



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:24 PM UTC

PDB ID : 7MUD / pdb_00007mud
EMDB ID : EMD-24005
Title : Legionella pneumophila Dot/Icm T4SS OMC
Authors : Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.
Deposited on : 2021-05-14
Resolution : 2.80 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:

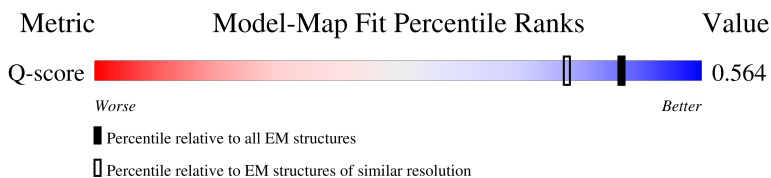
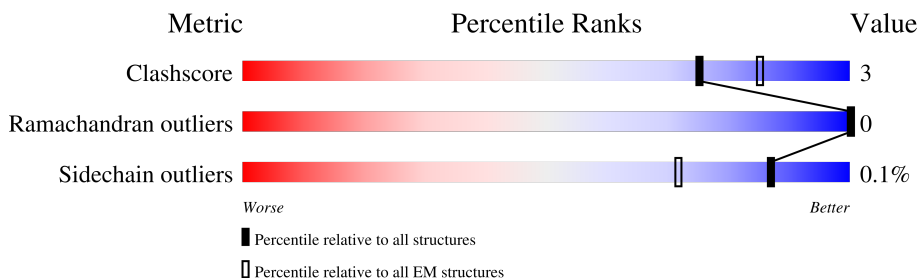
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.80 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	11806 (2.30 - 3.30)

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	AC	303	 64% 32%
1	BC	303	 64% 32%
1	CC	303	 62% 6% 32%
1	DC	303	 63% 5% 32%


























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Mol	Chain	Length	Quality of chain
1	EC	303	63% 5% 32%
1	FC	303	63% 5% 32%
1	GC	303	63% 5% 32%
1	HC	303	63% 5% 32%
1	IC	303	63% 5% 32%
1	JC	303	59% 9% 32%
1	KC	303	62% 6% 32%
1	LC	303	64% . 32%
1	MC	303	64% . 32%
2	AD	163	81% . 15%
2	Ad	163	81% . 17%
2	BD	163	78% 7% 15%
2	Bd	163	79% 5% 17%
2	CD	163	79% 6% 15%
2	Cd	163	79% . 17%
2	DD	163	82% . 15%
2	Dd	163	79% . 17%
2	ED	163	80% 5% 15%
2	Ed	163	76% 7% 17%
2	FD	163	77% 9% 15%
2	Fd	163	76% 7% 17%
2	GD	163	77% 8% 15%
2	Gd	163	77% 7% 17%
2	HD	163	79% 7% 15%
2	Hd	163	78% 6% 17%







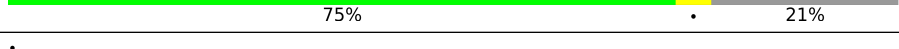
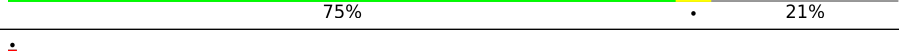
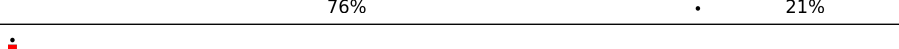
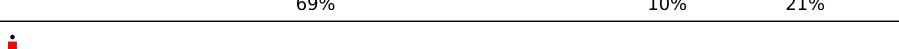
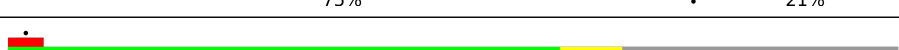

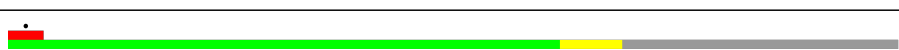

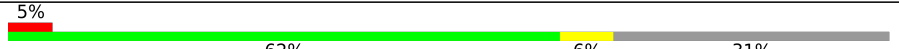





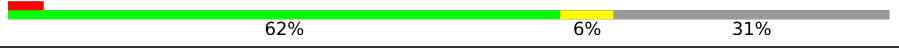
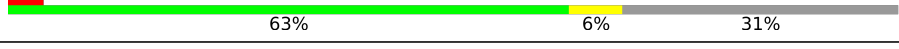



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Mol	Chain	Length	Quality of chain
2	ID	163	 80% 5% 15%
2	Id	163	 80% 5% 17%
2	JD	163	 77% 8% 15%
2	Jd	163	 80% 5% 17%
2	KD	163	 79% 6% 15%
2	Kd	163	 77% 6% 17%
2	LD	163	 81% 5% 15%
2	Ld	163	 78% 6% 17%
2	MD	163	 80% 5% 15%
2	Md	163	 82% 5% 17%
3	AH	361	 24% 5% 75%
3	BH	361	 22% 5% 75%
3	CH	361	 23% 5% 75%
3	DH	361	 24% 5% 75%
3	EH	361	 23% 5% 75%
3	FH	361	 24% 5% 75%
3	GH	361	 24% 5% 75%
3	HH	361	 23% 5% 75%
3	IH	361	 23% 5% 75%
3	JH	361	 24% 5% 75%
3	KH	361	 23% 5% 75%
3	LH	361	 24% 5% 75%
3	MH	361	 24% 5% 75%
4	AK	189	 72% 6% 21%
4	BK	189	 75% 5% 21%

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Mol	Chain	Length	Quality of chain
4	CK	189	 76% 21%
4	DK	189	 75% 21%
4	EK	189	 73% 6% 21%
4	FK	189	 76% 21%
4	GK	189	 72% 6% 21%
4	HK	189	 70% 8% 21%
4	IK	189	 75% 21%
4	JK	189	 75% 21%
4	KK	189	 76% 21%
4	LK	189	 69% 10% 21%
4	MK	189	 75% 21%
5	AL	249	 62% 7% 31%
5	BL	249	 62% 6% 31%
5	CL	249	 62% 7% 31%
5	DL	249	 63% 5% 31%
5	EL	249	 5% 62% 6% 31%
5	FL	249	 5% 62% 7% 31%
5	GL	249	 63% 6% 31%
5	HL	249	 63% 5% 31%
5	IL	249	 5% 63% 6% 31%
5	JL	249	 63% 6% 31%
5	KL	249	 62% 6% 31%
5	LL	249	 63% 6% 31%
5	ML	249	 63% 5% 31%
6	AM	320	 27% 73% 18% 9%

























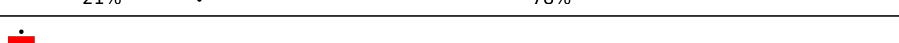
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Mol	Chain	Length	Quality of chain
6	BM	320	29% 76% 15% 9%
6	CM	320	29% 80% 11% 9%
6	DM	320	28% 79% 12% 9%
6	EM	320	28% 80% 12% 9%
6	FM	320	28% 77% 14% 9%
6	GM	320	28% 76% 15% 9%
6	HM	320	27% 76% 15% 9%
6	IM	320	27% 79% 12% 9%
6	JM	320	28% 76% 15% 9%
6	KM	320	29% 79% 12% 9%
6	LM	320	28% 79% 12% 9%
6	MM	320	28% 77% 15% 9%
7	AN	124	59% 39%
7	BN	124	57% 39%
7	CN	124	56% 6% 39%
7	DN	124	58% 39%
7	EN	124	58% 39%
7	FN	124	56% 5% 39%
7	GN	124	60% 39%
7	HN	124	57% 39%
7	IN	124	56% 5% 39%
7	JN	124	60% 39%
7	KN	124	58% 39%
7	LN	124	60% 39%
7	MN	124	57% 39%

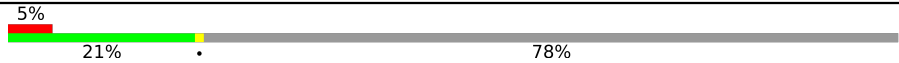
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Mol	Chain	Length	Quality of chain
8	AU	9	 100%
8	BU	9	 100%
8	CU	9	 100%
8	DU	9	 100%
8	EU	9	 100%
8	FU	9	 100%
8	GU	9	 100%
8	HU	9	 100%
8	IU	9	 100%
8	JU	9	 100%
8	KU	9	 100%
8	LU	9	 100%
8	MU	9	 100%
9	Af	269	 19% 78%
9	Bf	269	 21% 78%
9	Cf	269	 20% 78%
9	Df	269	 21% 78%
9	Ef	269	 19% 78%
9	Ff	269	 20% 78%
9	Gf	269	 20% 78%
9	Hf	269	 20% 78%
9	If	269	 21% 78%
9	Jf	269	 21% 78%
9	Kf	269	 21% 78%
9	Lf	269	 18% 78%

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Mol	Chain	Length	Quality of chain
9	Mf	269	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '5%', a green segment in the middle labeled '21%', and a grey segment on the right labeled '78%'. A small yellow dot is located at the end of the green segment.</p>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 134758 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 DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	BC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	CC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	DC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	EC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	FC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	GC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	HC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	IC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	JC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	KC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	LC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0
1	MC	206	Total 1634	C 1038	N 287	O 304	S 5	0	0

- Molecule 2 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AD	139	Total 1078	C 687	N 184	O 205	S 2	0	0
2	Ad	136	Total 1049	C 666	N 180	O 201	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Bd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	CD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Cd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	DD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Dd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	ED	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Ed	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	FD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Fd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	GD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Gd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	HD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Hd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	ID	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Id	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	JD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Jd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	KD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Kd	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	LD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ld	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
2	MD	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
2	Md	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		

- Molecule 3 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	BH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	CH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	DH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	EH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	FH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	GH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	HH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	IH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	JH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	KH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	LH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		
3	MH	91	Total	C	N	O	S	0	0
			690	440	121	125	4		

- Molecule 4 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	BK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	CK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	DK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	EK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	FK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	GK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	HK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	IK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	JK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	KK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	LK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
4	MK	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		

- Molecule 5 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	BL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	CL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	DL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	EL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	FL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	GL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	HL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	IL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	JL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	KL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	LL	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		
5	ML	171	Total	C	N	O	S	0	0
			1375	870	251	249	5		

- Molecule 6 is a protein called DUF2807 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	BM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	CM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	DM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	EM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	FM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	GM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	HM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	IM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	JM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	KM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	LM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		
6	MM	292	Total	C	N	O	S	0	0
			2320	1467	416	433	4		

- Molecule 7 is a protein called Neurogenic locus notch.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	BN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	CN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	DN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	EN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	FN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	GN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	HN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	IN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	JN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	KN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	LN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		
7	MN	76	Total	C	N	O	S	0	0
			565	347	96	109	13		

- Molecule 8 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AU	9	Total	C	N	O	0	0
			45	27	9	9		
8	BU	9	Total	C	N	O	0	0
			45	27	9	9		
8	CU	9	Total	C	N	O	0	0
			45	27	9	9		
8	DU	9	Total	C	N	O	0	0
			45	27	9	9		
8	EU	9	Total	C	N	O	0	0
			45	27	9	9		
8	FU	9	Total	C	N	O	0	0
			45	27	9	9		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	GU	9	45	27	9	9	0	0
8	HU	9	45	27	9	9	0	0
8	IU	9	45	27	9	9	0	0
8	JU	9	45	27	9	9	0	0
8	KU	9	45	27	9	9	0	0
8	LU	9	45	27	9	9	0	0
8	MU	9	45	27	9	9	0	0

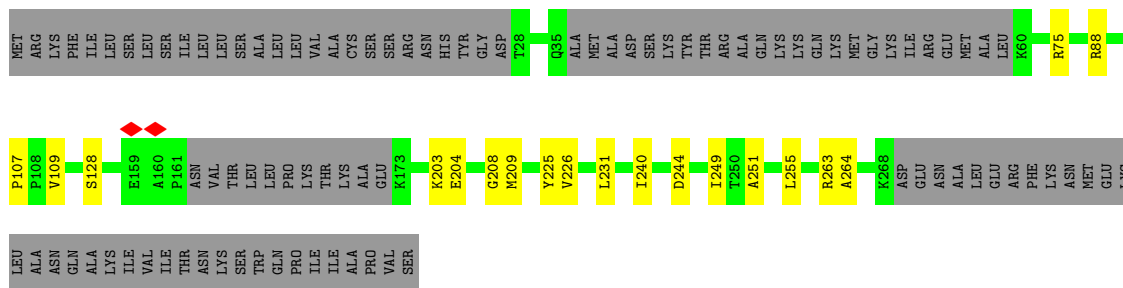
- Molecule 9 is a protein called DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Af	59	449	290	77	81	1	0	0
9	Bf	59	449	290	77	81	1	0	0
9	Cf	59	449	290	77	81	1	0	0
9	Df	59	449	290	77	81	1	0	0
9	Ef	59	449	290	77	81	1	0	0
9	Ff	59	449	290	77	81	1	0	0
9	Gf	59	449	290	77	81	1	0	0
9	Hf	59	449	290	77	81	1	0	0
9	If	59	449	290	77	81	1	0	0
9	Jf	59	449	290	77	81	1	0	0
9	Kf	59	449	290	77	81	1	0	0
9	Lf	59	449	290	77	81	1	0	0

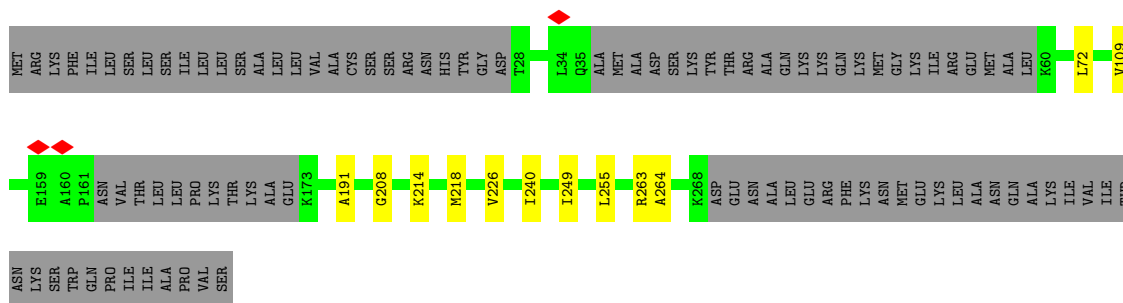
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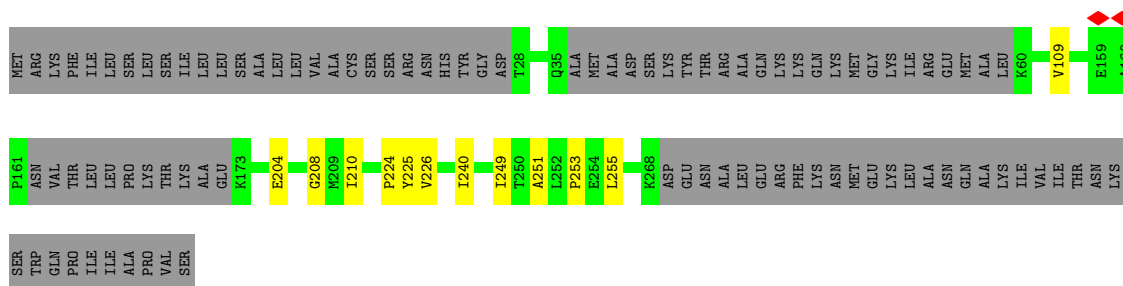
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Mf	59	449	290	77	81	1	0	0



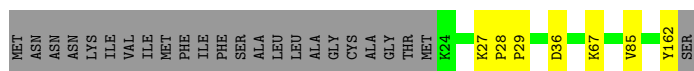
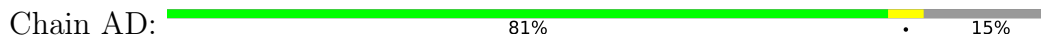
• Molecule 1: DotC



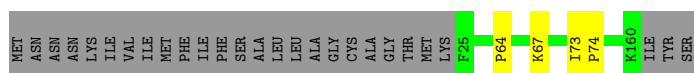
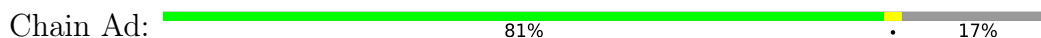
• Molecule 1: DotC



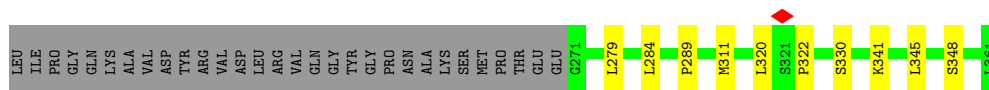
• Molecule 2: DotD



• Molecule 2: DotD



• Molecule 2: DotD



• Molecule 3: Type IV secretion protein IcmK

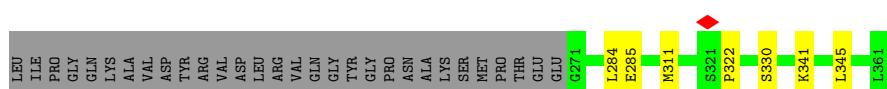


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GLY ASP GLY TYR ASN ASP ALA VAL VAL LYS SER THR GLN PRO GLN SER GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 ASP L279 ASP L284 GLN M311 P289 GLN L320 ARG S321 ARG S322 MET S330 LEU K341 VAL L345 SER S348 LEU L361 ALA

PRO LEU ASN PRO GLN VAL VAL LYS SER THR GLN PRO GLN SER GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 ASP L279 ASP L284 GLN M311 P289 GLN L320 ARG S321 ARG S322 MET S330 LEU K341 VAL L345 SER S348 LEU L361 ALA

PHE LEU ASP SER THR GLY ALA PRO PRO TRP ASP TRP ILE ILE TYR ASP GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 ASP L279 ASP L284 GLN M311 P289 GLN L320 ARG S321 ARG S322 MET S330 LEU K341 VAL L345 SER S348 LEU L361 ALA



• Molecule 3: Type IV secretion protein IcmK

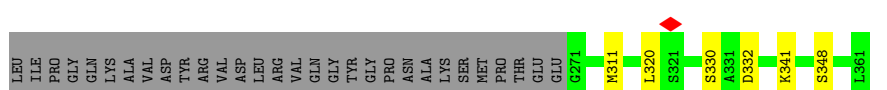


MET MET LYS LYS TYR GLN LYS ASP VAL ASP TRR ARG TRR CYS VAL ASP LEU ARG VAL ILE GLN GLN TYR PHE TYR SER PRO MET ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 ASP L284 E285 M311 S321 P322 S330 K341 L345 S348 L361 ALA

GLY ASP GLY TYR ASN ASP ALA VAL VAL LYS SER THR GLN PRO GLN SER GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 ASP L284 E285 M311 S321 P322 S330 K341 L345 S348 L361 ALA

PRO LEU ASN PRO GLN VAL VAL LYS SER THR GLN PRO GLN SER GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 ASP L284 E285 M311 S321 P322 S330 K341 L345 S348 L361 ALA

PHE LEU ASP SER THR GLY ALA PRO PRO TRP ASP TRP ILE ILE TYR ASP GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 ASP L284 E285 M311 S321 P322 S330 K341 L345 S348 L361 ALA



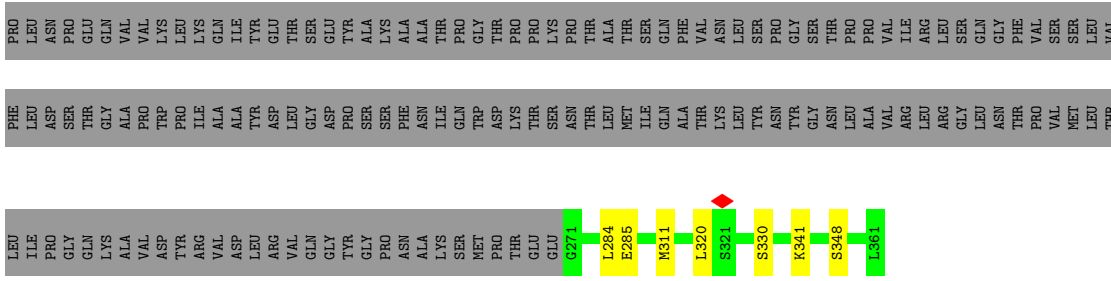
• Molecule 3: Type IV secretion protein IcmK



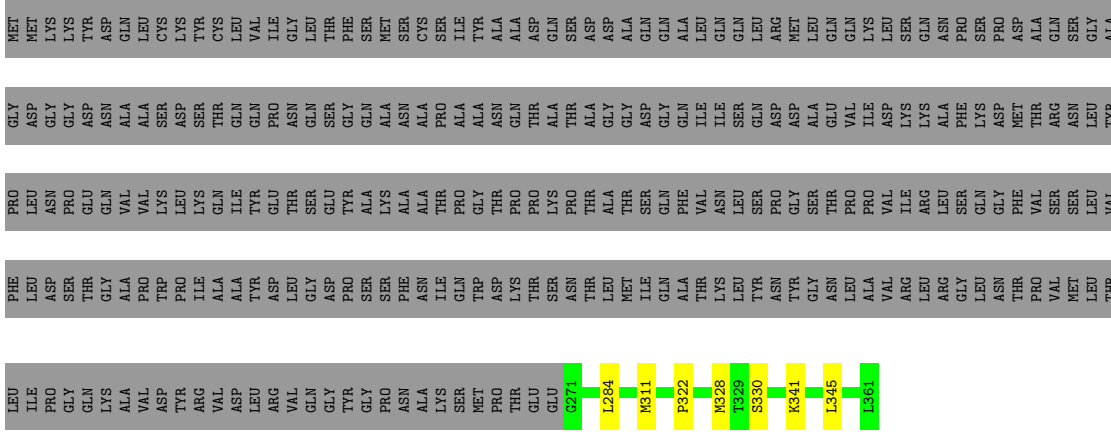
MET MET LYS LYS TYR GLN LYS ASP VAL ASP TRR ARG TRR CYS VAL ASP LEU ARG VAL ILE GLN GLN TYR PHE TYR SER PRO MET ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 M311 L320 S321 S330 D332 K341 S348 L361 ALA

GLY ASP GLY TYR ASN ASP ALA VAL VAL LYS SER THR GLN PRO GLN SER GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 M311 L320 S321 S330 D332 K341 S348 L361 ALA

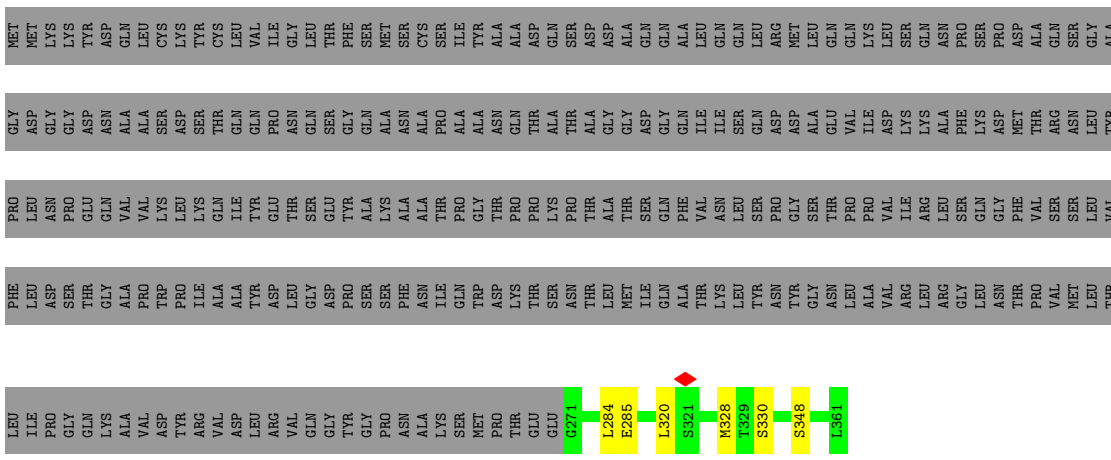
PRO LEU ASN PRO GLN VAL VAL LYS SER THR GLN PRO GLN SER GLY TYR PHE GLN MET LYS ASN CYS ALA CYS SER ILE MET TYR THR PRO THR GLU G271 M311 L320 S321 S330 D332 K341 S348 L361 ALA



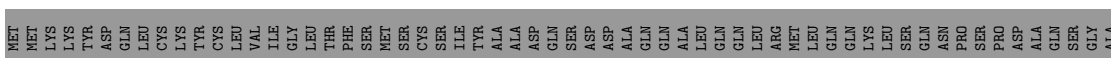
• Molecule 3: Type IV secretion protein IcmK

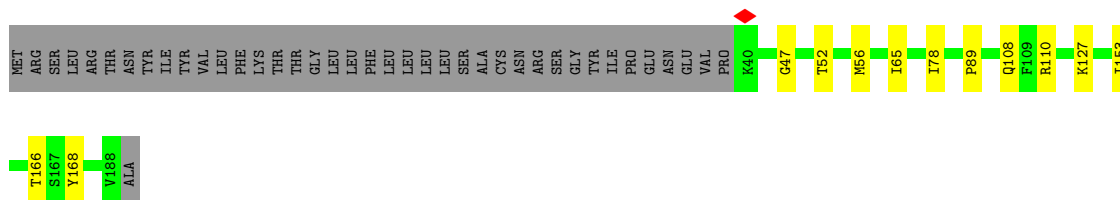


• Molecule 3: Type IV secretion protein IcmK

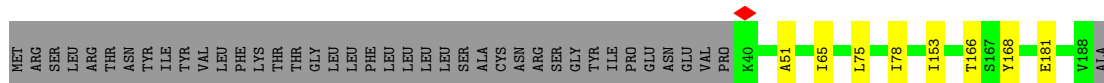
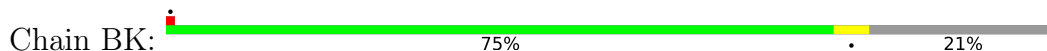


• Molecule 3: Type IV secretion protein IcmK

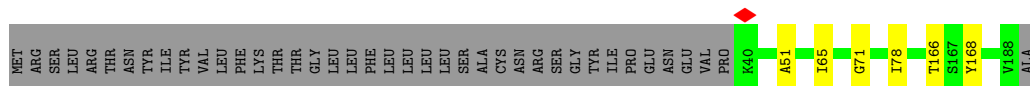
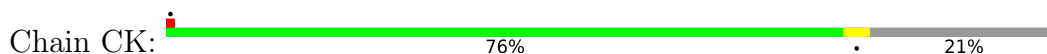




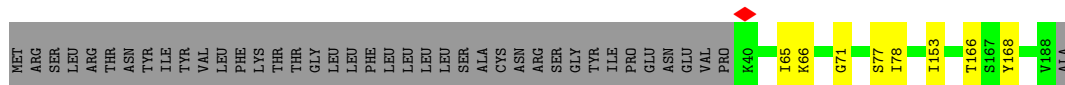
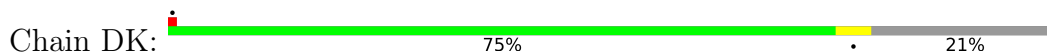
● Molecule 4: Inner membrane lipoprotein YiaD



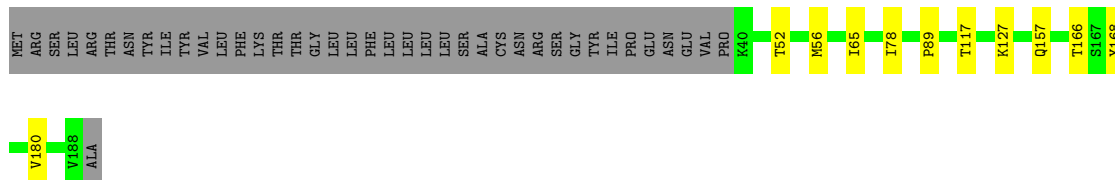
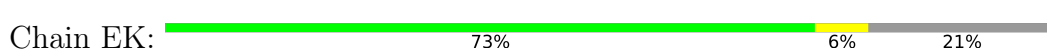
● Molecule 4: Inner membrane lipoprotein YiaD



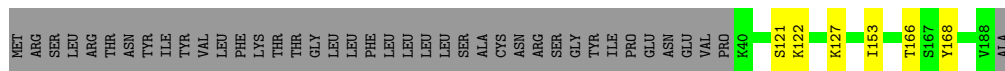
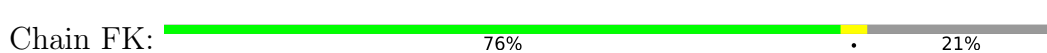
● Molecule 4: Inner membrane lipoprotein YiaD



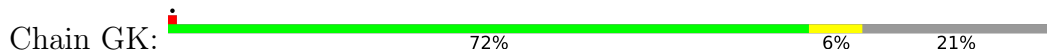
● Molecule 4: Inner membrane lipoprotein YiaD

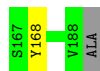
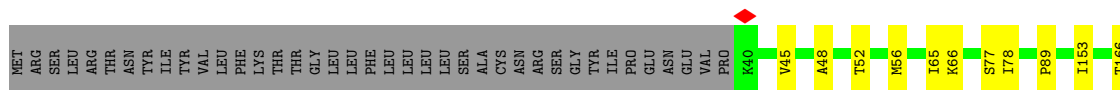


● Molecule 4: Inner membrane lipoprotein YiaD

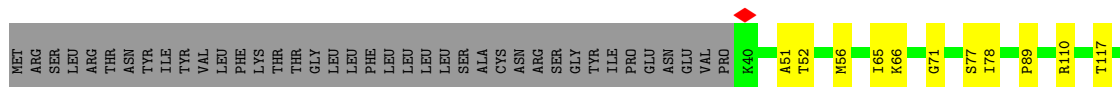


● Molecule 4: Inner membrane lipoprotein YiaD

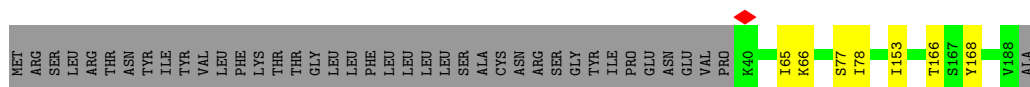
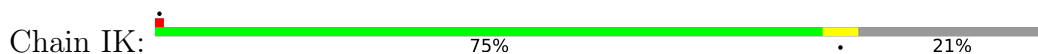




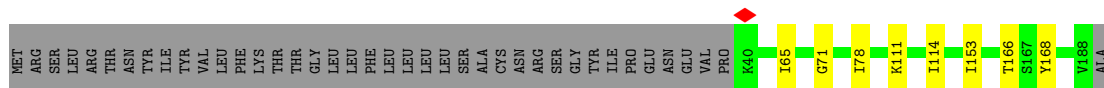
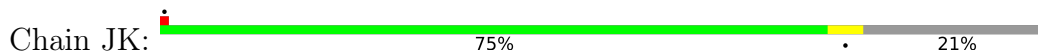
• Molecule 4: Inner membrane lipoprotein YiaD



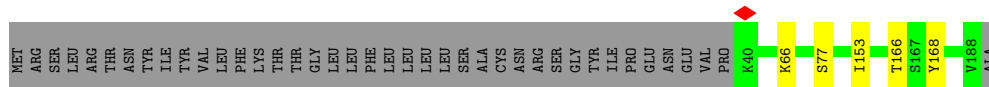
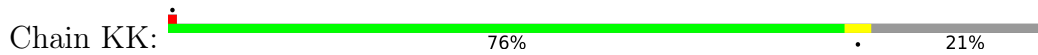
• Molecule 4: Inner membrane lipoprotein YiaD



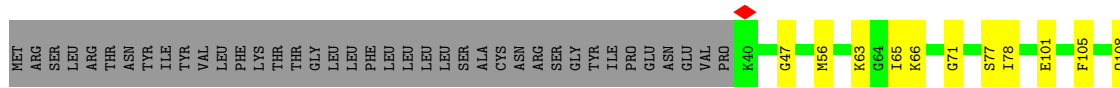
• Molecule 4: Inner membrane lipoprotein YiaD

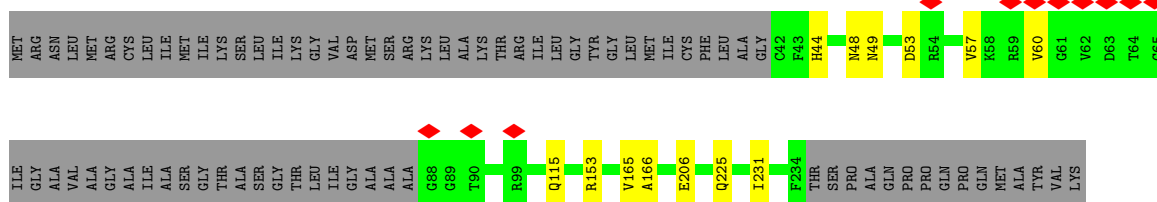


• Molecule 4: Inner membrane lipoprotein YiaD

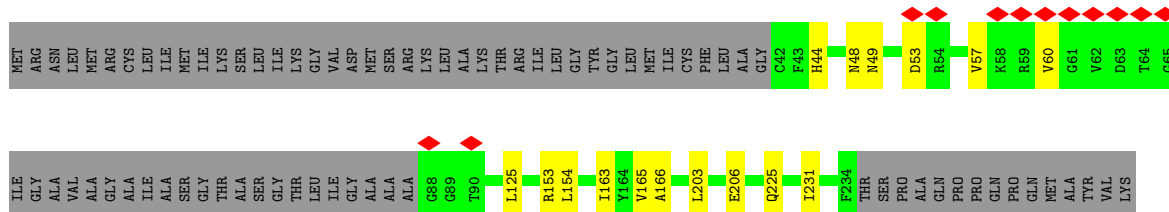


• Molecule 4: Inner membrane lipoprotein YiaD

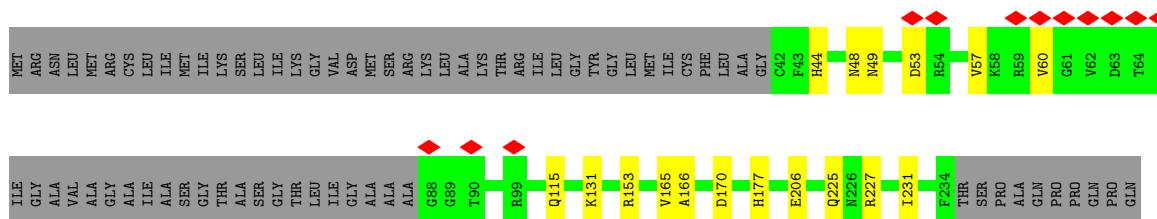




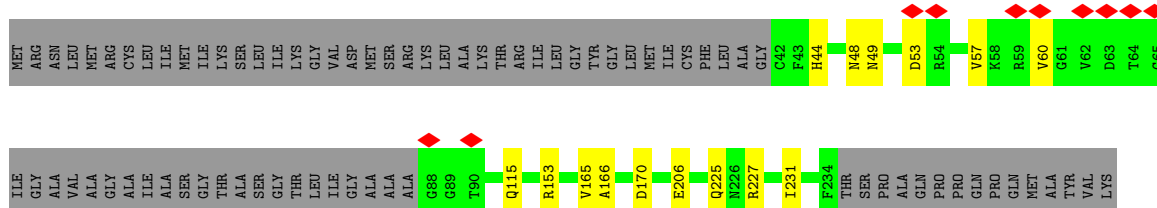
● Molecule 5: Outer membrane protein, OmpA family protein



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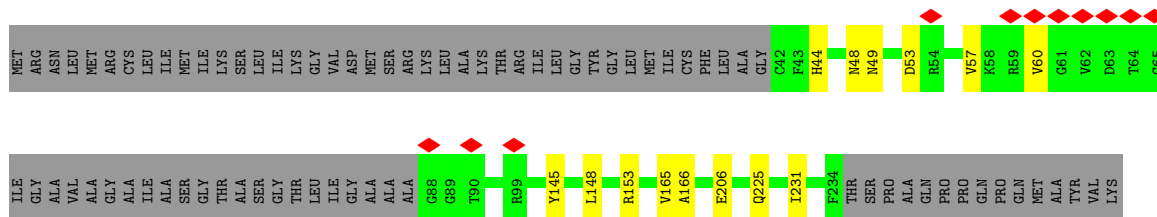


● Molecule 5: Outer membrane protein, OmpA family protein

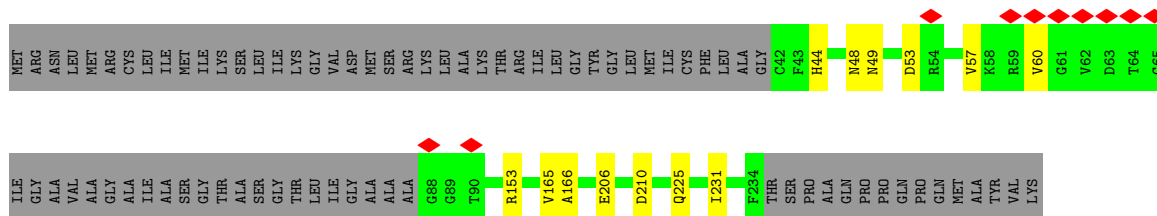


● Molecule 5: Outer membrane protein, OmpA family protein

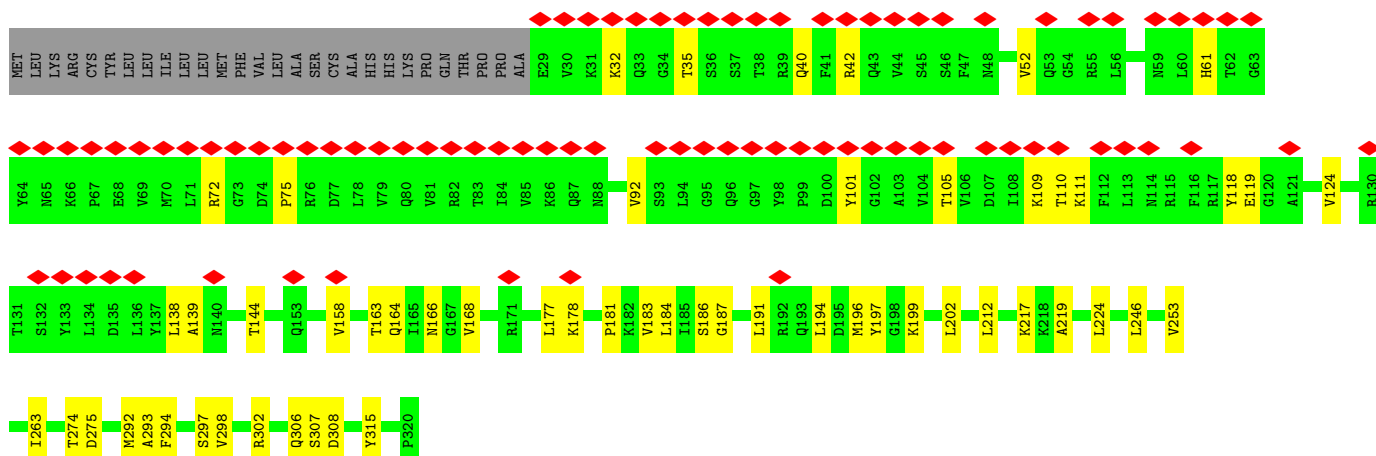
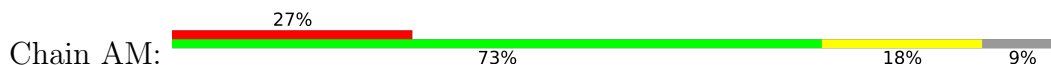




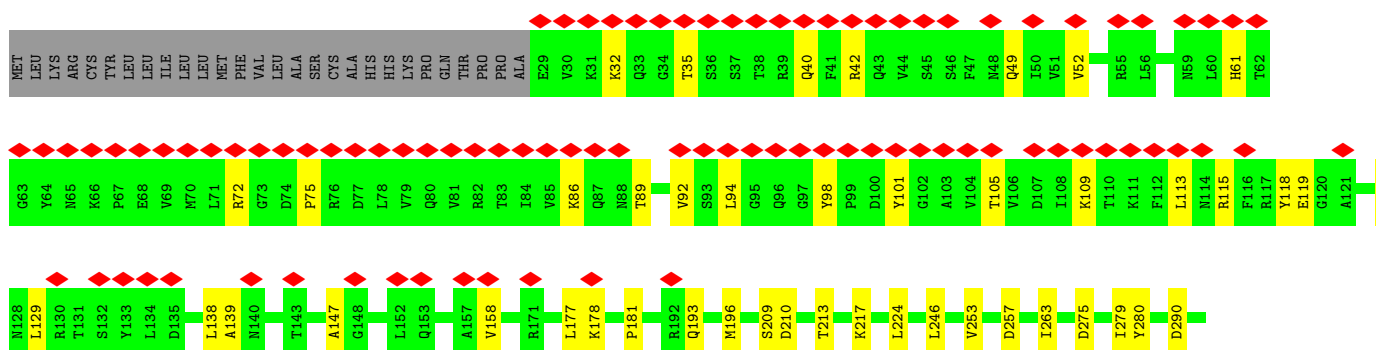
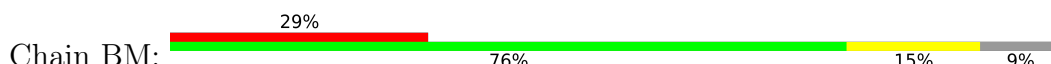
• Molecule 5: Outer membrane protein, OmpA family protein

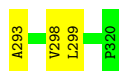


• Molecule 6: DUF2807 domain-containing protein

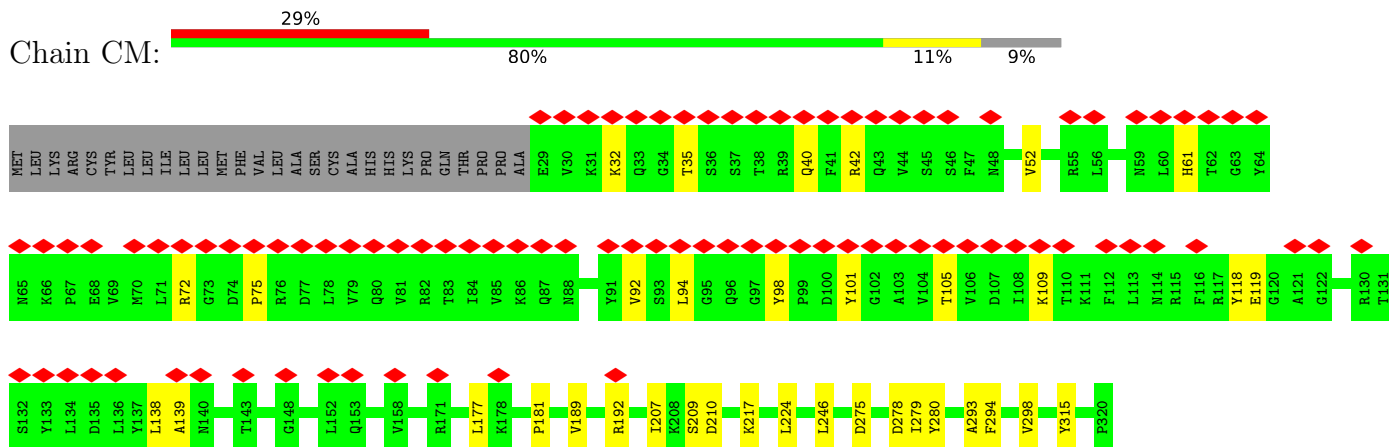


• Molecule 6: DUF2807 domain-containing protein

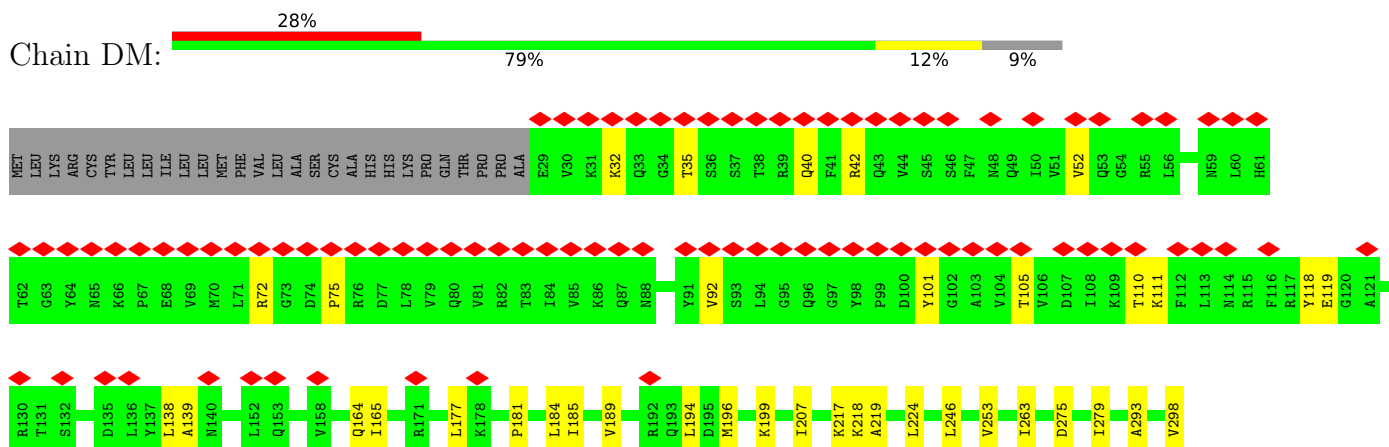




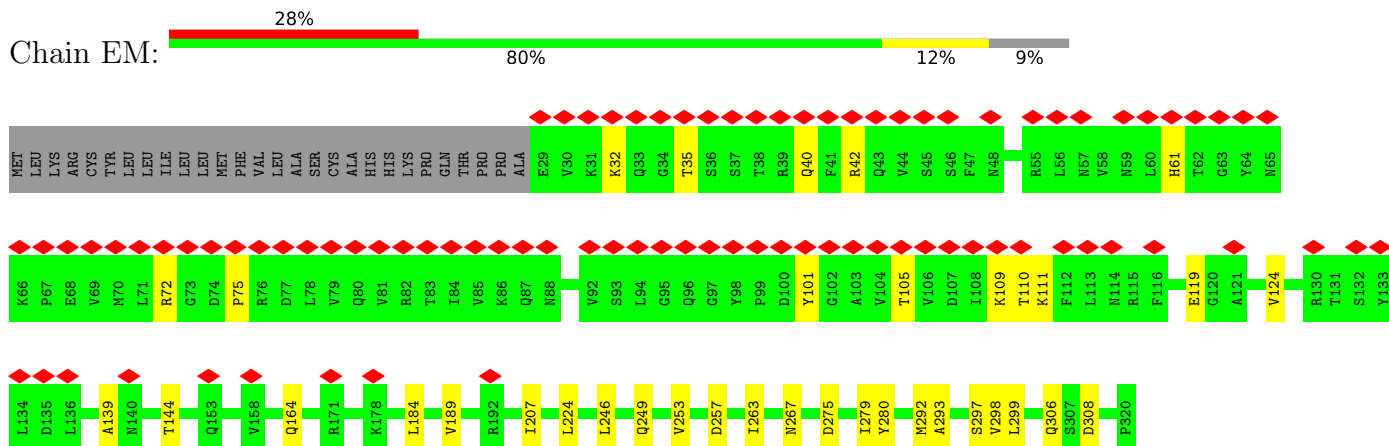
• Molecule 6: DUF2807 domain-containing protein



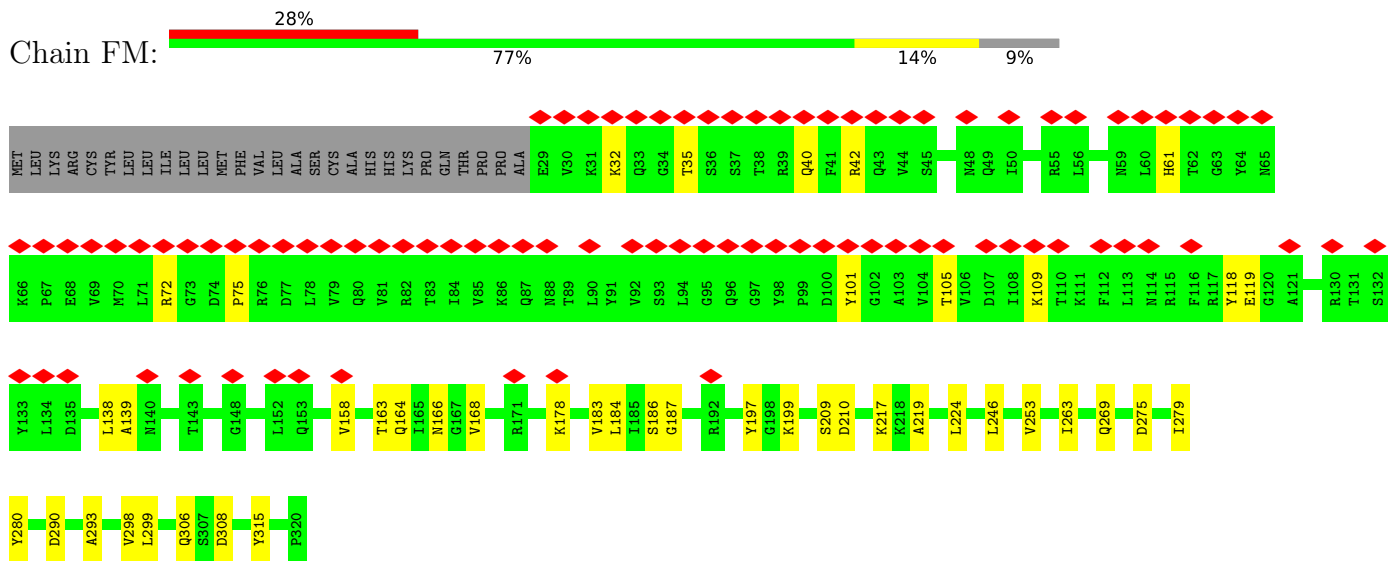
• Molecule 6: DUF2807 domain-containing protein



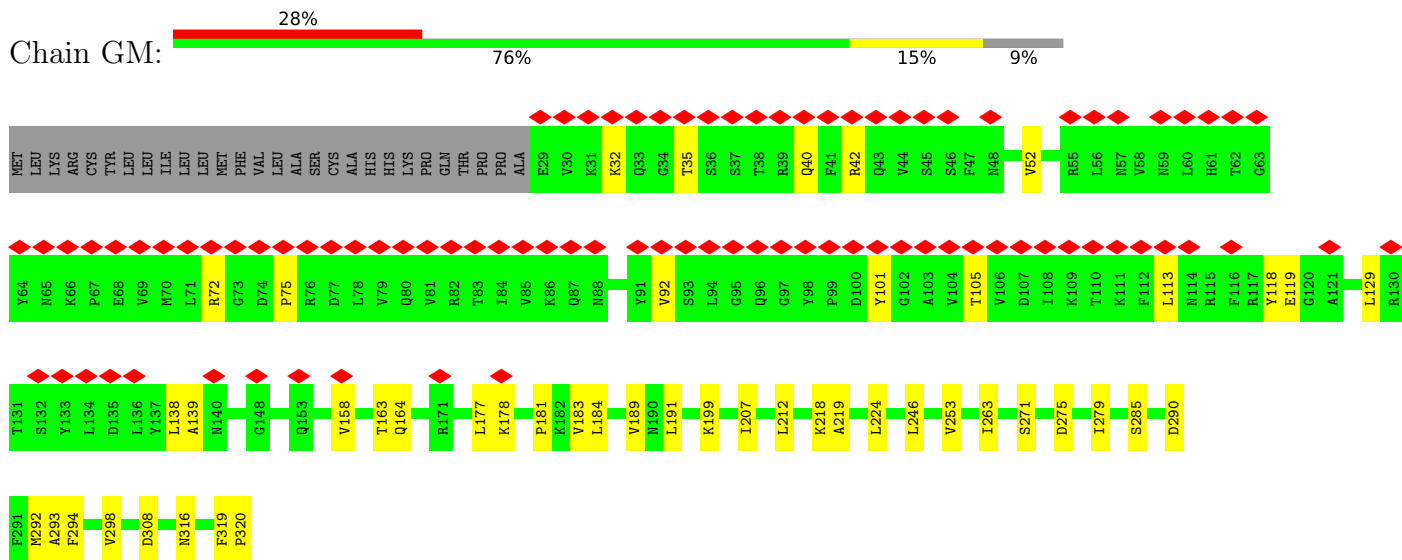
• Molecule 6: DUF2807 domain-containing protein



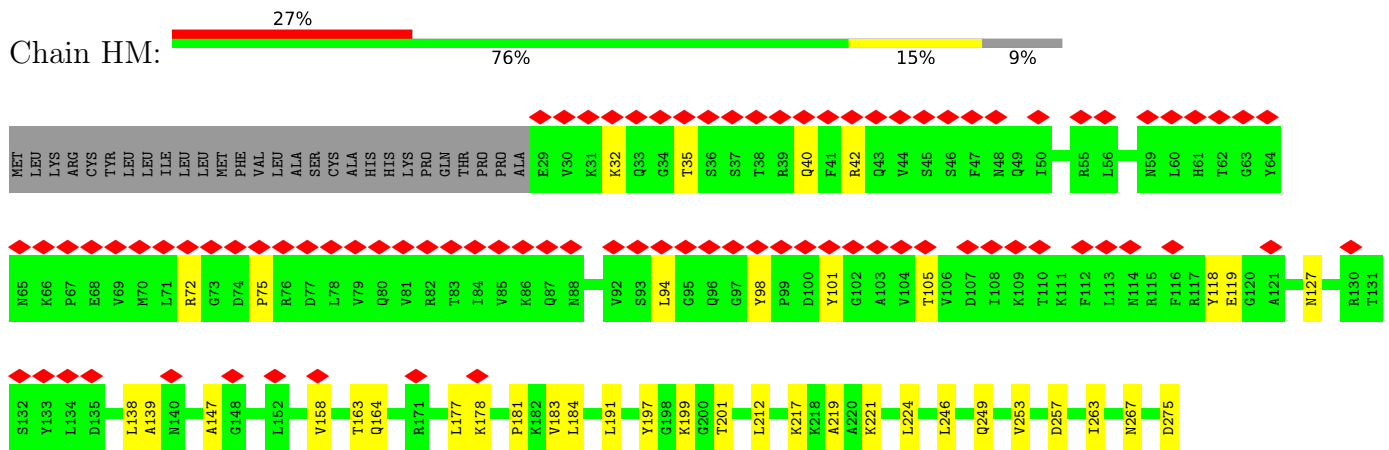
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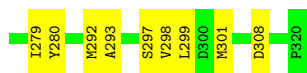


• Molecule 6: DUF2807 domain-containing protein

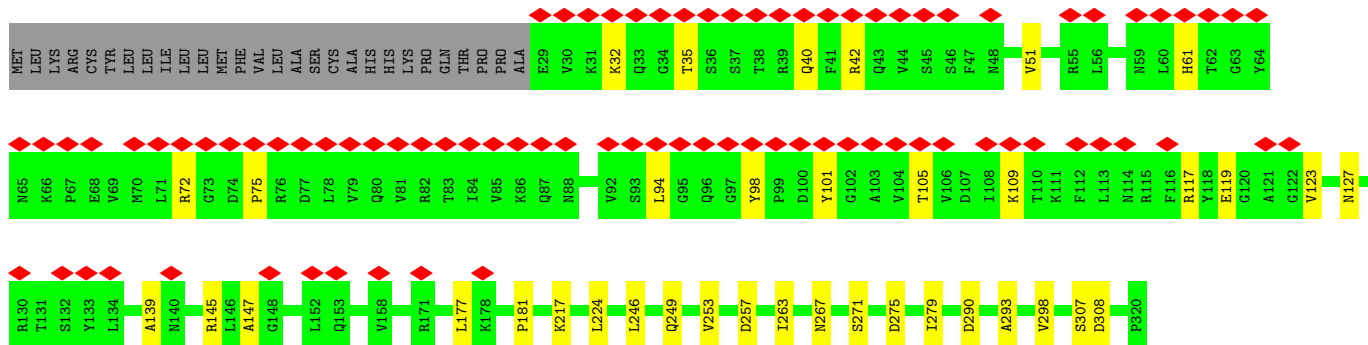
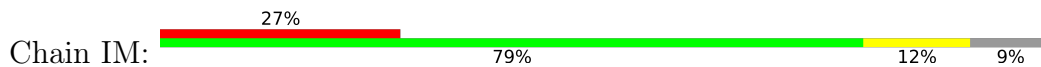


• Molecule 6: DUF2807 domain-containing protein

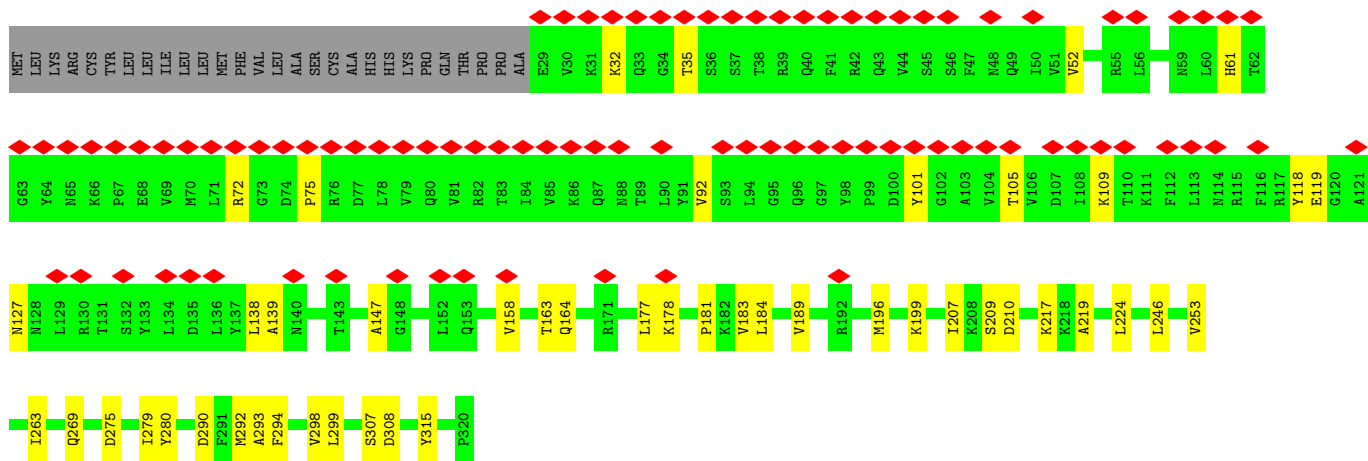
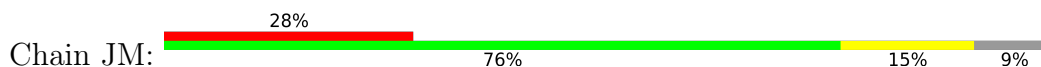




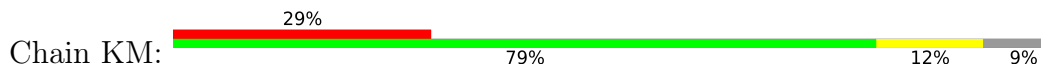
• Molecule 6: DUF2807 domain-containing protein



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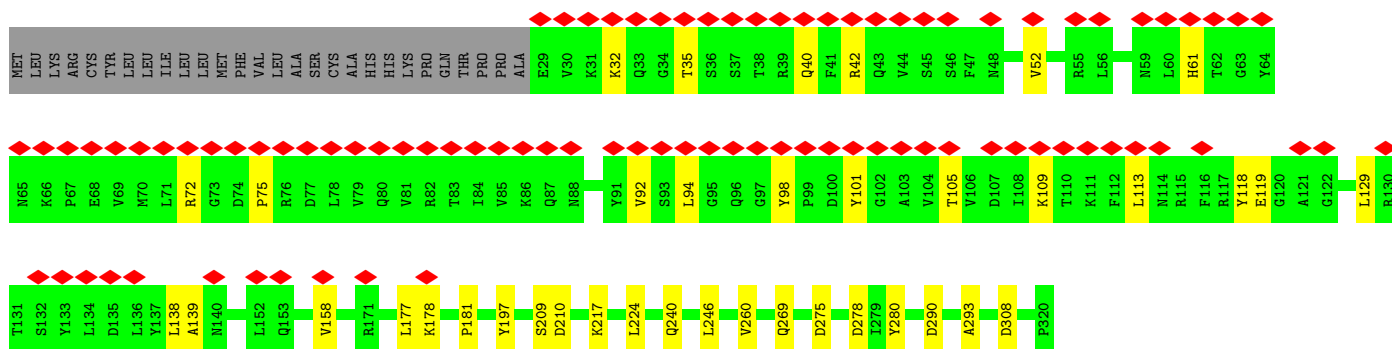
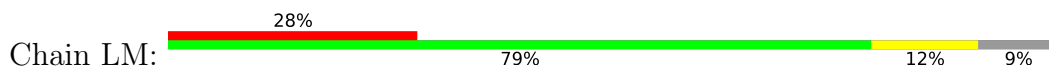


• Molecule 6: DUF2807 domain-containing protein

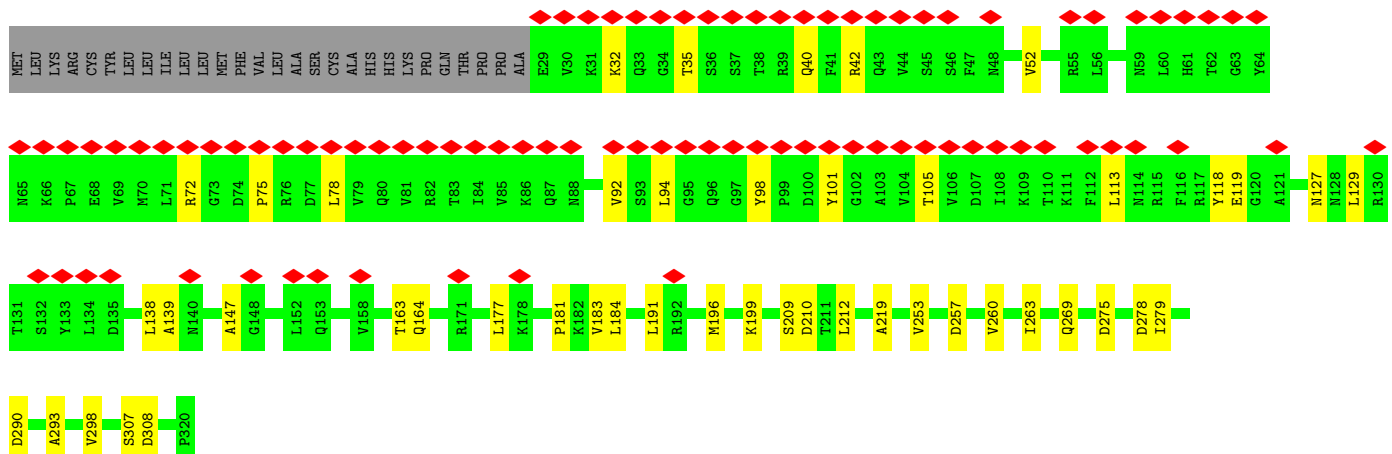
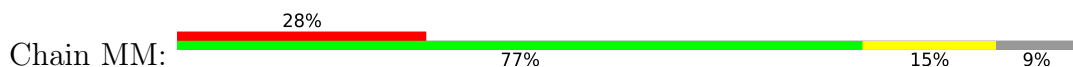


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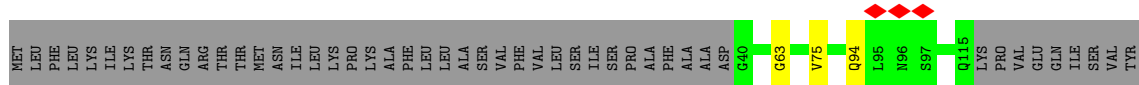
Molecule 6: DUF2807 domain-containing protein



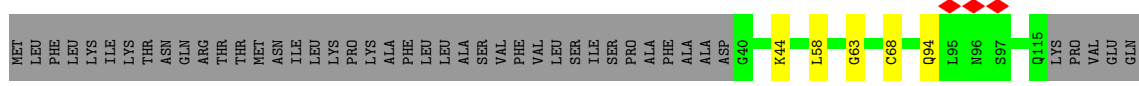
Molecule 6: DUF2807 domain-containing protein



Molecule 7: Neurogenic locus notch

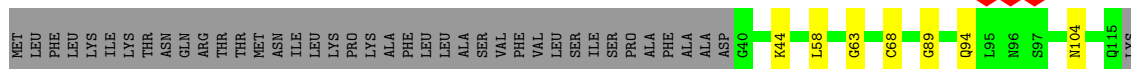


Molecule 7: Neurogenic locus notch



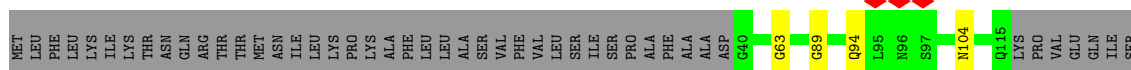
ILE
SER
VAL
TYR

• Molecule 7: Neurogenic locus notch



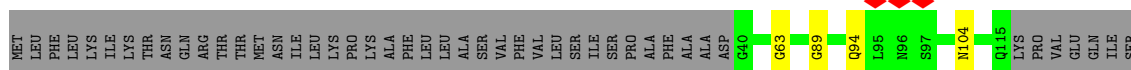
PRO
VAL
GLU
GLN
SER
VAL
TYR

• Molecule 7: Neurogenic locus notch



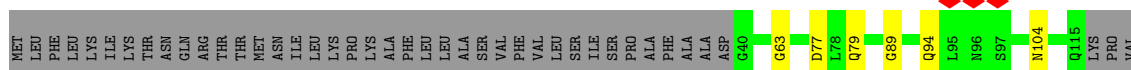
VAL
TYR

• Molecule 7: Neurogenic locus notch



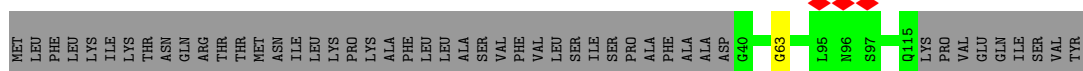
VAL
TYR

• Molecule 7: Neurogenic locus notch

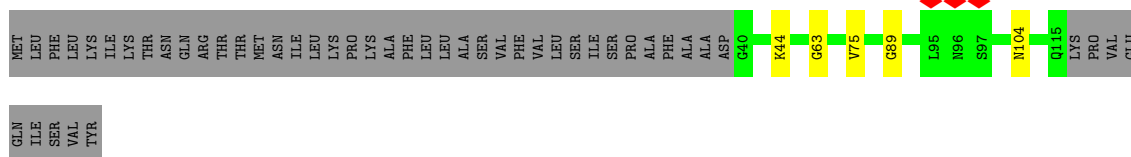


GLU
GLN
ILE
SER
VAL
TYR

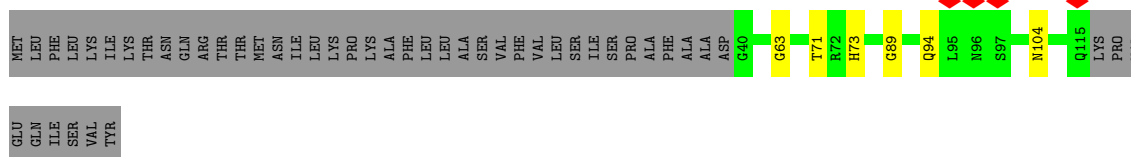
• Molecule 7: Neurogenic locus notch



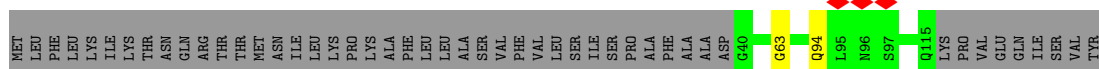
• Molecule 7: Neurogenic locus notch



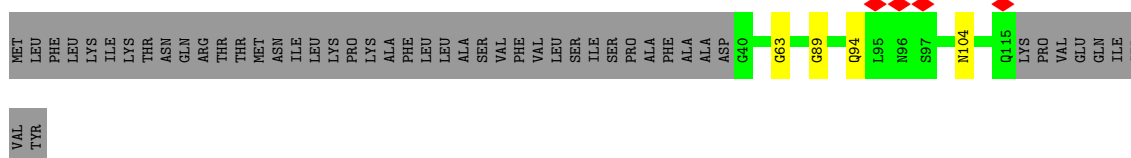
• Molecule 7: Neurogenic locus notch



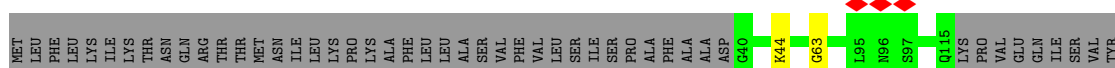
• Molecule 7: Neurogenic locus notch



• Molecule 7: Neurogenic locus notch

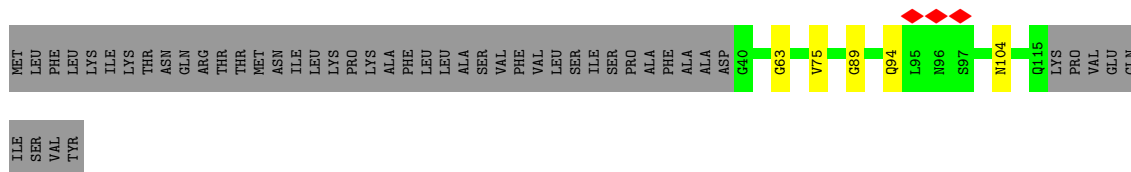


• Molecule 7: Neurogenic locus notch



• Molecule 7: Neurogenic locus notch





- Molecule 8: Unknown protein fragment

Chain AU:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Unknown protein fragment

Chain BU:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Unknown protein fragment

Chain CU:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Unknown protein fragment

Chain DU:  100%


There are no outlier residues recorded for this chain.

- Molecule 8: Unknown protein fragment

Chain EU:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Unknown protein fragment

Chain FU:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Unknown protein fragment

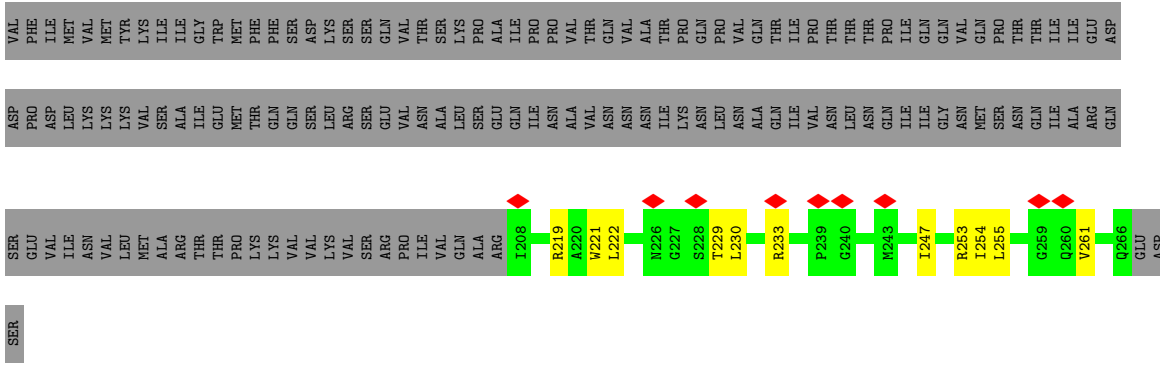
Chain GU:  100%

There are no outlier residues recorded for this chain.

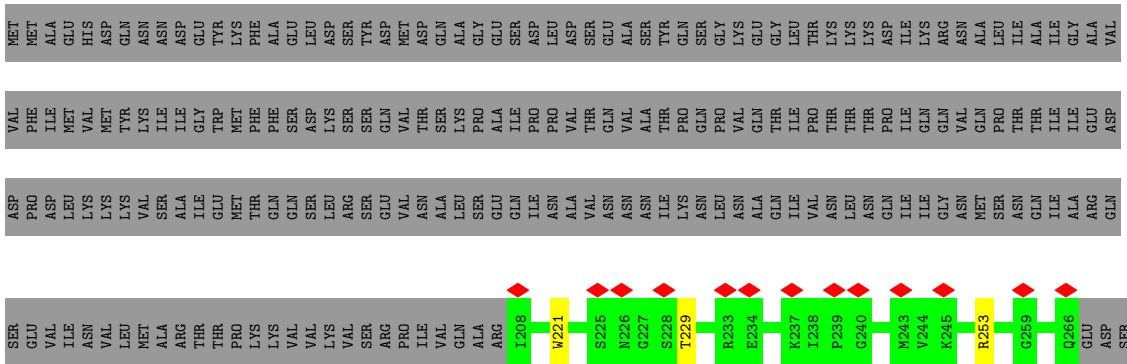
- Molecule 8: Unknown protein fragment

Chain HU:  100%

There are no outlier residues recorded for this chain.



• Molecule 9: DotF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84886	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.174	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	561.0, 561.0, 561.0	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AC	0.19	0/1666	0.37	0/2262
1	BC	0.18	0/1666	0.37	0/2262
1	CC	0.19	0/1666	0.37	0/2262
1	DC	0.19	0/1666	0.37	0/2262
1	EC	0.18	0/1666	0.38	0/2262
1	FC	0.19	0/1666	0.40	0/2262
1	GC	0.20	0/1666	0.38	0/2262
1	HC	0.18	0/1666	0.37	0/2262
1	IC	0.18	0/1666	0.36	0/2262
1	JC	0.20	0/1666	0.39	0/2262
1	KC	0.20	0/1666	0.38	0/2262
1	LC	0.18	0/1666	0.37	0/2262
1	MC	0.18	0/1666	0.36	0/2262
2	AD	0.22	0/1099	0.49	0/1492
2	Ad	0.18	0/1069	0.42	0/1452
2	BD	0.22	0/1099	0.50	0/1492
2	Bd	0.18	0/1069	0.45	2/1452 (0.1%)
2	CD	0.21	0/1099	0.49	0/1492
2	Cd	0.18	0/1069	0.43	2/1452 (0.1%)
2	DD	0.22	0/1099	0.51	0/1492
2	Dd	0.19	0/1069	0.46	2/1452 (0.1%)
2	ED	0.22	0/1099	0.52	2/1492 (0.1%)
2	Ed	0.18	0/1069	0.43	0/1452
2	FD	0.21	0/1099	0.49	0/1492
2	Fd	0.18	0/1069	0.43	2/1452 (0.1%)
2	GD	0.22	0/1099	0.49	0/1492
2	Gd	0.19	0/1069	0.47	2/1452 (0.1%)
2	HD	0.21	0/1099	0.48	0/1492
2	Hd	0.20	0/1069	0.46	0/1452
2	ID	0.22	0/1099	0.50	0/1492
2	Id	0.19	0/1069	0.46	2/1452 (0.1%)
2	JD	0.21	0/1099	0.49	0/1492
2	Jd	0.19	0/1069	0.43	0/1452
2	KD	0.21	0/1099	0.49	0/1492

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Kd	0.17	0/1069	0.40	0/1452
2	LD	0.21	0/1099	0.49	0/1492
2	Ld	0.17	0/1069	0.40	0/1452
2	MD	0.21	0/1099	0.48	0/1492
2	Md	0.19	0/1069	0.44	0/1452
3	AH	0.15	0/707	0.38	0/963
3	BH	0.16	0/707	0.41	0/963
3	CH	0.15	0/707	0.40	0/963
3	DH	0.16	0/707	0.41	0/963
3	EH	0.15	0/707	0.41	0/963
3	FH	0.15	0/707	0.39	0/963
3	GH	0.14	0/707	0.38	0/963
3	HH	0.15	0/707	0.39	0/963
3	IH	0.15	0/707	0.38	0/963
3	JH	0.15	0/707	0.40	0/963
3	KH	0.15	0/707	0.39	0/963
3	LH	0.14	0/707	0.37	0/963
3	MH	0.14	0/707	0.39	0/963
4	AK	0.16	0/1180	0.38	0/1594
4	BK	0.16	0/1180	0.39	0/1594
4	CK	0.16	0/1180	0.38	0/1594
4	DK	0.17	0/1180	0.39	0/1594
4	EK	0.16	0/1180	0.37	0/1594
4	FK	0.16	0/1180	0.37	0/1594
4	GK	0.16	0/1180	0.37	0/1594
4	HK	0.15	0/1180	0.38	0/1594
4	IK	0.16	0/1180	0.38	0/1594
4	JK	0.15	0/1180	0.35	0/1594
4	KK	0.16	0/1180	0.38	0/1594
4	LK	0.16	0/1180	0.38	0/1594
4	MK	0.16	0/1180	0.38	0/1594
5	AL	0.20	0/1404	0.47	0/1894
5	BL	0.20	0/1404	0.47	0/1894
5	CL	0.19	0/1404	0.45	0/1894
5	DL	0.20	0/1404	0.46	0/1894
5	EL	0.18	0/1404	0.44	0/1894
5	FL	0.19	0/1404	0.45	0/1894
5	GL	0.19	0/1404	0.44	0/1894
5	HL	0.19	0/1404	0.46	0/1894
5	IL	0.19	0/1404	0.45	0/1894
5	JL	0.18	0/1404	0.44	0/1894
5	KL	0.19	0/1404	0.45	0/1894
5	LL	0.20	0/1404	0.47	0/1894

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	ML	0.19	0/1404	0.44	0/1894
6	AM	0.17	0/2359	0.50	0/3183
6	BM	0.17	0/2359	0.46	0/3183
6	CM	0.17	0/2359	0.48	0/3183
6	DM	0.17	0/2359	0.46	0/3183
6	EM	0.17	0/2359	0.46	0/3183
6	FM	0.17	0/2359	0.47	0/3183
6	GM	0.17	0/2359	0.47	0/3183
6	HM	0.16	0/2359	0.47	0/3183
6	IM	0.16	0/2359	0.45	0/3183
6	JM	0.17	0/2359	0.49	0/3183
6	KM	0.17	0/2359	0.47	0/3183
6	LM	0.16	0/2359	0.46	0/3183
6	MM	0.17	0/2359	0.48	0/3183
7	AN	0.15	0/576	0.43	0/777
7	BN	0.16	0/576	0.44	0/777
7	CN	0.15	0/576	0.45	0/777
7	DN	0.15	0/576	0.44	0/777
7	EN	0.18	0/576	0.46	0/777
7	FN	0.15	0/576	0.43	0/777
7	GN	0.16	0/576	0.44	0/777
7	HN	0.16	0/576	0.44	0/777
7	IN	0.16	0/576	0.44	0/777
7	JN	0.16	0/576	0.44	0/777
7	KN	0.17	0/576	0.46	0/777
7	LN	0.16	0/576	0.43	0/777
7	MN	0.16	0/576	0.43	0/777
9	Af	0.15	0/456	0.41	0/615
9	Bf	0.19	0/456	0.44	0/615
9	Cf	0.14	0/456	0.44	0/615
9	Df	0.16	0/456	0.41	0/615
9	Ef	0.15	0/456	0.39	0/615
9	Ff	0.16	0/456	0.47	0/615
9	Gf	0.13	0/456	0.35	0/615
9	Hf	0.15	0/456	0.40	0/615
9	If	0.16	0/456	0.49	0/615
9	Jf	0.16	0/456	0.44	0/615
9	Kf	0.13	0/456	0.37	0/615
9	Lf	0.17	0/456	0.41	0/615
9	Mf	0.13	0/456	0.39	0/615
All	All	0.18	0/136708	0.43	14/185016 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	ED	77	TYR	CA-C-N	6.01	130.92	122.08
2	ED	77	TYR	C-N-CA	6.01	130.92	122.08
2	Cd	74	PRO	CA-C-N	5.28	131.62	121.54
2	Cd	74	PRO	C-N-CA	5.28	131.62	121.54
2	Id	74	PRO	CA-C-N	5.25	131.58	121.54
2	Id	74	PRO	C-N-CA	5.25	131.58	121.54
2	Bd	74	PRO	CA-C-N	5.25	131.57	121.54
2	Bd	74	PRO	C-N-CA	5.25	131.57	121.54
2	Gd	74	PRO	CA-C-N	5.22	131.52	121.54
2	Gd	74	PRO	C-N-CA	5.22	131.52	121.54
2	Fd	74	PRO	CA-C-N	5.21	131.50	121.54
2	Fd	74	PRO	C-N-CA	5.21	131.50	121.54
2	Dd	74	PRO	CA-C-N	5.12	131.33	121.54
2	Dd	74	PRO	C-N-CA	5.12	131.33	121.54

There are no chirality outliers.

There are no planarity outliers.

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	AC	1634	0	1638	9	0
1	BC	1634	0	1638	7	0
1	CC	1634	0	1638	12	0
1	DC	1634	0	1638	10	0
1	EC	1634	0	1638	10	0
1	FC	1634	0	1638	10	0
1	GC	1634	0	1638	10	0
1	HC	1634	0	1638	11	0
1	IC	1634	0	1638	11	0
1	JC	1634	0	1638	19	0
1	KC	1634	0	1638	13	0
1	LC	1634	0	1638	7	0
1	MC	1634	0	1638	8	0
2	AD	1078	0	1112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ad	1049	0	1079	3	0
2	BD	1078	0	1112	10	0
2	Bd	1049	0	1079	5	0
2	CD	1078	0	1112	9	0
2	Cd	1049	0	1079	6	0
2	DD	1078	0	1112	8	0
2	Dd	1049	0	1079	5	0
2	ED	1078	0	1112	7	0
2	Ed	1049	0	1079	7	0
2	FD	1078	0	1112	13	0
2	Fd	1049	0	1079	10	0
2	GD	1078	0	1112	12	0
2	Gd	1049	0	1079	7	0
2	HD	1078	0	1112	10	0
2	Hd	1049	0	1079	8	0
2	ID	1078	0	1112	10	0
2	Id	1049	0	1079	5	0
2	JD	1078	0	1112	10	0
2	Jd	1049	0	1079	6	0
2	KD	1078	0	1112	10	0
2	Kd	1049	0	1079	8	0
2	LD	1078	0	1112	6	0
2	Ld	1049	0	1079	7	0
2	MD	1078	0	1112	8	0
2	Md	1049	0	1079	3	0
3	AH	690	0	703	3	0
3	BH	690	0	703	6	0
3	CH	690	0	703	4	0
3	DH	690	0	703	3	0
3	EH	690	0	703	4	0
3	FH	690	0	703	3	0
3	GH	690	0	703	3	0
3	HH	690	0	703	4	0
3	IH	690	0	703	4	0
3	JH	690	0	703	4	0
3	KH	690	0	703	5	0
3	LH	690	0	703	3	0
3	MH	690	0	703	3	0
4	AK	1161	0	1205	8	0
4	BK	1161	0	1205	5	0
4	CK	1161	0	1205	4	0
4	DK	1161	0	1205	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EK	1161	0	1205	7	0
4	FK	1161	0	1205	4	0
4	GK	1161	0	1205	7	0
4	HK	1161	0	1205	11	0
4	IK	1161	0	1205	4	0
4	JK	1161	0	1205	5	0
4	KK	1161	0	1205	3	0
4	LK	1161	0	1205	11	0
4	MK	1161	0	1205	5	0
5	AL	1375	0	1366	11	0
5	BL	1375	0	1366	9	0
5	CL	1375	0	1366	11	0
5	DL	1375	0	1366	8	0
5	EL	1375	0	1366	10	0
5	FL	1375	0	1366	12	0
5	GL	1375	0	1366	9	0
5	HL	1375	0	1366	8	0
5	IL	1375	0	1366	10	0
5	JL	1375	0	1366	11	0
5	KL	1375	0	1366	12	0
5	LL	1375	0	1366	9	0
5	ML	1375	0	1366	9	0
6	AM	2320	0	2343	34	0
6	BM	2320	0	2343	27	0
6	CM	2320	0	2343	21	0
6	DM	2320	0	2343	23	0
6	EM	2320	0	2343	22	0
6	FM	2320	0	2343	25	0
6	GM	2320	0	2343	27	0
6	HM	2320	0	2343	30	0
6	IM	2320	0	2343	22	0
6	JM	2320	0	2343	29	0
6	KM	2320	0	2343	24	0
6	LM	2320	0	2343	22	0
6	MM	2320	0	2343	27	0
7	AN	565	0	513	2	0
7	BN	565	0	513	3	0
7	CN	565	0	513	4	0
7	DN	565	0	513	2	0
7	EN	565	0	513	2	0
7	FN	565	0	513	3	0
7	GN	565	0	513	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	HN	565	0	513	4	0
7	IN	565	0	513	3	0
7	JN	565	0	513	1	0
7	KN	565	0	513	2	0
7	LN	565	0	513	2	0
7	MN	565	0	513	3	0
8	AU	45	0	12	0	0
8	BU	45	0	12	0	0
8	CU	45	0	12	0	0
8	DU	45	0	12	0	0
8	EU	45	0	12	0	0
8	FU	45	0	12	0	0
8	GU	45	0	12	0	0
8	HU	45	0	12	0	0
8	IU	45	0	12	0	0
8	JU	45	0	12	0	0
8	KU	45	0	12	0	0
8	LU	45	0	12	0	0
8	MU	45	0	12	0	0
9	Af	449	0	474	5	0
9	Bf	449	0	474	1	0
9	Cf	449	0	474	2	0
9	Df	449	0	474	2	0
9	Ef	449	0	474	4	0
9	Ff	449	0	474	2	0
9	Gf	449	0	474	2	0
9	Hf	449	0	474	3	0
9	If	449	0	474	2	0
9	Jf	449	0	474	2	0
9	Kf	449	0	474	1	0
9	Lf	449	0	474	6	0
9	Mf	449	0	474	2	0
All	All	134758	0	135785	831	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:240:ILE:HG12	1:MC:255:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:240:ILE:HG12	1:BC:255:LEU:HD13	1.75	0.68
1:CC:240:ILE:HG12	1:DC:255:LEU:HD13	1.75	0.68
6:BM:49:GLN:HG3	6:BM:115:ARG:HB3	1.76	0.68
1:KC:240:ILE:HG12	1:LC:255:LEU:HD13	1.75	0.67
1:DC:240:ILE:HG12	1:EC:255:LEU:HD13	1.76	0.67
1:EC:240:ILE:HG12	1:FC:255:LEU:HD13	1.76	0.67
7:JN:63:GLY:HA3	2:KD:27:LYS:HB2	1.78	0.66
1:AC:255:LEU:HD13	1:MC:240:ILE:HG12	1.78	0.65
1:JC:116:THR:HG22	3:JH:328:MET:HG2	1.77	0.65
2:AD:27:LYS:HB2	7:MN:63:GLY:HA3	1.77	0.65
6:JM:177:LEU:HD13	6:JM:181:PRO:HG2	1.78	0.65
7:IN:63:GLY:HA3	2:JD:27:LYS:HB2	1.79	0.65
1:FC:240:ILE:HG12	1:GC:255:LEU:HD13	1.79	0.65
7:BN:63:GLY:HA3	2:CD:27:LYS:HB2	1.78	0.64
7:EN:63:GLY:HA3	2:FD:27:LYS:HB2	1.79	0.64
7:FN:63:GLY:HA3	2:GD:27:LYS:HB2	1.80	0.64
7:GN:63:GLY:HA3	2:HD:27:LYS:HB2	1.80	0.64
2:HD:29:PRO:HG2	5:HL:225:GLN:HA	1.79	0.64
2:CD:29:PRO:HG2	5:CL:225:GLN:HA	1.80	0.64
1:JC:226:VAL:HG22	1:JC:249:ILE:HG22	1.80	0.63
7:KN:63:GLY:HA3	2:LD:27:LYS:HB2	1.79	0.63
2:GD:29:PRO:HG2	5:GL:225:GLN:HA	1.81	0.63
6:HM:279:ILE:O	6:HM:298:VAL:HA	2.00	0.62
2:LD:29:PRO:HG2	5:LL:225:GLN:HA	1.80	0.62
2:BD:29:PRO:HG2	5:BL:225:GLN:HA	1.82	0.62
1:KC:226:VAL:HG22	1:KC:249:ILE:HG22	1.81	0.62
6:BM:177:LEU:HD13	6:BM:181:PRO:HG2	1.80	0.62
7:AN:63:GLY:HA3	2:BD:27:LYS:HB2	1.81	0.61
7:HN:63:GLY:HA3	2:ID:27:LYS:HB2	1.82	0.61
6:MM:177:LEU:HD13	6:MM:181:PRO:HG2	1.83	0.61
2:DD:29:PRO:HG2	5:DL:225:GLN:HA	1.83	0.61
1:HC:240:ILE:HG12	1:IC:255:LEU:HD13	1.83	0.61
7:LN:63:GLY:HA3	2:MD:27:LYS:HB2	1.83	0.61
4:EK:166:THR:HG22	4:EK:168:TYR:H	1.66	0.60
4:BK:166:THR:HG22	4:BK:168:TYR:H	1.66	0.60
4:EK:52:THR:HG22	4:EK:56:MET:HE2	1.83	0.60
1:AC:226:VAL:HG22	1:AC:249:ILE:HG22	1.84	0.60
4:GK:52:THR:HG22	4:GK:56:MET:HE2	1.84	0.60
6:KM:199:LYS:HG2	6:KM:219:ALA:HB3	1.83	0.60
5:IL:165:VAL:HG12	5:IL:231:ILE:HG12	1.84	0.60
1:LC:226:VAL:HG22	1:LC:249:ILE:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:GK:166:THR:HG22	4:GK:168:TYR:H	1.66	0.60
6:JM:292:MET:HE2	6:JM:298:VAL:H	1.66	0.60
2:ED:29:PRO:HG2	5:EL:225:GLN:HA	1.84	0.60
1:FC:107:PRO:HG2	1:FC:209:MET:HG2	1.82	0.60
4:MK:166:THR:HG22	4:MK:168:TYR:H	1.67	0.60
1:FC:226:VAL:HG22	1:FC:249:ILE:HG22	1.84	0.60
4:FK:166:THR:HG22	4:FK:168:TYR:H	1.66	0.60
4:KK:166:THR:HG22	4:KK:168:TYR:H	1.67	0.59
7:DN:63:GLY:HA3	2:ED:27:LYS:HB2	1.83	0.59
4:IK:166:THR:HG22	4:IK:168:TYR:H	1.66	0.59
5:ML:165:VAL:HG12	5:ML:231:ILE:HG12	1.84	0.59
1:HC:226:VAL:HG22	1:HC:249:ILE:HG22	1.84	0.59
6:AM:177:LEU:HD13	6:AM:181:PRO:HG2	1.85	0.59
3:EH:284:LEU:HD22	3:EH:330:SER:HB3	1.85	0.59
6:EM:32:LYS:HG2	6:EM:101:TYR:HA	1.85	0.59
5:AL:165:VAL:HG12	5:AL:231:ILE:HG12	1.83	0.59
6:CM:32:LYS:HG2	6:CM:101:TYR:HA	1.85	0.59
1:EC:263:ARG:NH1	1:EC:264:ALA:O	2.36	0.59
2:HD:85:VAL:HG23	4:HK:153:ILE:HG12	1.85	0.59
6:IM:177:LEU:HD13	6:IM:181:PRO:HG2	1.83	0.59
2:KD:29:PRO:HG2	5:KL:225:GLN:HA	1.83	0.58
6:FM:32:LYS:HG2	6:FM:101:TYR:HA	1.85	0.58
6:MM:32:LYS:HG2	6:MM:101:TYR:HA	1.84	0.58
2:GD:85:VAL:HG23	4:GK:153:ILE:HG12	1.84	0.58
4:AK:166:THR:HG22	4:AK:168:TYR:H	1.67	0.58
6:HM:177:LEU:HD13	6:HM:181:PRO:HG2	1.85	0.58
2:JD:85:VAL:HG23	4:JK:153:ILE:HG12	1.86	0.58
5:CL:165:VAL:HG12	5:CL:231:ILE:HG12	1.86	0.58
4:HK:166:THR:HG22	4:HK:168:TYR:H	1.68	0.58
6:KM:32:LYS:HG2	6:KM:101:TYR:HA	1.84	0.58
1:BC:240:ILE:HG12	1:CC:255:LEU:HD13	1.85	0.58
5:EL:165:VAL:HG12	5:EL:231:ILE:HG12	1.85	0.58
5:HL:165:VAL:HG12	5:HL:231:ILE:HG12	1.85	0.58
2:FD:85:VAL:HG23	4:FK:153:ILE:HG12	1.85	0.58
5:FL:44:HIS:HB2	5:FL:48:ASN:HA	1.85	0.58
1:GC:240:ILE:HG12	1:HC:255:LEU:HD13	1.85	0.58
5:JL:165:VAL:HG12	5:JL:231:ILE:HG12	1.86	0.58
6:BM:32:LYS:HG2	6:BM:101:TYR:HA	1.84	0.58
6:BM:40:GLN:HE22	6:BM:42:ARG:HH21	1.52	0.58
4:CK:166:THR:HG22	4:CK:168:TYR:H	1.67	0.58
1:CC:109:VAL:HG13	1:CC:208:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FL:165:VAL:HG12	5:FL:231:ILE:HG12	1.86	0.57
6:GM:177:LEU:HD13	6:GM:181:PRO:HG2	1.85	0.57
2:LD:85:VAL:HG23	4:LK:153:ILE:HG12	1.85	0.57
6:HM:32:LYS:HG2	6:HM:101:TYR:HA	1.86	0.57
5:AL:44:HIS:HB2	5:AL:48:ASN:HA	1.85	0.57
2:Ed:127:SER:HB3	2:Ed:130:GLU:HG3	1.85	0.57
6:KM:177:LEU:HB2	6:KM:196:MET:HG2	1.86	0.57
5:ML:44:HIS:HB2	5:ML:48:ASN:HA	1.87	0.57
6:JM:72:ARG:HB3	6:JM:105:THR:HB	1.87	0.57
5:DL:165:VAL:HG12	5:DL:231:ILE:HG12	1.86	0.57
3:GH:284:LEU:HD22	3:GH:330:SER:HB3	1.86	0.57
9:Bf:221:TRP:HE1	9:Bf:229:THR:HB	1.69	0.57
6:EM:279:ILE:O	6:EM:298:VAL:HA	2.04	0.57
4:JK:166:THR:HG22	4:JK:168:TYR:H	1.70	0.57
6:AM:194:LEU:HD21	6:AM:196:MET:HE3	1.86	0.57
6:AM:292:MET:HE2	6:AM:298:VAL:H	1.70	0.57
6:IM:61:HIS:HB2	6:IM:109:LYS:HG2	1.87	0.57
6:KM:163:THR:HB	6:KM:183:VAL:HG23	1.87	0.57
6:LM:32:LYS:HG2	6:LM:101:TYR:HA	1.87	0.57
6:CM:61:HIS:HB2	6:CM:109:LYS:HG2	1.85	0.57
6:HM:35:THR:HB	6:HM:75:PRO:HD2	1.87	0.57
6:FM:253:VAL:HG21	6:FM:263:ILE:HG21	1.87	0.56
1:IC:109:VAL:HG13	1:IC:208:GLY:HA3	1.86	0.56
2:KD:85:VAL:HG23	4:KK:153:ILE:HG12	1.85	0.56
5:KL:165:VAL:HG12	5:KL:231:ILE:HG12	1.86	0.56
6:AM:253:VAL:HG21	6:AM:263:ILE:HG21	1.87	0.56
1:DC:109:VAL:HG13	1:DC:208:GLY:HA3	1.88	0.56
1:DC:226:VAL:HG22	1:DC:249:ILE:HG22	1.88	0.56
5:DL:166:ALA:HA	5:DL:206:GLU:O	2.06	0.56
6:FM:199:LYS:HG3	6:FM:219:ALA:HB3	1.87	0.56
1:MC:226:VAL:HG22	1:MC:249:ILE:HG22	1.86	0.56
6:MM:307:SER:OG	9:Mf:253:ARG:NH2	2.39	0.56
6:AM:32:LYS:HG2	6:AM:101:TYR:HA	1.86	0.56
5:CL:44:HIS:HB2	5:CL:48:ASN:HA	1.87	0.56
6:FM:119:GLU:HG2	6:FM:139:ALA:HB3	1.87	0.56
5:IL:166:ALA:HA	5:IL:206:GLU:O	2.05	0.56
5:CL:166:ALA:HA	5:CL:206:GLU:O	2.06	0.56
5:GL:44:HIS:HB2	5:GL:48:ASN:HA	1.87	0.56
5:HL:44:HIS:HB2	5:HL:48:ASN:HA	1.88	0.56
5:IL:44:HIS:HB2	5:IL:48:ASN:HA	1.87	0.56
6:JM:32:LYS:HG2	6:JM:101:TYR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:KL:44:HIS:HB2	5:KL:48:ASN:HA	1.87	0.56
5:EL:44:HIS:HB2	5:EL:48:ASN:HA	1.87	0.56
9:Lf:219:ARG:HB3	9:Lf:233:ARG:HH11	1.72	0.55
2:MD:29:PRO:HG2	5:ML:225:GLN:HA	1.87	0.55
6:GM:32:LYS:HG2	6:GM:101:TYR:HA	1.88	0.55
3:FH:284:LEU:HD22	3:FH:330:SER:HB3	1.88	0.55
6:KM:40:GLN:HE22	6:KM:42:ARG:HH21	1.54	0.55
5:GL:165:VAL:HG12	5:GL:231:ILE:HG12	1.88	0.55
1:IC:240:ILE:HG12	1:JC:255:LEU:HD13	1.87	0.55
6:IM:32:LYS:HG2	6:IM:101:TYR:HA	1.87	0.55
3:AH:284:LEU:HD22	3:AH:330:SER:HB3	1.88	0.55
5:DL:44:HIS:HB2	5:DL:48:ASN:HA	1.88	0.55
5:KL:166:ALA:HA	5:KL:206:GLU:O	2.06	0.55
2:DD:85:VAL:HG23	4:DK:153:ILE:HG12	1.89	0.55
6:DM:32:LYS:HG2	6:DM:101:TYR:HA	1.88	0.55
6:HM:119:GLU:HG2	6:HM:139:ALA:HB3	1.89	0.55
6:IM:253:VAL:HG21	6:IM:263:ILE:HG21	1.89	0.55
1:EC:109:VAL:HG13	1:EC:208:GLY:HA3	1.89	0.55
1:GC:204:GLU:HG3	3:GH:285:GLU:HG3	1.89	0.55
6:LM:35:THR:HB	6:LM:75:PRO:HD2	1.87	0.55
5:BL:44:HIS:HB2	5:BL:48:ASN:HA	1.88	0.55
9:Jf:221:TRP:HE1	9:Jf:229:THR:HB	1.72	0.55
6:KM:119:GLU:HG2	6:KM:139:ALA:HB3	1.88	0.55
5:BL:165:VAL:HG12	5:BL:231:ILE:HG12	1.89	0.54
1:GC:226:VAL:HG22	1:GC:249:ILE:HG22	1.89	0.54
1:LC:109:VAL:HG13	1:LC:208:GLY:HA3	1.89	0.54
9:Lf:221:TRP:HE1	9:Lf:229:THR:HB	1.72	0.54
7:CN:63:GLY:HA3	2:DD:27:LYS:HB2	1.89	0.54
1:BC:109:VAL:HG13	1:BC:208:GLY:HA3	1.88	0.54
5:GL:166:ALA:HA	5:GL:206:GLU:O	2.06	0.54
6:IM:307:SER:OG	9:If:253:ARG:NH2	2.36	0.54
1:JC:107:PRO:HG2	1:JC:209:MET:HG2	1.89	0.54
1:CC:226:VAL:HG22	1:CC:249:ILE:HG22	1.88	0.54
6:CM:119:GLU:HG2	6:CM:139:ALA:HB3	1.88	0.54
5:LL:165:VAL:HG12	5:LL:231:ILE:HG12	1.89	0.54
1:CC:65:SER:O	1:CC:69:GLN:NE2	2.40	0.54
2:BD:85:VAL:HG23	4:BK:153:ILE:HG12	1.89	0.54
4:DK:166:THR:HG22	4:DK:168:TYR:H	1.72	0.54
5:EL:166:ALA:HA	5:EL:206:GLU:O	2.07	0.54
1:HC:104:ASN:ND2	2:HD:162:TYR:OH	2.41	0.54
1:MC:225:TYR:HD1	1:MC:251:ALA:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:67:LYS:HE3	2:Ad:64:PRO:HD3	1.90	0.54
1:BC:226:VAL:HG22	1:BC:249:ILE:HG22	1.89	0.54
1:EC:226:VAL:HG22	1:EC:249:ILE:HG22	1.90	0.54
6:EM:253:VAL:HG21	6:EM:263:ILE:HG21	1.89	0.54
4:HK:51:ALA:HB1	7:HN:44:LYS:HD3	1.90	0.54
5:ML:166:ALA:HA	5:ML:206:GLU:O	2.07	0.54
6:AM:119:GLU:HG2	6:AM:139:ALA:HB3	1.88	0.54
9:Cf:219:ARG:HG3	9:Cf:233:ARG:HD2	1.90	0.54
6:LM:308:ASP:OD2	9:Lf:253:ARG:NH2	2.41	0.54
5:AL:166:ALA:HA	5:AL:206:GLU:O	2.07	0.53
6:BM:61:HIS:HB2	6:BM:109:LYS:HG2	1.90	0.53
6:MM:40:GLN:HE22	6:MM:42:ARG:HH21	1.55	0.53
1:DC:107:PRO:HG2	1:DC:209:MET:HG2	1.88	0.53
3:HH:284:LEU:HD22	3:HH:330:SER:HB3	1.90	0.53
6:KM:253:VAL:HG21	6:KM:263:ILE:HG21	1.89	0.53
9:Kf:221:TRP:HE1	9:Kf:229:THR:HB	1.73	0.53
2:ED:140:GLY:O	2:Ed:60:LYS:NZ	2.42	0.53
6:FM:163:THR:HB	6:FM:183:VAL:HG23	1.90	0.53
1:GC:109:VAL:HG13	1:GC:208:GLY:HA3	1.91	0.53
6:IM:119:GLU:HG2	6:IM:139:ALA:HB3	1.91	0.53
6:MM:253:VAL:HG21	6:MM:263:ILE:HG21	1.90	0.53
6:AM:307:SER:OG	9:Af:253:ARG:NH2	2.38	0.53
6:EM:119:GLU:HG2	6:EM:139:ALA:HB3	1.91	0.53
6:EM:292:MET:HE2	6:EM:298:VAL:H	1.73	0.53
1:KC:109:VAL:HG13	1:KC:208:GLY:HA3	1.90	0.53
2:CD:67:LYS:HE3	2:Cd:64:PRO:HD3	1.91	0.53
6:HM:253:VAL:HG21	6:HM:263:ILE:HG21	1.90	0.53
6:JM:253:VAL:HG21	6:JM:263:ILE:HG21	1.91	0.53
3:LH:284:LEU:HD22	3:LH:330:SER:HB3	1.91	0.53
5:BL:166:ALA:HA	5:BL:206:GLU:O	2.09	0.53
6:GM:40:GLN:HE22	6:GM:42:ARG:HH21	1.57	0.53
5:HL:166:ALA:HA	5:HL:206:GLU:O	2.08	0.53
1:KC:107:PRO:HG2	1:KC:209:MET:HG2	1.91	0.53
1:LC:214:LYS:HG2	1:LC:218:MET:HE2	1.91	0.53
5:LL:166:ALA:HA	5:LL:206:GLU:O	2.08	0.53
6:IM:249:GLN:OE1	6:IM:267:ASN:ND2	2.42	0.53
6:LM:119:GLU:HG2	6:LM:139:ALA:HB3	1.90	0.53
1:AC:109:VAL:HG13	1:AC:208:GLY:HA3	1.90	0.52
2:CD:36:ASP:N	2:CD:36:ASP:OD1	2.42	0.52
4:LK:63:LYS:NZ	4:LK:101:GLU:OE1	2.43	0.52
6:MM:119:GLU:HG2	6:MM:139:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BM:72:ARG:HB3	6:BM:105:THR:HB	1.92	0.52
6:DM:119:GLU:HG2	6:DM:139:ALA:HB3	1.91	0.52
6:MM:35:THR:HB	6:MM:75:PRO:HD2	1.90	0.52
6:BM:253:VAL:HG21	6:BM:263:ILE:HG21	1.91	0.52
2:CD:140:GLY:O	2:Cd:60:LYS:NZ	2.43	0.52
2:DD:36:ASP:OD1	2:DD:36:ASP:N	2.42	0.52
6:EM:40:GLN:HE22	6:EM:42:ARG:HH21	1.56	0.52
9:Ef:222:LEU:HD12	9:Ef:230:LEU:HD22	1.92	0.52
4:HK:128:ARG:HA	6:HM:301:MET:HE1	1.90	0.52
1:JC:240:ILE:HG12	1:KC:255:LEU:HD13	1.91	0.52
6:LM:61:HIS:HB2	6:LM:109:LYS:HG2	1.90	0.52
9:Mf:221:TRP:HE1	9:Mf:229:THR:HB	1.74	0.52
1:GC:104:ASN:ND2	2:GD:162:TYR:OH	2.43	0.52
5:LL:44:HIS:HB2	5:LL:48:ASN:HA	1.90	0.52
6:HM:40:GLN:HE22	6:HM:42:ARG:HH21	1.56	0.52
2:BD:67:LYS:HE3	2:Bd:64:PRO:HD3	1.92	0.52
6:CM:279:ILE:HB	6:CM:298:VAL:HG22	1.92	0.52
2:DD:67:LYS:HE3	2:Dd:64:PRO:HD3	1.92	0.52
6:FM:279:ILE:O	6:FM:298:VAL:HA	2.10	0.52
2:KD:140:GLY:O	2:Kd:60:LYS:NZ	2.43	0.52
6:KM:158:VAL:HA	6:KM:178:LYS:HZ3	1.75	0.52
6:JM:119:GLU:HG2	6:JM:139:ALA:HB3	1.92	0.52
9:Af:219:ARG:HB3	9:Af:233:ARG:HH11	1.75	0.52
9:Cf:221:TRP:HE1	9:Cf:229:THR:HB	1.75	0.52
6:DM:194:LEU:HD21	6:DM:196:MET:HE3	1.92	0.52
5:JL:44:HIS:HB2	5:JL:48:ASN:HA	1.91	0.52
6:DM:199:LYS:HD2	6:DM:219:ALA:HB3	1.92	0.51
6:DM:279:ILE:HB	6:DM:298:VAL:HG22	1.91	0.51
9:Df:219:ARG:HB3	9:Df:233:ARG:HH11	1.74	0.51
9:Ef:221:TRP:HE1	9:Ef:229:THR:HB	1.75	0.51
2:FD:140:GLY:O	2:Fd:60:LYS:NZ	2.44	0.51
5:GL:53:ASP:OD2	5:GL:153:ARG:NH1	2.44	0.51
6:GM:35:THR:HB	6:GM:75:PRO:HD2	1.91	0.51
5:HL:49:ASN:ND2	6:HM:293:ALA:O	2.39	0.51
2:ID:67:LYS:HE3	2:Id:64:PRO:HD3	1.92	0.51
9:Lf:222:LEU:HD12	9:Lf:230:LEU:HD22	1.92	0.51
2:GD:67:LYS:HE3	2:Gd:64:PRO:HD3	1.93	0.51
6:GM:119:GLU:HG2	6:GM:139:ALA:HB3	1.92	0.51
9:Af:221:TRP:HE1	9:Af:229:THR:HB	1.76	0.51
1:JC:109:VAL:HG13	1:JC:208:GLY:HA3	1.92	0.51
1:KC:204:GLU:HG3	3:KH:285:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LM:177:LEU:HD13	6:LM:181:PRO:HG2	1.91	0.51
1:JC:104:ASN:ND2	2:JD:162:TYR:OH	2.42	0.51
6:JM:308:ASP:OD1	6:JM:308:ASP:N	2.44	0.51
5:KL:49:ASN:ND2	6:KM:293:ALA:O	2.38	0.51
6:LM:72:ARG:HB3	6:LM:105:THR:HB	1.91	0.51
1:MC:109:VAL:HG13	1:MC:208:GLY:HA3	1.92	0.51
6:MM:94:LEU:HD22	6:MM:98:TYR:HB2	1.91	0.51
5:IL:53:ASP:OD2	5:IL:153:ARG:NH1	2.44	0.51
6:BM:177:LEU:HD12	6:BM:196:MET:HE2	1.93	0.51
6:BM:224:LEU:HB2	6:BM:246:LEU:HD22	1.93	0.51
1:CC:75:ARG:NH2	2:CD:36:ASP:OD1	2.43	0.51
1:CC:204:GLU:HG3	3:CH:285:GLU:HG3	1.91	0.51
6:DM:307:SER:HG	9:Df:253:ARG:HH22	1.53	0.51
6:EM:61:HIS:HB2	6:EM:109:LYS:HG2	1.91	0.51
2:FD:67:LYS:HE3	2:Fd:64:PRO:HD3	1.93	0.51
2:HD:67:LYS:HE3	2:Hd:64:PRO:HD3	1.93	0.51
1:IC:226:VAL:HG22	1:IC:249:ILE:HG22	1.92	0.51
6:FM:72:ARG:HB3	6:FM:105:THR:HB	1.91	0.51
5:JL:53:ASP:OD2	5:JL:153:ARG:NH1	2.44	0.51
5:LL:53:ASP:OD2	5:LL:153:ARG:NH1	2.44	0.50
6:BM:279:ILE:O	6:BM:298:VAL:HA	2.10	0.50
1:FC:214:LYS:HG2	1:FC:218:MET:HE2	1.94	0.50
1:GC:263:ARG:NH1	1:GC:264:ALA:O	2.43	0.50
5:FL:166:ALA:HA	5:FL:206:GLU:O	2.11	0.50
5:KL:53:ASP:OD1	5:KL:53:ASP:N	2.45	0.50
2:Kd:36:ASP:N	2:Kd:36:ASP:OD1	2.45	0.50
5:FL:53:ASP:OD2	5:FL:153:ARG:NH1	2.44	0.50
9:Ff:221:TRP:HE1	9:Ff:229:THR:HB	1.75	0.50
1:IC:75:ARG:NH2	2:ID:36:ASP:OD1	2.44	0.50
6:MM:164:GLN:HG2	6:MM:184:LEU:HD11	1.94	0.50
6:MM:199:LYS:HG3	6:MM:219:ALA:HB3	1.94	0.50
4:CK:71:GLY:O	2:DD:27:LYS:NZ	2.38	0.50
6:JM:279:ILE:O	6:JM:298:VAL:HA	2.12	0.50
6:KM:224:LEU:HB2	6:KM:246:LEU:HD22	1.94	0.50
5:ML:53:ASP:OD2	5:ML:153:ARG:NH1	2.45	0.50
5:CL:49:ASN:ND2	6:CM:293:ALA:O	2.39	0.50
5:CL:53:ASP:OD2	5:CL:153:ARG:NH1	2.44	0.50
6:DM:35:THR:HB	6:DM:75:PRO:HD2	1.93	0.50
5:IL:49:ASN:ND2	6:IM:293:ALA:O	2.40	0.50
5:JL:166:ALA:HA	5:JL:206:GLU:O	2.11	0.50
5:JL:170:ASP:OD2	5:JL:227:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:JM:35:THR:HB	6:JM:75:PRO:HD2	1.93	0.50
2:Ld:36:ASP:OD1	2:Ld:36:ASP:N	2.45	0.50
5:AL:53:ASP:OD2	5:AL:153:ARG:NH1	2.45	0.50
2:CD:62:ILE:HG22	2:CD:63:THR:HG23	1.94	0.50
6:CM:224:LEU:HB2	6:CM:246:LEU:HD22	1.94	0.50
6:HM:308:ASP:OD2	9:Hf:253:ARG:NH2	2.44	0.50
6:LM:40:GLN:HE22	6:LM:42:ARG:HH21	1.58	0.50
3:CH:284:LEU:HD22	3:CH:330:SER:HB3	1.94	0.49
6:JM:280:TYR:HD1	6:JM:299:LEU:HB2	1.78	0.49
4:AK:52:THR:HG22	4:AK:56:MET:HE2	1.94	0.49
2:BD:130:GLU:OE1	2:BD:133:ARG:NH1	2.45	0.49
6:DM:224:LEU:HB2	6:DM:246:LEU:HD22	1.95	0.49
2:Ed:82:ARG:NH1	2:Ed:125:ASP:OD2	2.45	0.49
9:Ef:247:ILE:HA	9:Ef:254:ILE:HG12	1.92	0.49
1:FC:231:LEU:HB2	1:FC:244:ASP:HB2	1.95	0.49
6:FM:35:THR:HB	6:FM:75:PRO:HD2	1.94	0.49
1:JC:263:ARG:NH1	1:JC:264:ALA:O	2.45	0.49
2:Md:64:PRO:HG2	2:Md:67:LYS:HG2	1.95	0.49
1:AC:231:LEU:HB2	1:AC:244:ASP:HB2	1.93	0.49
6:CM:35:THR:HB	6:CM:75:PRO:HD2	1.94	0.49
3:DH:320:LEU:HD11	3:DH:348:SER:HB2	1.94	0.49
5:IL:170:ASP:OD1	5:IL:227:ARG:NH1	2.42	0.49
6:AM:164:GLN:HG2	6:AM:184:LEU:HD11	1.94	0.49
2:Dd:64:PRO:HG2	2:Dd:67:LYS:HG2	1.94	0.49
1:EC:231:LEU:HB2	1:EC:244:ASP:HB2	1.94	0.49
5:EL:53:ASP:OD2	5:EL:153:ARG:NH1	2.45	0.49
4:HK:110:ARG:NH1	7:HN:75:VAL:O	2.42	0.49
2:JD:130:GLU:OE2	2:JD:133:ARG:NH1	2.45	0.49
5:ML:49:ASN:ND2	6:MM:293:ALA:O	2.39	0.49
5:ML:210:ASP:OD1	5:ML:210:ASP:N	2.43	0.49
3:BH:322:PRO:HG2	3:BH:345:LEU:HD23	1.93	0.49
6:CM:177:LEU:HD13	6:CM:181:PRO:HG2	1.94	0.49
2:Fd:127:SER:HB3	2:Fd:130:GLU:HG3	1.93	0.49
6:GM:72:ARG:HB3	6:GM:105:THR:HB	1.94	0.49
2:Hd:36:ASP:OD1	2:Hd:36:ASP:N	2.43	0.49
2:Id:64:PRO:HG2	2:Id:67:LYS:HG2	1.94	0.49
6:KM:72:ARG:HB3	6:KM:105:THR:HB	1.93	0.49
3:AH:280:LEU:HB2	3:AH:328:MET:HE3	1.94	0.49
6:BM:119:GLU:HG2	6:BM:139:ALA:HB3	1.94	0.49
5:IL:53:ASP:OD1	5:IL:53:ASP:N	2.45	0.49
5:KL:53:ASP:OD2	5:KL:153:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ad:64:PRO:HG2	2:Ad:67:LYS:HG2	1.95	0.49
2:HD:36:ASP:OD1	2:HD:36:ASP:N	2.45	0.49
6:IM:72:ARG:HB3	6:IM:105:THR:HB	1.94	0.49
5:JL:177:HIS:HD1	6:JM:315:TYR:HH	1.61	0.49
2:Bd:64:PRO:HG2	2:Bd:67:LYS:HG2	1.94	0.49
6:EM:72:ARG:HB3	6:EM:105:THR:HB	1.93	0.49
6:GM:308:ASP:OD1	6:GM:308:ASP:N	2.45	0.49
1:HC:204:GLU:HG3	3:HH:285:GLU:HG3	1.95	0.49
2:HD:140:GLY:O	2:Hd:60:LYS:NZ	2.45	0.49
1:JC:204:GLU:HG3	3:JH:285:GLU:HG3	1.95	0.49
6:AM:72:ARG:HB3	6:AM:105:THR:HB	1.95	0.49
2:Hd:64:PRO:HG2	2:Hd:67:LYS:HG2	1.94	0.49
2:JD:67:LYS:HE3	2:Jd:64:PRO:HD3	1.95	0.49
5:LL:49:ASN:ND2	6:LM:293:ALA:O	2.41	0.49
2:Bd:82:ARG:NH1	2:Bd:125:ASP:OD2	2.46	0.48
2:Cd:64:PRO:HG2	2:Cd:67:LYS:HG2	1.95	0.48
6:FM:280:TYR:HD1	6:FM:299:LEU:HB2	1.78	0.48
2:Fd:64:PRO:HG2	2:Fd:67:LYS:HG2	1.94	0.48
5:JL:49:ASN:ND2	6:JM:293:ALA:O	2.40	0.48
6:JM:189:VAL:HB	6:JM:207:ILE:HG22	1.94	0.48
2:KD:34:SER:OG	2:Kd:36:ASP:OD1	2.31	0.48
2:MD:67:LYS:HE3	2:Md:64:PRO:HD3	1.95	0.48
6:AM:40:GLN:HE22	6:AM:42:ARG:HH21	1.59	0.48
6:AM:158:VAL:HA	6:AM:178:LYS:HZ3	1.78	0.48
6:HM:163:THR:HB	6:HM:183:VAL:HG23	1.94	0.48
2:Jd:36:ASP:OD1	2:Jd:36:ASP:N	2.45	0.48
5:AL:177:HIS:ND1	6:AM:315:TYR:OH	2.44	0.48
6:EM:35:THR:HB	6:EM:75:PRO:HD2	1.93	0.48
6:FM:164:GLN:HG2	6:FM:184:LEU:HD11	1.94	0.48
2:HD:28:PRO:HG3	5:HL:115:GLN:HB2	1.94	0.48
6:HM:197:TYR:HA	6:HM:217:LYS:HB3	1.95	0.48
6:EM:280:TYR:HD1	6:EM:299:LEU:HB2	1.79	0.48
2:HD:34:SER:OG	2:Hd:36:ASP:OD1	2.31	0.48
2:BD:62:ILE:HG22	2:BD:63:THR:HG23	1.96	0.48
6:EM:224:LEU:HB2	6:EM:246:LEU:HD22	1.96	0.48
2:KD:67:LYS:HE3	2:Kd:64:PRO:HD3	1.96	0.48
3:DH:311:MET:HE2	3:DH:341:LYS:HA	1.96	0.48
1:FC:75:ARG:NH2	2:FD:36:ASP:OD1	2.46	0.48
6:GM:158:VAL:HA	6:GM:178:LYS:HZ3	1.78	0.48
6:GM:253:VAL:HG21	6:GM:263:ILE:HG21	1.95	0.48
1:CC:263:ARG:NH1	1:CC:264:ALA:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:JM:61:HIS:HB2	6:JM:109:LYS:HG2	1.95	0.48
2:Jd:64:PRO:HG2	2:Jd:67:LYS:HG2	1.94	0.48
6:CM:118:TYR:HB3	6:CM:138:LEU:HD13	1.96	0.48
7:IN:71:THR:HG22	7:IN:73:HIS:H	1.79	0.48
2:JD:62:ILE:HG22	2:JD:63:THR:HG23	1.94	0.48
3:BH:284:LEU:HD22	3:BH:330:SER:HB3	1.95	0.48
6:BM:94:LEU:HD22	6:BM:98:TYR:HB2	1.94	0.48
2:GD:36:ASP:OD1	2:GD:36:ASP:N	2.45	0.48
5:GL:170:ASP:OD2	5:GL:227:ARG:NH1	2.45	0.48
9:Hf:221:TRP:HE1	9:Hf:229:THR:HB	1.78	0.48
6:MM:177:LEU:HD12	6:MM:196:MET:HE3	1.96	0.48
6:AM:163:THR:HB	6:AM:183:VAL:HG23	1.95	0.48
6:HM:72:ARG:HB3	6:HM:105:THR:HB	1.95	0.48
6:HM:292:MET:HE2	6:HM:298:VAL:H	1.79	0.48
3:IH:311:MET:HG3	3:IH:341:LYS:HA	1.96	0.48
6:KM:279:ILE:HB	6:KM:298:VAL:HG22	1.96	0.48
2:Kd:64:PRO:HG2	2:Kd:67:LYS:HG2	1.95	0.48
6:AM:35:THR:HB	6:AM:75:PRO:HD2	1.96	0.47
3:BH:320:LEU:HD11	3:BH:348:SER:HB2	1.95	0.47
6:BM:209:SER:OG	6:BM:210:ASP:N	2.47	0.47
6:DM:118:TYR:HB3	6:DM:138:LEU:HD13	1.96	0.47
2:GD:155:GLU:OE1	2:Gd:133:ARG:NH2	2.46	0.47
6:IM:35:THR:HB	6:IM:75:PRO:HD2	1.95	0.47
1:JC:225:TYR:HD1	1:JC:251:ALA:HB3	1.79	0.47
6:JM:224:LEU:HB2	6:JM:246:LEU:HD22	1.96	0.47
6:DM:72:ARG:HB3	6:DM:105:THR:HB	1.95	0.47
1:EC:104:ASN:OD1	2:ED:162:TYR:OH	2.33	0.47
2:FD:29:PRO:HG3	5:FL:225:GLN:HA	1.96	0.47
1:IC:263:ARG:NH1	1:IC:264:ALA:O	2.47	0.47
6:BM:35:THR:HB	6:BM:75:PRO:HD2	1.96	0.47
6:BM:280:TYR:HD1	6:BM:299:LEU:HB2	1.79	0.47
9:Ff:246:LEU:HD23	9:Ff:255:LEU:HD13	1.96	0.47
5:HL:53:ASP:OD2	5:HL:153:ARG:NH1	2.45	0.47
9:If:221:TRP:HE1	9:If:229:THR:HB	1.79	0.47
6:KM:164:GLN:HG2	6:KM:184:LEU:HD11	1.96	0.47
4:AK:89:PRO:HG2	6:AM:292:MET:HE1	1.95	0.47
5:BL:49:ASN:ND2	6:BM:293:ALA:O	2.40	0.47
4:DK:65:ILE:HD12	4:DK:78:ILE:HG23	1.95	0.47
6:JM:163:THR:HB	6:JM:183:VAL:HG23	1.96	0.47
6:JM:209:SER:OG	6:JM:210:ASP:N	2.48	0.47
2:MD:155:GLU:OE1	2:MD:157:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:MM:308:ASP:OD1	6:MM:308:ASP:N	2.48	0.47
2:AD:85:VAL:HG23	4:AK:153:ILE:HG12	1.96	0.47
1:DC:75:ARG:NH2	2:DD:36:ASP:OD1	2.47	0.47
4:EK:89:PRO:HG2	6:EM:292:MET:HE1	1.95	0.47
5:EL:49:ASN:ND2	6:EM:293:ALA:O	2.38	0.47
6:MM:72:ARG:HB3	6:MM:105:THR:HB	1.96	0.47
1:AC:104:ASN:ND2	2:AD:162:TYR:OH	2.42	0.47
6:AM:118:TYR:HB3	6:AM:138:LEU:HD13	1.97	0.47
5:GL:49:ASN:ND2	6:GM:293:ALA:O	2.40	0.47
6:HM:164:GLN:HG2	6:HM:184:LEU:HD11	1.97	0.47
1:IC:72:LEU:HD12	1:IC:191:ALA:HB2	1.97	0.47
5:KL:177:HIS:HD1	6:KM:315:TYR:HH	1.62	0.47
2:LD:62:ILE:HG22	2:LD:63:THR:HG23	1.95	0.47
6:AM:199:LYS:HD2	6:AM:219:ALA:HB3	1.97	0.47
1:BC:107:PRO:HG2	1:BC:209:MET:HG2	1.97	0.47
1:BC:263:ARG:NH1	1:BC:264:ALA:O	2.48	0.47
3:BH:279:LEU:HD11	3:BH:289:PRO:HB3	1.95	0.47
4:BK:75:LEU:HD11	4:BK:181:GLU:HG2	1.97	0.47
5:BL:53:ASP:OD2	5:BL:153:ARG:NH1	2.48	0.47
1:GC:72:LEU:HD12	1:GC:191:ALA:HB2	1.97	0.47
9:Gf:221:TRP:HE1	9:Gf:229:THR:HB	1.80	0.47
1:HC:214:LYS:HG2	1:HC:218:MET:HE2	1.96	0.47
6:HM:158:VAL:HA	6:HM:178:LYS:HZ3	1.78	0.47
6:HM:280:TYR:HD1	6:HM:299:LEU:HB2	1.80	0.47
1:JC:95:ASP:HB3	2:Jd:52:MET:HE3	1.95	0.47
5:KL:118:GLU:HG3	5:KL:123:ARG:HG3	1.97	0.47
5:LL:53:ASP:OD1	5:LL:53:ASP:N	2.47	0.47
2:JD:29:PRO:HG3	5:JL:225:GLN:HA	1.97	0.47
1:KC:225:TYR:HD2	1:KC:251:ALA:HB3	1.79	0.47
9:Lf:247:ILE:HA	9:Lf:254:ILE:HG12	1.96	0.47
4:AK:110:ARG:NH1	7:AN:75:VAL:O	2.47	0.47
3:EH:322:PRO:HG2	3:EH:345:LEU:HD23	1.97	0.47
2:Ed:92:GLU:OE2	2:Ed:158:TYR:OH	2.33	0.47
5:FL:49:ASN:ND2	6:FM:293:ALA:O	2.40	0.47
9:Hf:247:ILE:HA	9:Hf:254:ILE:HG12	1.97	0.47
6:IM:308:ASP:OD1	6:IM:308:ASP:N	2.47	0.47
6:KM:118:TYR:HB3	6:KM:138:LEU:HD13	1.97	0.47
1:AC:75:ARG:NH2	2:AD:36:ASP:OD1	2.48	0.46
6:CM:72:ARG:HB3	6:CM:105:THR:HB	1.96	0.46
4:DK:71:GLY:O	2:ED:27:LYS:NZ	2.39	0.46
1:HC:263:ARG:NH1	1:HC:264:ALA:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:IM:224:LEU:HB2	6:IM:246:LEU:HD22	1.98	0.46
3:JH:320:LEU:HD11	3:JH:348:SER:HB2	1.96	0.46
6:KM:35:THR:HB	6:KM:75:PRO:HD2	1.96	0.46
6:LM:118:TYR:HB3	6:LM:138:LEU:HD13	1.98	0.46
1:DC:72:LEU:HD12	1:DC:191:ALA:HB2	1.97	0.46
6:AM:306:GLN:NE2	6:AM:308:ASP:OD2	2.41	0.46
4:BK:51:ALA:HB1	7:BN:44:LYS:HD3	1.97	0.46
9:Gf:241:TYR:HB3	9:Gf:256:THR:HG21	1.98	0.46
1:IC:243:ASP:O	1:JC:128:SER:HA	2.14	0.46
6:DM:253:VAL:HG21	6:DM:263:ILE:HG21	1.96	0.46
6:GM:199:LYS:HD2	6:GM:219:ALA:HB3	1.97	0.46
6:HM:257:ASP:OD1	6:HM:257:ASP:N	2.46	0.46
6:IM:40:GLN:HE22	6:IM:42:ARG:HH21	1.63	0.46
6:LM:94:LEU:HD22	6:LM:98:TYR:HB2	1.98	0.46
1:MC:224:PRO:HB3	1:MC:253:PRO:HD3	1.97	0.46
5:DL:53:ASP:OD2	5:DL:153:ARG:NH1	2.48	0.46
6:JM:118:TYR:HB3	6:JM:138:LEU:HD13	1.97	0.46
4:LK:117:THR:HG23	4:LK:157:GLN:HG3	1.97	0.46
9:Lf:255:LEU:HG	9:Lf:261:VAL:HG22	1.98	0.46
3:MH:320:LEU:HD11	3:MH:348:SER:HB2	1.96	0.46
5:ML:53:ASP:OD1	5:ML:53:ASP:N	2.44	0.46
6:AM:52:VAL:HA	6:AM:92:VAL:O	2.15	0.46
6:BM:257:ASP:OD1	6:BM:257:ASP:N	2.46	0.46
2:Dd:82:ARG:NH1	2:Dd:125:ASP:OD2	2.44	0.46
2:Ed:147:VAL:HG22	2:Ed:154:VAL:HG12	1.98	0.46
6:GM:271:SER:OG	6:GM:290:ASP:OD1	2.34	0.46
6:JM:199:LYS:HD2	6:JM:219:ALA:HB3	1.98	0.46
6:FM:269:GLN:NE2	6:FM:290:ASP:OD1	2.48	0.46
5:JL:177:HIS:ND1	6:JM:315:TYR:OH	2.47	0.46
6:JM:164:GLN:HG2	6:JM:184:LEU:HD11	1.98	0.46
1:KC:75:ARG:NH2	2:KD:36:ASP:OD1	2.48	0.46
6:MM:191:LEU:HB3	6:MM:212:LEU:HD21	1.98	0.46
6:CM:278:ASP:OD2	6:CM:280:TYR:OH	2.29	0.46
1:FC:109:VAL:HG13	1:FC:208:GLY:HA3	1.97	0.46
4:HK:89:PRO:HG2	6:HM:292:MET:HE1	1.97	0.46
6:HM:199:LYS:HG3	6:HM:219:ALA:HB3	1.97	0.46
4:JK:65:ILE:HD12	4:JK:78:ILE:HG23	1.98	0.46
6:JM:307:SER:HG	9:Jf:253:ARG:HH22	1.60	0.46
6:AM:61:HIS:HB2	6:AM:109:LYS:HG2	1.97	0.46
1:CC:107:PRO:HG2	1:CC:209:MET:HG2	1.98	0.46
1:MC:204:GLU:HG3	3:MH:285:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:72:LEU:HD12	1:JC:191:ALA:HB2	1.97	0.46
3:MH:284:LEU:HD22	3:MH:330:SER:HB3	1.97	0.46
6:BM:118:TYR:HB3	6:BM:138:LEU:HD13	1.98	0.45
7:FN:77:ASP:OD1	7:FN:79:GLN:NE2	2.47	0.45
1:GC:77:LYS:NZ	1:GC:81:GLU:OE2	2.45	0.45
6:MM:163:THR:HB	6:MM:183:VAL:HG23	1.97	0.45
6:FM:118:TYR:HB3	6:FM:138:LEU:HD13	1.97	0.45
1:AC:263:ARG:NH1	1:AC:264:ALA:O	2.49	0.45
3:BH:311:MET:HE2	3:BH:341:LYS:HA	1.99	0.45
4:CK:51:ALA:HB1	7:CN:44:LYS:HD3	1.98	0.45
3:DH:330:SER:OG	3:DH:332:ASP:OD1	2.33	0.45
6:EM:257:ASP:OD1	6:EM:257:ASP:N	2.49	0.45
3:GH:320:LEU:HD11	3:GH:348:SER:HB2	1.97	0.45
6:LM:278:ASP:OD2	6:LM:280:TYR:OH	2.30	0.45
2:ED:67:LYS:HE3	2:Ed:64:PRO:HD3	1.97	0.45
1:JC:77:LYS:NZ	1:JC:81:GLU:OE2	2.46	0.45
2:JD:34:SER:OG	2:Jd:36:ASP:OD1	2.33	0.45
4:LK:71:GLY:O	2:MD:27:LYS:NZ	2.41	0.45
6:LM:224:LEU:HB2	6:LM:246:LEU:HD22	1.97	0.45
4:AK:127:LYS:NZ	6:AM:302:ARG:O	2.41	0.45
6:AM:307:SER:HG	9:Af:253:ARG:HH22	1.59	0.45
1:DC:214:LYS:HG2	1:DC:218:MET:HE2	1.99	0.45
1:EC:72:LEU:HD12	1:EC:191:ALA:HB2	1.98	0.45
6:FM:166:ASN:HA	6:FM:186:SER:HB3	1.98	0.45
4:HK:71:GLY:O	2:ID:27:LYS:NZ	2.41	0.45
2:Kd:147:VAL:HG22	2:Kd:154:VAL:HG12	1.99	0.45
4:LK:65:ILE:HD12	4:LK:78:ILE:HG23	1.99	0.45
6:MM:279:ILE:O	6:MM:298:VAL:HA	2.16	0.45
6:CM:94:LEU:HD22	6:CM:98:TYR:HB2	1.98	0.45
6:EM:124:VAL:HB	6:EM:144:THR:HG23	1.98	0.45
2:FD:155:GLU:OE2	2:Fd:133:ARG:NH2	2.49	0.45
6:HM:118:TYR:HB3	6:HM:138:LEU:HD13	1.98	0.45
2:AD:27:LYS:NZ	4:MK:71:GLY:O	2.39	0.45
2:AD:29:PRO:HG3	5:AL:225:GLN:HA	1.98	0.45
6:AM:191:LEU:HB3	6:AM:212:LEU:HD21	1.99	0.45
2:Ed:105:ARG:HB2	2:Ed:153:VAL:HG23	1.98	0.45
1:GC:75:ARG:NH2	2:GD:36:ASP:OD1	2.49	0.45
6:DM:110:THR:OG1	6:DM:111:LYS:N	2.50	0.45
6:GM:164:GLN:HG2	6:GM:184:LEU:HD11	1.99	0.45
4:IK:65:ILE:HD12	4:IK:78:ILE:HG23	1.99	0.45
1:BC:104:ASN:OD1	2:BD:162:TYR:OH	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BM:217:LYS:HA	6:BM:217:LYS:HD3	1.85	0.44
5:CL:177:HIS:ND1	6:CM:315:TYR:OH	2.45	0.44
6:FM:61:HIS:HB2	6:FM:109:LYS:HG2	1.97	0.44
6:HM:224:LEU:HB2	6:HM:246:LEU:HD22	1.99	0.44
7:HN:89:GLY:HA3	7:HN:104:ASN:HB2	1.99	0.44
5:JL:57:VAL:HA	5:JL:60:VAL:HG22	1.99	0.44
6:MM:118:TYR:HB3	6:MM:138:LEU:HD13	1.99	0.44
6:AM:110:THR:OG1	6:AM:111:LYS:N	2.50	0.44
2:Cd:36:ASP:N	2:Cd:36:ASP:OD2	2.45	0.44
6:GM:218:LYS:HD3	6:GM:218:LYS:HA	1.78	0.44
2:ID:29:PRO:HG3	5:IL:225:GLN:HA	1.98	0.44
2:ID:155:GLU:OE2	2:Id:133:ARG:NH2	2.44	0.44
5:KL:210:ASP:OD1	5:KL:210:ASP:N	2.44	0.44
5:BL:170:ASP:OD2	5:BL:227:ARG:NH1	2.46	0.44
6:BM:113:LEU:HD12	6:BM:129:LEU:HD11	1.98	0.44
2:AD:28:PRO:HG3	5:AL:115:GLN:HB2	1.98	0.44
6:EM:189:VAL:HB	6:EM:207:ILE:HG22	2.00	0.44
4:HK:65:ILE:HD12	4:HK:78:ILE:HG23	1.98	0.44
6:HM:280:TYR:HB3	6:HM:301:MET:HG3	1.99	0.44
6:IM:217:LYS:HA	6:IM:217:LYS:HD3	1.83	0.44
4:LK:121:SER:OG	4:LK:122:LYS:N	2.50	0.44
6:EM:249:GLN:OE1	6:EM:267:ASN:ND2	2.51	0.44
6:LM:52:VAL:HA	6:LM:92:VAL:O	2.18	0.44
3:KH:284:LEU:HD22	3:KH:330:SER:HB3	2.00	0.44
6:KM:52:VAL:HA	6:KM:92:VAL:O	2.17	0.44
6:CM:192:ARG:HE	6:CM:192:ARG:HB2	1.58	0.44
2:DD:28:PRO:HG3	5:DL:115:GLN:HB2	2.00	0.44
6:JM:269:GLN:NE2	6:JM:290:ASP:OD1	2.50	0.44
4:KK:66:LYS:HB3	4:KK:77:SER:HB3	1.99	0.44
5:KL:177:HIS:ND1	6:KM:315:TYR:OH	2.44	0.44
3:HH:311:MET:HE2	3:HH:341:LYS:HA	2.00	0.44
6:HM:249:GLN:OE1	6:HM:267:ASN:ND2	2.51	0.44
3:JH:284:LEU:HD22	3:JH:330:SER:HB3	2.00	0.44
6:LM:209:SER:OG	6:LM:210:ASP:N	2.51	0.44
2:MD:140:GLY:O	2:Md:60:LYS:NZ	2.51	0.44
4:AK:65:ILE:HD12	4:AK:78:ILE:HG23	1.98	0.44
1:CC:225:TYR:HD2	1:CC:251:ALA:HB3	1.83	0.44
2:Dd:97:ARG:HA	2:Dd:97:ARG:HD3	1.84	0.44
6:GM:279:ILE:HB	6:GM:298:VAL:HG22	2.00	0.44
3:LH:320:LEU:HD11	3:LH:348:SER:HB2	1.99	0.44
4:LK:47:GLY:O	4:LK:108:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LM:275:ASP:N	6:LM:275:ASP:OD1	2.51	0.44
6:BM:52:VAL:HA	6:BM:92:VAL:O	2.18	0.43
5:EL:57:VAL:HA	5:EL:60:VAL:HG22	1.99	0.43
4:GK:89:PRO:HG2	6:GM:292:MET:HE1	1.99	0.43
3:KH:330:SER:OG	3:KH:332:ASP:OD1	2.36	0.43
2:CD:155:GLU:OE2	2:CD:157:ARG:NH2	2.44	0.43
2:Cd:110:GLY:HA3	2:Cd:158:TYR:HB2	1.99	0.43
6:DM:52:VAL:HA	6:DM:92:VAL:O	2.17	0.43
6:FM:40:GLN:HE22	6:FM:42:ARG:HH21	1.64	0.43
1:IC:116:THR:HG23	3:IH:328:MET:HG2	2.00	0.43
2:ID:28:PRO:HG3	5:IL:115:GLN:HB2	2.00	0.43
7:KN:89:GLY:HA3	7:KN:104:ASN:HB2	1.99	0.43
3:CH:322:PRO:HG2	3:CH:345:LEU:HD23	2.00	0.43
5:CL:53:ASP:OD1	5:CL:53:ASP:N	2.52	0.43
6:FM:224:LEU:HB2	6:FM:246:LEU:HD22	2.00	0.43
2:BD:36:ASP:OD1	2:BD:36:ASP:N	2.50	0.43
2:ED:130:GLU:OE1	2:ED:133:ARG:NH1	2.46	0.43
6:HM:275:ASP:OD1	6:HM:275:ASP:N	2.51	0.43
3:LH:330:SER:OG	3:LH:332:ASP:OD1	2.35	0.43
3:CH:311:MET:HE2	3:CH:341:LYS:HA	2.01	0.43
6:DM:165:ILE:HD12	6:DM:185:ILE:HG12	2.01	0.43
2:FD:62:ILE:HG22	2:FD:63:THR:HG23	2.00	0.43
3:FH:279:LEU:HD11	3:FH:289:PRO:HB3	1.99	0.43
6:FM:217:LYS:HA	6:FM:217:LYS:HD3	1.80	0.43
6:GM:118:TYR:HB3	6:GM:138:LEU:HD13	1.99	0.43
1:HC:72:LEU:HD12	1:HC:191:ALA:HB2	2.00	0.43
2:Hd:82:ARG:NH1	2:Hd:125:ASP:OD1	2.51	0.43
2:Id:97:ARG:HA	2:Id:97:ARG:HD3	1.74	0.43
4:LK:166:THR:HG22	4:LK:168:TYR:H	1.83	0.43
4:AK:47:GLY:O	4:AK:108:GLN:NE2	2.51	0.43
5:AL:49:ASN:ND2	6:AM:293:ALA:O	2.39	0.43
6:DM:40:GLN:HE22	6:DM:42:ARG:HH21	1.65	0.43
2:Dd:111:LYS:HE2	2:Dd:111:LYS:HB3	1.78	0.43
2:FD:28:PRO:HG3	5:FL:115:GLN:HB2	2.00	0.43
4:FK:127:LYS:HB3	4:FK:127:LYS:HE3	1.85	0.43
4:GK:45:VAL:HG23	4:GK:48:ALA:HB3	2.01	0.43
2:HD:62:ILE:HG22	2:HD:63:THR:HG23	2.01	0.43
6:IM:257:ASP:OD1	6:IM:257:ASP:N	2.50	0.43
1:AC:204:GLU:HG3	3:AH:285:GLU:HG3	2.00	0.43
6:AM:224:LEU:HB2	6:AM:246:LEU:HD22	2.01	0.43
7:CN:58:LEU:HD12	7:CN:68:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DK:66:LYS:HB3	4:DK:77:SER:HB3	2.00	0.43
4:EK:65:ILE:HD12	4:EK:78:ILE:HG23	2.01	0.43
2:FD:107:ARG:NH1	2:Fd:130:GLU:OE2	2.48	0.43
6:FM:158:VAL:HA	6:FM:178:LYS:HZ3	1.84	0.43
4:GK:66:LYS:HB3	4:GK:77:SER:HB3	2.01	0.43
1:HC:88:ARG:HD2	1:HC:88:ARG:HA	1.81	0.43
6:HM:94:LEU:HD22	6:HM:98:TYR:HB2	2.01	0.43
7:IN:89:GLY:HA3	7:IN:104:ASN:HB2	2.00	0.43
1:KC:88:ARG:HD2	1:KC:88:ARG:HA	1.81	0.43
5:KL:57:VAL:HA	5:KL:60:VAL:HG22	2.01	0.43
5:AL:57:VAL:HA	5:AL:60:VAL:HG22	2.00	0.43
6:BM:158:VAL:HA	6:BM:178:LYS:HZ3	1.83	0.43
2:GD:50:ASP:HA	2:GD:53:LEU:HB2	2.01	0.43
3:HH:320:LEU:HD11	3:HH:348:SER:HB2	2.01	0.43
2:Ld:64:PRO:HG2	2:Ld:67:LYS:HG2	2.01	0.43
6:CM:217:LYS:HD3	6:CM:217:LYS:HA	1.82	0.43
2:GD:28:PRO:HG3	5:GL:115:GLN:HB2	2.00	0.43
2:GD:52:MET:HE3	2:GD:52:MET:HB3	1.85	0.43
4:HK:117:THR:HG23	4:HK:157:GLN:HG3	2.00	0.43
2:Hd:110:GLY:HA3	2:Hd:158:TYR:HB2	1.99	0.43
6:AM:197:TYR:HA	6:AM:217:LYS:HB3	2.01	0.43
4:BK:65:ILE:HD12	4:BK:78:ILE:HG23	2.00	0.43
6:CM:52:VAL:HA	6:CM:92:VAL:O	2.19	0.43
4:EK:127:LYS:HB3	4:EK:127:LYS:HE3	1.87	0.43
6:EM:292:MET:HE2	6:EM:297:SER:HA	2.01	0.43
4:FK:121:SER:OG	4:FK:122:LYS:N	2.51	0.43
1:JC:210:ILE:HG23	2:JD:55:MET:HG2	2.01	0.43
1:KC:231:LEU:HB2	1:KC:244:ASP:HB2	2.01	0.43
2:KD:130:GLU:OE2	2:KD:133:ARG:NH1	2.51	0.43
6:MM:52:VAL:HA	6:MM:92:VAL:O	2.19	0.43
2:BD:34:SER:OG	2:Bd:36:ASP:OD2	2.37	0.42
6:BM:290:ASP:HB3	6:BM:298:VAL:HG21	2.00	0.42
5:DL:57:VAL:HA	5:DL:60:VAL:HG22	2.01	0.42
6:DM:275:ASP:N	6:DM:275:ASP:OD1	2.52	0.42
6:FM:306:GLN:NE2	6:FM:308:ASP:OD1	2.44	0.42
6:GM:189:VAL:HB	6:GM:207:ILE:HG22	2.01	0.42
6:KM:191:LEU:HB3	6:KM:212:LEU:HD21	2.01	0.42
5:AL:125:LEU:HD11	5:AL:154:LEU:HD23	2.01	0.42
6:CM:40:GLN:HE22	6:CM:42:ARG:HH21	1.67	0.42
6:DM:177:LEU:HD13	6:DM:181:PRO:HG2	2.01	0.42
6:GM:163:THR:HB	6:GM:183:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:IK:66:LYS:HB3	4:IK:77:SER:HB3	2.02	0.42
6:JM:177:LEU:HD12	6:JM:196:MET:HE2	1.99	0.42
2:Kd:150:ASN:OD1	2:Kd:151:SER:N	2.49	0.42
5:LL:145:TYR:HA	5:LL:148:LEU:HD12	2.00	0.42
6:LM:269:GLN:NE2	6:LM:290:ASP:OD1	2.51	0.42
4:MK:117:THR:HG23	4:MK:157:GLN:HG3	2.01	0.42
6:MM:113:LEU:HD12	6:MM:129:LEU:HD11	2.01	0.42
6:GM:285:SER:O	6:GM:316:ASN:ND2	2.52	0.42
6:HM:191:LEU:HB3	6:HM:212:LEU:HD21	2.01	0.42
2:ID:34:SER:OG	2:Id:36:ASP:OD1	2.34	0.42
1:JC:88:ARG:HD2	1:JC:88:ARG:HA	1.89	0.42
6:DM:164:GLN:HG2	6:DM:184:LEU:HD11	2.01	0.42
6:EM:306:GLN:NE2	6:EM:308:ASP:OD1	2.42	0.42
5:FL:53:ASP:OD1	5:FL:53:ASP:N	2.44	0.42
6:HM:292:MET:HE2	6:HM:297:SER:HA	2.01	0.42
6:IM:51:VAL:HA	6:IM:117:ARG:HB3	2.02	0.42
7:LN:44:LYS:HA	7:LN:44:LYS:HD3	1.74	0.42
2:Bd:110:GLY:HA3	2:Bd:158:TYR:HB2	2.00	0.42
6:CM:279:ILE:O	6:CM:298:VAL:HA	2.19	0.42
7:CN:89:GLY:HA3	7:CN:104:ASN:HB2	2.01	0.42
1:EC:221:VAL:HG12	1:EC:255:LEU:HD23	2.02	0.42
6:FM:275:ASP:OD1	6:FM:275:ASP:N	2.52	0.42
3:IH:322:PRO:HG2	3:IH:345:LEU:HD23	2.00	0.42
1:KC:263:ARG:NH1	1:KC:264:ALA:O	2.52	0.42
3:KH:320:LEU:HD11	3:KH:348:SER:HB2	2.01	0.42
3:KH:322:PRO:HB2	3:KH:339:MET:HE1	2.00	0.42
4:LK:56:MET:HE1	4:LK:108:GLN:HG3	2.02	0.42
6:MM:257:ASP:N	6:MM:257:ASP:OD1	2.51	0.42
5:FL:57:VAL:HA	5:FL:60:VAL:HG22	2.01	0.42
4:GK:65:ILE:HD12	4:GK:78:ILE:HG23	2.02	0.42
6:KM:275:ASP:OD1	6:KM:275:ASP:N	2.53	0.42
6:LM:217:LYS:HA	6:LM:217:LYS:HD3	1.78	0.42
6:MM:275:ASP:OD1	6:MM:275:ASP:N	2.53	0.42
5:CL:57:VAL:HA	5:CL:60:VAL:HG22	2.01	0.42
6:EM:110:THR:OG1	6:EM:111:LYS:N	2.51	0.42
5:FL:170:ASP:OD2	5:FL:227:ARG:NH1	2.48	0.42
5:GL:57:VAL:HA	5:GL:60:VAL:HG22	2.02	0.42
2:LD:34:SER:OG	2:Ld:36:ASP:OD1	2.38	0.42
6:AM:292:MET:HE2	6:AM:297:SER:HA	2.01	0.42
1:CC:77:LYS:NZ	1:CC:81:GLU:OE2	2.43	0.42
3:EH:320:LEU:HD11	3:EH:348:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:203:LYS:NZ	2:FD:47:SER:OG	2.35	0.42
6:FM:209:SER:OG	6:FM:210:ASP:N	2.53	0.42
2:Fd:112:SER:HA	2:Fd:113:PRO:HD3	1.93	0.42
2:Ld:111:LYS:HE2	2:Ld:111:LYS:HB3	1.83	0.42
9:Af:222:LEU:HD12	9:Af:230:LEU:HD22	2.02	0.42
6:GM:191:LEU:HB3	6:GM:212:LEU:HD21	2.01	0.42
2:Gd:148:TYR:HB2	2:Gd:153:VAL:HG12	2.02	0.42
4:HK:66:LYS:HB3	4:HK:77:SER:HB3	2.02	0.42
2:ID:36:ASP:OD1	2:ID:36:ASP:N	2.51	0.42
6:IM:127:ASN:HB3	6:IM:147:ALA:HB3	2.00	0.42
4:MK:110:ARG:NH1	7:MN:75:VAL:O	2.43	0.42
2:CD:34:SER:OG	2:Cd:36:ASP:OD2	2.38	0.42
6:CM:275:ASP:HB3	6:CM:294:PHE:HB2	2.01	0.42
3:EH:311:MET:HE2	3:EH:341:LYS:HA	2.00	0.42
6:EM:275:ASP:OD1	6:EM:275:ASP:N	2.52	0.42
6:HM:127:ASN:HB3	6:HM:147:ALA:HB3	2.01	0.42
6:HM:201:THR:HG22	6:HM:221:LYS:HB2	2.02	0.42
5:IL:57:VAL:HA	5:IL:60:VAL:HG22	2.02	0.42
5:BL:57:VAL:HA	5:BL:60:VAL:HG22	2.01	0.41
6:DM:189:VAL:HB	6:DM:207:ILE:HG22	2.02	0.41
6:DM:279:ILE:O	6:DM:298:VAL:HA	2.19	0.41
6:IM:275:ASP:N	6:IM:275:ASP:OD1	2.51	0.41
6:LM:240:GLN:HA	6:LM:260:VAL:O	2.19	0.41
1:CC:243:ASP:O	1:DC:128:SER:HA	2.19	0.41
6:CM:209:SER:OG	6:CM:210:ASP:N	2.53	0.41
5:DL:49:ASN:ND2	6:DM:293:ALA:O	2.41	0.41
6:FM:197:TYR:HA	6:FM:217:LYS:HB3	2.02	0.41
2:Fd:150:ASN:OD1	2:Fd:150:ASN:N	2.51	0.41
6:GM:113:LEU:HD12	6:GM:129:LEU:HD11	2.03	0.41
4:JK:111:LYS:HD2	4:JK:114:ILE:HD11	2.02	0.41
1:KC:203:LYS:HZ1	2:KD:47:SER:HB2	1.84	0.41
6:MM:75:PRO:HA	6:MM:78:LEU:HG	2.01	0.41
1:DC:234:THR:OG1	1:DC:244:ASP:OD2	2.36	0.41
4:HK:52:THR:HG22	4:HK:56:MET:HE3	2.02	0.41
4:LK:56:MET:HE3	4:LK:105:PHE:HD1	1.85	0.41
2:MD:85:VAL:HG23	4:MK:153:ILE:HG12	2.01	0.41
7:BN:58:LEU:HD12	7:BN:68:CYS:HB2	2.03	0.41
2:ID:85:VAL:HG23	4:IK:153:ILE:HG12	2.02	0.41
6:KM:78:LEU:HD23	6:KM:78:LEU:HA	1.95	0.41
6:LM:158:VAL:HA	6:LM:178:LYS:HZ3	1.85	0.41
4:CK:65:ILE:HD12	4:CK:78:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DN:89:GLY:HA3	7:DN:104:ASN:HB2	2.03	0.41
5:EL:163:ILE:HB	5:EL:203:LEU:HD23	2.03	0.41
6:EM:164:GLN:HG2	6:EM:184:LEU:HD11	2.02	0.41
3:FH:279:LEU:HD21	3:FH:289:PRO:HB3	2.01	0.41
2:Gd:110:GLY:HA3	2:Gd:158:TYR:HB2	2.01	0.41
1:HC:107:PRO:HG2	1:HC:209:MET:HG2	2.03	0.41
6:KM:217:LYS:HD3	6:KM:217:LYS:HA	1.87	0.41
1:LC:263:ARG:NH1	1:LC:264:ALA:O	2.54	0.41
6:MM:127:ASN:HB3	6:MM:147:ALA:HB3	2.02	0.41
2:Ad:73:ILE:HA	2:Ad:74:PRO:HD3	1.93	0.41
6:GM:52:VAL:HA	6:GM:92:VAL:O	2.21	0.41
6:GM:275:ASP:N	6:GM:275:ASP:OD1	2.51	0.41
2:Gd:67:LYS:HE2	2:Gd:67:LYS:HB3	1.94	0.41
5:HL:57:VAL:HA	5:HL:60:VAL:HG22	2.02	0.41
6:IM:94:LEU:HD22	6:IM:98:TYR:HB2	2.02	0.41
6:IM:123:VAL:HG13	6:IM:145:ARG:HH12	1.85	0.41
6:LM:197:TYR:HA	6:LM:217:LYS:HB3	2.02	0.41
5:ML:57:VAL:HA	5:ML:60:VAL:HG22	2.02	0.41
6:BM:193:GLN:HG3	6:BM:213:THR:HB	2.03	0.41
4:EK:117:THR:HG23	4:EK:157:GLN:HG3	2.03	0.41
5:EL:53:ASP:OD1	5:EL:53:ASP:N	2.47	0.41
7:FN:89:GLY:HA3	7:FN:104:ASN:HB2	2.03	0.41
1:IC:234:THR:OG1	1:IC:244:ASP:OD2	2.34	0.41
4:JK:71:GLY:O	2:KD:27:LYS:NZ	2.40	0.41
6:JM:127:ASN:HB3	6:JM:147:ALA:HB3	2.02	0.41
6:MM:269:GLN:NE2	6:MM:290:ASP:OD1	2.53	0.41
5:BL:163:ILE:HB	5:BL:203:LEU:HD23	2.02	0.41
6:CM:189:VAL:HB	6:CM:207:ILE:HG22	2.02	0.41
6:DM:217:LYS:HA	6:DM:217:LYS:HD3	1.78	0.41
5:EL:125:LEU:HD11	5:EL:154:LEU:HD23	2.03	0.41
9:Ef:219:ARG:HG3	9:Ef:233:ARG:HD2	2.02	0.41
5:FL:131:LYS:HE2	5:FL:131:LYS:HB3	1.91	0.41
1:JC:243:ASP:O	1:KC:128:SER:HA	2.20	0.41
2:JD:155:GLU:OE2	2:JD:157:ARG:NH2	2.43	0.41
5:JL:53:ASP:OD1	5:JL:53:ASP:N	2.53	0.41
4:LK:66:LYS:HB3	4:LK:77:SER:HB3	2.03	0.41
5:AL:210:ASP:OD1	5:AL:210:ASP:N	2.44	0.41
6:AM:166:ASN:HA	6:AM:186:SER:HB3	2.02	0.41
6:AM:274:THR:HA	6:AM:293:ALA:HB3	2.03	0.41
3:BH:279:LEU:HD21	3:BH:289:PRO:HB3	2.03	0.41
6:BM:275:ASP:OD1	6:BM:275:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CL:163:ILE:HB	5:CL:203:LEU:HD23	2.03	0.41
6:DM:218:LYS:HA	6:DM:218:LYS:HD3	1.95	0.41
1:FC:144:PRO:HA	1:FC:145:PRO:HD3	1.98	0.41
2:FD:52:MET:HE3	2:FD:52:MET:HB3	1.73	0.41
5:FL:177:HIS:HD1	6:FM:315:TYR:HH	1.68	0.41
6:IM:279:ILE:O	6:IM:298:VAL:HA	2.21	0.41
6:JM:158:VAL:HA	6:JM:178:LYS:HZ3	1.86	0.41
6:JM:275:ASP:HB3	6:JM:294:PHE:HB2	2.03	0.41
2:Jd:112:SER:HA	2:Jd:113:PRO:HD3	1.94	0.41
6:KM:197:TYR:HA	6:KM:217:LYS:HB3	2.02	0.41
2:Kd:73:ILE:HA	2:Kd:74:PRO:HD3	1.95	0.41
2:LD:111:LYS:HA	2:LD:111:LYS:HD2	1.89	0.41
2:Ld:112:SER:HA	2:Ld:113:PRO:HD3	1.94	0.41
6:MM:260:VAL:HG22	6:MM:278:ASP:HB2	2.02	0.41
6:AM:168:VAL:H	6:AM:187:GLY:HA3	1.85	0.41
2:BD:53:LEU:HD12	2:BD:53:LEU:HA	1.97	0.41
6:BM:86:LYS:O	6:BM:89:THR:OG1	2.37	0.41
6:BM:127:ASN:HB3	6:BM:147:ALA:HB3	2.03	0.41
7:EN:89:GLY:HA3	7:EN:104:ASN:HB2	2.03	0.41
2:Gd:112:SER:HA	2:Gd:113:PRO:HD3	1.94	0.41
1:HC:213:ARG:NH2	2:Hd:59:GLU:OE1	2.53	0.41
1:IC:88:ARG:HA	1:IC:88:ARG:HD2	1.88	0.41
6:KM:94:LEU:HD22	6:KM:98:TYR:HB2	2.02	0.41
6:LM:113:LEU:HD12	6:LM:129:LEU:HD11	2.03	0.41
2:Gd:111:LYS:HE2	2:Gd:111:LYS:HB3	1.76	0.40
1:JC:114:ARG:HG2	1:JC:130:ARG:HG2	2.02	0.40
6:JM:52:VAL:HA	6:JM:92:VAL:O	2.21	0.40
1:EC:144:PRO:HA	1:EC:145:PRO:HD3	1.98	0.40
6:FM:168:VAL:H	6:FM:187:GLY:HA3	1.87	0.40
6:GM:224:LEU:HB2	6:GM:246:LEU:HD22	2.03	0.40
6:GM:275:ASP:HB3	6:GM:294:PHE:HB2	2.03	0.40
1:MC:210:ILE:HG23	2:MD:55:MET:HG2	2.04	0.40
7:MN:89:GLY:HA3	7:MN:104:ASN:HB2	2.02	0.40
6:AM:183:VAL:O	6:AM:202:LEU:HA	2.21	0.40
2:FD:34:SER:OG	2:Fd:36:ASP:OD1	2.39	0.40
6:GM:319:PHE:HA	6:GM:320:PRO:HD2	1.98	0.40
1:JC:178:ILE:HG23	1:JC:179:TYR:HD1	1.87	0.40
1:LC:72:LEU:HD12	1:LC:191:ALA:HB2	2.02	0.40
6:AM:124:VAL:HB	6:AM:144:THR:HG23	2.02	0.40
6:AM:275:ASP:HB3	6:AM:294:PHE:HB2	2.02	0.40
4:EK:78:ILE:HB	4:EK:180:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Fd:97:ARG:HA	2:Fd:97:ARG:HD3	1.86	0.40
2:GD:62:ILE:HG22	2:GD:63:THR:HG23	2.04	0.40
6:JM:217:LYS:HA	6:JM:217:LYS:HD3	1.81	0.40
5:LL:57:VAL:HA	5:LL:60:VAL:HG22	2.02	0.40
2:Ld:97:ARG:HD3	2:Ld:97:ARG:HA	1.85	0.40
2:Ld:110:GLY:HA3	2:Ld:158:TYR:HB2	2.03	0.40
5:CL:99:ARG:HA	5:CL:104:LYS:HG2	2.03	0.40
3:IH:284:LEU:HD22	3:IH:330:SER:HB3	2.04	0.40
6:IM:271:SER:OG	6:IM:290:ASP:OD1	2.40	0.40
6:MM:209:SER:OG	6:MM:210:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	200/303 (66%)	193 (96%)	7 (4%)	0	100	100
1	BC	200/303 (66%)	193 (96%)	7 (4%)	0	100	100
1	CC	200/303 (66%)	194 (97%)	6 (3%)	0	100	100
1	DC	200/303 (66%)	192 (96%)	8 (4%)	0	100	100
1	EC	200/303 (66%)	193 (96%)	7 (4%)	0	100	100
1	FC	200/303 (66%)	192 (96%)	8 (4%)	0	100	100
1	GC	200/303 (66%)	194 (97%)	6 (3%)	0	100	100
1	HC	200/303 (66%)	194 (97%)	6 (3%)	0	100	100
1	IC	200/303 (66%)	192 (96%)	8 (4%)	0	100	100
1	JC	200/303 (66%)	194 (97%)	6 (3%)	0	100	100
1	KC	200/303 (66%)	192 (96%)	8 (4%)	0	100	100
1	LC	200/303 (66%)	192 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MC	200/303 (66%)	194 (97%)	6 (3%)	0	100	100
2	AD	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Ad	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	BD	137/163 (84%)	135 (98%)	2 (2%)	0	100	100
2	Bd	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	CD	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Cd	134/163 (82%)	128 (96%)	6 (4%)	0	100	100
2	DD	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
2	Dd	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	ED	137/163 (84%)	133 (97%)	4 (3%)	0	100	100
2	Ed	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	FD	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Fd	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	GD	137/163 (84%)	133 (97%)	4 (3%)	0	100	100
2	Gd	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	HD	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Hd	134/163 (82%)	127 (95%)	7 (5%)	0	100	100
2	ID	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Id	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	JD	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Jd	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	KD	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Kd	134/163 (82%)	128 (96%)	6 (4%)	0	100	100
2	LD	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
2	Ld	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	MD	137/163 (84%)	133 (97%)	4 (3%)	0	100	100
2	Md	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
3	AH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	BH	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
3	CH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	DH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	FH	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
3	GH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	HH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	IH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	JH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	KH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
3	LH	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
3	MH	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
4	AK	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
4	BK	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
4	CK	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
4	DK	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
4	EK	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
4	FK	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
4	GK	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
4	HK	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
4	IK	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
4	JK	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
4	KK	147/189 (78%)	142 (97%)	5 (3%)	0	100	100
4	LK	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
4	MK	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
5	AL	167/249 (67%)	160 (96%)	7 (4%)	0	100	100
5	BL	167/249 (67%)	159 (95%)	8 (5%)	0	100	100
5	CL	167/249 (67%)	160 (96%)	7 (4%)	0	100	100
5	DL	167/249 (67%)	159 (95%)	8 (5%)	0	100	100
5	EL	167/249 (67%)	161 (96%)	6 (4%)	0	100	100
5	FL	167/249 (67%)	159 (95%)	8 (5%)	0	100	100
5	GL	167/249 (67%)	160 (96%)	7 (4%)	0	100	100
5	HL	167/249 (67%)	159 (95%)	8 (5%)	0	100	100
5	IL	167/249 (67%)	159 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	JL	167/249 (67%)	161 (96%)	6 (4%)	0	100	100
5	KL	167/249 (67%)	161 (96%)	6 (4%)	0	100	100
5	LL	167/249 (67%)	158 (95%)	9 (5%)	0	100	100
5	ML	167/249 (67%)	160 (96%)	7 (4%)	0	100	100
6	AM	290/320 (91%)	268 (92%)	22 (8%)	0	100	100
6	BM	290/320 (91%)	272 (94%)	18 (6%)	0	100	100
6	CM	290/320 (91%)	266 (92%)	24 (8%)	0	100	100
6	DM	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
6	EM	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
6	FM	290/320 (91%)	268 (92%)	22 (8%)	0	100	100
6	GM	290/320 (91%)	267 (92%)	23 (8%)	0	100	100
6	HM	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
6	IM	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
6	JM	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
6	KM	290/320 (91%)	267 (92%)	23 (8%)	0	100	100
6	LM	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
6	MM	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
7	AN	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
7	BN	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
7	CN	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
7	DN	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
7	EN	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
7	FN	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
7	GN	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
7	HN	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
7	IN	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
7	JN	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
7	KN	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
7	LN	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
7	MN	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
9	Af	57/269 (21%)	53 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Bf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
9	Cf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
9	Df	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
9	Ef	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
9	Ff	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
9	Gf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
9	Hf	57/269 (21%)	56 (98%)	1 (2%)	0	100	100
9	If	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
9	Jf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
9	Kf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
9	Lf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
9	Mf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
All	All	16835/27833 (60%)	16046 (95%)	789 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	173/257 (67%)	173 (100%)	0	100	100
1	BC	173/257 (67%)	173 (100%)	0	100	100
1	CC	173/257 (67%)	173 (100%)	0	100	100
1	DC	173/257 (67%)	173 (100%)	0	100	100
1	EC	173/257 (67%)	173 (100%)	0	100	100
1	FC	173/257 (67%)	173 (100%)	0	100	100
1	GC	173/257 (67%)	173 (100%)	0	100	100
1	HC	173/257 (67%)	173 (100%)	0	100	100
1	IC	173/257 (67%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JC	173/257 (67%)	173 (100%)	0	100	100
1	KC	173/257 (67%)	173 (100%)	0	100	100
1	LC	173/257 (67%)	173 (100%)	0	100	100
1	MC	173/257 (67%)	173 (100%)	0	100	100
2	AD	120/139 (86%)	120 (100%)	0	100	100
2	Ad	117/139 (84%)	117 (100%)	0	100	100
2	BD	120/139 (86%)	120 (100%)	0	100	100
2	Bd	117/139 (84%)	117 (100%)	0	100	100
2	CD	120/139 (86%)	120 (100%)	0	100	100
2	Cd	117/139 (84%)	117 (100%)	0	100	100
2	DD	120/139 (86%)	120 (100%)	0	100	100
2	Dd	117/139 (84%)	117 (100%)	0	100	100
2	ED	120/139 (86%)	120 (100%)	0	100	100
2	Ed	117/139 (84%)	117 (100%)	0	100	100
2	FD	120/139 (86%)	120 (100%)	0	100	100
2	Fd	117/139 (84%)	117 (100%)	0	100	100
2	GD	120/139 (86%)	120 (100%)	0	100	100
2	Gd	117/139 (84%)	117 (100%)	0	100	100
2	HD	120/139 (86%)	120 (100%)	0	100	100
2	Hd	117/139 (84%)	117 (100%)	0	100	100
2	ID	120/139 (86%)	120 (100%)	0	100	100
2	Id	117/139 (84%)	117 (100%)	0	100	100
2	JD	120/139 (86%)	120 (100%)	0	100	100
2	Jd	117/139 (84%)	117 (100%)	0	100	100
2	KD	120/139 (86%)	120 (100%)	0	100	100
2	Kd	117/139 (84%)	117 (100%)	0	100	100
2	LD	120/139 (86%)	120 (100%)	0	100	100
2	Ld	117/139 (84%)	117 (100%)	0	100	100
2	MD	120/139 (86%)	120 (100%)	0	100	100
2	Md	117/139 (84%)	117 (100%)	0	100	100
3	AH	76/300 (25%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BH	76/300 (25%)	76 (100%)	0	100	100
3	CH	76/300 (25%)	76 (100%)	0	100	100
3	DH	76/300 (25%)	76 (100%)	0	100	100
3	EH	76/300 (25%)	76 (100%)	0	100	100
3	FH	76/300 (25%)	76 (100%)	0	100	100
3	GH	76/300 (25%)	76 (100%)	0	100	100
3	HH	76/300 (25%)	76 (100%)	0	100	100
3	IH	76/300 (25%)	76 (100%)	0	100	100
3	JH	76/300 (25%)	76 (100%)	0	100	100
3	KH	76/300 (25%)	76 (100%)	0	100	100
3	LH	76/300 (25%)	76 (100%)	0	100	100
3	MH	76/300 (25%)	76 (100%)	0	100	100
4	AK	127/163 (78%)	127 (100%)	0	100	100
4	BK	127/163 (78%)	127 (100%)	0	100	100
4	CK	127/163 (78%)	127 (100%)	0	100	100
4	DK	127/163 (78%)	127 (100%)	0	100	100
4	EK	127/163 (78%)	127 (100%)	0	100	100
4	FK	127/163 (78%)	127 (100%)	0	100	100
4	GK	127/163 (78%)	127 (100%)	0	100	100
4	HK	127/163 (78%)	127 (100%)	0	100	100
4	IK	127/163 (78%)	127 (100%)	0	100	100
4	JK	127/163 (78%)	127 (100%)	0	100	100
4	KK	127/163 (78%)	127 (100%)	0	100	100
4	LK	127/163 (78%)	127 (100%)	0	100	100
4	MK	127/163 (78%)	127 (100%)	0	100	100
5	AL	146/203 (72%)	146 (100%)	0	100	100
5	BL	146/203 (72%)	146 (100%)	0	100	100
5	CL	146/203 (72%)	146 (100%)	0	100	100
5	DL	146/203 (72%)	146 (100%)	0	100	100
5	EL	146/203 (72%)	146 (100%)	0	100	100
5	FL	146/203 (72%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	GL	146/203 (72%)	146 (100%)	0	100	100
5	HL	146/203 (72%)	146 (100%)	0	100	100
5	IL	146/203 (72%)	146 (100%)	0	100	100
5	JL	146/203 (72%)	146 (100%)	0	100	100
5	KL	146/203 (72%)	146 (100%)	0	100	100
5	LL	146/203 (72%)	146 (100%)	0	100	100
5	ML	146/203 (72%)	146 (100%)	0	100	100
6	AM	251/276 (91%)	251 (100%)	0	100	100
6	BM	251/276 (91%)	251 (100%)	0	100	100
6	CM	251/276 (91%)	251 (100%)	0	100	100
6	DM	251/276 (91%)	251 (100%)	0	100	100
6	EM	251/276 (91%)	251 (100%)	0	100	100
6	FM	251/276 (91%)	251 (100%)	0	100	100
6	GM	251/276 (91%)	251 (100%)	0	100	100
6	HM	251/276 (91%)	251 (100%)	0	100	100
6	IM	251/276 (91%)	251 (100%)	0	100	100
6	JM	251/276 (91%)	251 (100%)	0	100	100
6	KM	251/276 (91%)	251 (100%)	0	100	100
6	LM	251/276 (91%)	251 (100%)	0	100	100
6	MM	251/276 (91%)	251 (100%)	0	100	100
7	AN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	BN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	CN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	DN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	EN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	FN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	GN	64/107 (60%)	64 (100%)	0	100	100
7	HN	64/107 (60%)	64 (100%)	0	100	100
7	IN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	JN	64/107 (60%)	63 (98%)	1 (2%)	55	83
7	KN	64/107 (60%)	63 (98%)	1 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LN	64/107 (60%)	64 (100%)	0	100	100
7	MN	64/107 (60%)	63 (98%)	1 (2%)	55	83
9	Af	49/237 (21%)	49 (100%)	0	100	100
9	Bf	49/237 (21%)	49 (100%)	0	100	100
9	Cf	49/237 (21%)	49 (100%)	0	100	100
9	Df	49/237 (21%)	49 (100%)	0	100	100
9	Ef	49/237 (21%)	49 (100%)	0	100	100
9	Ff	49/237 (21%)	49 (100%)	0	100	100
9	Gf	49/237 (21%)	49 (100%)	0	100	100
9	Hf	49/237 (21%)	49 (100%)	0	100	100
9	If	49/237 (21%)	49 (100%)	0	100	100
9	Jf	49/237 (21%)	49 (100%)	0	100	100
9	Kf	49/237 (21%)	49 (100%)	0	100	100
9	Lf	49/237 (21%)	49 (100%)	0	100	100
9	Mf	49/237 (21%)	49 (100%)	0	100	100
All	All	14599/23673 (62%)	14589 (100%)	10 (0%)	87	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	AN	94	GLN
7	BN	94	GLN
7	CN	94	GLN
7	DN	94	GLN
7	EN	94	GLN
7	FN	94	GLN
7	IN	94	GLN
7	JN	94	GLN
7	KN	94	GLN
7	MN	94	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	AC	82	GLN
1	AC	104	ASN

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Mol	Chain	Res	Type
1	AC	137	GLN
2	AD	32	ASN
2	AD	152	GLN
3	AH	335	HIS
6	AM	40	GLN
6	AM	57	ASN
6	AM	80	GLN
2	Ad	80	GLN
2	BD	32	ASN
2	BD	80	GLN
2	BD	138	GLN
4	BK	72	GLN
6	BM	40	GLN
6	BM	57	ASN
6	BM	80	GLN
6	BM	316	ASN
2	Bd	146	HIS
9	Bf	213	GLN
1	CC	69	GLN
1	CC	82	GLN
1	CC	123	GLN
2	CD	32	ASN
2	CD	78	ASN
5	CL	160	GLN
5	CL	183	GLN
6	CM	40	GLN
6	CM	57	ASN
6	CM	316	ASN
2	Cd	80	GLN
1	DC	35	GLN
1	DC	190	GLN
2	DD	32	ASN
3	DH	335	HIS
4	DK	157	GLN
6	DM	40	GLN
6	DM	80	GLN
6	DM	190	ASN
6	DM	316	ASN
7	DN	73	HIS
7	DN	115	GLN
2	Dd	146	HIS
1	EC	35	GLN

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Mol	Chain	Res	Type
1	EC	82	GLN
1	EC	123	GLN
2	ED	31	ASN
2	ED	32	ASN
5	EL	160	GLN
6	EM	40	GLN
6	EM	80	GLN
2	Ed	31	ASN
1	FC	69	GLN
1	FC	82	GLN
1	FC	149	GLN
2	FD	32	ASN
2	FD	80	GLN
2	FD	138	GLN
4	FK	157	GLN
6	FM	40	GLN
6	FM	57	ASN
6	FM	80	GLN
9	Ff	213	GLN
1	GC	82	GLN
2	GD	32	ASN
2	GD	138	GLN
3	GH	335	HIS
3	GH	340	GLN
5	GL	110	GLN
6	GM	40	GLN
6	GM	57	ASN
6	GM	316	ASN
2	Gd	31	ASN
2	Gd	80	GLN
1	HC	35	GLN
1	HC	103	HIS
2	HD	32	ASN
2	HD	152	GLN
6	HM	40	GLN
6	HM	57	ASN
6	HM	80	GLN
9	Hf	260	GLN
9	Hf	266	GLN
1	IC	82	GLN
2	ID	32	ASN
2	ID	138	GLN

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Mol	Chain	Res	Type
2	ID	152	GLN
4	IK	157	GLN
6	IM	40	GLN
6	IM	80	GLN
6	IM	190	ASN
6	IM	316	ASN
2	Id	80	GLN
2	Id	146	HIS
1	JC	82	GLN
1	JC	104	ASN
1	JC	149	GLN
2	JD	32	ASN
6	JM	48	ASN
6	JM	57	ASN
6	JM	80	GLN
9	Jf	213	GLN
1	KC	149	GLN
2	KD	32	ASN
2	KD	138	GLN
5	KL	51	GLN
5	KL	160	GLN
6	KM	40	GLN
6	KM	80	GLN
6	KM	190	ASN
2	Kd	80	GLN
2	Kd	146	HIS
9	Kf	213	GLN
1	LC	69	GLN
2	LD	32	ASN
2	LD	78	ASN
3	LH	340	GLN
6	LM	40	GLN
6	LM	57	ASN
6	LM	80	GLN
7	LN	73	HIS
1	MC	82	GLN
2	MD	32	ASN
2	MD	80	GLN
2	MD	138	GLN
3	MH	340	GLN
5	ML	51	GLN
5	ML	183	GLN

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Mol	Chain	Res	Type
5	ML	232	GLN
6	MM	40	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

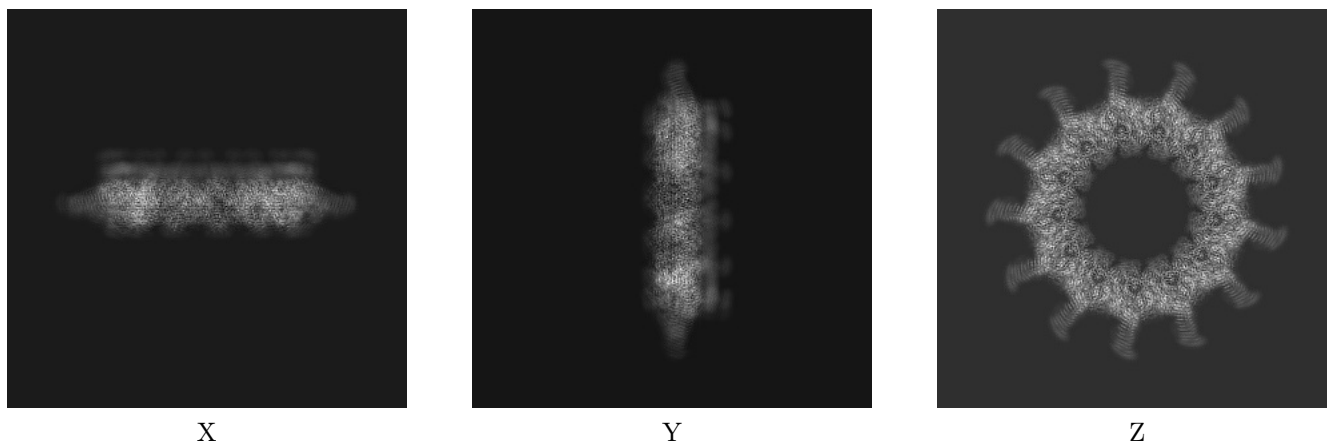
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24005. 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](#)

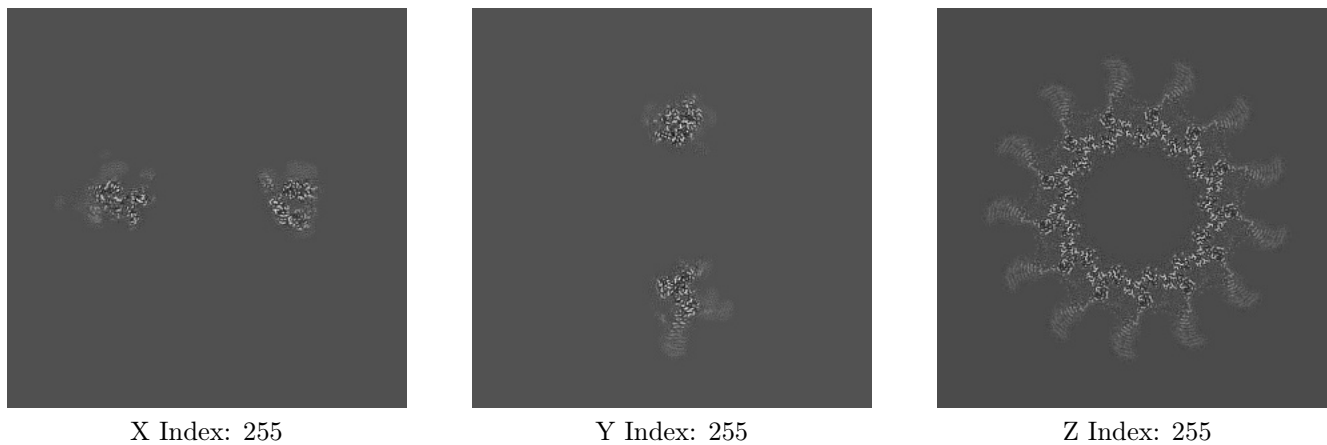
6.1.1 Primary map



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

6.2 Central slices [i](#)

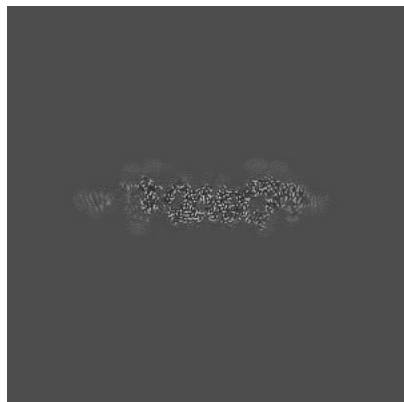
6.2.1 Primary map



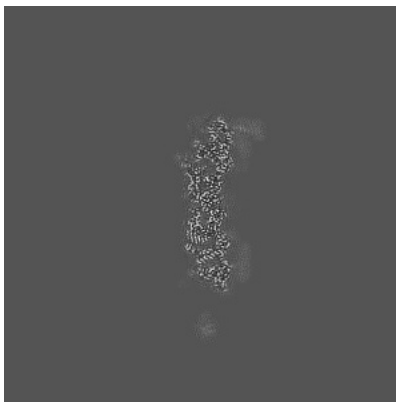
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

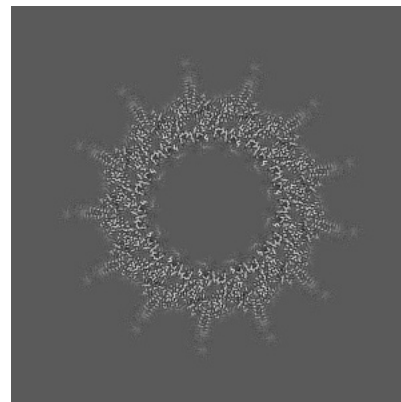
6.3.1 Primary map



X Index: 164



Y Index: 344

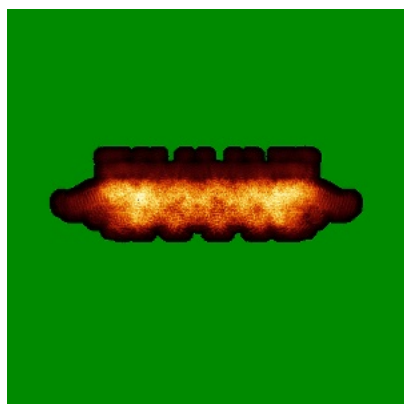


Z Index: 273

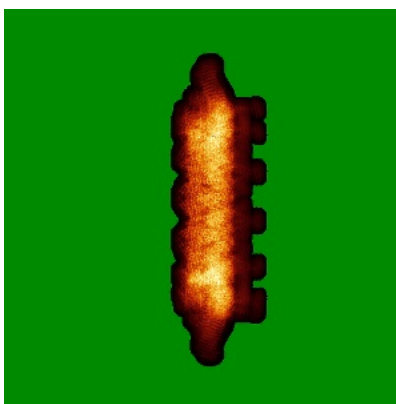
The images above show the largest variance slices of the map in three orthogonal directions.

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

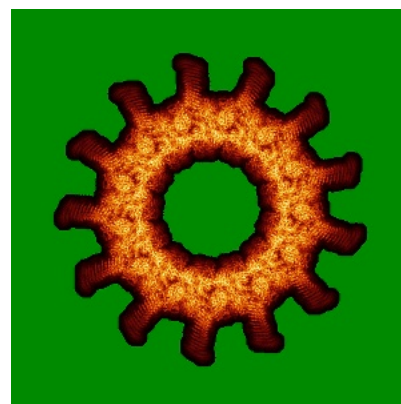
6.4.1 Primary map



X



Y

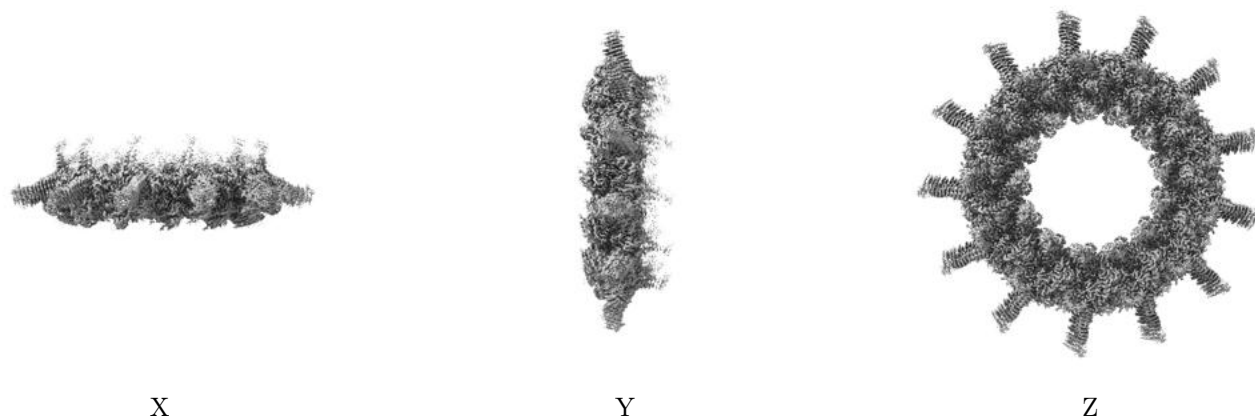


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

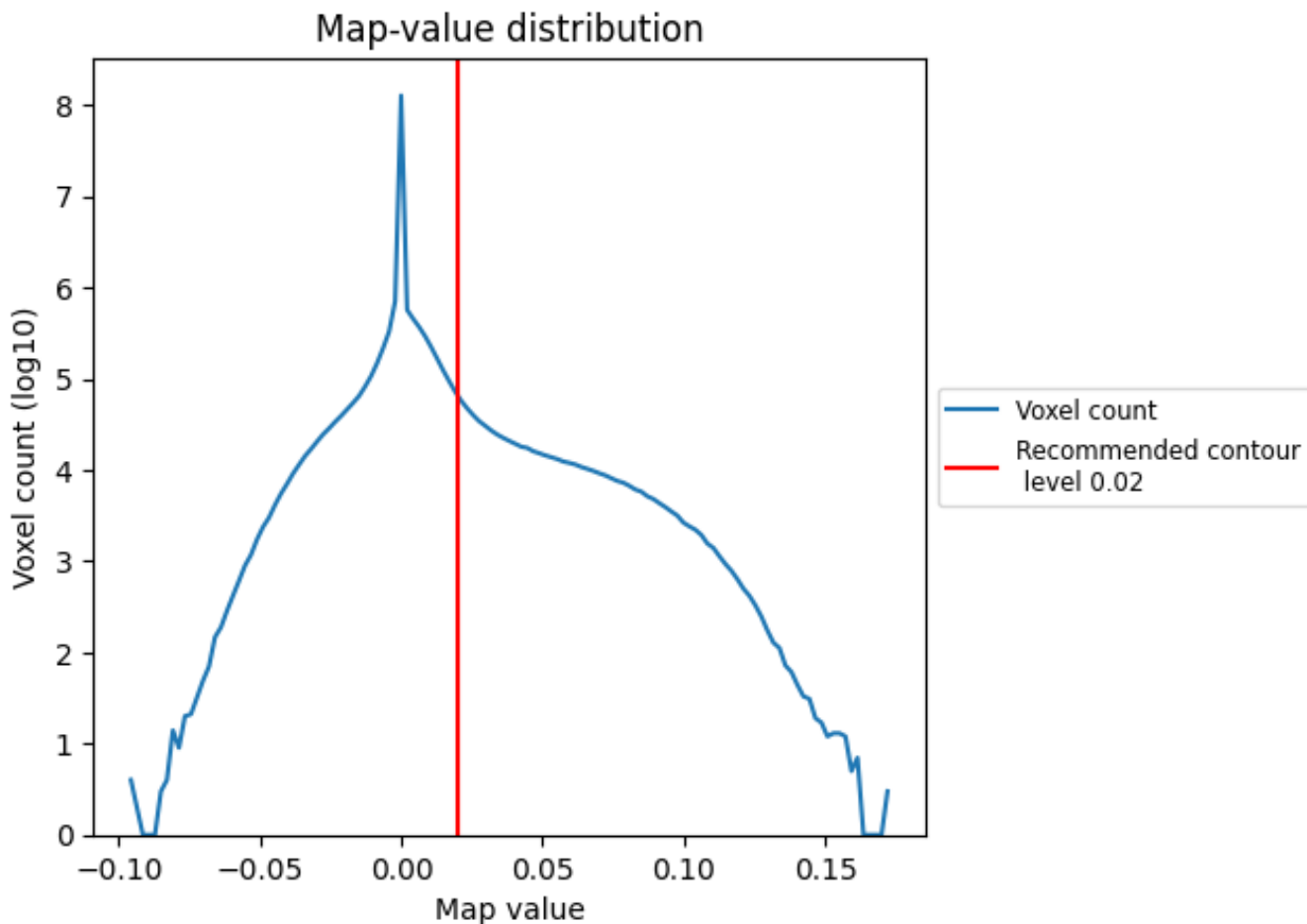
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

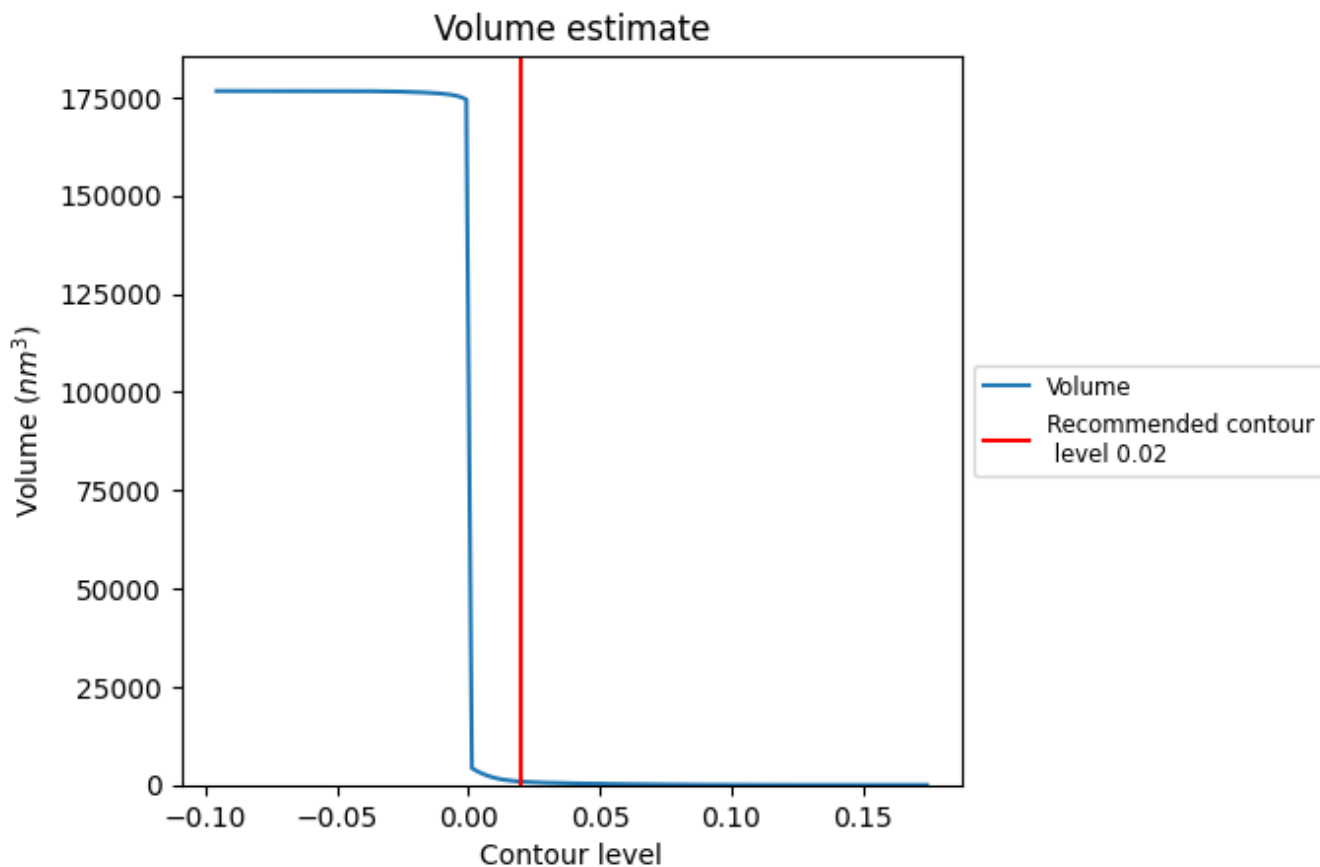
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

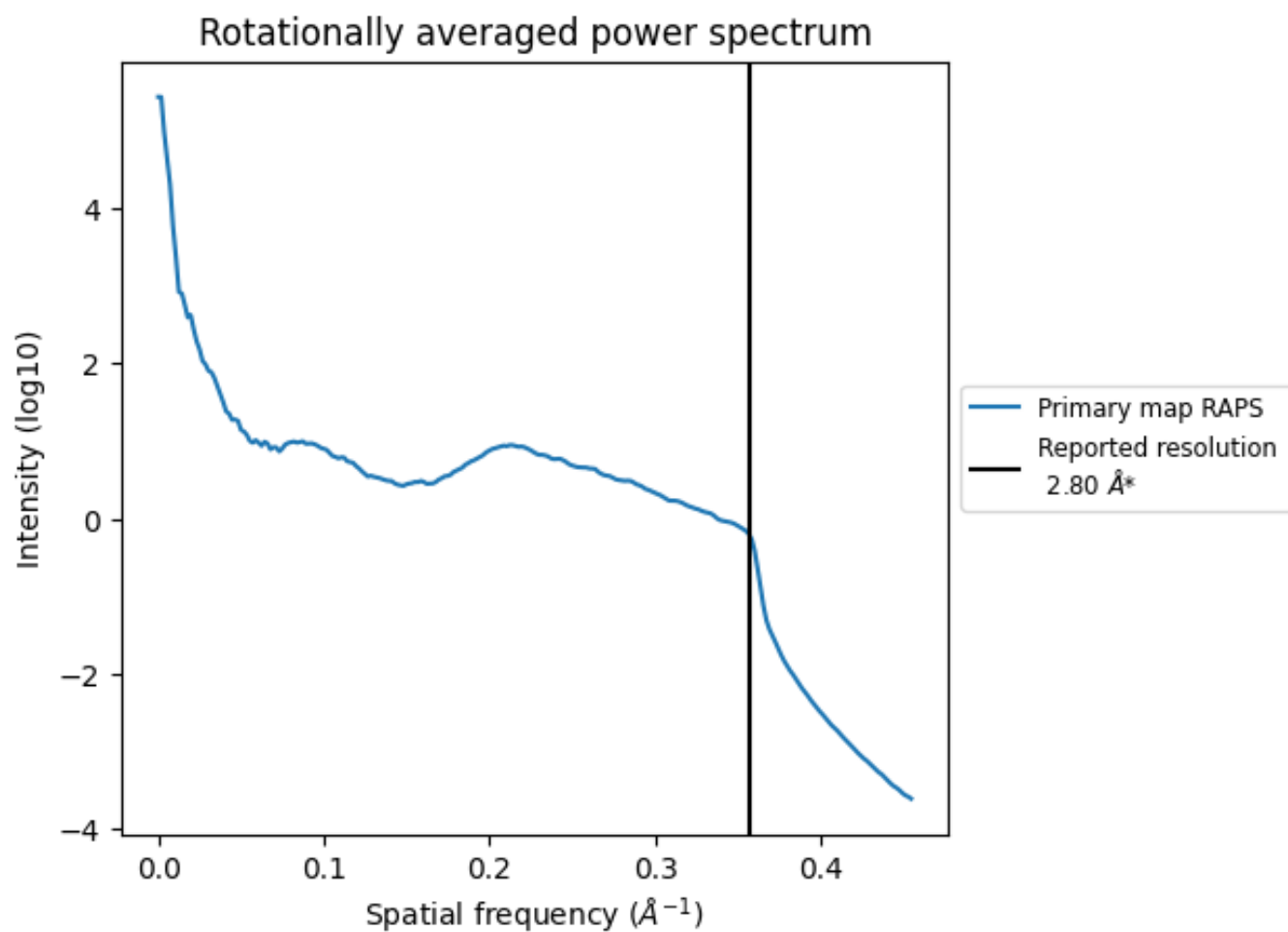
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 856 nm^3 ; this corresponds to an approximate mass of 773 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.357\AA^{-1}

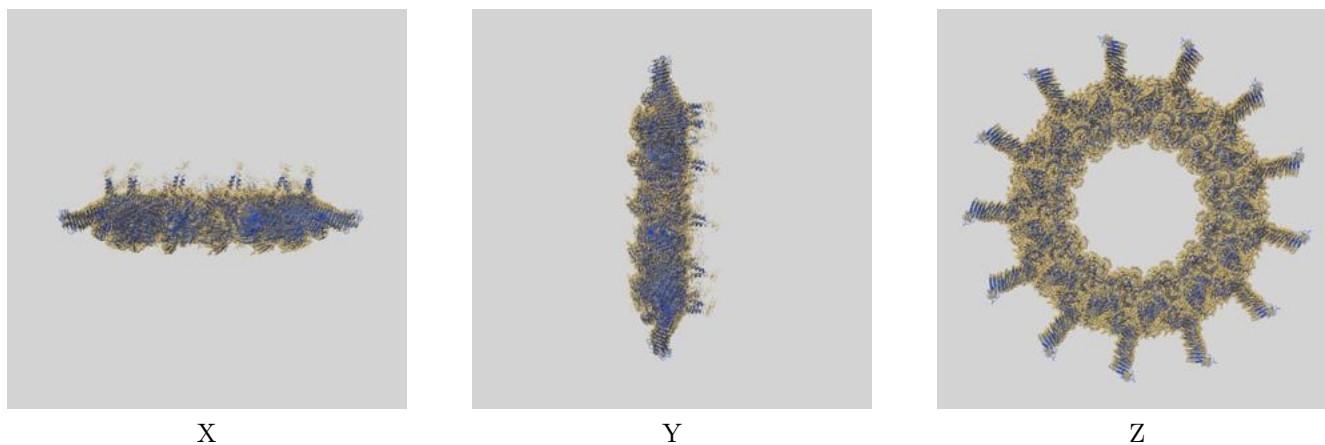
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

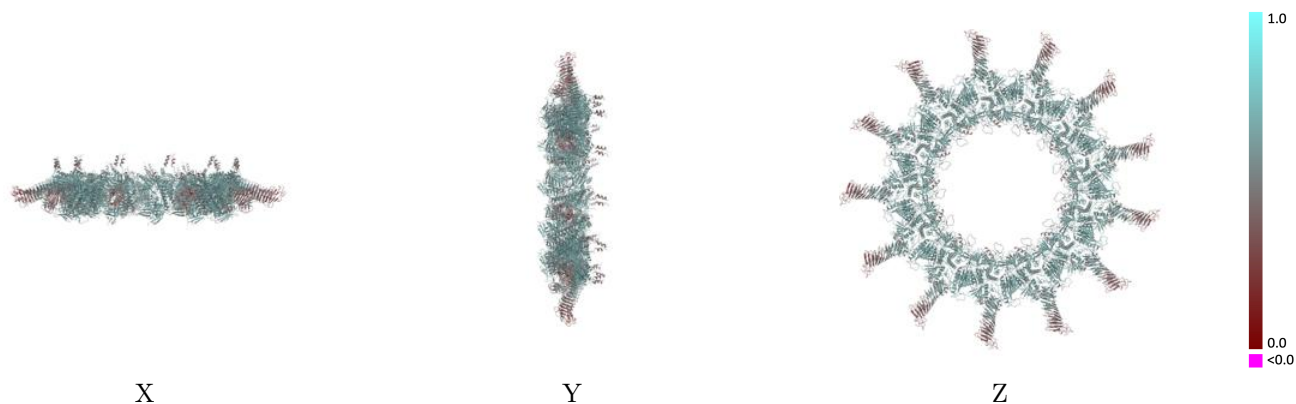
This section contains information regarding the fit between EMDB map EMD-24005 and PDB model 7MUD. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



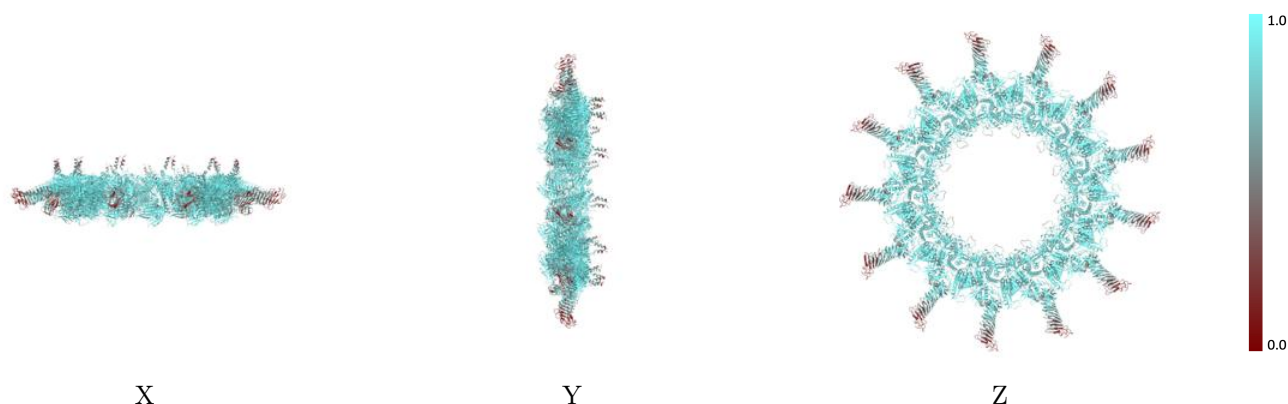
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



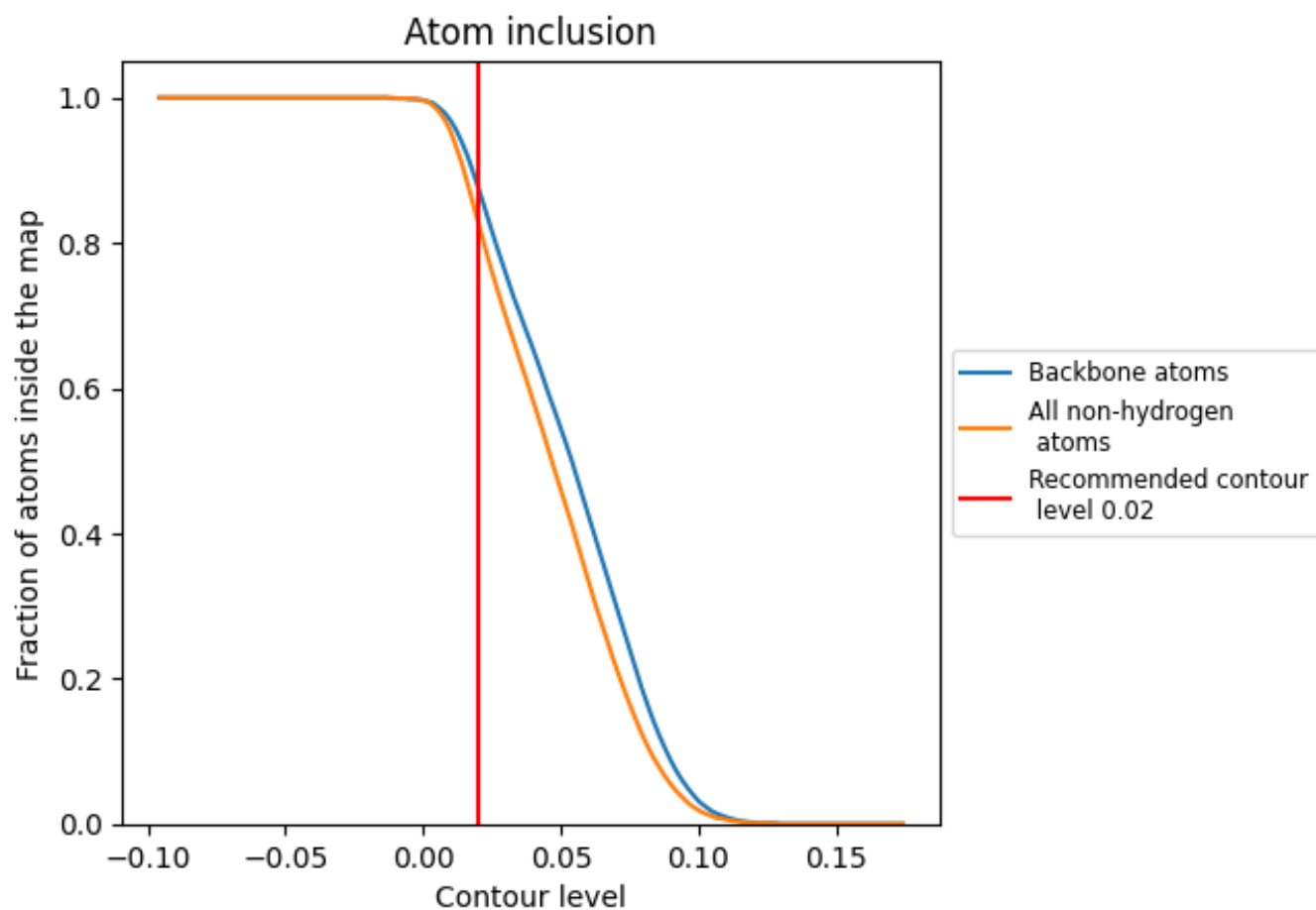
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8290	0.5640
AC	0.9180	0.6000
AD	0.9200	0.6080
AH	0.9540	0.6300
AK	0.9380	0.6160
AL	0.8740	0.5860
AM	0.6070	0.4590
AN	0.9060	0.5970
AU	0.9330	0.5480
Ad	0.8700	0.5850
Af	0.6200	0.4870
BC	0.9160	0.5980
BD	0.9260	0.6100
BH	0.9510	0.6290
BK	0.9370	0.6110
BL	0.8750	0.5880
BM	0.6040	0.4600
BN	0.9030	0.5980
BU	0.9560	0.5490
Bd	0.8700	0.5830
Bf	0.6010	0.4740
CC	0.9150	0.5980
CD	0.9240	0.6110
CH	0.9470	0.6290
CK	0.9370	0.6130
CL	0.8770	0.5860
CM	0.6040	0.4590
CN	0.9030	0.5960
CU	0.9330	0.5530
Cd	0.8740	0.5830
Cf	0.6080	0.4770
DC	0.9170	0.6010
DD	0.9230	0.6110
DH	0.9510	0.6300
DK	0.9370	0.6190























































































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Chain	Atom inclusion	Q-score
DL	 0.8790	 0.5890
DM	 0.6080	 0.4570
DN	 0.8970	 0.5940
DU	 0.8890	 0.5600
Dd	 0.8720	 0.5790
Df	 0.6060	 0.4800
EC	 0.9200	 0.6000
ED	 0.9250	 0.6100
EH	 0.9530	 0.6290
EK	 0.9440	 0.6120
EL	 0.8770	 0.5910
EM	 0.6090	 0.4590
EN	 0.8940	 0.5930
EU	 0.9330	 0.5410
Ed	 0.8710	 0.5850
Ef	 0.6130	 0.4770
FC	 0.9170	 0.6010
FD	 0.9260	 0.6140
FH	 0.9480	 0.6300
FK	 0.9360	 0.6180
FL	 0.8780	 0.5890
FM	 0.6000	 0.4600
FN	 0.9030	 0.5980
FU	 0.9110	 0.5510
Fd	 0.8740	 0.5840
Ff	 0.6130	 0.4740
GC	 0.9160	 0.5980
GD	 0.9220	 0.6100
GH	 0.9510	 0.6300
GK	 0.9390	 0.6150
GL	 0.8770	 0.5890
GM	 0.6040	 0.4540
GN	 0.9080	 0.5950
GU	 0.9330	 0.5470
Gd	 0.8770	 0.5820
Gf	 0.6060	 0.4790
HC	 0.9170	 0.6010
HD	 0.9250	 0.6100
HH	 0.9530	 0.6340
HK	 0.9410	 0.6150
HL	 0.8750	 0.5890
HM	 0.6090	 0.4570

























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Chain	Atom inclusion	Q-score
HN	 0.8990	 0.5950
HU	 0.9110	 0.5480
Hd	 0.8780	 0.5830
Hf	 0.6060	 0.4740
IC	 0.9170	 0.6000
ID	 0.9200	 0.6110
IH	 0.9540	 0.6350
IK	 0.9470	 0.6170
IL	 0.8780	 0.5910
IM	 0.6090	 0.4560
IN	 0.8990	 0.5940
IU	 0.9330	 0.5410
Id	 0.8700	 0.5860
If	 0.6220	 0.4800
JC	 0.9180	 0.6010
JD	 0.9240	 0.6100
JH	 0.9470	 0.6270
JK	 0.9400	 0.6150
JL	 0.8770	 0.5910
JM	 0.6100	 0.4590
JN	 0.8950	 0.5940
JU	 0.9330	 0.5470
Jd	 0.8690	 0.5820
Jf	 0.5950	 0.4760
KC	 0.9100	 0.6000
KD	 0.9210	 0.6110
KH	 0.9450	 0.6240
KK	 0.9390	 0.6140
KL	 0.8760	 0.5920
KM	 0.6060	 0.4590
KN	 0.8950	 0.5950
KU	 0.9330	 0.5420
Kd	 0.8690	 0.5800
Kf	 0.6060	 0.4830
LC	 0.9120	 0.5990
LD	 0.9190	 0.6120
LH	 0.9530	 0.6280
LK	 0.9380	 0.6140
LL	 0.8760	 0.5890
LM	 0.6030	 0.4520
LN	 0.8990	 0.5960
LU	 0.9560	 0.5410

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Chain	Atom inclusion	Q-score
Ld	 0.8760	 0.5840
Lf	 0.6130	 0.4770
MC	 0.9190	 0.5980
MD	 0.9240	 0.6090
MH	 0.9510	 0.6270
MK	 0.9400	 0.6150
ML	 0.8770	 0.5870
MM	 0.6030	 0.4570
MN	 0.8920	 0.5970
MU	 0.9330	 0.5510
Md	 0.8720	 0.5830
Mf	 0.5920	 0.4900