN:NE2	2.29	0.64
2:P:39:ASP:H	2:P:69:THR:HG22	1.63	0.64
2:J:149:VAL:HG21	2:J:159:VAL:HG11	1.79	0.64
2:N:149:VAL:HG21	2:N:159:VAL:HG21	1.80	0.63
8:BC:9:LEU:HD11	8:BC:65:VAL:HG23	1.79	0.63
1:AF:112:ARG:NH1	1:AJ:84:GLU:OE2	2.32	0.63
3:k:323:VAL:HG12	3:k:355:VAL:HG12	1.80	0.63
5:5:13:VAL:HG13	7:AM:81:VAL:HG21	1.81	0.62
8:BC:12:VAL:HA	8:BC:15:LYS:HD2	1.80	0.62
1:s:184:SER:HB3	1:t:173:ASN:HD22	1.65	0.62
2:A:137:PRO:HD2	2:Q:97:GLN:HE21	1.64	0.61
2:Q:149:VAL:HG21	2:Q:159:VAL:HG11	1.80	0.61
1:v:72:ILE:HD13	1:v:77:LEU:HB2	1.81	0.61
3:a:232:ILE:HD11	3:a:248:ILE:HG21	1.83	0.61
2:A:36:VAL:HG22	2:A:71:ASN:HD22	1.64	0.61
1:AI:139:ASN:HB3	1:AI:141:ARG:HG2	1.83	0.61
4:O:206:ASP:OD1	5:5:175:ASN:ND2	2.33	0.61
2:I:38:LYS:NZ	3:j:369:ARG:O	2.34	0.60
8:AZ:20:VAL:HG21	8:AZ:24:GLN:HE21	1.65	0.60
2:C:39:ASP:H	2:C:69:THR:HG22	1.66	0.60
5:5:64:PRO:HB2	5:5:160:MET:HE3	1.83	0.60
3:f:256:PRO:HG2	3:f:289:VAL:HG12	1.83	0.60
7:AN:54:ARG:NH1	7:AN:66:GLU:OE2	2.35	0.60
1:AL:85:ILE:HB	1:AL:107:SER:HB2	1.83	0.60
2:K:38:LYS:NZ	3:m:369:ARG:O	2.33	0.60
6:9:29:ILE:HD12	6:9:51:ILE:HG22	1.84	0.60
1:AD:24:LEU:HB3	1:AD:27:LEU:HD21	1.83	0.59
1:AE:135:ASP:OD1	1:o:102:LYS:NZ	2.35	0.59
2:A:149:VAL:HG11	2:A:159:VAL:HG21	1.84	0.59
3:U:336:ILE:HD11	1:s:165:SER:HB3	1.84	0.59
3:U:310:GLN:O	3:U:338:ARG:NH1	2.36	0.59
3:l:317:ARG:HB2	3:l:324:THR:HG23	1.84	0.59
4:2:214:GLY:HA3	6:7:83:LEU:HD13	1.84	0.59
4:3:15:THR:HG22	7:AP:90:LYS:HD2	1.85	0.59
3:a:335:GLU:OE2	3:a:338:ARG:NH2	2.35	0.59
2:D:97:GLN:HE21	2:F:137:PRO:HD2	1.68	0.59
3:E:361:LEU:HD13	1:o:165:SER:HB2	1.84	0.59
1:AH:34:GLU:OE2	1:AI:73:LYS:NZ	2.35	0.59
8:AS:78:ASN:HA	8:AT:80:ARG:HH21	1.67	0.58
1:y:71:TRP:HA	1:y:74:THR:HG22	1.84	0.58
8:AY:55:ASN:O	8:AY:59:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:85:ILE:HB	1:AC:107:SER:HB2	1.85	0.58
1:u:168:LYS:O	1:u:172:LYS:HB2	2.02	0.58
1:AA:85:ILE:HB	1:AA:107:SER:HB2	1.85	0.58
2:L:169:GLN:HE22	2:M:115:ARG:HA	1.67	0.58
3:c:349:THR:HG1	3:c:350:TRP:CD1	2.22	0.58
1:x:169:ARG:NH1	1:x:180:TYR:OH	2.36	0.58
3:c:256:PRO:HG2	3:c:289:VAL:HG12	1.85	0.58
3:f:371:PHE:HE1	3:f:380:LYS:HG2	1.69	0.58
3:l:363:ASP:OD1	3:l:363:ASP:N	2.37	0.58
1:z:21:LYS:NZ	1:z:62:GLU:OE1	2.35	0.58
1:AJ:34:GLU:OE2	1:AJ:34:GLU:HA	2.03	0.58
3:f:316:ARG:HH21	3:f:318:ASN:HD21	1.52	0.57
8:AS:63:ASN:OD1	8:AY:80:ARG:NH1	2.36	0.57
2:A:114:LEU:HD13	2:A:117:VAL:HG13	1.86	0.57
3:T:190:ARG:NH1	3:T:286:ALA:O	2.37	0.57
4:0:97:ASP:OD2	4:0:100:ARG:NH1	2.36	0.57
6:8:60:LEU:O	6:8:64:SER:HB3	2.03	0.57
3:j:173:LEU:HD12	3:j:194:LEU:HD23	1.86	0.57
3:m:262:ARG:HA	3:m:293:LEU:HD23	1.85	0.57
7:AQ:53:ASN:HA	7:AQ:56:GLU:HG3	1.85	0.57
4:2:25:THR:OG1	4:2:26:CYS:N	2.37	0.57
8:AX:26:GLN:OE1	8:AX:50:LYS:NZ	2.36	0.57
1:y:179:ASP:OD1	1:y:179:ASP:N	2.36	0.57
3:E:304:GLU:OE1	3:E:316:ARG:NH1	2.37	0.57
1:s:20:ASP:OD1	1:s:20:ASP:N	2.38	0.57
3:R:229:ASN:HD21	3:R:248:ILE:H	1.53	0.57
3:f:326:VAL:HA	3:f:358:ALA:HB3	1.86	0.57
1:p:139:ASN:HB2	1:p:141:ARG:HG2	1.87	0.57
4:0:5:ILE:HD12	4:0:8:ILE:HD13	1.87	0.57
3:V:356:GLN:NE2	3:W:310:GLN:OE1	2.38	0.56
1:r:85:ILE:HB	1:r:107:SER:HB2	1.87	0.56
1:y:99:ARG:NH2	1:y:138:GLU:OE2	2.38	0.56
3:l:362:LYS:NZ	3:m:332:ASP:OD2	2.38	0.56
4:3:5:ILE:HG12	7:AQ:44:THR:HG21	1.87	0.56
1:AD:98:PRO:HA	1:AD:101:GLU:HG2	1.88	0.56
3:Y:261:SER:O	3:Y:265:ASN:ND2	2.39	0.56
8:AS:60:ALA:HB2	8:AY:76:ILE:HD13	1.87	0.56
2:A:115:ARG:HG2	2:Q:169:GLN:HE22	1.71	0.56
3:V:263:GLN:NE2	3:V:295:ASP:OD2	2.38	0.56
2:G:161:ASN:HA	2:G:164:THR:HG22	1.88	0.56
2:L:149:VAL:HG21	2:L:159:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:333:ASP:OD2	3:m:333:ASP:N	2.39	0.56
2:C:113:SER:HA	2:C:145:GLY:O	2.06	0.56
1:AJ:39:LEU:HD22	1:AJ:44:ILE:HD11	1.86	0.56
4:0:5:ILE:HG21	7:AN:41:ALA:HA	1.86	0.56
1:v:25:LYS:NZ	1:w:56:TYR:OH	2.36	0.56
5:5:39:SER:OG	5:5:40:GLY:N	2.39	0.56
3:h:262:ARG:NH1	3:h:295:ASP:OD1	2.39	0.55
3:T:206:TRP:O	1:q:43:ASN:ND2	2.37	0.55
1:AI:177:ASP:N	1:AI:177:ASP:OD2	2.39	0.55
3:e:356:GLN:NE2	3:f:310:GLN:OE1	2.36	0.55
1:s:127:ARG:O	1:s:150:ALA:HA	2.07	0.55
1:AL:169:ARG:NH1	1:AL:180:TYR:OH	2.37	0.55
3:f:173:LEU:HA	3:f:176:LEU:HD12	1.87	0.55
4:3:34:PHE:HB3	4:3:52:LEU:HD22	1.87	0.55
5:5:83:MET:HG2	5:5:165:PRO:HB3	1.89	0.55
5:5:206:ALA:HB1	6:9:38:THR:HG21	1.88	0.55
3:d:316:ARG:HH21	3:d:318:ASN:HD21	1.54	0.55
2:G:97:GLN:HE22	2:H:139:ARG:HE	1.55	0.55
2:L:33:SER:OG	2:L:34:GLY:N	2.38	0.55
8:AX:16:PHE:HB3	8:AX:57:TYR:HE1	1.71	0.55
3:E:365:TRP:HD1	3:E:390:SER:HB2	1.71	0.55
4:2:30:PHE:HB3	4:2:56:ALA:HB1	1.89	0.55
7:AO:31:ASP:OD1	7:AO:31:ASP:N	2.38	0.55
1:AF:24:LEU:HB3	1:AF:27:LEU:HD21	1.89	0.54
3:W:258:PHE:HB3	3:W:291:ILE:HG12	1.90	0.54
3:f:363:ASP:OD1	3:f:363:ASP:N	2.38	0.54
1:u:139:ASN:HD22	1:u:141:ARG:HH11	1.53	0.54
1:u:177:ASP:OD2	1:u:177:ASP:N	2.38	0.54
7:AO:66:GLU:HA	7:AO:69:ILE:HG22	1.88	0.54
3:S:196:VAL:HB	3:S:222:VAL:HG12	1.90	0.54
3:c:316:ARG:HH21	3:c:318:ASN:HD21	1.56	0.54
2:O:38:LYS:NZ	3:U:369:ARG:O	2.36	0.54
3:T:191:ASP:OD1	3:T:191:ASP:N	2.41	0.54
1:p:191:SER:OG	1:p:192:ASP:N	2.40	0.54
1:r:169:ARG:NH1	1:r:180:TYR:OH	2.39	0.54
8:AT:39:SER:HB2	8:BE:9:LEU:HD23	1.87	0.54
8:AV:60:ALA:HB2	8:BB:76:ILE:HD11	1.88	0.54
3:X:200:ASN:O	3:X:204:THR:OG1	2.23	0.54
1:w:38:VAL:HG11	1:w:77:LEU:HD11	1.89	0.54
1:AC:38:VAL:HG11	1:AC:77:LEU:HD11	1.89	0.54
3:e:174:ASP:N	3:e:174:ASP:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:304:GLU:OE1	3:l:316:ARG:NH1	2.40	0.54
8:AV:59:ASN:O	8:AV:63:ASN:ND2	2.36	0.54
8:AX:21:ASP:N	8:AX:21:ASP:OD1	2.41	0.54
3:S:173:LEU:HD12	3:S:194:LEU:HD23	1.88	0.54
3:Y:263:GLN:NE2	3:Y:295:ASP:OD1	2.40	0.54
8:AZ:24:GLN:NE2	8:AZ:57:TYR:OH	2.41	0.54
3:b:360:GLU:HG2	3:c:334:VAL:HG21	1.90	0.54
3:c:224:ASN:HB3	3:c:227:GLU:HG2	1.90	0.54
8:AZ:72:ASP:OD1	8:AZ:72:ASP:N	2.39	0.54
8:BD:13:SER:OG	8:BD:61:GLN:NE2	2.41	0.54
3:R:221:ARG:NH1	3:S:182:GLU:OE2	2.41	0.54
3:d:256:PRO:HG2	3:d:289:VAL:HG12	1.90	0.54
3:n:245:TYR:OH	3:n:353:ARG:NH2	2.41	0.54
4:2:218:GLN:NE2	6:7:83:LEU:O	2.41	0.54
8:AY:27:VAL:HG12	8:AY:50:LYS:HB3	1.90	0.54
3:g:356:GLN:NE2	3:h:310:GLN:OE1	2.41	0.54
3:S:316:ARG:HH21	3:S:318:ASN:HD21	1.56	0.53
3:Y:310:GLN:O	3:Y:338:ARG:NH1	2.41	0.53
3:c:262:ARG:NH1	3:c:295:ASP:OD1	2.40	0.53
2:F:114:LEU:HD21	2:F:163:ALA:HB1	1.90	0.53
2:B:114:LEU:HD21	2:B:163:ALA:HB1	1.91	0.53
1:v:64:ASP:OD2	1:v:64:ASP:N	2.38	0.53
4:2:38:ARG:NH1	4:2:48:SER:O	2.42	0.53
5:5:176:GLN:OE1	5:5:179:GLN:NE2	2.41	0.53
3:E:316:ARG:NE	3:E:318:ASN:OD1	2.41	0.53
1:AA:165:SER:HB2	3:c:361:LEU:HD13	1.91	0.53
1:AI:39:LEU:HD22	1:AI:44:ILE:HD11	1.90	0.53
3:h:204:THR:HB	3:h:224:ASN:HD21	1.73	0.53
4:4:147:LEU:HA	4:4:150:TYR:HB3	1.91	0.53
1:AD:71:TRP:HA	1:AD:74:THR:HG22	1.89	0.53
1:t:25:LYS:H	1:u:29:GLN:HE21	1.56	0.53
1:t:184:SER:HB3	1:u:173:ASN:HD22	1.72	0.53
4:1:143:ILE:HD12	4:1:146:LEU:HD11	1.90	0.53
4:4:36:MET:HE3	5:5:37:VAL:HG23	1.90	0.53
5:5:76:GLN:HE22	5:5:162:GLU:HG2	1.74	0.53
6:7:37:GLN:HB3	6:7:41:GLN:HA	1.90	0.53
1:AE:99:ARG:HE	1:o:102:LYS:HZ3	1.57	0.53
3:W:271:GLU:HA	3:W:274:VAL:HG12	1.90	0.53
1:u:80:ARG:NH2	1:v:82:ARG:NH1	2.57	0.53
4:3:84:ASP:OD1	4:3:87:SER:N	2.42	0.53
1:AC:73:LYS:NZ	1:AL:34:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:39:ASP:H	2:O:69:THR:HB	1.74	0.53
4:O:25:THR:OG1	4:O:26:CYS:N	2.42	0.53
4:O:62:PHE:HB3	4:O:220:MET:HE1	1.89	0.53
1:AH:163:GLN:HE22	3:i:340:ARG:HH22	1.57	0.53
3:Z:258:PHE:HB3	3:Z:291:ILE:HG12	1.90	0.53
3:c:331:LEU:HD23	3:c:367:LYS:HD3	1.90	0.53
8:BC:9:LEU:HA	8:BC:12:VAL:HG12	1.91	0.53
3:S:356:GLN:HB2	3:T:309:GLN:HE21	1.74	0.52
1:AF:112:ARG:HG2	1:AJ:129:HIS:HE1	1.74	0.52
2:J:141:ASP:HB3	2:J:144:LYS:HB2	1.90	0.52
3:m:187:LEU:HD21	3:m:253:PRO:HB2	1.91	0.52
1:o:38:VAL:HG11	1:o:77:LEU:HD11	1.90	0.52
1:AK:31:GLN:NE2	1:AK:79:PRO:O	2.42	0.52
4:3:29:LYS:HG3	4:3:158:ALA:HB2	1.92	0.52
2:D:87:GLN:NE2	3:c:373:TYR:OH	2.42	0.52
3:X:202:ARG:NH2	1:u:41:MET:SD	2.78	0.52
4:2:48:SER:OG	4:2:51:THR:N	2.38	0.52
3:c:258:PHE:HB3	3:c:291:ILE:HG12	1.91	0.52
8:AS:32:ASP:N	8:AS:32:ASP:OD1	2.38	0.52
8:AY:22:ASN:OD1	8:AY:25:THR:OG1	2.28	0.52
8:BD:55:ASN:O	8:BD:59:ASN:ND2	2.43	0.52
1:AB:39:LEU:HD22	1:AB:44:ILE:HD11	1.90	0.52
3:V:363:ASP:OD2	3:V:363:ASP:N	2.42	0.52
1:AL:169:ARG:HH11	1:AL:180:TYR:HH	1.53	0.52
3:n:258:PHE:HB3	3:n:291:ILE:HG12	1.90	0.52
1:v:177:ASP:OD1	1:v:177:ASP:N	2.43	0.52
1:AA:71:TRP:HA	1:AA:74:THR:HG22	1.92	0.52
3:e:186:VAL:HG12	3:e:196:VAL:HG12	1.91	0.52
4:O:16:LEU:HD11	7:AN:95:VAL:HG11	1.91	0.52
4:1:200:VAL:HA	4:1:203:VAL:HG12	1.91	0.52
1:AE:98:PRO:HD3	6:7:77:GLN:HE21	1.73	0.52
1:o:99:ARG:HE	1:o:134:ILE:HD12	1.75	0.52
1:x:156:ARG:NH2	1:x:190:ARG:O	2.42	0.52
6:7:79:ILE:HD12	6:7:82:ALA:HB3	1.92	0.52
7:AO:28:SER:OG	7:AO:30:ASP:OD1	2.28	0.52
2:Q:36:VAL:HG23	3:X:373:TYR:HE1	1.74	0.52
1:z:71:TRP:HA	1:z:74:THR:HG22	1.91	0.52
3:h:201:GLU:HA	3:h:204:THR:HG22	1.92	0.52
2:J:40:ASP:OD2	2:J:44:THR:OG1	2.24	0.52
2:P:149:VAL:HG21	2:P:159:VAL:HG21	1.92	0.52
3:V:328:GLN:HG2	3:V:360:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:228:GLU:OE2	3:d:231:ARG:NE	2.43	0.52
3:m:310:GLN:O	3:m:338:ARG:NH1	2.43	0.52
1:AD:177:ASP:OD1	1:AD:177:ASP:N	2.43	0.51
3:X:217:ASP:OD2	3:X:217:ASP:N	2.43	0.51
3:f:186:VAL:HG22	3:f:196:VAL:HG12	1.92	0.51
1:AC:93:SER:OG	1:AC:94:LEU:N	2.41	0.51
2:H:33:SER:OG	2:H:34:GLY:N	2.41	0.51
3:a:268:SER:OG	3:a:269:LYS:N	2.43	0.51
4:3:176:VAL:HA	4:3:179:VAL:HG12	1.93	0.51
6:9:10:LYS:HE2	6:9:74:TYR:HE1	1.75	0.51
3:c:363:ASP:OD1	3:c:363:ASP:N	2.37	0.51
3:d:316:ARG:NE	3:d:318:ASN:OD1	2.38	0.51
8:AY:58:ARG:HH11	8:AY:61:GLN:HE22	1.58	0.51
1:AA:156:ARG:NH2	1:AA:190:ARG:O	2.42	0.51
1:AB:73:LYS:NZ	1:AC:34:GLU:OE2	2.42	0.51
3:h:364:ASP:OD1	3:h:364:ASP:N	2.43	0.51
8:AX:34:LEU:HD21	8:AX:47:TYR:HB2	1.92	0.51
3:W:371:PHE:HE1	3:W:380:LYS:HG2	1.76	0.51
3:m:246:TYR:OH	3:m:296:ASP:OD1	2.29	0.51
1:v:36:ILE:HD11	1:v:48:LYS:HB2	1.93	0.51
1:z:39:LEU:HD22	1:z:44:ILE:HD11	1.92	0.51
2:G:60:SER:OG	2:G:61:LYS:N	2.44	0.51
3:Z:326:VAL:HA	3:Z:358:ALA:HB3	1.92	0.51
1:AL:177:ASP:OD1	1:AL:177:ASP:N	2.41	0.51
1:AA:184:SER:HB3	1:AB:173:ASN:HD21	1.74	0.51
2:F:103:ASP:OD1	2:F:104:ALA:N	2.44	0.51
3:S:213:ARG:HD3	1:p:201:PRO:HB3	1.92	0.51
6:8:10:LYS:NZ	6:8:77:GLN:OE1	2.37	0.51
8:AU:63:ASN:OD1	8:BA:80:ARG:NH1	2.43	0.51
8:BA:9:LEU:HA	8:BA:12:VAL:HG12	1.92	0.51
1:AG:99:ARG:HE	1:AG:134:ILE:HD12	1.75	0.51
2:L:73:GLU:OE1	2:L:75:HIS:ND1	2.38	0.51
3:U:196:VAL:HG23	3:U:222:VAL:HG13	1.93	0.51
3:V:258:PHE:HB3	3:V:291:ILE:HG12	1.93	0.51
3:W:363:ASP:OD1	3:W:363:ASP:N	2.40	0.51
3:c:313:PRO:HG3	3:c:367:LYS:HD2	1.93	0.51
3:h:268:SER:OG	3:h:269:LYS:N	2.43	0.51
2:I:118:SER:OG	2:I:119:LEU:N	2.44	0.50
3:Y:332:ASP:OD1	3:Y:332:ASP:N	2.38	0.50
3:f:364:ASP:OD1	3:f:364:ASP:N	2.42	0.50
5:5:133:ALA:HA	5:5:136:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:3:ASP:OD1	6:9:3:ASP:N	2.43	0.50
1:AI:163:GLN:HE21	3:h:340:ARG:HH22	1.58	0.50
3:E:316:ARG:HH21	3:E:318:ASN:HD21	1.59	0.50
2:I:44:THR:HB	3:j:380:LYS:HE2	1.92	0.50
2:P:33:SER:OG	2:P:34:GLY:N	2.44	0.50
3:l:361:LEU:HD13	1:AJ:165:SER:HB2	1.92	0.50
8:AS:24:GLN:O	8:AS:28:THR:OG1	2.21	0.50
8:BD:70:ASP:HA	8:BD:73:ALA:HB3	1.93	0.50
1:AC:71:TRP:HA	1:AC:74:THR:HG22	1.92	0.50
1:AE:177:ASP:OD1	1:AE:177:ASP:N	2.44	0.50
3:W:200:ASN:O	3:W:204:THR:OG1	2.27	0.50
3:a:201:GLU:HA	3:a:204:THR:HG22	1.92	0.50
1:AC:184:SER:HB3	1:AL:173:ASN:HD21	1.75	0.50
1:AG:177:ASP:OD1	1:AG:177:ASP:N	2.45	0.50
3:W:180:GLU:OE2	3:W:183:ARG:NH2	2.42	0.50
5:5:233:PRO:HG2	5:5:234:VAL:HG23	1.93	0.50
6:7:33:VAL:HG21	6:7:48:PRO:HB3	1.93	0.50
2:L:40:ASP:HB2	2:L:44:THR:HG23	1.94	0.50
2:P:57:VAL:HG12	2:P:99:ILE:HB	1.93	0.50
3:X:246:TYR:OH	3:X:296:ASP:OD2	2.27	0.50
3:f:356:GLN:NE2	3:g:310:GLN:OE1	2.44	0.50
7:AP:89:ARG:O	7:AP:89:ARG:NH1	2.44	0.50
1:AH:177:ASP:OD2	1:AH:177:ASP:N	2.45	0.50
3:R:340:ARG:HH21	1:p:163:GLN:HE22	1.58	0.50
1:y:172:LYS:NZ	1:y:178:VAL:O	2.44	0.50
7:AO:64:PRO:HA	7:AO:67:LEU:HB2	1.93	0.50
3:U:316:ARG:HH21	3:U:318:ASN:HD21	1.60	0.50
3:a:202:ARG:HH22	1:x:194:GLN:HB2	1.76	0.50
1:AK:191:SER:OG	1:AK:192:ASP:N	2.43	0.50
2:H:57:VAL:HG12	2:H:99:ILE:HB	1.92	0.50
3:i:174:ASP:N	3:i:174:ASP:OD2	2.40	0.50
3:l:316:ARG:HH21	3:l:318:ASN:HD21	1.59	0.50
3:E:258:PHE:HB3	3:E:291:ILE:HG12	1.94	0.49
2:K:114:LEU:HD13	2:K:117:VAL:HB	1.93	0.49
3:i:332:ASP:OD1	3:i:332:ASP:N	2.36	0.49
3:n:200:ASN:N	3:n:200:ASN:OD1	2.44	0.49
1:AJ:112:ARG:NH1	1:AK:110:GLU:OE2	2.45	0.49
3:k:256:PRO:HG3	3:k:283:MET:HE1	1.95	0.49
1:u:99:ARG:NH2	1:u:135:ASP:OD1	2.44	0.49
1:AB:139:ASN:HD22	1:AB:141:ARG:HE	1.61	0.49
1:AI:126:ALA:HA	1:AI:151:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:169:GLN:HE22	2:Q:115:ARG:HA	1.77	0.49
3:Z:224:ASN:HB3	3:Z:227:GLU:HG2	1.94	0.49
3:m:256:PRO:HG2	3:m:289:VAL:HG12	1.95	0.49
3:T:333:ASP:OD1	3:T:333:ASP:N	2.43	0.49
1:AL:165:SER:HB2	3:f:361:LEU:HD13	1.94	0.49
3:e:215:ASP:OD1	3:e:215:ASP:N	2.45	0.49
3:m:268:SER:OG	3:m:269:LYS:N	2.46	0.49
4:0:84:ASP:OD2	4:0:86:SER:OG	2.28	0.49
4:3:200:VAL:HA	4:3:203:VAL:HG22	1.95	0.49
6:9:14:LEU:HD23	6:9:17:ILE:HD11	1.95	0.49
8:AV:29:GLU:O	8:AV:33:LYS:NZ	2.46	0.49
2:M:114:LEU:HD11	2:M:147:PHE:HE1	1.78	0.49
2:N:44:THR:HB	3:S:380:LYS:HE2	1.95	0.49
3:V:178:GLY:O	3:V:181:LYS:NZ	2.45	0.49
3:f:228:GLU:OE2	3:f:231:ARG:NH2	2.43	0.49
3:k:232:ILE:HD11	3:k:279:LEU:HD22	1.94	0.49
1:v:94:LEU:HG	1:v:95:VAL:HG23	1.94	0.49
1:AJ:173:ASN:HD21	1:AK:184:SER:HB3	1.77	0.49
4:4:97:ASP:OD1	4:4:140[A]:LYS:NZ	2.46	0.49
6:8:52:LYS:NZ	6:9:46:THR:OG1	2.44	0.49
7:AR:30:ASP:OD1	7:AR:30:ASP:N	2.45	0.49
1:AI:156:ARG:NH2	1:AI:192:ASP:OD1	2.45	0.49
1:AJ:64:ASP:OD2	1:AJ:64:ASP:N	2.44	0.49
8:AY:56:LEU:HD13	8:BE:72:ASP:HB2	1.94	0.49
2:F:57:VAL:HG12	2:F:99:ILE:HB	1.95	0.49
3:X:183:ARG:NH1	3:X:203:ASP:OD2	2.41	0.49
3:R:363:ASP:OD1	3:R:363:ASP:N	2.45	0.49
3:W:361:LEU:HD13	1:u:165:SER:HB2	1.94	0.49
3:c:246:TYR:OH	3:c:296:ASP:OD2	2.30	0.49
7:AR:47:ASP:HA	7:AR:50:THR:HG22	1.93	0.49
3:T:187:LEU:HD22	3:T:285:TYR:HB2	1.95	0.49
1:s:177:ASP:OD1	1:s:177:ASP:N	2.46	0.49
8:BB:76:ILE:HG13	8:BB:79:PHE:HE2	1.78	0.49
1:AA:166:ASP:N	1:AA:166:ASP:OD2	2.46	0.48
3:b:217:ASP:OD1	3:b:217:ASP:N	2.45	0.48
3:g:263:GLN:NE2	3:g:295:ASP:OD2	2.40	0.48
1:o:135:ASP:OD1	1:o:135:ASP:N	2.46	0.48
4:4:25:THR:OG1	4:4:26:CYS:N	2.46	0.48
7:AO:63:ASP:HB3	7:AO:66:GLU:HG2	1.94	0.48
7:AQ:31:ASP:OD2	7:AQ:31:ASP:N	2.45	0.48
2:A:118:SER:OG	2:A:121:GLU:OE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:SER:OG	2:D:61:LYS:N	2.44	0.48
2:M:39:ASP:H	2:M:69:THR:HB	1.77	0.48
3:W:229:ASN:HD22	3:W:247:ARG:HE	1.61	0.48
1:v:24:LEU:HD11	1:v:72:ILE:HD12	1.95	0.48
1:p:85:ILE:HB	1:p:107:SER:HB2	1.95	0.48
8:AY:23:LEU:HG	8:AY:54:TYR:HD1	1.77	0.48
1:AH:85:ILE:HB	1:AH:107:SER:HB2	1.94	0.48
3:T:228:GLU:OE2	3:T:231:ARG:NE	2.39	0.48
3:d:364:ASP:OD1	3:d:364:ASP:N	2.44	0.48
6:9:6:PHE:O	6:9:10:LYS:NZ	2.46	0.48
7:AP:26:ILE:HG21	7:AP:32:ARG:HE	1.78	0.48
8:AZ:24:GLN:OE1	8:AZ:58:ARG:NH2	2.46	0.48
3:R:271:GLU:HA	3:R:274:VAL:HG12	1.95	0.48
3:d:190:ARG:NH2	3:d:280:ARG:O	2.44	0.48
1:o:85:ILE:HB	1:o:107:SER:HB2	1.96	0.48
1:t:177:ASP:OD1	1:t:177:ASP:N	2.46	0.48
1:AJ:28:ASP:HB3	1:AJ:31:GLN:HG3	1.96	0.48
8:AV:27:VAL:HG13	8:AV:50:LYS:HE3	1.96	0.48
3:j:246:TYR:OH	3:j:296:ASP:OD2	2.28	0.48
5:5:99:GLY:HA2	5:5:102:ILE:HG22	1.95	0.48
1:AG:93:SER:OG	1:AG:95:VAL:O	2.29	0.48
3:V:316:ARG:HE	3:V:318:ASN:HD21	1.60	0.48
4:2:173:ASP:HA	4:2:176:VAL:HG22	1.94	0.48
3:R:304:GLU:OE1	3:R:316:ARG:NH1	2.47	0.48
3:Y:363:ASP:OD1	3:Y:363:ASP:N	2.46	0.48
3:i:263:GLN:NE2	3:i:295:ASP:OD1	2.47	0.48
1:y:114:GLU:HB3	1:y:128:VAL:HG12	1.94	0.48
1:z:174:SER:O	1:z:174:SER:OG	2.30	0.48
6:8:3:ASP:HA	6:8:6:PHE:HB3	1.94	0.48
7:AR:55:ILE:HG13	8:AW:64:THR:HG21	1.95	0.48
2:O:107:MET:HE2	2:O:151:GLY:HA2	1.95	0.48
2:P:141:ASP:HB3	2:P:144:LYS:HB2	1.95	0.48
4:4:25:THR:HG23	4:4:27:PHE:H	1.78	0.48
2:D:38:LYS:NZ	3:d:369:ARG:O	2.41	0.48
3:T:340:ARG:HH22	1:r:163:GLN:HE21	1.62	0.48
3:T:364:ASP:N	3:T:364:ASP:OD1	2.44	0.48
1:AL:28:ASP:OD1	1:AL:28:ASP:N	2.46	0.48
4:4:156:LYS:HG3	5:5:138:LEU:HG	1.96	0.48
3:X:316:ARG:HH21	3:X:318:ASN:HD21	1.62	0.47
3:Z:323:VAL:HG22	3:Z:355:VAL:HG12	1.96	0.47
2:F:149:VAL:HG21	2:F:159:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:340:ARG:HH22	1:u:163:GLN:HE21	1.61	0.47
3:h:366:LEU:HD11	3:h:379:ILE:HD13	1.96	0.47
4:4:191:VAL:O	4:4:195:THR:OG1	2.31	0.47
8:AX:31:LEU:HA	8:AX:34:LEU:HB2	1.96	0.47
4:2:93:ASP:OD1	4:2:93:ASP:N	2.46	0.47
4:3:35:VAL:HG13	4:3:38:ARG:HH21	1.79	0.47
8:AX:74:ALA:O	8:AX:78:ASN:ND2	2.47	0.47
8:BD:74:ALA:O	8:BD:78:ASN:ND2	2.47	0.47
3:l:364:ASP:OD1	3:l:364:ASP:N	2.48	0.47
1:w:20:ASP:N	1:w:20:ASP:OD1	2.46	0.47
8:AW:60:ALA:HA	8:BC:76:ILE:HD11	1.95	0.47
1:AF:173:ASN:HD21	1:AJ:184:SER:HB3	1.79	0.47
3:E:364:ASP:OD1	3:E:364:ASP:N	2.48	0.47
2:I:41:SER:O	2:I:41:SER:OG	2.28	0.47
4:0:173:ASP:N	4:0:173:ASP:OD1	2.43	0.47
7:AQ:13:ILE:HG13	7:AQ:15:GLN:HE22	1.79	0.47
1:AC:196:GLN:OE1	3:f:179:GLN:N	2.46	0.47
3:i:356:GLN:NE2	3:j:310:GLN:OE1	2.46	0.47
1:t:25:LYS:O	1:u:29:GLN:NE2	2.47	0.47
6:9:29:ILE:HD11	6:9:52:LYS:HA	1.97	0.47
2:A:97:GLN:HE21	2:B:137:PRO:HD2	1.78	0.47
2:C:116:ASN:ND2	2:C:170:ASN:O	2.48	0.47
2:G:107:MET:HE2	2:G:151:GLY:HA2	1.97	0.47
2:G:118:SER:OG	2:G:119:LEU:N	2.48	0.47
2:N:41:SER:O	2:N:41:SER:OG	2.30	0.47
2:Q:40:ASP:OD1	2:Q:44:THR:OG1	2.28	0.47
3:U:232:ILE:HD11	3:U:279:LEU:HD22	1.97	0.47
3:U:262:ARG:HA	3:U:293:LEU:HD23	1.97	0.47
3:m:364:ASP:OD1	3:m:364:ASP:N	2.41	0.47
1:r:69:VAL:HG12	1:s:37:ALA:HB2	1.96	0.47
1:s:69:VAL:HG12	1:t:37:ALA:HB2	1.96	0.47
1:y:99:ARG:HH22	1:y:138:GLU:HB3	1.79	0.47
4:1:180:LEU:HD12	4:1:190:PRO:HB3	1.95	0.47
6:7:60:LEU:O	6:7:64:SER:OG	2.26	0.47
7:AN:75:SER:HB3	8:AT:69:LYS:HD3	1.96	0.47
8:AS:48:GLN:NE2	8:BD:78:ASN:O	2.47	0.47
8:AU:32:ASP:OD2	8:AU:32:ASP:N	2.48	0.47
1:AD:85:ILE:HB	1:AD:107:SER:HB2	1.96	0.47
2:K:38:LYS:HG2	3:l:388:PHE:HE1	1.80	0.47
3:R:356:GLN:NE2	3:S:310:GLN:OE1	2.47	0.47
2:P:51:LEU:HD22	2:Q:87:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:363:ASP:OD1	3:h:363:ASP:N	2.47	0.47
1:AJ:159:PRO:HB2	1:AJ:162:HIS:HD2	1.80	0.47
7:AO:49:GLN:HG3	7:AO:53:ASN:HD21	1.79	0.47
8:AW:32:ASP:N	8:AW:32:ASP:OD1	2.48	0.47
8:BE:8:TYR:HA	8:BE:11:ASP:HB2	1.97	0.47
2:N:109:ASN:OD1	2:N:109:ASN:N	2.46	0.47
3:j:258:PHE:HB3	3:j:291:ILE:HG12	1.97	0.47
1:x:146:VAL:HG13	1:x:178:VAL:HG12	1.96	0.47
4:0:49:ASN:N	4:0:49:ASN:OD1	2.48	0.47
4:3:48:SER:OG	4:3:50:MET:N	2.48	0.47
5:5:89:SER:O	5:5:89:SER:OG	2.28	0.47
8:AY:9:LEU:HD21	8:AY:65:VAL:HG13	1.97	0.47
1:AE:107:SER:O	1:AE:111:GLN:NE2	2.49	0.46
1:AE:160:LEU:HD21	3:E:341:GLN:HE22	1.80	0.46
1:q:156:ARG:NH2	1:q:190:ARG:O	2.48	0.46
1:AJ:85:ILE:HB	1:AJ:107:SER:HB2	1.97	0.46
6:9:2:ASP:OD1	6:9:2:ASP:N	2.48	0.46
7:AO:90:LYS:NZ	8:AU:79:PHE:O	2.37	0.46
8:BD:13:SER:HA	8:BD:16:PHE:HD2	1.79	0.46
1:AB:85:ILE:HB	1:AB:107:SER:HB2	1.97	0.46
3:Z:229:ASN:HD21	3:Z:247:ARG:HG3	1.79	0.46
3:k:356:GLN:NE2	3:l:310:GLN:OE1	2.47	0.46
1:q:85:ILE:HB	1:q:107:SER:HB2	1.97	0.46
1:w:141:ARG:HH11	1:x:142:PRO:HA	1.81	0.46
7:AQ:72:GLU:O	7:AQ:75:SER:OG	2.31	0.46
2:I:108:ARG:HH12	2:I:153:PRO:HB3	1.80	0.46
2:L:118:SER:OG	2:L:119:LEU:N	2.49	0.46
3:e:268:SER:OG	3:e:271:GLU:OE1	2.31	0.46
1:q:51:SER:OG	1:q:55:GLY:O	2.31	0.46
4:4:171:VAL:HG23	6:9:15:VAL:HG13	1.96	0.46
3:n:235:TRP:HE3	3:n:236:LEU:HD12	1.81	0.46
4:4:201:LEU:HD11	6:9:71:LEU:HB3	1.96	0.46
1:AA:172:LYS:HD2	1:AA:180:TYR:CZ	2.51	0.46
1:o:107:SER:O	1:o:111:GLN:NE2	2.48	0.46
1:v:35:VAL:HG22	1:v:77:LEU:HD13	1.98	0.46
1:AJ:20:ASP:N	1:AJ:20:ASP:OD1	2.48	0.46
1:AK:53:LYS:HE3	1:AK:53:LYS:HB3	1.76	0.46
1:AF:20:ASP:N	1:AF:20:ASP:OD1	2.48	0.46
1:AG:190:ARG:NH1	1:AG:191:SER:O	2.48	0.46
3:R:257:VAL:HG12	3:R:290:ASN:HB3	1.98	0.46
3:T:326:VAL:HA	3:T:358:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:326:VAL:HA	3:W:358:ALA:HB3	1.97	0.46
3:h:196:VAL:HB	3:h:222:VAL:HG12	1.98	0.46
1:AE:147:HIS:NE2	1:o:176:ALA:O	2.49	0.46
1:AF:39:LEU:HD22	1:AF:44:ILE:HD11	1.96	0.46
3:c:228:GLU:HG3	3:c:231:ARG:HE	1.81	0.46
4:0:188:MET:HE2	4:0:188:MET:HB3	1.80	0.46
4:2:191:VAL:O	4:2:195:THR:OG1	2.23	0.46
7:AQ:55:ILE:HD12	7:AQ:55:ILE:HA	1.88	0.46
8:AW:41:PRO:HG2	8:BC:54:TYR:HE2	1.81	0.46
1:AE:147:HIS:HB3	1:o:173:ASN:HB2	1.98	0.46
1:q:31:GLN:NE2	1:q:79:PRO:O	2.48	0.46
1:x:38:VAL:HG11	1:x:77:LEU:HD11	1.97	0.46
4:3:25:THR:OG1	4:3:26:CYS:N	2.48	0.46
5:5:102:ILE:HD11	5:5:223:ALA:HB1	1.97	0.46
5:5:224:VAL:HG13	6:9:16:LEU:HD12	1.97	0.46
3:g:229:ASN:HD21	3:g:247:ARG:HD2	1.81	0.46
2:B:141:ASP:HB3	2:B:144:LYS:HB2	1.97	0.46
3:E:256:PRO:HG2	3:E:289:VAL:HG12	1.97	0.46
3:b:381:MET:HE1	3:c:392:LEU:HD12	1.97	0.46
4:4:5:ILE:HG22	4:4:8:ILE:HD12	1.97	0.46
7:AO:51:ILE:HG22	7:AO:73:MET:HE3	1.97	0.46
7:AQ:24:THR:OG1	7:AQ:25:ASP:N	2.48	0.46
8:AU:24:GLN:O	8:AU:28:THR:OG1	2.29	0.46
8:BA:17:ASP:OD1	8:BA:57:TYR:OH	2.34	0.46
8:BA:74:ALA:O	8:BA:78:ASN:ND2	2.49	0.46
2:K:169:GLN:HE22	2:L:115:ARG:HA	1.81	0.45
2:O:36:VAL:HG23	3:U:373:TYR:HE1	1.81	0.45
2:P:114:LEU:HD13	2:P:117:VAL:HB	1.98	0.45
2:P:116:ASN:OD1	2:P:116:ASN:N	2.50	0.45
3:R:217:ASP:OD1	3:R:217:ASP:N	2.40	0.45
3:Y:196:VAL:HB	3:Y:222:VAL:HG12	1.98	0.45
3:e:334:VAL:HG23	3:e:338:ARG:HH21	1.79	0.45
4:1:190:PRO:O	4:1:194:SER:HB3	2.15	0.45
2:A:108:ARG:HG3	2:A:156:VAL:HG21	1.98	0.45
2:K:76:ASP:HA	2:K:77:PRO:HD3	1.86	0.45
3:U:200:ASN:O	3:U:204:THR:OG1	2.26	0.45
4:3:113:GLN:O	4:3:117:ASN:ND2	2.48	0.45
4:4:10:LEU:HD21	7:AQ:87:LEU:HD21	1.98	0.45
8:AW:58:ARG:HA	8:AW:58:ARG:HD3	1.73	0.45
1:AB:177:ASP:N	1:AB:177:ASP:OD1	2.48	0.45
2:L:97:GLN:HE22	2:M:139:ARG:HE	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:69:VAL:HG21	1:p:36:ILE:HG23	1.98	0.45
4:0:213:LYS:HA	4:0:216:ILE:HG22	1.97	0.45
2:P:58:ILE:HD13	2:Q:105:SER:HA	1.97	0.45
3:S:217:ASP:N	3:S:217:ASP:OD1	2.44	0.45
3:i:364:ASP:OD1	3:i:364:ASP:N	2.49	0.45
3:m:380:LYS:HE3	3:m:380:LYS:HB3	1.66	0.45
6:8:25:VAL:HA	6:8:28:ILE:HG12	1.98	0.45
1:AH:29:GLN:NE2	1:AI:25:LYS:O	2.49	0.45
2:F:63:ALA:HB2	2:F:103:ASP:HB2	1.99	0.45
3:U:380:LYS:HE3	3:U:380:LYS:HB3	1.70	0.45
3:l:340:ARG:HH22	1:AJ:163:GLN:HE21	1.64	0.45
1:p:98:PRO:HA	1:p:101:GLU:HG2	1.98	0.45
4:3:192:THR:HG23	4:3:193:ILE:HG13	1.98	0.45
1:AA:39:LEU:HD22	1:AA:44:ILE:HD11	1.98	0.45
1:AA:160:LEU:HD12	3:d:337:LEU:HD21	1.99	0.45
2:D:168:LYS:HA	2:D:168:LYS:HD3	1.76	0.45
2:F:60:SER:OG	2:F:61:LYS:N	2.48	0.45
3:T:173:LEU:HA	3:T:176:LEU:HD12	1.99	0.45
3:h:366:LEU:HD13	3:h:366:LEU:HA	1.72	0.45
1:o:99:ARG:NH1	1:p:101:GLU:OE2	2.40	0.45
1:AA:169:ARG:NE	3:c:333:ASP:OD1	2.41	0.45
1:AF:92:ASP:OD1	1:AF:92:ASP:N	2.49	0.45
1:p:155:GLU:OE2	1:p:156:ARG:N	2.50	0.45
1:z:177:ASP:N	1:z:177:ASP:OD1	2.48	0.45
5:5:52:LEU:HD23	5:5:52:LEU:HA	1.87	0.45
5:5:166:SER:O	5:5:166:SER:OG	2.32	0.45
7:AR:69:ILE:HG22	7:AR:73:MET:HE1	1.99	0.45
8:AU:76:ILE:H	8:AU:76:ILE:HG12	1.42	0.45
2:N:76:ASP:OD1	2:N:76:ASP:N	2.49	0.45
3:X:200:ASN:N	3:X:200:ASN:OD1	2.49	0.45
1:q:110:GLU:OE1	1:r:112:ARG:NE	2.49	0.45
4:4:188:MET:HE3	4:4:189:SER:H	1.82	0.45
1:AA:20:ASP:OD1	1:AA:20:ASP:N	2.50	0.45
2:A:76:ASP:OD1	2:A:76:ASP:N	2.50	0.45
3:d:372:GLN:O	3:d:377:GLY:HA2	2.16	0.45
3:l:326:VAL:HA	3:l:358:ALA:HB3	1.98	0.45
1:t:24:LEU:HB3	1:t:27:LEU:HD11	1.99	0.45
8:AZ:55:ASN:HA	8:BE:71:ILE:HD11	1.99	0.45
8:AZ:72:ASP:HA	8:AZ:75:ILE:HD12	1.99	0.45
1:AF:112:ARG:NE	1:AJ:110:GLU:OE2	2.50	0.45
2:K:125:PHE:HD1	2:L:141:ASP:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:174:SER:O	1:t:174:SER:OG	2.33	0.45
2:B:36:VAL:HG23	3:a:373:TYR:HE1	1.81	0.44
2:I:28:ILE:HD11	3:j:389:PRO:HG3	1.99	0.44
2:M:114:LEU:HD21	2:M:163:ALA:HB1	1.98	0.44
2:O:114:LEU:HD21	2:O:163:ALA:HB1	1.99	0.44
3:S:333:ASP:OD1	3:S:333:ASP:N	2.49	0.44
3:U:217:ASP:OD2	3:U:217:ASP:N	2.50	0.44
4:1:113:GLN:HA	4:1:116:GLU:HG3	1.99	0.44
4:3:82:PHE:HB2	4:3:88:LEU:HG	1.99	0.44
1:AA:152:ALA:HB3	1:AA:187:LEU:HB3	1.99	0.44
1:AI:99:ARG:HG3	1:AI:134:ILE:HG21	1.99	0.44
2:N:114:LEU:HD13	2:N:117:VAL:HG13	2.00	0.44
3:R:247:ARG:NH1	3:R:348:ARG:O	2.50	0.44
3:e:263:GLN:NE2	3:e:295:ASP:OD1	2.50	0.44
3:h:191:ASP:OD1	3:h:191:ASP:N	2.49	0.44
3:i:326:VAL:HA	3:i:358:ALA:HB3	1.98	0.44
4:0:186:MET:HE3	4:0:186:MET:HB3	1.85	0.44
6:8:37:GLN:HE21	6:8:43:GLN:HA	1.82	0.44
3:Z:364:ASP:OD1	3:Z:364:ASP:N	2.50	0.44
4:0:86:SER:HA	4:0:89:SER:HB3	1.99	0.44
5:5:56:PRO:HD3	5:5:154:TYR:CD2	2.52	0.44
2:I:28:ILE:HG12	3:j:379:ILE:HD11	1.98	0.44
3:h:242:GLN:HE22	3:i:294:MET:HE1	1.82	0.44
1:v:71:TRP:HA	1:v:71:TRP:CE3	2.52	0.44
1:x:39:LEU:HD22	1:x:44:ILE:HD11	2.00	0.44
1:AC:191:SER:OG	1:AC:192:ASP:N	2.51	0.44
2:H:138:LEU:HD22	2:H:149:VAL:HG12	1.99	0.44
3:b:200:ASN:OD1	3:b:200:ASN:N	2.49	0.44
7:AN:63:ASP:OD1	7:AN:66:GLU:N	2.44	0.44
8:BD:9:LEU:HD11	8:BD:65:VAL:HG13	1.99	0.44
2:C:40:ASP:HB3	2:C:44:THR:HG23	1.99	0.44
2:D:52:GLN:HG3	2:D:74:PHE:HB2	2.00	0.44
3:R:219:ASN:HD21	3:S:181:LYS:HE2	1.82	0.44
3:b:191:ASP:OD1	3:b:191:ASP:N	2.49	0.44
6:8:14:LEU:HA	6:8:17:ILE:HG22	1.99	0.44
2:N:57:VAL:HG12	2:N:99:ILE:HB	1.98	0.44
3:g:190:ARG:NH1	3:g:286:ALA:O	2.50	0.44
3:g:270:LYS:HA	3:g:270:LYS:HD3	1.78	0.44
3:k:200:ASN:O	3:k:204:THR:OG1	2.22	0.44
1:r:172:LYS:HD2	1:r:180:TYR:CZ	2.53	0.44
4:4:52:LEU:HA	4:4:55:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:VAL:HG22	2:B:148:TYR:HD1	1.83	0.44
3:Y:316:ARG:HE	3:Y:318:ASN:HD21	1.66	0.44
1:s:85:ILE:HB	1:s:107:SER:HB2	2.00	0.44
4:2:173:ASP:OD1	4:2:173:ASP:N	2.43	0.44
8:BD:64:THR:HA	8:BD:67:VAL:HG22	2.00	0.44
1:AH:173:ASN:HB2	1:AI:147:HIS:HB3	2.00	0.44
3:E:228:GLU:OE2	3:E:231:ARG:NH2	2.48	0.44
2:P:87:GLN:HE22	3:U:376:GLU:HB3	1.83	0.44
3:g:262:ARG:HA	3:g:293:LEU:HD23	1.99	0.44
3:h:221:ARG:HE	3:h:221:ARG:HB3	1.61	0.44
3:n:188:PRO:HA	3:n:194:LEU:HD12	1.98	0.44
4:2:7:LEU:HD21	7:AO:83:MET:HE1	2.00	0.44
8:AW:22:ASN:HD21	8:BC:5:TRP:HE1	1.63	0.44
1:AA:173:ASN:OD1	1:AA:173:ASN:N	2.47	0.43
3:U:334:VAL:HG13	3:U:338:ARG:HH21	1.83	0.43
3:m:173:LEU:HD23	3:m:173:LEU:HA	1.85	0.43
4:2:48:SER:OG	4:2:50:MET:N	2.49	0.43
5:5:202:LEU:HD12	5:5:202:LEU:HA	1.91	0.43
8:BE:9:LEU:HA	8:BE:12:VAL:HG22	1.99	0.43
1:AH:39:LEU:HD22	1:AH:44:ILE:HD11	1.99	0.43
2:C:61:LYS:NZ	7:AR:25:ASP:OD1	2.49	0.43
2:J:38:LYS:HA	2:J:69:THR:HG23	1.99	0.43
3:a:258:PHE:HB3	3:a:291:ILE:HG12	2.00	0.43
3:i:190:ARG:NH1	3:i:286:ALA:O	2.43	0.43
1:v:51:SER:HB2	1:v:55:GLY:O	2.18	0.43
4:2:176:VAL:HA	4:2:179:VAL:HG22	2.00	0.43
2:C:107:MET:HE2	2:C:151:GLY:HA2	2.01	0.43
2:J:97:GLN:HE22	2:K:139:ARG:HE	1.66	0.43
2:N:144:LYS:HD2	2:N:144:LYS:HA	1.89	0.43
3:R:244:ALA:HB3	3:R:265:ASN:HD21	1.84	0.43
3:T:208:ARG:HG2	3:T:222:VAL:HG21	2.00	0.43
3:X:333:ASP:OD1	3:X:333:ASP:N	2.51	0.43
4:0:208:TRP:HB2	5:5:175:ASN:CG	2.43	0.43
7:AP:75:SER:HA	8:AV:69:LYS:HE3	2.00	0.43
1:AE:95:VAL:HG11	6:7:70:VAL:HG23	2.01	0.43
2:L:144:LYS:HD3	2:L:144:LYS:HA	1.87	0.43
2:P:50:ALA:HB2	2:P:57:VAL:HG22	2.01	0.43
3:m:362:LYS:HE2	3:m:362:LYS:HB3	1.86	0.43
1:w:23:LEU:HD23	1:w:23:LEU:HA	1.85	0.43
6:7:66:TRP:HA	6:7:69:GLU:HG2	1.98	0.43
8:AZ:21:ASP:OD1	8:AZ:21:ASP:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:25:LYS:H	1:AC:29:GLN:NE2	2.17	0.43
1:AD:148:LEU:HD22	1:AD:171:LEU:HD13	1.99	0.43
1:AI:78:PRO:HA	1:AI:79:PRO:HD3	1.91	0.43
2:G:63:ALA:HB2	2:G:103:ASP:HB2	1.99	0.43
2:H:42:LEU:HD22	2:H:66:LYS:HB2	2.00	0.43
2:I:76:ASP:HA	2:I:77:PRO:HD3	1.80	0.43
2:L:63:ALA:HB2	2:L:103:ASP:HB3	2.01	0.43
3:T:364:ASP:HA	3:T:390:SER:HB3	1.99	0.43
3:W:249:HIS:HB2	3:W:257:VAL:HG22	2.01	0.43
3:a:304:GLU:OE1	3:a:316:ARG:NH1	2.51	0.43
3:f:174:ASP:OD1	3:f:174:ASP:N	2.51	0.43
3:h:294:MET:HE3	3:h:294:MET:HB2	1.68	0.43
1:s:93:SER:O	1:s:93:SER:OG	2.35	0.43
1:AJ:177:ASP:OD2	1:AJ:177:ASP:N	2.50	0.43
4:1:52:LEU:HA	4:1:55:VAL:HG22	2.00	0.43
4:2:106:TYR:OH	4:2:218:GLN:O	2.31	0.43
1:AD:20:ASP:OD1	1:AD:20:ASP:N	2.51	0.43
2:H:107:MET:HE2	2:H:151:GLY:HA2	2.00	0.43
2:N:114:LEU:HD21	2:N:163:ALA:HB1	2.00	0.43
3:R:229:ASN:ND2	3:R:248:ILE:O	2.52	0.43
3:Y:316:ARG:HH21	3:Y:318:ASN:HD21	1.66	0.43
1:AL:191:SER:OG	1:AL:192:ASP:N	2.51	0.43
3:e:271:GLU:HA	3:e:274:VAL:HG22	1.99	0.43
3:n:271:GLU:HA	3:n:274:VAL:HG22	2.01	0.43
1:x:160:LEU:HD12	1:x:187:LEU:HD12	2.01	0.43
1:AJ:94:LEU:HG	1:AJ:95:VAL:HG23	2.00	0.43
3:i:221:ARG:HE	3:i:221:ARG:HB3	1.65	0.43
3:l:313:PRO:HG3	3:l:367:LYS:HD3	2.01	0.43
3:n:307:LEU:HD12	3:n:307:LEU:HA	1.87	0.43
4:0:97:ASP:HA	4:0:100:ARG:HB3	2.01	0.43
4:3:27:PHE:O	4:3:31:SER:OG	2.27	0.43
2:K:112:VAL:HG23	7:AP:16:ALA:HB2	2.00	0.43
3:U:260:LEU:HD13	3:U:291:ILE:HG23	2.01	0.43
3:Z:340:ARG:HH22	1:x:163:GLN:HE21	1.66	0.43
1:p:203:LYS:HD2	1:p:203:LYS:HA	1.88	0.43
1:t:110:GLU:OE2	1:u:112:ARG:NE	2.51	0.43
1:u:93:SER:OG	1:u:95:VAL:O	2.31	0.43
8:AT:58:ARG:HA	8:AT:58:ARG:HD3	1.75	0.43
1:AE:146:VAL:HG23	1:AE:178:VAL:HG12	2.00	0.43
2:M:44:THR:HB	3:R:380:LYS:HE2	2.00	0.43
3:S:243:LEU:HD12	3:S:243:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:78:PRO:HA	1:AL:79:PRO:HD3	1.94	0.43
3:c:332:ASP:OD2	3:c:332:ASP:N	2.43	0.43
3:g:258:PHE:HB3	3:g:291:ILE:HG12	2.01	0.43
5:5:83:MET:HE3	5:5:87:LEU:HD21	2.01	0.43
7:AP:86:THR:HG22	8:AU:78:ASN:HD21	1.83	0.43
8:AS:58:ARG:HA	8:AS:58:ARG:HD3	1.87	0.43
2:G:168:LYS:HE2	2:G:168:LYS:HB3	1.77	0.43
3:Y:188:PRO:HA	3:Y:194:LEU:HD12	2.01	0.43
6:6:6:PHE:HE1	6:6:77:GLN:HE22	1.66	0.43
7:AR:57:ASP:OD1	7:AR:60:LEU:N	2.52	0.43
8:BA:75:ILE:HA	8:BA:78:ASN:HB2	2.01	0.43
2:A:156:VAL:HA	2:A:159:VAL:HG22	2.01	0.42
3:W:333:ASP:OD1	1:u:169:ARG:NE	2.49	0.42
3:W:365:TRP:HD1	3:W:390:SER:HB2	1.84	0.42
3:X:258:PHE:HB3	3:X:291:ILE:HG12	2.01	0.42
3:g:249:HIS:HB2	3:g:257:VAL:HG22	2.01	0.42
1:x:151:LEU:HD21	1:y:120:MET:HE2	2.01	0.42
4:4:167:LEU:HD23	4:4:167:LEU:HA	1.85	0.42
1:AA:151:LEU:HD21	1:AB:120:MET:HE2	2.00	0.42
2:K:115:ARG:HH12	7:AP:13:ILE:C	2.27	0.42
3:S:363:ASP:N	3:S:363:ASP:OD1	2.47	0.42
3:Y:232:ILE:HD11	3:Y:279:LEU:HD22	2.00	0.42
3:k:380:LYS:HE3	3:k:380:LYS:HB3	1.80	0.42
3:l:364:ASP:HA	3:l:390:SER:HB2	2.01	0.42
3:m:228:GLU:OE2	3:m:231:ARG:NH2	2.45	0.42
4:3:172:VAL:HA	4:3:175:VAL:HG12	2.01	0.42
5:5:56:PRO:HG3	5:5:154:TYR:HB3	2.01	0.42
1:AC:171:LEU:HD23	1:AC:171:LEU:HA	1.87	0.42
3:X:260:LEU:HD13	3:X:291:ILE:HG23	2.02	0.42
1:AL:139:ASN:HD22	1:AL:139:ASN:HA	1.70	0.42
3:c:249:HIS:HB2	3:c:257:VAL:HG23	2.02	0.42
3:k:363:ASP:OD2	3:k:363:ASP:N	2.51	0.42
1:w:177:ASP:N	1:w:177:ASP:OD1	2.49	0.42
1:z:23:LEU:HD12	1:z:24:LEU:HG	2.02	0.42
8:AS:56:LEU:HD13	8:AS:56:LEU:HA	1.87	0.42
1:AA:147:HIS:NE2	1:AB:176:ALA:O	2.52	0.42
1:AA:151:LEU:HA	1:AA:186:VAL:O	2.18	0.42
2:I:36:VAL:HG23	3:j:373:TYR:HE1	1.84	0.42
3:X:252:GLU:HA	3:X:253:PRO:HD3	1.90	0.42
3:h:332:ASP:N	3:h:332:ASP:OD1	2.36	0.42
3:l:200:ASN:O	3:l:204:THR:OG1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:334:VAL:HG12	3:m:338:ARG:HE	1.83	0.42
1:u:73:LYS:NZ	1:v:34:GLU:OE2	2.52	0.42
4:0:59:LEU:HD23	4:0:59:LEU:HA	1.91	0.42
1:AC:126:ALA:HA	1:AC:151:LEU:O	2.20	0.42
3:T:361:LEU:HD13	1:r:165:SER:HB2	2.02	0.42
3:e:223:ILE:HD13	3:e:223:ILE:HG21	1.87	0.42
1:s:153:VAL:HA	1:s:188:SER:O	2.20	0.42
4:2:90:LYS:HE3	4:2:90:LYS:HB3	1.82	0.42
4:3:161:ILE:HG13	6:8:82:ALA:HB1	2.02	0.42
8:AS:76:ILE:H	8:AS:76:ILE:HG12	1.48	0.42
1:AC:36:ILE:HD11	1:AC:48:LYS:HB2	2.01	0.42
1:AE:78:PRO:HA	1:AE:79:PRO:HD3	1.94	0.42
1:AF:51:SER:HB3	1:AF:55:GLY:O	2.20	0.42
3:E:188:PRO:HA	3:E:194:LEU:HD12	2.01	0.42
2:M:120:ASN:O	2:M:124:ASN:ND2	2.48	0.42
3:R:202:ARG:NH1	1:o:192:ASP:O	2.53	0.42
3:Y:245:TYR:OH	3:Y:353:ARG:NH1	2.53	0.42
3:g:200:ASN:O	3:g:204:THR:OG1	2.31	0.42
4:2:176:VAL:HG21	4:2:194:SER:HB2	2.01	0.42
8:AU:48:GLN:HA	8:AU:51:LEU:HD23	2.02	0.42
8:AU:58:ARG:HD3	8:AU:58:ARG:HA	1.78	0.42
1:AF:36:ILE:HD11	1:AF:48:LYS:HB2	2.01	0.42
3:R:249:HIS:HB2	3:R:257:VAL:HG23	2.01	0.42
3:W:279:LEU:HD23	3:W:279:LEU:HA	1.85	0.42
3:g:200:ASN:OD1	3:g:200:ASN:N	2.52	0.42
3:g:236:LEU:HD12	3:g:236:LEU:HA	1.93	0.42
3:h:200:ASN:OD1	3:h:200:ASN:N	2.52	0.42
1:q:20:ASP:OD1	1:q:20:ASP:N	2.51	0.42
4:2:163:PHE:HB2	4:3:199:LEU:HD11	2.02	0.42
4:3:97:ASP:OD1	4:3:100:ARG:NH1	2.52	0.42
4:4:152:LEU:HB3	5:5:143:LEU:HD13	2.01	0.42
7:AN:48:LYS:O	7:AN:52:THR:OG1	2.26	0.42
2:F:116:ASN:OD1	2:F:116:ASN:N	2.53	0.42
2:M:165:MET:HE2	7:AO:15:GLN:HB2	2.02	0.42
3:U:232:ILE:O	3:U:236:LEU:HB2	2.20	0.42
3:W:304:GLU:OE1	3:W:316:ARG:NH1	2.53	0.42
3:b:200:ASN:O	3:b:204:THR:OG1	2.32	0.42
1:r:154:TYR:HE2	1:r:187:LEU:HD22	1.85	0.42
1:AJ:139:ASN:HD22	1:AJ:141:ARG:NH1	2.17	0.42
4:1:96:LEU:HD11	4:1:100:ARG:HH21	1.85	0.42
8:AS:60:ALA:O	8:AS:64:THR:OG1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:63:ALA:HB2	2:O:103:ASP:HB3	2.01	0.42
3:V:380:LYS:HE2	3:V:380:LYS:HB3	1.87	0.42
3:Z:217:ASP:OD1	3:Z:217:ASP:N	2.46	0.42
1:q:107:SER:O	1:q:111:GLN:NE2	2.50	0.42
1:r:117:LEU:HD23	1:r:117:LEU:HA	1.89	0.42
1:t:85:ILE:HB	1:t:107:SER:HB2	2.01	0.42
1:v:85:ILE:HB	1:v:107:SER:HB3	2.02	0.42
5:5:51:ALA:HA	5:5:54:VAL:HG22	2.01	0.42
8:AS:26:GLN:HG3	8:AS:50:LYS:HZ1	1.85	0.42
1:AC:177:ASP:OD2	1:AC:177:ASP:N	2.52	0.42
2:B:76:ASP:HA	2:B:77:PRO:HD3	1.80	0.42
2:Q:158:MET:HE3	2:Q:158:MET:HB3	1.88	0.42
3:S:236:LEU:HD23	3:S:236:LEU:HA	1.92	0.42
3:U:204:THR:OG1	3:U:224:ASN:ND2	2.53	0.42
3:X:372:GLN:O	3:X:377:GLY:HA2	2.19	0.42
3:Z:195:TYR:HE1	3:Z:221:ARG:HH11	1.66	0.42
3:b:208:ARG:HG3	3:b:222:VAL:HG11	2.02	0.42
3:k:306:GLY:O	3:k:310:GLN:NE2	2.53	0.42
1:w:39:LEU:HD22	1:w:44:ILE:HD11	2.01	0.42
7:AQ:42:ILE:HD13	7:AQ:42:ILE:HA	1.92	0.42
1:AE:85:ILE:HB	1:AE:107:SER:HB3	2.02	0.41
2:C:84:LEU:O	2:C:88:LEU:HB2	2.20	0.41
3:S:307:LEU:HD12	3:S:307:LEU:HA	1.91	0.41
3:U:372:GLN:O	3:U:377:GLY:HA2	2.20	0.41
3:X:363:ASP:N	3:X:363:ASP:OD1	2.43	0.41
3:f:245:TYR:OH	3:f:353:ARG:NH1	2.53	0.41
3:m:235:TRP:CD2	3:m:282:LEU:HD11	2.55	0.41
1:u:39:LEU:HD22	1:u:44:ILE:HD11	2.02	0.41
1:u:147:HIS:NE2	1:v:176:ALA:O	2.53	0.41
1:AK:153:VAL:HA	1:AK:188:SER:O	2.19	0.41
4:3:160:LYS:HB2	4:4:203:VAL:HG21	2.02	0.41
5:5:95:MET:HG3	5:5:129:LEU:HB3	2.02	0.41
8:AS:69:LYS:HD3	8:AS:69:LYS:HA	1.78	0.41
1:AE:41:MET:HE3	1:AE:41:MET:HB2	1.85	0.41
1:AG:94:LEU:HD13	6:8:17:ILE:HD11	2.02	0.41
3:E:274:VAL:HG12	3:E:278:LYS:HE2	2.01	0.41
3:E:343:VAL:HG11	1:o:162:HIS:CE1	2.55	0.41
3:Z:315:SER:HB3	3:Z:326:VAL:HG23	2.01	0.41
3:k:318:ASN:HA	3:k:323:VAL:HG23	2.01	0.41
1:AK:203:LYS:HB3	1:AK:203:LYS:HE2	1.83	0.41
4:2:36:MET:HE3	4:2:36:MET:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2:171:VAL:HG23	6:7:15:VAL:HG22	2.02	0.41
8:AU:56:LEU:HD13	8:AU:56:LEU:HA	1.86	0.41
2:D:39:ASP:H	2:D:69:THR:HB	1.84	0.41
2:F:152:PRO:HA	2:F:153:PRO:HD3	1.96	0.41
2:I:107:MET:HE2	2:I:151:GLY:HA2	2.02	0.41
3:g:363:ASP:N	3:g:363:ASP:OD1	2.43	0.41
1:p:99:ARG:HE	1:p:134:ILE:HB	1.85	0.41
1:s:169:ARG:NH1	1:s:180:TYR:OH	2.53	0.41
1:w:88:MET:HB3	1:w:88:MET:HE2	1.76	0.41
1:x:107:SER:O	1:x:107:SER:OG	2.37	0.41
7:AR:85:SER:OG	7:AR:86:THR:N	2.53	0.41
8:AX:37:LYS:HA	8:AX:37:LYS:HD3	1.82	0.41
1:AA:146:VAL:HB	1:AA:178:VAL:HG12	2.03	0.41
1:AF:108:ALA:HB2	1:AJ:88:MET:HG3	2.03	0.41
2:Q:141:ASP:HB3	2:Q:144:LYS:HB2	2.01	0.41
3:X:180:GLU:H	3:X:180:GLU:HG2	1.64	0.41
3:a:256:PRO:HG2	3:a:289:VAL:HG12	2.01	0.41
3:i:272:LEU:HD23	3:i:272:LEU:HA	1.93	0.41
3:m:200:ASN:N	3:m:200:ASN:OD1	2.52	0.41
4:0:111:LEU:HD23	4:0:115:PHE:HE2	1.85	0.41
8:BB:72:ASP:HA	8:BB:75:ILE:HG12	2.02	0.41
2:B:109:ASN:OD1	2:B:109:ASN:N	2.54	0.41
2:D:40:ASP:OD2	2:D:44:THR:OG1	2.31	0.41
2:K:116:ASN:OD1	2:K:116:ASN:N	2.53	0.41
3:S:213:ARG:NH2	1:p:43:ASN:O	2.52	0.41
3:U:190:ARG:NH2	3:U:284:PRO:HA	2.35	0.41
1:r:78:PRO:HA	1:r:79:PRO:HD3	1.91	0.41
1:v:203:LYS:HE3	1:v:203:LYS:HB3	1.95	0.41
1:y:85:ILE:HB	1:y:107:SER:HB2	2.03	0.41
1:AJ:34:GLU:HG2	1:AJ:79:PRO:HG2	2.03	0.41
1:AJ:198:PRO:HD3	1:AK:66:THR:HG21	2.01	0.41
5:5:92:PHE:HB3	5:5:130:ASN:HD21	1.86	0.41
7:AN:67:LEU:HD23	7:AN:67:LEU:HA	1.90	0.41
8:AS:49:SER:OG	8:AY:10:ASP:OD1	2.30	0.41
8:AT:59:ASN:O	8:AT:63:ASN:ND2	2.43	0.41
8:BE:12:VAL:HA	8:BE:15:LYS:HE2	2.02	0.41
2:C:141:ASP:HB3	2:C:144:LYS:HB2	2.03	0.41
2:I:144:LYS:HA	2:I:144:LYS:HD3	1.88	0.41
2:M:97:GLN:OE1	2:N:150:SER:OG	2.37	0.41
2:O:166:MET:HE2	2:O:166:MET:HB3	1.95	0.41
3:V:260:LEU:HD12	3:V:260:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:356:GLN:HB2	3:Z:309:GLN:HE21	1.86	0.41
3:i:295:ASP:HB3	3:i:298:THR:HG22	2.02	0.41
3:k:229:ASN:HD21	3:k:248:ILE:H	1.67	0.41
3:k:381:MET:HE3	3:k:381:MET:HB3	1.91	0.41
4:2:186:MET:SD	4:2:186:MET:N	2.91	0.41
7:AR:83:MET:HG3	8:AX:76:ILE:HD12	2.02	0.41
1:AD:69:VAL:HG11	1:AI:36:ILE:HG22	2.03	0.41
1:AG:75:TYR:HB3	1:AG:77:LEU:HD13	2.03	0.41
2:O:109:ASN:OD1	2:O:109:ASN:N	2.52	0.41
3:X:193:MET:HG3	3:X:219:ASN:HB2	2.03	0.41
3:g:310:GLN:HB2	3:g:312:LEU:HD23	2.03	0.41
1:o:173:ASN:OD1	1:o:173:ASN:N	2.49	0.41
1:u:155:GLU:OE1	1:u:156:ARG:N	2.53	0.41
1:w:104:ARG:HH11	1:w:104:ARG:HD3	1.74	0.41
5:5:192:LEU:HD22	5:5:219:LYS:HG2	2.02	0.41
6:7:25:VAL:HA	6:7:28:ILE:HG22	2.02	0.41
8:AW:24:GLN:O	8:AW:28:THR:OG1	2.33	0.41
1:AD:72:ILE:HD13	1:AD:72:ILE:HA	1.94	0.41
2:J:113:SER:HA	2:J:146:THR:HA	2.03	0.41
2:M:152:PRO:HA	2:M:153:PRO:HD3	1.96	0.41
2:O:49:MET:HE2	2:O:49:MET:HB3	1.82	0.41
3:S:258:PHE:HB3	3:S:291:ILE:HG12	2.03	0.41
3:T:173:LEU:HD12	3:T:176:LEU:HD12	2.01	0.41
1:AL:164:ILE:HG12	1:AL:187:LEU:HD21	2.01	0.41
3:j:364:ASP:OD1	3:j:364:ASP:N	2.46	0.41
1:o:20:ASP:OD1	1:o:20:ASP:N	2.54	0.41
1:o:151:LEU:HD23	1:o:186:VAL:HB	2.02	0.41
4:2:103:LEU:HD12	4:2:103:LEU:HA	1.89	0.41
7:AQ:58:PRO:HB2	8:BB:5:TRP:CZ2	2.55	0.41
8:AV:27:VAL:O	8:AV:50:LYS:NZ	2.51	0.41
8:BE:14:ALA:O	8:BE:18:THR:OG1	2.31	0.41
1:AG:194:GLN:HB2	3:k:202:ARG:NH2	2.36	0.41
2:C:161:ASN:HD22	7:AR:19:ILE:HG22	1.84	0.41
3:E:340:ARG:NH2	1:o:163:GLN:HE21	2.18	0.41
2:L:116:ASN:OD1	2:L:116:ASN:N	2.54	0.41
2:P:113:SER:HB2	2:P:146:THR:HG22	2.03	0.41
3:V:196:VAL:HG13	3:V:222:VAL:HG13	2.02	0.41
3:Y:272:LEU:HD23	3:Y:272:LEU:HA	1.95	0.41
3:a:243:LEU:HD12	3:a:243:LEU:HA	1.94	0.41
3:b:327:ILE:HB	3:b:359:ILE:HG22	2.03	0.41
3:e:380:LYS:HE3	3:e:380:LYS:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:310:GLN:HB2	3:h:312:LEU:HG	2.03	0.41
3:h:380:LYS:HB3	3:h:380:LYS:HE3	1.86	0.41
3:i:260:LEU:O	3:i:293:LEU:HA	2.21	0.41
3:j:217:ASP:OD1	3:j:217:ASP:N	2.50	0.41
1:z:38:VAL:HG11	1:z:77:LEU:HD11	2.03	0.41
4:3:36:MET:HE2	4:3:36:MET:HB3	1.81	0.41
6:8:35:LEU:HA	6:8:38:THR:HG22	2.03	0.41
7:AN:81:VAL:HA	7:AN:84:VAL:HG12	2.03	0.41
8:AV:31:LEU:HD13	8:BA:15:LYS:HE3	2.03	0.41
8:AZ:62:SER:HA	8:AZ:65:VAL:HG12	2.01	0.41
2:O:27:LYS:HB2	2:O:27:LYS:HE3	1.89	0.41
3:c:364:ASP:OD1	3:c:364:ASP:N	2.53	0.41
3:e:217:ASP:N	3:e:217:ASP:OD1	2.42	0.41
3:e:316:ARG:HH21	3:e:318:ASN:HD21	1.69	0.41
3:f:333:ASP:OD1	3:f:333:ASP:N	2.53	0.41
4:1:171:VAL:HG13	6:6:15:VAL:HG12	2.02	0.41
4:4:8:ILE:HG12	8:AW:75:ILE:HG21	2.02	0.41
4:4:96:LEU:HD23	4:4:96:LEU:HA	1.92	0.41
4:4:132:LYS:HA	4:4:132:LYS:HD3	1.79	0.41
6:9:37:GLN:HE21	6:9:47:LEU:HD23	1.85	0.41
8:AS:59:ASN:O	8:AS:63:ASN:ND2	2.42	0.41
3:E:228:GLU:HG3	3:E:231:ARG:HE	1.86	0.40
3:i:307:LEU:HD12	3:i:307:LEU:HA	1.90	0.40
3:j:255:LYS:HB3	3:j:255:LYS:HE3	1.85	0.40
3:n:328:GLN:HG2	3:n:360:GLU:HB3	2.02	0.40
1:w:53:LYS:HD3	1:w:53:LYS:HA	1.90	0.40
4:3:194:SER:O	4:3:198:LYS:N	2.54	0.40
2:C:60:SER:OG	2:C:61:LYS:N	2.54	0.40
2:F:109:ASN:OD1	2:F:109:ASN:N	2.54	0.40
3:T:243:LEU:HD12	3:T:243:LEU:HA	1.90	0.40
3:a:235:TRP:CD2	3:a:282:LEU:HD11	2.57	0.40
3:f:356:GLN:HB2	3:g:309:GLN:HE21	1.85	0.40
3:j:245:TYR:OH	3:j:353:ARG:NH1	2.54	0.40
3:l:316:ARG:NH2	3:l:318:ASN:HD21	2.18	0.40
1:s:139:ASN:ND2	4:0:110:GLU:OE1	2.54	0.40
4:2:20:ILE:HD13	4:2:20:ILE:HA	1.92	0.40
4:2:200:VAL:HA	4:2:203:VAL:HG12	2.02	0.40
8:AU:35:ALA:HB1	8:AZ:19:GLY:HA3	2.03	0.40
8:AY:40:ASP:HA	8:AY:41:PRO:HD3	1.94	0.40
8:BD:7:GLY:H	8:BD:10:ASP:HB2	1.85	0.40
1:AB:23:LEU:HD12	1:AB:24:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:176:ALA:O	1:AF:147:HIS:NE2	2.54	0.40
1:AH:163:GLN:NE2	3:i:340:ARG:HH22	2.20	0.40
2:B:114:LEU:HD13	2:B:117:VAL:HG13	2.03	0.40
2:J:112:VAL:HG11	2:J:160:VAL:HG23	2.03	0.40
2:M:158:MET:HB3	2:M:158:MET:HE3	1.80	0.40
3:T:196:VAL:HB	3:T:222:VAL:HG12	2.02	0.40
3:X:192:LYS:HE2	3:X:192:LYS:HB2	1.96	0.40
3:b:205:LEU:HD23	3:b:205:LEU:HA	1.90	0.40
3:d:304:GLU:OE1	3:d:316:ARG:NH1	2.53	0.40
1:t:134:ILE:HG21	1:u:105:LEU:HD22	2.03	0.40
1:v:80:ARG:H	1:v:80:ARG:HG2	1.66	0.40
1:x:78:PRO:HD2	1:y:30:GLU:OE2	2.21	0.40
4:2:113:GLN:HA	4:2:116:GLU:HG2	2.01	0.40
5:5:227:MET:HE3	5:5:227:MET:HB2	1.89	0.40
7:AN:51:ILE:HA	7:AN:54:ARG:HB3	2.03	0.40
7:AN:63:ASP:OD2	7:AN:65:LYS:NZ	2.55	0.40
1:AH:173:ASN:HD21	1:AI:184:SER:HB3	1.86	0.40
2:D:158:MET:HB3	2:D:158:MET:HE3	1.89	0.40
3:E:246:TYR:OH	3:E:296:ASP:OD1	2.38	0.40
2:G:40:ASP:HB3	2:G:44:THR:HG23	2.04	0.40
2:L:55:GLU:HG3	2:L:94:PHE:CE1	2.56	0.40
3:U:333:ASP:HA	3:U:336:ILE:HG22	2.03	0.40
1:r:158:SER:OG	1:r:163:GLN:NE2	2.55	0.40
1:z:85:ILE:H	1:z:85:ILE:HG12	1.75	0.40
1:AK:117:LEU:HD23	1:AK:117:LEU:HA	1.89	0.40
4:0:187:MET:HA	4:1:187:MET:HE3	2.04	0.40
4:3:101:ASP:OD1	4:3:140:LYS:NZ	2.47	0.40
1:AF:203:LYS:HA	1:AF:203:LYS:HD2	1.89	0.40
2:C:152:PRO:HA	2:C:153:PRO:HD3	1.95	0.40
3:U:333:ASP:OD2	1:r:185:VAL:N	2.54	0.40
3:b:245:TYR:OH	3:b:353:ARG:NH2	2.51	0.40
3:g:174:ASP:OD1	3:g:174:ASP:N	2.54	0.40
3:g:364:ASP:OD1	3:g:364:ASP:N	2.40	0.40
3:i:245:TYR:HB3	3:i:260:LEU:HD12	2.04	0.40
3:i:335:GLU:OE1	3:i:335:GLU:N	2.55	0.40
1:u:25:LYS:HB3	1:u:25:LYS:HE2	1.88	0.40
1:AJ:102:LYS:HE3	1:AJ:102:LYS:HB2	1.95	0.40
5:5:91:PRO:HA	5:5:94:VAL:HG12	2.04	0.40
7:AN:85:SER:OG	7:AN:86:THR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	AB	155/215 (72%)	155 (100%)	0	100	100
1	AC	155/215 (72%)	155 (100%)	0	100	100
1	AD	155/215 (72%)	155 (100%)	0	100	100
1	AE	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	AF	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	AG	155/215 (72%)	155 (100%)	0	100	100
1	AH	155/215 (72%)	155 (100%)	0	100	100
1	AI	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	AJ	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	AK	155/215 (72%)	155 (100%)	0	100	100
1	AL	155/215 (72%)	155 (100%)	0	100	100
1	o	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	p	155/215 (72%)	155 (100%)	0	100	100
1	q	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	r	155/215 (72%)	154 (99%)	1 (1%)	78	80
1	s	155/215 (72%)	155 (100%)	0	100	100
1	t	155/215 (72%)	155 (100%)	0	100	100
1	u	155/215 (72%)	155 (100%)	0	100	100
1	v	155/215 (72%)	153 (99%)	2 (1%)	61	72
1	w	155/215 (72%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	155/215 (72%)	155 (100%)	0	100	100
1	y	155/215 (72%)	155 (100%)	0	100	100
1	z	155/215 (72%)	155 (100%)	0	100	100
2	A	119/477 (25%)	118 (99%)	1 (1%)	73	77
2	B	125/477 (26%)	125 (100%)	0	100	100
2	C	119/477 (25%)	119 (100%)	0	100	100
2	D	124/477 (26%)	123 (99%)	1 (1%)	73	77
2	F	119/477 (25%)	118 (99%)	1 (1%)	73	77
2	G	125/477 (26%)	124 (99%)	1 (1%)	73	77
2	H	119/477 (25%)	118 (99%)	1 (1%)	73	77
2	I	125/477 (26%)	125 (100%)	0	100	100
2	J	119/477 (25%)	118 (99%)	1 (1%)	73	77
2	K	125/477 (26%)	125 (100%)	0	100	100
2	L	119/477 (25%)	118 (99%)	1 (1%)	73	77
2	M	75/477 (16%)	74 (99%)	1 (1%)	61	72
2	N	119/477 (25%)	118 (99%)	1 (1%)	73	77
2	O	125/477 (26%)	125 (100%)	0	100	100
2	P	119/477 (25%)	118 (99%)	1 (1%)	73	77
2	Q	125/477 (26%)	124 (99%)	1 (1%)	73	77
3	E	190/337 (56%)	190 (100%)	0	100	100
3	R	97/337 (29%)	97 (100%)	0	100	100
3	Z	156/337 (46%)	154 (99%)	2 (1%)	61	72
3	a	189/337 (56%)	188 (100%)	1 (0%)	81	82
3	b	188/337 (56%)	187 (100%)	1 (0%)	81	82
3	c	190/337 (56%)	190 (100%)	0	100	100
3	d	189/337 (56%)	188 (100%)	1 (0%)	81	82
3	e	188/337 (56%)	187 (100%)	1 (0%)	81	82
3	f	190/337 (56%)	190 (100%)	0	100	100
3	g	189/337 (56%)	185 (98%)	4 (2%)	47	65
3	h	188/337 (56%)	188 (100%)	0	100	100
3	i	190/337 (56%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	j	189/337 (56%)	187 (99%)	2 (1%)	65	74
3	k	188/337 (56%)	187 (100%)	1 (0%)	81	82
3	l	163/337 (48%)	161 (99%)	2 (1%)	63	73
3	m	189/337 (56%)	185 (98%)	4 (2%)	47	65
3	n	188/337 (56%)	187 (100%)	1 (0%)	81	82
4	0	175/199 (88%)	172 (98%)	3 (2%)	53	68
4	1	177/199 (89%)	177 (100%)	0	100	100
4	2	175/199 (88%)	175 (100%)	0	100	100
4	3	180/199 (90%)	179 (99%)	1 (1%)	78	80
4	4	197/199 (99%)	197 (100%)	0	100	100
5	5	205/219 (94%)	204 (100%)	1 (0%)	81	82
6	6	41/71 (58%)	41 (100%)	0	100	100
6	7	69/71 (97%)	69 (100%)	0	100	100
6	8	69/71 (97%)	69 (100%)	0	100	100
6	9	70/71 (99%)	70 (100%)	0	100	100
7	AM	34/88 (39%)	33 (97%)	1 (3%)	37	58
7	AN	71/88 (81%)	71 (100%)	0	100	100
7	AO	76/88 (86%)	76 (100%)	0	100	100
7	AP	77/88 (88%)	76 (99%)	1 (1%)	61	72
7	AQ	77/88 (88%)	77 (100%)	0	100	100
7	AR	76/88 (86%)	76 (100%)	0	100	100
8	AS	50/67 (75%)	46 (92%)	4 (8%)	11	33
8	AT	50/67 (75%)	44 (88%)	6 (12%)	5	20
8	AU	50/67 (75%)	45 (90%)	5 (10%)	7	26
8	AV	50/67 (75%)	45 (90%)	5 (10%)	7	26
8	AW	50/67 (75%)	44 (88%)	6 (12%)	5	20
8	AX	62/67 (92%)	62 (100%)	0	100	100
8	AY	66/67 (98%)	66 (100%)	0	100	100
8	AZ	51/67 (76%)	51 (100%)	0	100	100
8	BA	48/67 (72%)	47 (98%)	1 (2%)	47	65
8	BB	42/67 (63%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BC	42/67 (63%)	42 (100%)	0	100	100
8	BD	42/67 (63%)	42 (100%)	0	100	100
8	BE	37/67 (55%)	37 (100%)	0	100	100
All	All	11091/21418 (52%)	11016 (99%)	75 (1%)	73	79

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	166	ASP
1	AE	34	GLU
1	AF	92	ASP
1	AI	60	VAL
2	A	111	VAL
2	D	40	ASP
2	F	111	VAL
2	G	121	GLU
2	H	36	VAL
2	J	40	ASP
2	L	111	VAL
2	M	126	LEU
2	N	111	VAL
2	P	111	VAL
2	Q	40	ASP
3	Z	222	VAL
3	Z	334	VAL
3	a	366	LEU
3	b	355	VAL
3	d	366	LEU
3	e	361	LEU
3	g	194	LEU
3	g	312	LEU
3	g	355	VAL
3	g	366	LEU
3	j	222	VAL
3	j	355	VAL
3	k	222	VAL
3	l	196	VAL
3	l	355	VAL
3	m	279	LEU
3	m	333	ASP
3	m	355	VAL

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Mol	Chain	Res	Type
3	m	366	LEU
3	n	355	VAL
1	o	202	VAL
1	q	24	LEU
1	r	60	VAL
1	v	72	ILE
1	v	82	ARG
1	AJ	77	LEU
4	0	46	ILE
4	0	81	THR
4	0	152	LEU
4	3	211	LEU
5	5	68	VAL
7	AM	87	LEU
7	AP	98	LEU
8	AS	28	THR
8	AS	56	LEU
8	AS	64	THR
8	AS	76	ILE
8	AT	28	THR
8	AT	51	LEU
8	AT	56	LEU
8	AT	64	THR
8	AT	72	ASP
8	AT	76	ILE
8	AU	28	THR
8	AU	51	LEU
8	AU	56	LEU
8	AU	64	THR
8	AU	76	ILE
8	AV	31	LEU
8	AV	44	LEU
8	AV	56	LEU
8	AV	67	VAL
8	AV	76	ILE
8	AW	28	THR
8	AW	44	LEU
8	AW	51	LEU
8	AW	56	LEU
8	AW	64	THR
8	AW	76	ILE
8	BA	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	29	GLN
1	AB	33	ASN
1	AB	139	ASN
1	AE	31	GLN
1	AE	162	HIS
1	AF	47	ASN
1	AF	162	HIS
1	AH	29	GLN
1	AH	31	GLN
1	AI	162	HIS
1	AI	163	GLN
2	A	71	ASN
2	A	87	GLN
2	B	75	HIS
2	B	87	GLN
2	B	170	ASN
2	C	123	ASN
2	C	161	ASN
2	D	87	GLN
3	E	199	GLN
3	E	249	HIS
3	E	341	GLN
2	F	71	ASN
2	G	97	GLN
2	G	123	ASN
2	G	124	ASN
2	G	169	GLN
2	G	170	ASN
2	H	97	GLN
2	I	169	GLN
2	I	170	ASN
2	J	97	GLN
2	J	124	ASN
2	K	123	ASN
2	L	71	ASN
2	L	87	GLN
2	L	123	ASN
2	L	169	GLN
2	M	123	ASN
2	M	142	ASN
2	M	161	ASN

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Mol	Chain	Res	Type
2	M	169	GLN
2	N	123	ASN
2	N	169	GLN
2	N	170	ASN
2	P	71	ASN
2	P	87	GLN
2	P	169	GLN
2	Q	97	GLN
2	Q	169	GLN
3	R	219	ASN
3	R	229	ASN
3	Z	249	HIS
3	Z	265	ASN
3	Z	290	ASN
3	Z	309	GLN
3	Z	356	GLN
1	AL	40	GLN
1	AL	162	HIS
3	a	209	GLN
3	a	229	ASN
3	a	290	ASN
3	a	310	GLN
3	a	318	ASN
3	b	219	ASN
3	b	249	HIS
3	c	219	ASN
3	c	263	GLN
3	c	318	ASN
3	d	209	GLN
3	d	263	GLN
3	d	290	ASN
3	d	356	GLN
3	e	219	ASN
3	e	310	GLN
3	e	318	ASN
3	f	249	HIS
3	f	356	GLN
3	g	209	GLN
3	g	229	ASN
3	g	290	ASN
3	g	309	GLN
3	g	310	GLN

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Mol	Chain	Res	Type
3	g	319	HIS
3	g	372	GLN
3	h	209	GLN
3	h	224	ASN
3	h	318	ASN
3	i	318	ASN
3	j	263	GLN
3	j	328	GLN
3	k	209	GLN
3	k	310	GLN
3	k	356	GLN
3	l	310	GLN
3	l	341	GLN
3	m	219	ASN
3	m	318	ASN
3	m	372	GLN
3	n	224	ASN
1	o	115	GLN
1	o	162	HIS
1	p	31	GLN
1	p	47	ASN
1	p	139	ASN
1	p	163	GLN
1	q	47	ASN
1	r	163	GLN
1	s	162	HIS
1	s	163	GLN
1	t	33	ASN
1	t	162	HIS
1	t	163	GLN
1	t	173	ASN
1	u	29	GLN
1	u	139	ASN
1	u	173	ASN
1	v	29	GLN
1	v	111	GLN
1	v	139	ASN
1	v	162	HIS
1	w	129	HIS
1	x	162	HIS
1	x	163	GLN
1	z	47	ASN

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Mol	Chain	Res	Type
1	z	162	HIS
1	AJ	47	ASN
1	AJ	139	ASN
1	AJ	162	HIS
1	AJ	163	GLN
1	AK	139	ASN
4	1	3	ASN
4	2	44	GLN
4	2	69	HIS
4	3	117	ASN
4	4	44	GLN
4	4	91	HIS
5	5	76	GLN
5	5	104	ASN
5	5	105	GLN
5	5	130	ASN
5	5	139	GLN
5	5	161	ASN
5	5	210	ASN
5	5	238	ASN
5	5	245	GLN
6	7	37	GLN
6	7	77	GLN
6	8	9	ASN
6	8	37	GLN
6	8	41	GLN
6	8	43	GLN
6	9	9	ASN
6	9	37	GLN
7	AN	71	GLN
7	AN	78	ASN
7	AO	53	ASN
7	AP	49	GLN
7	AP	53	ASN
7	AP	59	ASN
7	AP	71	GLN
7	AQ	59	ASN
7	AQ	71	GLN
7	AR	53	ASN
7	AR	71	GLN
8	AS	26	GLN
8	AS	48	GLN

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Mol	Chain	Res	Type
8	AT	26	GLN
8	AT	61	GLN
8	AT	78	ASN
8	AU	78	ASN
8	AW	22	ASN
8	AW	63	ASN
8	AX	61	GLN
8	AX	78	ASN
8	AY	63	ASN
8	AZ	26	GLN
8	AZ	78	ASN
8	BB	78	ASN
8	BC	55	ASN
8	BD	59	ASN
8	BD	61	GLN
8	BD	78	ASN
8	BE	61	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

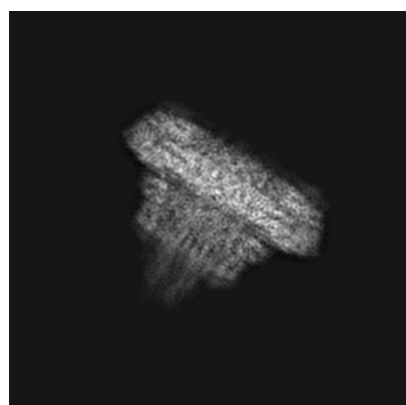
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20556. These allow visual inspection of the internal detail of the map and identification of artifacts.

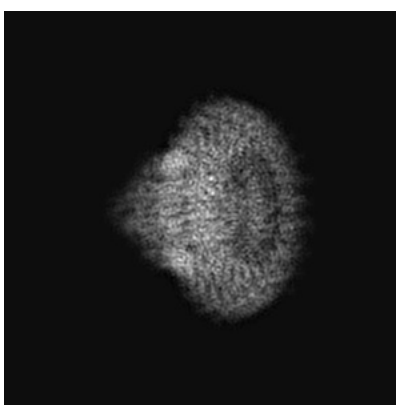
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

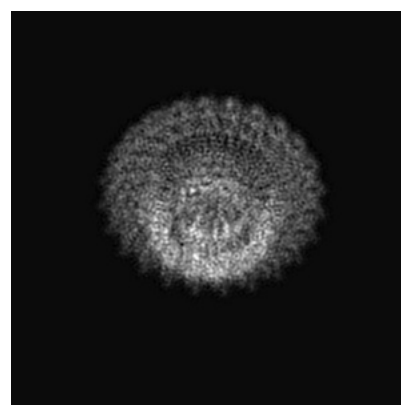
6.1.1 Primary map



X



Y

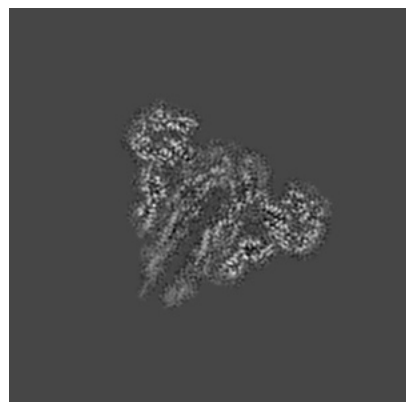


Z

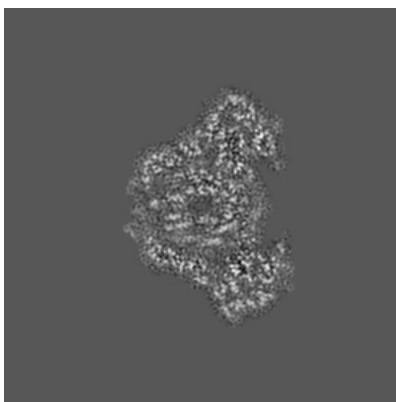
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

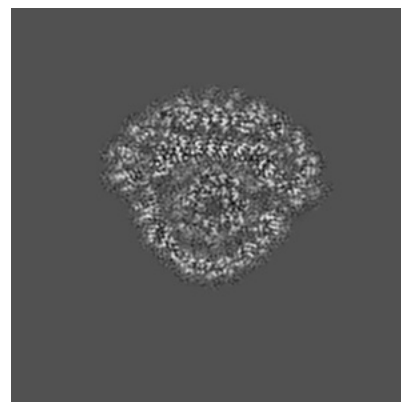
6.2.1 Primary map



X Index: 125



Y Index: 125



Z Index: 125

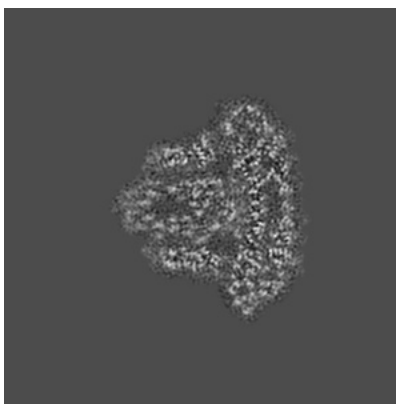
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

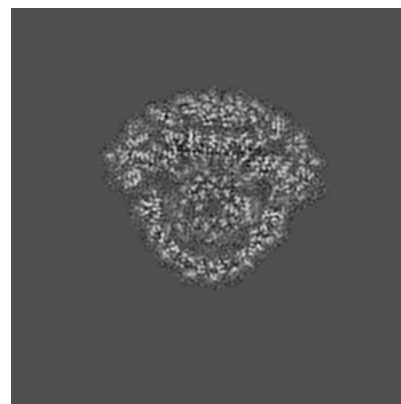
6.3.1 Primary map



X Index: 114



Y Index: 112

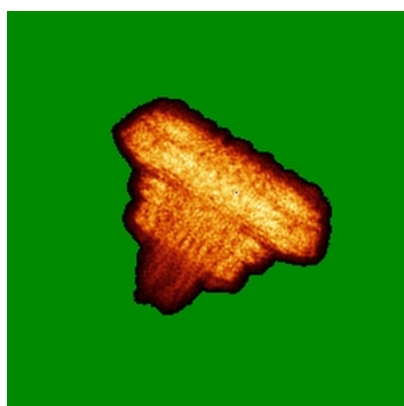


Z Index: 123

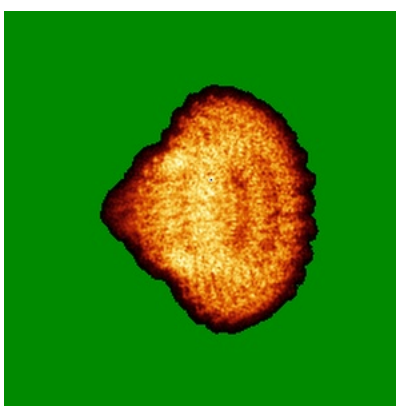
The images above show the largest variance slices of the map in three orthogonal directions.

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

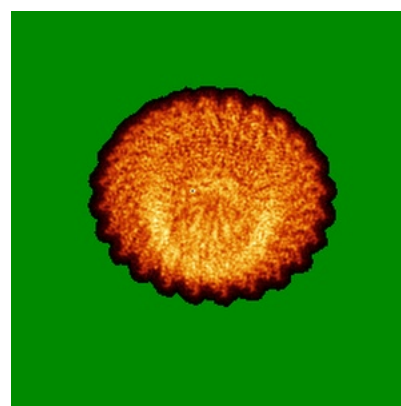
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

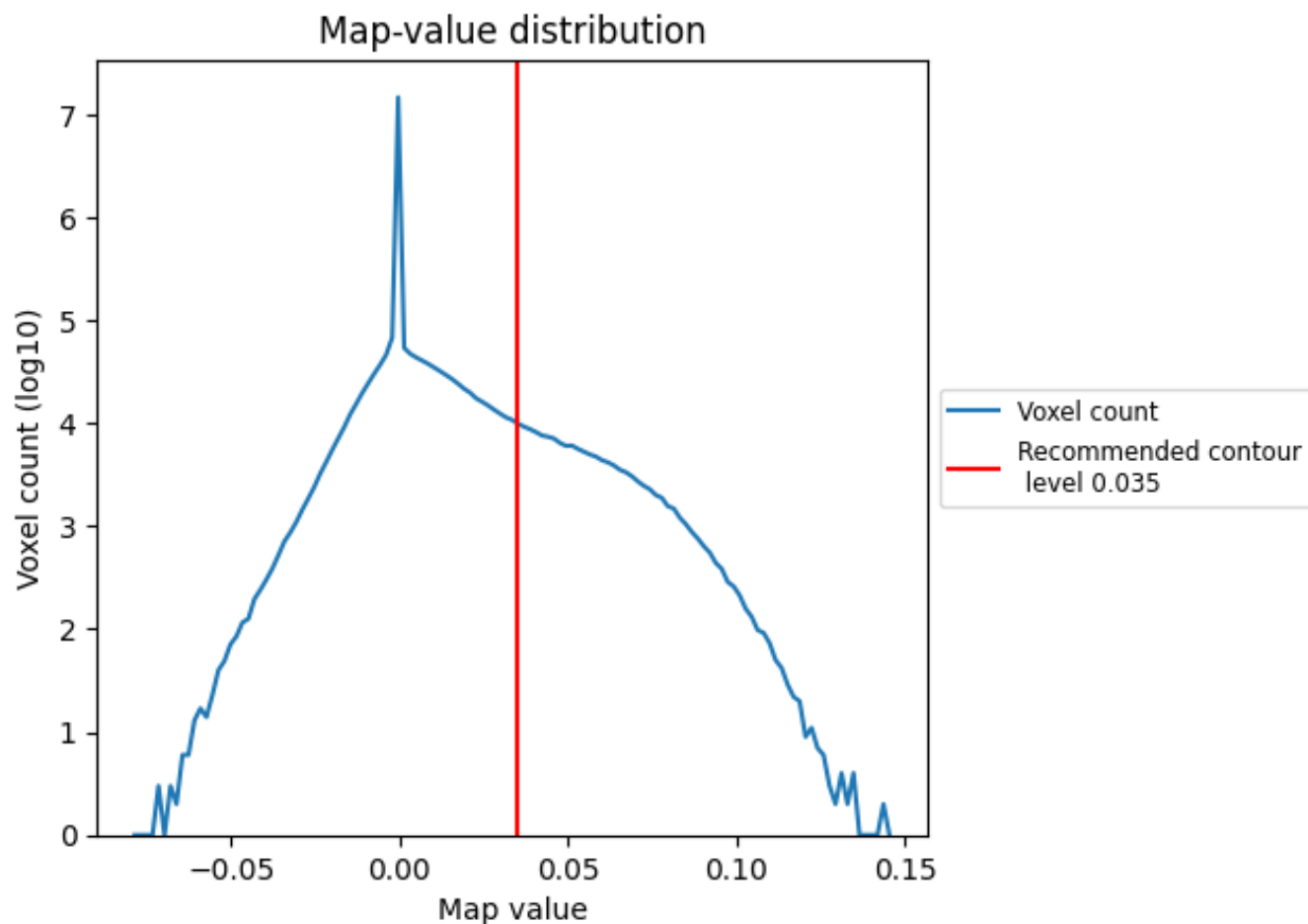
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

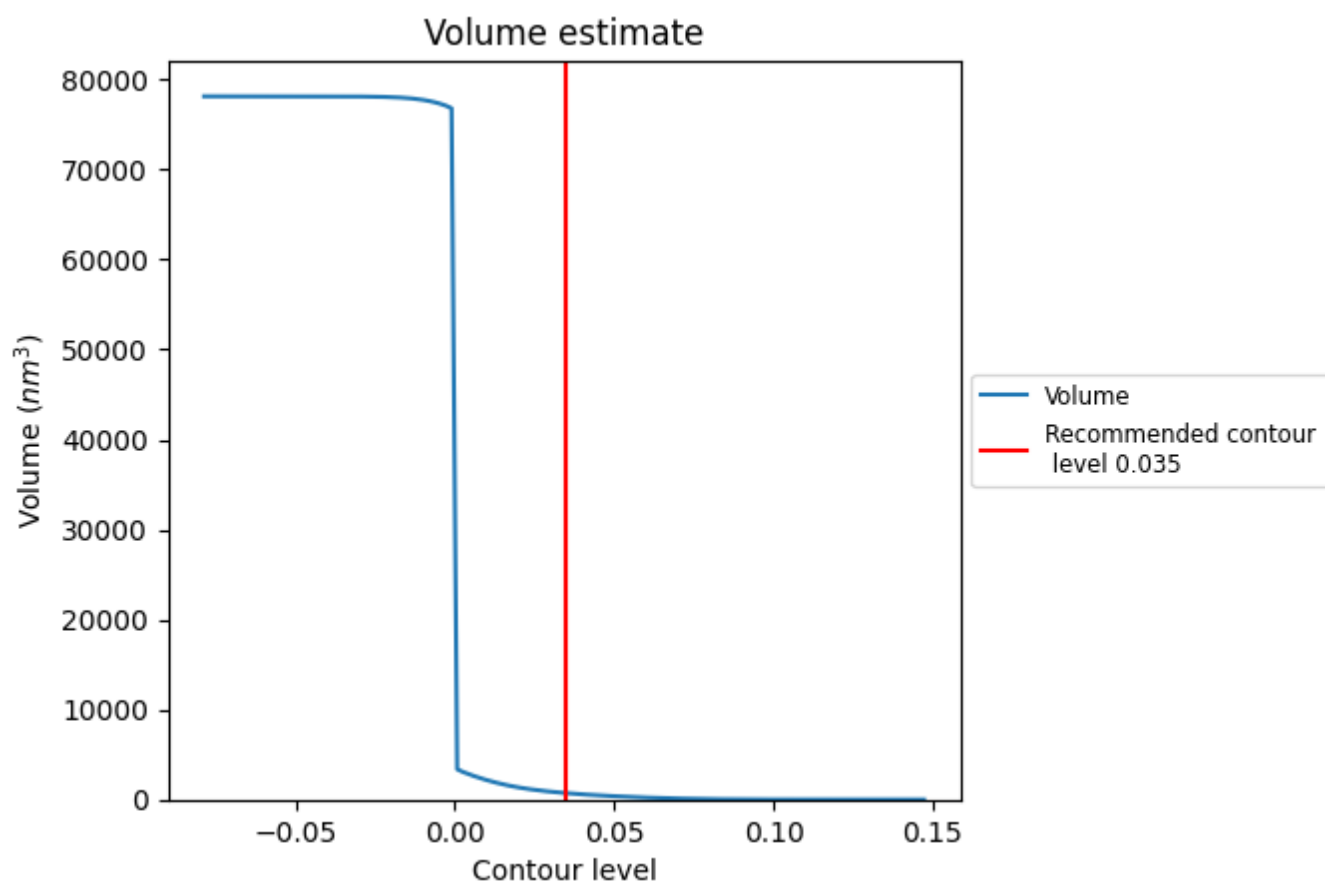
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

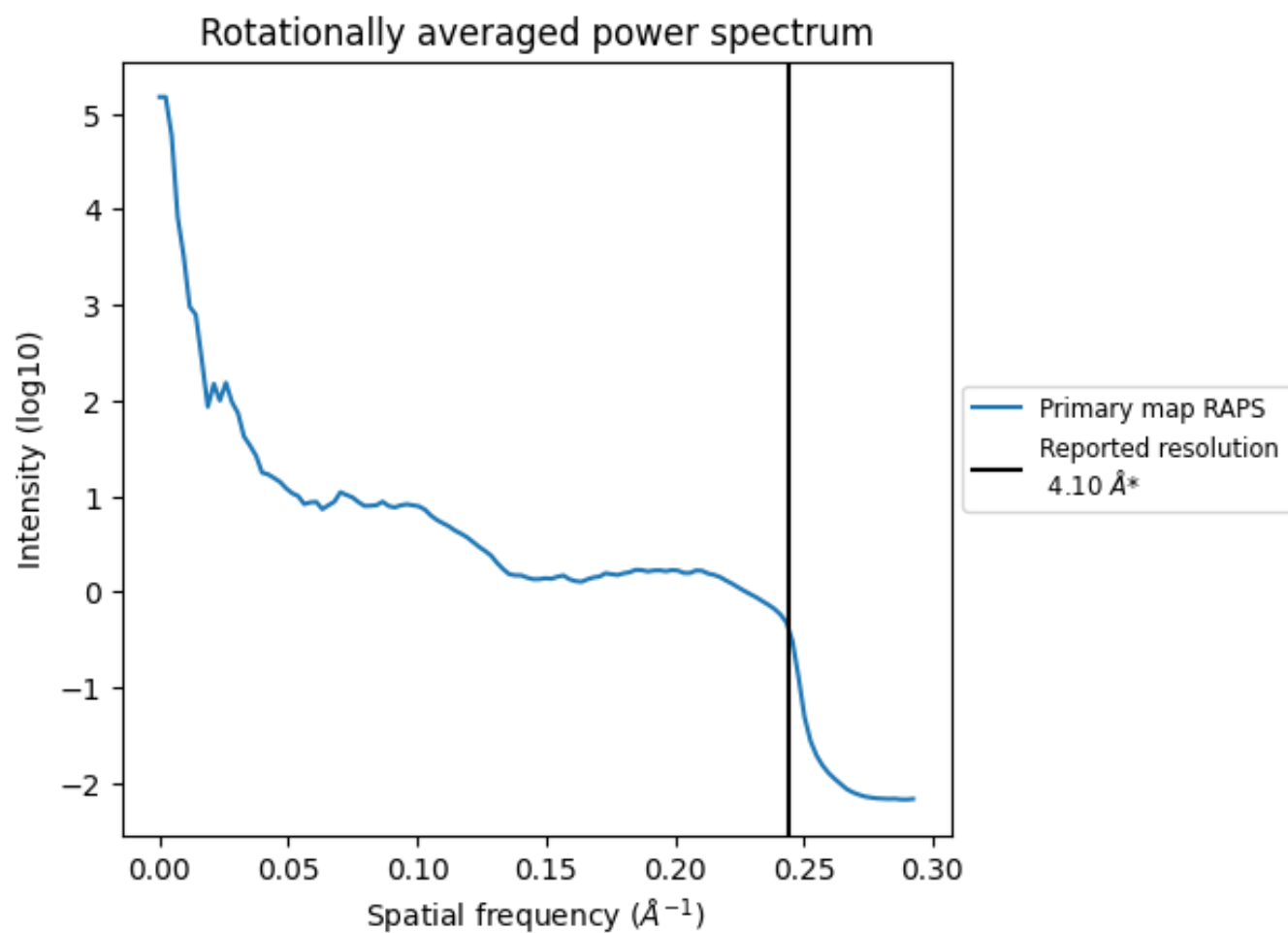
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 715 nm³; this corresponds to an approximate mass of 646 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 0.244 Å⁻¹

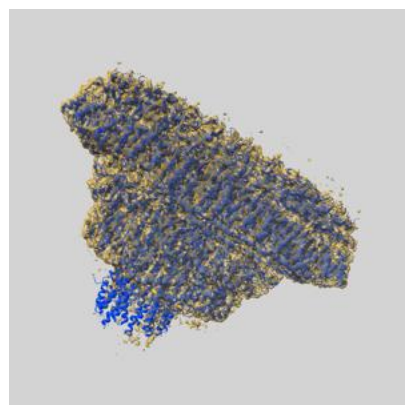
8 Fourier-Shell correlation ⓘ

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

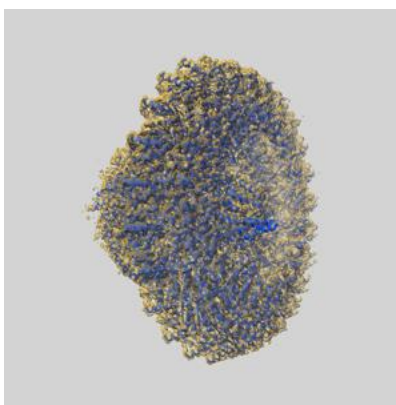
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20556 and PDB model 6Q16. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

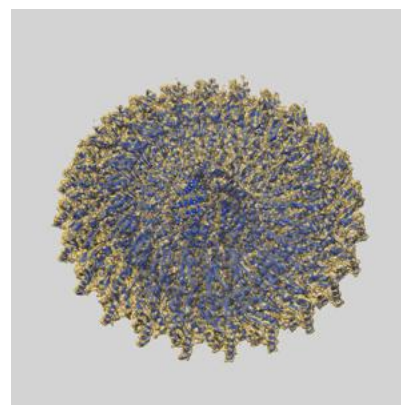
9.1 Map-model overlay [i](#)



X



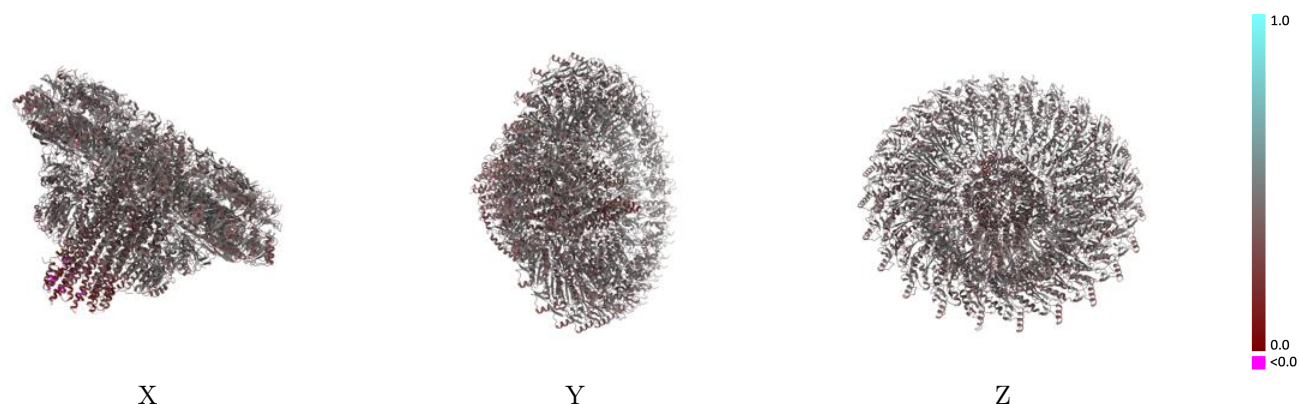
Y



Z

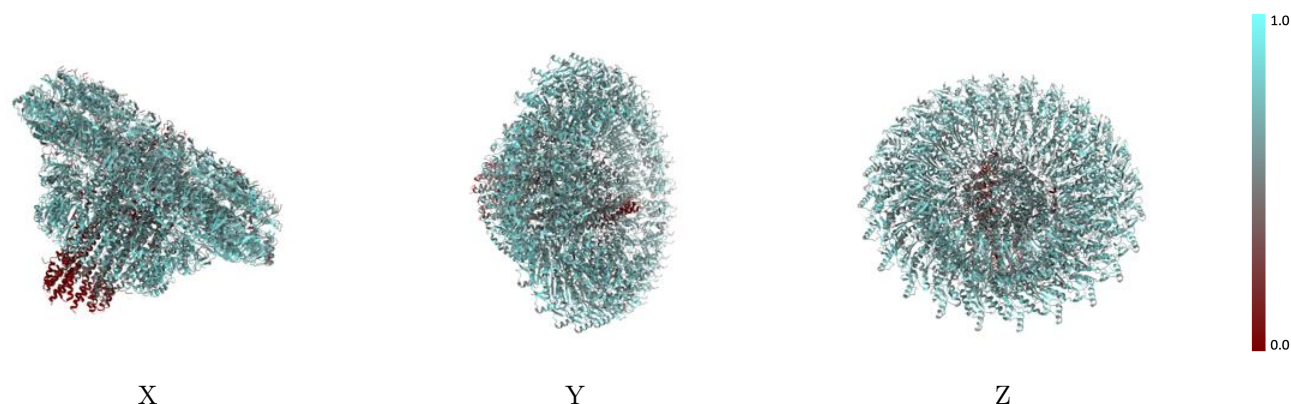
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



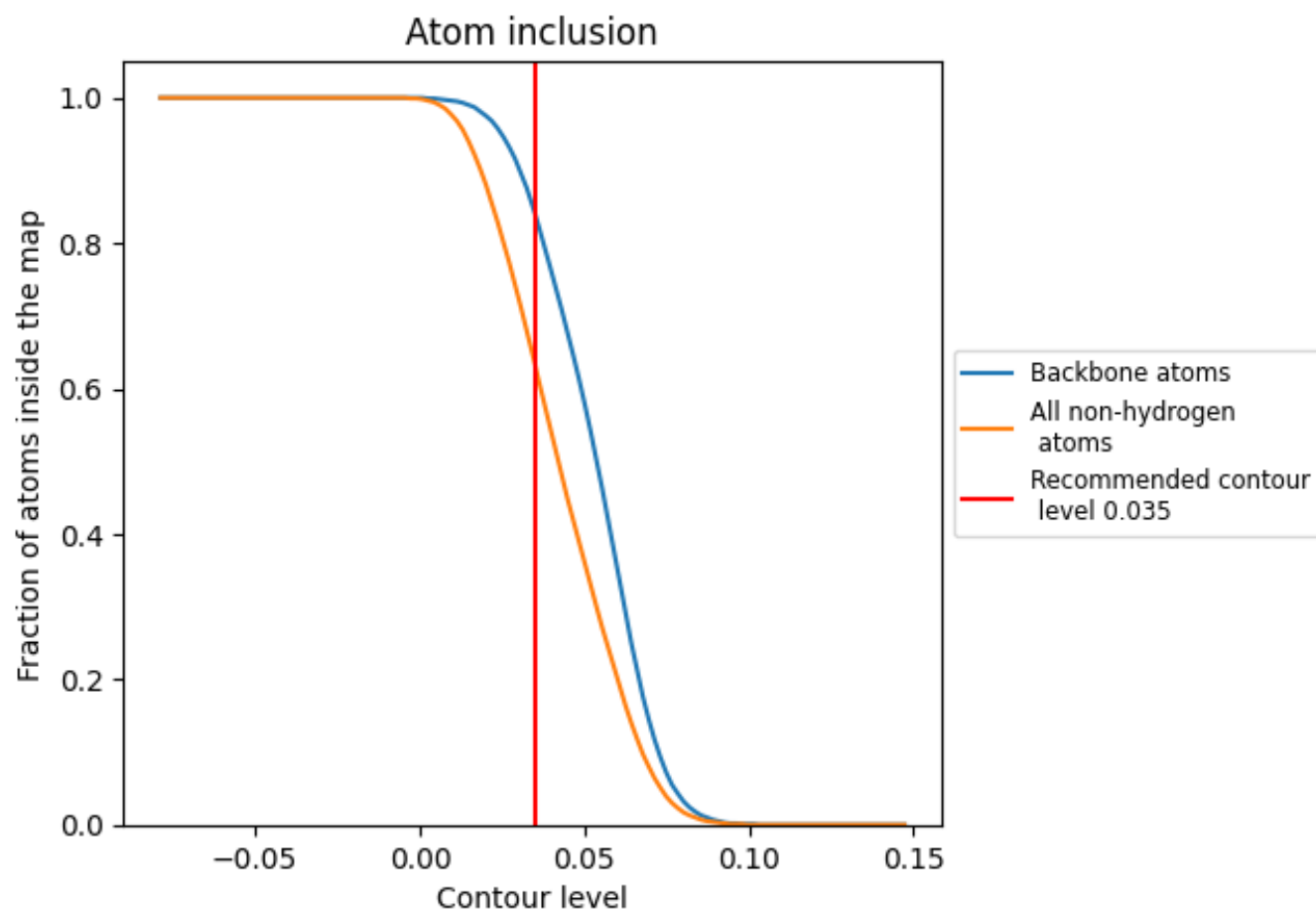
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 63% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6340	 0.4040
0	 0.5530	 0.3700
1	 0.5440	 0.3610
2	 0.5420	 0.3690
3	 0.5660	 0.3750
4	 0.5500	 0.3790
5	 0.6250	 0.4070
6	 0.2590	 0.3530
7	 0.3120	 0.3520
8	 0.4930	 0.3670
9	 0.5500	 0.3760
A	 0.7020	 0.4050
AA	 0.6490	 0.4220
AB	 0.6600	 0.4270
AC	 0.6740	 0.4340
AD	 0.6530	 0.4250
AE	 0.6660	 0.4250
AF	 0.6490	 0.4340
AG	 0.6650	 0.4230
AH	 0.6550	 0.4280
AI	 0.6610	 0.4230
AJ	 0.6460	 0.4260
AK	 0.6520	 0.4200
AL	 0.6710	 0.4290
AM	 0.5000	 0.3590
AN	 0.4840	 0.3490
AO	 0.4990	 0.3630
AP	 0.5130	 0.3510
AQ	 0.5020	 0.3480
AR	 0.4460	 0.3380
AS	 0.4200	 0.3130
AT	 0.4790	 0.2900
AU	 0.4640	 0.3050
AV	 0.4490	 0.2850
AW	 0.3640	 0.2910



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Chain	Atom inclusion	Q-score
AX	 0.0990	 0.2850
AY	 0.2520	 0.2530
AZ	 0.3190	 0.2720
B	 0.6950	 0.4010
BA	 0.3150	 0.2660
BB	 0.2760	 0.2440
BC	 0.0660	 0.2520
BD	 0.0260	 0.2330
BE	 0.0500	 0.1660
C	 0.7160	 0.4140
D	 0.6910	 0.4050
E	 0.6390	 0.3980
F	 0.7000	 0.4120
G	 0.6950	 0.4180
H	 0.7220	 0.4150
I	 0.6920	 0.4060
J	 0.7120	 0.4160
K	 0.6890	 0.4050
L	 0.7250	 0.4150
M	 0.6940	 0.4100
N	 0.7120	 0.4160
O	 0.6950	 0.4080
P	 0.7000	 0.4010
Q	 0.6930	 0.4000
R	 0.6950	 0.4100
S	 0.6930	 0.4120
T	 0.6500	 0.4110
U	 0.6840	 0.4200
V	 0.6810	 0.4160
W	 0.6290	 0.4120
X	 0.6900	 0.4150
Y	 0.6880	 0.4200
Z	 0.6350	 0.4150
a	 0.6790	 0.4200
b	 0.6940	 0.4240
c	 0.6660	 0.4180
d	 0.7110	 0.4240
e	 0.6930	 0.4110
f	 0.6700	 0.4150
g	 0.6890	 0.4160
h	 0.6940	 0.4150
i	 0.6620	 0.4160

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Chain	Atom inclusion	Q-score
j	 0.6930	 0.4180
k	 0.6980	 0.4150
l	 0.6540	 0.4130
m	 0.6910	 0.4140
n	 0.7010	 0.4220
o	 0.6520	 0.4300
p	 0.6420	 0.4230
q	 0.6450	 0.4220
r	 0.6410	 0.4270
s	 0.6340	 0.4220
t	 0.6320	 0.4230
u	 0.6380	 0.4220
v	 0.6290	 0.4140
w	 0.6410	 0.4230
x	 0.6620	 0.4300
y	 0.6620	 0.4170
z	 0.6540	 0.4280