



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:08 AM UTC

PDB ID : 6X65 / pdb_00006x65
EMDB ID : EMD-22070
Title : Legionella pneumophila Dot/Icm T4SS
Authors : Durie, C.L.; Sheedlo, M.J.; Chung, J.M.; Byrne, B.G.; Su, M.; Knight, T.; Swanson, M.S.; Lacy, D.B.; Ohi, M.D.
Deposited on : 2020-05-27
Resolution : 3.70 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

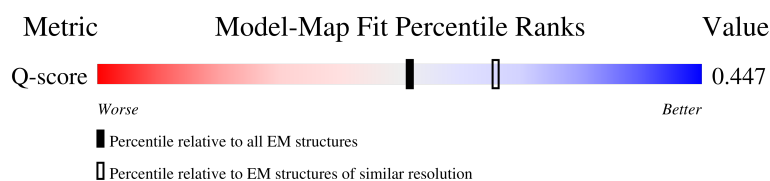
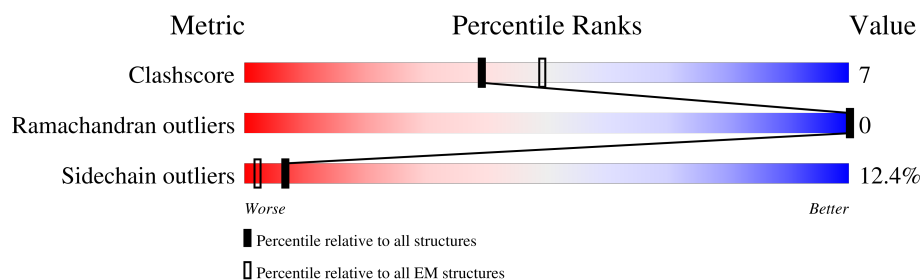
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	AV	228	61% 37%
1	AW	228	14% 86%
1	AX	228	9% 90% 10%
1	AY	228	23% 77%

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Mol	Chain	Length	Quality of chain
1	AZ	228	
1	BV	228	
1	BW	228	
1	BX	228	
1	BY	228	
1	BZ	228	
1	CV	228	
1	CW	228	
1	CX	228	
1	CY	228	
1	CZ	228	
1	DV	228	
1	DW	228	
1	DX	228	
1	DY	228	
1	DZ	228	
1	EV	228	
1	EW	228	
1	EX	228	
1	EY	228	
1	EZ	228	
1	FV	228	
1	FW	228	
1	FX	228	
1	FY	228	

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Mol	Chain	Length	Quality of chain
1	FZ	228	
1	GV	228	
1	GW	228	
1	GX	228	
1	GY	228	
1	GZ	228	
1	HV	228	
1	HW	228	
1	HX	228	
1	HY	228	
1	HZ	228	
1	IV	228	
1	IW	228	
1	IX	228	
1	IY	228	
1	IZ	228	
1	JV	228	
1	JW	228	
1	JX	228	
1	JY	228	
1	JZ	228	
1	KV	228	
1	KW	228	
1	KX	228	
1	KY	228	

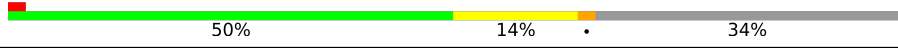
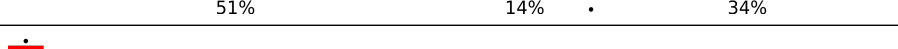
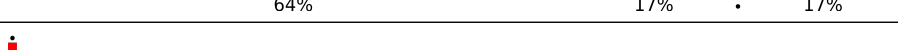
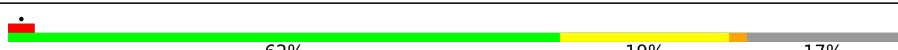
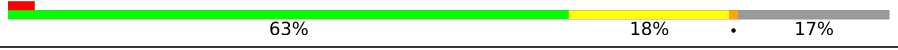
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Mol	Chain	Length	Quality of chain
1	KZ	228	
1	LV	228	
1	LW	228	
1	LX	228	
1	LY	228	
1	LZ	228	
1	MV	228	
1	MW	228	
1	MX	228	
1	MY	228	
1	MZ	228	
1	NV	228	
1	NW	228	
1	OV	228	
1	OW	228	
1	PV	228	
1	PW	228	
1	QV	228	
1	QW	228	
1	RV	228	
1	RW	228	
2	AC	303	
2	BC	303	
2	CC	303	
2	DC	303	

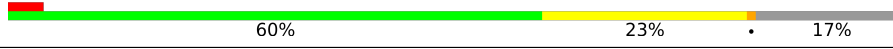
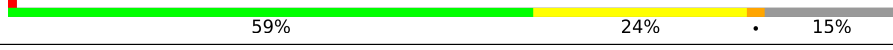
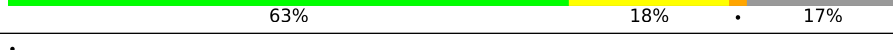
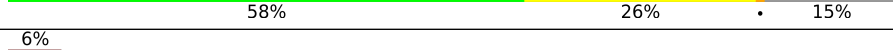
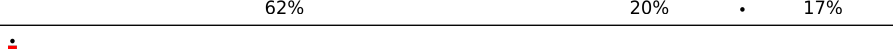
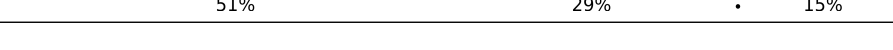
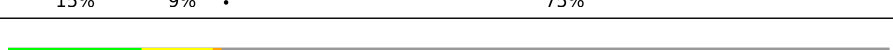
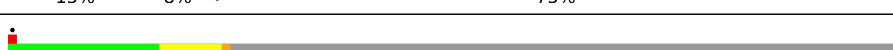
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Mol	Chain	Length	Quality of chain
2	EC	303	
2	FC	303	
2	GC	303	
2	HC	303	
2	IC	303	
2	JC	303	
2	KC	303	
2	LC	303	
2	MC	303	
3	AD	163	
3	Ad	163	
3	BD	163	
3	Bd	163	
3	CD	163	
3	Cd	163	
3	DD	163	
3	Dd	163	
3	ED	163	
3	Ed	163	
3	FD	163	
3	Fd	163	
3	GD	163	
3	Gd	163	
3	HD	163	
3	Hd	163	

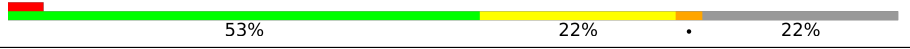
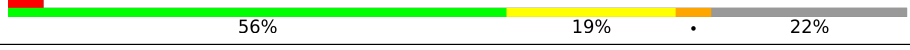
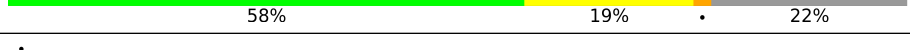
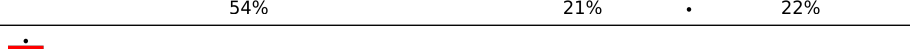
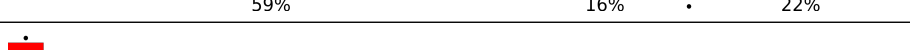
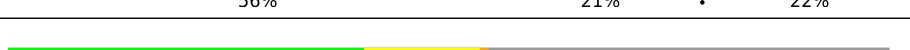
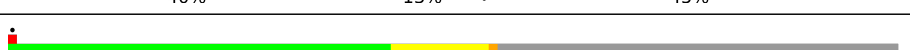
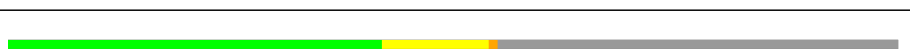
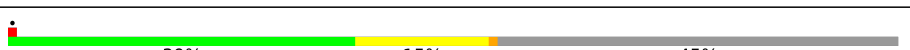
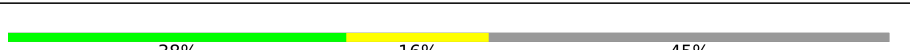
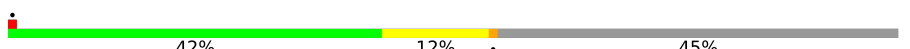
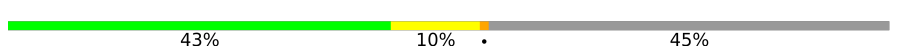
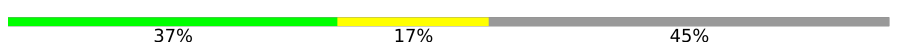
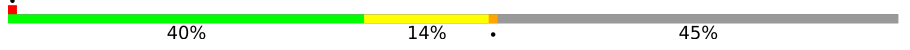
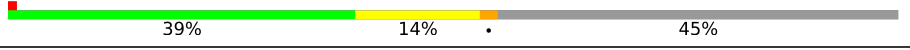
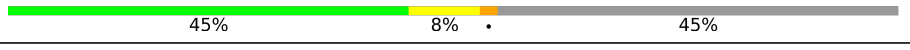
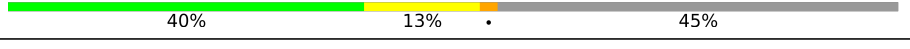
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Mol	Chain	Length	Quality of chain
3	ID	163	
3	Id	163	
3	JD	163	
3	Jd	163	
3	KD	163	
3	Kd	163	
3	LD	163	
3	Ld	163	
3	MD	163	
3	Md	163	
4	AH	361	
4	BH	361	
4	CH	361	
4	DH	361	
4	EH	361	
4	FH	361	
4	GH	361	
4	HH	361	
4	IH	361	
4	JH	361	
4	KH	361	
4	LH	361	
4	MH	361	
5	AK	189	
5	BK	189	

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Mol	Chain	Length	Quality of chain
5	CK	189	
5	DK	189	
5	EK	189	
5	FK	189	
5	GK	189	
5	HK	189	
5	IK	189	
5	JK	189	
5	KK	189	
5	LK	189	
5	MK	189	
6	N	249	
6	O	249	
6	P	249	
6	Q	249	
6	R	249	
6	S	249	
6	T	249	
6	U	249	
6	V	249	
6	W	249	
6	X	249	
6	Y	249	
6	Z	249	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 124910 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 Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AV	144	Total	C	N	O	0	0
			720	432	144	144		
1	AW	32	Total	C	N	O	0	0
			160	96	32	32		
1	BV	144	Total	C	N	O	0	0
			720	432	144	144		
1	BW	32	Total	C	N	O	0	0
			160	96	32	32		
1	CV	144	Total	C	N	O	0	0
			720	432	144	144		
1	CW	32	Total	C	N	O	0	0
			160	96	32	32		
1	DV	144	Total	C	N	O	0	0
			720	432	144	144		
1	DW	32	Total	C	N	O	0	0
			160	96	32	32		
1	EV	144	Total	C	N	O	0	0
			720	432	144	144		
1	EW	32	Total	C	N	O	0	0
			160	96	32	32		
1	FV	144	Total	C	N	O	0	0
			720	432	144	144		
1	FW	32	Total	C	N	O	0	0
			160	96	32	32		
1	GV	144	Total	C	N	O	0	0
			720	432	144	144		
1	GW	32	Total	C	N	O	0	0
			160	96	32	32		
1	HV	144	Total	C	N	O	0	0
			720	432	144	144		
1	HW	32	Total	C	N	O	0	0
			160	96	32	32		
1	IV	144	Total	C	N	O	0	0
			720	432	144	144		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	IW	32	Total	C	N	O	0	0
			160	96	32	32		
1	JV	144	Total	C	N	O	0	0
			720	432	144	144		
1	JW	32	Total	C	N	O	0	0
			160	96	32	32		
1	KV	144	Total	C	N	O	0	0
			720	432	144	144		
1	KW	32	Total	C	N	O	0	0
			160	96	32	32		
1	LV	144	Total	C	N	O	0	0
			720	432	144	144		
1	LW	32	Total	C	N	O	0	0
			160	96	32	32		
1	MV	144	Total	C	N	O	0	0
			720	432	144	144		
1	MW	32	Total	C	N	O	0	0
			160	96	32	32		
1	NV	144	Total	C	N	O	0	0
			720	432	144	144		
1	NW	32	Total	C	N	O	0	0
			160	96	32	32		
1	OV	144	Total	C	N	O	0	0
			720	432	144	144		
1	OW	32	Total	C	N	O	0	0
			160	96	32	32		
1	PV	144	Total	C	N	O	0	0
			720	432	144	144		
1	PW	32	Total	C	N	O	0	0
			160	96	32	32		
1	QV	144	Total	C	N	O	0	0
			720	432	144	144		
1	QW	32	Total	C	N	O	0	0
			160	96	32	32		
1	RV	144	Total	C	N	O	0	0
			720	432	144	144		
1	RW	32	Total	C	N	O	0	0
			160	96	32	32		
1	AX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	AY	52	Total	C	N	O	0	0
			260	156	52	52		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	AZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	BX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	BY	52	Total	C	N	O	0	0
			260	156	52	52		
1	BZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	CX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	CY	52	Total	C	N	O	0	0
			260	156	52	52		
1	CZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	DX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	DY	52	Total	C	N	O	0	0
			260	156	52	52		
1	DZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	EX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	EY	52	Total	C	N	O	0	0
			260	156	52	52		
1	EZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	FX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	FY	52	Total	C	N	O	0	0
			260	156	52	52		
1	FZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	GX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	GY	52	Total	C	N	O	0	0
			260	156	52	52		
1	GZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	HX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	HY	52	Total	C	N	O	0	0
			260	156	52	52		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	HZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	IX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	IY	52	Total	C	N	O	0	0
			260	156	52	52		
1	IZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	JX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	JY	52	Total	C	N	O	0	0
			260	156	52	52		
1	JZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	KX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	KY	52	Total	C	N	O	0	0
			260	156	52	52		
1	KZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	LX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	LY	52	Total	C	N	O	0	0
			260	156	52	52		
1	LZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	MX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	MY	52	Total	C	N	O	0	0
			260	156	52	52		
1	MZ	70	Total	C	N	O	0	0
			350	210	70	70		

- Molecule 2 is a protein called DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	BC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	CC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	EC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	FC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	GC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	HC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	IC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	JC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	KC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	LC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	MC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		

- Molecule 3 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Ad	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	BD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Bd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	CD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Cd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	DD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Dd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	ED	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ed	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	FD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Fd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	GD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Gd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	HD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Hd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	ID	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Id	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	JD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Jd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	KD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Kd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	LD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Ld	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	MD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Md	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		

- Molecule 4 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	BH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	CH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	DH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	EH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	FH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	GH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	HH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	IH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	JH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	KH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	LH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	MH	89	Total 678	C 432	N 119	O 123	S 4	0	0

- Molecule 5 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	BK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	CK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	DK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	EK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	FK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	GK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	HK	148	Total 1152	C 731	N 205	O 212	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	IK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	JK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	KK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	LK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	MK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

- Molecule 6 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	O	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	P	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	Q	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	R	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	S	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	T	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	U	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	V	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	W	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	X	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	Y	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	Z	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		

3 Residue-property plots [i](#)

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

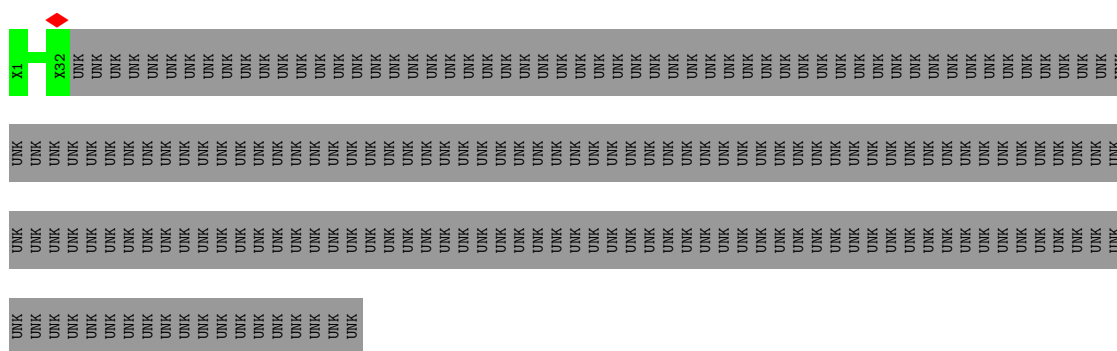
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AV: 



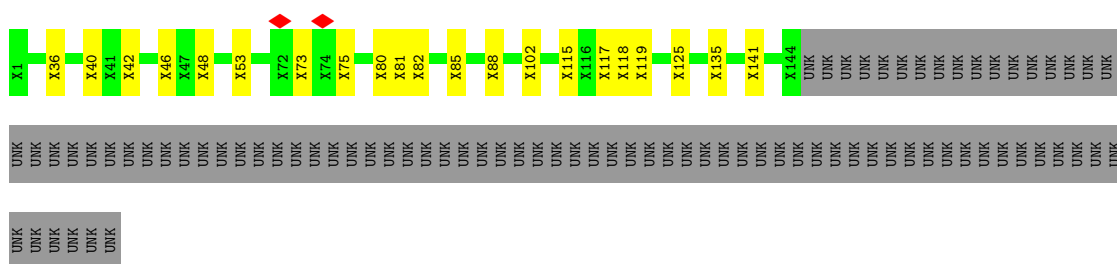
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AW: 



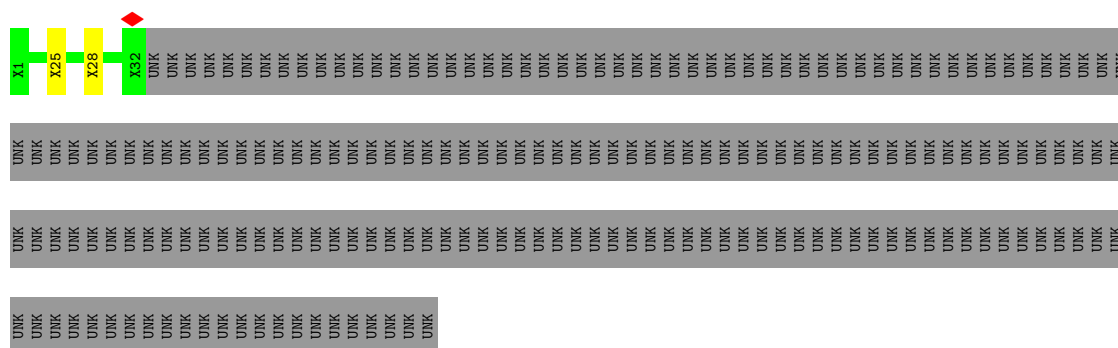
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BV: 



- Molecule 1: Type IV secretion system unknown protein fragment

Chain BW:  13% 86%



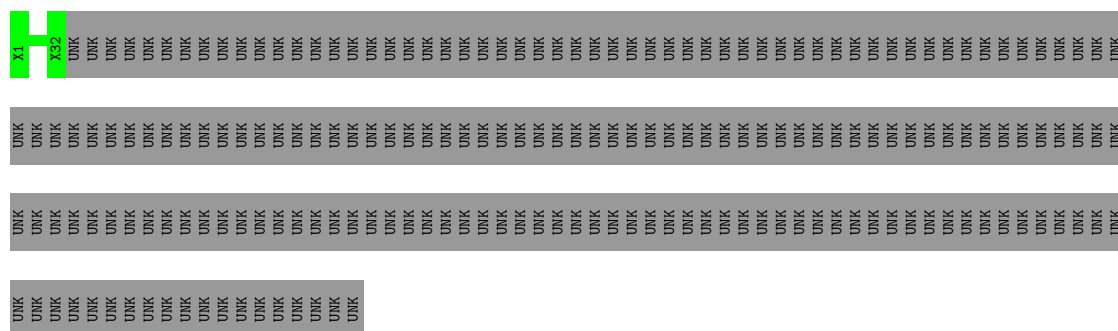
- Molecule 1: Type IV secretion system unknown protein fragment

Chain CV:  59% 37%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain CW:  14% 86%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain DV:  61% 37%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain DW: 14% 86%



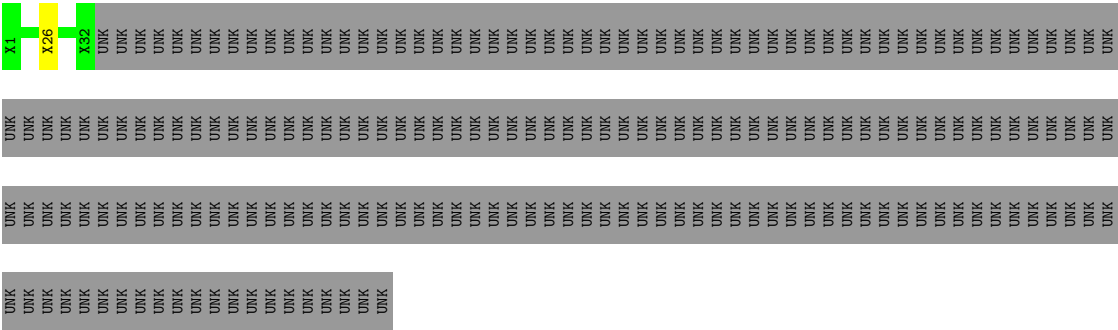
• Molecule 1: Type IV secretion system unknown protein fragment

Chain EV: 60% 37%



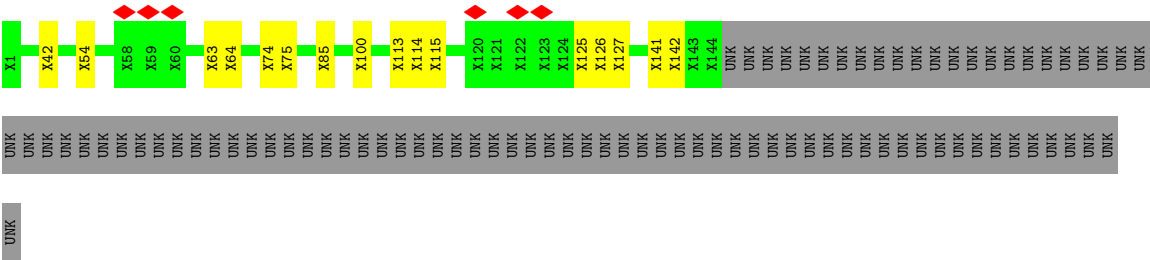
• Molecule 1: Type IV secretion system unknown protein fragment

Chain EW: 14% 86%

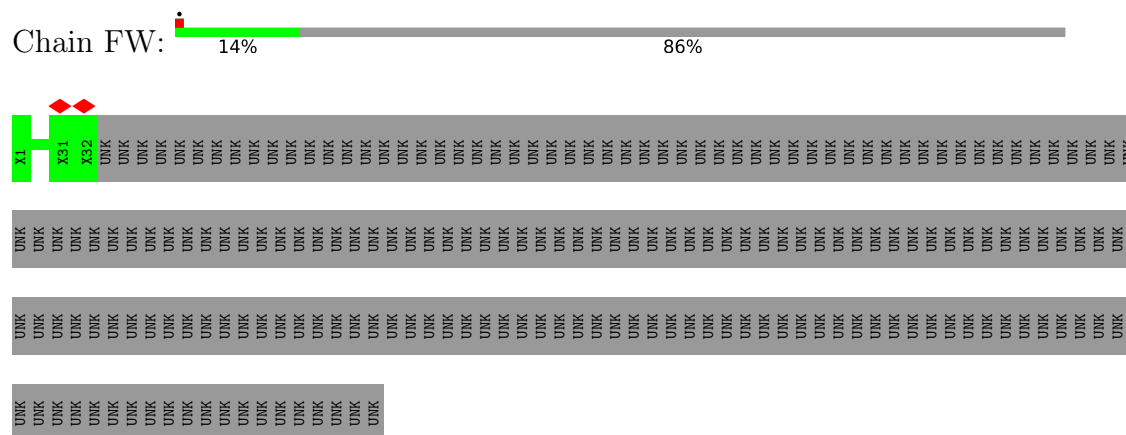


• Molecule 1: Type IV secretion system unknown protein fragment

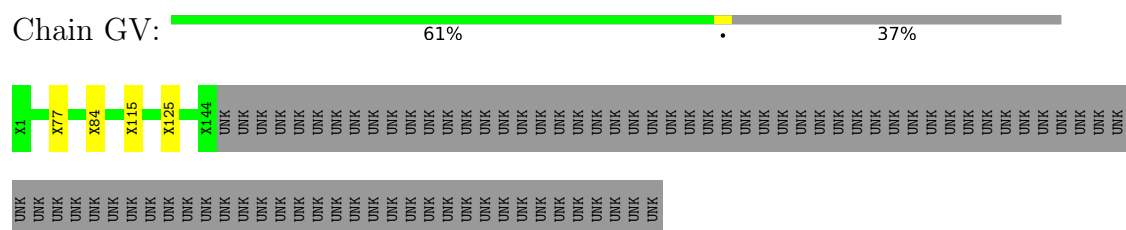
Chain FV: 56% 7% 37%



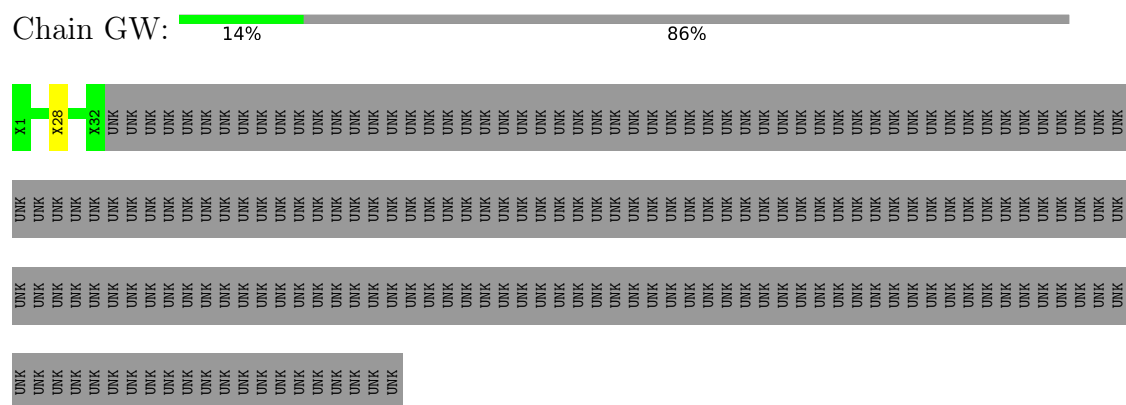
• Molecule 1: Type IV secretion system unknown protein fragment



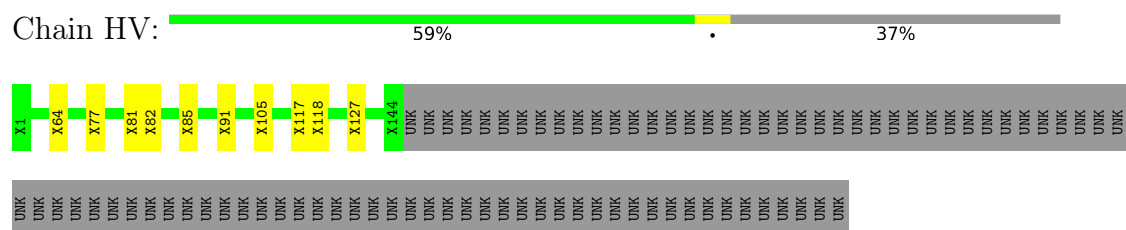
- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

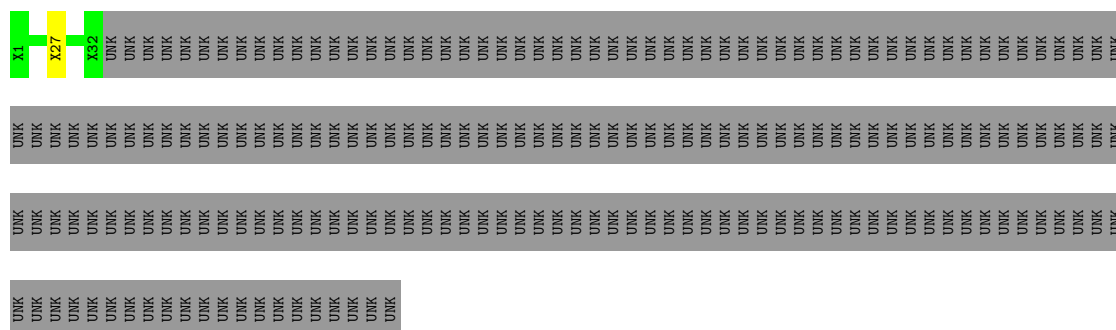


- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

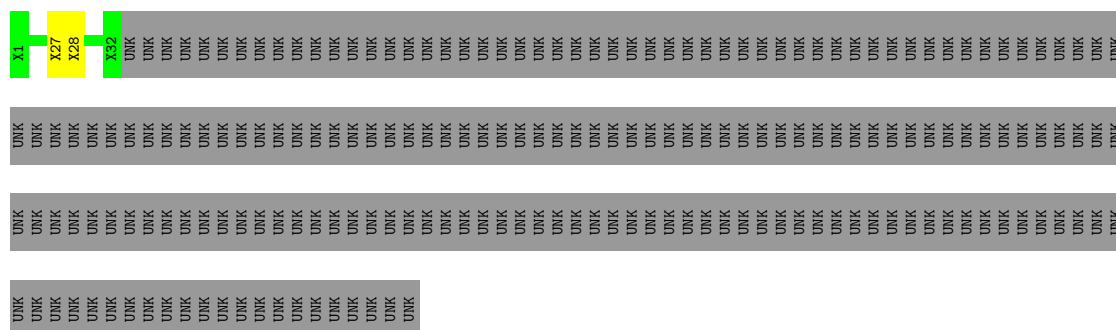




- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

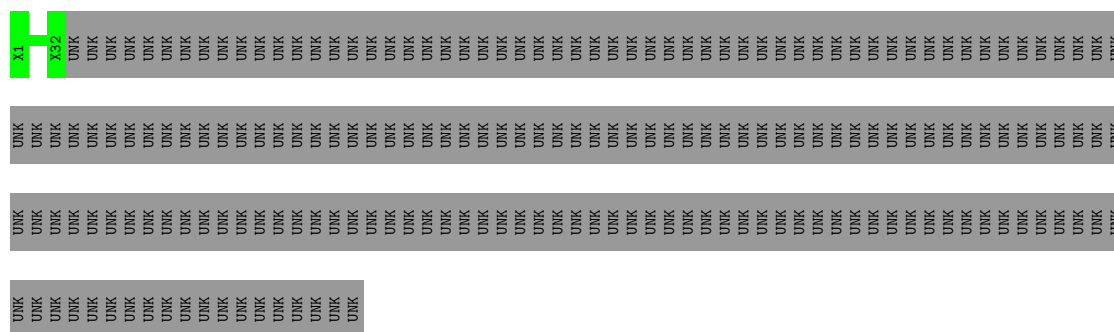


- Molecule 1: Type IV secretion system unknown protein fragment

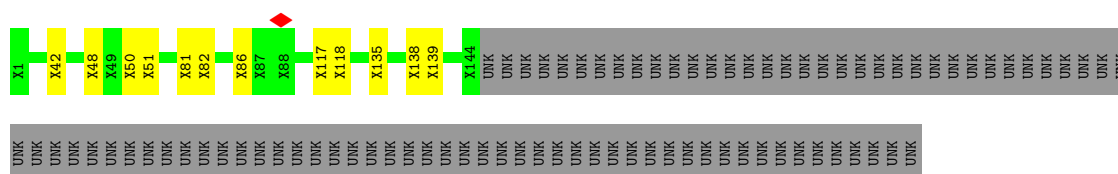


- Molecule 1: Type IV secretion system unknown protein fragment

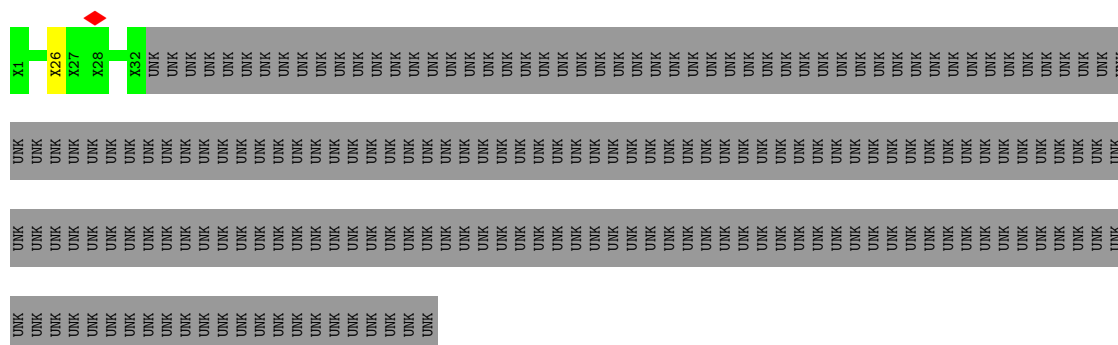




- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

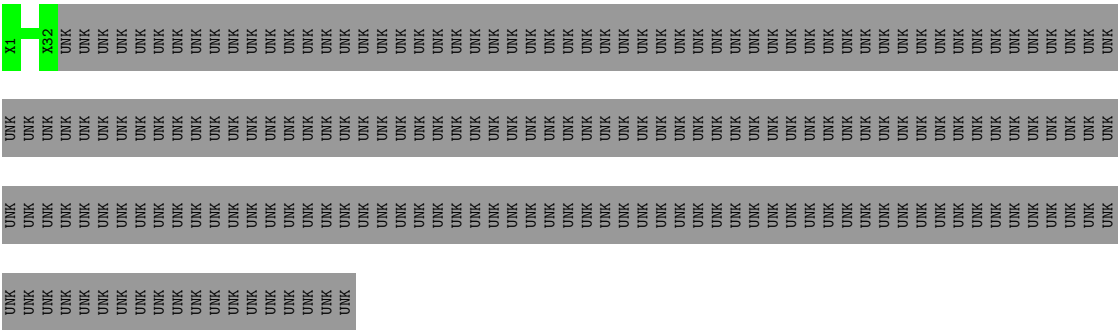


- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment





● Molecule 1: Type IV secretion system unknown protein fragment



● Molecule 1: Type IV secretion system unknown protein fragment



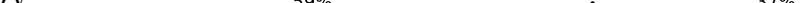
● Molecule 1: Type IV secretion system unknown protein fragment



● Molecule 1: Type IV secretion system unknown protein fragment



UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Chain OV: 

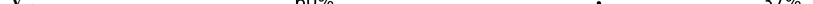
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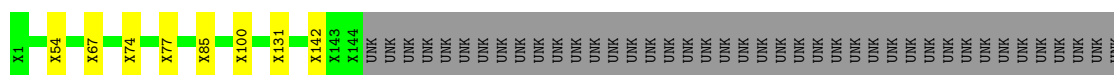
- Chain OW: 14% 86%

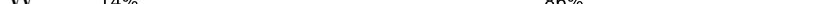


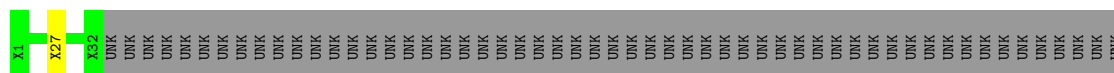
UNK

[illegible][illegible]

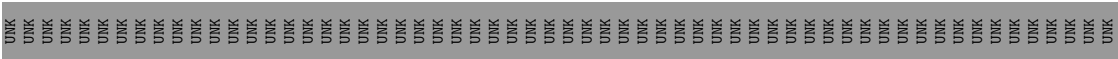
- Chain PV: 

[illegible]

- Chain PW:  14% 86%



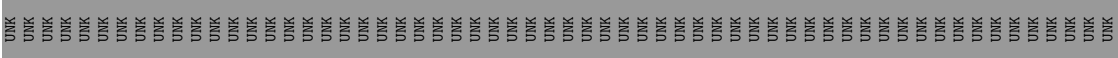
UNK



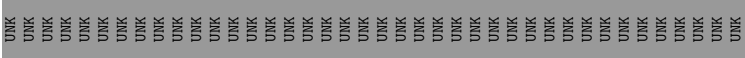
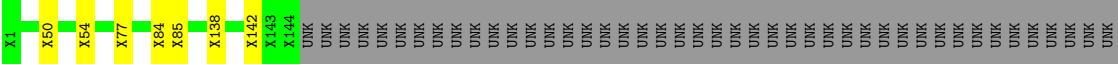
● Molecule 1: Type IV secretion system unknown protein fragment



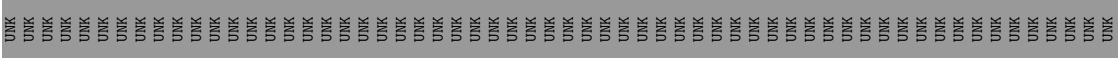
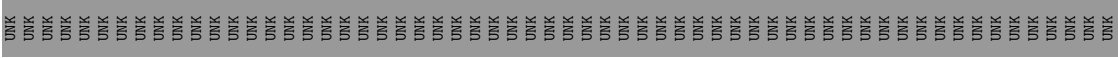
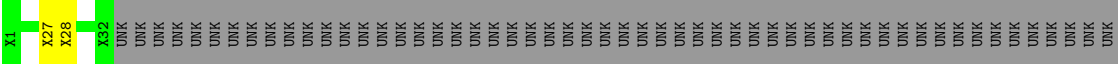
● Molecule 1: Type IV secretion system unknown protein fragment

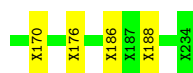


● Molecule 1: Type IV secretion system unknown protein fragment

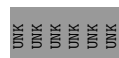


● Molecule 1: Type IV secretion system unknown protein fragment

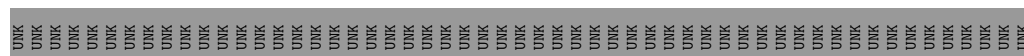




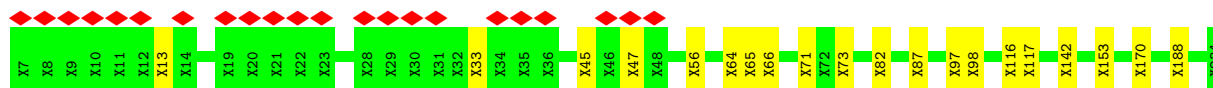
- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment



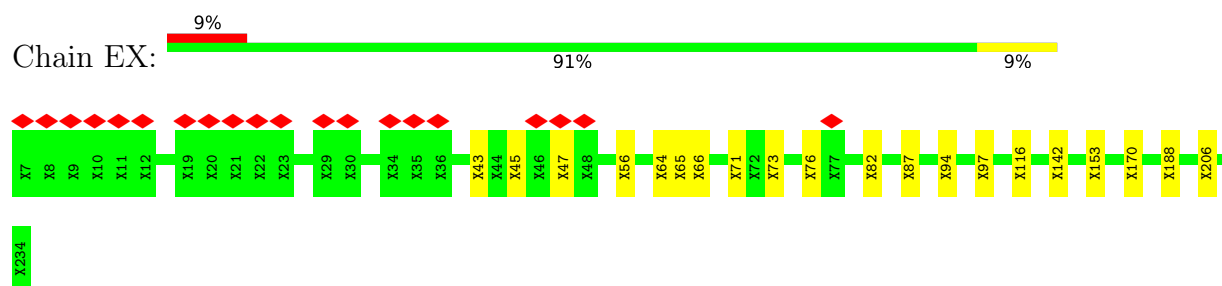
- Molecule 1: Type IV secretion system unknown protein fragment



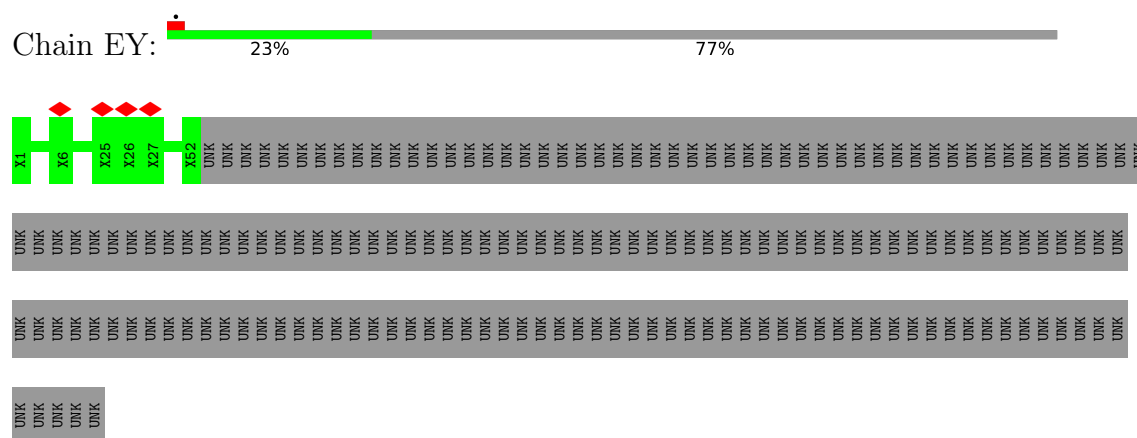
- Molecule 1: Type IV secretion system unknown protein fragment



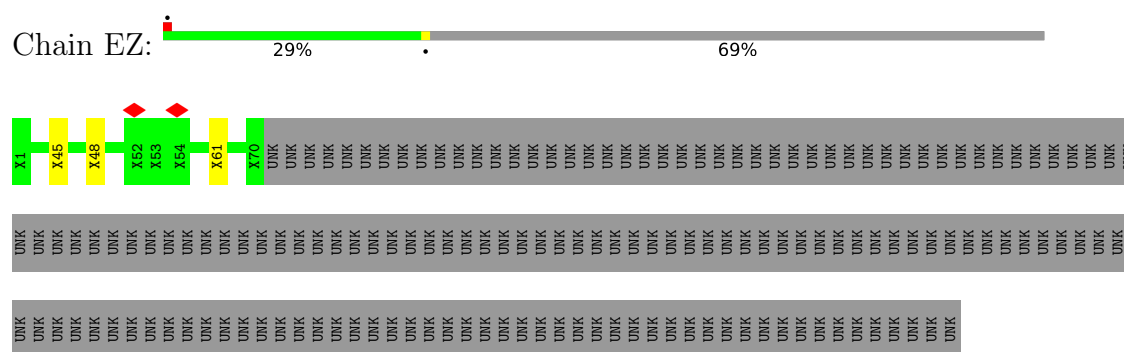
- Molecule 1: Type IV secretion system unknown protein fragment



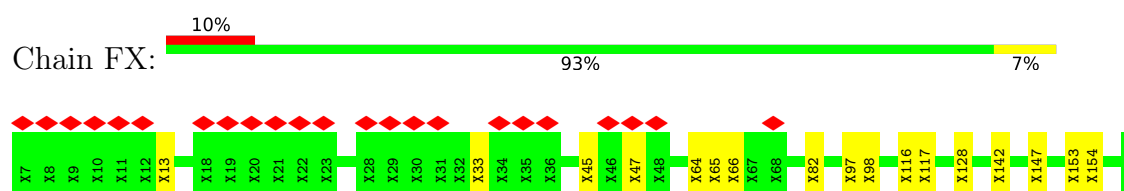
- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

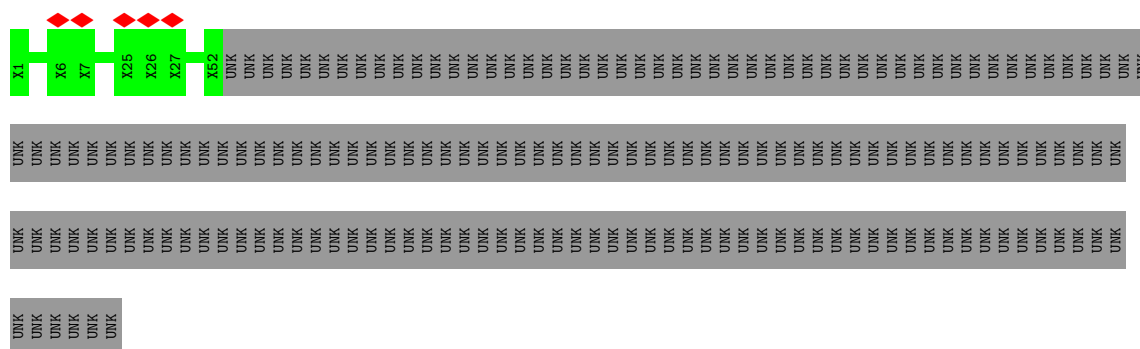


- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

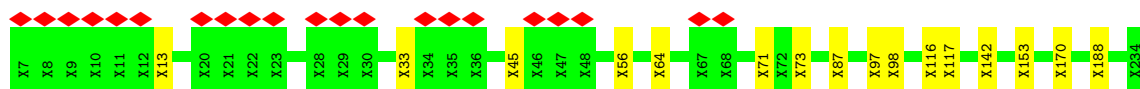




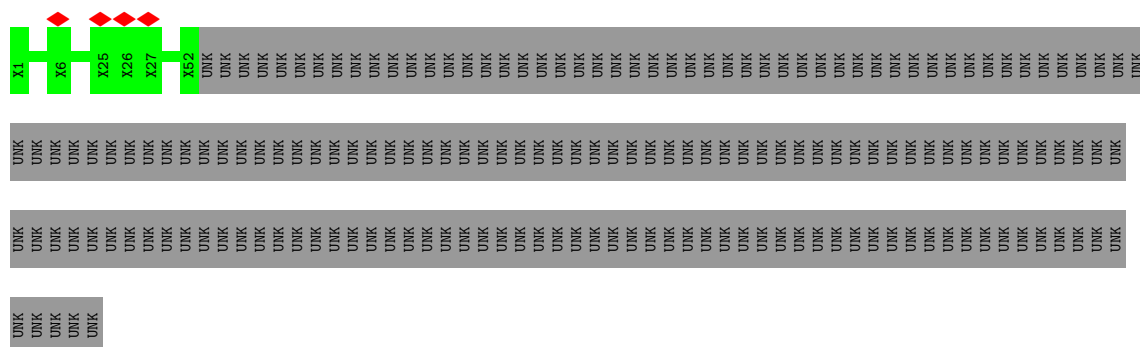
- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

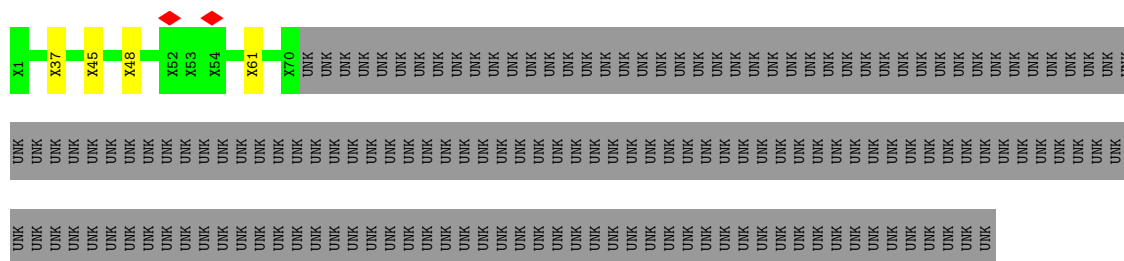


- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

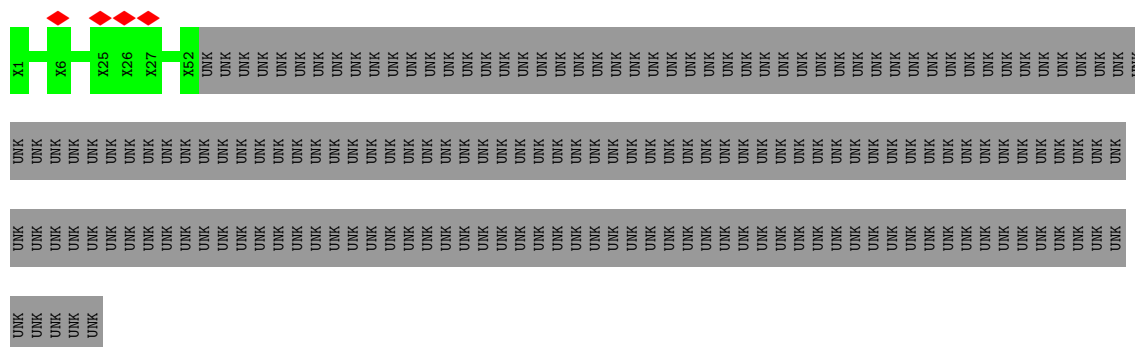




- Molecule 1: Type IV secretion system unknown protein fragment



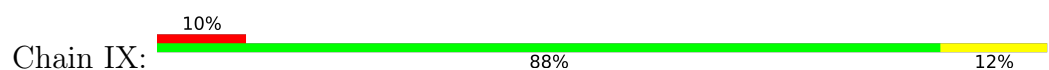
- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment





- Molecule 1: Type IV secretion system unknown protein fragment

Chain IY: 23% 77%



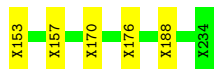
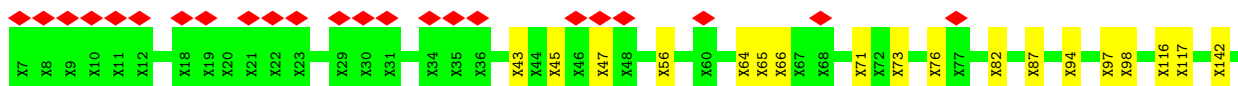
- Molecule 1: Type IV secretion system unknown protein fragment

Chain IZ: 29% 69%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain JX: 10% 90% 10%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain JY: 23% 77%



UNK

-
- | Category | Count |
|----------|-------|
| X7 | 100 |
| X8 | 100 |
| X9 | 100 |
| X10 | 100 |
| X11 | 100 |
| X12 | 100 |
| X18 | 100 |
| X19 | 100 |
| X20 | 100 |
| X21 | 100 |
| X22 | 100 |
| X23 | 100 |
| X28 | 100 |
| X29 | 100 |
| X30 | 100 |
| X34 | 100 |
| X35 | 100 |
| X45 | 100 |
| X46 | 100 |
| X47 | 100 |
| X48 | 100 |
| X64 | 100 |
| X65 | 100 |
| X66 | 100 |
| X67 | 100 |
| X68 | 100 |
| X71 | 100 |
| X76 | 100 |
| X82 | 100 |
| X87 | 100 |
| X94 | 100 |
| X97 | 100 |
| X116 | 100 |
| X142 | 100 |
| X153 | 100 |
| X154 | 100 |
| X170 | 100 |
| X198 | 100 |
| X204 | 100 |

- [illegible]

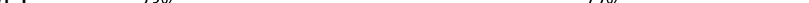
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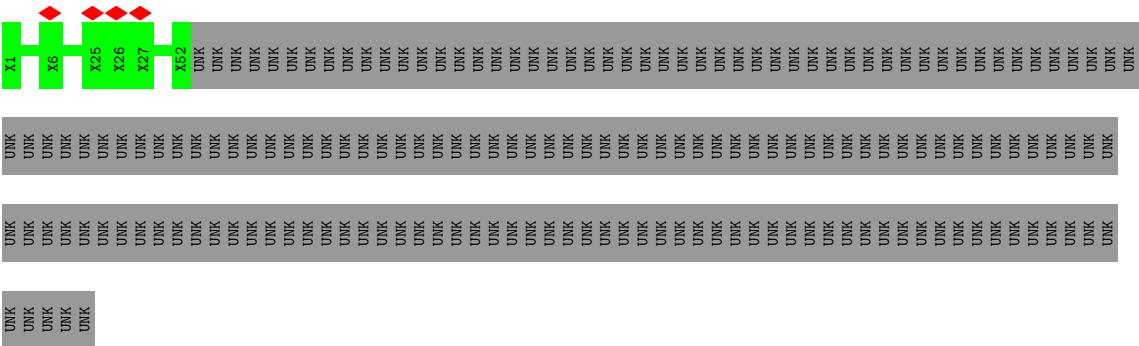
UNK UNK UNK UNK UNK

-
- | Item | Category | Value (approx.) |
|------|----------|-----------------|
| X1 | Yellow | 1.5 |
| X2 | Yellow | 1.5 |
| X3 | Yellow | 1.5 |
| X4 | Yellow | 1.5 |
| X5 | Yellow | 1.5 |
| X6 | Yellow | 1.5 |
| X7 | Yellow | 1.5 |
| X8 | Yellow | 1.5 |
| X9 | Yellow | 1.5 |
| X10 | Yellow | 1.5 |
| X11 | Yellow | 1.5 |
| X12 | Yellow | 1.5 |
| X13 | Yellow | 1.5 |
| X14 | Yellow | 1.5 |
| X15 | Yellow | 1.5 |
| X16 | Yellow | 1.5 |
| X17 | Grey | 0.5 |
| X18 | Grey | 0.5 |
| X19 | Grey | 0.5 |
| X20 | Grey | 0.5 |
| X21 | Grey | 0.5 |
| X22 | Grey | 0.5 |
| X23 | Grey | 0.5 |
| X24 | Grey | 0.5 |
| X25 | Grey | 0.5 |
| X26 | Grey | 0.5 |
| X27 | Grey | 0.5 |
| X28 | Grey | 0.5 |
| X29 | Grey | 0.5 |
| X30 | Grey | 0.5 |
| X31 | Grey | 0.5 |
| X32 | Grey | 0.5 |

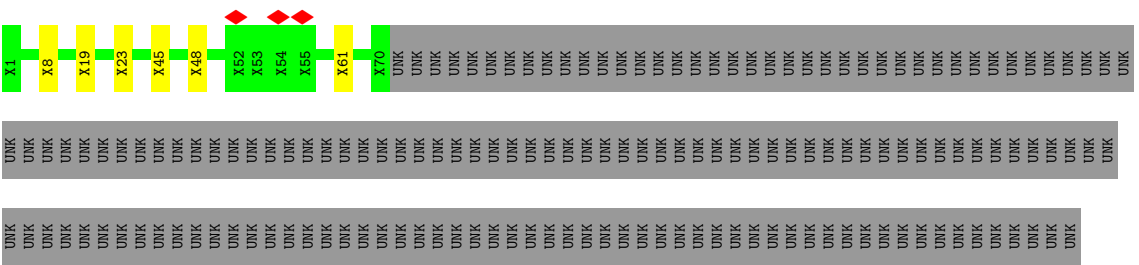
[illegible][illegible]

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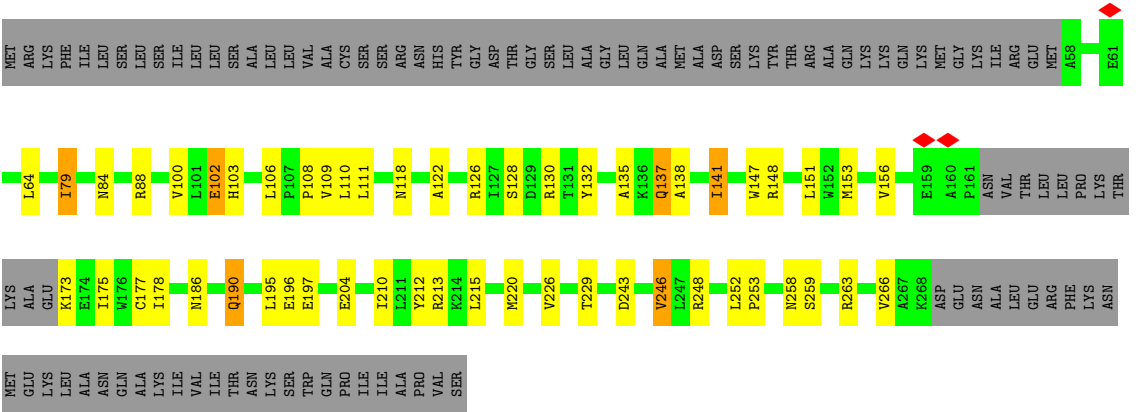
- Chain MY:  23% 77%



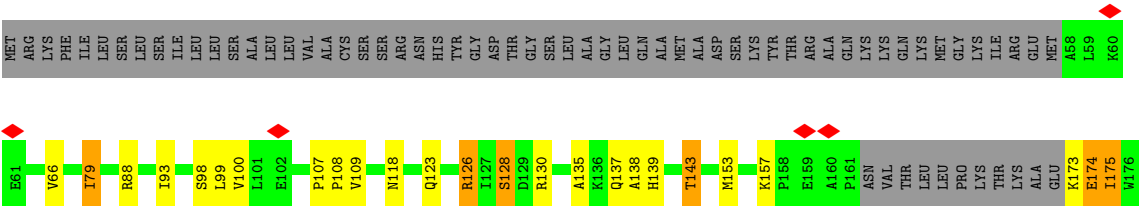
• Molecule 1: Type IV secretion system unknown protein fragment

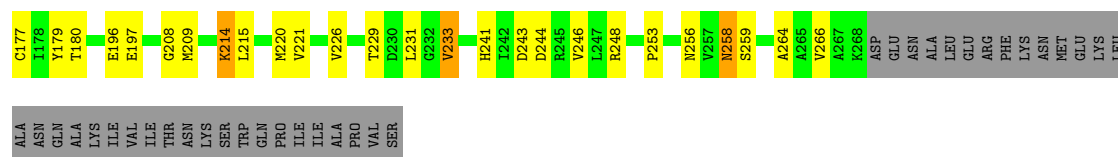


• Molecule 2: DotC

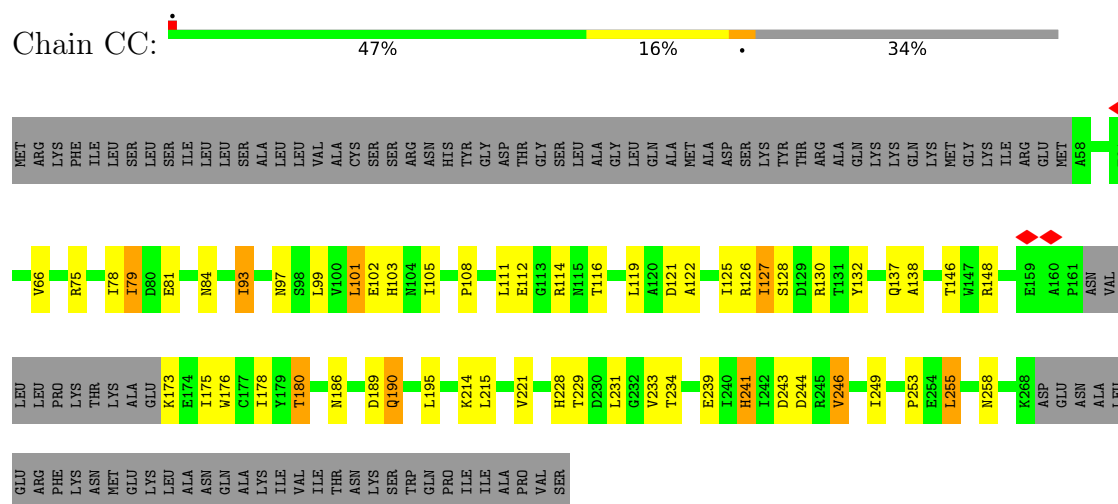


• Molecule 2: DotC

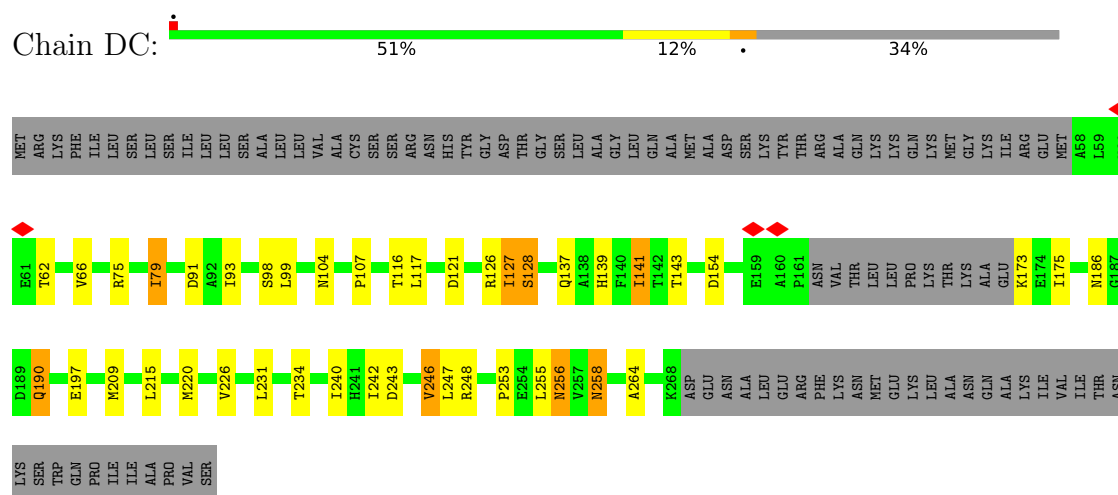




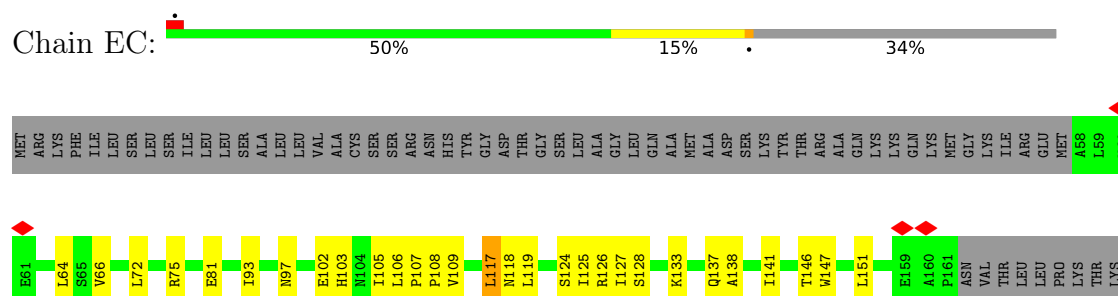
• Molecule 2: DotC

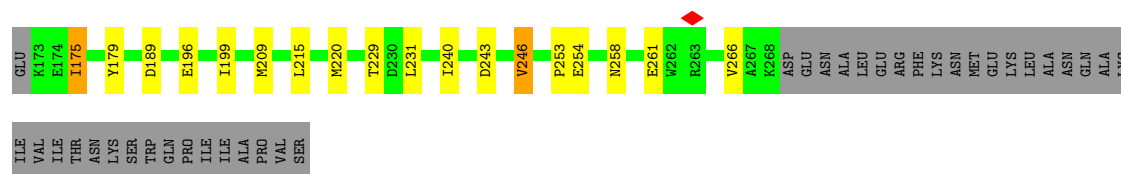


• Molecule 2: DotC

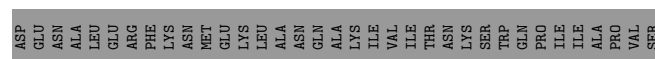
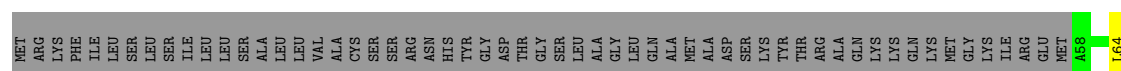


• Molecule 2: DotC

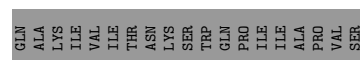
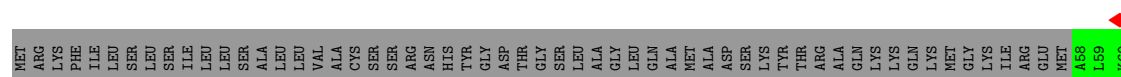




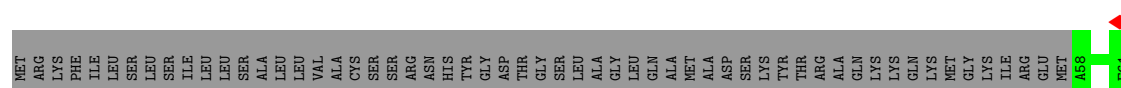
• Molecule 2: DotC

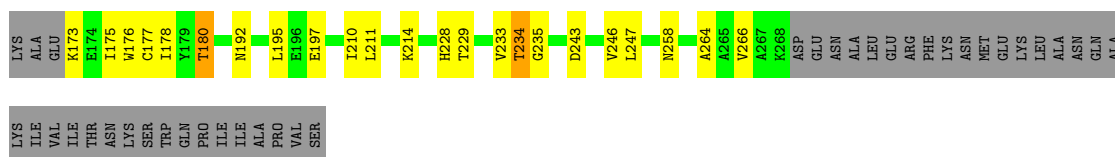


• Molecule 2: DotC

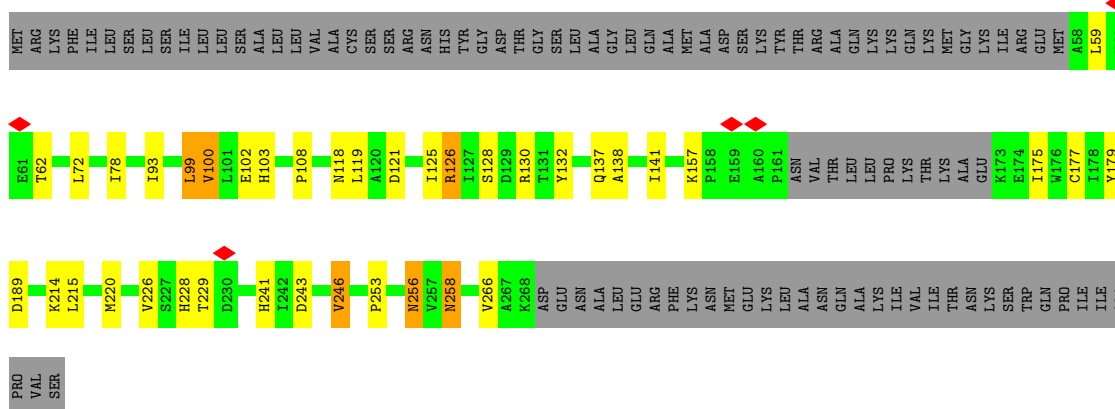


• Molecule 2: DotC

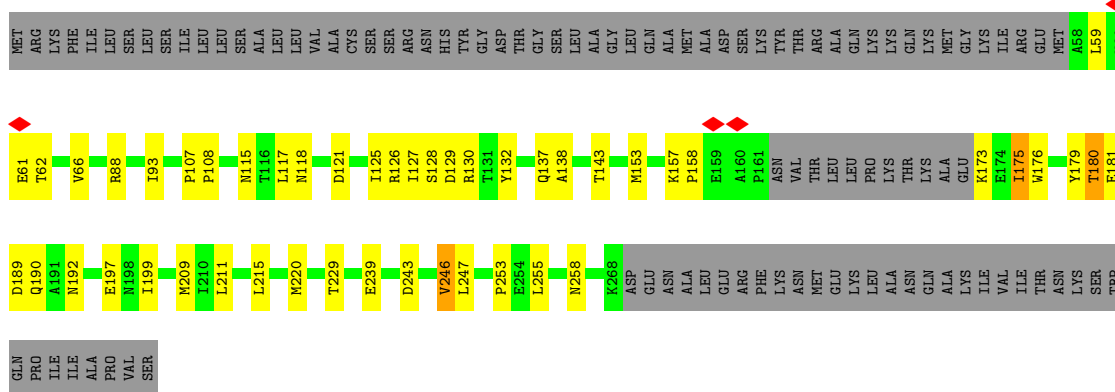




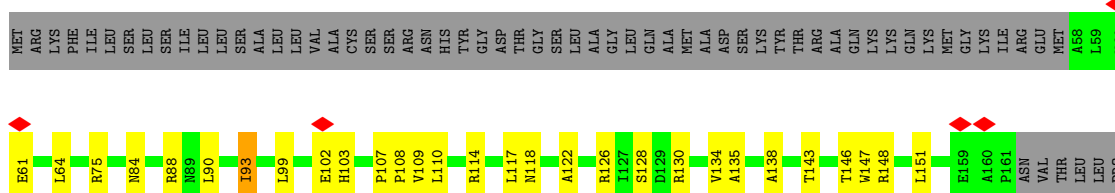
● Molecule 2: DotC

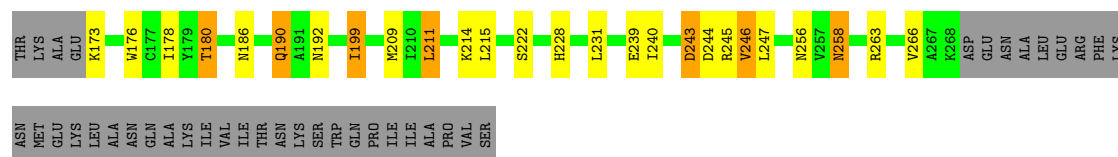


● Molecule 2: DotC

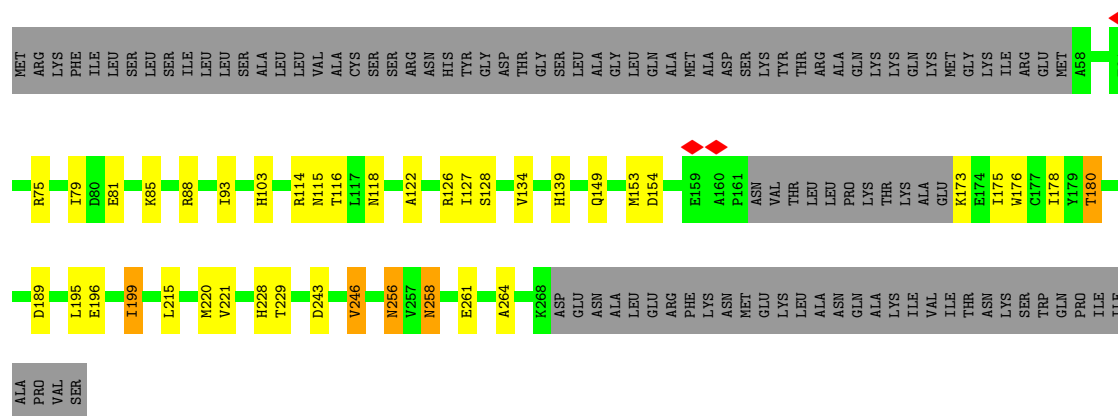


● Molecule 2: DotC

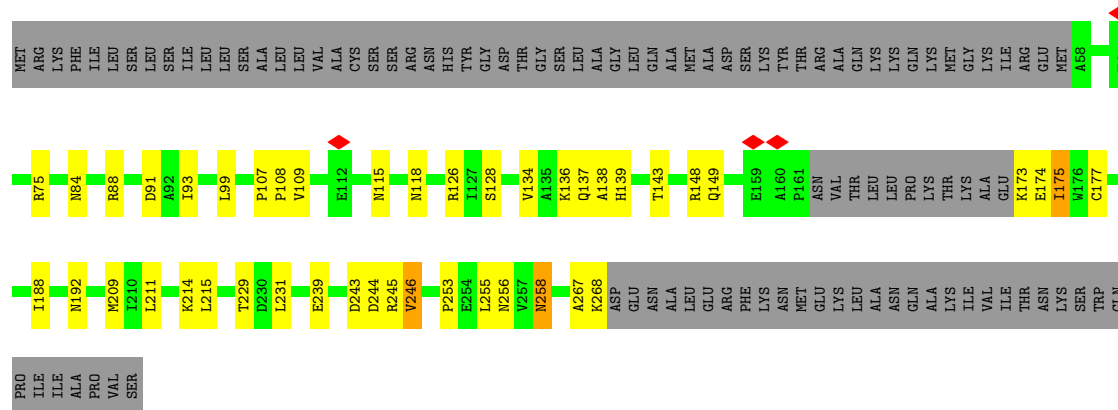




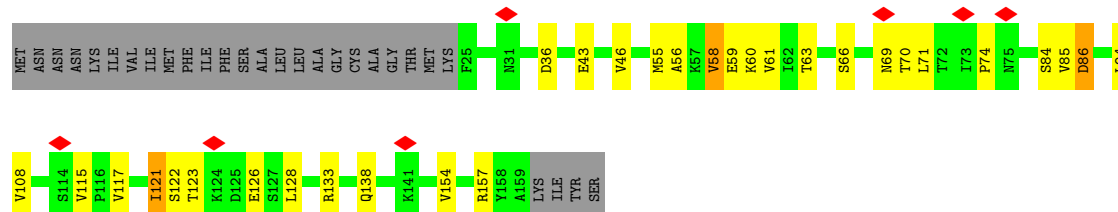
• Molecule 2: DotC



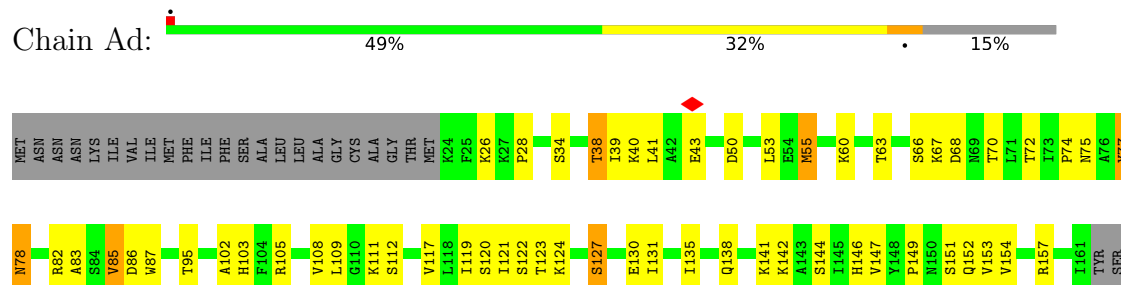
• Molecule 2: DotC



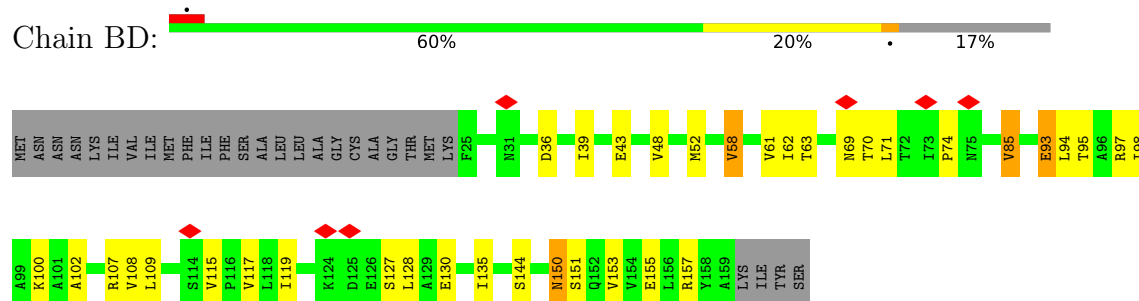
• Molecule 3: DotD



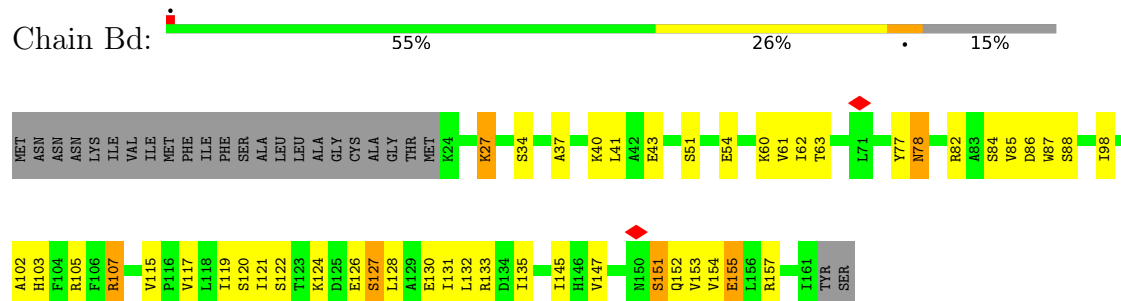
- Molecule 3: DotD



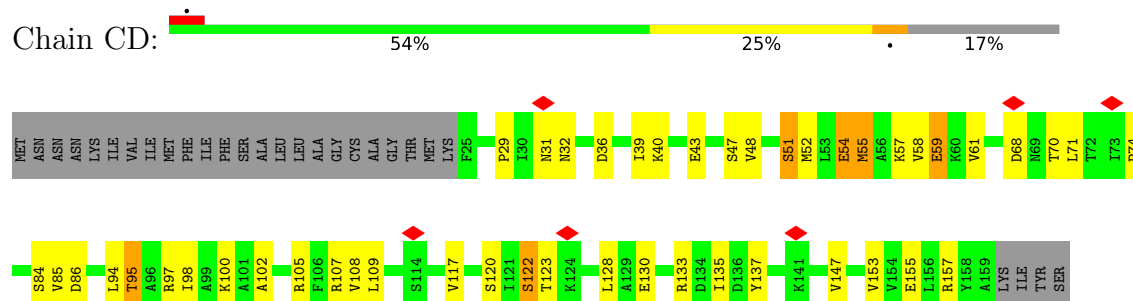
- Molecule 3: DotD



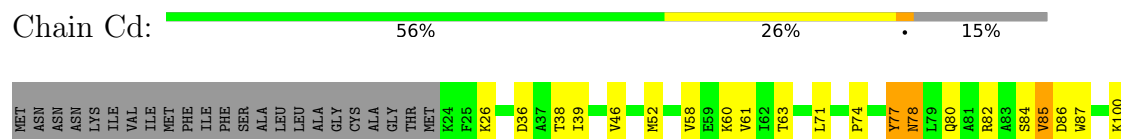
- Molecule 3: DotD



- Molecule 3: DotD



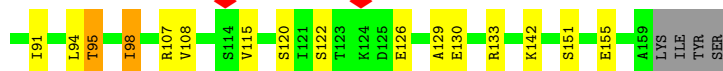
- Molecule 3: DotD





• Molecule 3: DotD

Chain DD: 62% 19% 17%



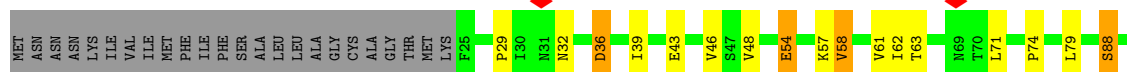
• Molecule 3: DotD

Chain Dd: 54% 29% 15%



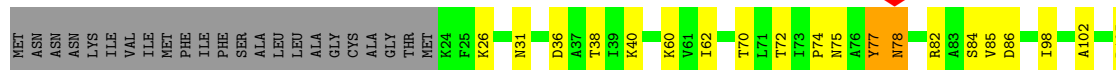
• Molecule 3: DotD

Chain ED: 60% 18% 17%



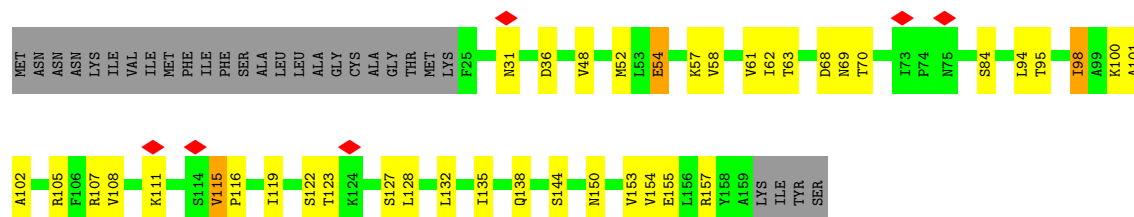
• Molecule 3: DotD

Chain Ed: 63% 20% 15%

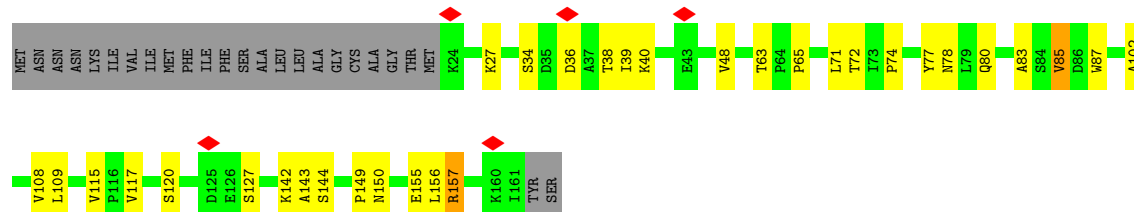


• Molecule 3: DotD

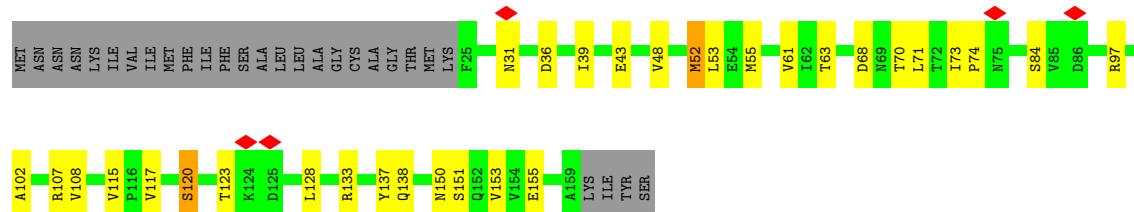
Chain FD: 58% 23% 17%



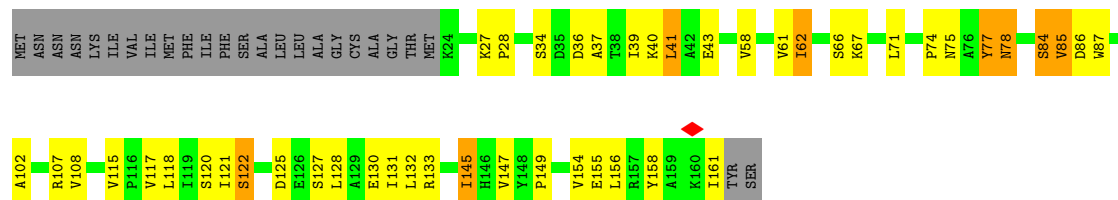
• Molecule 3: DotD



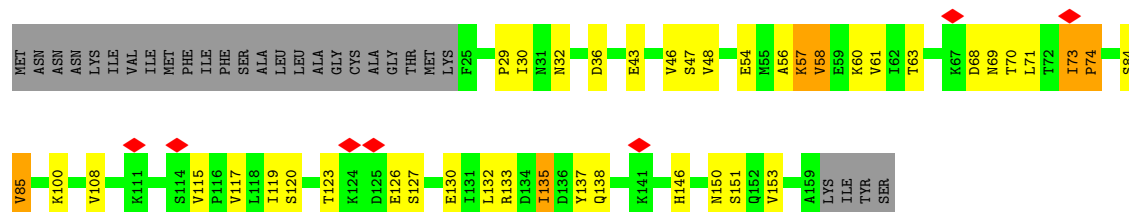
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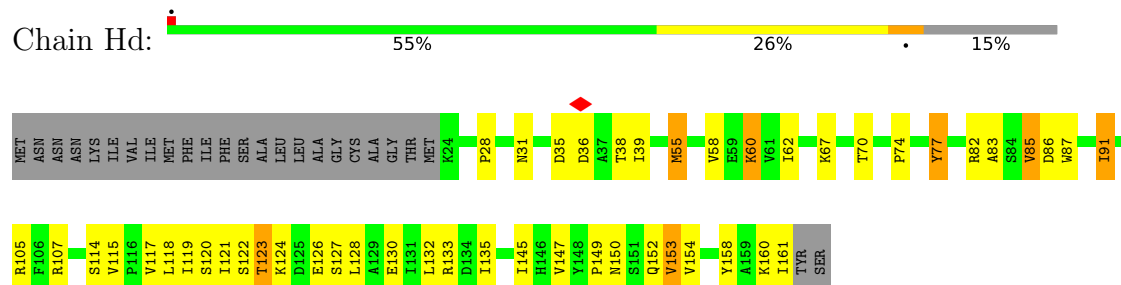
• Molecule 3: DotD



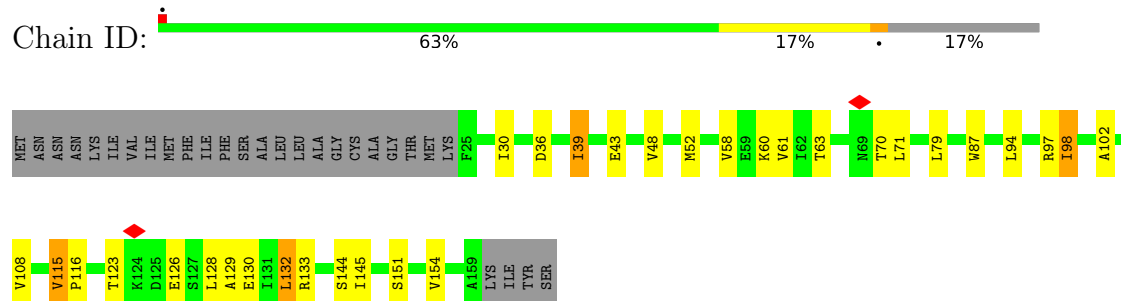
• Molecule 3: DotD



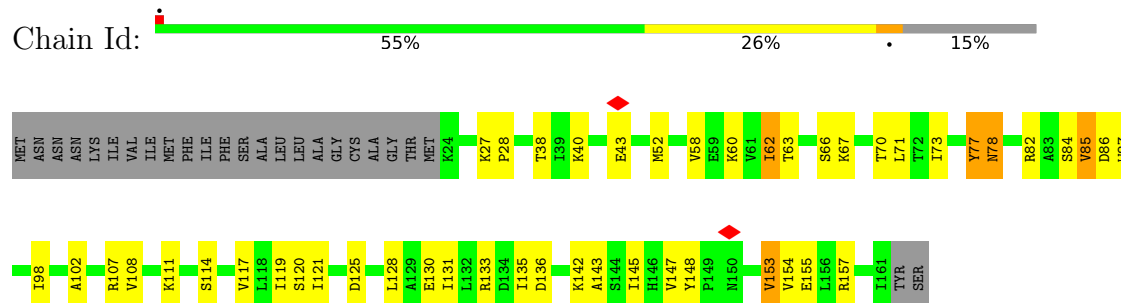
- Molecule 3: DotD



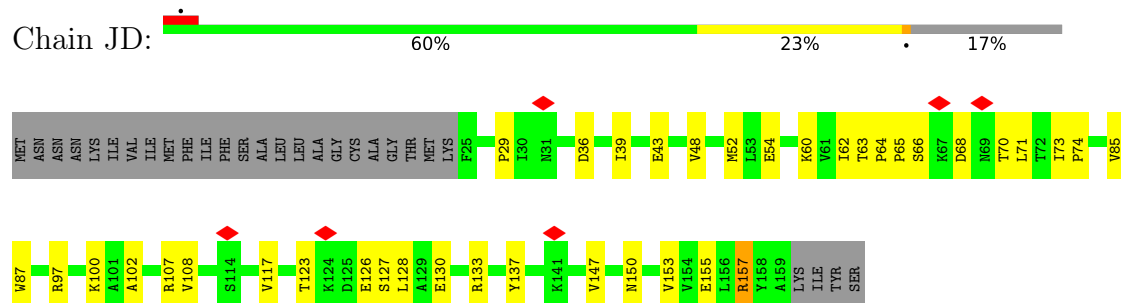
- Molecule 3: DotD



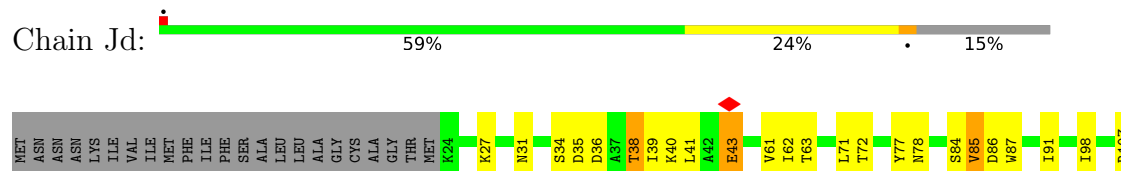
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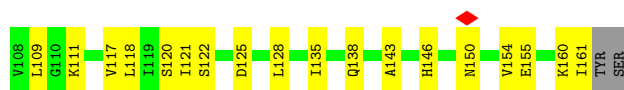


- Molecule 3: DotD

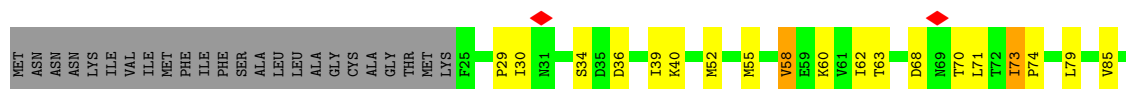


- Molecule 3: DotD





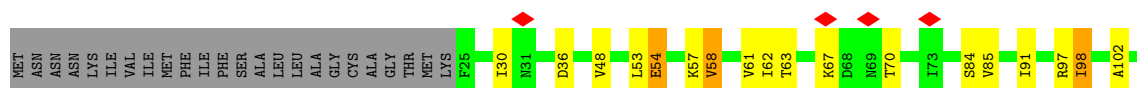
• Molecule 3: DotD



• Molecule 3: DotD



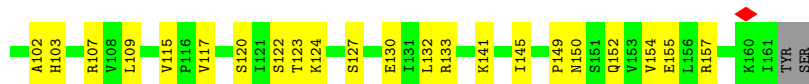
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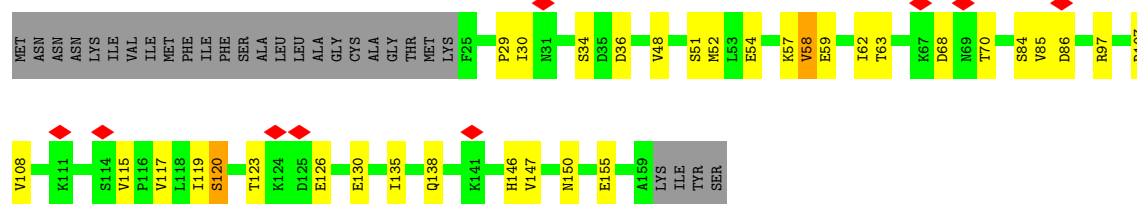


• Molecule 3: DotD

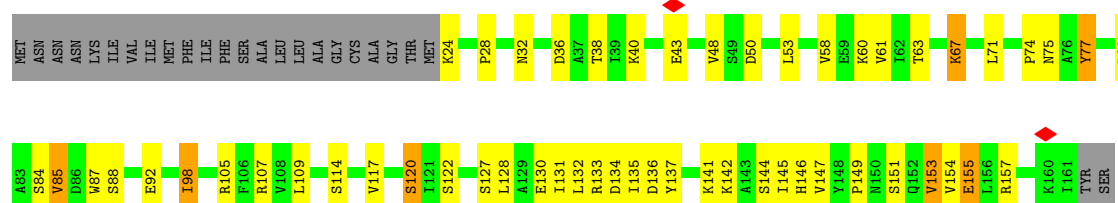


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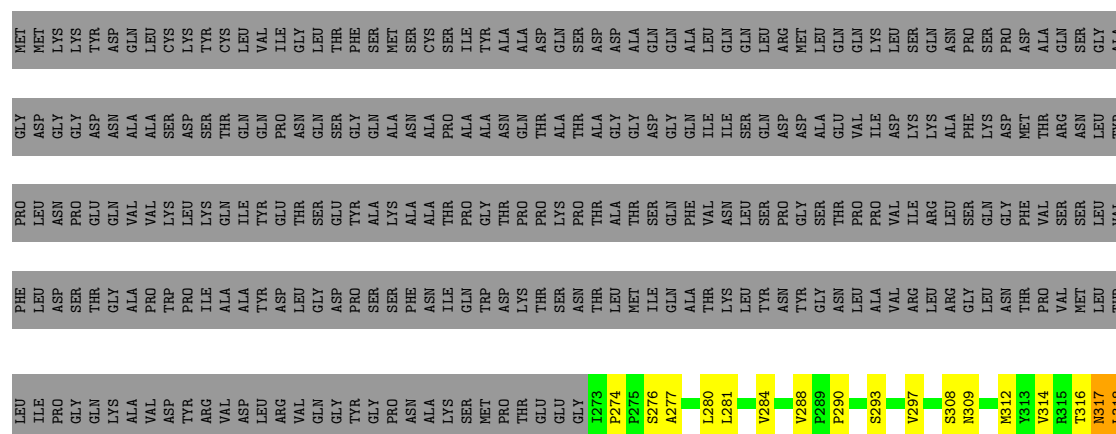




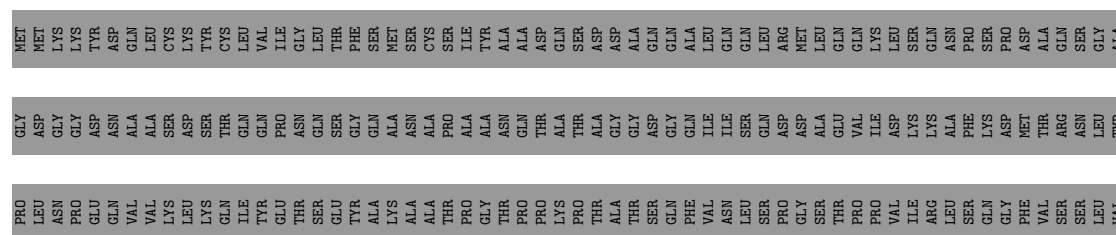
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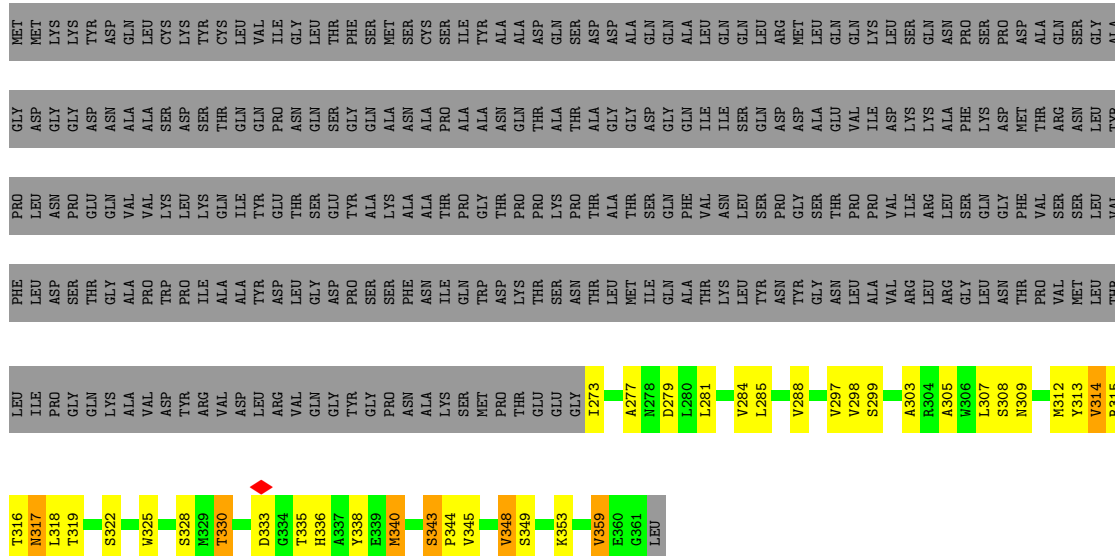


• Molecule 4: Type IV secretion protein IcmK

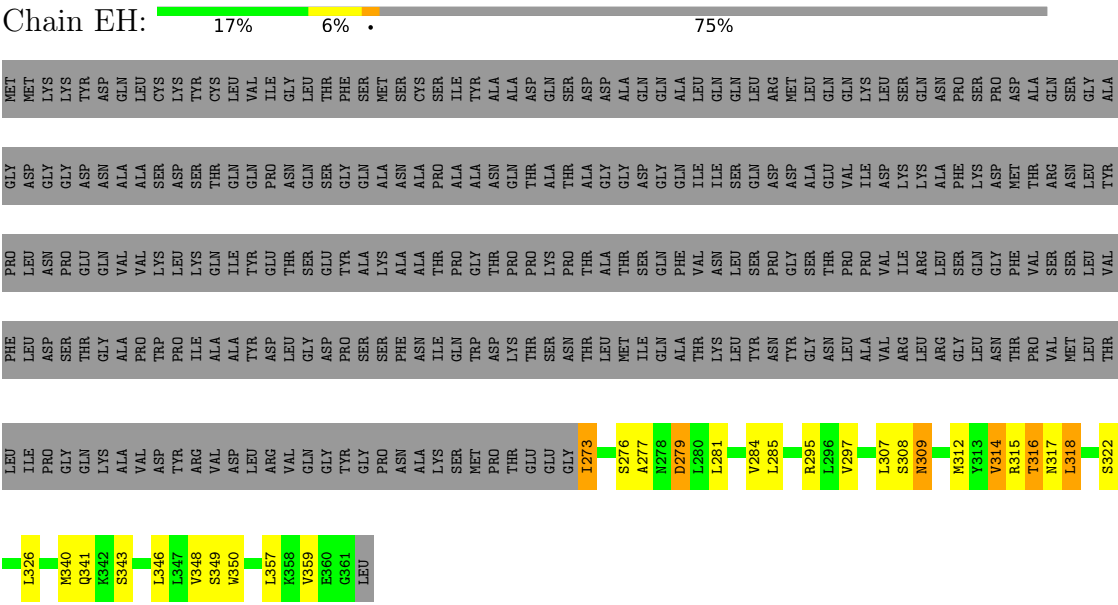


• Molecule 4: Type IV secretion protein IcmK

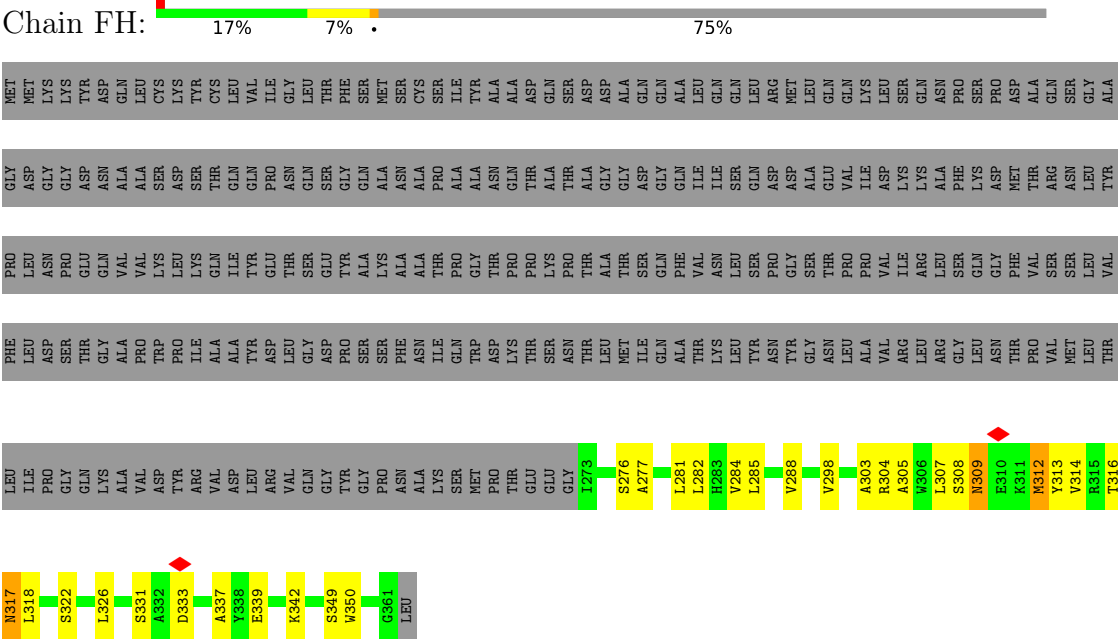




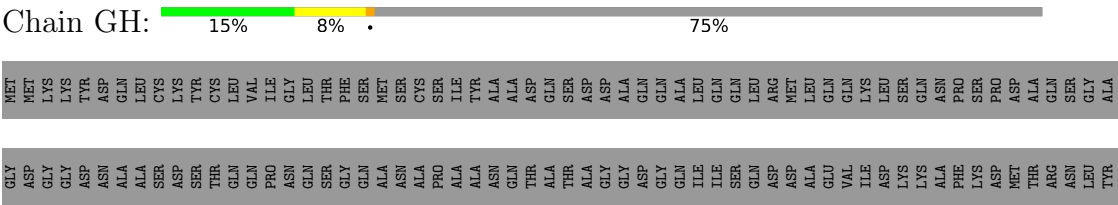
• Molecule 4: Type IV secretion protein IcmK

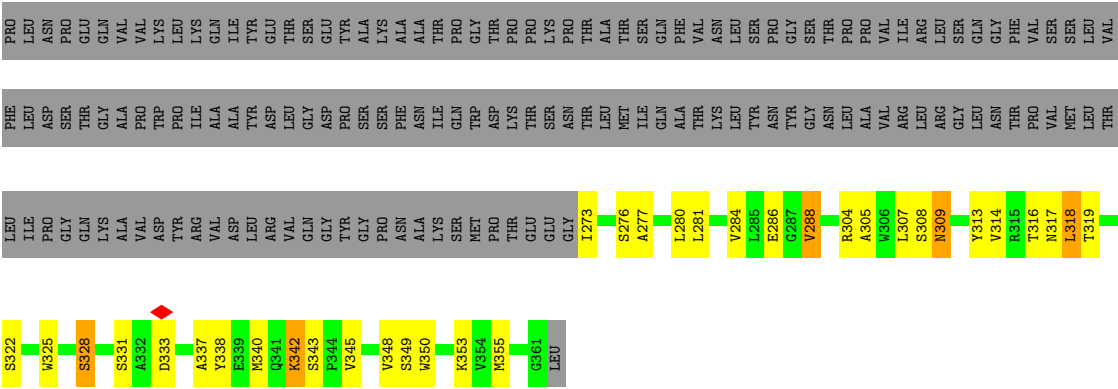


• Molecule 4: Type IV secretion protein IcmK

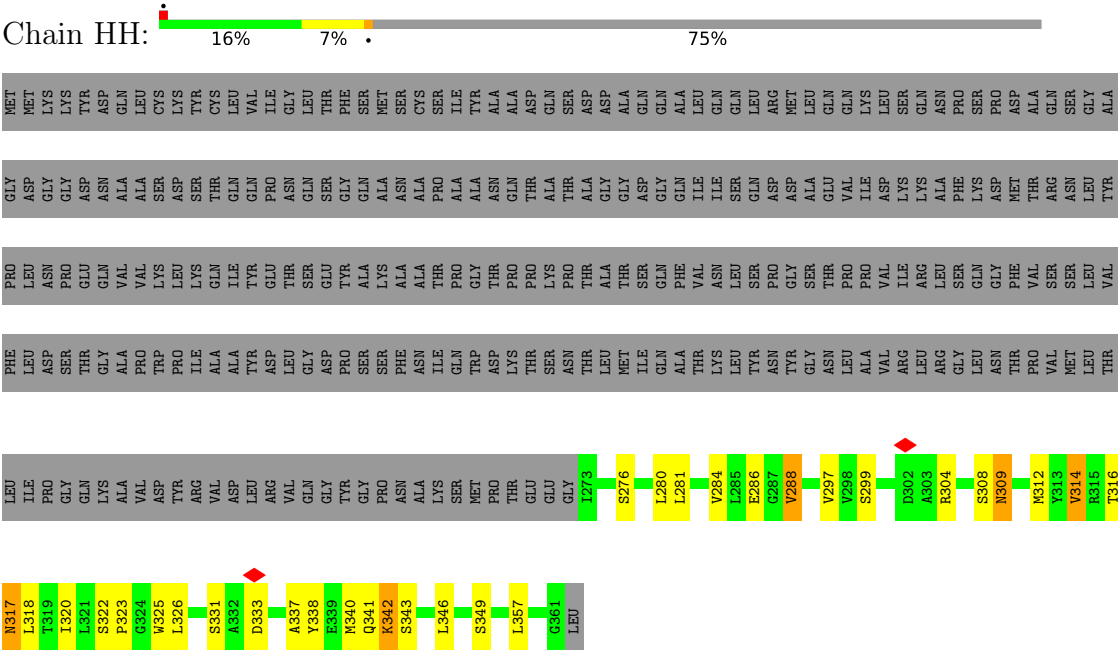


• Molecule 4: Type IV secretion protein IcmK

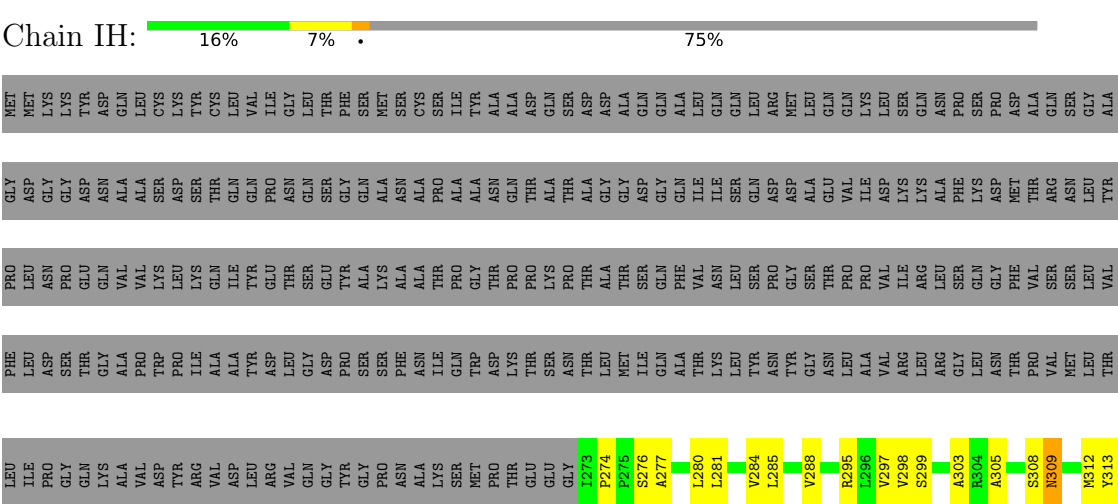


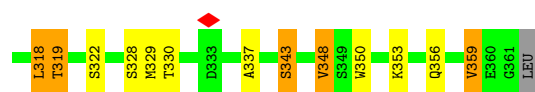


• Molecule 4: Type IV secretion protein IcmK

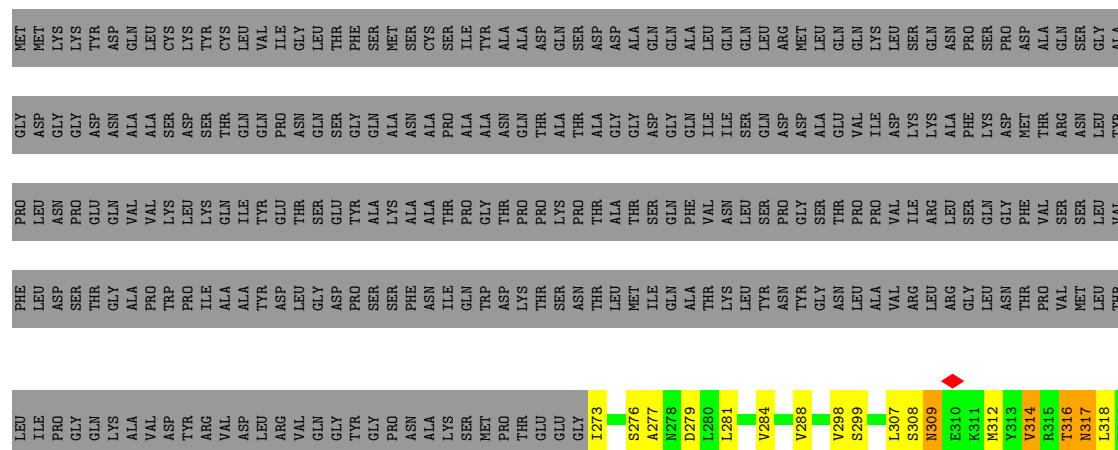


• Molecule 4: Type IV secretion protein IcmK

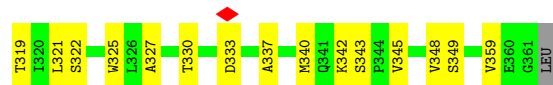
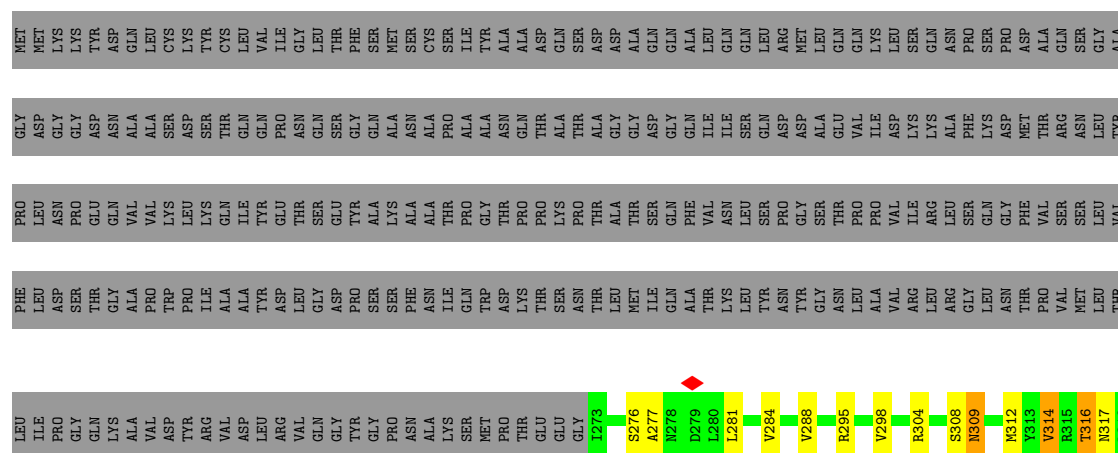




• Molecule 4: Type IV secretion protein IcmK

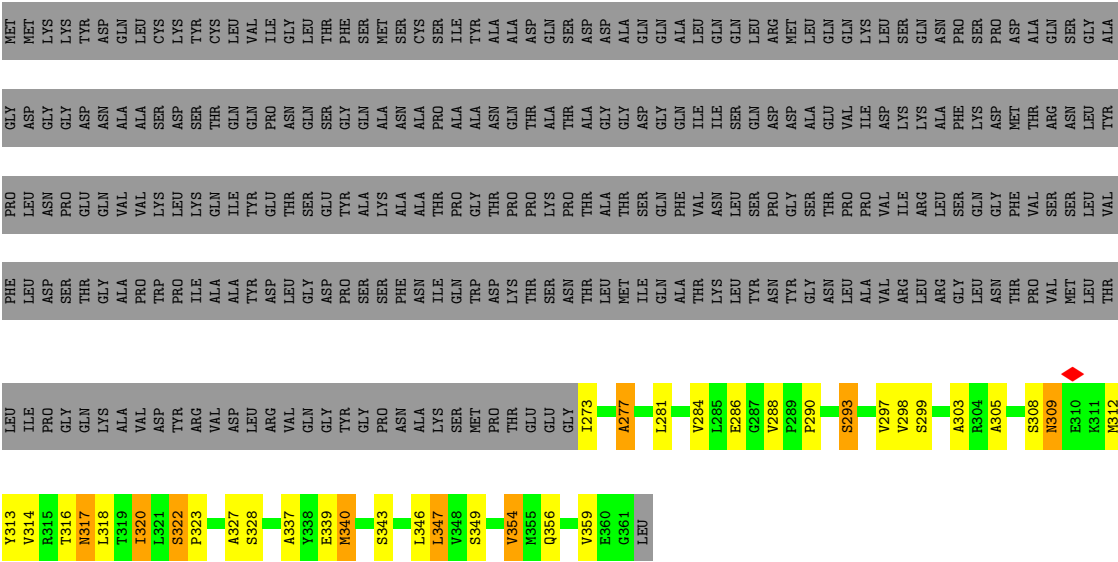


• Molecule 4: Type IV secretion protein IcmK



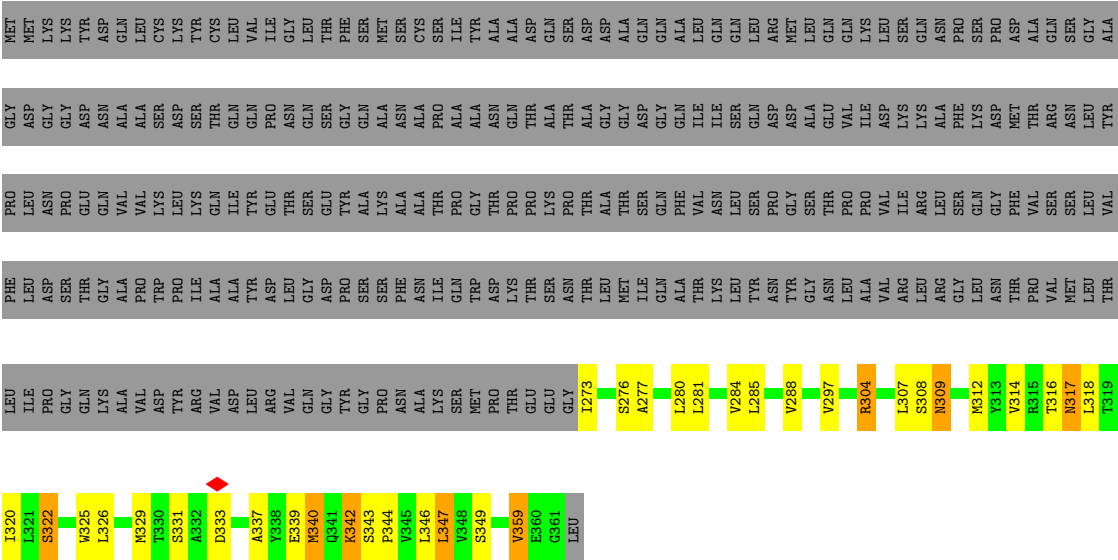
• Molecule 4: Type IV secretion protein IcmK





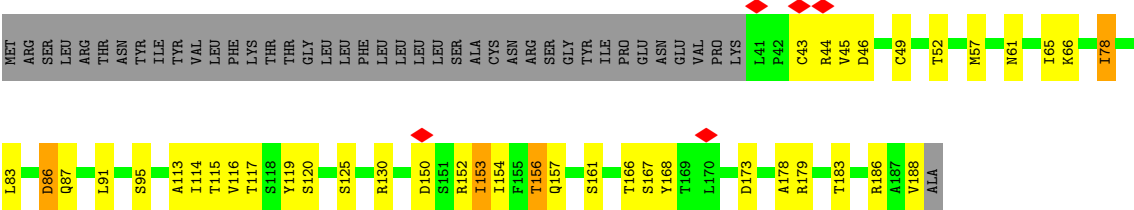
• Molecule 4: Type IV secretion protein IcmK

Chain MH: 15% 7% 75%



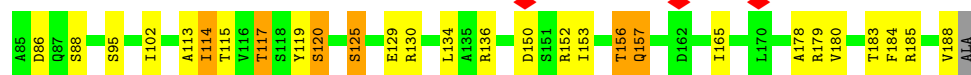
• Molecule 5: Inner membrane lipoprotein YiaD

Chain AK: 57% 20% 22%



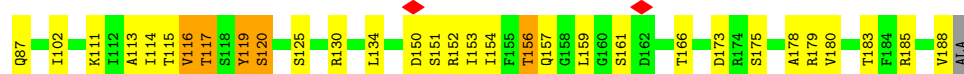
• Molecule 5: Inner membrane lipoprotein YiaD

Frequency	Percentage
Daily	57%
Weekly	17%
Monthly	5%
Never	22%



- Molecule 5: Inner membrane lipoprotein YiaD

Frequency	Percentage
Daily	56%
Weekly	19%
Monthly	22%
Other	3%



- Molecule 5: Inner membrane lipoprotein YiaD

Frequency	Percentage
Daily	54%
Often	23%
Sometimes	22%
Never	3%



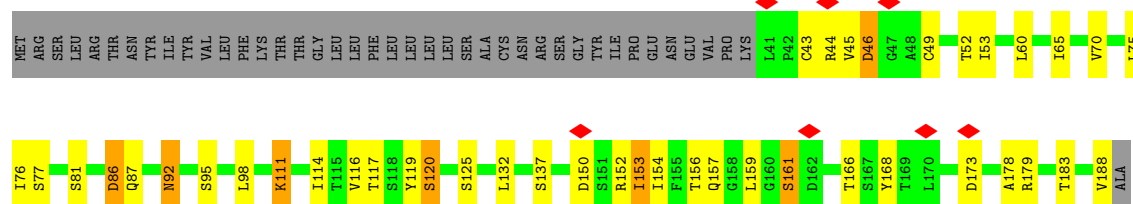
- Molecule 5: Inner membrane lipoprotein YiaD

Frequency	Percentage
Daily	53%
Weekly	22%
Monthly	22%
Other	3%



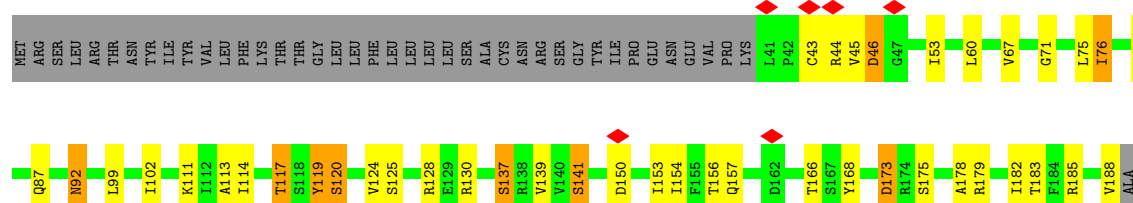
- Molecule 5: Inner membrane lipoprotein YiaD

Chain FK: 



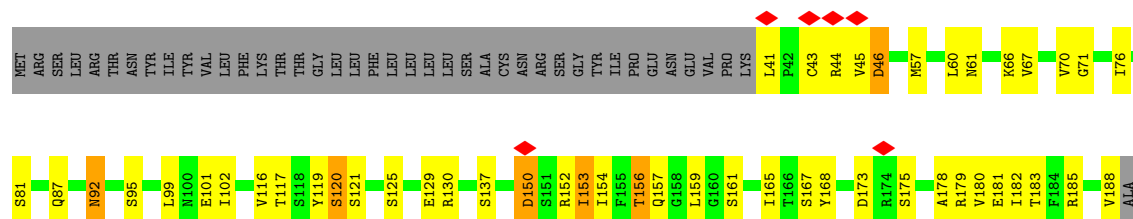
- Molecule 5: Inner membrane lipoprotein YiaD

Chain GK: 



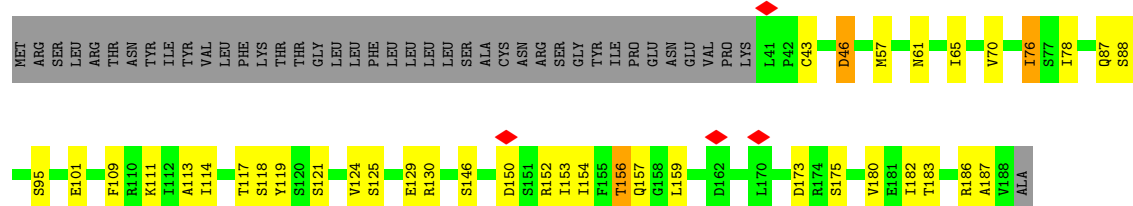
- Molecule 5: Inner membrane lipoprotein YiaD

Chain HK: 



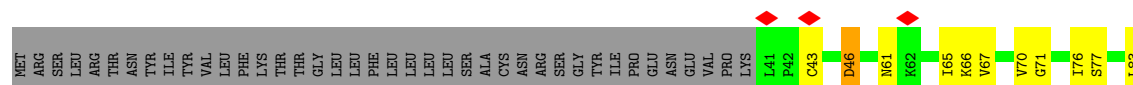
- Molecule 5: Inner membrane lipoprotein YiaD

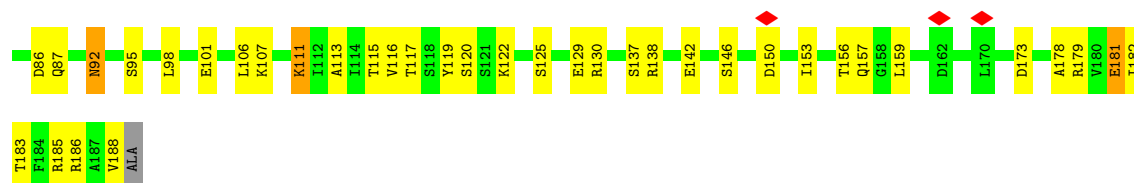
Chain IK: 



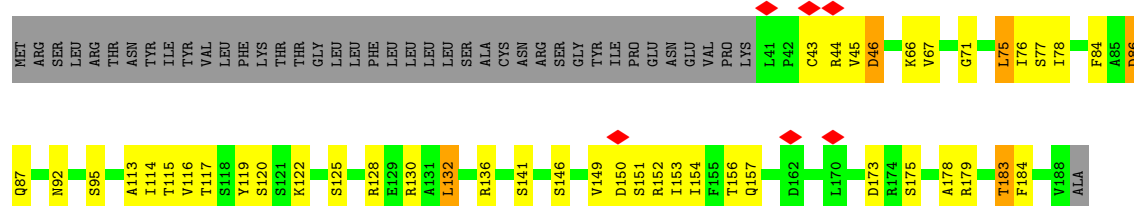
- Molecule 5: Inner membrane lipoprotein YiaD

Chain JK: 

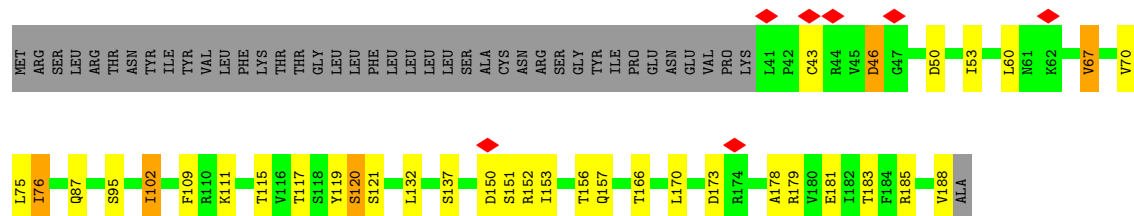




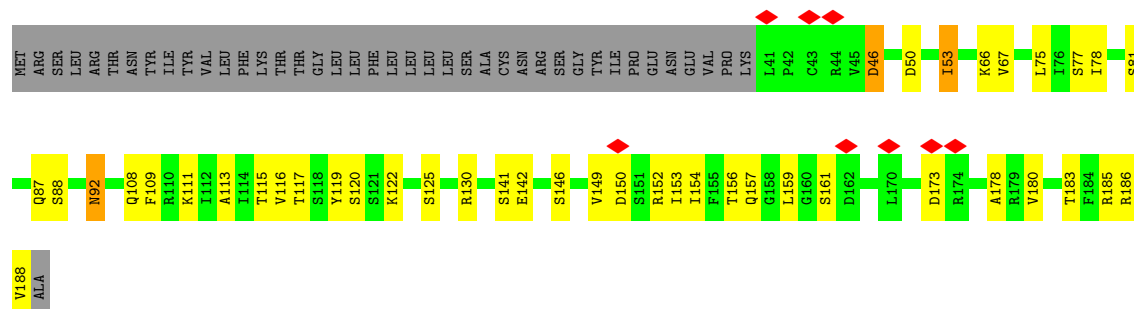
• Molecule 5: Inner membrane lipoprotein YiaD



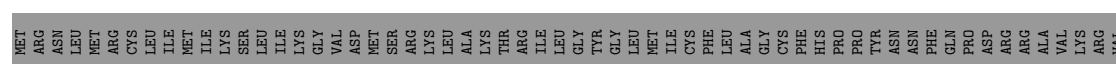
• Molecule 5: Inner membrane lipoprotein YiaD



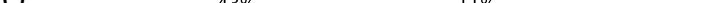
• Molecule 5: Inner membrane lipoprotein YiaD

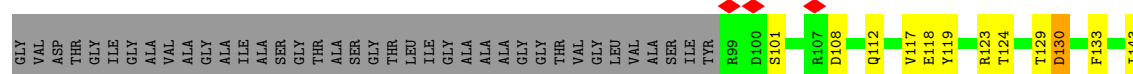


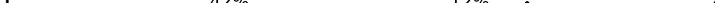
• Molecule 6: Outer membrane protein, OmpA family protein

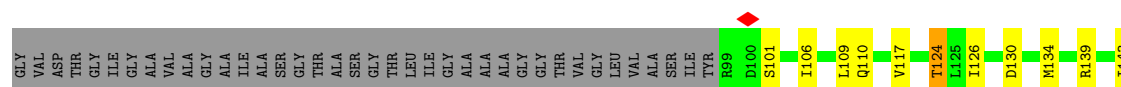
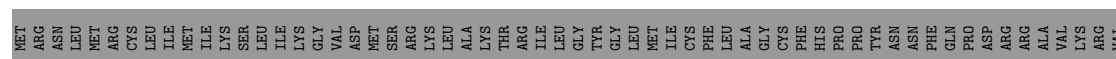




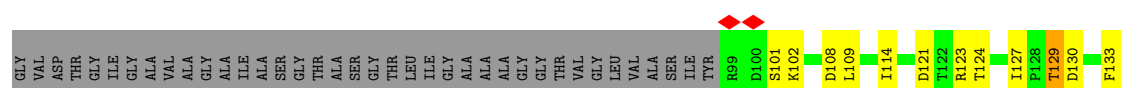
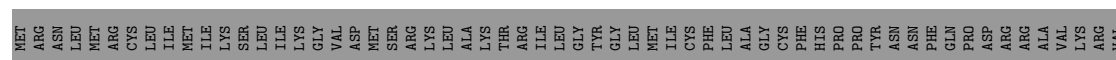
- Chain O:  43% 11% 45%



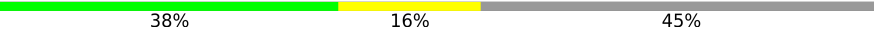
- Chain P:  42% 12% 45%

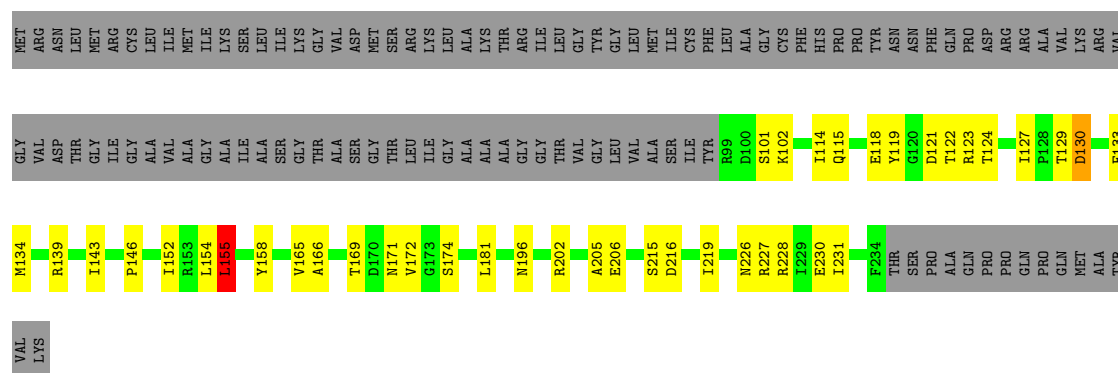


- Chain Q:

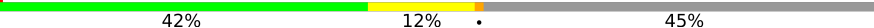


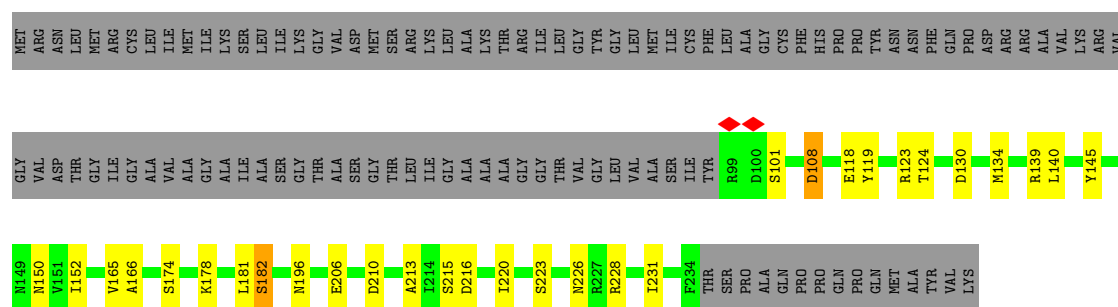
- WORLDWIDE
PDB
PROTEIN DATA BANK

Chain R: 

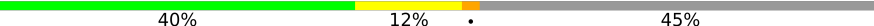


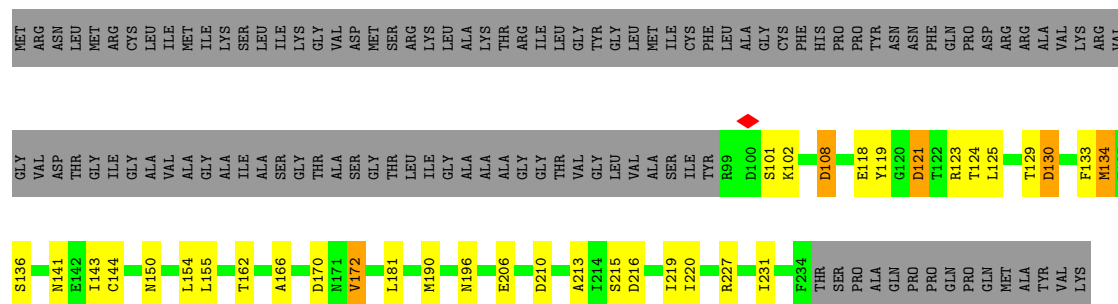
- Molecule 6: Outer membrane protein, OmpA family protein

Chain S: 

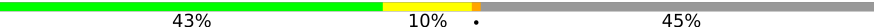


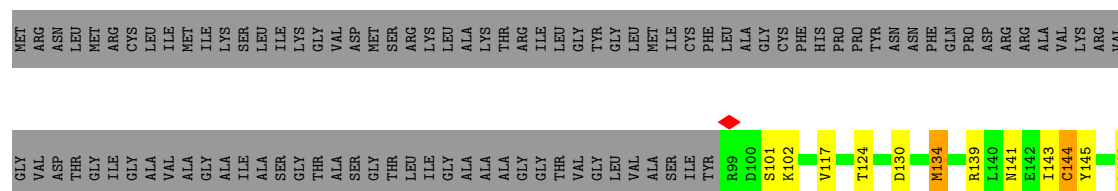
- Molecule 6: Outer membrane protein, OmpA family protein

Chain T: 



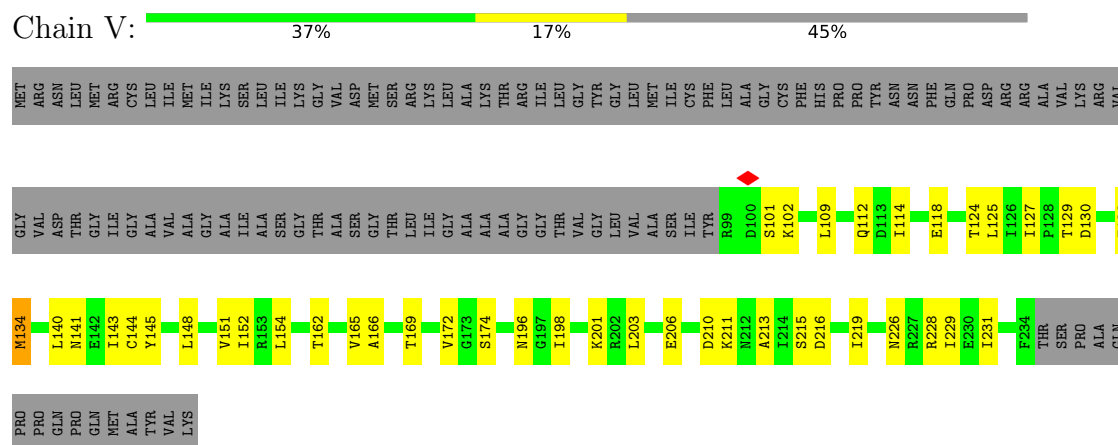
- Molecule 6: Outer membrane protein, OmpA family protein

Chain U: 

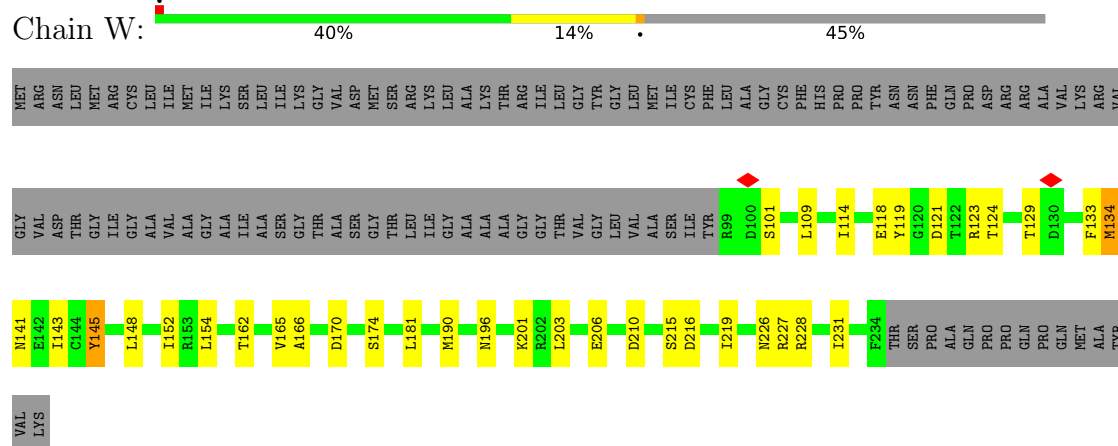




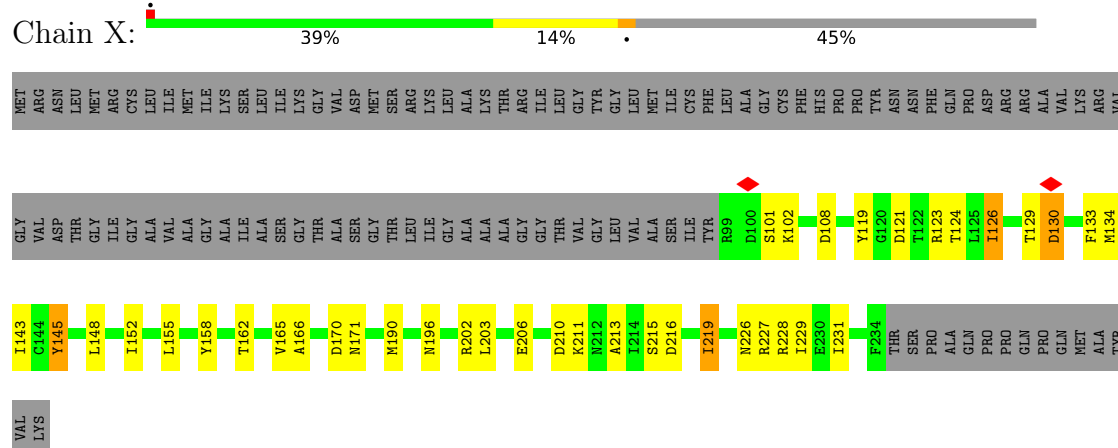
- Molecule 6: Outer membrane protein, OmpA family protein



- Molecule 6: Outer membrane protein, OmpA family protein



- Molecule 6: Outer membrane protein, OmpA family protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12200	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 ($e^-/\text{\AA}^2$)	58.1	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	42.385	Depositor
Minimum map value	-19.636	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.109	Depositor
Recommended contour level	9	Depositor
Map size (Å)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	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
2	AC	0.52	0/1629	0.72	0/2214
2	BC	0.54	0/1629	0.81	0/2214
2	CC	0.53	0/1629	0.82	2/2214 (0.1%)
2	DC	0.51	0/1629	0.77	0/2214
2	EC	0.56	0/1629	0.81	0/2214
2	FC	0.53	0/1629	0.78	0/2214
2	GC	0.54	0/1629	0.83	2/2214 (0.1%)
2	HC	0.55	0/1629	0.83	1/2214 (0.0%)
2	IC	0.54	0/1629	0.78	0/2214
2	JC	0.52	0/1629	0.84	0/2214
2	KC	0.56	0/1629	0.80	1/2214 (0.0%)
2	LC	0.55	0/1629	0.79	0/2214
2	MC	0.55	0/1629	0.80	0/2214
3	AD	0.48	0/1060	0.84	3/1441 (0.2%)
3	Ad	0.52	0/1086	0.93	4/1474 (0.3%)
3	BD	0.49	0/1060	0.87	3/1441 (0.2%)
3	Bd	0.51	0/1086	0.90	0/1474
3	CD	0.49	0/1060	0.95	5/1441 (0.3%)
3	Cd	0.52	0/1086	0.95	4/1474 (0.3%)
3	DD	0.48	0/1060	0.86	2/1441 (0.1%)
3	Dd	0.53	0/1086	0.95	2/1474 (0.1%)
3	ED	0.49	0/1060	0.85	2/1441 (0.1%)
3	Ed	0.51	0/1086	0.89	2/1474 (0.1%)
3	FD	0.49	0/1060	0.88	2/1441 (0.1%)
3	Fd	0.53	0/1086	0.88	0/1474
3	GD	0.49	0/1060	0.88	0/1441
3	Gd	0.50	0/1086	0.89	3/1474 (0.2%)
3	HD	0.54	0/1060	0.92	6/1441 (0.4%)
3	Hd	0.53	0/1086	0.91	3/1474 (0.2%)
3	ID	0.47	0/1060	0.85	0/1441
3	Id	0.52	0/1086	0.97	5/1474 (0.3%)
3	JD	0.48	0/1060	0.83	0/1441
3	Jd	0.52	0/1086	0.95	3/1474 (0.2%)
3	KD	0.50	0/1060	0.88	1/1441 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Kd	0.51	0/1086	0.93	2/1474 (0.1%)
3	LD	0.52	0/1060	0.90	1/1441 (0.1%)
3	Ld	0.50	0/1086	0.88	2/1474 (0.1%)
3	MD	0.49	0/1060	0.86	0/1441
3	Md	0.52	0/1086	0.92	4/1474 (0.3%)
4	AH	0.61	0/695	0.84	0/947
4	BH	0.60	0/695	0.88	0/947
4	CH	0.61	0/695	0.87	0/947
4	DH	0.58	0/695	0.82	0/947
4	EH	0.61	0/695	0.82	0/947
4	FH	0.59	0/695	0.79	0/947
4	GH	0.59	0/695	0.81	0/947
4	HH	0.57	0/695	0.79	0/947
4	IH	0.58	0/695	0.80	0/947
4	JH	0.65	0/695	0.85	0/947
4	KH	0.59	0/695	0.83	0/947
4	LH	0.63	0/695	0.83	0/947
4	MH	0.61	0/695	0.83	0/947
5	AK	0.54	0/1171	0.81	0/1583
5	BK	0.50	0/1171	0.81	0/1583
5	CK	0.50	0/1171	0.80	0/1583
5	DK	0.52	0/1171	0.77	0/1583
5	EK	0.51	0/1171	0.77	0/1583
5	FK	0.50	0/1171	0.80	0/1583
5	GK	0.52	0/1171	0.81	0/1583
5	HK	0.50	0/1171	0.79	0/1583
5	IK	0.51	0/1171	0.79	3/1583 (0.2%)
5	JK	0.52	0/1171	0.79	0/1583
5	KK	0.51	0/1171	0.80	0/1583
5	LK	0.50	0/1171	0.75	0/1583
5	MK	0.49	0/1171	0.75	0/1583
6	N	0.49	0/1130	0.82	1/1522 (0.1%)
6	O	0.49	0/1130	0.79	0/1522
6	P	0.52	0/1130	0.84	1/1522 (0.1%)
6	Q	0.47	0/1130	0.79	0/1522
6	R	0.48	0/1130	0.85	2/1522 (0.1%)
6	S	0.47	0/1130	0.79	1/1522 (0.1%)
6	T	0.51	0/1130	0.80	0/1522
6	U	0.47	0/1130	0.81	0/1522
6	V	0.47	0/1130	0.83	1/1522 (0.1%)
6	W	0.49	0/1130	0.81	1/1522 (0.1%)
6	X	0.50	0/1130	0.82	2/1522 (0.1%)
6	Y	0.51	0/1130	0.81	0/1522

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Z	0.46	0/1130	0.82	3/1522 (0.2%)
All	All	0.52	0/88023	0.84	80/119353 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AX	0	2
1	AZ	0	2
1	BV	0	2
1	BX	0	2
1	BZ	0	2
1	CV	0	1
1	CX	0	2
1	CZ	0	1
1	DX	0	3
1	DZ	0	2
1	EX	0	3
1	EZ	0	1
1	FV	0	1
1	FX	0	3
1	FZ	0	1
1	GV	0	1
1	GX	0	2
1	GZ	0	1
1	HV	0	1
1	HX	0	2
1	HZ	0	1
1	IV	0	1
1	IX	0	2
1	IZ	0	1
1	JX	0	3
1	JZ	0	1
1	KV	0	1
1	KX	0	3
1	KZ	0	1
1	LX	0	3
1	LZ	0	2
1	MX	0	3
1	MZ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	NV	0	1
1	OV	0	2
1	PV	0	1
1	RV	0	1
2	BC	0	1
3	Bd	0	1
3	Ed	0	1
3	Fd	0	1
3	Id	0	1
3	Jd	0	1
3	Kd	0	1
3	Md	0	1
4	AH	0	1
4	BH	0	1
4	DH	0	2
4	EH	0	1
4	FH	0	1
4	GH	0	1
4	HH	0	1
4	IH	0	1
4	JH	0	1
4	KH	0	1
4	LH	0	1
5	DK	0	1
6	N	0	2
6	O	0	2
6	Q	0	2
6	T	0	1
6	V	0	2
6	W	0	1
6	X	0	1
6	Z	0	1
All	All	0	96

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Id	111	LYS	CA-C-N	8.64	132.40	120.39
3	Id	111	LYS	C-N-CA	8.64	132.40	120.39
3	Cd	111	LYS	CA-C-N	8.30	132.54	120.51
3	Cd	111	LYS	C-N-CA	8.30	132.54	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Kd	111	LYS	CA-C-N	7.70	131.10	120.39
3	Kd	111	LYS	C-N-CA	7.70	131.10	120.39
3	Ed	77	TYR	CA-C-N	7.01	132.38	122.08
3	Ed	77	TYR	C-N-CA	7.01	132.38	122.08
6	Z	145	TYR	N-CA-C	6.78	122.93	113.57
3	BD	69	ASN	N-CA-CB	-6.65	106.59	114.17
2	CC	101	LEU	CA-C-N	6.52	129.34	120.54
2	CC	101	LEU	C-N-CA	6.52	129.34	120.54
2	HC	117	LEU	CA-CB-CG	6.46	138.92	116.30
6	X	155	LEU	CA-CB-CG	6.28	138.26	116.30
3	CD	59	GLU	CA-CB-CG	6.16	126.42	114.10
3	CD	74	PRO	CA-C-N	6.15	131.11	122.08
3	CD	74	PRO	C-N-CA	6.15	131.11	122.08
3	BD	74	PRO	CA-C-N	6.09	131.03	122.08
3	BD	74	PRO	C-N-CA	6.09	131.03	122.08
3	HD	73	ILE	CB-CA-C	6.06	116.58	110.94
3	DD	74	PRO	CA-C-N	6.03	130.94	122.08
3	DD	74	PRO	C-N-CA	6.03	130.94	122.08
3	HD	74	PRO	CA-C-N	6.02	130.93	122.08
3	HD	74	PRO	C-N-CA	6.02	130.93	122.08
3	Hd	77	TYR	CA-C-N	6.01	136.78	126.32
3	Hd	77	TYR	C-N-CA	6.01	136.78	126.32
3	Ld	77	TYR	CA-C-N	6.00	136.76	126.32
3	Ld	77	TYR	C-N-CA	6.00	136.76	126.32
3	HD	68	ASP	CA-C-N	5.94	132.89	121.54
3	HD	68	ASP	C-N-CA	5.94	132.89	121.54
3	AD	69	ASN	N-CA-CB	-5.87	107.48	114.17
6	X	145	TYR	N-CA-C	5.86	121.65	113.57
3	Md	77	TYR	CA-C-N	5.83	135.27	125.02
3	Md	77	TYR	C-N-CA	5.83	135.27	125.02
3	Ad	77	TYR	CA-C-N	5.81	136.41	125.66
3	Ad	77	TYR	C-N-CA	5.81	136.41	125.66
3	Ad	142	LYS	N-CA-C	-5.81	106.11	113.43
3	HD	69	ASN	CA-CB-CG	5.76	118.36	112.60
6	V	145	TYR	N-CA-C	5.75	122.52	109.81
6	N	145	TYR	N-CA-C	5.74	122.50	109.81
2	GC	117	LEU	CA-CB-CG	5.71	136.30	116.30
5	IK	124	VAL	N-CA-C	-5.62	108.02	113.53
3	LD	67	LYS	CA-CB-CG	5.62	125.33	114.10
3	Ad	28	PRO	N-CA-C	5.56	117.49	110.70
6	S	119	TYR	CA-CB-CG	-5.50	104.00	113.90
3	Dd	77	TYR	CA-C-N	5.47	135.79	125.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Dd	77	TYR	C-N-CA	5.47	135.79	125.66
3	Gd	77	TYR	CA-C-N	5.47	136.14	126.45
3	Gd	77	TYR	C-N-CA	5.47	136.14	126.45
3	Id	28	PRO	N-CA-C	5.34	117.21	110.70
3	Gd	28	PRO	N-CA-C	5.27	117.13	110.70
3	KD	73	ILE	CB-CA-C	5.24	115.82	110.94
2	GC	119	LEU	CA-CB-CG	5.21	134.54	116.30
3	Cd	77	TYR	CA-C-N	5.21	135.66	126.45
3	Cd	77	TYR	C-N-CA	5.21	135.66	126.45
2	KC	64	LEU	CA-CB-CG	5.20	134.50	116.30
3	Id	77	TYR	CA-C-N	5.19	135.63	126.45
3	Id	77	TYR	C-N-CA	5.19	135.63	126.45
6	R	155	LEU	CA-CB-CG	5.17	134.41	116.30
3	ED	74	PRO	CA-C-N	5.17	130.68	122.61
3	ED	74	PRO	C-N-CA	5.17	130.68	122.61
3	Md	28	PRO	N-CA-C	5.15	116.98	110.70
3	Jd	111	LYS	CA-C-N	5.13	128.48	120.68
3	Jd	111	LYS	C-N-CA	5.13	128.48	120.68
6	Z	144	CYS	CA-C-N	5.12	126.16	120.06
6	Z	144	CYS	C-N-CA	5.12	126.16	120.06
3	FD	68	ASP	CA-C-N	5.09	131.25	121.54
3	FD	68	ASP	C-N-CA	5.09	131.25	121.54
3	AD	74	PRO	CA-C-N	5.07	130.52	122.61
3	AD	74	PRO	C-N-CA	5.07	130.52	122.61
3	Md	142	LYS	N-CA-C	-5.07	107.75	114.04
6	P	146	PRO	CA-N-CD	-5.07	104.90	112.00
6	R	146	PRO	CA-N-CD	-5.07	104.90	112.00
3	Jd	43	GLU	CA-CB-CG	5.04	124.19	114.10
6	W	145	TYR	N-CA-C	5.04	120.32	113.16
3	CD	68	ASP	CA-C-N	5.03	131.15	121.54
3	CD	68	ASP	C-N-CA	5.03	131.15	121.54
5	IK	187	ALA	CA-C-N	5.01	130.72	121.70
5	IK	187	ALA	C-N-CA	5.01	130.72	121.70
3	Hd	28	PRO	N-CA-C	5.01	116.81	110.70

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AH	322	SER	Peptide
1	AX	142	UNK	Peptide
1	AX	153	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	AZ	20	UNK	Peptide
1	AZ	45	UNK	Peptide
2	BC	233	VAL	Peptide
4	BH	277	ALA	Peptide
1	BV	42	UNK	Peptide
1	BV	46	UNK	Peptide
1	BX	142	UNK	Peptide
1	BX	153	UNK	Peptide
1	BZ	20	UNK	Peptide
1	BZ	45	UNK	Peptide
3	Bd	27	LYS	Peptide
1	CV	77	UNK	Peptide
1	CX	142	UNK	Peptide
1	CX	153	UNK	Peptide
1	CZ	45	UNK	Peptide
4	DH	277	ALA	Peptide
4	DH	322	SER	Peptide
5	DK	148	GLY	Peptide
1	DX	142	UNK	Peptide
1	DX	153	UNK	Peptide
1	DX	219	UNK	Peptide
1	DZ	20	UNK	Peptide
1	DZ	45	UNK	Peptide
4	EH	322	SER	Peptide
1	EX	142	UNK	Peptide
1	EX	153	UNK	Peptide
1	EX	43	UNK	Peptide
1	EZ	45	UNK	Peptide
3	Ed	78	ASN	Peptide
4	FH	322	SER	Peptide
1	FV	42	UNK	Peptide
1	FX	142	UNK	Peptide
1	FX	153	UNK	Peptide
1	FX	154	UNK	Peptide
1	FZ	45	UNK	Peptide
3	Fd	85	VAL	Peptide
4	GH	322	SER	Peptide
1	GV	77	UNK	Peptide
1	GX	142	UNK	Peptide
1	GX	153	UNK	Peptide
1	GZ	45	UNK	Peptide
4	HH	322	SER	Peptide

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Mol	Chain	Res	Type	Group
1	HV	77	UNK	Peptide
1	HX	142	UNK	Peptide
1	HX	153	UNK	Peptide
1	HZ	45	UNK	Peptide
4	IH	322	SER	Peptide
1	IV	77	UNK	Peptide
1	IX	142	UNK	Peptide
1	IX	153	UNK	Peptide
1	IZ	45	UNK	Peptide
3	Id	85	VAL	Peptide
4	JH	322	SER	Peptide
1	JX	142	UNK	Peptide
1	JX	153	UNK	Peptide
1	JX	43	UNK	Peptide
1	JZ	45	UNK	Peptide
3	Jd	85	VAL	Peptide
4	KH	322	SER	Peptide
1	KV	42	UNK	Peptide
1	KX	142	UNK	Peptide
1	KX	153	UNK	Peptide
1	KX	43	UNK	Peptide
1	KZ	45	UNK	Peptide
3	Kd	78	ASN	Peptide
4	LH	277	ALA	Peptide
1	LX	142	UNK	Peptide
1	LX	153	UNK	Peptide
1	LX	154	UNK	Peptide
1	LZ	20	UNK	Peptide
1	LZ	45	UNK	Peptide
1	MX	142	UNK	Peptide
1	MX	153	UNK	Peptide
1	MX	43	UNK	Peptide
1	MZ	45	UNK	Peptide
3	Md	85	VAL	Peptide
6	N	134	MET	Peptide
6	N	196	ASN	Peptide
1	NV	42	UNK	Peptide
6	O	112	GLN	Peptide
6	O	155	LEU	Peptide
1	OV	41	UNK	Peptide
1	OV	42	UNK	Peptide
1	PV	77	UNK	Peptide

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Mol	Chain	Res	Type	Group
6	Q	134	MET	Peptide
6	Q	212	ASN	Peptide
1	RV	77	UNK	Peptide
6	T	134	MET	Peptide
6	V	134	MET	Peptide
6	V	196	ASN	Peptide
6	W	134	MET	Peptide
6	X	134	MET	Peptide
6	Z	196	ASN	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	AV	720	0	168	3	0
1	AW	160	0	34	0	0
1	AX	1140	0	256	11	0
1	AY	260	0	62	0	0
1	AZ	350	0	75	5	0
1	BV	720	0	164	11	0
1	BW	160	0	35	2	0
1	BX	1140	0	260	13	0
1	BY	260	0	62	0	0
1	BZ	350	0	75	1	0
1	CV	720	0	159	4	0
1	CW	160	0	35	0	0
1	CX	1140	0	256	9	0
1	CY	260	0	60	0	0
1	CZ	350	0	75	2	0
1	DV	720	0	160	3	0
1	DW	160	0	36	1	0
1	DX	1140	0	256	8	0
1	DY	260	0	61	0	0
1	DZ	350	0	75	3	0
1	EV	720	0	159	5	0
1	EW	160	0	35	1	0
1	EX	1140	0	258	9	0
1	EY	260	0	62	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EZ	350	0	76	1	0
1	FV	720	0	162	8	0
1	FW	160	0	34	0	0
1	FX	1140	0	257	8	0
1	FY	260	0	62	0	0
1	FZ	350	0	75	2	0
1	GV	720	0	165	2	0
1	GW	160	0	35	1	0
1	GX	1140	0	257	9	0
1	GY	260	0	62	0	0
1	GZ	350	0	74	2	0
1	HV	720	0	160	5	0
1	HW	160	0	36	1	0
1	HX	1140	0	258	9	0
1	HY	260	0	62	0	0
1	HZ	350	0	75	1	0
1	IV	720	0	161	5	0
1	IW	160	0	35	2	0
1	IX	1140	0	256	13	0
1	IY	260	0	62	0	0
1	IZ	350	0	75	3	0
1	JV	720	0	160	4	0
1	JW	160	0	35	0	0
1	JX	1140	0	257	10	0
1	JY	260	0	61	0	0
1	JZ	350	0	74	2	0
1	KV	720	0	167	6	0
1	KW	160	0	36	1	0
1	KX	1140	0	254	10	0
1	KY	260	0	62	0	0
1	KZ	350	0	76	3	0
1	LV	720	0	161	5	0
1	LW	160	0	35	0	0
1	LX	1140	0	259	7	0
1	LY	260	0	62	0	0
1	LZ	350	0	75	3	0
1	MV	720	0	161	4	0
1	MW	160	0	35	1	0
1	MX	1140	0	259	7	0
1	MY	260	0	61	0	0
1	MZ	350	0	74	3	0
1	NV	720	0	163	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	NW	160	0	36	0	0
1	OV	720	0	157	4	0
1	OW	160	0	35	1	0
1	PV	720	0	158	4	0
1	PW	160	0	35	1	0
1	QV	720	0	161	1	0
1	QW	160	0	35	0	0
1	RV	720	0	162	4	0
1	RW	160	0	35	2	0
2	AC	1596	0	1602	32	0
2	BC	1596	0	1602	33	0
2	CC	1596	0	1602	34	0
2	DC	1596	0	1602	26	0
2	EC	1596	0	1602	24	0
2	FC	1596	0	1602	30	0
2	GC	1596	0	1602	27	0
2	HC	1596	0	1602	33	0
2	IC	1596	0	1602	23	0
2	JC	1596	0	1602	29	0
2	KC	1596	0	1602	36	0
2	LC	1596	0	1602	27	0
2	MC	1596	0	1602	28	0
3	AD	1040	0	1066	12	0
3	Ad	1066	0	1103	34	0
3	BD	1040	0	1066	21	0
3	Bd	1066	0	1103	29	0
3	CD	1040	0	1066	23	0
3	Cd	1066	0	1103	28	0
3	DD	1040	0	1066	16	0
3	Dd	1066	0	1103	27	0
3	ED	1040	0	1066	18	0
3	Ed	1066	0	1103	20	0
3	FD	1040	0	1066	13	0
3	Fd	1066	0	1103	12	0
3	GD	1040	0	1066	16	0
3	Gd	1066	0	1103	23	0
3	HD	1040	0	1066	18	0
3	Hd	1066	0	1103	34	0
3	ID	1040	0	1066	16	0
3	Id	1066	0	1103	30	0
3	JD	1040	0	1066	17	0
3	Jd	1066	0	1103	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	KD	1040	0	1066	18	0
3	Kd	1066	0	1103	26	0
3	LD	1040	0	1066	13	0
3	Ld	1066	0	1103	21	0
3	MD	1040	0	1066	17	0
3	Md	1066	0	1103	26	0
4	AH	678	0	689	17	0
4	BH	678	0	689	22	0
4	CH	678	0	689	16	0
4	DH	678	0	689	19	0
4	EH	678	0	689	14	0
4	FH	678	0	689	16	0
4	GH	678	0	689	21	0
4	HH	678	0	689	17	0
4	IH	678	0	689	18	0
4	JH	678	0	689	17	0
4	KH	678	0	689	16	0
4	LH	678	0	689	19	0
4	MH	678	0	689	21	0
5	AK	1152	0	1192	18	0
5	BK	1152	0	1192	16	0
5	CK	1152	0	1192	22	0
5	DK	1152	0	1192	21	0
5	EK	1152	0	1192	23	0
5	FK	1152	0	1192	20	0
5	GK	1152	0	1192	22	0
5	HK	1152	0	1192	24	0
5	IK	1152	0	1192	16	0
5	JK	1152	0	1192	22	0
5	KK	1152	0	1192	24	0
5	LK	1152	0	1192	18	0
5	MK	1152	0	1192	17	0
6	N	1108	0	1107	21	0
6	O	1108	0	1107	15	0
6	P	1108	0	1107	14	0
6	Q	1108	0	1107	19	0
6	R	1108	0	1107	23	0
6	S	1108	0	1107	12	0
6	T	1108	0	1107	19	0
6	U	1108	0	1107	12	0
6	V	1108	0	1107	18	0
6	W	1108	0	1107	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	1108	0	1107	20	0
6	Y	1108	0	1107	12	0
6	Z	1108	0	1107	14	0
All	All	124910	0	96525	1589	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 7.

All (1589) 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)
2:GC:176:TRP:O	2:GC:180:THR:HB	1.77	0.85
2:FC:176:TRP:O	2:FC:180:THR:HB	1.76	0.83
3:Hd:86:ASP:HA	3:Hd:121:ILE:O	1.79	0.81
1:BV:53:UNK:O	1:BV:141:UNK:HA	1.82	0.80
2:CC:176:TRP:O	2:CC:180:THR:HB	1.82	0.78
2:HC:176:TRP:O	2:HC:180:THR:HB	1.82	0.78
2:KC:176:TRP:O	2:KC:180:THR:HB	1.83	0.78
3:ID:39:ILE:O	3:ID:43:GLU:HB2	1.84	0.77
3:Jd:86:ASP:HA	3:Jd:121:ILE:O	1.85	0.76
1:FV:74:UNK:O	1:FV:100:UNK:HA	1.86	0.76
1:LV:48:UNK:HA	1:LV:135:UNK:O	1.87	0.75
1:EV:85:UNK:O	1:EV:114:UNK:HA	1.86	0.75
2:EC:128:SER:HA	2:FC:243:ASP:O	1.86	0.75
1:FV:63:UNK:O	1:FV:126:UNK:HA	1.87	0.74
6:Q:129:THR:O	6:Q:133:PHE:HB2	1.90	0.71
6:Z:129:THR:O	6:Z:133:PHE:HB2	1.90	0.71
6:W:166:ALA:HA	6:W:206:GLU:O	1.90	0.71
6:W:124:THR:HA	6:W:231:ILE:O	1.90	0.71
1:NV:54:UNK:HA	1:NV:142:UNK:O	1.91	0.70
2:FC:128:SER:HA	2:GC:243:ASP:O	1.91	0.70
2:IC:128:SER:HA	2:JC:243:ASP:O	1.91	0.70
3:Ad:86:ASP:HA	3:Ad:121:ILE:O	1.91	0.70
3:Id:87:TRP:O	3:Id:120:SER:HA	1.93	0.69
3:BD:39:ILE:O	3:BD:43:GLU:HB2	1.91	0.69
6:O:124:THR:HA	6:O:231:ILE:O	1.92	0.69
6:S:166:ALA:HA	6:S:206:GLU:O	1.92	0.69
1:KV:48:UNK:HA	1:KV:135:UNK:O	1.92	0.69
2:JC:176:TRP:O	2:JC:180:THR:HB	1.93	0.69
6:Z:166:ALA:HA	6:Z:206:GLU:O	1.92	0.69
2:DC:128:SER:HA	2:EC:243:ASP:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cd:86:ASP:HA	3:Cd:121:ILE:O	1.92	0.68
1:FV:85:UNK:O	1:FV:114:UNK:HA	1.93	0.68
1:FX:128:UNK:HA	1:FX:147:UNK:O	1.93	0.68
5:HK:117:THR:HA	5:HK:157:GLN:O	1.94	0.68
6:Z:124:THR:HA	6:Z:231:ILE:O	1.94	0.68
1:EV:84:UNK:HA	1:EV:115:UNK:O	1.94	0.67
2:AC:128:SER:HA	2:BC:243:ASP:O	1.95	0.67
6:R:124:THR:HA	6:R:231:ILE:O	1.95	0.67
1:JX:76:UNK:HA	1:JX:94:UNK:O	1.95	0.67
1:DV:49:UNK:O	1:DV:136:UNK:HA	1.95	0.67
1:RV:84:UNK:O	1:RW:28:UNK:HA	1.95	0.66
6:N:166:ALA:HA	6:N:206:GLU:O	1.95	0.66
6:N:124:THR:HA	6:N:231:ILE:O	1.95	0.66
4:DH:281:LEU:O	4:DH:285:LEU:HB2	1.96	0.66
2:BC:109:VAL:HB	2:BC:135:ALA:O	1.96	0.66
2:GC:128:SER:HA	2:HC:243:ASP:O	1.96	0.66
2:AC:109:VAL:HB	2:AC:135:ALA:O	1.96	0.65
2:AC:243:ASP:O	2:MC:128:SER:HA	1.97	0.65
1:RV:85:UNK:HA	1:RW:27:UNK:O	1.96	0.65
5:HK:125:SER:O	5:HK:129:GLU:HB2	1.96	0.65
1:JX:98:UNK:O	1:JX:117:UNK:HA	1.97	0.65
3:MD:107:ARG:O	3:MD:155:GLU:HA	1.97	0.64
6:P:124:THR:HA	6:P:231:ILE:O	1.97	0.64
6:Q:166:ALA:HA	6:Q:206:GLU:O	1.98	0.64
2:BC:128:SER:HA	2:CC:243:ASP:O	1.98	0.64
6:Q:124:THR:HA	6:Q:231:ILE:O	1.97	0.64
6:R:166:ALA:HA	6:R:206:GLU:O	1.98	0.64
6:T:166:ALA:HA	6:T:206:GLU:O	1.97	0.64
6:V:166:ALA:HA	6:V:206:GLU:O	1.98	0.64
6:O:166:ALA:HA	6:O:206:GLU:O	1.97	0.63
3:FD:107:ARG:O	3:FD:155:GLU:HA	1.99	0.63
1:BX:97:UNK:HA	1:BX:116:UNK:O	1.98	0.63
1:KX:98:UNK:O	1:KX:117:UNK:HA	1.98	0.63
6:R:129:THR:O	6:R:133:PHE:HB2	1.99	0.63
1:KV:86:UNK:O	1:KW:26:UNK:HA	1.99	0.63
1:JV:51:UNK:O	1:JV:139:UNK:HA	1.99	0.62
6:P:166:ALA:HA	6:P:206:GLU:O	2.00	0.62
3:Ad:72:THR:HG1	3:Ad:146:HIS:HD1	1.48	0.62
6:V:124:THR:HA	6:V:231:ILE:O	1.99	0.62
6:V:129:THR:O	6:V:133:PHE:HB2	2.00	0.62
1:FX:97:UNK:HA	1:FX:116:UNK:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:166:ALA:HA	6:Y:206:GLU:O	2.00	0.62
1:GX:97:UNK:HA	1:GX:116:UNK:O	1.99	0.61
5:IK:117:THR:HA	5:IK:157:GLN:O	1.99	0.61
2:JC:128:SER:HA	2:KC:243:ASP:O	2.00	0.61
1:KX:65:UNK:HA	1:KX:82:UNK:O	2.00	0.61
1:MX:97:UNK:HA	1:MX:116:UNK:O	2.00	0.61
2:KC:128:SER:HA	2:LC:243:ASP:O	1.99	0.61
5:KK:117:THR:HA	5:KK:157:GLN:O	2.00	0.61
3:Ld:87:TRP:O	3:Ld:120:SER:HA	2.01	0.61
2:HC:109:VAL:HB	2:HC:135:ALA:O	2.00	0.61
1:IX:76:UNK:HA	1:IX:94:UNK:O	2.01	0.61
1:JX:97:UNK:HA	1:JX:116:UNK:O	2.01	0.61
3:Bd:86:ASP:HA	3:Bd:121:ILE:O	2.00	0.61
1:BX:157:UNK:HA	1:BX:176:UNK:O	2.01	0.60
2:AC:186:ASN:O	2:AC:190:GLN:HB2	2.01	0.60
5:BK:113:ALA:HA	5:BK:153:ILE:O	2.02	0.60
2:FC:186:ASN:O	2:FC:190:GLN:HB2	2.02	0.60
2:JC:215:LEU:HB3	2:JC:220:MET:HB2	1.83	0.60
2:CC:101:LEU:HB2	2:CC:105:ILE:HB	1.84	0.60
6:T:124:THR:HA	6:T:231:ILE:O	2.00	0.60
5:AK:117:THR:HA	5:AK:157:GLN:O	2.00	0.60
3:DD:43:GLU:HB3	6:Q:172:VAL:HG21	1.82	0.60
3:Dd:87:TRP:O	3:Dd:120:SER:HA	2.02	0.60
4:LH:322:SER:HB3	4:LH:347:LEU:HB3	1.84	0.60
5:CK:113:ALA:HA	5:CK:153:ILE:O	2.02	0.59
3:LD:48:VAL:HG23	3:Ld:52:MET:HG2	1.85	0.59
1:JX:45:UNK:O	1:JX:64:UNK:HA	2.02	0.59
1:BX:98:UNK:O	1:BX:117:UNK:HA	2.02	0.59
3:FD:94:LEU:O	3:FD:98:ILE:HB	2.02	0.59
3:Gd:87:TRP:O	3:Gd:120:SER:HA	2.03	0.59
1:KX:97:UNK:HA	1:KX:116:UNK:O	2.03	0.59
1:CX:97:UNK:HA	1:CX:116:UNK:O	2.03	0.59
1:IX:97:UNK:HA	1:IX:116:UNK:O	2.03	0.59
3:Kd:86:ASP:HA	3:Kd:121:ILE:O	2.02	0.59
2:BC:79:ILE:HD12	3:Bd:37:ALA:HB2	1.85	0.58
3:AD:43:GLU:HG3	6:N:172:VAL:HG21	1.84	0.58
5:CK:117:THR:HA	5:CK:157:GLN:O	2.02	0.58
2:GC:126:ARG:HG2	4:HH:276:SER:HA	1.85	0.58
2:KC:109:VAL:HB	2:KC:135:ALA:O	2.03	0.58
5:MK:117:THR:HA	5:MK:157:GLN:O	2.02	0.58
1:LV:50:UNK:HA	1:LV:138:UNK:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BK:125:SER:O	5:BK:129:GLU:HB2	2.04	0.58
6:U:166:ALA:HA	6:U:206:GLU:O	2.03	0.58
2:HC:88:ARG:HH21	3:Hd:122:SER:HB3	1.69	0.57
4:IH:281:LEU:HA	4:IH:284:VAL:HG22	1.86	0.57
2:AC:210:ILE:HG23	3:Ad:55:MET:HG2	1.86	0.57
1:HX:97:UNK:HA	1:HX:116:UNK:O	2.03	0.57
3:Dd:107:ARG:O	3:Dd:155:GLU:HA	2.04	0.57
5:BK:117:THR:HA	5:BK:157:GLN:O	2.03	0.57
3:Bd:87:TRP:O	3:Bd:120:SER:HA	2.04	0.57
3:Ed:98:ILE:HG23	3:Ed:128:LEU:HD22	1.86	0.57
4:JH:325:TRP:HB3	4:JH:340:MET:HE2	1.86	0.57
1:GX:98:UNK:O	1:GX:117:UNK:HA	2.05	0.57
3:Gd:85:VAL:O	3:Gd:122:SER:HA	2.04	0.57
4:GH:281:LEU:HA	4:GH:284:VAL:HG22	1.87	0.57
3:Gd:37:ALA:O	3:Gd:41:LEU:HB2	2.05	0.57
1:KX:45:UNK:O	1:KX:64:UNK:HA	2.05	0.57
4:EH:312:MET:HE1	4:EH:359:VAL:HG21	1.87	0.56
2:HC:128:SER:HA	2:IC:243:ASP:O	2.04	0.56
3:Kd:107:ARG:O	3:Kd:155:GLU:HA	2.05	0.56
2:KC:108:PRO:HD3	2:KC:138:ALA:HB2	1.86	0.56
3:Md:87:TRP:O	3:Md:120:SER:HA	2.04	0.56
6:S:178:LYS:O	6:S:182:SER:HB3	2.05	0.56
6:U:124:THR:HA	6:U:231:ILE:O	2.04	0.56
2:DC:186:ASN:O	2:DC:190:GLN:HB2	2.05	0.56
1:DX:97:UNK:HA	1:DX:116:UNK:O	2.05	0.56
5:HK:153:ILE:HG23	3:Hd:85:VAL:HB	1.88	0.56
3:Hd:105:ARG:O	3:Hd:153:VAL:HA	2.06	0.56
3:ID:48:VAL:HG23	3:Id:52:MET:HG2	1.87	0.56
2:HC:210:ILE:HG23	3:Hd:55:MET:HG2	1.87	0.56
1:IZ:8:UNK:HA	1:IZ:19:UNK:HA	1.88	0.56
1:MV:84:UNK:O	1:MW:28:UNK:HA	2.05	0.55
3:HD:132:LEU:HD23	3:HD:135:ILE:HD11	1.89	0.55
3:Md:98:ILE:HG23	3:Md:128:LEU:HD22	1.88	0.55
5:FK:114:ILE:O	5:FK:154:ILE:HA	2.05	0.55
5:GK:60:LEU:HD21	5:GK:102:ILE:HG22	1.89	0.55
3:Hd:132:LEU:HD23	3:Hd:135:ILE:HD11	1.88	0.55
5:JK:125:SER:O	5:JK:129:GLU:HB2	2.05	0.55
4:DH:281:LEU:HA	4:DH:284:VAL:HG12	1.88	0.55
1:HX:47:UNK:O	1:HX:66:UNK:HA	2.06	0.55
1:LX:97:UNK:HA	1:LX:116:UNK:O	2.06	0.55
1:CX:65:UNK:HA	1:CX:82:UNK:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KC:243:ASP:OD2	2:KC:243:ASP:N	2.39	0.55
4:KH:281:LEU:HA	4:KH:284:VAL:HG22	1.89	0.55
4:LH:312:MET:HE1	4:LH:359:VAL:HG21	1.89	0.55
5:EK:117:THR:HA	5:EK:157:GLN:O	2.06	0.55
1:HX:76:UNK:HA	1:HX:94:UNK:O	2.07	0.55
5:KK:113:ALA:HA	5:KK:153:ILE:O	2.07	0.55
6:Z:127:ILE:HB	6:Z:229:ILE:HB	1.89	0.55
1:IX:45:UNK:O	1:IX:64:UNK:HA	2.07	0.55
3:Cd:132:LEU:HD22	3:Cd:145:ILE:HG21	1.89	0.55
3:ID:102:ALA:HB2	3:ID:128:LEU:HD11	1.88	0.55
3:Ld:107:ARG:O	3:Ld:155:GLU:HA	2.06	0.55
3:Dd:147:VAL:HG22	3:Dd:154:VAL:HG22	1.88	0.54
1:EX:97:UNK:HA	1:EX:116:UNK:O	2.06	0.54
3:Id:98:ILE:HG23	3:Id:128:LEU:HD22	1.88	0.54
2:CC:102:GLU:HB3	2:CC:103:HIS:HD2	1.72	0.54
6:Q:165:VAL:HG23	6:Q:231:ILE:HG12	1.89	0.54
1:EV:86:UNK:O	1:EW:26:UNK:HA	2.08	0.54
5:LK:153:ILE:HG23	3:Ld:85:VAL:HG22	1.88	0.54
1:KV:82:UNK:N	1:KV:117:UNK:O	2.41	0.54
2:BC:231:LEU:HB2	2:BC:244:ASP:HB3	1.90	0.54
5:HK:44:ARG:HE	5:HK:45:VAL:HG23	1.72	0.54
1:HX:98:UNK:O	1:HX:117:UNK:HA	2.08	0.54
1:LX:65:UNK:HA	1:LX:82:UNK:O	2.08	0.54
3:Hd:91:ILE:HD12	3:Hd:119:ILE:HD13	1.89	0.54
6:P:134:MET:SD	6:P:139:ARG:NH2	2.81	0.54
5:JK:76:ILE:HB	5:JK:182:ILE:HB	1.90	0.54
1:JX:170:UNK:HA	1:JX:188:UNK:O	2.07	0.54
2:AC:246:VAL:HB	2:MC:126:ARG:HD2	1.89	0.54
5:AK:113:ALA:HA	5:AK:153:ILE:O	2.07	0.54
3:FD:132:LEU:HD23	3:FD:135:ILE:HD11	1.89	0.54
6:S:124:THR:HA	6:S:231:ILE:O	2.07	0.54
6:W:129:THR:O	6:W:133:PHE:HB2	2.08	0.54
1:KV:81:UNK:HA	1:KV:118:UNK:HA	1.89	0.53
4:BH:281:LEU:HA	4:BH:284:VAL:HG22	1.91	0.53
5:DK:117:THR:HA	5:DK:157:GLN:O	2.08	0.53
6:R:101:SER:OG	6:R:102:LYS:N	2.41	0.53
6:X:124:THR:HA	6:X:231:ILE:O	2.08	0.53
6:N:215:SER:OG	6:N:216:ASP:N	2.42	0.53
6:U:134:MET:SD	6:U:139:ARG:NH2	2.81	0.53
2:CC:186:ASN:O	2:CC:190:GLN:HB2	2.09	0.53
2:CC:231:LEU:HB2	2:CC:244:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FC:126:ARG:HG2	4:GH:276:SER:HA	1.90	0.53
3:JD:102:ALA:HB2	3:JD:128:LEU:HD11	1.91	0.53
3:Jd:107:ARG:O	3:Jd:155:GLU:HA	2.08	0.53
2:EC:119:LEU:HA	2:EC:125:ILE:HG22	1.91	0.53
1:EX:76:UNK:HA	1:EX:94:UNK:O	2.09	0.53
2:HC:126:ARG:HG2	4:IH:276:SER:HA	1.90	0.53
5:KK:153:ILE:HG23	3:Kd:85:VAL:HB	1.89	0.53
4:LH:320:ILE:HG21	4:LH:340:MET:HE1	1.88	0.53
4:MH:281:LEU:O	4:MH:285:LEU:HB2	2.08	0.53
3:Fd:87:TRP:O	3:Fd:120:SER:HA	2.07	0.53
3:JD:43:GLU:OE2	6:W:227:ARG:NH1	2.42	0.53
5:EK:153:ILE:HG23	3:Ed:85:VAL:HG22	1.89	0.53
1:EX:45:UNK:O	1:EX:64:UNK:HA	2.07	0.53
5:GK:117:THR:HA	5:GK:157:GLN:O	2.09	0.53
1:IV:49:UNK:O	1:IV:136:UNK:HA	2.09	0.53
3:Ed:78:ASN:ND2	3:Ed:102:ALA:O	2.42	0.53
6:V:101:SER:OG	6:V:102:LYS:N	2.41	0.53
2:CC:128:SER:HA	2:DC:243:ASP:O	2.09	0.53
2:EC:215:LEU:HB3	2:EC:220:MET:HB2	1.91	0.53
5:FK:117:THR:HA	5:FK:157:GLN:O	2.09	0.53
1:FX:98:UNK:O	1:FX:117:UNK:HA	2.09	0.53
2:JC:192:ASN:ND2	3:Jd:36:ASP:OD2	2.41	0.53
2:MC:75:ARG:NH1	3:Md:36:ASP:OD1	2.42	0.53
6:R:215:SER:OG	6:R:216:ASP:N	2.41	0.53
6:X:129:THR:O	6:X:133:PHE:HB2	2.08	0.53
2:DC:79:ILE:HD12	3:Dd:37:ALA:HB2	1.90	0.53
3:FD:102:ALA:HB2	3:FD:128:LEU:HD11	1.91	0.53
2:JC:88:ARG:HH21	3:Jd:122:SER:HG	1.56	0.53
4:AH:325:TRP:HA	4:AH:340:MET:HB3	1.91	0.52
1:AX:47:UNK:O	1:AX:66:UNK:HA	2.09	0.52
4:CH:298:VAL:HG11	4:CH:303:ALA:HB3	1.90	0.52
1:IX:65:UNK:HA	1:IX:82:UNK:O	2.09	0.52
6:T:215:SER:OG	6:T:216:ASP:N	2.42	0.52
1:BV:81:UNK:HA	1:BV:118:UNK:HA	1.89	0.52
3:Bd:98:ILE:HG23	3:Bd:128:LEU:HD22	1.92	0.52
5:HK:150:ASP:OD2	5:HK:150:ASP:N	2.43	0.52
2:IC:118:ASN:HB2	4:JH:277:ALA:HA	1.91	0.52
5:IK:113:ALA:HA	5:IK:153:ILE:O	2.10	0.52
5:AK:179:ARG:NH2	6:Z:119:TYR:OH	2.42	0.52
5:FK:153:ILE:HG23	3:Fd:85:VAL:HG22	1.92	0.52
2:LC:128:SER:HA	2:MC:243:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:101:SER:OG	6:Q:102:LYS:N	2.43	0.52
5:AK:44:ARG:HE	5:AK:45:VAL:HG13	1.74	0.52
1:AX:76:UNK:HA	1:AX:94:UNK:O	2.08	0.52
3:BD:58:VAL:HG21	3:Bd:60:LYS:HA	1.90	0.52
2:CC:99:LEU:HG	3:CD:52:MET:HE1	1.90	0.52
6:Y:117:VAL:HG23	6:Y:124:THR:HG23	1.92	0.52
2:EC:126:ARG:HG2	4:FH:276:SER:HA	1.92	0.52
3:HD:43:GLU:OE2	6:U:227:ARG:NH1	2.43	0.52
4:HH:281:LEU:HA	4:HH:284:VAL:HG22	1.92	0.52
5:MK:46:ASP:OD1	5:MK:46:ASP:N	2.43	0.52
5:AK:153:ILE:HG23	3:Ad:85:VAL:HB	1.92	0.52
1:AX:97:UNK:HA	1:AX:116:UNK:O	2.10	0.52
4:GH:309:ASN:OD1	4:GH:309:ASN:N	2.43	0.52
1:GV:84:UNK:O	1:GW:28:UNK:HA	2.10	0.52
4:BH:304:ARG:O	4:BH:314:VAL:HA	2.10	0.52
5:CK:179:ARG:NH2	6:O:119:TYR:OH	2.43	0.52
2:FC:84:ASN:OD1	2:FC:148:ARG:NH1	2.43	0.52
3:Ld:78:ASN:ND2	3:Ld:102:ALA:O	2.43	0.52
6:U:101:SER:OG	6:U:102:LYS:N	2.42	0.52
1:MV:82:UNK:N	1:MV:117:UNK:O	2.43	0.52
4:DH:317:ASN:OD1	4:DH:317:ASN:N	2.42	0.52
5:FK:86:ASP:OD2	5:FK:86:ASP:N	2.43	0.52
6:O:129:THR:O	6:O:133:PHE:HB2	2.10	0.52
6:W:215:SER:OG	6:W:216:ASP:N	2.42	0.52
2:AC:108:PRO:HD3	2:AC:138:ALA:HB2	1.91	0.52
5:AK:86:ASP:OD2	5:AK:86:ASP:N	2.38	0.52
2:BC:215:LEU:HB3	2:BC:220:MET:HB2	1.92	0.52
3:ED:79:LEU:HB3	3:ED:129:ALA:HB2	1.90	0.52
3:HD:58:VAL:HG21	3:Hd:60:LYS:HA	1.92	0.52
5:HK:179:ARG:NH2	6:T:119:TYR:OH	2.43	0.52
4:JH:314:VAL:HG23	4:JH:338:TYR:HB2	1.92	0.52
5:MK:185:ARG:NH2	6:Y:213:ALA:O	2.43	0.52
6:O:215:SER:OG	6:O:216:ASP:N	2.43	0.52
6:Y:101:SER:OG	6:Y:102:LYS:N	2.43	0.52
3:AD:84:SER:HB3	2:MC:267:ALA:HB3	1.92	0.51
4:FH:281:LEU:HA	4:FH:284:VAL:HG22	1.92	0.51
4:HH:316:THR:OG1	4:HH:317:ASN:N	2.43	0.51
4:JH:316:THR:OG1	4:JH:317:ASN:N	2.43	0.51
6:P:215:SER:OG	6:P:216:ASP:N	2.43	0.51
6:T:101:SER:OG	6:T:102:LYS:N	2.43	0.51
2:GC:117:LEU:HD21	3:Hd:115:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:GK:111:LYS:NZ	5:GK:150:ASP:OD2	2.43	0.51
2:HC:126:ARG:NH1	4:IH:274:PRO:O	2.43	0.51
4:HH:346:LEU:HB2	4:HH:357:LEU:HB2	1.92	0.51
3:Id:78:ASN:ND2	3:Id:102:ALA:O	2.44	0.51
4:JH:281:LEU:HA	4:JH:284:VAL:HG22	1.91	0.51
5:KK:114:ILE:HG23	5:KK:184:PHE:HB3	1.92	0.51
6:S:108:ASP:OD1	6:S:150:ASN:ND2	2.43	0.51
3:Ad:105:ARG:O	3:Ad:153:VAL:HA	2.09	0.51
4:CH:281:LEU:HA	4:CH:284:VAL:HG22	1.92	0.51
5:CK:60:LEU:HD21	5:CK:102:ILE:HG22	1.92	0.51
3:Ed:105:ARG:O	3:Ed:153:VAL:HA	2.10	0.51
5:GK:76:ILE:HG12	5:GK:182:ILE:HB	1.92	0.51
3:ID:79:LEU:HB3	3:ID:129:ALA:HB2	1.92	0.51
2:MC:108:PRO:HD3	2:MC:138:ALA:HB2	1.91	0.51
6:R:226:ASN:O	6:R:228:ARG:NH1	2.44	0.51
6:T:108:ASP:OD1	6:T:150:ASN:ND2	2.44	0.51
1:BX:47:UNK:O	1:BX:66:UNK:HA	2.11	0.51
2:CC:255:LEU:HD13	2:DC:240:ILE:HG12	1.91	0.51
3:CD:29:PRO:HB2	3:CD:32:ASN:HB2	1.93	0.51
4:GH:305:ALA:HA	4:GH:313:TYR:O	2.09	0.51
3:CD:102:ALA:HB2	3:CD:128:LEU:HD11	1.92	0.51
3:GD:43:GLU:HB3	6:T:172:VAL:HG21	1.93	0.51
4:HH:317:ASN:N	4:HH:317:ASN:OD1	2.43	0.51
4:KH:325:TRP:HA	4:KH:340:MET:HB3	1.93	0.51
3:Kd:98:ILE:HG23	3:Kd:128:LEU:HD22	1.93	0.51
5:LK:60:LEU:HD21	5:LK:102:ILE:HG22	1.92	0.51
2:AC:110:LEU:HD13	2:AC:215:LEU:HD12	1.93	0.51
2:BC:88:ARG:HH21	3:Bd:122:SER:HB2	1.76	0.51
3:CD:130:GLU:OE2	3:Cd:107:ARG:NH2	2.44	0.51
5:GK:46:ASP:N	5:GK:46:ASP:OD1	2.44	0.51
5:GK:114:ILE:HB	5:GK:154:ILE:HG12	1.92	0.51
5:IK:114:ILE:HB	5:IK:154:ILE:HG12	1.92	0.51
3:JD:137:TYR:O	3:Jd:160:LYS:NZ	2.44	0.51
6:V:127:ILE:HB	6:V:229:ILE:HB	1.93	0.51
2:DC:75:ARG:NH1	3:Dd:36:ASP:OD2	2.44	0.51
5:JK:117:THR:HA	5:JK:157:GLN:O	2.10	0.51
2:KC:114:ARG:HG2	2:KC:130:ARG:HD3	1.92	0.51
4:AH:277:ALA:HA	2:MC:118:ASN:HB2	1.92	0.51
5:BK:179:ARG:NH2	6:N:119:TYR:OH	2.44	0.51
5:BK:185:ARG:NH2	6:N:213:ALA:O	2.44	0.51
3:Bd:82:ARG:HA	3:Bd:127:SER:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CC:258:ASN:OD1	2:CC:258:ASN:N	2.43	0.51
3:ED:43:GLU:HG3	6:R:172:VAL:HG21	1.92	0.51
5:HK:46:ASP:OD1	5:HK:46:ASP:N	2.43	0.51
2:LC:196:GLU:OE1	4:MH:304:ARG:NH1	2.44	0.51
4:MH:316:THR:OG1	4:MH:317:ASN:N	2.43	0.51
6:X:101:SER:OG	6:X:102:LYS:N	2.43	0.51
4:FH:309:ASN:OD1	4:FH:309:ASN:N	2.44	0.51
4:GH:316:THR:OG1	4:GH:317:ASN:N	2.43	0.51
2:LC:176:TRP:O	2:LC:180:THR:HB	2.11	0.51
2:LC:256:ASN:ND2	2:LC:258:ASN:O	2.44	0.51
4:LH:281:LEU:HA	4:LH:284:VAL:HG22	1.93	0.51
4:LH:305:ALA:HA	4:LH:313:TYR:O	2.11	0.51
3:CD:48:VAL:HG23	3:Cd:52:MET:HG2	1.93	0.51
5:CK:66:LYS:NZ	6:O:118:GLU:O	2.44	0.51
3:Dd:98:ILE:HG23	3:Dd:128:LEU:HD22	1.92	0.51
5:EK:114:ILE:O	5:EK:154:ILE:HA	2.10	0.51
1:KX:170:UNK:HA	1:KX:188:UNK:O	2.11	0.51
5:LK:150:ASP:OD2	5:LK:150:ASP:N	2.44	0.51
1:LX:47:UNK:O	1:LX:66:UNK:HA	2.11	0.51
2:MC:93:ILE:HA	3:MD:48:VAL:HG11	1.93	0.51
5:MK:142:GLU:OE1	6:Z:139:ARG:NH1	2.44	0.51
6:N:155:LEU:HD11	6:N:193:LEU:HD22	1.92	0.51
1:BV:82:UNK:N	1:BV:117:UNK:O	2.45	0.50
2:AC:88:ARG:NH2	3:Ad:122:SER:OG	2.43	0.50
2:AC:122:ALA:HB1	2:BC:139:HIS:HB2	1.92	0.50
2:BC:264:ALA:O	3:CD:97:ARG:NH1	2.44	0.50
2:CC:111:LEU:O	2:CC:132:TYR:HA	2.11	0.50
4:CH:356:GLN:HG3	1:CZ:37:UNK:HA	1.93	0.50
2:HC:192:ASN:ND2	3:Hd:36:ASP:OD1	2.44	0.50
2:IC:214:LYS:HG3	3:Id:58:VAL:HG11	1.93	0.50
2:KC:102:GLU:HG2	2:KC:103:HIS:HD2	1.76	0.50
2:MC:192:ASN:ND2	3:Md:36:ASP:OD2	2.44	0.50
4:AH:276:SER:HA	2:MC:126:ARG:HG2	1.92	0.50
3:Cd:105:ARG:O	3:Cd:153:VAL:HA	2.11	0.50
5:EK:114:ILE:HB	5:EK:154:ILE:HG12	1.93	0.50
3:GD:43:GLU:OE2	6:T:227:ARG:NH1	2.44	0.50
3:Gd:40:LYS:HA	3:Gd:43:GLU:HG2	1.93	0.50
3:Jd:87:TRP:O	3:Jd:120:SER:HA	2.11	0.50
3:Ld:103:HIS:O	3:Ld:152:GLN:NE2	2.44	0.50
6:W:165:VAL:HG23	6:W:231:ILE:HG12	1.94	0.50
6:Y:108:ASP:OD1	6:Y:150:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BK:46:ASP:N	5:BK:46:ASP:OD1	2.45	0.50
3:DD:79:LEU:HB3	3:DD:129:ALA:HB2	1.92	0.50
5:DK:114:ILE:HG23	5:DK:184:PHE:HB3	1.93	0.50
3:KD:79:LEU:HB3	3:KD:129:ALA:HB2	1.94	0.50
3:Kd:147:VAL:HG22	3:Kd:154:VAL:HG22	1.92	0.50
4:LH:309:ASN:N	4:LH:309:ASN:OD1	2.45	0.50
6:X:166:ALA:HA	6:X:206:GLU:O	2.11	0.50
1:IV:81:UNK:HA	1:IV:118:UNK:HA	1.94	0.50
5:CK:185:ARG:NH2	6:O:213:ALA:O	2.45	0.50
3:Cd:84:SER:HB2	3:Cd:125:ASP:H	1.75	0.50
4:IH:309:ASN:OD1	4:IH:309:ASN:N	2.44	0.50
3:KD:132:LEU:HD23	3:KD:135:ILE:HD11	1.92	0.50
3:AD:58:VAL:HG21	3:Ad:60:LYS:HA	1.93	0.50
2:CC:75:ARG:NH1	3:Cd:36:ASP:OD2	2.44	0.50
4:CH:325:TRP:HA	4:CH:340:MET:HB3	1.93	0.50
5:GK:87:GLN:NE2	5:GK:173:ASP:OD1	2.44	0.50
3:Gd:147:VAL:HG22	3:Gd:154:VAL:HG22	1.93	0.50
4:HH:309:ASN:N	4:HH:309:ASN:OD1	2.44	0.50
3:Hd:74:PRO:HG2	3:Hd:149:PRO:HG3	1.93	0.50
1:JX:65:UNK:HA	1:JX:82:UNK:O	2.12	0.50
4:MH:309:ASN:OD1	4:MH:309:ASN:N	2.44	0.50
5:MK:113:ALA:HA	5:MK:153:ILE:O	2.12	0.50
3:Md:40:LYS:HA	3:Md:43:GLU:HG3	1.94	0.50
6:V:165:VAL:HG22	6:V:231:ILE:HG12	1.93	0.50
4:BH:317:ASN:OD1	4:BH:317:ASN:N	2.44	0.50
3:Bd:126:GLU:HG2	3:Bd:131:ILE:HG13	1.94	0.50
2:CC:84:ASN:OD1	2:CC:148:ARG:NH1	2.44	0.50
4:CH:284:VAL:HG23	4:CH:337:ALA:HB1	1.94	0.50
3:Cd:120:SER:O	3:Cd:138:GLN:NE2	2.45	0.50
4:DH:309:ASN:OD1	4:DH:309:ASN:N	2.44	0.50
3:ED:36:ASP:HB3	3:Ed:31:ASN:HD22	1.75	0.50
2:FC:267:ALA:HB3	3:GD:84:SER:HB3	1.93	0.50
2:JC:93:ILE:HA	3:JD:48:VAL:HG11	1.93	0.50
2:KC:75:ARG:NH1	3:Kd:36:ASP:OD1	2.44	0.50
2:LC:93:ILE:HA	3:LD:48:VAL:HG11	1.93	0.50
5:LK:46:ASP:OD1	5:LK:46:ASP:N	2.45	0.50
6:R:121:ASP:O	6:R:123:ARG:NH1	2.45	0.50
6:X:126:ILE:HA	6:X:229:ILE:O	2.11	0.50
3:Ad:78:ASN:ND2	3:Ad:102:ALA:O	2.44	0.50
3:Ad:82:ARG:HA	3:Ad:127:SER:HA	1.93	0.50
2:FC:215:LEU:HB3	2:FC:220:MET:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HC:234:THR:OG1	2:HC:235:GLY:N	2.45	0.50
4:HH:314:VAL:HG22	4:HH:338:TYR:HB2	1.94	0.50
4:BH:314:VAL:HG23	4:BH:338:TYR:HB2	1.94	0.50
5:BK:44:ARG:HE	5:BK:45:VAL:HG13	1.77	0.50
5:BK:150:ASP:O	5:BK:152:ARG:NH2	2.44	0.50
5:EK:185:ARG:NH2	6:Q:213:ALA:O	2.41	0.50
3:FD:36:ASP:OD1	3:FD:36:ASP:N	2.45	0.50
2:GC:256:ASN:ND2	2:GC:258:ASN:O	2.45	0.50
3:Gd:78:ASN:ND2	3:Gd:102:ALA:O	2.45	0.50
2:HC:133:LYS:NZ	2:HC:134:VAL:O	2.45	0.50
5:JK:111:LYS:NZ	5:JK:150:ASP:OD2	2.44	0.50
5:JK:185:ARG:NH2	6:V:213:ALA:O	2.45	0.50
4:AH:317:ASN:N	4:AH:317:ASN:OD1	2.43	0.50
2:BC:130:ARG:O	2:CC:241:HIS:HA	2.12	0.50
3:Bd:155:GLU:OE1	3:Bd:157:ARG:NH2	2.44	0.50
3:CD:94:LEU:HD23	3:CD:135:ILE:HD12	1.94	0.50
5:DK:67:VAL:HG13	5:DK:76:ILE:HG22	1.94	0.50
3:Hd:132:LEU:HD22	3:Hd:145:ILE:HG21	1.93	0.50
3:Id:130:GLU:OE2	3:Id:107:ARG:NH2	2.45	0.50
5:IK:87:GLN:NE2	5:IK:173:ASP:OD1	2.45	0.50
5:IK:125:SER:O	5:IK:129:GLU:HB2	2.12	0.50
3:Id:130:GLU:OE1	3:Id:133:ARG:NH2	2.45	0.50
3:Ld:132:LEU:HD22	3:Ld:145:ILE:HG21	1.93	0.50
3:MD:120:SER:H	3:MD:138:GLN:HE22	1.60	0.50
5:AK:65:ILE:HD12	5:AK:78:ILE:HG23	1.94	0.49
2:DC:99:LEU:HG	3:DD:52:MET:HE1	1.93	0.49
2:FC:75:ARG:NH1	3:Fd:36:ASP:OD2	2.45	0.49
5:FK:111:LYS:NZ	5:FK:150:ASP:OD2	2.45	0.49
3:Jd:150:ASN:OD1	3:Jd:150:ASN:N	2.45	0.49
4:KH:319:THR:O	4:KH:348:VAL:HA	2.12	0.49
5:KK:46:ASP:OD1	5:KK:46:ASP:N	2.44	0.49
6:Q:215:SER:OG	6:Q:216:ASP:N	2.44	0.49
6:W:145:TYR:HA	6:W:148:LEU:HD12	1.92	0.49
6:Z:158:TYR:O	6:Z:202:ARG:NH2	2.45	0.49
1:BV:73:UNK:HA	1:BV:102:UNK:HA	1.94	0.49
2:BC:93:ILE:HA	3:BD:48:VAL:HG11	1.95	0.49
5:EK:156:THR:HG23	3:Ed:82:ARG:HB2	1.94	0.49
5:GK:114:ILE:O	5:GK:154:ILE:HA	2.13	0.49
5:HK:87:GLN:NE2	5:HK:173:ASP:OD1	2.46	0.49
2:JC:126:ARG:HD3	4:KH:276:SER:HA	1.94	0.49
5:LK:185:ARG:NH2	6:X:213:ALA:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MH:317:ASN:N	4:MH:317:ASN:OD1	2.45	0.49
3:BD:43:GLU:OE1	6:O:227:ARG:NH1	2.45	0.49
4:BH:308:SER:OG	4:BH:309:ASN:N	2.46	0.49
1:CX:45:UNK:O	1:CX:64:UNK:HA	2.13	0.49
3:Cd:151:SER:OG	3:Cd:152:GLN:N	2.45	0.49
3:Dd:103:HIS:O	3:Dd:152:GLN:NE2	2.45	0.49
4:GH:319:THR:O	4:GH:348:VAL:HA	2.13	0.49
4:HH:308:SER:OG	4:HH:309:ASN:N	2.46	0.49
2:IC:93:ILE:HA	3:ID:48:VAL:HG11	1.94	0.49
5:IK:46:ASP:N	5:IK:46:ASP:OD1	2.44	0.49
6:S:215:SER:OG	6:S:216:ASP:N	2.44	0.49
6:Y:124:THR:HB	6:Y:232:GLN:HG2	1.93	0.49
4:AH:316:THR:OG1	4:AH:317:ASN:N	2.44	0.49
4:CH:308:SER:OG	4:CH:309:ASN:N	2.45	0.49
5:CK:150:ASP:O	5:CK:152:ARG:NH2	2.45	0.49
3:HD:130:GLU:OE2	3:Hd:107:ARG:NH2	2.45	0.49
5:IK:76:ILE:HG13	5:IK:182:ILE:HB	1.94	0.49
5:IK:111:LYS:NZ	5:IK:150:ASP:OD1	2.45	0.49
1:IX:170:UNK:HA	1:IX:188:UNK:O	2.12	0.49
3:JD:155:GLU:OE2	3:JD:157:ARG:NH2	2.46	0.49
4:JH:308:SER:OG	4:JH:309:ASN:N	2.44	0.49
3:Ld:130:GLU:OE2	3:Ld:133:ARG:NH2	2.45	0.49
6:N:130:ASP:N	6:N:130:ASP:OD2	2.44	0.49
1:RV:50:UNK:HA	1:RV:138:UNK:O	2.12	0.49
1:AX:56:UNK:O	1:AX:73:UNK:N	2.46	0.49
4:BH:312:MET:HE1	4:BH:359:VAL:HG21	1.93	0.49
3:ED:95:THR:HG23	3:ED:135:ILE:HD13	1.93	0.49
3:Id:147:VAL:HG23	3:Id:154:VAL:HG22	1.95	0.49
6:Q:170:ASP:OD2	6:Q:227:ARG:NH1	2.45	0.49
6:S:226:ASN:O	6:S:228:ARG:NH1	2.45	0.49
6:V:226:ASN:O	6:V:228:ARG:NH1	2.45	0.49
1:CX:47:UNK:O	1:CX:66:UNK:HA	2.12	0.49
2:DC:255:LEU:HD13	2:EC:240:ILE:HG12	1.94	0.49
5:DK:76:ILE:HG12	5:DK:182:ILE:HB	1.93	0.49
3:Fd:27:LYS:NZ	5:GK:71:GLY:O	2.45	0.49
5:LK:111:LYS:NZ	5:LK:150:ASP:OD2	2.45	0.49
1:MV:81:UNK:HA	1:MV:118:UNK:HA	1.95	0.49
5:CK:119:TYR:OH	5:CK:179:ARG:NH1	2.45	0.49
4:EH:318:LEU:HD12	4:EH:350:TRP:HA	1.94	0.49
5:JK:46:ASP:OD1	5:JK:46:ASP:N	2.45	0.49
4:LH:316:THR:OG1	4:LH:317:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:226:ASN:O	6:U:228:ARG:NH1	2.45	0.49
3:Bd:132:LEU:HB3	3:Bd:145:ILE:HG21	1.94	0.49
5:DK:153:ILE:HG23	3:Dd:85:VAL:HG22	1.95	0.49
2:EC:118:ASN:HB2	4:FH:277:ALA:HA	1.93	0.49
3:FD:155:GLU:OE2	3:FD:157:ARG:NH2	2.46	0.49
3:KD:40:LYS:HE2	3:Kd:46:VAL:HG11	1.95	0.49
4:MH:281:LEU:HA	4:MH:284:VAL:HG22	1.93	0.49
5:MK:87:GLN:NE2	5:MK:173:ASP:OD1	2.45	0.49
1:BV:115:UNK:HA	1:BV:125:UNK:HA	1.94	0.49
3:DD:48:VAL:HG23	3:Dd:52:MET:HG2	1.94	0.49
4:DH:308:SER:OG	4:DH:309:ASN:N	2.46	0.49
5:EK:124:VAL:HB	5:EK:128:ARG:HG2	1.94	0.49
1:EX:47:UNK:O	1:EX:66:UNK:HA	2.12	0.49
5:GK:130:ARG:NH2	3:Gd:77:TYR:OH	2.46	0.49
5:JK:66:LYS:NZ	6:V:118:GLU:O	2.45	0.49
3:KD:58:VAL:HG21	3:Kd:60:LYS:HA	1.94	0.49
5:KK:66:LYS:HB3	5:KK:77:SER:HB3	1.94	0.49
6:U:170:ASP:OD1	6:U:170:ASP:N	2.45	0.49
2:AC:84:ASN:OD1	2:AC:148:ARG:NH1	2.46	0.49
5:BK:60:LEU:HD21	5:BK:102:ILE:HG22	1.94	0.49
3:Bd:78:ASN:ND2	3:Bd:102:ALA:O	2.45	0.49
5:CK:67:VAL:HG13	5:CK:76:ILE:HG23	1.95	0.49
3:Fd:78:ASN:ND2	3:Fd:102:ALA:O	2.46	0.49
2:GC:248:ARG:HH22	4:GH:273:ILE:HD13	1.78	0.49
2:HC:118:ASN:HB2	4:IH:277:ALA:HA	1.94	0.49
2:IC:228:HIS:HA	2:IC:246:VAL:O	2.13	0.49
4:IH:356:GLN:NE2	1:IZ:37:UNK:O	2.46	0.49
2:KC:107:PRO:HG2	2:KC:209:MET:HG2	1.95	0.49
5:LK:117:THR:HA	5:LK:157:GLN:O	2.13	0.49
2:MC:256:ASN:ND2	2:MC:258:ASN:O	2.46	0.49
2:BC:175:ILE:O	2:BC:179:TYR:HB2	2.13	0.48
2:DC:107:PRO:HG2	2:DC:209:MET:HG2	1.95	0.48
2:DC:226:VAL:HA	2:DC:248:ARG:O	2.13	0.48
3:ED:130:GLU:OE2	3:Ed:107:ARG:NH2	2.46	0.48
5:EK:120:SER:OG	5:EK:121:SER:N	2.45	0.48
5:GK:67:VAL:HG13	5:GK:76:ILE:HG22	1.95	0.48
1:JX:47:UNK:O	1:JX:66:UNK:HA	2.13	0.48
2:LC:126:ARG:NH1	2:MC:244:ASP:OD1	2.46	0.48
5:LK:151:SER:OG	5:LK:152:ARG:N	2.46	0.48
6:P:170:ASP:OD1	6:P:170:ASP:N	2.46	0.48
6:T:121:ASP:O	6:T:123:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:108:ASP:OD1	6:Z:150:ASN:ND2	2.46	0.48
1:BV:80:UNK:O	1:BV:119:UNK:N	2.46	0.48
1:CX:98:UNK:O	1:CX:117:UNK:HA	2.13	0.48
3:Gd:132:LEU:HD22	3:Gd:145:ILE:HG21	1.95	0.48
2:KC:258:ASN:N	2:KC:258:ASN:OD1	2.46	0.48
6:N:165:VAL:HG23	6:N:231:ILE:HG12	1.95	0.48
6:R:130:ASP:OD2	6:R:130:ASP:N	2.44	0.48
6:T:130:ASP:OD2	6:T:130:ASP:N	2.45	0.48
1:JV:82:UNK:N	1:JV:117:UNK:O	2.46	0.48
2:AC:84:ASN:ND2	1:AZ:37:UNK:O	2.45	0.48
2:AC:147:TRP:HD1	2:AC:151:LEU:HD12	1.78	0.48
4:DH:312:MET:HE1	4:DH:359:VAL:HG21	1.96	0.48
3:GD:150:ASN:OD1	3:GD:150:ASN:N	2.46	0.48
2:HC:106:LEU:HB2	2:HC:141:ILE:HG12	1.96	0.48
3:Hd:130:GLU:HA	3:Hd:133:ARG:HB2	1.94	0.48
4:KH:309:ASN:OD1	4:KH:309:ASN:N	2.46	0.48
3:Kd:130:GLU:OE1	3:Kd:133:ARG:NH2	2.46	0.48
3:MD:58:VAL:HG21	3:Md:60:LYS:HA	1.93	0.48
3:BD:97:ARG:HA	3:BD:100:LYS:HG2	1.94	0.48
2:CC:116:THR:O	2:CC:127:ILE:HA	2.13	0.48
2:CC:126:ARG:HD3	2:DC:246:VAL:HB	1.95	0.48
5:CK:87:GLN:NE2	5:CK:173:ASP:OD1	2.46	0.48
3:DD:130:GLU:OE2	3:Dd:107:ARG:NH2	2.46	0.48
3:Gd:107:ARG:O	3:Gd:155:GLU:HA	2.14	0.48
5:HK:66:LYS:NZ	6:T:118:GLU:O	2.44	0.48
3:ID:36:ASP:OD1	3:ID:36:ASP:N	2.46	0.48
4:JH:298:VAL:HG22	4:JH:359:VAL:HG12	1.94	0.48
3:Jd:72:THR:OG1	3:Jd:146:HIS:ND1	2.45	0.48
2:MC:149:GLN:NE2	4:MH:322:SER:O	2.46	0.48
4:MH:276:SER:OG	4:MH:277:ALA:N	2.46	0.48
3:Md:24:LYS:O	6:Z:110:GLN:NE2	2.47	0.48
6:Z:170:ASP:OD1	6:Z:170:ASP:N	2.43	0.48
1:NV:81:UNK:HA	1:NV:118:UNK:HA	1.93	0.48
1:PV:54:UNK:HA	1:PV:142:UNK:O	2.14	0.48
3:CD:43:GLU:OE1	6:P:227:ARG:NH1	2.46	0.48
3:Cd:78:ASN:ND2	3:Cd:102:ALA:O	2.47	0.48
3:Cd:130:GLU:OE2	3:Cd:133:ARG:NH2	2.45	0.48
4:JH:317:ASN:N	4:JH:317:ASN:OD1	2.44	0.48
5:JK:87:GLN:NE2	5:JK:173:ASP:OD1	2.46	0.48
3:KD:130:GLU:OE2	3:Kd:105:ARG:NH1	2.47	0.48
1:KX:47:UNK:O	1:KX:66:UNK:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MX:56:UNK:O	1:MX:73:UNK:N	2.46	0.48
2:FC:126:ARG:NH1	2:GC:244:ASP:OD1	2.46	0.48
2:IC:130:ARG:NH2	2:IC:132:TYR:OH	2.44	0.48
3:Jd:34:SER:OG	3:Jd:35:ASP:N	2.47	0.48
2:LC:122:ALA:HB1	2:MC:139:HIS:HB2	1.95	0.48
3:LD:102:ALA:HB2	3:LD:128:LEU:HD11	1.95	0.48
3:LD:130:GLU:OE1	3:Ld:107:ARG:NH2	2.47	0.48
5:LK:109:PHE:O	5:LK:111:LYS:NZ	2.46	0.48
6:W:134:MET:HE2	6:W:141:ASN:HA	1.95	0.48
1:KV:51:UNK:O	1:KV:139:UNK:HA	2.13	0.48
2:AC:258:ASN:OD1	2:AC:258:ASN:N	2.47	0.48
4:BH:325:TRP:HA	4:BH:340:MET:HB3	1.96	0.48
5:CK:114:ILE:O	5:CK:154:ILE:HA	2.13	0.48
3:Cd:126:GLU:HG2	3:Cd:131:ILE:HG13	1.96	0.48
3:Ed:26:LYS:O	6:R:115:GLN:NE2	2.46	0.48
3:Ed:130:GLU:OE1	3:Ed:133:ARG:NH2	2.47	0.48
1:IX:128:UNK:HA	1:IX:147:UNK:O	2.14	0.48
4:KH:308:SER:OG	4:KH:309:ASN:N	2.46	0.48
5:KK:84:PHE:HB2	5:KK:136:ARG:HH21	1.79	0.48
6:U:155:LEU:HD11	6:U:193:LEU:HD22	1.96	0.48
5:DK:46:ASP:N	5:DK:46:ASP:OD1	2.46	0.48
2:FC:256:ASN:ND2	2:FC:258:ASN:O	2.47	0.48
4:FH:284:VAL:HG23	4:FH:337:ALA:HB1	1.94	0.48
5:FK:120:SER:HA	5:FK:178:ALA:HA	1.96	0.48
4:GH:304:ARG:O	4:GH:314:VAL:HA	2.13	0.48
3:Id:86:ASP:HA	3:Id:121:ILE:O	2.14	0.48
2:JC:130:ARG:NH2	2:JC:132:TYR:OH	2.47	0.48
5:KK:128:ARG:HH22	5:KK:132:LEU:HD13	1.78	0.48
5:LK:67:VAL:HB	5:LK:76:ILE:HG23	1.95	0.48
2:MC:109:VAL:HG22	2:MC:136:LYS:HB2	1.94	0.48
3:Md:147:VAL:HG22	3:Md:154:VAL:HG22	1.95	0.48
1:OV:115:UNK:HA	1:OV:125:UNK:HA	1.94	0.48
5:CK:111:LYS:NZ	5:CK:150:ASP:OD2	2.47	0.48
4:FH:281:LEU:O	4:FH:285:LEU:HB2	2.13	0.48
5:HK:185:ARG:NH2	6:T:213:ALA:O	2.46	0.48
1:HX:170:UNK:HA	1:HX:188:UNK:O	2.13	0.48
5:KK:67:VAL:HG13	5:KK:76:ILE:HG22	1.96	0.48
6:Y:130:ASP:OD2	6:Y:130:ASP:N	2.43	0.48
4:CH:281:LEU:O	4:CH:285:LEU:HB2	2.14	0.48
4:DH:316:THR:OG1	4:DH:317:ASN:N	2.46	0.48
1:DX:45:UNK:O	1:DX:64:UNK:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EH:285:LEU:O	4:EH:315:ARG:NH1	2.45	0.48
4:EH:308:SER:OG	4:EH:309:ASN:N	2.45	0.48
5:EK:116:VAL:O	5:EK:156:THR:HA	2.14	0.48
5:FK:166:THR:HG22	5:FK:168:TYR:H	1.78	0.48
5:LK:87:GLN:NE2	5:LK:173:ASP:OD1	2.47	0.48
6:R:134:MET:HE3	6:R:139:ARG:HB3	1.95	0.48
6:V:215:SER:OG	6:V:216:ASP:N	2.46	0.48
6:Z:121:ASP:O	6:Z:123:ARG:NH1	2.47	0.48
1:AV:54:UNK:HA	1:AV:142:UNK:O	2.13	0.47
1:AV:74:UNK:O	1:AV:100:UNK:HA	2.14	0.47
5:AK:57:MET:O	5:AK:61:ASN:ND2	2.47	0.47
5:AK:150:ASP:O	5:AK:152:ARG:NH2	2.47	0.47
3:Ad:109:LEU:HB2	3:Ad:157:ARG:HB3	1.96	0.47
1:BX:128:UNK:HA	1:BX:147:UNK:O	2.14	0.47
2:CC:93:ILE:HA	3:CD:48:VAL:HG11	1.96	0.47
4:DH:298:VAL:HG11	4:DH:303:ALA:HB3	1.96	0.47
2:EC:258:ASN:ND2	2:EC:261:GLU:OE2	2.47	0.47
3:ED:102:ALA:HB2	3:ED:128:LEU:HD11	1.96	0.47
5:FK:46:ASP:OD1	5:FK:46:ASP:N	2.47	0.47
5:FK:92:ASN:OD1	5:FK:92:ASN:N	2.46	0.47
5:KK:130:ARG:NH2	3:Kd:77:TYR:OH	2.47	0.47
2:LC:118:ASN:HB2	4:MH:277:ALA:HA	1.95	0.47
3:LD:58:VAL:HG21	3:Ld:60:LYS:HA	1.94	0.47
2:AC:137:GLN:HE22	2:AC:252:LEU:HB3	1.79	0.47
3:Ad:151:SER:OG	3:Ad:152:GLN:N	2.45	0.47
1:CX:56:UNK:O	1:CX:73:UNK:N	2.47	0.47
2:DC:141:ILE:HD12	2:DC:141:ILE:HA	1.86	0.47
4:DH:305:ALA:HA	4:DH:313:TYR:O	2.14	0.47
1:DX:56:UNK:O	1:DX:73:UNK:N	2.47	0.47
4:EH:309:ASN:N	4:EH:309:ASN:OD1	2.46	0.47
5:GK:113:ALA:HA	5:GK:153:ILE:O	2.14	0.47
3:ID:58:VAL:HG21	3:Id:60:LYS:HA	1.96	0.47
5:JK:179:ARG:HH21	5:JK:181:GLU:HG2	1.79	0.47
3:Kd:103:HIS:O	3:Kd:152:GLN:NE2	2.47	0.47
2:LC:258:ASN:OD1	2:LC:258:ASN:N	2.42	0.47
2:MC:88:ARG:HH21	3:Md:122:SER:HB2	1.80	0.47
2:AC:266:VAL:HG23	3:BD:85:VAL:HB	1.96	0.47
3:BD:98:ILE:HG13	3:BD:128:LEU:HD12	1.95	0.47
5:BK:130:ARG:NH2	3:Bd:77:TYR:OH	2.47	0.47
3:CD:36:ASP:N	3:CD:36:ASP:OD1	2.47	0.47
3:Cd:103:HIS:O	3:Cd:152:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DC:126:ARG:HD3	2:EC:246:VAL:HB	1.96	0.47
1:DX:47:UNK:O	1:DX:66:UNK:HA	2.14	0.47
3:ED:43:GLU:OE2	6:R:227:ARG:NH1	2.47	0.47
5:EK:111:LYS:NZ	5:EK:150:ASP:OD2	2.44	0.47
3:Ed:150:ASN:OD1	3:Ed:150:ASN:N	2.45	0.47
3:Gd:128:LEU:HA	3:Gd:131:ILE:HD12	1.96	0.47
3:JD:36:ASP:OD1	3:JD:36:ASP:N	2.44	0.47
3:JD:48:VAL:O	3:JD:52:MET:HB2	2.15	0.47
2:LC:114:ARG:NH2	3:MD:86:ASP:OD2	2.46	0.47
4:LH:356:GLN:HG3	1:LZ:37:UNK:HA	1.96	0.47
3:Md:109:LEU:O	3:Md:157:ARG:HA	2.13	0.47
1:BV:85:UNK:HA	1:BW:28:UNK:HA	1.96	0.47
5:HK:154:ILE:O	3:Hd:83:ALA:HA	2.15	0.47
1:HZ:8:UNK:HA	1:HZ:19:UNK:HA	1.96	0.47
4:LH:298:VAL:HG11	4:LH:303:ALA:HB3	1.97	0.47
1:MX:45:UNK:O	1:MX:64:UNK:HA	2.14	0.47
2:AC:111:LEU:O	2:AC:132:TYR:HA	2.14	0.47
4:AH:309:ASN:OD1	4:AH:309:ASN:N	2.46	0.47
4:BH:318:LEU:HD12	4:BH:350:TRP:HA	1.97	0.47
3:Bd:103:HIS:O	3:Bd:152:GLN:NE2	2.48	0.47
2:CC:116:THR:HA	4:DH:328:SER:O	2.14	0.47
5:EK:46:ASP:OD1	5:EK:46:ASP:N	2.47	0.47
4:HH:326:LEU:HD11	4:HH:341:GLN:HG2	1.97	0.47
2:JC:197:GLU:OE2	4:KH:295:ARG:NE	2.47	0.47
4:JH:309:ASN:N	4:JH:309:ASN:OD1	2.47	0.47
3:Ld:38:THR:HA	3:Ld:41:LEU:HB2	1.96	0.47
3:Md:105:ARG:O	3:Md:153:VAL:HA	2.15	0.47
6:N:121:ASP:O	6:N:123:ARG:NH1	2.48	0.47
6:Q:130:ASP:OD2	6:Q:130:ASP:N	2.47	0.47
6:Y:190:MET:HE3	6:Y:190:MET:HB3	1.84	0.47
2:AC:263:ARG:NH1	3:BD:93:GLU:OE2	2.48	0.47
2:CC:119:LEU:HA	2:CC:125:ILE:HG22	1.97	0.47
2:DC:93:ILE:HA	3:DD:48:VAL:HG11	1.96	0.47
5:HK:130:ARG:NH2	3:Hd:77:TYR:OH	2.47	0.47
5:KK:179:ARG:NH2	6:W:119:TYR:OH	2.47	0.47
1:KZ:48:UNK:O	1:KZ:61:UNK:N	2.48	0.47
3:Ld:150:ASN:N	3:Ld:150:ASN:OD1	2.47	0.47
1:FV:113:UNK:HA	1:FV:127:UNK:HA	1.96	0.47
1:LV:72:UNK:O	1:LV:102:UNK:HA	2.15	0.47
2:AC:196:GLU:OE1	3:Ad:40:LYS:NZ	2.45	0.47
4:AH:281:LEU:HA	4:AH:284:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CH:309:ASN:N	4:CH:309:ASN:OD1	2.47	0.47
3:CD:26:LYS:NZ	6:P:110:GLN:O	2.47	0.47
3:CD:36:ASP:HA	3:CD:39:ILE:HB	1.95	0.47
3:DD:71:LEU:O	3:DD:133:ARG:NE	2.47	0.47
4:DH:325:TRP:HA	4:DH:340:MET:HB3	1.96	0.47
5:DK:116:VAL:HG22	5:DK:182:ILE:HG12	1.97	0.47
2:FC:121:ASP:OD1	2:FC:121:ASP:N	2.48	0.47
2:HC:175:ILE:HA	2:HC:178:ILE:HG22	1.97	0.47
3:ID:143:ALA:HA	3:ID:157:ARG:O	2.15	0.47
3:MD:34:SER:OG	3:MD:32:ASN:ND2	2.48	0.47
5:MK:149:VAL:HG21	5:MK:154:ILE:HD11	1.95	0.47
6:N:108:ASP:OD2	6:N:150:ASN:ND2	2.48	0.47
1:HV:64:UNK:HA	1:HV:127:UNK:O	2.15	0.47
2:AC:118:ASN:HB2	4:BH:277:ALA:HA	1.97	0.47
5:AK:130:ARG:NH2	3:AD:77:TYR:OH	2.48	0.47
3:BD:94:LEU:O	3:BD:98:ILE:HB	2.15	0.47
1:BX:170:UNK:HA	1:BX:188:UNK:O	2.15	0.47
3:GD:27:LYS:NZ	5:HK:71:GLY:O	2.44	0.47
2:IC:126:ARG:HG2	4:JH:276:SER:HA	1.96	0.47
2:IC:137:GLN:NE2	2:IC:253:PRO:O	2.45	0.47
5:KK:75:LEU:HD12	5:KK:183:THR:HB	1.95	0.47
6:Z:101:SER:OG	6:Z:102:LYS:N	2.45	0.47
3:AD:103:HIS:O	3:AD:152:GLN:NE2	2.48	0.47
3:AD:123:THR:OG1	3:AD:124:LYS:N	2.47	0.47
3:DD:74:PRO:HG2	3:DD:149:PRO:HG3	1.97	0.47
4:GH:318:LEU:HD12	4:GH:350:TRP:HA	1.96	0.47
3:HD:36:ASP:HB3	3:HD:31:ASN:HD22	1.80	0.47
3:ID:107:ARG:O	3:ID:155:GLU:HA	2.15	0.47
2:MC:99:LEU:HG	3:MD:52:MET:HE1	1.97	0.47
5:MK:92:ASN:OD1	5:MK:92:ASN:N	2.48	0.47
6:X:165:VAL:HG22	6:X:231:ILE:HG12	1.96	0.47
1:PV:74:UNK:O	1:PV:100:UNK:HA	2.14	0.47
4:BH:316:THR:HG22	4:BH:318:LEU:H	1.78	0.47
4:BH:321:LEU:HB2	4:BH:347:LEU:HD23	1.96	0.47
4:CH:321:LEU:HB2	4:CH:347:LEU:HD23	1.97	0.47
2:DC:256:ASN:ND2	2:DC:258:ASN:O	2.48	0.47
5:DK:130:ARG:NH2	3:DD:77:TYR:OH	2.48	0.47
2:FC:199:ILE:O	2:FC:203:LYS:HB2	2.15	0.47
2:JC:125:ILE:HD11	2:KC:247:LEU:HD22	1.97	0.47
2:JC:137:GLN:NE2	2:JC:253:PRO:O	2.48	0.47
3:KD:147:VAL:HG22	3:KD:154:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ld:74:PRO:HG2	3:Ld:149:PRO:HG3	1.97	0.47
4:MH:308:SER:OG	4:MH:309:ASN:N	2.47	0.47
6:O:130:ASP:OD1	6:O:130:ASP:N	2.40	0.47
3:AD:36:ASP:OD1	3:AD:36:ASP:N	2.43	0.46
4:AH:308:SER:OG	4:AH:309:ASN:N	2.49	0.46
5:BK:114:ILE:HG23	5:BK:184:PHE:HB3	1.96	0.46
3:DD:36:ASP:OD1	3:DD:36:ASP:N	2.48	0.46
4:KH:304:ARG:O	4:KH:314:VAL:HA	2.16	0.46
5:MK:66:LYS:HB3	5:MK:77:SER:HB3	1.97	0.46
3:Md:74:PRO:HG2	3:Md:149:PRO:HG3	1.97	0.46
6:W:170:ASP:OD1	6:W:170:ASP:N	2.46	0.46
6:W:170:ASP:OD2	6:W:227:ARG:NH1	2.47	0.46
6:X:226:ASN:O	6:X:228:ARG:NH1	2.48	0.46
3:AD:56:ALA:O	3:AD:60:LYS:HB2	2.15	0.46
3:Ad:39:ILE:HG23	6:N:220:ILE:HG13	1.96	0.46
2:BC:108:PRO:HD3	2:BC:138:ALA:HB2	1.96	0.46
3:ED:150:ASN:OD1	3:ED:150:ASN:N	2.47	0.46
2:FC:137:GLN:NE2	2:FC:253:PRO:O	2.46	0.46
3:Gd:130:GLU:OE2	3:Gd:133:ARG:NH2	2.47	0.46
4:HH:312:MET:HG2	4:HH:342:LYS:HA	1.96	0.46
2:IC:102:GLU:HG2	2:IC:103:HIS:HD2	1.81	0.46
2:IC:108:PRO:HD3	2:IC:138:ALA:HB2	1.97	0.46
4:IH:281:LEU:O	4:IH:285:LEU:HB2	2.16	0.46
6:N:226:ASN:O	6:N:228:ARG:NH1	2.47	0.46
1:CZ:48:UNK:O	1:CZ:61:UNK:N	2.49	0.46
2:EC:266:VAL:HG21	3:FD:101:ALA:HB2	1.96	0.46
2:HC:75:ARG:NH1	3:Hd:36:ASP:OD2	2.47	0.46
3:ID:71:LEU:O	3:ID:133:ARG:NE	2.47	0.46
6:Q:158:TYR:O	6:Q:202:ARG:NH2	2.48	0.46
1:MV:91:UNK:HA	1:MV:105:UNK:HA	1.98	0.46
3:CD:95:THR:HG23	3:CD:135:ILE:HD13	1.98	0.46
2:DC:116:THR:O	2:DC:127:ILE:HA	2.16	0.46
4:DH:333:ASP:OD1	4:DH:333:ASP:N	2.44	0.46
1:DX:71:UNK:HA	1:DX:87:UNK:HA	1.97	0.46
3:ED:43:GLU:HA	3:ED:46:VAL:HG12	1.98	0.46
2:GC:88:ARG:NE	3:Gd:86:ASP:OD1	2.48	0.46
2:HC:228:HIS:HB3	2:HC:247:LEU:HG	1.98	0.46
3:HD:56:ALA:O	3:HD:60:LYS:HB2	2.15	0.46
1:HX:56:UNK:O	1:HX:73:UNK:N	2.48	0.46
3:ID:98:ILE:HG12	3:ID:128:LEU:HD12	1.96	0.46
5:JK:113:ALA:HA	5:JK:153:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MH:325:TRP:HA	4:MH:340:MET:HB3	1.97	0.46
5:MK:150:ASP:O	5:MK:152:ARG:NH2	2.47	0.46
3:Md:146:HIS:HB2	3:Md:155:GLU:HG2	1.97	0.46
6:Q:170:ASP:N	6:Q:170:ASP:OD1	2.48	0.46
6:S:152:ILE:HG12	6:S:196:ASN:HB3	1.97	0.46
6:T:118:GLU:OE2	6:T:123:ARG:NE	2.49	0.46
6:X:215:SER:OG	6:X:216:ASP:N	2.47	0.46
2:AC:106:LEU:HB2	2:AC:141:ILE:HG12	1.97	0.46
3:Ed:151:SER:OG	3:Ed:152:GLN:N	2.47	0.46
2:GC:266:VAL:HG23	3:HD:85:VAL:HB	1.96	0.46
4:HH:323:PRO:HG2	4:HH:346:LEU:HD23	1.98	0.46
1:HX:97:UNK:C	1:HX:116:UNK:O	2.64	0.46
2:JC:108:PRO:HD3	2:JC:138:ALA:HB2	1.97	0.46
3:JD:68:ASP:OD2	3:JD:68:ASP:N	2.48	0.46
2:KC:99:LEU:HG	3:KD:52:MET:HE1	1.98	0.46
2:KC:151:LEU:HD21	2:KC:199:ILE:HG13	1.98	0.46
3:KD:109:LEU:O	3:KD:157:ARG:HA	2.14	0.46
6:P:130:ASP:N	6:P:130:ASP:OD2	2.48	0.46
6:T:125:LEU:HD11	6:T:154:LEU:HD23	1.96	0.46
1:NV:82:UNK:N	1:NV:117:UNK:O	2.48	0.46
3:AD:71:LEU:O	3:AD:133:ARG:NE	2.45	0.46
2:BC:137:GLN:NE2	2:BC:253:PRO:O	2.48	0.46
3:CD:40:LYS:HE2	3:Cd:46:VAL:HG11	1.97	0.46
3:Cd:146:HIS:HB2	3:Cd:155:GLU:HG2	1.98	0.46
5:DK:185:ARG:NH2	6:P:213:ALA:O	2.43	0.46
3:Ed:107:ARG:O	3:Ed:155:GLU:HA	2.15	0.46
3:FD:105:ARG:HB3	3:FD:153:VAL:HG23	1.97	0.46
2:GC:263:ARG:HE	3:Gd:62:ILE:HD11	1.80	0.46
4:GH:307:LEU:HD11	4:GH:342:LYS:HD2	1.97	0.46
2:HC:264:ALA:O	3:ID:97:ARG:NE	2.48	0.46
3:Hd:127:SER:OG	3:Hd:128:LEU:N	2.47	0.46
2:JC:121:ASP:OD1	2:JC:121:ASP:N	2.48	0.46
1:JX:71:UNK:HA	1:JX:87:UNK:HA	1.96	0.46
5:KK:86:ASP:OD1	5:KK:86:ASP:N	2.42	0.46
6:Y:124:THR:HA	6:Y:231:ILE:O	2.15	0.46
1:DV:73:UNK:HA	1:DV:102:UNK:HA	1.98	0.46
2:AC:213:ARG:NH2	3:AD:59:GLU:OE2	2.46	0.46
4:AH:326:LEU:N	4:AH:339:GLU:O	2.47	0.46
5:AK:186:ARG:NH1	1:AZ:23:UNK:O	2.49	0.46
2:BC:196:GLU:OE1	3:Bd:40:LYS:NZ	2.45	0.46
3:Bd:130:GLU:HA	3:Bd:133:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:GK:173:ASP:OD1	5:GK:173:ASP:N	2.48	0.46
3:Hd:147:VAL:HG22	3:Hd:154:VAL:HG22	1.98	0.46
3:JD:130:GLU:OE2	3:Jd:107:ARG:NH2	2.48	0.46
1:FV:75:UNK:O	1:FV:141:UNK:N	2.49	0.46
1:KV:50:UNK:HA	1:KV:138:UNK:O	2.16	0.46
1:BX:56:UNK:O	1:BX:73:UNK:N	2.49	0.46
5:DK:57:MET:O	5:DK:61:ASN:ND2	2.48	0.46
5:DK:87:GLN:NE2	5:DK:173:ASP:OD1	2.49	0.46
3:Dd:34:SER:OG	3:Dd:35:ASP:N	2.48	0.46
3:Dd:128:LEU:HD23	3:Dd:131:ILE:HD11	1.98	0.46
2:FC:93:ILE:HA	3:FD:48:VAL:HG11	1.97	0.46
5:GK:185:ARG:NH2	6:S:213:ALA:O	2.49	0.46
4:JH:312:MET:HE1	4:JH:359:VAL:HG21	1.98	0.46
3:KD:34:SER:OG	3:Kd:32:ASN:ND2	2.49	0.46
5:KK:150:ASP:O	5:KK:152:ARG:NH2	2.49	0.46
3:MD:119:ILE:HG21	3:MD:135:ILE:HG22	1.98	0.46
1:BX:76:UNK:HA	1:BX:94:UNK:O	2.16	0.46
2:EC:137:GLN:NE2	2:EC:253:PRO:O	2.44	0.46
5:EK:120:SER:HA	5:EK:178:ALA:HA	1.97	0.46
1:EX:71:UNK:HA	1:EX:87:UNK:HA	1.98	0.46
1:FX:65:UNK:HA	1:FX:82:UNK:O	2.16	0.46
2:GC:84:ASN:ND2	1:GZ:37:UNK:O	2.48	0.46
2:HC:93:ILE:HA	3:HD:48:VAL:HG11	1.98	0.46
2:IC:126:ARG:HD3	2:JC:246:VAL:HB	1.97	0.46
4:IH:318:LEU:HD12	4:IH:350:TRP:HA	1.97	0.46
5:JK:120:SER:HA	5:JK:178:ALA:HA	1.97	0.46
1:LX:170:UNK:HA	1:LX:188:UNK:O	2.15	0.46
4:MH:331:SER:OG	4:MH:333:ASP:OD1	2.34	0.46
6:X:152:ILE:HG12	6:X:196:ASN:HB3	1.98	0.46
1:AX:71:UNK:HA	1:AX:87:UNK:HA	1.96	0.46
1:FX:45:UNK:O	1:FX:64:UNK:HA	2.15	0.46
3:HD:137:TYR:O	3:Hd:160:LYS:NZ	2.46	0.46
4:IH:305:ALA:HA	4:IH:313:TYR:O	2.16	0.46
1:IX:71:UNK:HA	1:IX:87:UNK:HA	1.98	0.46
5:KK:151:SER:OG	5:KK:152:ARG:N	2.47	0.46
4:MH:312:MET:HG2	4:MH:342:LYS:HA	1.97	0.46
3:Md:136:ASP:HB2	3:Md:145:ILE:HB	1.97	0.46
6:Q:145:TYR:HA	6:Q:148:LEU:HD12	1.97	0.46
6:T:190:MET:HB3	6:T:190:MET:HE3	1.82	0.46
1:HV:81:UNK:HA	1:HV:118:UNK:HA	1.98	0.45
1:JV:81:UNK:HA	1:JV:118:UNK:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ad:26:LYS:NZ	6:N:110:GLN:O	2.48	0.45
2:BC:126:ARG:HG3	2:CC:246:VAL:HB	1.98	0.45
2:CC:108:PRO:HD3	2:CC:138:ALA:HB2	1.98	0.45
2:GC:121:ASP:N	2:GC:121:ASP:OD1	2.49	0.45
2:KC:88:ARG:NH2	3:Kd:122:SER:OG	2.43	0.45
4:LH:308:SER:OG	4:LH:309:ASN:N	2.49	0.45
3:Md:36:ASP:OD1	3:Md:36:ASP:N	2.44	0.45
6:N:170:ASP:N	6:N:170:ASP:OD1	2.49	0.45
6:N:170:ASP:OD2	6:N:227:ARG:NH1	2.48	0.45
6:O:155:LEU:HD11	6:O:193:LEU:HD22	1.97	0.45
4:CH:331:SER:OG	4:CH:333:ASP:OD2	2.35	0.45
1:CX:170:UNK:HA	1:CX:188:UNK:O	2.16	0.45
4:IH:308:SER:OG	4:IH:309:ASN:N	2.48	0.45
3:Id:84:SER:HB2	3:Id:125:ASP:H	1.80	0.45
3:JD:29:PRO:HG3	5:JK:146:SER:HB2	1.97	0.45
3:KD:60:LYS:NZ	3:Kd:143:ALA:O	2.49	0.45
3:Kd:40:LYS:HA	3:Kd:43:GLU:HG2	1.97	0.45
5:LK:120:SER:HA	5:LK:178:ALA:HA	1.98	0.45
6:Y:126:ILE:HA	6:Y:229:ILE:O	2.16	0.45
1:LV:81:UNK:HA	1:LV:118:UNK:HA	1.98	0.45
1:PV:85:UNK:HA	1:PW:27:UNK:O	2.16	0.45
3:BD:150:ASN:OD1	3:BD:150:ASN:N	2.47	0.45
4:BH:309:ASN:N	4:BH:309:ASN:OD1	2.48	0.45
3:CD:58:VAL:HG21	3:Cd:60:LYS:HA	1.99	0.45
4:CH:322:SER:HB3	4:CH:347:LEU:HB3	1.98	0.45
3:Cd:87:TRP:O	3:Cd:120:SER:HA	2.15	0.45
5:EK:60:LEU:HD21	5:EK:102:ILE:HG22	1.97	0.45
5:EK:130:ARG:NH2	3:Ed:77:TYR:OH	2.49	0.45
5:EK:150:ASP:O	5:EK:152:ARG:NH2	2.48	0.45
5:FK:114:ILE:HB	5:FK:154:ILE:HG12	1.98	0.45
5:GK:92:ASN:N	5:GK:92:ASN:OD1	2.49	0.45
4:HH:284:VAL:HG23	4:HH:337:ALA:HB1	1.98	0.45
3:ID:94:LEU:O	3:ID:98:ILE:HB	2.17	0.45
5:JK:138:ARG:O	5:JK:142:GLU:HB2	2.16	0.45
2:LC:215:LEU:HB3	2:LC:220:MET:HB2	1.98	0.45
6:R:171:ASN:OD1	6:R:171:ASN:N	2.49	0.45
6:U:141:ASN:HD22	6:U:144:CYS:HB2	1.81	0.45
1:BV:48:UNK:HA	1:BV:135:UNK:O	2.16	0.45
2:AC:137:GLN:NE2	2:AC:253:PRO:O	2.49	0.45
3:Ad:120:SER:O	3:Ad:138:GLN:NE2	2.50	0.45
2:BC:175:ILE:H	2:BC:175:ILE:HG13	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:45:UNK:O	1:BX:64:UNK:HA	2.16	0.45
2:DC:215:LEU:HB3	2:DC:220:MET:HB2	1.99	0.45
2:EC:93:ILE:HA	3:ED:48:VAL:HG11	1.98	0.45
2:EC:147:TRP:HD1	2:EC:151:LEU:HD12	1.81	0.45
4:EH:326:LEU:HD11	4:EH:341:GLN:HE21	1.81	0.45
5:EK:57:MET:O	5:EK:61:ASN:ND2	2.46	0.45
5:GK:137:SER:O	5:GK:141:SER:OG	2.33	0.45
2:HC:121:ASP:OD1	2:HC:121:ASP:N	2.49	0.45
2:IC:99:LEU:HB3	3:ID:52:MET:HE1	1.97	0.45
5:IK:57:MET:O	5:IK:61:ASN:ND2	2.48	0.45
1:IX:56:UNK:O	1:IX:73:UNK:N	2.49	0.45
2:JC:118:ASN:HB2	4:KH:277:ALA:HA	1.98	0.45
3:LD:98:ILE:HB	3:LD:128:LEU:HD12	1.98	0.45
2:MC:75:ARG:HB2	2:MC:188:ILE:HG12	1.99	0.45
5:MK:186:ARG:NH1	1:MZ:23:UNK:O	2.44	0.45
6:R:152:ILE:HG12	6:R:196:ASN:HB3	1.97	0.45
3:Ad:38:THR:HA	3:Ad:41:LEU:HB2	1.98	0.45
3:Ad:147:VAL:HG22	3:Ad:154:VAL:HG22	1.99	0.45
1:BX:65:UNK:HA	1:BX:82:UNK:O	2.16	0.45
4:CH:317:ASN:OD1	4:CH:317:ASN:N	2.50	0.45
2:EC:196:GLU:OE1	3:Ed:40:LYS:NZ	2.49	0.45
4:FH:305:ALA:HA	4:FH:313:TYR:O	2.16	0.45
5:FK:150:ASP:OD2	5:FK:150:ASP:N	2.47	0.45
5:HK:156:THR:HG23	3:Hd:82:ARG:HB2	1.99	0.45
4:IH:312:MET:HE3	4:IH:343:SER:H	1.81	0.45
1:IX:58:UNK:O	1:IX:75:UNK:HA	2.16	0.45
3:KD:71:LEU:O	3:KD:133:ARG:NE	2.50	0.45
4:MH:284:VAL:HG23	4:MH:337:ALA:HB1	1.97	0.45
6:T:141:ASN:HD22	6:T:144:CYS:HB2	1.81	0.45
1:NV:91:UNK:HA	1:NV:104:UNK:O	2.15	0.45
5:BK:165:ILE:HG22	6:N:120:GLY:HA3	1.97	0.45
3:Bd:40:LYS:HE2	3:Bd:40:LYS:HB3	1.81	0.45
3:GD:102:ALA:HB2	3:GD:128:LEU:HD11	1.98	0.45
5:GK:44:ARG:HE	5:GK:45:VAL:HG13	1.82	0.45
3:ID:60:LYS:NZ	3:Id:143:ALA:O	2.50	0.45
5:IK:118:SER:HB2	5:IK:180:VAL:HG12	1.98	0.45
3:Id:66:SER:OG	3:Id:67:LYS:NZ	2.50	0.45
6:R:165:VAL:HG22	6:R:231:ILE:HG12	1.99	0.45
4:AH:312:MET:HE1	4:AH:359:VAL:HG21	1.98	0.45
5:CK:153:ILE:HG23	3:Cd:85:VAL:HB	1.98	0.45
5:CK:156:THR:HG23	3:Cd:82:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:HH:320:ILE:HD12	4:HH:346:LEU:HD22	1.99	0.45
4:HH:325:TRP:HA	4:HH:340:MET:HB3	1.99	0.45
5:HK:120:SER:HA	5:HK:178:ALA:HA	1.99	0.45
4:IH:298:VAL:HG11	4:IH:303:ALA:HB3	1.98	0.45
4:IH:319:THR:O	4:IH:348:VAL:HA	2.17	0.45
5:IK:156:THR:HG23	3:Id:82:ARG:HB2	1.99	0.45
3:JD:107:ARG:O	3:JD:155:GLU:HA	2.15	0.45
2:KC:199:ILE:HD13	3:Kd:40:LYS:HG3	1.98	0.45
2:LC:127:ILE:HD11	2:MC:245:ARG:HD3	1.99	0.45
6:Z:145:TYR:HA	6:Z:148:LEU:HD12	1.99	0.45
3:Ad:74:PRO:HG2	3:Ad:149:PRO:HG3	1.98	0.45
2:BC:197:GLU:OE2	4:CH:295:ARG:NE	2.50	0.45
3:Bd:151:SER:OG	3:Bd:152:GLN:N	2.49	0.45
2:CC:121:ASP:OD1	2:CC:121:ASP:N	2.49	0.45
4:CH:308:SER:OG	4:CH:309:ASN:OD1	2.35	0.45
4:FH:317:ASN:OD1	4:FH:317:ASN:N	2.50	0.45
4:GH:325:TRP:HA	4:GH:340:MET:HB3	1.97	0.45
3:KD:36:ASP:OD1	3:KD:36:ASP:N	2.45	0.45
2:LC:175:ILE:HA	2:LC:178:ILE:HG22	1.99	0.45
3:Ld:109:LEU:HD12	3:Ld:157:ARG:HG2	1.98	0.45
2:MC:175:ILE:H	2:MC:175:ILE:HG13	1.63	0.45
6:P:106:ILE:HA	6:P:109:LEU:HB2	1.98	0.45
2:BC:107:PRO:HG2	2:BC:209:MET:HG2	1.98	0.45
4:EH:312:MET:HG3	4:EH:340:MET:HG3	1.99	0.45
2:FC:72:LEU:HG	2:FC:191:ALA:HB2	1.98	0.45
2:GC:109:VAL:O	2:GC:134:VAL:HA	2.17	0.45
5:HK:57:MET:O	5:HK:61:ASN:ND2	2.50	0.45
5:HK:179:ARG:HH21	5:HK:181:GLU:HB3	1.80	0.45
4:IH:312:MET:HE1	4:IH:359:VAL:HG21	1.98	0.45
3:Jd:36:ASP:HA	3:Jd:39:ILE:HB	1.99	0.45
2:KC:146:THR:OG1	2:KC:147:TRP:N	2.49	0.45
1:KX:76:UNK:HA	1:KX:94:UNK:O	2.17	0.45
3:Md:130:GLU:OE2	3:Md:133:ARG:NH2	2.50	0.45
6:X:130:ASP:OD1	6:X:130:ASP:N	2.44	0.45
4:AH:318:LEU:HD12	4:AH:350:TRP:HA	1.98	0.45
4:BH:306:TRP:O	4:BH:312:MET:HA	2.17	0.45
5:DK:124:VAL:HB	5:DK:128:ARG:HG2	1.98	0.45
5:EK:87:GLN:NE2	5:EK:173:ASP:OD1	2.50	0.45
3:Ed:74:PRO:HG2	3:Ed:149:PRO:HG3	1.99	0.45
4:GH:286:GLU:HB2	4:GH:288:VAL:HG12	1.99	0.45
6:N:145:TYR:HA	6:N:148:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:198:ILE:HB	6:V:203:LEU:HD11	1.99	0.45
2:AC:79:ILE:HD13	2:AC:195:LEU:HD22	1.98	0.44
2:AC:197:GLU:OE2	4:BH:295:ARG:NE	2.49	0.44
2:BC:123:GLN:HA	2:CC:249:ILE:HD12	1.99	0.44
4:GH:284:VAL:HG21	4:GH:313:TYR:HB3	1.99	0.44
2:HC:197:GLU:OE2	4:IH:295:ARG:NE	2.47	0.44
3:Kd:87:TRP:O	3:Kd:120:SER:HA	2.17	0.44
2:MC:137:GLN:NE2	2:MC:253:PRO:O	2.46	0.44
6:T:170:ASP:OD1	6:T:170:ASP:N	2.48	0.44
1:BV:75:UNK:O	1:BV:141:UNK:N	2.50	0.44
2:AC:215:LEU:HB3	2:AC:220:MET:HB2	1.98	0.44
1:AX:101:UNK:HA	1:AX:120:UNK:O	2.18	0.44
1:AZ:8:UNK:HA	1:AZ:19:UNK:HA	1.99	0.44
2:BC:99:LEU:HG	3:BD:52:MET:HE1	1.98	0.44
3:BD:102:ALA:HB2	3:BD:128:LEU:HD11	1.98	0.44
3:Dd:40:LYS:HA	3:Dd:43:GLU:HG3	1.99	0.44
1:GX:45:UNK:O	1:GX:64:UNK:HA	2.17	0.44
3:Hd:150:ASN:OD1	3:Hd:150:ASN:N	2.46	0.44
2:JC:153:MET:HE2	2:JC:153:MET:HB3	1.86	0.44
5:JK:65:ILE:HD11	5:JK:98:LEU:HD21	1.99	0.44
3:MD:54:GLU:HA	3:MD:57:LYS:HB2	1.99	0.44
6:X:121:ASP:O	6:X:123:ARG:NH1	2.51	0.44
2:CC:130:ARG:HB2	2:DC:242:ILE:HD12	1.99	0.44
3:ED:88:SER:O	3:ED:88:SER:OG	2.34	0.44
4:EH:314:VAL:HG11	4:EH:346:LEU:HD11	1.99	0.44
5:EK:67:VAL:HG22	5:EK:76:ILE:HG22	1.99	0.44
1:EX:170:UNK:HA	1:EX:188:UNK:O	2.17	0.44
3:Gd:74:PRO:HG2	3:Gd:149:PRO:HG3	1.98	0.44
5:HK:92:ASN:OD1	5:HK:92:ASN:N	2.50	0.44
5:JK:66:LYS:HB3	5:JK:77:SER:HB3	2.00	0.44
3:Jd:40:LYS:HB3	3:Jd:40:LYS:HE2	1.78	0.44
3:LD:54:GLU:HA	3:LD:57:LYS:HB2	1.98	0.44
5:LK:50:ASP:HA	5:LK:53:ILE:HD12	1.98	0.44
5:MK:130:ARG:NH2	3:Md:77:TYR:OH	2.50	0.44
4:AH:274:PRO:O	2:MC:126:ARG:NH1	2.48	0.44
3:Ad:112:SER:O	2:MC:115:ASN:ND2	2.49	0.44
2:CC:137:GLN:NE2	2:CC:253:PRO:O	2.47	0.44
3:Dd:86:ASP:HA	3:Dd:121:ILE:O	2.17	0.44
3:ED:29:PRO:HB2	3:ED:32:ASN:HB2	2.00	0.44
2:GC:117:LEU:HD23	3:Hd:114:SER:HB2	1.99	0.44
3:GD:71:LEU:O	3:GD:133:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:KK:115:THR:HG23	5:KK:183:THR:HG23	1.99	0.44
6:R:219:ILE:HD12	6:R:219:ILE:HA	1.89	0.44
1:DV:85:UNK:HA	1:DW:27:UNK:O	2.17	0.44
1:AX:65:UNK:HA	1:AX:82:UNK:O	2.17	0.44
4:BH:308:SER:OG	4:BH:309:ASN:OD1	2.36	0.44
5:DK:134:LEU:HD11	3:Dd:82:ARG:HG3	1.99	0.44
4:GH:284:VAL:HG23	4:GH:337:ALA:HB1	1.97	0.44
4:HH:286:GLU:HB2	4:HH:288:VAL:HG12	1.99	0.44
2:IC:175:ILE:O	2:IC:179:TYR:HB2	2.17	0.44
3:Id:40:LYS:HB3	3:Id:40:LYS:HE2	1.79	0.44
3:Jd:120:SER:O	3:Jd:138:GLN:NE2	2.50	0.44
2:KC:110:LEU:HB2	2:KC:211:LEU:HB3	1.98	0.44
1:KX:97:UNK:C	1:KX:116:UNK:O	2.65	0.44
4:LH:347:LEU:HD11	4:LH:354:VAL:HB	2.00	0.44
3:CD:47:SER:O	3:CD:51:SER:OG	2.33	0.44
1:DZ:8:UNK:HA	1:DZ:19:UNK:HA	1.98	0.44
4:FH:312:MET:HG2	4:FH:342:LYS:HA	2.00	0.44
2:JC:126:ARG:HG3	2:KC:246:VAL:HB	2.00	0.44
4:KH:284:VAL:HG23	4:KH:337:ALA:HB1	2.00	0.44
1:MZ:8:UNK:HA	1:MZ:19:UNK:HA	1.99	0.44
6:Z:109:LEU:HD22	6:Z:114:ILE:HB	1.98	0.44
2:BC:157:LYS:HA	2:BC:157:LYS:HD2	1.88	0.44
3:BD:109:LEU:O	3:BD:157:ARG:HA	2.17	0.44
3:BD:130:GLU:OE2	3:Bd:107:ARG:NH2	2.50	0.44
5:DK:154:ILE:O	3:Dd:83:ALA:HA	2.18	0.44
4:EH:276:SER:OG	4:EH:277:ALA:N	2.49	0.44
2:FC:116:THR:HG21	2:FC:131:THR:HG23	1.99	0.44
2:HC:97:ASN:ND2	3:Hd:118:LEU:O	2.44	0.44
2:HC:116:THR:HA	4:IH:328:SER:O	2.17	0.44
4:HH:331:SER:OG	4:HH:333:ASP:OD2	2.36	0.44
5:JK:153:ILE:HG23	3:Jd:85:VAL:HG22	1.99	0.44
4:KH:312:MET:HE3	4:KH:342:LYS:HA	1.99	0.44
5:AK:154:ILE:O	3:Ad:83:ALA:HA	2.18	0.44
4:BH:352:GLY:O	3:Bd:88:SER:OG	2.36	0.44
3:CD:109:LEU:O	3:CD:157:ARG:HA	2.18	0.44
2:DC:137:GLN:NE2	2:DC:253:PRO:O	2.44	0.44
5:FK:154:ILE:O	3:Fd:83:ALA:HA	2.17	0.44
5:GK:153:ILE:HD12	3:Gd:85:VAL:HB	1.98	0.44
2:IC:121:ASP:N	2:IC:121:ASP:OD1	2.49	0.44
3:ID:132:LEU:HD12	3:ID:145:ILE:HG21	2.00	0.44
2:KC:126:ARG:HG3	2:LC:246:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MX:47:UNK:O	1:MX:66:UNK:HA	2.18	0.44
6:Q:121:ASP:O	6:Q:123:ARG:NH1	2.50	0.44
1:FV:115:UNK:HA	1:FV:125:UNK:HA	2.00	0.44
1:HV:85:UNK:HA	1:HW:27:UNK:O	2.18	0.44
1:IV:54:UNK:HA	1:IV:142:UNK:O	2.18	0.44
2:BC:173:LYS:HB2	2:BC:174:GLU:H	1.69	0.44
4:CH:307:LEU:HD11	4:CH:342:LYS:HD2	1.99	0.44
4:DH:344:PRO:HA	4:DH:359:VAL:HG22	1.99	0.44
2:GC:108:PRO:HD3	2:GC:138:ALA:HB2	2.00	0.44
4:IH:284:VAL:HG23	4:IH:337:ALA:HB1	1.99	0.44
3:JD:36:ASP:HB3	3:Jd:31:ASN:HD22	1.82	0.44
5:JK:92:ASN:OD1	5:JK:92:ASN:N	2.50	0.44
5:JK:116:VAL:HG22	5:JK:182:ILE:HG12	1.99	0.44
2:KC:84:ASN:ND2	1:KZ:37:UNK:O	2.51	0.44
1:LZ:48:UNK:O	1:LZ:61:UNK:N	2.50	0.44
2:MC:214:LYS:HG3	3:Md:58:VAL:HG11	2.00	0.44
6:N:190:MET:HB3	6:N:190:MET:HE3	1.85	0.44
6:V:112:GLN:HE21	6:V:112:GLN:HB2	1.62	0.44
6:W:152:ILE:HG12	6:W:196:ASN:HB3	2.00	0.44
6:X:170:ASP:OD1	6:X:170:ASP:N	2.51	0.44
3:DD:31:ASN:OD1	3:DD:31:ASN:N	2.45	0.43
2:EC:107:PRO:HG2	2:EC:209:MET:HG2	2.00	0.43
5:HK:120:SER:OG	5:HK:121:SER:N	2.50	0.43
5:HK:152:ARG:O	3:Hd:85:VAL:HA	2.18	0.43
3:Hd:87:TRP:O	3:Hd:120:SER:HA	2.17	0.43
2:IC:258:ASN:N	2:IC:258:ASN:OD1	2.49	0.43
3:Id:128:LEU:HD23	3:Id:131:ILE:HD11	1.99	0.43
2:KC:186:ASN:O	2:KC:190:GLN:HB2	2.18	0.43
2:KC:245:ARG:HH22	3:Kd:161:ILE:HG22	1.83	0.43
4:LH:284:VAL:HG23	4:LH:337:ALA:HB1	2.00	0.43
1:LX:45:UNK:O	1:LX:64:UNK:HA	2.18	0.43
6:R:118:GLU:OE2	6:R:123:ARG:NE	2.51	0.43
6:V:125:LEU:HD13	6:V:151:VAL:HG23	1.99	0.43
2:AC:204:GLU:HG3	4:BH:286:GLU:HG3	1.99	0.43
3:DD:94:LEU:O	3:DD:98:ILE:HB	2.18	0.43
3:ED:91:ILE:O	3:ED:95:THR:OG1	2.34	0.43
5:GK:99:LEU:HA	5:GK:102:ILE:HG12	2.00	0.43
5:HK:150:ASP:O	5:HK:152:ARG:NH2	2.51	0.43
4:JH:325:TRP:HA	4:JH:340:MET:HB3	2.00	0.43
3:Md:132:LEU:HD22	3:Md:145:ILE:HG21	1.99	0.43
1:OV:54:UNK:HA	1:OV:142:UNK:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:226:VAL:HA	2:AC:248:ARG:O	2.18	0.43
4:BH:328:SER:HA	4:BH:337:ALA:O	2.19	0.43
3:Bd:84:SER:HB2	3:Bd:124:LYS:HA	1.99	0.43
4:DH:279:ASP:OD2	4:DH:279:ASP:N	2.44	0.43
1:IX:157:UNK:HA	1:IX:176:UNK:O	2.19	0.43
3:Id:73:ILE:HA	3:Id:147:VAL:HG12	2.01	0.43
3:Jd:84:SER:HB2	3:Jd:125:ASP:H	1.83	0.43
2:KC:90:LEU:HA	2:KC:93:ILE:HG22	2.00	0.43
3:KD:70:THR:HG21	3:Kd:157:ARG:HH12	1.84	0.43
5:MK:109:PHE:O	5:MK:111:LYS:NZ	2.43	0.43
6:X:130:ASP:OD2	6:X:227:ARG:NE	2.51	0.43
6:X:145:TYR:HA	6:X:148:LEU:HD12	2.00	0.43
6:X:219:ILE:HD12	6:X:219:ILE:HA	1.88	0.43
3:Ad:40:LYS:HA	3:Ad:43:GLU:HG3	1.99	0.43
3:BD:70:THR:OG1	3:BD:71:LEU:N	2.52	0.43
3:Dd:40:LYS:HE2	3:Dd:40:LYS:HB3	1.91	0.43
3:Ed:70:THR:HA	3:Ed:133:ARG:HE	1.82	0.43
3:GD:68:ASP:OD2	3:GD:68:ASP:N	2.49	0.43
3:HD:137:TYR:OH	3:Hd:158:TYR:O	2.34	0.43
1:HX:71:UNK:HA	1:HX:87:UNK:HA	2.00	0.43
3:Id:148:TYR:HB2	3:Id:153:VAL:HG22	2.00	0.43
4:JH:279:ASP:OD1	4:JH:279:ASP:N	2.47	0.43
1:JX:56:UNK:O	1:JX:73:UNK:N	2.51	0.43
2:KC:192:ASN:ND2	3:Kd:36:ASP:OD2	2.52	0.43
3:KD:29:PRO:HG3	5:KK:146:SER:HB2	2.00	0.43
5:KK:120:SER:HA	5:KK:178:ALA:HA	1.99	0.43
3:Kd:84:SER:HB2	3:Kd:124:LYS:HA	2.01	0.43
2:LC:79:ILE:HD12	2:LC:195:LEU:HD13	2.00	0.43
1:LX:76:UNK:HA	1:LX:94:UNK:O	2.19	0.43
3:MD:68:ASP:OD2	3:MD:68:ASP:N	2.50	0.43
3:Md:134:ASP:HA	3:Md:137:TYR:HB2	2.00	0.43
1:AZ:48:UNK:O	1:AZ:61:UNK:N	2.51	0.43
3:Ad:50:ASP:HA	3:Ad:53:LEU:HB3	1.99	0.43
3:CD:71:LEU:O	3:CD:133:ARG:NE	2.51	0.43
5:CK:114:ILE:HB	5:CK:154:ILE:HG12	2.01	0.43
2:DC:197:GLU:OE2	4:EH:295:ARG:NE	2.49	0.43
3:DD:36:ASP:HA	3:DD:39:ILE:HD12	1.99	0.43
1:FZ:8:UNK:HA	1:FZ:19:UNK:HA	2.00	0.43
2:GC:97:ASN:HB2	2:GC:144:PRO:HG3	2.00	0.43
2:GC:106:LEU:HB2	2:GC:141:ILE:HG12	2.01	0.43
5:IK:114:ILE:O	5:IK:154:ILE:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Kd:146:HIS:HB2	3:Kd:155:GLU:HG2	2.00	0.43
2:MC:84:ASN:OD1	2:MC:148:ARG:NH1	2.51	0.43
2:MC:107:PRO:HG2	2:MC:209:MET:HG2	2.00	0.43
1:MZ:48:UNK:O	1:MZ:61:UNK:N	2.51	0.43
6:V:201:LYS:HA	6:V:201:LYS:HD3	1.92	0.43
1:IV:85:UNK:HA	1:IW:27:UNK:O	2.19	0.43
3:Ad:87:TRP:O	3:Ad:120:SER:HA	2.19	0.43
2:CC:122:ALA:HB1	2:DC:139:HIS:HB2	2.00	0.43
5:DK:122:LYS:HA	5:DK:122:LYS:HD2	1.91	0.43
2:JC:107:PRO:HG2	2:JC:209:MET:HG2	2.01	0.43
2:KC:118:ASN:HB2	4:LH:277:ALA:HA	2.01	0.43
2:LC:258:ASN:ND2	2:LC:261:GLU:OE2	2.52	0.43
4:LH:314:VAL:HG21	4:LH:346:LEU:HD11	1.99	0.43
5:MK:120:SER:HA	5:MK:178:ALA:HA	2.01	0.43
1:EV:71:UNK:HA	1:EV:103:UNK:O	2.18	0.43
5:AK:49:CYS:O	5:AK:52:THR:OG1	2.36	0.43
3:Ad:131:ILE:HD12	3:Ad:131:ILE:HA	1.84	0.43
4:BH:331:SER:OG	4:BH:333:ASP:OD2	2.36	0.43
3:Bd:37:ALA:O	3:Bd:41:LEU:HB2	2.19	0.43
3:Bd:147:VAL:HG22	3:Bd:154:VAL:HG22	2.01	0.43
2:EC:117:LEU:HB2	2:EC:127:ILE:HG22	2.00	0.43
3:ED:58:VAL:HG21	3:Ed:60:LYS:HA	1.99	0.43
4:EH:273:ILE:HD13	4:EH:273:ILE:HA	1.91	0.43
4:FH:308:SER:OG	4:FH:309:ASN:N	2.51	0.43
5:FK:65:ILE:HG13	5:FK:98:LEU:HD11	2.01	0.43
2:GC:147:TRP:HD1	2:GC:151:LEU:HD12	1.83	0.43
3:GD:39:ILE:O	3:GD:43:GLU:HB2	2.18	0.43
3:HD:29:PRO:HB2	3:HD:32:ASN:HB2	2.01	0.43
3:Hd:123:THR:OG1	3:Hd:124:LYS:N	2.50	0.43
2:JC:255:LEU:HD13	2:KC:240:ILE:HG12	1.99	0.43
2:KC:84:ASN:OD1	2:KC:148:ARG:NH1	2.51	0.43
2:KC:231:LEU:HB2	2:KC:244:ASP:O	2.18	0.43
2:LC:75:ARG:NH1	3:Ld:36:ASP:OD1	2.51	0.43
3:LD:36:ASP:OD1	3:LD:36:ASP:N	2.46	0.43
4:LH:327:ALA:HB3	4:LH:339:GLU:HB3	1.99	0.43
5:LK:179:ARG:HH21	5:LK:181:GLU:HB3	1.84	0.43
3:MD:62:ILE:HB	3:Md:67:LYS:HZ3	1.84	0.43
1:AX:97:UNK:C	1:AX:116:UNK:O	2.66	0.43
2:DC:75:ARG:HD3	2:DC:188:ILE:HG23	1.99	0.43
4:DH:343:SER:OG	4:DH:345:VAL:O	2.36	0.43
3:Dd:84:SER:HB2	3:Dd:125:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:ED:54:GLU:HA	3:ED:57:LYS:HB2	2.01	0.43
5:EK:94:ALA:O	5:EK:97:SER:OG	2.37	0.43
4:FH:307:LEU:HD11	4:FH:342:LYS:HD2	2.01	0.43
3:Gd:66:SER:OG	3:Gd:67:LYS:NZ	2.52	0.43
2:HC:146:THR:OG1	2:HC:147:TRP:N	2.51	0.43
3:HD:43:GLU:HA	3:HD:46:VAL:HG12	1.99	0.43
2:JC:175:ILE:O	2:JC:179:TYR:HB2	2.19	0.43
3:JD:60:LYS:NZ	3:Jd:143:ALA:O	2.52	0.43
6:R:158:TYR:O	6:R:202:ARG:NH2	2.51	0.43
6:W:219:ILE:HD12	6:W:219:ILE:HA	1.84	0.43
3:Bd:107:ARG:O	3:Bd:155:GLU:HA	2.19	0.43
2:CC:79:ILE:HD12	2:CC:195:LEU:HD22	2.01	0.43
5:DK:150:ASP:O	5:DK:152:ARG:NH2	2.52	0.43
1:DX:128:UNK:HA	1:DX:147:UNK:O	2.19	0.43
1:EX:56:UNK:O	1:EX:73:UNK:N	2.52	0.43
2:FC:108:PRO:HD3	2:FC:138:ALA:HB2	2.00	0.43
4:FH:298:VAL:HG11	4:FH:303:ALA:HB3	2.00	0.43
1:FX:47:UNK:O	1:FX:66:UNK:HA	2.18	0.43
4:GH:308:SER:OG	4:GH:309:ASN:N	2.52	0.43
3:Gd:84:SER:HB3	3:Gd:125:ASP:H	1.84	0.43
2:HC:117:LEU:HD23	3:Id:114:SER:HB2	2.01	0.43
6:T:129:THR:O	6:T:133:PHE:HB2	2.18	0.43
6:V:109:LEU:HD22	6:V:114:ILE:HB	2.00	0.43
2:AC:110:LEU:HD12	2:AC:212:TYR:HA	2.01	0.43
1:CX:71:UNK:HA	1:CX:87:UNK:HA	2.00	0.43
3:Fd:74:PRO:HG2	3:Fd:149:PRO:HG3	2.01	0.43
2:IC:78:ILE:HD13	2:IC:78:ILE:HA	1.94	0.43
4:JH:322:SER:H	4:JH:347:LEU:HB3	1.84	0.43
5:KK:87:GLN:NE2	5:KK:173:ASP:OD1	2.52	0.43
3:LD:62:ILE:HG13	3:Ld:67:LYS:HZ3	1.83	0.43
4:MH:326:LEU:N	4:MH:339:GLU:O	2.51	0.43
6:R:165:VAL:O	6:R:205:ALA:HA	2.18	0.43
6:W:109:LEU:HD22	6:W:114:ILE:HB	2.01	0.43
1:CV:91:UNK:HA	1:CV:105:UNK:HA	2.01	0.42
3:AD:86:ASP:HA	3:AD:122:SER:HA	2.00	0.42
4:AH:276:SER:OG	4:AH:277:ALA:N	2.51	0.42
4:AH:290:PRO:O	4:AH:293:SER:OG	2.36	0.42
2:CC:112:GLU:OE2	2:CC:114:ARG:NE	2.47	0.42
5:DK:92:ASN:OD1	5:DK:92:ASN:N	2.52	0.42
2:FC:88:ARG:HA	2:FC:88:ARG:HD2	1.85	0.42
5:GK:119:TYR:OH	5:GK:179:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Id:117:VAL:HG12	3:Id:142:LYS:HZ3	1.83	0.42
2:LC:126:ARG:HG3	2:MC:246:VAL:HB	2.00	0.42
4:MH:314:VAL:HG11	4:MH:346:LEU:HD11	2.01	0.42
6:U:215:SER:OG	6:U:222:GLY:O	2.36	0.42
6:W:201:LYS:HA	6:W:201:LYS:HD3	1.88	0.42
1:CV:50:UNK:HA	1:CV:138:UNK:O	2.19	0.42
3:BD:94:LEU:HD22	3:BD:135:ILE:HD12	2.01	0.42
1:DZ:48:UNK:O	1:DZ:61:UNK:N	2.52	0.42
3:Dd:152:GLN:HE21	3:Dd:152:GLN:HB3	1.64	0.42
2:FC:101:LEU:HB2	2:FC:105:ILE:HB	2.01	0.42
1:FZ:48:UNK:O	1:FZ:61:UNK:N	2.52	0.42
3:Id:70:THR:HA	3:Id:133:ARG:HE	1.85	0.42
1:JX:157:UNK:HA	1:JX:176:UNK:O	2.19	0.42
4:LH:323:PRO:HG2	4:LH:346:LEU:HD23	2.01	0.42
4:MH:322:SER:HB3	4:MH:347:LEU:HB3	2.01	0.42
6:O:118:GLU:OE2	6:O:123:ARG:NE	2.52	0.42
6:Q:219:ILE:HD12	6:Q:219:ILE:HA	1.84	0.42
1:LV:54:UNK:HA	1:LV:142:UNK:O	2.19	0.42
2:AC:130:ARG:O	2:BC:241:HIS:HA	2.19	0.42
4:AH:314:VAL:HG11	4:AH:346:LEU:HD11	2.01	0.42
3:BD:43:GLU:HB3	6:O:172:VAL:HG21	2.00	0.42
3:CD:107:ARG:O	3:CD:155:GLU:HA	2.20	0.42
5:CK:120:SER:HA	5:CK:178:ALA:HA	2.01	0.42
3:GD:48:VAL:O	3:GD:52:MET:HB2	2.18	0.42
2:JC:132:TYR:O	2:KC:239:GLU:HA	2.20	0.42
4:LH:273:ILE:HD13	4:LH:273:ILE:HA	1.91	0.42
4:MH:320:ILE:HD13	4:MH:346:LEU:HD22	2.01	0.42
6:W:118:GLU:OE2	6:W:123:ARG:NE	2.52	0.42
4:DH:314:VAL:HG23	4:DH:338:TYR:HB2	2.01	0.42
2:EC:106:LEU:HB2	2:EC:141:ILE:HG12	2.00	0.42
2:EC:175:ILE:H	2:EC:175:ILE:HG13	1.62	0.42
5:FK:87:GLN:NE2	5:FK:173:ASP:OD1	2.52	0.42
5:FK:173:ASP:OD1	5:FK:173:ASP:N	2.52	0.42
4:GH:353:LYS:HG3	4:GH:355:MET:HG3	2.01	0.42
1:HX:65:UNK:HA	1:HX:82:UNK:O	2.18	0.42
5:IK:65:ILE:HG23	5:IK:78:ILE:HG13	2.02	0.42
2:JC:115:ASN:HB2	4:KH:330:THR:HG22	2.02	0.42
3:LD:97:ARG:HH11	3:LD:97:ARG:HD2	1.70	0.42
3:MD:130:GLU:OE2	3:Md:107:ARG:NH2	2.52	0.42
6:X:190:MET:HG2	6:X:203:LEU:HD22	2.01	0.42
1:GV:115:UNK:HA	1:GV:125:UNK:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AK:87:GLN:NE2	5:AK:173:ASP:OD1	2.52	0.42
1:AX:13:UNK:O	1:AX:33:UNK:N	2.53	0.42
5:BK:67:VAL:HB	5:BK:76:ILE:HG23	2.00	0.42
5:BK:120:SER:HA	5:BK:178:ALA:HA	2.02	0.42
5:CK:130:ARG:NH2	3:CD:77:TYR:OH	2.52	0.42
2:DC:264:ALA:O	3:ED:97:ARG:NH1	2.52	0.42
2:EC:102:GLU:HG2	2:EC:103:HIS:HD2	1.84	0.42
2:FC:225:TYR:HB2	2:FC:251:ALA:HB3	2.01	0.42
3:GD:36:ASP:OD1	3:GD:34:SER:OG	2.36	0.42
3:GD:73:ILE:HA	3:GD:74:PRO:HD3	1.89	0.42
3:Id:40:LYS:HA	3:Id:43:GLU:HG3	2.01	0.42
2:JC:115:ASN:N	2:JC:129:ASP:O	2.50	0.42
4:JH:320:ILE:HG21	4:JH:340:MET:HE1	2.01	0.42
3:Jd:27:LYS:NZ	5:KK:71:GLY:O	2.50	0.42
2:KC:143:THR:OG1	4:KH:321:LEU:O	2.32	0.42
2:KC:228:HIS:HB3	2:KC:247:LEU:HG	2.01	0.42
5:MK:67:VAL:HA	5:MK:75:LEU:O	2.18	0.42
6:V:141:ASN:HD22	6:V:144:CYS:HB2	1.83	0.42
5:AK:120:SER:HA	5:AK:178:ALA:HA	2.01	0.42
2:BC:118:ASN:HB2	4:CH:277:ALA:HA	2.00	0.42
2:CC:75:ARG:HA	2:CC:75:ARG:HD2	1.91	0.42
2:EC:146:THR:OG1	2:EC:147:TRP:N	2.53	0.42
1:EX:65:UNK:HA	1:EX:82:UNK:O	2.20	0.42
3:Fd:40:LYS:HB3	3:Fd:40:LYS:HE2	1.78	0.42
2:GC:93:ILE:HA	3:GD:48:VAL:HG11	2.01	0.42
2:LC:103:HIS:HE1	2:LC:228:HIS:HD2	1.68	0.42
3:MD:59:GLU:O	3:Md:141:LYS:NZ	2.46	0.42
4:MH:285:LEU:HD22	4:MH:329:MET:HB3	2.00	0.42
6:S:118:GLU:OE2	6:S:123:ARG:NE	2.52	0.42
1:AV:52:UNK:HA	1:AV:140:UNK:O	2.20	0.42
1:CV:54:UNK:HA	1:CV:142:UNK:O	2.19	0.42
5:AK:156:THR:HG23	3:Ad:82:ARG:HB2	2.02	0.42
1:AX:98:UNK:O	1:AX:117:UNK:HA	2.19	0.42
3:Bd:119:ILE:HD12	3:Bd:135:ILE:HG12	2.01	0.42
3:CD:55:MET:HE3	3:CD:55:MET:HB2	1.79	0.42
4:DH:319:THR:O	4:DH:348:VAL:HA	2.19	0.42
5:DK:165:ILE:N	5:DK:177:ASN:OD1	2.49	0.42
5:EK:92:ASN:O	5:EK:95:SER:OG	2.36	0.42
4:GH:313:TYR:HA	4:GH:338:TYR:O	2.19	0.42
1:GX:170:UNK:HA	1:GX:188:UNK:O	2.19	0.42
1:LX:71:UNK:HA	1:LX:87:UNK:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ld:43:GLU:HA	3:Ld:46:VAL:HG22	2.02	0.42
6:O:201:LYS:HA	6:O:201:LYS:HD3	1.91	0.42
6:R:152:ILE:HA	6:R:155:LEU:HD23	2.02	0.42
1:FV:54:UNK:HA	1:FV:142:UNK:O	2.20	0.42
1:BX:97:UNK:C	1:BX:116:UNK:O	2.67	0.42
2:CC:214:LYS:HG3	3:Cd:58:VAL:HG11	2.01	0.42
1:DX:18:UNK:O	1:DX:37:UNK:HA	2.20	0.42
3:Dd:130:GLU:OE1	3:Dd:133:ARG:NH2	2.53	0.42
3:ED:71:LEU:O	3:ED:133:ARG:NE	2.52	0.42
3:ED:119:ILE:HD13	3:ED:135:ILE:HG13	2.01	0.42
2:FC:98:SER:O	2:FC:98:SER:OG	2.38	0.42
4:FH:304:ARG:O	4:FH:314:VAL:HA	2.20	0.42
1:FX:13:UNK:O	1:FX:33:UNK:N	2.53	0.42
5:HK:99:LEU:HD23	5:HK:99:LEU:HA	1.92	0.42
1:IX:11:UNK:H	1:IX:30:UNK:HA	1.84	0.42
3:Id:136:ASP:HB2	3:Id:145:ILE:HB	2.00	0.42
2:KC:103:HIS:HE1	2:KC:228:HIS:HD2	1.66	0.42
5:KK:116:VAL:O	5:KK:156:THR:HA	2.20	0.42
1:KX:97:UNK:CA	1:KX:116:UNK:O	2.68	0.42
3:MD:29:PRO:HG3	5:MK:146:SER:HB2	2.02	0.42
3:MD:36:ASP:OD1	3:MD:36:ASP:N	2.43	0.42
6:X:171:ASN:OD1	6:X:171:ASN:N	2.53	0.42
1:HV:82:UNK:N	1:HV:117:UNK:O	2.52	0.42
2:BC:153:MET:HB3	2:BC:153:MET:HE2	1.84	0.42
1:CX:13:UNK:O	1:CX:33:UNK:N	2.53	0.42
2:DC:121:ASP:N	2:DC:121:ASP:OD1	2.51	0.42
2:FC:153:MET:HE2	2:FC:153:MET:HB3	1.86	0.42
4:FH:318:LEU:HD12	4:FH:350:TRP:HA	2.01	0.42
3:Fd:39:ILE:HG23	6:S:220:ILE:HG13	2.02	0.42
1:GX:97:UNK:CA	1:GX:116:UNK:O	2.67	0.42
2:HC:108:PRO:HD3	2:HC:138:ALA:HB2	2.02	0.42
2:HC:116:THR:HB	4:IH:329:MET:HG2	2.00	0.42
3:HD:54:GLU:HA	3:HD:57:LYS:HB2	2.02	0.42
5:HK:76:ILE:HB	5:HK:182:ILE:HB	2.02	0.42
2:IC:100:VAL:HG21	2:IC:141:ILE:HD11	2.02	0.42
1:IX:47:UNK:O	1:IX:66:UNK:HA	2.20	0.42
3:JD:73:ILE:HA	3:JD:74:PRO:HD3	1.91	0.42
4:JH:347:LEU:HD12	4:JH:356:GLN:HG2	2.02	0.42
3:Ld:40:LYS:HE2	3:Ld:40:LYS:HB3	1.81	0.42
3:Ld:123:THR:OG1	3:Ld:124:LYS:N	2.53	0.42
3:Ld:141:LYS:HB2	3:Ld:141:LYS:HE3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:145:TYR:HA	6:O:148:LEU:HD12	2.02	0.42
3:Ad:152:GLN:HE21	3:Ad:152:GLN:HB3	1.66	0.42
4:BH:343:SER:OG	4:BH:345:VAL:O	2.37	0.42
2:DC:154:ASP:HB3	1:DZ:42:UNK:HA	2.01	0.42
3:DD:91:ILE:O	3:DD:95:THR:OG1	2.35	0.42
4:EH:281:LEU:HA	4:EH:284:VAL:HG22	2.01	0.42
1:GZ:48:UNK:O	1:GZ:61:UNK:N	2.53	0.42
2:KC:214:LYS:HG3	3:Kd:58:VAL:HG11	2.01	0.42
5:KK:149:VAL:HG21	5:KK:154:ILE:HD11	2.01	0.42
2:LC:88:ARG:HD2	2:LC:88:ARG:HA	1.89	0.42
2:BC:266:VAL:HG21	3:CD:98:ILE:HG22	2.02	0.41
2:FC:147:TRP:HD1	2:FC:151:LEU:HD12	1.85	0.41
1:GX:56:UNK:O	1:GX:73:UNK:N	2.53	0.41
2:IC:215:LEU:HB3	2:IC:220:MET:HB2	2.00	0.41
5:IK:109:PHE:HB2	5:IK:111:LYS:HE3	2.02	0.41
4:KH:333:ASP:OD1	4:KH:333:ASP:N	2.45	0.41
4:MH:344:PRO:HA	4:MH:359:VAL:HG22	2.02	0.41
1:MX:128:UNK:HA	1:MX:147:UNK:O	2.20	0.41
2:AC:102:GLU:HG2	2:AC:103:HIS:HD2	1.85	0.41
2:EC:75:ARG:NH1	3:Ed:36:ASP:OD2	2.53	0.41
2:EC:175:ILE:O	2:EC:179:TYR:HB2	2.19	0.41
3:Ed:84:SER:HB2	3:Ed:124:LYS:HA	2.00	0.41
4:FH:326:LEU:N	4:FH:339:GLU:O	2.50	0.41
2:HC:79:ILE:HD13	2:HC:195:LEU:HD22	2.02	0.41
3:HD:71:LEU:O	3:HD:133:ARG:NE	2.52	0.41
3:Kd:87:TRP:CD1	3:Kd:89:GLY:H	2.38	0.41
1:MX:97:UNK:CA	1:MX:116:UNK:O	2.68	0.41
6:V:148:LEU:HA	6:V:151:VAL:HG12	2.02	0.41
2:BC:143:THR:OG1	4:BH:321:LEU:O	2.32	0.41
2:BC:226:VAL:HA	2:BC:248:ARG:O	2.21	0.41
3:Cd:74:PRO:HG2	3:Cd:149:PRO:HG3	2.02	0.41
5:DK:114:ILE:O	5:DK:154:ILE:HA	2.20	0.41
3:Fd:150:ASN:OD1	3:Fd:150:ASN:N	2.43	0.41
1:GX:13:UNK:O	1:GX:33:UNK:N	2.53	0.41
1:GX:97:UNK:C	1:GX:116:UNK:O	2.68	0.41
1:IX:13:UNK:O	1:IX:33:UNK:N	2.53	0.41
3:Jd:38:THR:HA	3:Jd:41:LEU:HB2	2.03	0.41
6:N:134:MET:HE3	6:N:134:MET:HB3	1.82	0.41
3:Bd:105:ARG:O	3:Bd:153:VAL:HA	2.20	0.41
2:CC:148:ARG:HH21	2:CC:148:ARG:HD2	1.75	0.41
3:Cd:100:LYS:HB3	3:Cd:100:LYS:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Dd:90:PRO:HA	3:Dd:118:LEU:HA	2.02	0.41
4:EH:279:ASP:OD2	4:EH:279:ASP:N	2.52	0.41
2:MC:173:LYS:HB2	2:MC:174:GLU:H	1.66	0.41
6:P:152:ILE:HG12	6:P:196:ASN:HB3	2.01	0.41
3:CD:55:MET:HA	3:CD:58:VAL:HG12	2.02	0.41
5:EK:78:ILE:HB	5:EK:180:VAL:HG23	2.02	0.41
2:FC:228:HIS:HB3	2:FC:247:LEU:HG	2.02	0.41
4:FH:331:SER:OG	4:FH:333:ASP:OD1	2.38	0.41
1:GX:71:UNK:HA	1:GX:87:UNK:HA	2.02	0.41
4:HH:304:ARG:O	4:HH:314:VAL:HA	2.21	0.41
5:JK:130:ARG:NH2	3:Jd:77:TYR:OH	2.53	0.41
5:LK:179:ARG:NH2	6:X:119:TYR:OH	2.54	0.41
1:EV:93:UNK:HA	1:EV:103:UNK:HA	2.01	0.41
3:AD:60:LYS:HZ2	3:Ad:141:LYS:H	1.67	0.41
3:AD:94:LEU:HD11	3:AD:121:ILE:HD11	2.03	0.41
3:Ad:68:ASP:HB2	3:Ad:70:THR:HG23	2.02	0.41
2:BC:214:LYS:NZ	3:Bd:54:GLU:OE2	2.53	0.41
3:CD:137:TYR:O	3:Cd:160:LYS:NZ	2.44	0.41
5:CK:151:SER:OG	5:CK:153:ILE:O	2.39	0.41
5:CK:173:ASP:OD1	5:CK:173:ASP:N	2.53	0.41
4:EH:316:THR:OG1	4:EH:317:ASN:N	2.54	0.41
2:FC:196:GLU:OE2	4:GH:304:ARG:NH1	2.53	0.41
1:FX:97:UNK:CA	1:FX:116:UNK:O	2.68	0.41
3:GD:55:MET:HE2	3:GD:55:MET:HB3	1.84	0.41
3:GD:107:ARG:O	3:GD:155:GLU:HA	2.21	0.41
2:HC:117:LEU:HD22	2:HC:125:ILE:HD12	2.02	0.41
3:HD:120:SER:H	3:HD:138:GLN:HE22	1.68	0.41
3:HD:150:ASN:OD1	3:HD:150:ASN:N	2.53	0.41
6:Q:190:MET:HG2	6:Q:203:LEU:HD22	2.02	0.41
1:NV:76:UNK:N	1:NV:99:UNK:O	2.53	0.41
1:OV:85:UNK:HA	1:OW:27:UNK:O	2.21	0.41
3:BD:36:ASP:OD1	3:BD:36:ASP:N	2.45	0.41
1:BZ:48:UNK:O	1:BZ:61:UNK:N	2.53	0.41
2:CC:125:ILE:HD11	2:DC:247:LEU:HD22	2.02	0.41
3:DD:27:LYS:HG3	5:DK:100:ASN:HD21	1.86	0.41
5:DK:120:SER:HA	5:DK:178:ALA:HA	2.02	0.41
2:EC:254:GLU:HB2	2:FC:237:GLY:HA3	2.03	0.41
5:EK:120:SER:O	5:EK:161:SER:OG	2.37	0.41
1:EX:188:UNK:HA	1:EX:206:UNK:O	2.21	0.41
1:EZ:48:UNK:O	1:EZ:61:UNK:N	2.54	0.41
2:FC:116:THR:HA	4:GH:328:SER:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GC:214:LYS:HG3	3:Gd:58:VAL:HG11	2.02	0.41
3:GD:137:TYR:OH	3:Gd:158:TYR:O	2.37	0.41
5:GK:124:VAL:HG22	5:GK:128:ARG:HG2	2.02	0.41
3:Gd:39:ILE:HG23	6:T:220:ILE:HG13	2.01	0.41
2:IC:125:ILE:HD11	2:JC:247:LEU:HD22	2.03	0.41
2:IC:256:ASN:ND2	2:IC:258:ASN:O	2.53	0.41
2:JC:59:LEU:HA	2:JC:62:THR:HG22	2.03	0.41
2:KC:122:ALA:HB1	2:LC:139:HIS:HB2	2.02	0.41
2:LC:85:LYS:HE3	2:LC:85:LYS:HB2	1.90	0.41
2:LC:115:ASN:O	3:Md:114:SER:OG	2.36	0.41
5:LK:67:VAL:HA	5:LK:75:LEU:O	2.21	0.41
1:HV:91:UNK:HA	1:HV:105:UNK:HA	2.02	0.41
1:OV:53:UNK:O	1:OV:141:UNK:HA	2.21	0.41
4:AH:330:THR:OG1	4:AH:336:HIS:ND1	2.49	0.41
4:AH:356:GLN:HG3	1:AZ:37:UNK:HA	2.03	0.41
3:BD:95:THR:HG23	3:BD:135:ILE:HD13	2.02	0.41
3:Fd:143:ALA:HA	3:Fd:157:ARG:O	2.21	0.41
2:GC:228:HIS:HB3	2:GC:247:LEU:HG	2.03	0.41
4:GH:276:SER:OG	4:GH:277:ALA:N	2.54	0.41
2:HC:112:GLU:HB2	2:HC:211:LEU:HD21	2.03	0.41
5:IK:186:ARG:NH1	1:IZ:23:UNK:O	2.53	0.41
5:KK:44:ARG:HE	5:KK:45:VAL:HG13	1.85	0.41
1:KZ:8:UNK:HA	1:KZ:19:UNK:HA	2.03	0.41
3:Kd:120:SER:O	3:Kd:138:GLN:NE2	2.54	0.41
3:Ld:84:SER:HB2	3:Ld:124:LYS:HA	2.02	0.41
6:O:202:ARG:H	6:O:202:ARG:HG3	1.75	0.41
6:U:145:TYR:HA	6:U:148:LEU:HD12	2.01	0.41
1:BV:88:UNK:N	1:BW:25:UNK:O	2.54	0.41
1:IV:84:UNK:O	1:IW:28:UNK:HA	2.21	0.41
1:PV:67:UNK:O	1:PV:131:UNK:N	2.54	0.41
1:QV:93:UNK:HA	1:QV:103:UNK:HA	2.03	0.41
2:AC:153:MET:HE2	2:AC:153:MET:HB3	1.92	0.41
1:AX:45:UNK:O	1:AX:64:UNK:HA	2.21	0.41
1:BX:97:UNK:CA	1:BX:116:UNK:O	2.67	0.41
3:Bd:27:LYS:NZ	5:CK:71:GLY:O	2.47	0.41
5:CK:77:SER:HB3	5:CK:179:ARG:HH21	1.86	0.41
5:CK:116:VAL:O	5:CK:156:THR:HA	2.21	0.41
4:DH:330:THR:OG1	4:DH:336:HIS:ND1	2.48	0.41
3:Dd:150:ASN:OD1	3:Dd:150:ASN:N	2.51	0.41
2:EC:108:PRO:HD3	2:EC:138:ALA:HB2	2.02	0.41
3:FD:58:VAL:HA	3:Fd:65:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FK:120:SER:O	5:FK:161:SER:OG	2.35	0.41
2:GC:137:GLN:NE2	2:GC:253:PRO:O	2.46	0.41
2:GC:186:ASN:O	2:GC:190:GLN:HB2	2.20	0.41
2:GC:215:LEU:HB3	2:GC:220:MET:HB2	2.03	0.41
4:GH:331:SER:OG	4:GH:333:ASP:OD1	2.39	0.41
5:GK:120:SER:HA	5:GK:178:ALA:HA	2.03	0.41
3:HD:73:ILE:HA	3:HD:74:PRO:HD3	1.81	0.41
3:HD:130:GLU:OE1	3:Hd:105:ARG:NH1	2.43	0.41
2:IC:157:LYS:HD2	2:IC:157:LYS:HA	1.86	0.41
3:Id:62:ILE:HD12	3:Id:62:ILE:HA	1.92	0.41
3:JD:71:LEU:O	3:JD:133:ARG:NE	2.53	0.41
4:JH:320:ILE:HD12	4:JH:346:LEU:HD22	2.02	0.41
5:JK:186:ARG:NH1	1:JZ:23:UNK:O	2.49	0.41
2:KC:263:ARG:HA	2:KC:263:ARG:HD2	1.87	0.41
3:KD:55:MET:HE2	3:KD:55:MET:HB3	1.85	0.41
3:KD:68:ASP:OD2	3:KD:68:ASP:N	2.52	0.41
3:KD:73:ILE:HA	3:KD:74:PRO:HD3	1.82	0.41
2:LC:264:ALA:O	3:MD:97:ARG:NH1	2.54	0.41
3:LD:107:ARG:NH2	3:LD:155:GLU:OE2	2.46	0.41
5:LK:120:SER:OG	5:LK:121:SER:N	2.53	0.41
1:LZ:8:UNK:HA	1:LZ:19:UNK:HA	2.03	0.41
6:P:168:PHE:HE2	6:P:230:GLU:HB3	1.85	0.41
6:Q:109:LEU:HD22	6:Q:114:ILE:HB	2.03	0.41
6:Y:219:ILE:HD12	6:Y:219:ILE:HA	1.85	0.41
1:BV:36:UNK:O	1:BV:40:UNK:CB	2.68	0.41
1:JV:53:UNK:O	1:JV:142:UNK:CB	2.69	0.41
4:BH:286:GLU:HB2	4:BH:288:VAL:HG12	2.01	0.41
5:BK:84:PHE:HB2	5:BK:136:ARG:HH21	1.86	0.41
3:Bd:40:LYS:HA	3:Bd:43:GLU:HG2	2.03	0.41
3:CD:86:ASP:HA	3:CD:122:SER:HA	2.02	0.41
3:DD:55:MET:HE2	3:DD:55:MET:HB3	1.87	0.41
4:DH:285:LEU:O	4:DH:315:ARG:NH1	2.53	0.41
3:Dd:134:ASP:HA	3:Dd:137:TYR:HB2	2.03	0.41
3:FD:150:ASN:OD1	3:FD:150:ASN:N	2.53	0.41
2:HC:119:LEU:HA	2:HC:125:ILE:HG22	2.03	0.41
5:HK:173:ASP:OD1	5:HK:173:ASP:N	2.54	0.41
3:Hd:82:ARG:HA	3:Hd:127:SER:HA	2.03	0.41
2:IC:59:LEU:HA	2:IC:62:THR:HG22	2.02	0.41
2:LC:149:GLN:NE2	4:LH:322:SER:O	2.53	0.41
3:Md:50:ASP:HA	3:Md:53:LEU:HB3	2.03	0.41
6:N:134:MET:O	6:N:137:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:232:GLN:HE21	6:Q:232:GLN:HB2	1.74	0.41
6:X:158:TYR:O	6:X:202:ARG:NH2	2.49	0.41
3:AD:55:MET:HE2	3:AD:55:MET:HB3	1.88	0.40
5:AK:114:ILE:O	5:AK:154:ILE:HA	2.21	0.40
3:Ad:144:SER:HB3	3:Ad:157:ARG:HG3	2.03	0.40
2:BC:256:ASN:ND2	2:BC:258:ASN:OD1	2.51	0.40
2:CC:78:ILE:HD13	2:CC:78:ILE:HA	1.97	0.40
3:DD:107:ARG:O	3:DD:155:GLU:HA	2.22	0.40
3:Dd:72:THR:OG1	3:Dd:146:HIS:ND1	2.49	0.40
2:FC:131:THR:HA	2:GC:240:ILE:O	2.21	0.40
2:FC:199:ILE:HA	2:FC:202:ILE:HG22	2.03	0.40
5:FK:44:ARG:HE	5:FK:45:VAL:HG13	1.86	0.40
2:HC:258:ASN:N	2:HC:258:ASN:OD1	2.53	0.40
3:Hd:36:ASP:HA	3:Hd:39:ILE:HB	2.03	0.40
3:Hd:70:THR:HA	3:Hd:133:ARG:HE	1.85	0.40
5:IK:130:ARG:NH2	3:Id:77:TYR:OH	2.55	0.40
3:Id:52:MET:HE2	3:Id:52:MET:HB2	1.93	0.40
2:JC:117:LEU:O	4:KH:327:ALA:HA	2.20	0.40
3:LD:132:LEU:HD22	3:LD:145:ILE:HG21	2.02	0.40
3:MD:62:ILE:HD13	3:MD:62:ILE:HA	1.96	0.40
6:R:134:MET:HE3	6:R:134:MET:HB2	1.89	0.40
6:W:190:MET:HG2	6:W:203:LEU:HD22	2.02	0.40
1:RV:54:UNK:HA	1:RV:142:UNK:O	2.21	0.40
5:AK:166:THR:HG22	5:AK:168:TYR:H	1.87	0.40
3:Ad:40:LYS:HB3	3:Ad:40:LYS:HE2	1.76	0.40
3:Ad:119:ILE:HD12	3:Ad:135:ILE:HG12	2.02	0.40
5:BK:156:THR:HG23	3:Bd:82:ARG:HB2	2.03	0.40
3:Dd:151:SER:OG	3:Dd:152:GLN:N	2.54	0.40
3:Ed:40:LYS:HB3	3:Ed:40:LYS:HE2	1.83	0.40
5:FK:150:ASP:O	5:FK:152:ARG:NH2	2.54	0.40
3:GD:120:SER:H	3:GD:138:GLN:HE22	1.69	0.40
3:KD:139:ALA:HB1	3:KD:143:ALA:HB3	2.03	0.40
4:KH:316:THR:OG1	4:KH:317:ASN:N	2.53	0.40
1:KX:167:UNK:O	1:KX:186:UNK:CB	2.69	0.40
5:LK:156:THR:O	5:LK:156:THR:OG1	2.40	0.40
6:P:148:LEU:HA	6:P:151:VAL:HG22	2.03	0.40
6:V:152:ILE:HD12	6:V:152:ILE:HA	1.94	0.40
1:CV:72:UNK:O	1:CV:102:UNK:HA	2.21	0.40
2:BC:109:VAL:HG13	2:BC:208:GLY:HA3	2.02	0.40
3:BD:107:ARG:O	3:BD:155:GLU:HA	2.22	0.40
3:Cd:147:VAL:HG22	3:Cd:154:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DX:188:UNK:HA	1:DX:206:UNK:O	2.21	0.40
5:FK:49:CYS:O	5:FK:52:THR:OG1	2.35	0.40
2:GC:95:ASP:OD1	2:GC:95:ASP:N	2.45	0.40
2:HC:98:SER:O	2:HC:98:SER:OG	2.34	0.40
3:ID:115:VAL:HA	3:ID:116:PRO:HD3	1.97	0.40
2:LC:196:GLU:HA	2:LC:199:ILE:HB	2.03	0.40
4:LH:290:PRO:O	4:LH:293:SER:OG	2.39	0.40
1:MX:65:UNK:HA	1:MX:82:UNK:O	2.21	0.40
6:R:114:ILE:HG12	6:R:127:ILE:HA	2.02	0.40
6:S:145:TYR:HA	6:S:148:LEU:HD12	2.03	0.40
2:BC:98:SER:HB2	3:BD:52:MET:HE3	2.02	0.40
1:BX:167:UNK:O	1:BX:186:UNK:CB	2.70	0.40
2:CC:97:ASN:ND2	3:Cd:118:LEU:O	2.46	0.40
5:EK:57:MET:HG2	5:EK:67:VAL:HG11	2.04	0.40
3:Gd:40:LYS:HE2	3:Gd:40:LYS:HB3	1.93	0.40
3:Id:27:LYS:NZ	5:JK:71:GLY:O	2.52	0.40
3:Id:119:ILE:HD12	3:Id:135:ILE:HG12	2.03	0.40
2:JC:175:ILE:H	2:JC:175:ILE:HG13	1.56	0.40
5:JK:61:ASN:HD21	5:JK:67:VAL:HB	1.87	0.40
1:JZ:8:UNK:HA	1:JZ:19:UNK:HA	2.04	0.40
3:LD:91:ILE:HD12	3:LD:119:ILE:HD11	2.03	0.40
6:Q:127:ILE:HB	6:Q:229:ILE:HB	2.02	0.40
6:S:134:MET:HE2	6:S:139:ARG:HH22	1.86	0.40
6:U:183:GLN:O	6:U:187:GLU:HB2	2.21	0.40
6:W:226:ASN:O	6:W:228:ARG:NH1	2.54	0.40
1:FV:64:UNK:HA	1:FV:127:UNK:O	2.22	0.40
3:AD:43:GLU:HA	3:AD:46:VAL:HG22	2.04	0.40
3:CD:54:GLU:HA	3:CD:57:LYS:HB2	2.03	0.40
3:DD:79:LEU:HD23	3:DD:79:LEU:HA	1.95	0.40
3:FD:54:GLU:HA	3:FD:57:LYS:HB2	2.04	0.40
3:FD:115:VAL:HA	3:FD:116:PRO:HD3	1.95	0.40
5:FK:179:ARG:NH2	6:R:119:TYR:OH	2.55	0.40
2:HC:214:LYS:HG3	3:Hd:58:VAL:HG11	2.03	0.40
2:JC:157:LYS:HD2	2:JC:158:PRO:HD2	2.03	0.40
3:JD:64:PRO:HA	3:JD:65:PRO:HD3	1.96	0.40
3:JD:97:ARG:HE	3:JD:100:LYS:HZ1	1.70	0.40
3:Jd:98:ILE:HG23	3:Jd:128:LEU:HD22	2.04	0.40
5:KK:92:ASN:OD1	5:KK:92:ASN:N	2.54	0.40
4:MH:273:ILE:HD13	4:MH:273:ILE:HA	1.92	0.40
5:MK:53:ILE:HD11	5:MK:108:GLN:HB3	2.03	0.40
6:P:126:ILE:HA	6:P:229:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:215:SER:OG	6:Y:216:ASP:N	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	196/303 (65%)	190 (97%)	6 (3%)	0	100	100
2	BC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	CC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	DC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	EC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	FC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	GC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	HC	196/303 (65%)	190 (97%)	6 (3%)	0	100	100
2	IC	196/303 (65%)	191 (97%)	5 (3%)	0	100	100
2	JC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	KC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	LC	196/303 (65%)	188 (96%)	8 (4%)	0	100	100
2	MC	196/303 (65%)	191 (97%)	5 (3%)	0	100	100
3	AD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
3	Ad	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	BD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Bd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
3	CD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Cd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	DD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Dd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
3	ED	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Ed	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
3	FD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Fd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	GD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Gd	136/163 (83%)	128 (94%)	8 (6%)	0	100	100
3	HD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Hd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	ID	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
3	Id	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	JD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Jd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
3	KD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
3	Kd	136/163 (83%)	130 (96%)	6 (4%)	0	100	100
3	LD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Ld	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	MD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Md	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
4	AH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	BH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	CH	87/361 (24%)	77 (88%)	10 (12%)	0	100	100
4	DH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	EH	87/361 (24%)	76 (87%)	11 (13%)	0	100	100
4	FH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	GH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	HH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	IH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	JH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
4	KH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LH	87/361 (24%)	77 (88%)	10 (12%)	0	100	100
4	MH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
5	AK	146/189 (77%)	142 (97%)	4 (3%)	0	100	100
5	BK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	CK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	DK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	EK	146/189 (77%)	139 (95%)	7 (5%)	0	100	100
5	FK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
5	GK	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
5	HK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	IK	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
5	JK	146/189 (77%)	141 (97%)	5 (3%)	0	100	100
5	KK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
5	LK	146/189 (77%)	139 (95%)	7 (5%)	0	100	100
5	MK	146/189 (77%)	136 (93%)	10 (7%)	0	100	100
6	N	134/249 (54%)	123 (92%)	11 (8%)	0	100	100
6	O	134/249 (54%)	124 (92%)	10 (8%)	0	100	100
6	P	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	Q	134/249 (54%)	127 (95%)	7 (5%)	0	100	100
6	R	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	S	134/249 (54%)	127 (95%)	7 (5%)	0	100	100
6	T	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	U	134/249 (54%)	128 (96%)	6 (4%)	0	100	100
6	V	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	W	134/249 (54%)	124 (92%)	10 (8%)	0	100	100
6	X	134/249 (54%)	125 (93%)	9 (7%)	0	100	100
6	Y	134/249 (54%)	125 (93%)	9 (7%)	0	100	100
6	Z	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
All	All	10816/18564 (58%)	10205 (94%)	611 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	169/257 (66%)	153 (90%)	16 (10%)	8	31
2	BC	169/257 (66%)	152 (90%)	17 (10%)	7	29
2	CC	169/257 (66%)	147 (87%)	22 (13%)	4	20
2	DC	169/257 (66%)	150 (89%)	19 (11%)	6	25
2	EC	169/257 (66%)	153 (90%)	16 (10%)	8	31
2	FC	169/257 (66%)	150 (89%)	19 (11%)	6	25
2	GC	169/257 (66%)	151 (89%)	18 (11%)	6	27
2	HC	169/257 (66%)	153 (90%)	16 (10%)	8	31
2	IC	169/257 (66%)	155 (92%)	14 (8%)	10	35
2	JC	169/257 (66%)	153 (90%)	16 (10%)	8	31
2	KC	169/257 (66%)	152 (90%)	17 (10%)	7	29
2	LC	169/257 (66%)	154 (91%)	15 (9%)	9	33
2	MC	169/257 (66%)	154 (91%)	15 (9%)	9	33
3	AD	116/139 (84%)	99 (85%)	17 (15%)	3	17
3	Ad	119/139 (86%)	104 (87%)	15 (13%)	4	21
3	BD	116/139 (84%)	101 (87%)	15 (13%)	4	21
3	Bd	119/139 (86%)	106 (89%)	13 (11%)	6	26
3	CD	116/139 (84%)	96 (83%)	20 (17%)	2	13
3	Cd	119/139 (86%)	110 (92%)	9 (8%)	12	38
3	DD	116/139 (84%)	99 (85%)	17 (15%)	3	17
3	Dd	119/139 (86%)	105 (88%)	14 (12%)	5	23
3	ED	116/139 (84%)	96 (83%)	20 (17%)	2	13
3	Ed	119/139 (86%)	109 (92%)	10 (8%)	10	35
3	FD	116/139 (84%)	94 (81%)	22 (19%)	1	10
3	Fd	119/139 (86%)	101 (85%)	18 (15%)	3	16
3	GD	116/139 (84%)	102 (88%)	14 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Gd	119/139 (86%)	100 (84%)	19 (16%)	2	15
3	HD	116/139 (84%)	95 (82%)	21 (18%)	2	12
3	Hd	119/139 (86%)	105 (88%)	14 (12%)	5	23
3	ID	116/139 (84%)	101 (87%)	15 (13%)	4	21
3	Id	119/139 (86%)	111 (93%)	8 (7%)	15	42
3	JD	116/139 (84%)	99 (85%)	17 (15%)	3	17
3	Jd	119/139 (86%)	105 (88%)	14 (12%)	5	23
3	KD	116/139 (84%)	104 (90%)	12 (10%)	7	29
3	Kd	119/139 (86%)	106 (89%)	13 (11%)	6	26
3	LD	116/139 (84%)	99 (85%)	17 (15%)	3	17
3	Ld	119/139 (86%)	107 (90%)	12 (10%)	7	29
3	MD	116/139 (84%)	100 (86%)	16 (14%)	3	19
3	Md	119/139 (86%)	97 (82%)	22 (18%)	1	10
4	AH	75/300 (25%)	64 (85%)	11 (15%)	3	17
4	BH	75/300 (25%)	66 (88%)	9 (12%)	5	23
4	CH	75/300 (25%)	64 (85%)	11 (15%)	3	17
4	DH	75/300 (25%)	59 (79%)	16 (21%)	1	7
4	EH	75/300 (25%)	63 (84%)	12 (16%)	2	15
4	FH	75/300 (25%)	68 (91%)	7 (9%)	8	32
4	GH	75/300 (25%)	66 (88%)	9 (12%)	5	23
4	HH	75/300 (25%)	64 (85%)	11 (15%)	3	17
4	IH	75/300 (25%)	63 (84%)	12 (16%)	2	15
4	JH	75/300 (25%)	61 (81%)	14 (19%)	1	10
4	KH	75/300 (25%)	66 (88%)	9 (12%)	5	23
4	LH	75/300 (25%)	59 (79%)	16 (21%)	1	7
4	MH	75/300 (25%)	60 (80%)	15 (20%)	1	9
5	AK	126/163 (77%)	108 (86%)	18 (14%)	3	18
5	BK	126/163 (77%)	102 (81%)	24 (19%)	1	10
5	CK	126/163 (77%)	104 (82%)	22 (18%)	2	12
5	DK	126/163 (77%)	107 (85%)	19 (15%)	3	16
5	EK	126/163 (77%)	106 (84%)	20 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	FK	126/163 (77%)	101 (80%)	25 (20%)	1	9
5	GK	126/163 (77%)	105 (83%)	21 (17%)	2	14
5	HK	126/163 (77%)	99 (79%)	27 (21%)	1	7
5	IK	126/163 (77%)	111 (88%)	15 (12%)	5	23
5	JK	126/163 (77%)	106 (84%)	20 (16%)	2	15
5	KK	126/163 (77%)	113 (90%)	13 (10%)	7	29
5	LK	126/163 (77%)	110 (87%)	16 (13%)	4	21
5	MK	126/163 (77%)	107 (85%)	19 (15%)	3	16
6	N	118/203 (58%)	109 (92%)	9 (8%)	12	38
6	O	118/203 (58%)	107 (91%)	11 (9%)	8	32
6	P	118/203 (58%)	108 (92%)	10 (8%)	10	35
6	Q	118/203 (58%)	109 (92%)	9 (8%)	12	38
6	R	118/203 (58%)	109 (92%)	9 (8%)	12	38
6	S	118/203 (58%)	108 (92%)	10 (8%)	10	35
6	T	118/203 (58%)	105 (89%)	13 (11%)	6	26
6	U	118/203 (58%)	109 (92%)	9 (8%)	12	38
6	V	118/203 (58%)	106 (90%)	12 (10%)	7	29
6	W	118/203 (58%)	110 (93%)	8 (7%)	14	42
6	X	118/203 (58%)	110 (93%)	8 (7%)	14	42
6	Y	118/203 (58%)	105 (89%)	13 (11%)	6	26
6	Z	118/203 (58%)	105 (89%)	13 (11%)	6	26
All	All	9399/15613 (60%)	8230 (88%)	1169 (12%)	7	22

All (1169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AC	64	LEU
2	AC	79	ILE
2	AC	100	VAL
2	AC	102	GLU
2	AC	126	ARG
2	AC	137	GLN
2	AC	141	ILE
2	AC	156	VAL
2	AC	173	LYS

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Mol	Chain	Res	Type
2	AC	175	ILE
2	AC	177	CYS
2	AC	178	ILE
2	AC	190	GLN
2	AC	229	THR
2	AC	246	VAL
2	AC	259	SER
3	AD	58	VAL
3	AD	61	VAL
3	AD	63	THR
3	AD	66	SER
3	AD	70	THR
3	AD	85	VAL
3	AD	86	ASP
3	AD	108	VAL
3	AD	115	VAL
3	AD	117	VAL
3	AD	121	ILE
3	AD	123	THR
3	AD	126	GLU
3	AD	128	LEU
3	AD	138	GLN
3	AD	154	VAL
3	AD	157	ARG
4	AH	280	LEU
4	AH	288	VAL
4	AH	297	VAL
4	AH	317	ASN
4	AH	318	LEU
4	AH	321	LEU
4	AH	328	SER
4	AH	333	ASP
4	AH	343	SER
4	AH	349	SER
4	AH	358	LYS
5	AK	43	CYS
5	AK	46	ASP
5	AK	66	LYS
5	AK	78	ILE
5	AK	83	LEU
5	AK	86	ASP
5	AK	91	LEU

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Mol	Chain	Res	Type
5	AK	95	SER
5	AK	115	THR
5	AK	116	VAL
5	AK	119	TYR
5	AK	125	SER
5	AK	153	ILE
5	AK	156	THR
5	AK	161	SER
5	AK	167	SER
5	AK	183	THR
5	AK	188	VAL
3	Ad	34	SER
3	Ad	38	THR
3	Ad	55	MET
3	Ad	63	THR
3	Ad	66	SER
3	Ad	67	LYS
3	Ad	75	ASN
3	Ad	78	ASN
3	Ad	85	VAL
3	Ad	95	THR
3	Ad	108	VAL
3	Ad	111	LYS
3	Ad	117	VAL
3	Ad	127	SER
3	Ad	130	GLU
2	BC	66	VAL
2	BC	79	ILE
2	BC	100	VAL
2	BC	126	ARG
2	BC	128	SER
2	BC	143	THR
2	BC	174	GLU
2	BC	175	ILE
2	BC	177	CYS
2	BC	180	THR
2	BC	214	LYS
2	BC	221	VAL
2	BC	229	THR
2	BC	233	VAL
2	BC	246	VAL
2	BC	258	ASN

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Mol	Chain	Res	Type
2	BC	259	SER
3	BD	58	VAL
3	BD	61	VAL
3	BD	62	ILE
3	BD	63	THR
3	BD	85	VAL
3	BD	93	GLU
3	BD	108	VAL
3	BD	115	VAL
3	BD	117	VAL
3	BD	119	ILE
3	BD	127	SER
3	BD	144	SER
3	BD	150	ASN
3	BD	151	SER
3	BD	153	VAL
4	BH	273	ILE
4	BH	276	SER
4	BH	288	VAL
4	BH	298	VAL
4	BH	318	LEU
4	BH	319	THR
4	BH	328	SER
4	BH	340	MET
4	BH	349	SER
5	BK	41	LEU
5	BK	43	CYS
5	BK	46	ASP
5	BK	66	LYS
5	BK	67	VAL
5	BK	70	VAL
5	BK	75	LEU
5	BK	76	ILE
5	BK	78	ILE
5	BK	86	ASP
5	BK	88	SER
5	BK	95	SER
5	BK	114	ILE
5	BK	115	THR
5	BK	117	THR
5	BK	119	TYR
5	BK	120	SER

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Mol	Chain	Res	Type
5	BK	125	SER
5	BK	134	LEU
5	BK	156	THR
5	BK	157	GLN
5	BK	180	VAL
5	BK	183	THR
5	BK	188	VAL
3	Bd	34	SER
3	Bd	51	SER
3	Bd	61	VAL
3	Bd	62	ILE
3	Bd	63	THR
3	Bd	78	ASN
3	Bd	85	VAL
3	Bd	107	ARG
3	Bd	115	VAL
3	Bd	117	VAL
3	Bd	127	SER
3	Bd	151	SER
3	Bd	155	GLU
2	CC	66	VAL
2	CC	79	ILE
2	CC	81	GLU
2	CC	93	ILE
2	CC	127	ILE
2	CC	146	THR
2	CC	173	LYS
2	CC	175	ILE
2	CC	178	ILE
2	CC	180	THR
2	CC	189	ASP
2	CC	190	GLN
2	CC	215	LEU
2	CC	221	VAL
2	CC	228	HIS
2	CC	229	THR
2	CC	233	VAL
2	CC	234	THR
2	CC	239	GLU
2	CC	241	HIS
2	CC	246	VAL
2	CC	255	LEU

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Mol	Chain	Res	Type
3	CD	31	ASN
3	CD	39	ILE
3	CD	51	SER
3	CD	54	GLU
3	CD	55	MET
3	CD	59	GLU
3	CD	61	VAL
3	CD	70	THR
3	CD	84	SER
3	CD	85	VAL
3	CD	95	THR
3	CD	100	LYS
3	CD	105	ARG
3	CD	108	VAL
3	CD	117	VAL
3	CD	120	SER
3	CD	122	SER
3	CD	123	THR
3	CD	147	VAL
3	CD	153	VAL
4	CH	280	LEU
4	CH	288	VAL
4	CH	309	ASN
4	CH	314	VAL
4	CH	316	THR
4	CH	319	THR
4	CH	322	SER
4	CH	328	SER
4	CH	342	LYS
4	CH	349	SER
4	CH	353	LYS
5	CK	41	LEU
5	CK	43	CYS
5	CK	46	ASP
5	CK	67	VAL
5	CK	76	ILE
5	CK	81	SER
5	CK	86	ASP
5	CK	115	THR
5	CK	116	VAL
5	CK	117	THR
5	CK	119	TYR

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Mol	Chain	Res	Type
5	CK	120	SER
5	CK	125	SER
5	CK	134	LEU
5	CK	156	THR
5	CK	159	LEU
5	CK	161	SER
5	CK	166	THR
5	CK	175	SER
5	CK	180	VAL
5	CK	183	THR
5	CK	188	VAL
3	Cd	38	THR
3	Cd	61	VAL
3	Cd	63	THR
3	Cd	71	LEU
3	Cd	78	ASN
3	Cd	80	GLN
3	Cd	85	VAL
3	Cd	131	ILE
3	Cd	135	ILE
2	DC	62	THR
2	DC	66	VAL
2	DC	79	ILE
2	DC	91	ASP
2	DC	98	SER
2	DC	104	ASN
2	DC	117	LEU
2	DC	127	ILE
2	DC	128	SER
2	DC	141	ILE
2	DC	143	THR
2	DC	173	LYS
2	DC	175	ILE
2	DC	190	GLN
2	DC	231	LEU
2	DC	234	THR
2	DC	246	VAL
2	DC	256	ASN
2	DC	258	ASN
3	DD	30	ILE
3	DD	31	ASN
3	DD	51	SER

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Mol	Chain	Res	Type
3	DD	54	GLU
3	DD	62	ILE
3	DD	63	THR
3	DD	70	THR
3	DD	85	VAL
3	DD	95	THR
3	DD	98	ILE
3	DD	108	VAL
3	DD	115	VAL
3	DD	120	SER
3	DD	122	SER
3	DD	126	GLU
3	DD	142	LYS
3	DD	151	SER
4	DH	273	ILE
4	DH	288	VAL
4	DH	297	VAL
4	DH	299	SER
4	DH	307	LEU
4	DH	314	VAL
4	DH	317	ASN
4	DH	318	LEU
4	DH	330	THR
4	DH	335	THR
4	DH	340	MET
4	DH	343	SER
4	DH	348	VAL
4	DH	349	SER
4	DH	353	LYS
4	DH	359	VAL
5	DK	43	CYS
5	DK	46	ASP
5	DK	75	LEU
5	DK	81	SER
5	DK	88	SER
5	DK	92	ASN
5	DK	95	SER
5	DK	111	LYS
5	DK	115	THR
5	DK	119	TYR
5	DK	137	SER
5	DK	151	SER

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Mol	Chain	Res	Type
5	DK	156	THR
5	DK	159	LEU
5	DK	161	SER
5	DK	165	ILE
5	DK	166	THR
5	DK	183	THR
5	DK	188	VAL
3	Dd	38	THR
3	Dd	53	LEU
3	Dd	61	VAL
3	Dd	62	ILE
3	Dd	63	THR
3	Dd	68	ASP
3	Dd	75	ASN
3	Dd	108	VAL
3	Dd	117	VAL
3	Dd	118	LEU
3	Dd	144	SER
3	Dd	151	SER
3	Dd	156	LEU
3	Dd	161	ILE
2	EC	64	LEU
2	EC	66	VAL
2	EC	72	LEU
2	EC	81	GLU
2	EC	97	ASN
2	EC	105	ILE
2	EC	109	VAL
2	EC	117	LEU
2	EC	124	SER
2	EC	133	LYS
2	EC	175	ILE
2	EC	189	ASP
2	EC	199	ILE
2	EC	229	THR
2	EC	231	LEU
2	EC	246	VAL
3	ED	36	ASP
3	ED	39	ILE
3	ED	54	GLU
3	ED	58	VAL
3	ED	61	VAL

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Mol	Chain	Res	Type
3	ED	62	ILE
3	ED	63	THR
3	ED	88	SER
3	ED	91	ILE
3	ED	94	LEU
3	ED	95	THR
3	ED	98	ILE
3	ED	108	VAL
3	ED	119	ILE
3	ED	123	THR
3	ED	124	LYS
3	ED	126	GLU
3	ED	127	SER
3	ED	151	SER
3	ED	153	VAL
4	EH	273	ILE
4	EH	279	ASP
4	EH	297	VAL
4	EH	307	LEU
4	EH	309	ASN
4	EH	314	VAL
4	EH	316	THR
4	EH	318	LEU
4	EH	343	SER
4	EH	348	VAL
4	EH	349	SER
4	EH	357	LEU
5	EK	43	CYS
5	EK	46	ASP
5	EK	53	ILE
5	EK	86	ASP
5	EK	111	LYS
5	EK	115	THR
5	EK	119	TYR
5	EK	120	SER
5	EK	125	SER
5	EK	129	GLU
5	EK	141	SER
5	EK	156	THR
5	EK	161	SER
5	EK	165	ILE
5	EK	166	THR

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Mol	Chain	Res	Type
5	EK	167	SER
5	EK	175	SER
5	EK	180	VAL
5	EK	183	THR
5	EK	188	VAL
3	Ed	38	THR
3	Ed	62	ILE
3	Ed	72	THR
3	Ed	75	ASN
3	Ed	86	ASP
3	Ed	115	VAL
3	Ed	131	ILE
3	Ed	135	ILE
3	Ed	153	VAL
3	Ed	161	ILE
2	FC	64	LEU
2	FC	66	VAL
2	FC	72	LEU
2	FC	81	GLU
2	FC	97	ASN
2	FC	115	ASN
2	FC	124	SER
2	FC	134	VAL
2	FC	143	THR
2	FC	157	LYS
2	FC	175	ILE
2	FC	178	ILE
2	FC	180	THR
2	FC	190	GLN
2	FC	199	ILE
2	FC	221	VAL
2	FC	233	VAL
2	FC	241	HIS
2	FC	246	VAL
3	FD	31	ASN
3	FD	52	MET
3	FD	54	GLU
3	FD	61	VAL
3	FD	62	ILE
3	FD	63	THR
3	FD	69	ASN
3	FD	70	THR

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Mol	Chain	Res	Type
3	FD	84	SER
3	FD	95	THR
3	FD	98	ILE
3	FD	100	LYS
3	FD	108	VAL
3	FD	111	LYS
3	FD	115	VAL
3	FD	119	ILE
3	FD	122	SER
3	FD	123	THR
3	FD	127	SER
3	FD	138	GLN
3	FD	144	SER
3	FD	154	VAL
4	FH	282	LEU
4	FH	288	VAL
4	FH	309	ASN
4	FH	312	MET
4	FH	316	THR
4	FH	317	ASN
4	FH	349	SER
5	FK	43	CYS
5	FK	46	ASP
5	FK	53	ILE
5	FK	60	LEU
5	FK	70	VAL
5	FK	75	LEU
5	FK	76	ILE
5	FK	77	SER
5	FK	81	SER
5	FK	86	ASP
5	FK	92	ASN
5	FK	95	SER
5	FK	111	LYS
5	FK	116	VAL
5	FK	119	TYR
5	FK	120	SER
5	FK	125	SER
5	FK	132	LEU
5	FK	137	SER
5	FK	153	ILE
5	FK	156	THR

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Mol	Chain	Res	Type
5	FK	159	LEU
5	FK	161	SER
5	FK	183	THR
5	FK	188	VAL
3	Fd	34	SER
3	Fd	38	THR
3	Fd	48	VAL
3	Fd	63	THR
3	Fd	71	LEU
3	Fd	72	THR
3	Fd	77	TYR
3	Fd	80	GLN
3	Fd	108	VAL
3	Fd	109	LEU
3	Fd	115	VAL
3	Fd	117	VAL
3	Fd	127	SER
3	Fd	142	LYS
3	Fd	144	SER
3	Fd	155	GLU
3	Fd	156	LEU
3	Fd	157	ARG
2	GC	97	ASN
2	GC	100	VAL
2	GC	109	VAL
2	GC	117	LEU
2	GC	134	VAL
2	GC	141	ILE
2	GC	173	LYS
2	GC	175	ILE
2	GC	178	ILE
2	GC	180	THR
2	GC	189	ASP
2	GC	190	GLN
2	GC	199	ILE
2	GC	221	VAL
2	GC	233	VAL
2	GC	234	THR
2	GC	241	HIS
2	GC	246	VAL
3	GD	31	ASN
3	GD	52	MET

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Mol	Chain	Res	Type
3	GD	53	LEU
3	GD	61	VAL
3	GD	63	THR
3	GD	70	THR
3	GD	97	ARG
3	GD	108	VAL
3	GD	115	VAL
3	GD	117	VAL
3	GD	120	SER
3	GD	123	THR
3	GD	151	SER
3	GD	153	VAL
4	GH	280	LEU
4	GH	288	VAL
4	GH	309	ASN
4	GH	318	LEU
4	GH	328	SER
4	GH	342	LYS
4	GH	343	SER
4	GH	345	VAL
4	GH	349	SER
5	GK	43	CYS
5	GK	46	ASP
5	GK	53	ILE
5	GK	75	LEU
5	GK	76	ILE
5	GK	81	SER
5	GK	92	ASN
5	GK	117	THR
5	GK	119	TYR
5	GK	120	SER
5	GK	125	SER
5	GK	137	SER
5	GK	139	VAL
5	GK	141	SER
5	GK	156	THR
5	GK	166	THR
5	GK	168	TYR
5	GK	173	ASP
5	GK	175	SER
5	GK	183	THR
5	GK	188	VAL

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Mol	Chain	Res	Type
3	Gd	36	ASP
3	Gd	41	LEU
3	Gd	61	VAL
3	Gd	62	ILE
3	Gd	71	LEU
3	Gd	75	ASN
3	Gd	78	ASN
3	Gd	84	SER
3	Gd	85	VAL
3	Gd	108	VAL
3	Gd	115	VAL
3	Gd	117	VAL
3	Gd	118	LEU
3	Gd	121	ILE
3	Gd	122	SER
3	Gd	127	SER
3	Gd	145	ILE
3	Gd	156	LEU
3	Gd	161	ILE
2	HC	64	LEU
2	HC	72	LEU
2	HC	81	GLU
2	HC	99	LEU
2	HC	116	THR
2	HC	117	LEU
2	HC	133	LYS
2	HC	141	ILE
2	HC	173	LYS
2	HC	177	CYS
2	HC	180	THR
2	HC	229	THR
2	HC	233	VAL
2	HC	234	THR
2	HC	246	VAL
2	HC	266	VAL
3	HD	30	ILE
3	HD	47	SER
3	HD	57	LYS
3	HD	58	VAL
3	HD	61	VAL
3	HD	63	THR
3	HD	70	THR

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Mol	Chain	Res	Type
3	HD	84	SER
3	HD	85	VAL
3	HD	100	LYS
3	HD	108	VAL
3	HD	115	VAL
3	HD	117	VAL
3	HD	119	ILE
3	HD	123	THR
3	HD	126	GLU
3	HD	127	SER
3	HD	135	ILE
3	HD	146	HIS
3	HD	151	SER
3	HD	153	VAL
4	HH	280	LEU
4	HH	288	VAL
4	HH	297	VAL
4	HH	299	SER
4	HH	309	ASN
4	HH	314	VAL
4	HH	317	ASN
4	HH	318	LEU
4	HH	342	LYS
4	HH	343	SER
4	HH	349	SER
5	HK	41	LEU
5	HK	43	CYS
5	HK	46	ASP
5	HK	60	LEU
5	HK	67	VAL
5	HK	70	VAL
5	HK	81	SER
5	HK	92	ASN
5	HK	95	SER
5	HK	101	GLU
5	HK	102	ILE
5	HK	116	VAL
5	HK	119	TYR
5	HK	120	SER
5	HK	137	SER
5	HK	150	ASP
5	HK	153	ILE

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Mol	Chain	Res	Type
5	HK	156	THR
5	HK	159	LEU
5	HK	161	SER
5	HK	165	ILE
5	HK	167	SER
5	HK	168	TYR
5	HK	175	SER
5	HK	180	VAL
5	HK	183	THR
5	HK	188	VAL
3	Hd	35	ASP
3	Hd	38	THR
3	Hd	55	MET
3	Hd	60	LYS
3	Hd	62	ILE
3	Hd	67	LYS
3	Hd	85	VAL
3	Hd	91	ILE
3	Hd	117	VAL
3	Hd	123	THR
3	Hd	126	GLU
3	Hd	152	GLN
3	Hd	153	VAL
3	Hd	161	ILE
2	IC	72	LEU
2	IC	99	LEU
2	IC	100	VAL
2	IC	119	LEU
2	IC	126	ARG
2	IC	177	CYS
2	IC	189	ASP
2	IC	226	VAL
2	IC	229	THR
2	IC	241	HIS
2	IC	246	VAL
2	IC	256	ASN
2	IC	258	ASN
2	IC	266	VAL
3	ID	30	ILE
3	ID	39	ILE
3	ID	61	VAL
3	ID	63	THR

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Mol	Chain	Res	Type
3	ID	70	THR
3	ID	87	TRP
3	ID	98	ILE
3	ID	108	VAL
3	ID	115	VAL
3	ID	123	THR
3	ID	126	GLU
3	ID	132	LEU
3	ID	144	SER
3	ID	151	SER
3	ID	154	VAL
4	IH	280	LEU
4	IH	288	VAL
4	IH	297	VAL
4	IH	299	SER
4	IH	309	ASN
4	IH	318	LEU
4	IH	319	THR
4	IH	330	THR
4	IH	343	SER
4	IH	348	VAL
4	IH	353	LYS
4	IH	359	VAL
5	IK	43	CYS
5	IK	46	ASP
5	IK	70	VAL
5	IK	76	ILE
5	IK	88	SER
5	IK	95	SER
5	IK	101	GLU
5	IK	119	TYR
5	IK	121	SER
5	IK	146	SER
5	IK	152	ARG
5	IK	156	THR
5	IK	159	LEU
5	IK	175	SER
5	IK	183	THR
3	Id	38	THR
3	Id	62	ILE
3	Id	63	THR
3	Id	71	LEU

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Mol	Chain	Res	Type
3	Id	78	ASN
3	Id	85	VAL
3	Id	108	VAL
3	Id	153	VAL
2	JC	61	GLU
2	JC	66	VAL
2	JC	127	ILE
2	JC	143	THR
2	JC	173	LYS
2	JC	175	ILE
2	JC	180	THR
2	JC	181	GLU
2	JC	189	ASP
2	JC	190	GLN
2	JC	199	ILE
2	JC	211	LEU
2	JC	229	THR
2	JC	239	GLU
2	JC	246	VAL
2	JC	258	ASN
3	JD	39	ILE
3	JD	54	GLU
3	JD	62	ILE
3	JD	63	THR
3	JD	66	SER
3	JD	70	THR
3	JD	85	VAL
3	JD	87	TRP
3	JD	108	VAL
3	JD	117	VAL
3	JD	123	THR
3	JD	126	GLU
3	JD	127	SER
3	JD	147	VAL
3	JD	150	ASN
3	JD	153	VAL
3	JD	157	ARG
4	JH	273	ILE
4	JH	288	VAL
4	JH	299	SER
4	JH	307	LEU
4	JH	309	ASN

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Mol	Chain	Res	Type
4	JH	314	VAL
4	JH	316	THR
4	JH	317	ASN
4	JH	318	LEU
4	JH	328	SER
4	JH	342	LYS
4	JH	343	SER
4	JH	345	VAL
4	JH	349	SER
5	JK	43	CYS
5	JK	46	ASP
5	JK	70	VAL
5	JK	83	LEU
5	JK	86	ASP
5	JK	92	ASN
5	JK	95	SER
5	JK	101	GLU
5	JK	106	LEU
5	JK	107	LYS
5	JK	111	LYS
5	JK	115	THR
5	JK	119	TYR
5	JK	122	LYS
5	JK	137	SER
5	JK	156	THR
5	JK	159	LEU
5	JK	181	GLU
5	JK	183	THR
5	JK	188	VAL
3	Jd	38	THR
3	Jd	43	GLU
3	Jd	61	VAL
3	Jd	62	ILE
3	Jd	63	THR
3	Jd	71	LEU
3	Jd	78	ASN
3	Jd	91	ILE
3	Jd	109	LEU
3	Jd	117	VAL
3	Jd	118	LEU
3	Jd	135	ILE
3	Jd	154	VAL

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Mol	Chain	Res	Type
3	Jd	161	ILE
2	KC	61	GLU
2	KC	93	ILE
2	KC	117	LEU
2	KC	134	VAL
2	KC	173	LYS
2	KC	178	ILE
2	KC	180	THR
2	KC	190	GLN
2	KC	199	ILE
2	KC	211	LEU
2	KC	215	LEU
2	KC	222	SER
2	KC	243	ASP
2	KC	246	VAL
2	KC	256	ASN
2	KC	258	ASN
2	KC	266	VAL
3	KD	30	ILE
3	KD	39	ILE
3	KD	58	VAL
3	KD	62	ILE
3	KD	63	THR
3	KD	85	VAL
3	KD	94	LEU
3	KD	108	VAL
3	KD	115	VAL
3	KD	117	VAL
3	KD	121	ILE
3	KD	127	SER
4	KH	288	VAL
4	KH	298	VAL
4	KH	309	ASN
4	KH	314	VAL
4	KH	316	THR
4	KH	343	SER
4	KH	345	VAL
4	KH	349	SER
4	KH	359	VAL
5	KK	43	CYS
5	KK	46	ASP
5	KK	75	LEU

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Mol	Chain	Res	Type
5	KK	78	ILE
5	KK	86	ASP
5	KK	95	SER
5	KK	119	TYR
5	KK	122	LYS
5	KK	125	SER
5	KK	132	LEU
5	KK	141	SER
5	KK	175	SER
5	KK	183	THR
3	Kd	38	THR
3	Kd	43	GLU
3	Kd	62	ILE
3	Kd	63	THR
3	Kd	72	THR
3	Kd	78	ASN
3	Kd	84	SER
3	Kd	85	VAL
3	Kd	86	ASP
3	Kd	115	VAL
3	Kd	120	SER
3	Kd	144	SER
3	Kd	161	ILE
2	LC	81	GLU
2	LC	116	THR
2	LC	134	VAL
2	LC	153	MET
2	LC	154	ASP
2	LC	173	LYS
2	LC	180	THR
2	LC	185	LYS
2	LC	189	ASP
2	LC	199	ILE
2	LC	221	VAL
2	LC	229	THR
2	LC	246	VAL
2	LC	256	ASN
2	LC	258	ASN
3	LD	30	ILE
3	LD	53	LEU
3	LD	54	GLU
3	LD	58	VAL

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Mol	Chain	Res	Type
3	LD	61	VAL
3	LD	63	THR
3	LD	70	THR
3	LD	84	SER
3	LD	85	VAL
3	LD	98	ILE
3	LD	108	VAL
3	LD	115	VAL
3	LD	123	THR
3	LD	127	SER
3	LD	147	VAL
3	LD	153	VAL
3	LD	157	ARG
4	LH	286	GLU
4	LH	288	VAL
4	LH	293	SER
4	LH	297	VAL
4	LH	299	SER
4	LH	309	ASN
4	LH	317	ASN
4	LH	318	LEU
4	LH	320	ILE
4	LH	322	SER
4	LH	328	SER
4	LH	340	MET
4	LH	343	SER
4	LH	347	LEU
4	LH	349	SER
4	LH	354	VAL
5	LK	43	CYS
5	LK	46	ASP
5	LK	67	VAL
5	LK	70	VAL
5	LK	76	ILE
5	LK	95	SER
5	LK	102	ILE
5	LK	115	THR
5	LK	119	TYR
5	LK	120	SER
5	LK	132	LEU
5	LK	137	SER
5	LK	166	THR

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Mol	Chain	Res	Type
5	LK	170	LEU
5	LK	183	THR
5	LK	188	VAL
3	Ld	34	SER
3	Ld	36	ASP
3	Ld	48	VAL
3	Ld	61	VAL
3	Ld	62	ILE
3	Ld	63	THR
3	Ld	72	THR
3	Ld	115	VAL
3	Ld	117	VAL
3	Ld	122	SER
3	Ld	127	SER
3	Ld	154	VAL
2	MC	91	ASP
2	MC	134	VAL
2	MC	143	THR
2	MC	175	ILE
2	MC	177	CYS
2	MC	180	THR
2	MC	211	LEU
2	MC	215	LEU
2	MC	229	THR
2	MC	231	LEU
2	MC	239	GLU
2	MC	246	VAL
2	MC	255	LEU
2	MC	258	ASN
2	MC	268	LYS
3	MD	30	ILE
3	MD	51	SER
3	MD	58	VAL
3	MD	63	THR
3	MD	70	THR
3	MD	84	SER
3	MD	85	VAL
3	MD	108	VAL
3	MD	115	VAL
3	MD	117	VAL
3	MD	120	SER
3	MD	123	THR

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Mol	Chain	Res	Type
3	MD	126	GLU
3	MD	146	HIS
3	MD	147	VAL
3	MD	150	ASN
4	MH	280	LEU
4	MH	288	VAL
4	MH	297	VAL
4	MH	304	ARG
4	MH	307	LEU
4	MH	309	ASN
4	MH	317	ASN
4	MH	318	LEU
4	MH	322	SER
4	MH	340	MET
4	MH	342	LYS
4	MH	343	SER
4	MH	347	LEU
4	MH	349	SER
4	MH	359	VAL
5	MK	46	ASP
5	MK	50	ASP
5	MK	53	ILE
5	MK	78	ILE
5	MK	81	SER
5	MK	88	SER
5	MK	92	ASN
5	MK	115	THR
5	MK	116	VAL
5	MK	119	TYR
5	MK	122	LYS
5	MK	125	SER
5	MK	141	SER
5	MK	156	THR
5	MK	159	LEU
5	MK	161	SER
5	MK	180	VAL
5	MK	183	THR
5	MK	188	VAL
3	Md	38	THR
3	Md	48	VAL
3	Md	61	VAL
3	Md	63	THR

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Mol	Chain	Res	Type
3	Md	67	LYS
3	Md	71	LEU
3	Md	75	ASN
3	Md	82	ARG
3	Md	84	SER
3	Md	85	VAL
3	Md	88	SER
3	Md	92	GLU
3	Md	98	ILE
3	Md	117	VAL
3	Md	120	SER
3	Md	127	SER
3	Md	131	ILE
3	Md	135	ILE
3	Md	144	SER
3	Md	151	SER
3	Md	153	VAL
3	Md	155	GLU
6	N	101	SER
6	N	130	ASP
6	N	134	MET
6	N	143	ILE
6	N	155	LEU
6	N	162	THR
6	N	169	THR
6	N	210	ASP
6	N	230	GLU
6	O	101	SER
6	O	108	ASP
6	O	117	VAL
6	O	130	ASP
6	O	143	ILE
6	O	155	LEU
6	O	162	THR
6	O	174	SER
6	O	202	ARG
6	O	219	ILE
6	O	226	ASN
6	P	101	SER
6	P	117	VAL
6	P	124	THR
6	P	143	ILE

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Mol	Chain	Res	Type
6	P	155	LEU
6	P	169	THR
6	P	174	SER
6	P	181	LEU
6	P	196	ASN
6	P	210	ASP
6	Q	108	ASP
6	Q	129	THR
6	Q	143	ILE
6	Q	162	THR
6	Q	174	SER
6	Q	181	LEU
6	Q	210	ASP
6	Q	219	ILE
6	Q	223	SER
6	R	122	THR
6	R	130	ASP
6	R	143	ILE
6	R	154	LEU
6	R	155	LEU
6	R	169	THR
6	R	174	SER
6	R	181	LEU
6	R	230	GLU
6	S	101	SER
6	S	108	ASP
6	S	130	ASP
6	S	140	LEU
6	S	165	VAL
6	S	174	SER
6	S	181	LEU
6	S	182	SER
6	S	210	ASP
6	S	223	SER
6	T	108	ASP
6	T	121	ASP
6	T	130	ASP
6	T	134	MET
6	T	136	SER
6	T	143	ILE
6	T	155	LEU
6	T	162	THR

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Mol	Chain	Res	Type
6	T	172	VAL
6	T	181	LEU
6	T	196	ASN
6	T	210	ASP
6	T	219	ILE
6	U	117	VAL
6	U	130	ASP
6	U	134	MET
6	U	143	ILE
6	U	144	CYS
6	U	155	LEU
6	U	169	THR
6	U	174	SER
6	U	210	ASP
6	V	130	ASP
6	V	134	MET
6	V	140	LEU
6	V	143	ILE
6	V	154	LEU
6	V	162	THR
6	V	169	THR
6	V	172	VAL
6	V	174	SER
6	V	210	ASP
6	V	211	LYS
6	V	219	ILE
6	W	101	SER
6	W	121	ASP
6	W	143	ILE
6	W	154	LEU
6	W	162	THR
6	W	174	SER
6	W	181	LEU
6	W	210	ASP
6	X	108	ASP
6	X	126	ILE
6	X	130	ASP
6	X	143	ILE
6	X	162	THR
6	X	210	ASP
6	X	211	LYS
6	X	219	ILE

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Mol	Chain	Res	Type
6	Y	108	ASP
6	Y	124	THR
6	Y	126	ILE
6	Y	129	THR
6	Y	130	ASP
6	Y	134	MET
6	Y	150	ASN
6	Y	155	LEU
6	Y	169	THR
6	Y	174	SER
6	Y	181	LEU
6	Y	219	ILE
6	Y	226	ASN
6	Z	101	SER
6	Z	108	ASP
6	Z	118	GLU
6	Z	130	ASP
6	Z	139	ARG
6	Z	140	LEU
6	Z	143	ILE
6	Z	162	THR
6	Z	165	VAL
6	Z	172	VAL
6	Z	174	SER
6	Z	181	LEU
6	Z	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
2	AC	82	GLN
2	AC	97	ASN
2	AC	103	HIS
2	AC	241	HIS
2	AC	256	ASN
3	AD	80	GLN
3	AD	152	GLN
5	AK	87	GLN
5	AK	147	GLN
3	Ad	152	GLN
2	BC	82	GLN
2	BC	103	HIS

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Mol	Chain	Res	Type
2	BC	104	ASN
3	BD	80	GLN
3	BD	138	GLN
3	BD	152	GLN
3	Bd	152	GLN
2	CC	228	HIS
2	CC	256	ASN
3	CD	152	GLN
5	CK	100	ASN
5	CK	147	GLN
3	Cd	75	ASN
3	Cd	78	ASN
3	Cd	152	GLN
2	DC	97	ASN
2	DC	103	HIS
2	DC	104	ASN
2	DC	190	GLN
3	DD	80	GLN
3	DD	152	GLN
5	DK	87	GLN
5	DK	100	ASN
5	DK	147	GLN
3	Dd	152	GLN
2	EC	103	HIS
2	EC	115	ASN
3	ED	80	GLN
3	ED	138	GLN
3	ED	152	GLN
5	EK	87	GLN
5	EK	100	ASN
5	EK	147	GLN
3	Ed	31	ASN
3	Ed	32	ASN
3	Ed	152	GLN
2	FC	256	ASN
2	FC	258	ASN
3	FD	80	GLN
3	FD	103	HIS
3	FD	138	GLN
3	FD	152	GLN
5	FK	108	GLN
5	FK	147	GLN

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Mol	Chain	Res	Type
3	Fd	32	ASN
2	GC	89	ASN
2	GC	103	HIS
2	GC	104	ASN
2	GC	190	GLN
2	GC	258	ASN
3	GD	80	GLN
3	GD	138	GLN
3	GD	152	GLN
4	GH	341	GLN
5	GK	100	ASN
5	GK	147	GLN
3	Gd	103	HIS
2	HC	82	GLN
2	HC	256	ASN
3	HD	80	GLN
3	HD	138	GLN
3	HD	152	GLN
5	HK	61	ASN
5	HK	147	GLN
3	Hd	31	ASN
2	IC	103	HIS
2	IC	118	ASN
3	ID	80	GLN
3	ID	138	GLN
3	ID	152	GLN
5	IK	72	GLN
5	IK	87	GLN
5	IK	108	GLN
5	IK	147	GLN
3	Id	80	GLN
3	Id	103	HIS
3	Id	152	GLN
2	JC	97	ASN
2	JC	103	HIS
2	JC	123	GLN
2	JC	256	ASN
3	JD	75	ASN
3	JD	138	GLN
3	JD	152	GLN
5	JK	87	GLN
5	JK	100	ASN

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Mol	Chain	Res	Type
5	JK	108	GLN
3	Jd	31	ASN
3	Jd	32	ASN
3	Jd	78	ASN
2	KC	97	ASN
2	KC	123	GLN
2	KC	228	HIS
3	KD	80	GLN
3	KD	138	GLN
5	KK	87	GLN
5	KK	108	GLN
5	KK	147	GLN
3	Kd	32	ASN
3	Kd	152	GLN
2	LC	97	ASN
2	LC	103	HIS
2	LC	123	GLN
2	LC	139	HIS
3	LD	75	ASN
3	LD	80	GLN
3	LD	138	GLN
3	LD	152	GLN
5	LK	87	GLN
5	LK	100	ASN
5	LK	147	GLN
3	Ld	32	ASN
3	Ld	152	GLN
2	MC	103	HIS
2	MC	192	ASN
3	MD	80	GLN
3	MD	138	GLN
4	MH	283	HIS
5	MK	108	GLN
5	MK	147	GLN
3	Md	32	ASN
3	Md	78	ASN
3	Md	150	ASN
6	N	115	GLN
6	N	141	ASN
6	N	150	ASN
6	N	156	ASN
6	N	177	HIS

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Mol	Chain	Res	Type
6	N	212	ASN
6	N	232	GLN
6	O	141	ASN
6	O	185	GLN
6	O	212	ASN
6	O	232	GLN
6	P	141	ASN
6	P	149	ASN
6	P	177	HIS
6	P	185	GLN
6	P	212	ASN
6	P	232	GLN
6	Q	150	ASN
6	Q	232	GLN
6	R	112	GLN
6	R	149	ASN
6	R	156	ASN
6	R	177	HIS
6	R	185	GLN
6	R	196	ASN
6	R	212	ASN
6	R	232	GLN
6	S	141	ASN
6	S	150	ASN
6	S	177	HIS
6	S	185	GLN
6	S	212	ASN
6	S	232	GLN
6	T	112	GLN
6	T	141	ASN
6	T	149	ASN
6	T	150	ASN
6	T	177	HIS
6	T	212	ASN
6	T	232	GLN
6	U	112	GLN
6	U	141	ASN
6	U	150	ASN
6	U	177	HIS
6	U	185	GLN
6	U	212	ASN
6	U	232	GLN

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Mol	Chain	Res	Type
6	V	112	GLN
6	V	150	ASN
6	V	177	HIS
6	V	212	ASN
6	V	232	GLN
6	W	112	GLN
6	W	177	HIS
6	W	185	GLN
6	W	212	ASN
6	W	221	HIS
6	W	232	GLN
6	X	112	GLN
6	X	149	ASN
6	X	150	ASN
6	X	177	HIS
6	X	185	GLN
6	X	196	ASN
6	X	212	ASN
6	X	232	GLN
6	Y	150	ASN
6	Y	185	GLN
6	Y	196	ASN
6	Y	212	ASN
6	Y	232	GLN
6	Z	112	GLN
6	Z	149	ASN
6	Z	212	ASN
6	Z	232	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

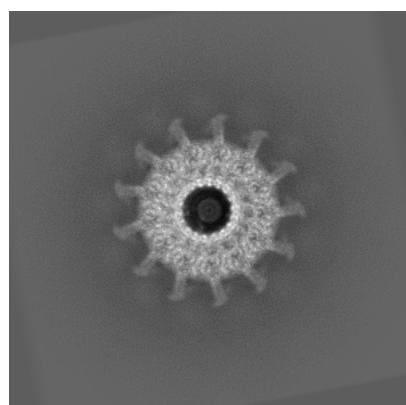
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22070. These allow visual inspection of the internal detail of the map and identification of artifacts.

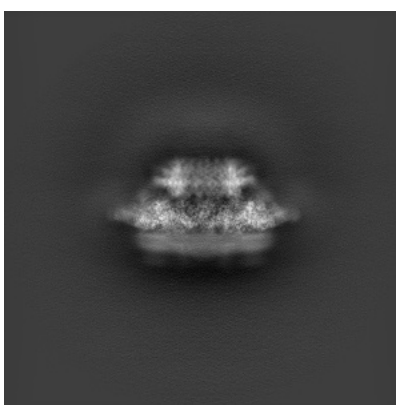
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

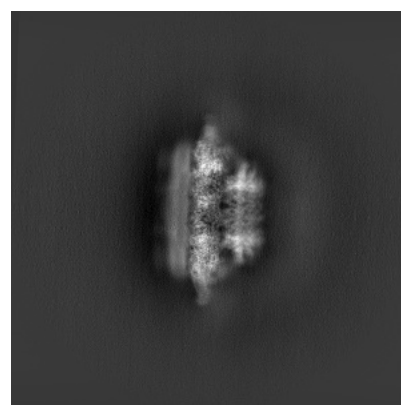
6.1.1 Primary map



X



Y

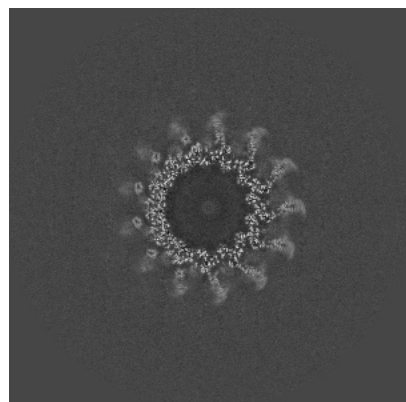


Z

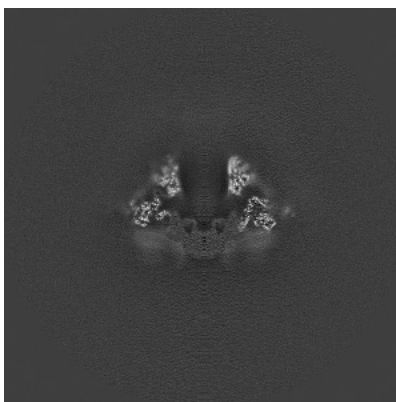
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

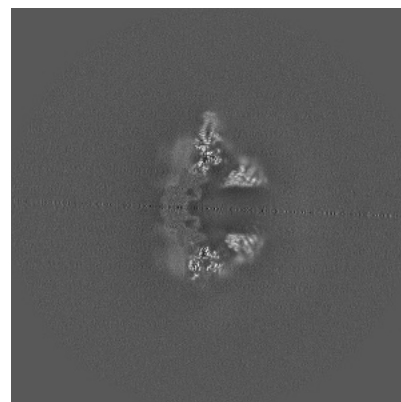
6.2.1 Primary map



X Index: 255



Y Index: 255

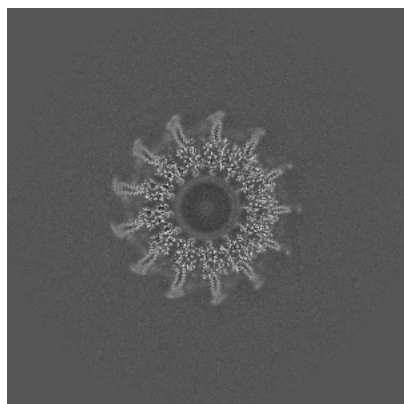


Z Index: 255

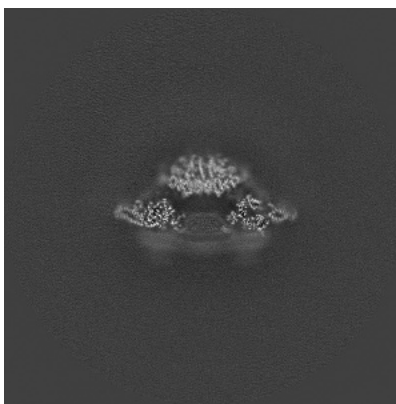
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

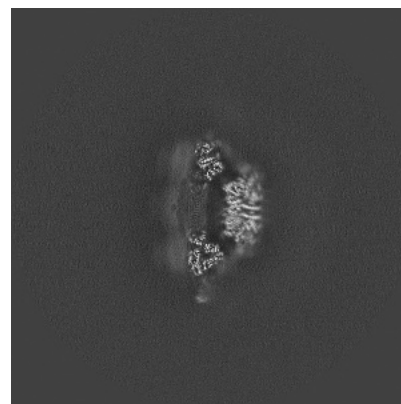
6.3.1 Primary map



X Index: 245



Y Index: 218

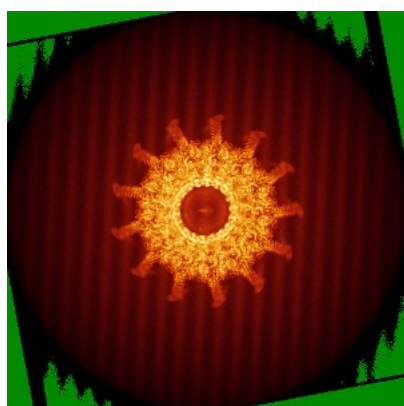


Z Index: 288

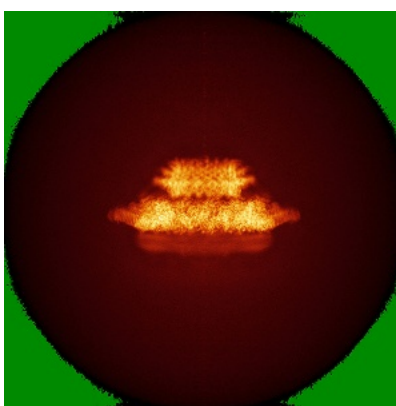
The images above show the largest variance slices of the map in three orthogonal directions.

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

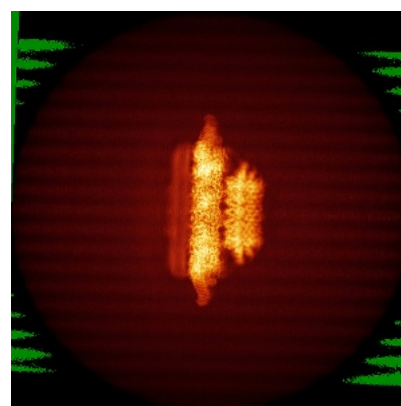
6.4.1 Primary map



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

This section was not generated.

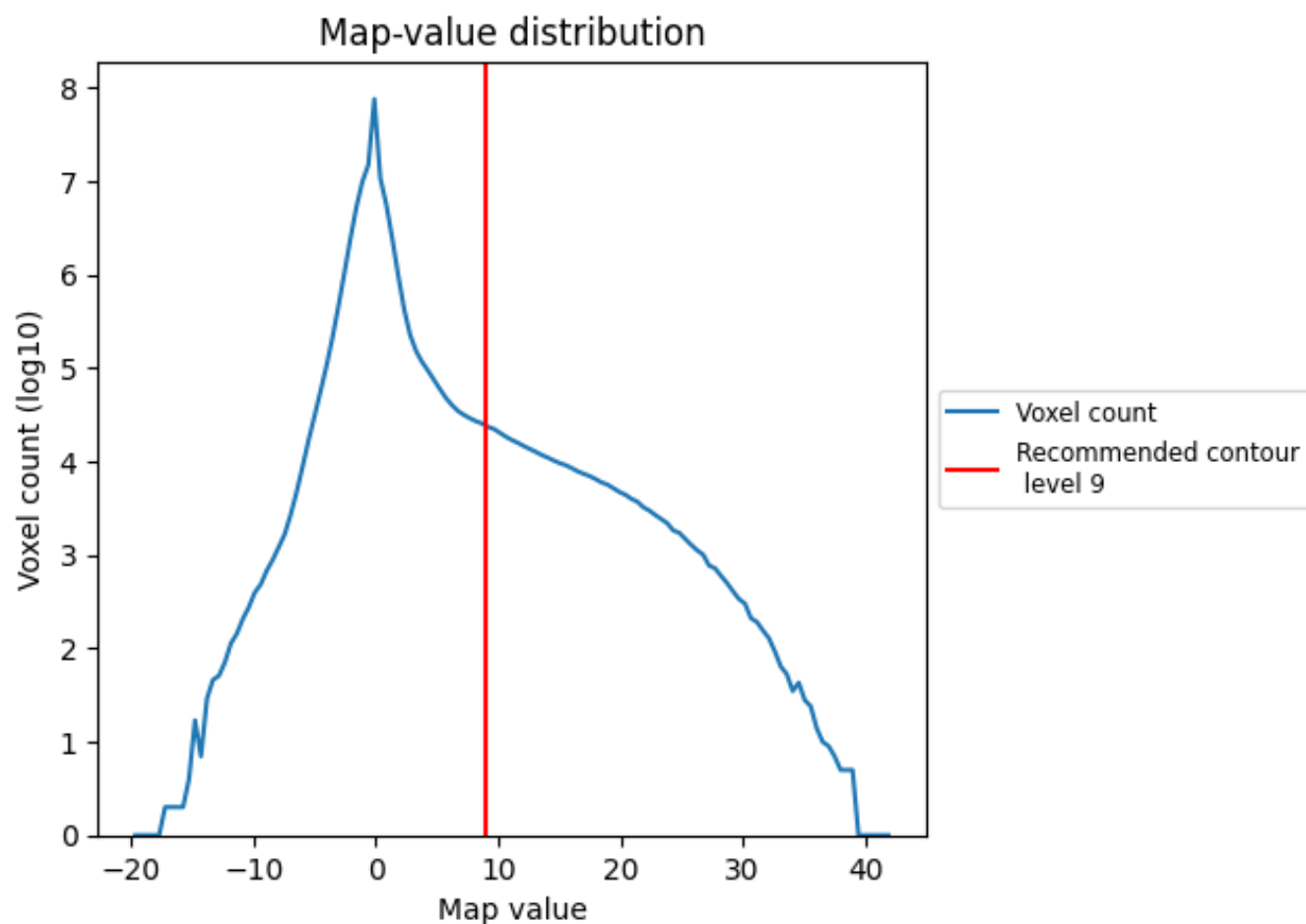
6.6 Mask visualisation

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

7 Map analysis [i](#)

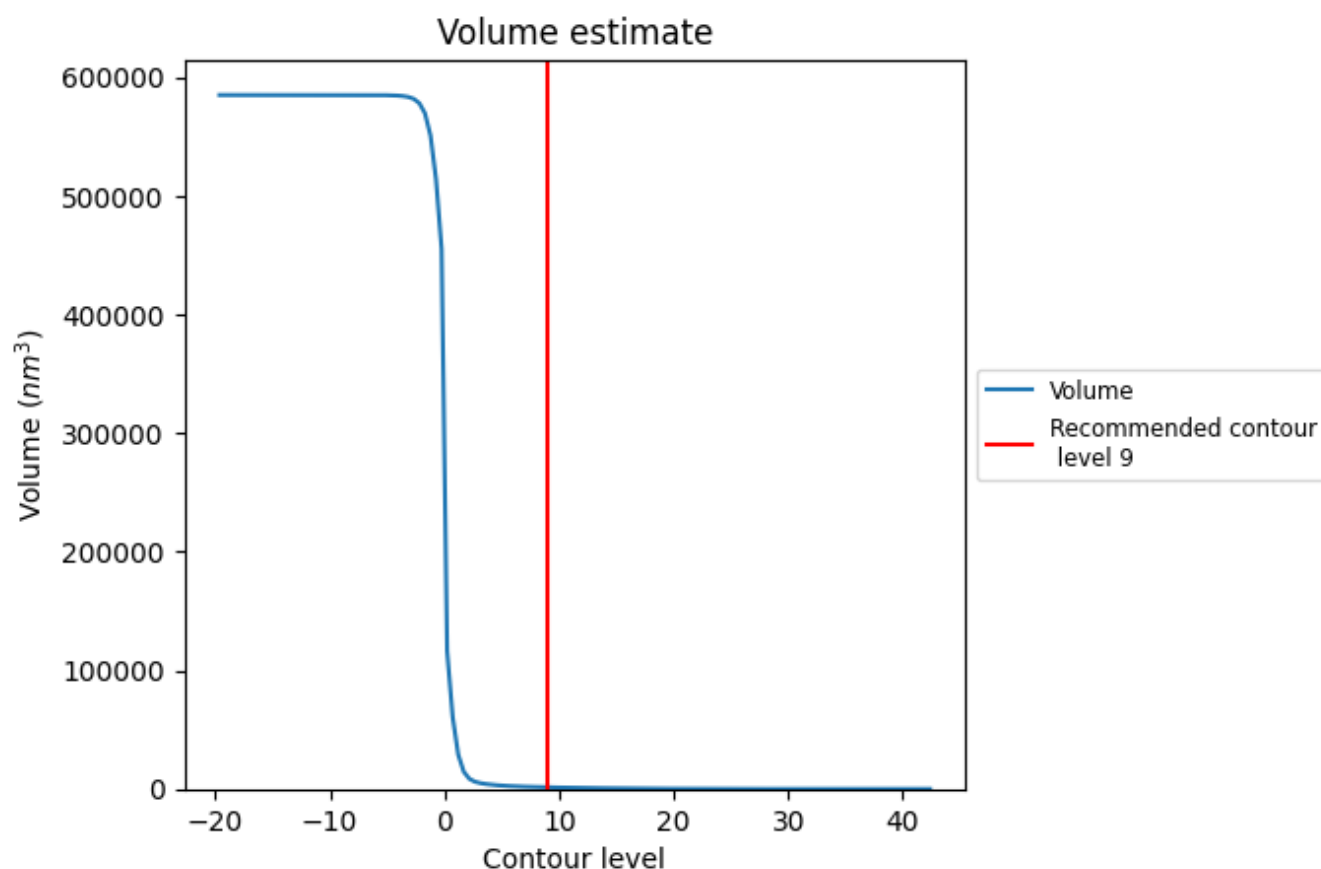
This section contains the results of statistical analysis of the map.

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.

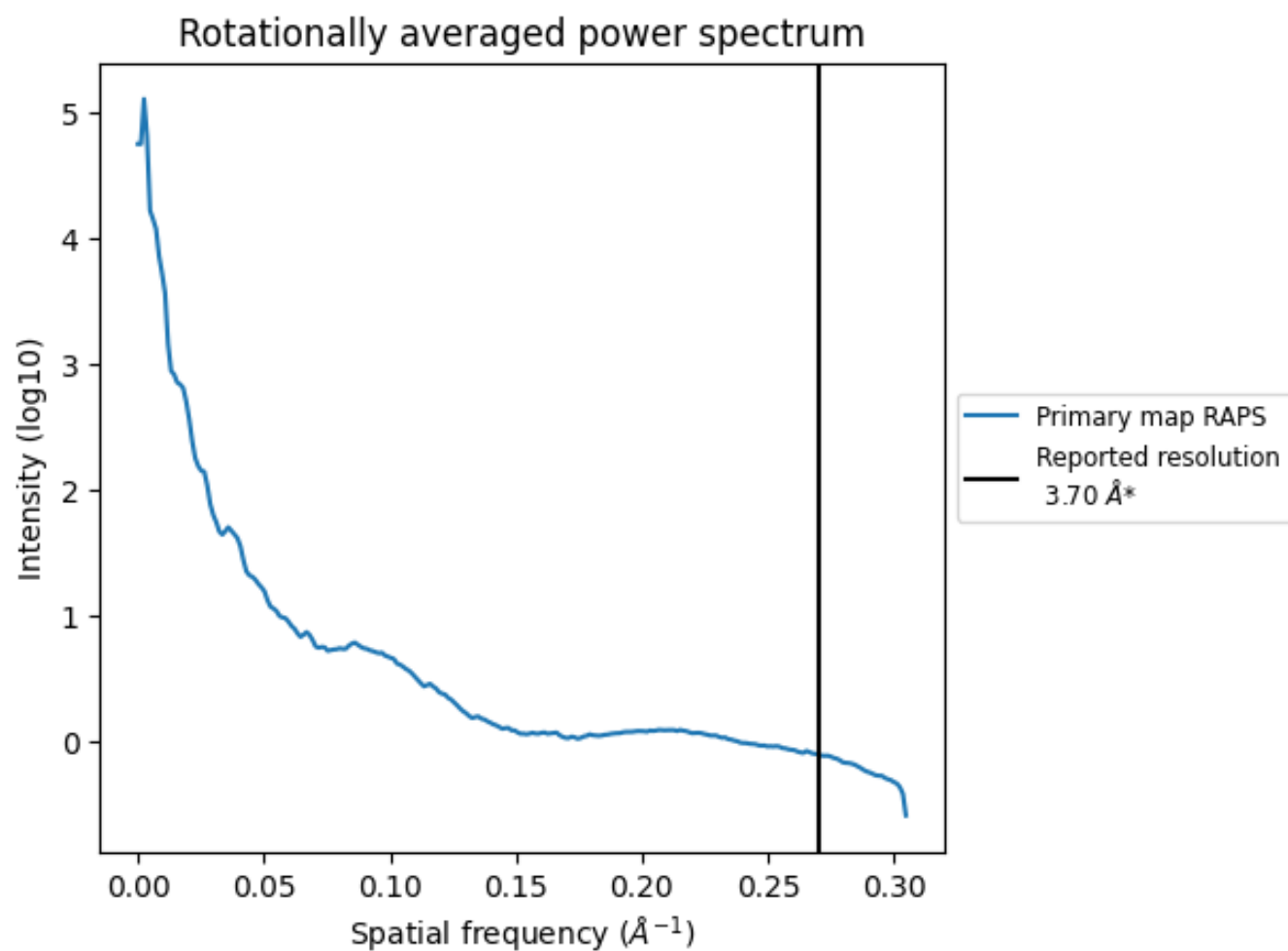
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1402 nm³; this corresponds to an approximate mass of 1266 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 0.270 Å⁻¹

8 Fourier-Shell correlation

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

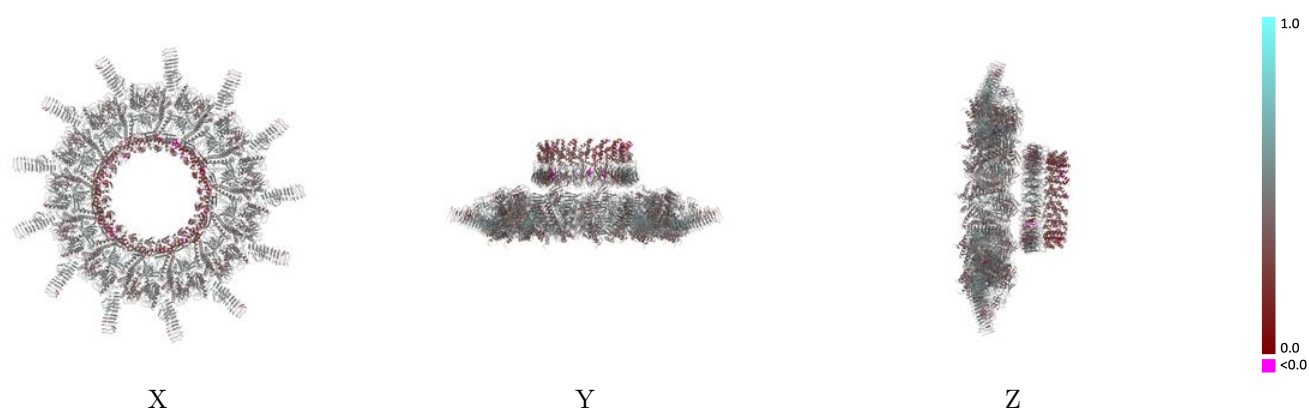
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22070 and PDB model 6X65. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)

This section was not generated.

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

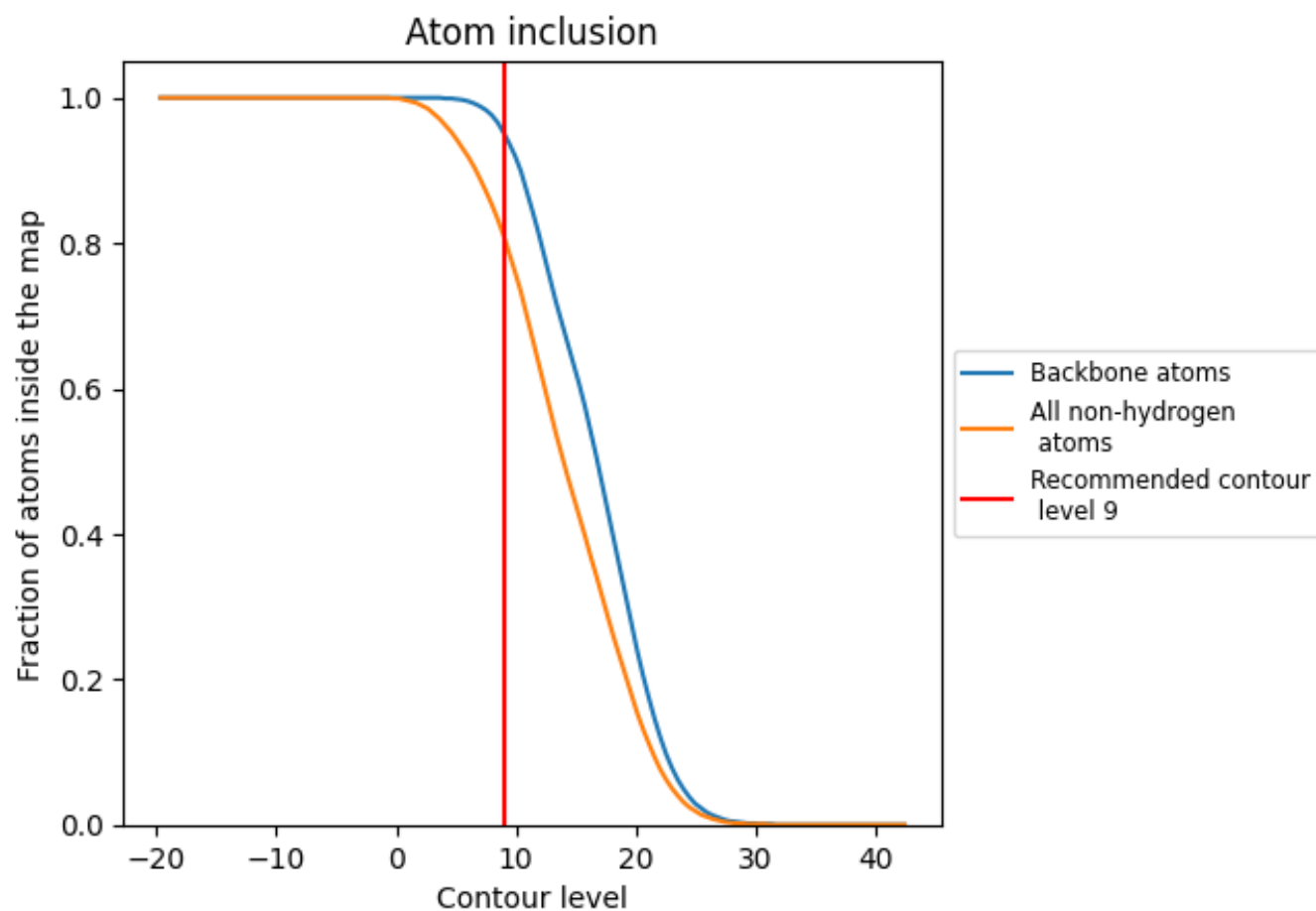


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.4470
AC	 0.7620	 0.4530
AD	 0.7180	 0.4220
AH	 0.8070	 0.5070
AK	 0.7700	 0.4580
AV	 0.9760	 0.3580
AW	 0.9810	 0.3400
AX	 0.8610	 0.4630
AY	 0.8460	 0.4500
AZ	 0.8860	 0.5180
Ad	 0.7510	 0.4540
BC	 0.7660	 0.4570
BD	 0.7250	 0.4290
BH	 0.8150	 0.5090
BK	 0.7620	 0.4450
BV	 0.9610	 0.2800
BW	 0.9630	 0.3040
BX	 0.8580	 0.4760
BY	 0.8420	 0.4470
BZ	 0.8970	 0.5160
Bd	 0.7500	 0.4560
CC	 0.7700	 0.4530
CD	 0.7230	 0.4170
CH	 0.7950	 0.5060
CK	 0.7660	 0.4510
CV	 0.9810	 0.3860
CW	 0.9750	 0.3280
CX	 0.8590	 0.4620
CY	 0.8580	 0.4410
CZ	 0.8910	 0.5130
Cd	 0.7430	 0.4470
DC	 0.7690	 0.4560
DD	 0.7290	 0.4350
DH	 0.8070	 0.5020
DK	 0.7620	 0.4540



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Chain	Atom inclusion	Q-score
DV	 0.9820	 0.3910
DW	 0.9380	 0.3030
DX	 0.8540	 0.4700
DY	 0.8500	 0.4410
DZ	 0.9030	 0.5150
Dd	 0.7640	 0.4570
EC	 0.7670	 0.4590
ED	 0.7260	 0.4310
EH	 0.7970	 0.4990
EK	 0.7700	 0.4520
EV	 0.9390	 0.2740
EW	 0.9690	 0.3310
EX	 0.8590	 0.4730
EY	 0.8500	 0.4540
EZ	 0.9090	 0.5190
Ed	 0.7430	 0.4570
FC	 0.7760	 0.4610
FD	 0.7150	 0.4230
FH	 0.7980	 0.5080
FK	 0.7700	 0.4530
FV	 0.9360	 0.2930
FW	 0.8750	 0.2360
FX	 0.8500	 0.4730
FY	 0.8350	 0.4580
FZ	 0.9060	 0.5080
Fd	 0.7460	 0.4580
GC	 0.7720	 0.4620
GD	 0.7200	 0.4230
GH	 0.7980	 0.5090
GK	 0.7740	 0.4550
GV	 0.9960	 0.4300
GW	 0.9560	 0.2900
GX	 0.8500	 0.4690
GY	 0.8460	 0.4480
GZ	 0.8860	 0.5140
Gd	 0.7550	 0.4670
HC	 0.7700	 0.4600
HD	 0.7350	 0.4330
HH	 0.8040	 0.5030
HK	 0.7660	 0.4490
HV	 0.9960	 0.4550
HW	 0.9440	 0.3390

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Chain	Atom inclusion	Q-score
HX	 0.8570	 0.4730
HY	 0.8540	 0.4360
HZ	 0.8890	 0.5010
Hd	 0.7470	 0.4510
IC	 0.7680	 0.4600
ID	 0.7170	 0.4300
IH	 0.7950	 0.4980
IK	 0.7720	 0.4530
IV	 0.9860	 0.4410
IW	 0.9940	 0.3720
IX	 0.8580	 0.4700
IY	 0.8540	 0.4480
IZ	 0.8860	 0.5150
Id	 0.7450	 0.4550
JC	 0.7660	 0.4510
JD	 0.7270	 0.4290
JH	 0.8010	 0.5050
JK	 0.7570	 0.4510
JV	 0.9460	 0.2930
JW	 0.9750	 0.3670
JX	 0.8490	 0.4680
JY	 0.8390	 0.4440
JZ	 0.8910	 0.5080
Jd	 0.7560	 0.4580
KC	 0.7680	 0.4570
KD	 0.7250	 0.4320
KH	 0.7980	 0.5070
KK	 0.7640	 0.4470
KV	 0.9690	 0.3160
KW	 0.9500	 0.3300
KX	 0.8580	 0.4710
KY	 0.8310	 0.4380
KZ	 0.9030	 0.5180
Kd	 0.7460	 0.4560
LC	 0.7750	 0.4550
LD	 0.7210	 0.4250
LH	 0.8060	 0.5050
LK	 0.7590	 0.4500
LV	 0.9940	 0.3760
LW	 0.9690	 0.3240
LX	 0.8610	 0.4700
LY	 0.8460	 0.4470

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Chain	Atom inclusion	Q-score
LZ	 0.8890	 0.5160
Ld	 0.7420	 0.4470
MC	 0.7610	 0.4620
MD	 0.7200	 0.4260
MH	 0.8150	 0.5050
MK	 0.7590	 0.4450
MV	 0.9960	 0.4090
MW	 0.9690	 0.3240
MX	 0.8550	 0.4660
MY	 0.8690	 0.4590
MZ	 0.8970	 0.5130
Md	 0.7490	 0.4500
N	 0.7830	 0.4560
NV	 0.9890	 0.3740
NW	 0.9500	 0.2530
O	 0.7820	 0.4500
OV	 0.9360	 0.3130
OW	 0.8870	 0.2990
P	 0.7900	 0.4660
PV	 0.9930	 0.4050
PW	 0.9560	 0.3400
Q	 0.7850	 0.4570
QV	 0.9970	 0.4140
QW	 0.9940	 0.3590
R	 0.7810	 0.4480
RV	 0.9960	 0.4260
RW	 0.9880	 0.3870
S	 0.7710	 0.4430
T	 0.7790	 0.4540
U	 0.7700	 0.4440
V	 0.7710	 0.4440
W	 0.7870	 0.4550
X	 0.7810	 0.4560
Y	 0.7880	 0.4600
Z	 0.7740	 0.4420