



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:45 AM UTC

PDB ID : 9OAD / pdb\_00009oad  
EMDB ID : EMD-70280  
Title : C1 reconstruction of the thermophilic bacteriophage P74-26 Portal and Portal Vertex  
Authors : Sedivy, E.L.; Agnello, E.; Song, K.; Xu, C.; Kelch, B.A.  
Deposited on : 2025-04-21  
Resolution : 3.56 Å(reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

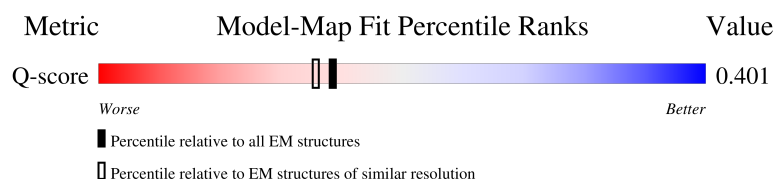
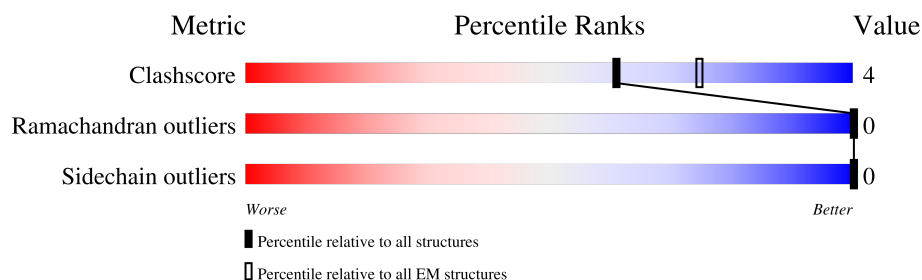
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.56 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.





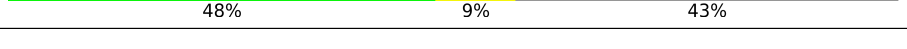
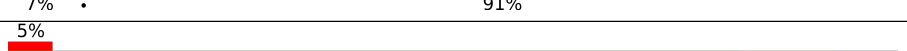

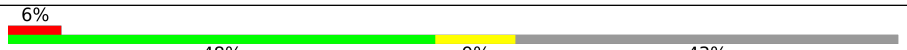


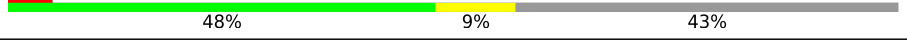
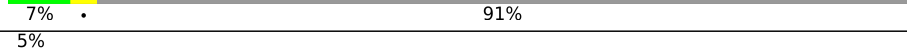
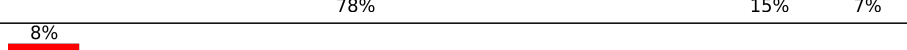






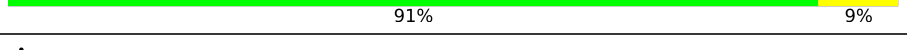
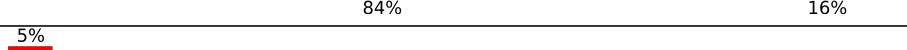




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12750 ( 3.06 - 4.06 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	409	 7% 91%
1	Ab	409	 9% 78% 15% 7%
1	Ac	409	 6% 83% 17%
1	Ad	409	 6% 51% 6% 43%

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Mol	Chain	Length	Quality of chain
1	Ae	409	
1	Af	409	
1	Ag	409	
1	Ah	409	
1	Ai	409	
1	Aj	409	
1	Ak	409	
1	Al	409	
1	Am	409	
1	An	409	
1	Ao	409	
1	Ap	409	
1	Aq	409	
1	Ar	409	
1	As	409	
1	At	409	
2	Ba	146	
2	Bb	146	
2	Bc	146	
2	Bd	146	
2	Be	146	
2	Bf	146	
2	Bg	146	
2	Bh	146	
2	Bi	146	

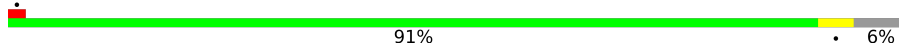






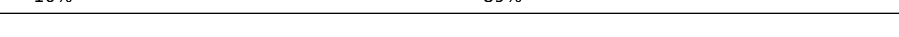
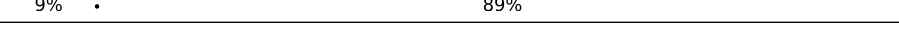





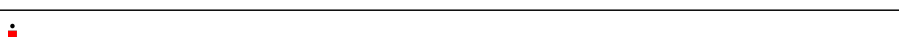
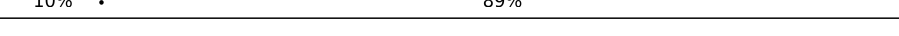
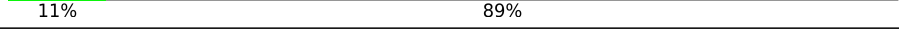

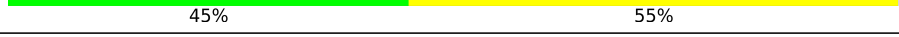
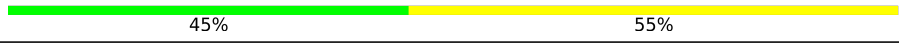





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Mol	Chain	Length	Quality of chain
2	Bj	146	
2	Bk	146	
2	Bl	146	
2	Bm	146	
2	Bn	146	
2	Bo	146	
2	Bp	146	
2	Bq	146	
2	Br	146	
2	Bs	146	
2	Bt	146	
3	Ca	73	
3	Cb	73	
3	Cc	73	
3	Cd	73	
3	Ce	73	
4	Da	448	
4	Db	448	
4	Dc	448	
4	Dd	448	
4	De	448	
4	Df	448	
4	Dg	448	
4	Dh	448	
4	Di	448	

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Mol	Chain	Length	Quality of chain
4	Dj	448	 91% 6%
4	Dk	448	 89% 5% 6%
4	Dl	448	 89% 5% 6%
5	Ea	130	 11% 89%
5	Eb	130	 11% 89%
5	Ec	130	 10% 89%
5	Ed	130	 10% 89%
5	Ee	130	 9% 89%
5	Ef	130	 10% 89%
5	Eg	130	 11% 89%
5	Eh	130	 11% 89%
5	Ei	130	 11% 89%
5	Ej	130	 10% 89%
5	Ek	130	 10% 89%
5	El	130	 11% 89%
6	Ja	31	 42% 58%
6	Jc	31	 45% 55%
6	Je	31	 45% 55%
6	Jg	31	 45% 55%
6	Ji	31	 6% 35% 65%
7	Jb	31	 48% 52%
7	Jd	31	 45% 55%
7	Jf	31	 52% 48%
7	Jh	31	 45% 55%
7	Jj	31	 45% 55%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 111630 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 Major head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	38	Total	C	N	O	S	0	0
			288	183	53	51	1		
1	Ab	382	Total	C	N	O	S	0	0
			3100	1999	527	569	5		
1	Ac	409	Total	C	N	O	S	0	0
			3303	2125	563	609	6		
1	Ad	233	Total	C	N	O	S	0	0
			1901	1232	320	346	3		
1	Ae	38	Total	C	N	O	S	0	0
			288	183	53	51	1		
1	Af	382	Total	C	N	O	S	0	0
			3100	1999	527	569	5		
1	Ag	409	Total	C	N	O	S	0	0
			3303	2125	563	609	6		
1	Ah	233	Total	C	N	O	S	0	0
			1901	1232	320	346	3		
1	Ai	38	Total	C	N	O	S	0	0
			288	183	53	51	1		
1	Aj	382	Total	C	N	O	S	0	0
			3100	1999	527	569	5		
1	Ak	409	Total	C	N	O	S	0	0
			3303	2125	563	609	6		
1	Al	233	Total	C	N	O	S	0	0
			1901	1232	320	346	3		
1	Am	38	Total	C	N	O	S	0	0
			288	183	53	51	1		
1	An	382	Total	C	N	O	S	0	0
			3100	1999	527	569	5		
1	Ao	409	Total	C	N	O	S	0	0
			3303	2125	563	609	6		
1	Ap	233	Total	C	N	O	S	0	0
			1901	1232	320	346	3		
1	Aq	38	Total	C	N	O	S	0	0
			288	183	53	51	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	382	Total	C	N	O	S	0	0
			3100	1999	527	569	5		
1	As	409	Total	C	N	O	S	0	0
			3303	2125	563	609	6		
1	At	233	Total	C	N	O	S	0	0
			1901	1232	320	346	3		

- Molecule 2 is a protein called P74-26 Head Decoration Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ba	26	Total	C	N	O	S	0	0
			225	147	38	39	1		
2	Bb	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bc	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bd	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Be	26	Total	C	N	O	S	0	0
			225	147	38	39	1		
2	Bf	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bg	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bh	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bi	26	Total	C	N	O	S	0	0
			225	147	38	39	1		
2	Bj	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bk	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bl	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bm	26	Total	C	N	O	S	0	0
			225	147	38	39	1		
2	Bn	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bo	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bp	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bq	26	Total	C	N	O	S	0	0
			225	147	38	39	1		
2	Br	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bs	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		
2	Bt	146	Total	C	N	O	S	0	0
			1161	756	197	205	3		

- Molecule 3 is a protein called Portal Vertex Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ca	73	Total	C	N	O	S	0	0
			595	374	107	113	1		
3	Cb	73	Total	C	N	O	S	0	0
			595	374	107	113	1		
3	Cc	73	Total	C	N	O	S	0	0
			595	374	107	113	1		
3	Cd	73	Total	C	N	O	S	0	0
			595	374	107	113	1		
3	Ce	73	Total	C	N	O	S	0	0
			595	374	107	113	1		

- Molecule 4 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Da	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Db	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Dc	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Dd	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	De	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Df	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Dg	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Dh	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Di	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Dj	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Dk	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
4	Dl	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		

- Molecule 5 is a protein called Adaptor (P74p90).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Ea	14	Total	C	N	O	0	0
			113	74	15	24		
5	Eb	14	Total	C	N	O	0	0
			113	74	15	24		
5	Ec	14	Total	C	N	O	0	0
			113	74	15	24		
5	Ed	14	Total	C	N	O	0	0
			113	74	15	24		
5	Ee	14	Total	C	N	O	0	0
			113	74	15	24		
5	Ef	14	Total	C	N	O	0	0
			113	74	15	24		
5	Eg	14	Total	C	N	O	0	0
			113	74	15	24		
5	Eh	14	Total	C	N	O	0	0
			113	74	15	24		
5	Ei	14	Total	C	N	O	0	0
			113	74	15	24		
5	Ej	14	Total	C	N	O	0	0
			113	74	15	24		
5	Ek	14	Total	C	N	O	0	0
			113	74	15	24		
5	El	14	Total	C	N	O	0	0
			113	74	15	24		

- Molecule 6 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ja	31	Total	C	N	O	P	0	0
			620	310	62	217	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Jc	31	Total 620	C 310	N 62	O 217	P 31	0	0
6	Je	31	Total 620	C 310	N 62	O 217	P 31	0	0
6	Jg	31	Total 620	C 310	N 62	O 217	P 31	0	0
6	Ji	31	Total 620	C 310	N 62	O 217	P 31	0	0

- Molecule 7 is a DNA chain called DNA (31-MER).


Mol	Chain	Residues	Atoms					AltConf	Trace
7	Jb	31	Total 651	C 310	N 155	O 155	P 31	0	0
7	Jd	31	Total 651	C 310	N 155	O 155	P 31	0	0
7	Jf	31	Total 651	C 310	N 155	O 155	P 31	0	0
7	Jh	31	Total 651	C 310	N 155	O 155	P 31	0	0
7	Jj	31	Total 651	C 310	N 155	O 155	P 31	0	0

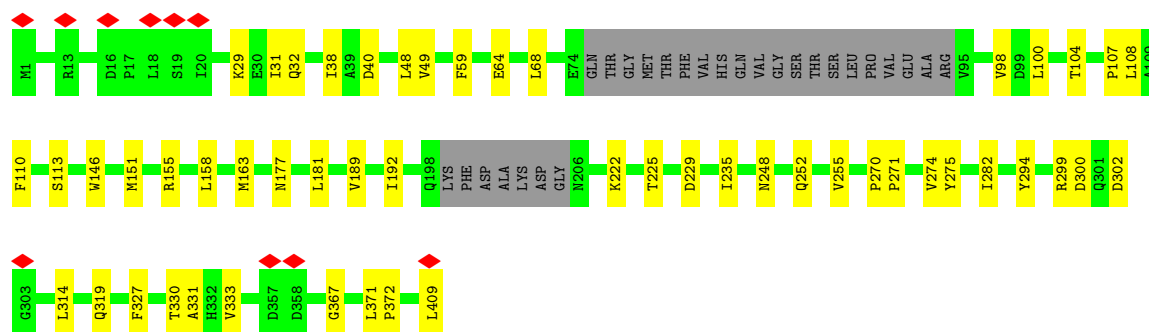





[illegible]

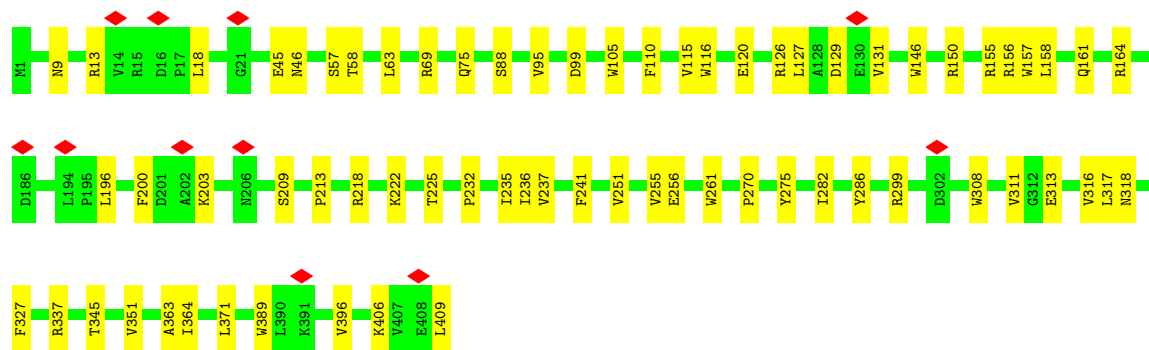
- Molecule 1: Major head protein

Chain Aff: 



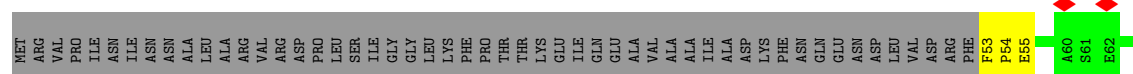
- Molecule 1: Major head protein

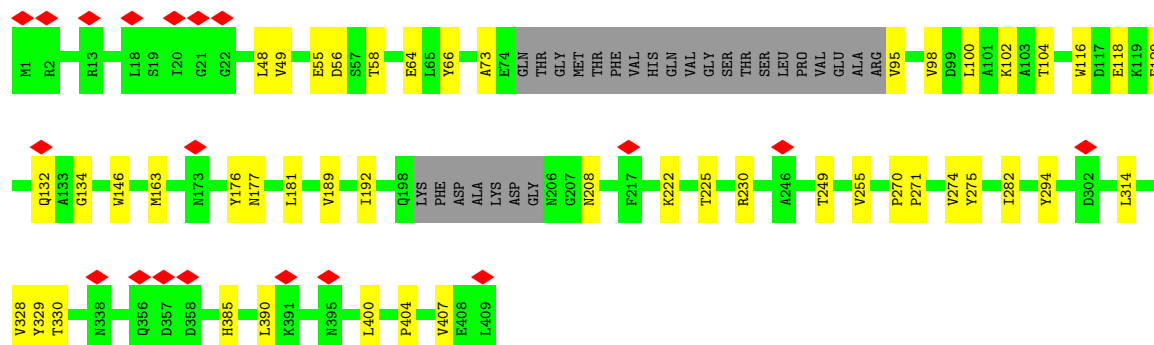
Chain Ag:  83% 17%



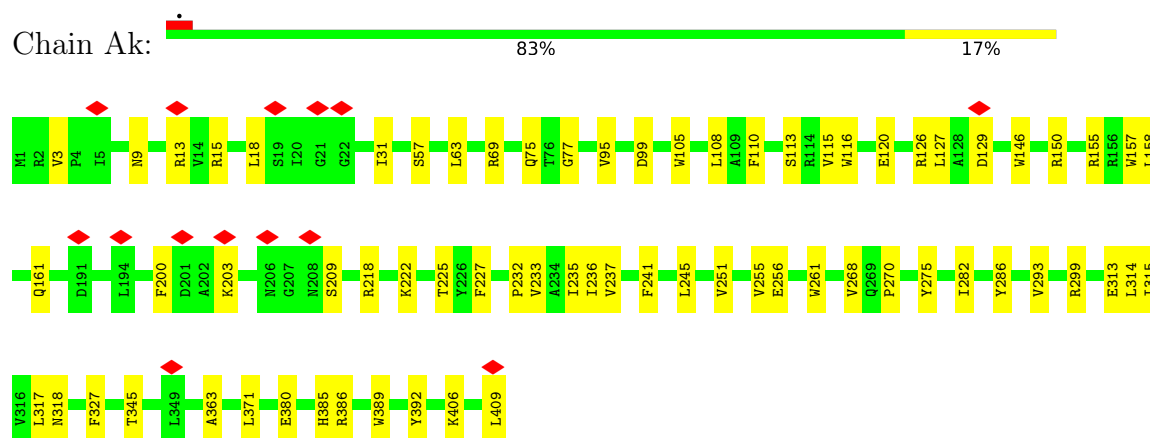
- Molecule 1: Major head protein

Chain Ah: 

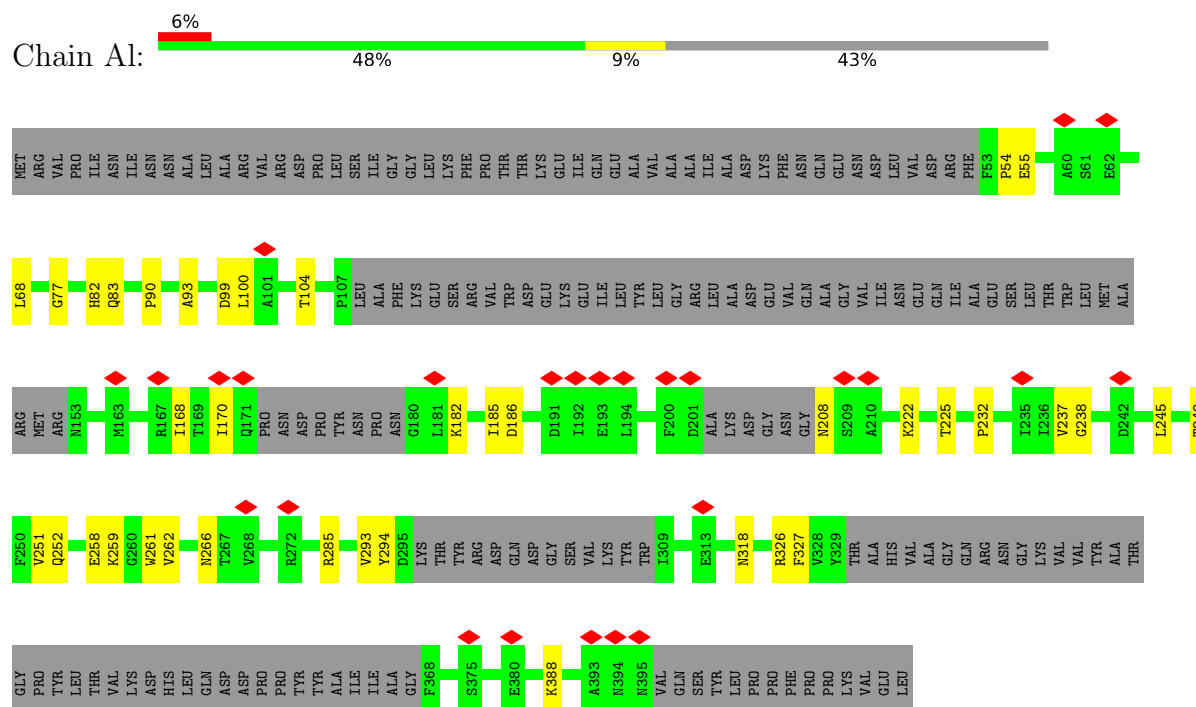




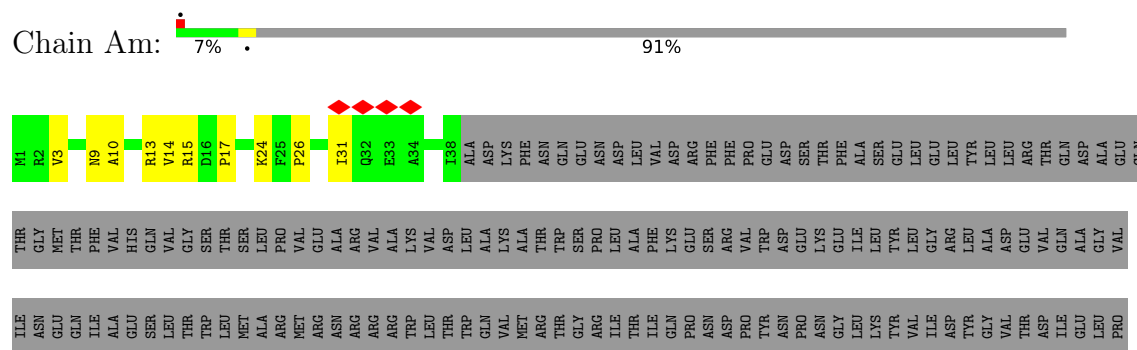
- Molecule 1: Major head protein

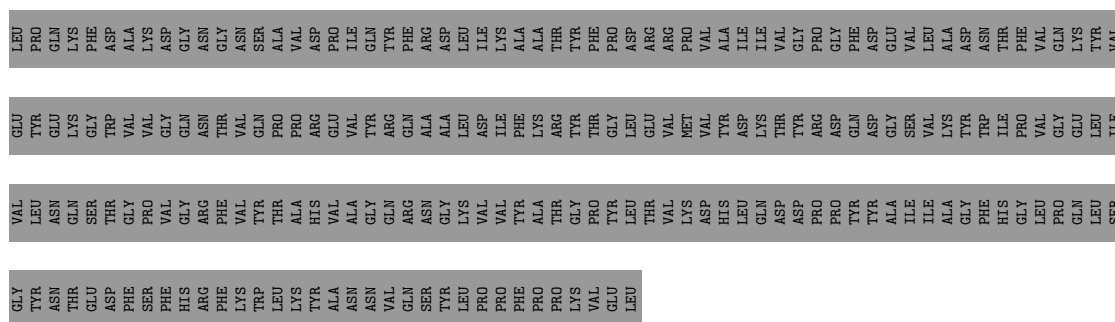


- Molecule 1: Major head protein

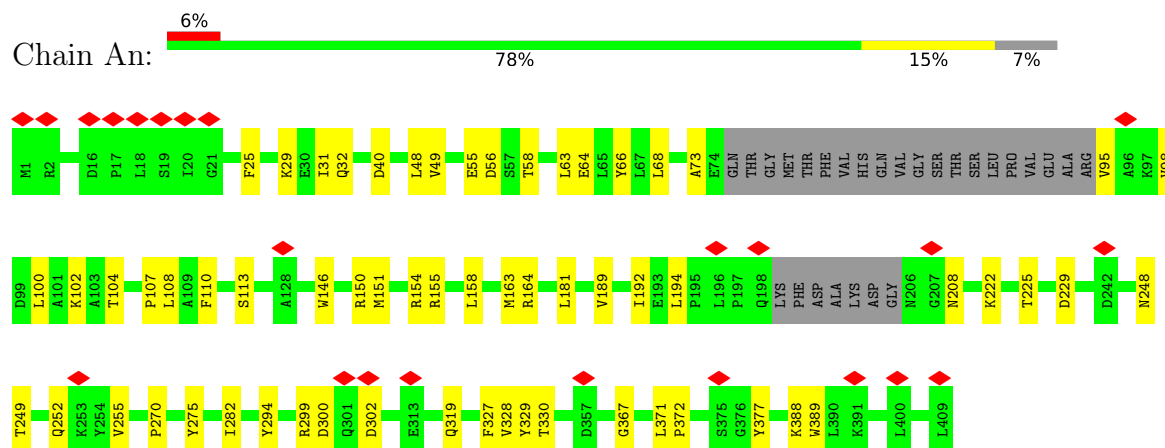


- Molecule 1: Major head protein

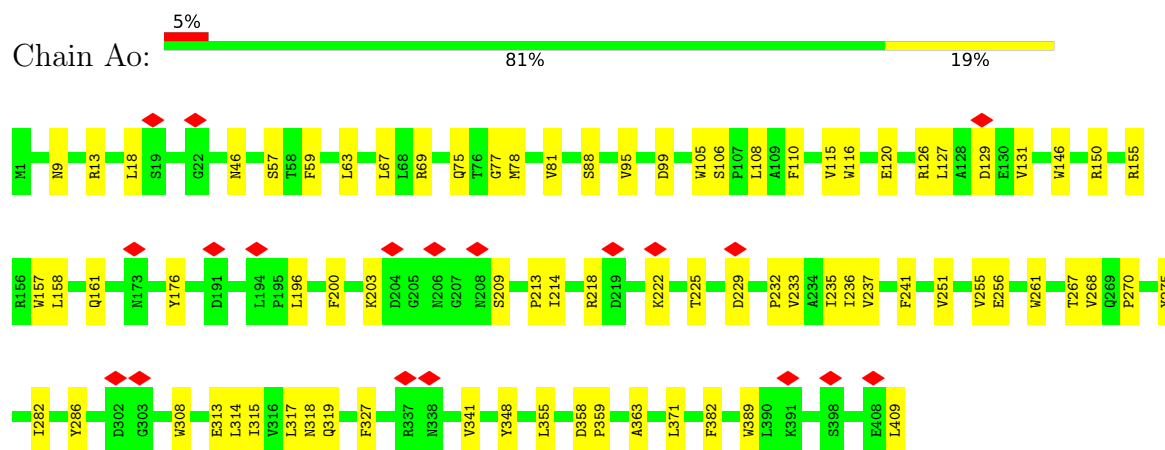




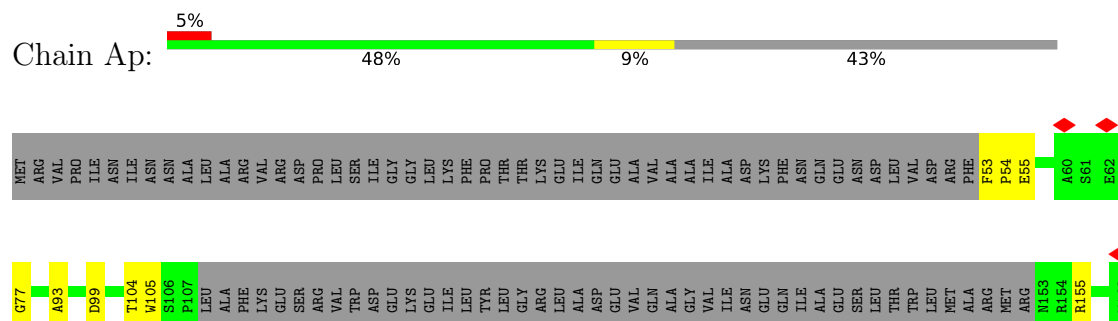
- Molecule 1: Major head protein



- Molecule 1: Major head protein

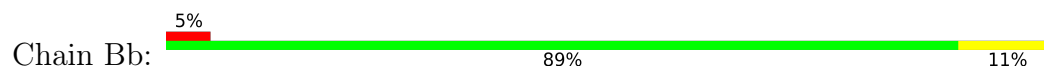


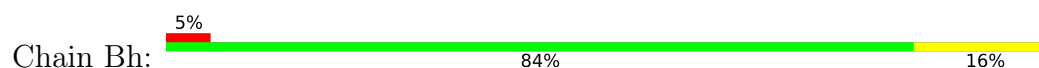
- Molecule 1: Major head protein

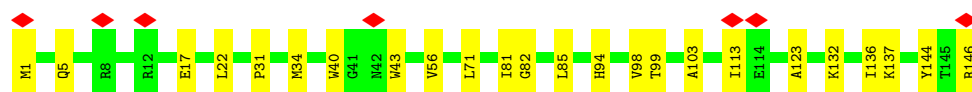




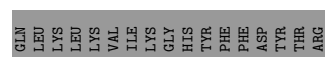
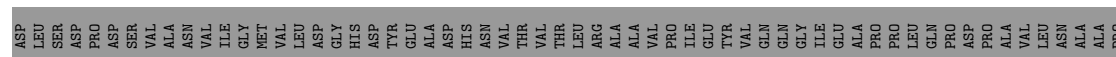
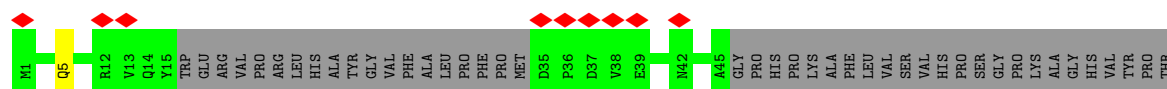








• Molecule 2: P74-26 Head Decoration Protein



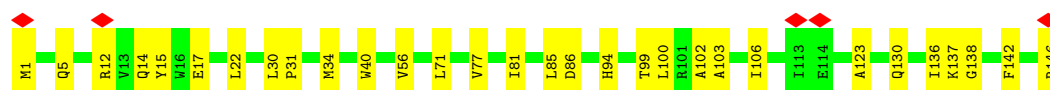
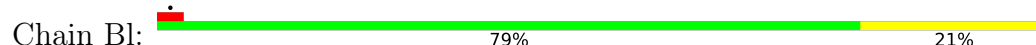
• Molecule 2: P74-26 Head Decoration Protein



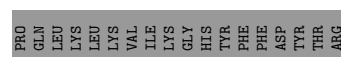
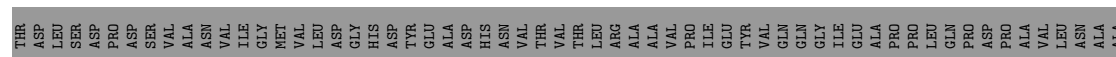
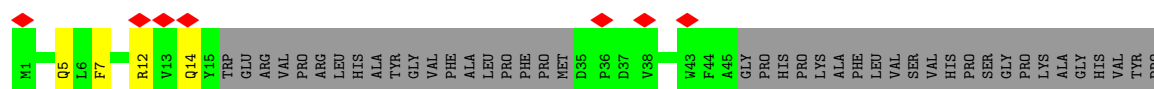
• Molecule 2: P74-26 Head Decoration Protein



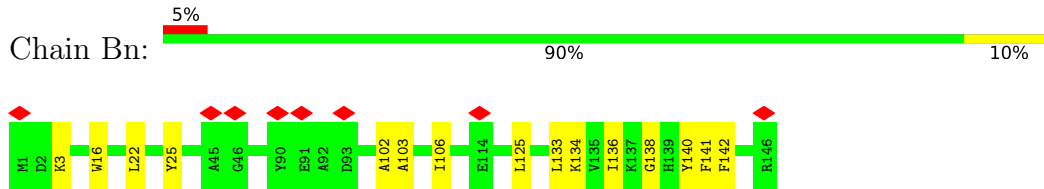
• Molecule 2: P74-26 Head Decoration Protein



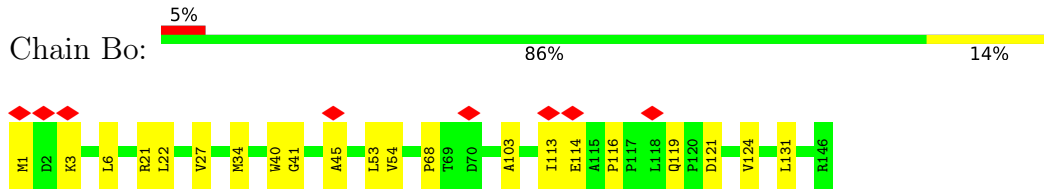
• Molecule 2: P74-26 Head Decoration Protein



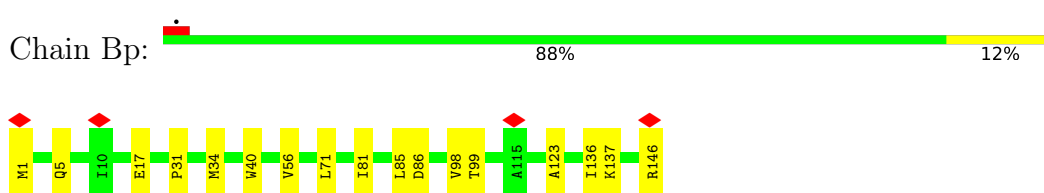
- Molecule 2: P74-26 Head Decoration Protein



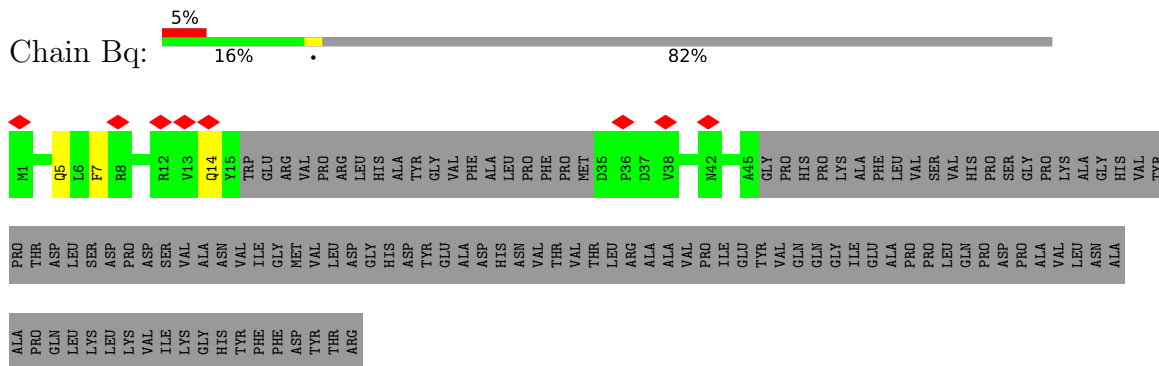
- Molecule 2: P74-26 Head Decoration Protein



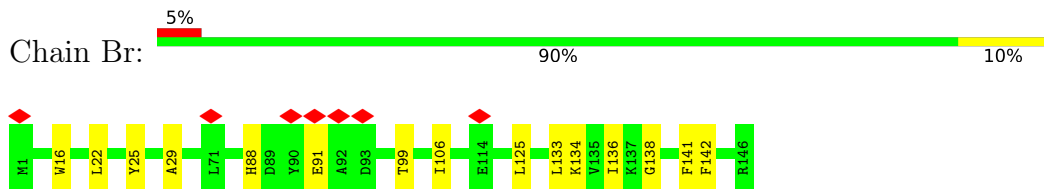
- Molecule 2: P74-26 Head Decoration Protein



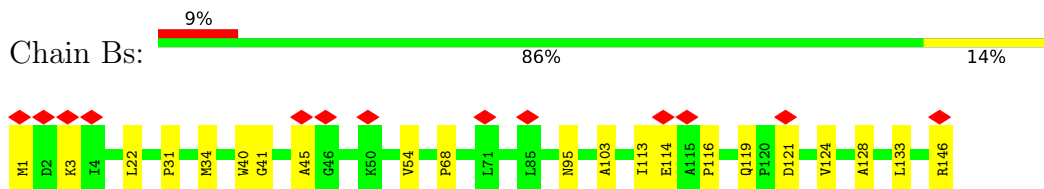
- Molecule 2: P74-26 Head Decoration Protein



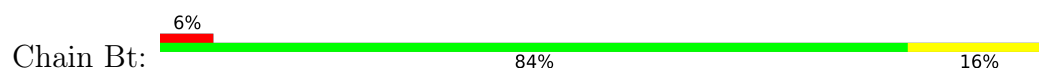
- Molecule 2: P74-26 Head Decoration Protein



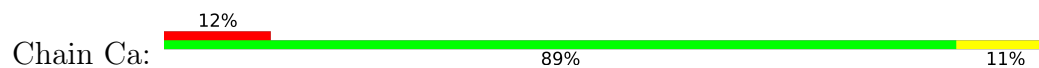
- Molecule 2: P74-26 Head Decoration Protein



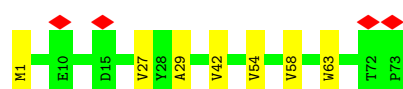
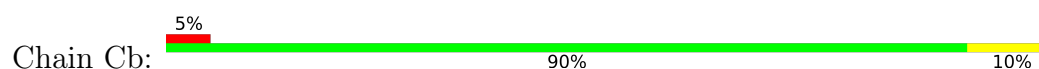
- Molecule 2: P74-26 Head Decoration Protein



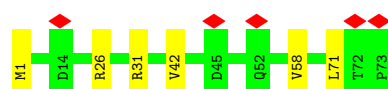
- Molecule 3: Portal Vertex Protein



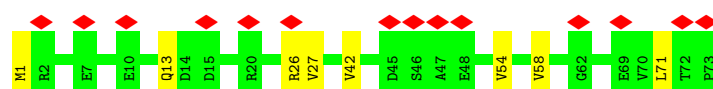
- Molecule 3: Portal Vertex Protein



- Molecule 3: Portal Vertex Protein



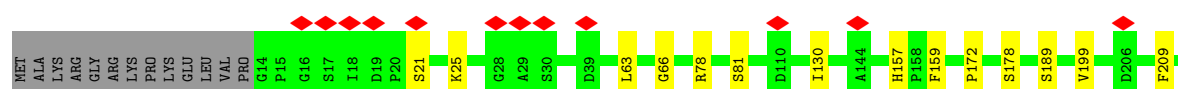
- Molecule 3: Portal Vertex Protein



- Molecule 3: Portal Vertex Protein

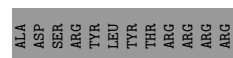
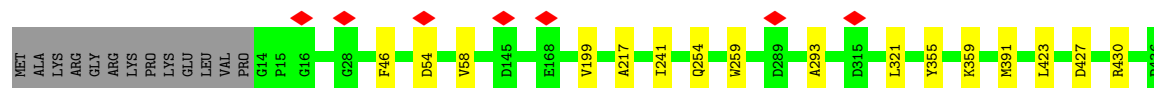


- Molecule 4: Portal protein

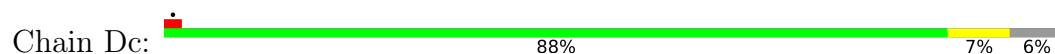




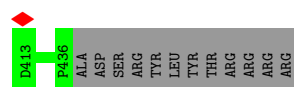
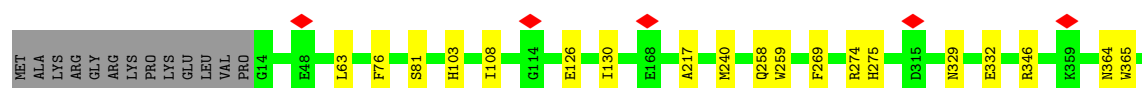
• Molecule 4: Portal protein



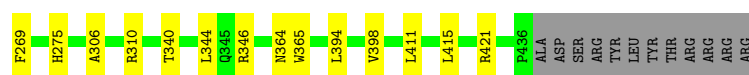
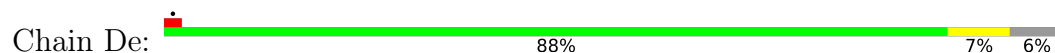
• Molecule 4: Portal protein



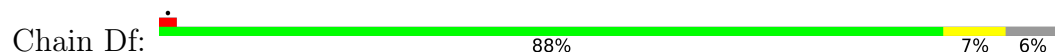
• Molecule 4: Portal protein

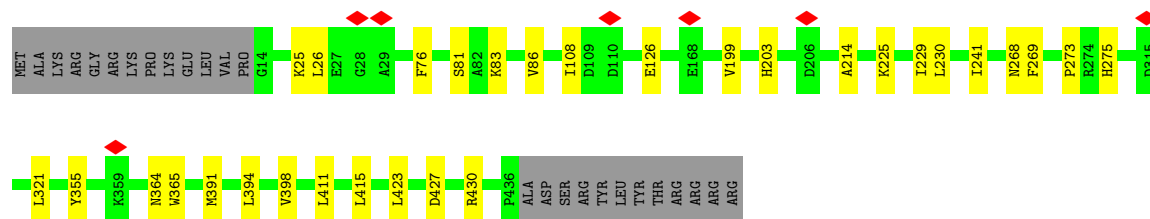


• Molecule 4: Portal protein



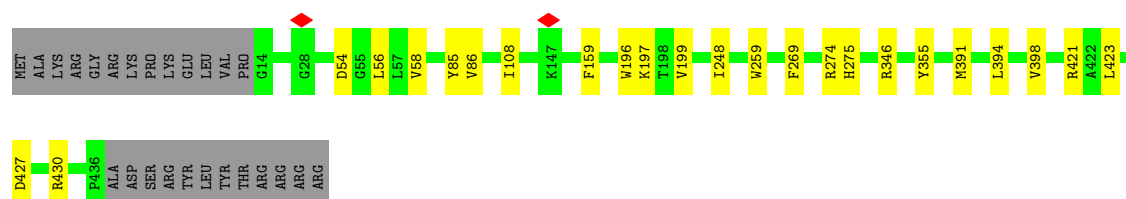
• Molecule 4: Portal protein





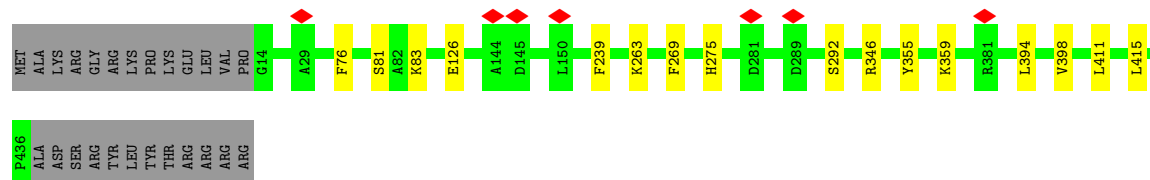
- Molecule 4: Portal protein

Chain Dg: 89% 5% 6%



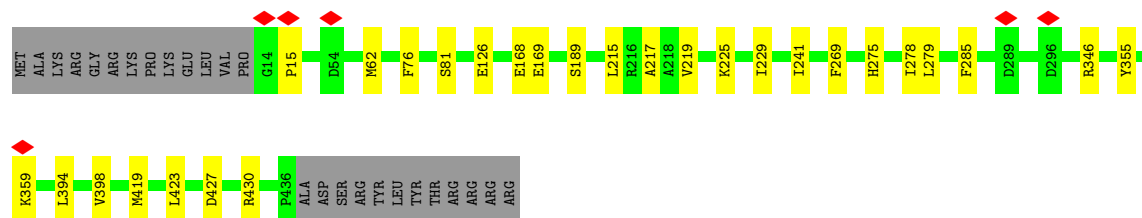
- Molecule 4: Portal protein

Chain Dh: 91% 6% 6%



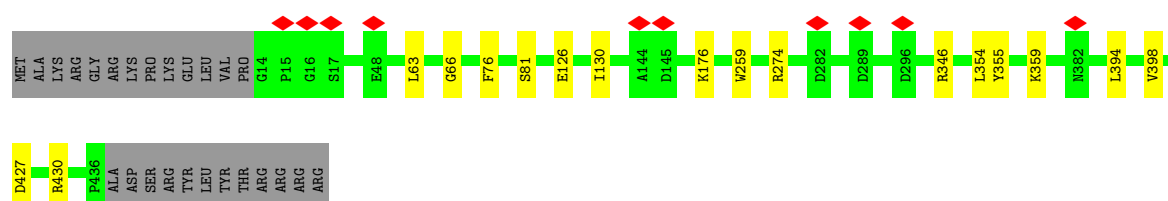
- Molecule 4: Portal protein

Chain Di: 88% 6% 6%



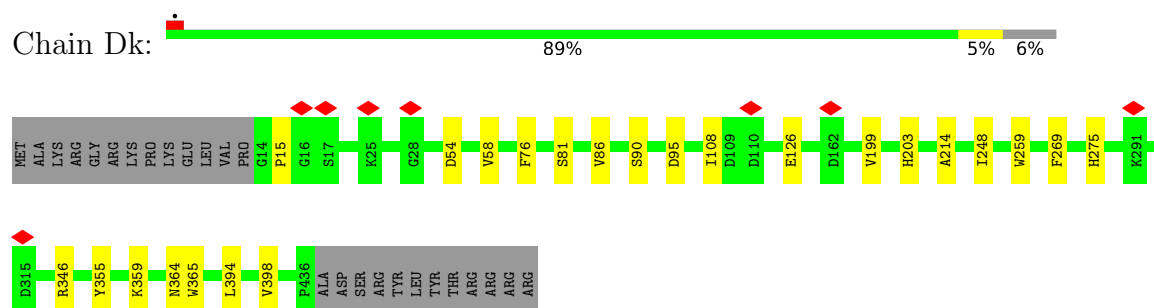
- Molecule 4: Portal protein

Chain Dj: 91% 6% 6%

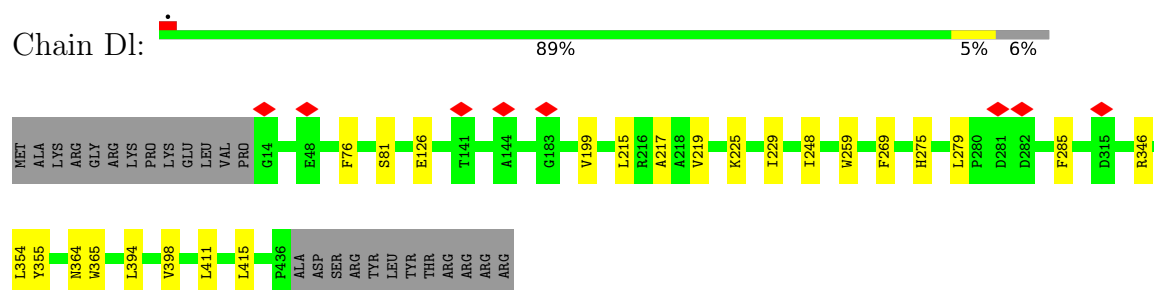




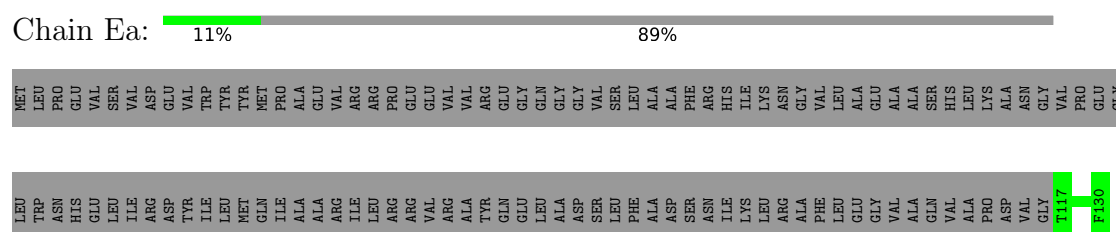
## • Molecule 4: Portal protein



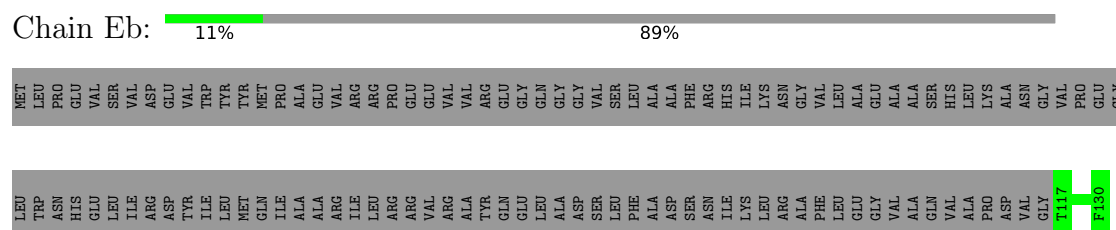
## • Molecule 4: Portal protein



## • Molecule 5: Adaptor (P74p90)



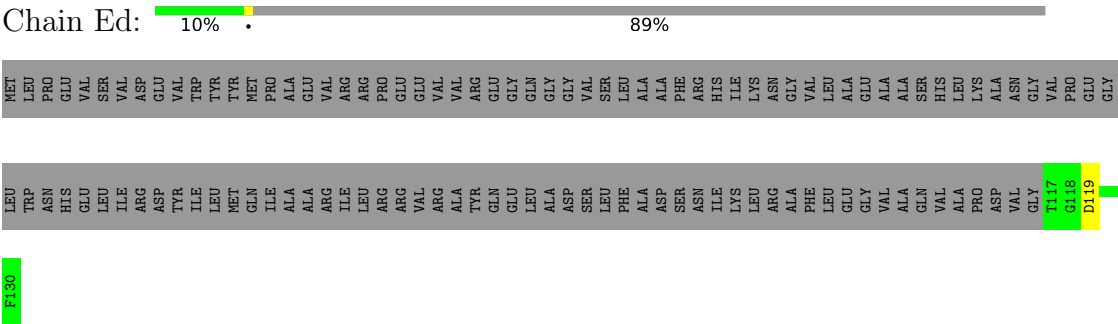
## • Molecule 5: Adaptor (P74p90)



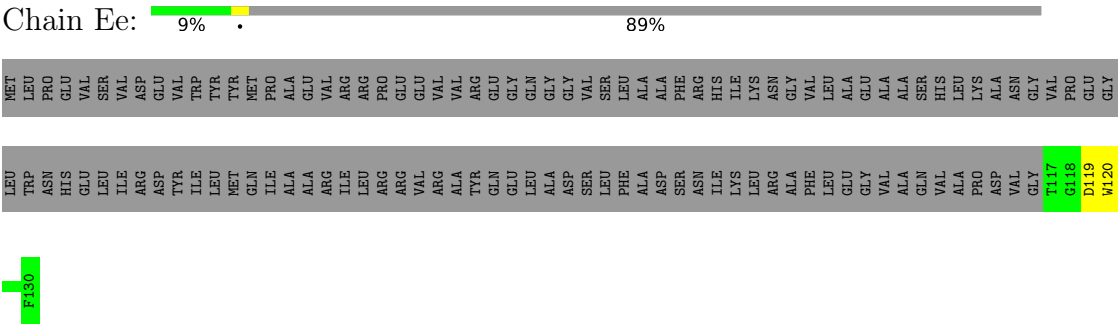
## • Molecule 5: Adaptor (P74p90)



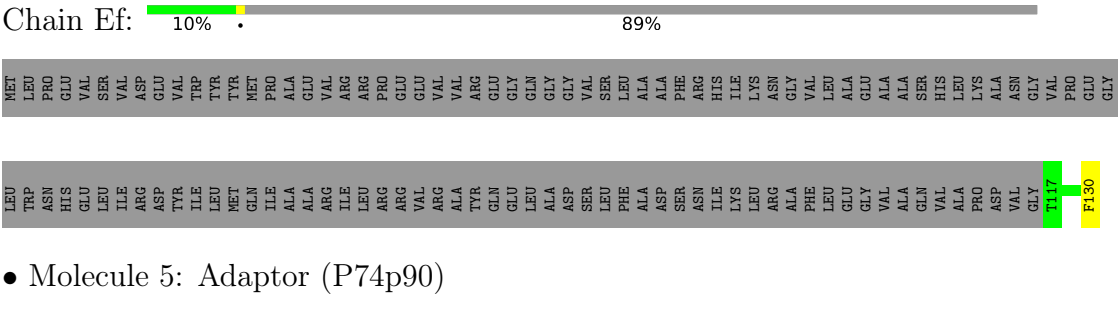
• Molecule 5: Adaptor (P74p90)



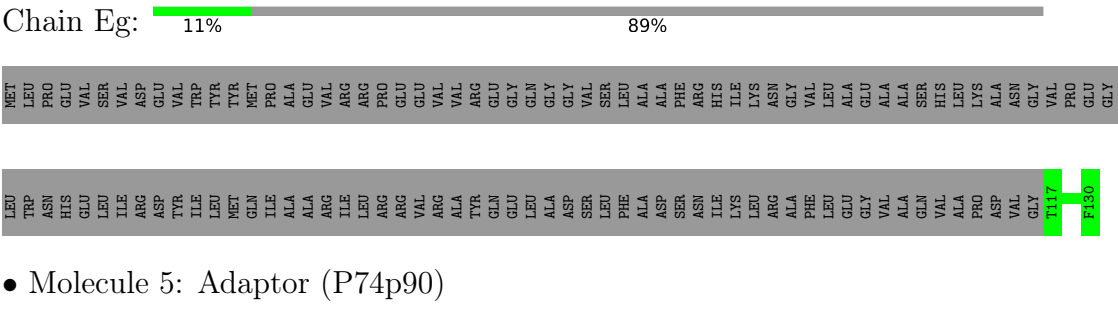
• Molecule 5: Adaptor (P74p90)



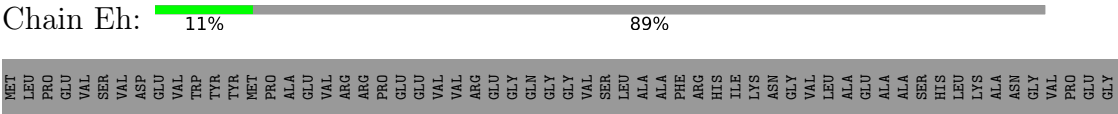
• Molecule 5: Adaptor (P74p90)



• Molecule 5: Adaptor (P74p90)



• Molecule 5: Adaptor (P74p90)



LEU	TRP	ASN	HIS	GLU	LEU	ILE	ARG	ASP	TYR	ILE	LEU	MET	GLN	ILE	ALA	ALA	ARG	ILE	LEU	ARG	ARG	VAL	VAL	ALA	ALA	TYR	GLN	GLU	LEU	ALA	ASP	SER	SER	ASN	ILE	LYS	LEU	ARG	ALA	PHE	LEU	GLU	GLY	VAL	ALA	GLN	VAL	ALA	PRO	ASP	VAL	GLY	T117	F130
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● Molecule 5: Adaptor (P74p90)

Chain Ei: 11% 89%

MET	LEU	PRO	ASN	GLU	VAL	SER	VAL	ASP	GLU	TYR	TRP	ILE	TYR	MET	PRO	ILE	ALA	ALA	GLU	VAL	ARG	ARG	PRO	GLU	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	LEU	ALA	GLU	GLY	VAL	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY
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LEU	TRP	ASN	HIS	GLU	LEU	ILE	ARG	ASP	TYR	ILE	LEU	MET	GLN	ILE	ALA	ALA	GLU	VAL	ARG	ILE	LEU	ARG	PRO	GLU	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	PHE	LEU	GLU	GLY	VAL	ALA	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY	T117	F130
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● Molecule 5: Adaptor (P74p90)

Chain Ej: 10% 89%

MET	LEU	PRO	ASN	GLU	VAL	SER	VAL	ASP	GLU	TYR	TRP	ILE	TYR	MET	PRO	ILE	ALA	ALA	GLU	VAL	ARG	ARG	PRO	GLU	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	LEU	ALA	GLU	GLY	VAL	ALA	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY
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LEU	TRP	ASN	HIS	GLU	LEU	ILE	ARG	ASP	GLU	TYR	TRP	ILE	TYR	MET	GLN	ILE	ALA	ALA	GLU	VAL	ARG	ILE	LEU	ARG	PRO	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	PHE	LEU	GLU	GLY	VAL	ALA	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY	T117	G118	D119
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F130
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● Molecule 5: Adaptor (P74p90)

Chain Ek: 10% 89%

MET	LEU	PRO	ASN	GLU	VAL	SER	VAL	ASP	GLU	TYR	TRP	ILE	TYR	MET	GLN	ILE	ALA	ALA	GLU	VAL	ARG	ARG	PRO	GLU	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	LEU	ALA	GLU	GLY	VAL	ALA	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY
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LEU	TRP	ASN	HIS	GLU	LEU	ILE	ARG	ASP	GLU	TYR	TRP	ILE	TYR	MET	GLN	ILE	ALA	ALA	GLU	VAL	ARG	ILE	LEU	ARG	PRO	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	PHE	LEU	GLU	GLY	VAL	ALA	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY	T117	G118	D119
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F130
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● Molecule 5: Adaptor (P74p90)

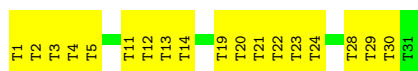
Chain El: 11% 89%

MET	LEU	PRO	ASN	GLU	VAL	SER	VAL	ASP	GLU	TYR	TRP	ILE	TYR	MET	PRO	ILE	ALA	ALA	GLU	VAL	ARG	ARG	PRO	GLU	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	PHE	LEU	GLU	GLY	VAL	ALA	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY
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LEU	TRP	ASN	HIS	GLU	LEU	ILE	ARG	ASP	TYR	ILE	LEU	MET	GLN	ILE	ALA	ALA	GLU	VAL	ARG	ILE	LEU	ARG	PRO	GLU	GLU	VAL	VAL	ALA	TYR	GLN	GLU	GLY	GLY	VAL	SER	LEU	PHE	ALA	ALA	ASP	SER	PHE	ASN	ARG	HIS	ILE	LYS	LEU	ASN	GLY	VAL	PHE	LEU	GLU	GLY	VAL	ALA	ALA	ALA	SER	HIS	VAL	ALA	PRO	LYS	ALA	ASN	GLY	VAL	PRO	GLU	GLY	T117	F130
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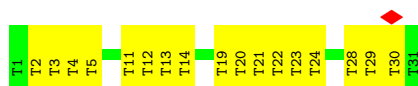
● Molecule 6: DNA (31-MER)

Chain Ja:  42% 58%



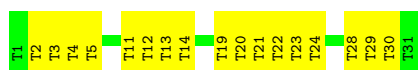
- Molecule 6: DNA (31-MER)

Chain Jc:  45% 55%



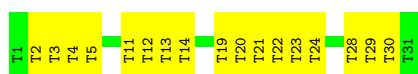
- Molecule 6: DNA (31-MER)

Chain Je:  45% 55%



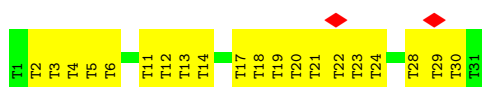
- Molecule 6: DNA (31-MER)

Chain Jg:  45% 55%



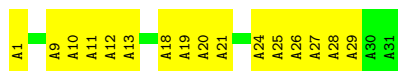
- Molecule 6: DNA (31-MER)

Chain Ji:  6% 35% 65%



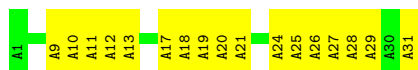
- Molecule 7: DNA (31-MER)

Chain Jb:  48% 52%

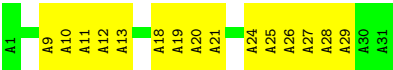


- Molecule 7: DNA (31-MER)

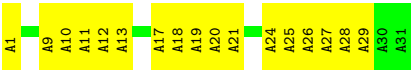
Chain Jd:  45% 55%



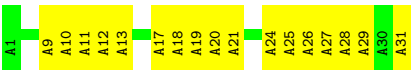
- Molecule 7: DNA (31-MER)



● Molecule 7: DNA (31-MER)



● Molecule 7: DNA (31-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39382	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.0571	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.525	Depositor
Minimum map value	-0.302	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	Aa	0.14	0/291	0.37	0/394
1	Ab	0.18	0/3182	0.38	0/4333
1	Ac	0.21	0/3391	0.41	0/4618
1	Ad	0.17	0/1949	0.34	0/2647
1	Ae	0.15	0/291	0.36	0/394
1	Af	0.20	0/3182	0.37	0/4333
1	Ag	0.22	0/3391	0.42	0/4618
1	Ah	0.17	0/1949	0.34	0/2647
1	Ai	0.16	0/291	0.37	0/394
1	Aj	0.20	0/3182	0.39	0/4333
1	Ak	0.22	0/3391	0.42	0/4618
1	Al	0.16	0/1949	0.35	0/2647
1	Am	0.14	0/291	0.36	0/394
1	An	0.20	0/3182	0.38	0/4333
1	Ao	0.21	0/3391	0.41	0/4618
1	Ap	0.17	0/1949	0.34	0/2647
1	Aq	0.15	0/291	0.38	0/394
1	Ar	0.19	0/3182	0.38	0/4333
1	As	0.20	0/3391	0.42	0/4618
1	At	0.16	0/1949	0.35	0/2647
2	Ba	0.15	0/231	0.30	0/311
2	Bb	0.19	0/1203	0.35	0/1648
2	Bc	0.19	0/1203	0.35	0/1648
2	Bd	0.20	0/1203	0.36	0/1648
2	Be	0.14	0/231	0.25	0/311
2	Bf	0.21	0/1203	0.37	0/1648
2	Bg	0.21	0/1203	0.37	0/1648
2	Bh	0.21	0/1203	0.35	0/1648
2	Bi	0.14	0/231	0.28	0/311
2	Bj	0.21	0/1203	0.37	0/1648
2	Bk	0.20	0/1203	0.36	0/1648
2	Bl	0.20	0/1203	0.36	0/1648
2	Bm	0.15	0/231	0.25	0/311
2	Bn	0.20	0/1203	0.37	0/1648

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Bo	0.20	0/1203	0.34	0/1648
2	Bp	0.20	0/1203	0.35	0/1648
2	Bq	0.15	0/231	0.26	0/311
2	Br	0.20	0/1203	0.40	0/1648
2	Bs	0.19	0/1203	0.35	0/1648
2	Bt	0.19	0/1203	0.36	0/1648
3	Ca	0.19	0/609	0.41	0/826
3	Cb	0.21	0/609	0.43	0/826
3	Cc	0.21	0/609	0.44	0/826
3	Cd	0.19	0/609	0.44	0/826
3	Ce	0.19	0/609	0.43	0/826
4	Da	0.21	0/3361	0.39	0/4567
4	Db	0.21	0/3361	0.38	0/4567
4	Dc	0.22	0/3361	0.39	0/4567
4	Dd	0.22	0/3361	0.39	0/4567
4	De	0.22	0/3361	0.38	0/4567
4	Df	0.22	0/3361	0.38	0/4567
4	Dg	0.22	0/3361	0.39	0/4567
4	Dh	0.22	0/3361	0.38	0/4567
4	Di	0.22	0/3361	0.39	0/4567
4	Dj	0.21	0/3361	0.39	0/4567
4	Dk	0.21	0/3361	0.38	0/4567
4	Dl	0.22	0/3361	0.40	0/4567
5	Ea	0.21	0/117	0.41	0/160
5	Eb	0.19	0/117	0.36	0/160
5	Ec	0.19	0/117	0.40	0/160
5	Ed	0.20	0/117	0.41	0/160
5	Ee	0.18	0/117	0.48	0/160
5	Ef	0.18	0/117	0.51	0/160
5	Eg	0.20	0/117	0.51	0/160
5	Eh	0.18	0/117	0.48	0/160
5	Ei	0.19	0/117	0.48	0/160
5	Ej	0.17	0/117	0.42	0/160
5	Ek	0.18	0/117	0.39	0/160
5	El	0.15	0/117	0.33	0/160
6	Ja	0.27	0/681	0.60	0/1050
6	Jc	0.27	0/681	0.60	0/1050
6	Je	0.27	0/681	0.60	0/1050
6	Jg	0.27	0/681	0.60	0/1050
6	Ji	0.27	0/681	0.60	0/1050
7	Jb	0.24	0/743	0.44	0/1143
7	Jd	0.24	0/743	0.44	0/1143
7	Jf	0.24	0/743	0.44	0/1143



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	Jh	0.24	0/743	0.44	0/1143
7	Jj	0.24	0/743	0.44	0/1143
All	All	0.21	0/115166	0.40	0/158054

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	288	0	313	8	0
1	Ab	3100	0	3055	43	0
1	Ac	3303	0	3255	49	0
1	Ad	1901	0	1862	18	0
1	Ae	288	0	313	10	0
1	Af	3100	0	3055	36	0
1	Ag	3303	0	3255	46	0
1	Ah	1901	0	1862	22	0
1	Ai	288	0	313	10	0
1	Aj	3100	0	3055	31	0
1	Ak	3303	0	3255	54	0
1	Al	1901	0	1862	26	0
1	Am	288	0	313	9	0
1	An	3100	0	3055	43	0
1	Ao	3303	0	3255	57	0
1	Ap	1901	0	1862	25	0
1	Aq	288	0	313	11	0
1	Ar	3100	0	3055	41	0
1	As	3303	0	3255	53	0
1	At	1901	0	1862	26	0
2	Ba	225	0	212	2	0
2	Bb	1161	0	1129	12	0
2	Bc	1161	0	1129	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bd	1161	0	1129	15	0
2	Be	225	0	212	1	0
2	Bf	1161	0	1129	10	0
2	Bg	1161	0	1129	16	0
2	Bh	1161	0	1129	17	0
2	Bi	225	0	212	1	0
2	Bj	1161	0	1129	12	0
2	Bk	1161	0	1129	8	0
2	Bl	1161	0	1129	20	0
2	Bm	225	0	212	3	0
2	Bn	1161	0	1129	12	0
2	Bo	1161	0	1129	12	0
2	Bp	1161	0	1129	13	0
2	Bq	225	0	212	3	0
2	Br	1161	0	1129	11	0
2	Bs	1161	0	1129	13	0
2	Bt	1161	0	1129	16	0
3	Ca	595	0	584	5	0
3	Cb	595	0	584	5	0
3	Cc	595	0	584	4	0
3	Cd	595	0	584	6	0
3	Ce	595	0	584	6	0
4	Da	3287	0	3319	15	0
4	Db	3287	0	3319	11	0
4	Dc	3287	0	3319	21	0
4	Dd	3287	0	3319	14	0
4	De	3287	0	3319	22	0
4	Df	3287	0	3319	21	0
4	Dg	3287	0	3319	16	0
4	Dh	3287	0	3319	10	0
4	Di	3287	0	3319	19	0
4	Dj	3287	0	3319	13	0
4	Dk	3287	0	3319	15	0
4	Dl	3287	0	3319	14	0
5	Ea	113	0	98	0	0
5	Eb	113	0	98	0	0
5	Ec	113	0	98	1	0
5	Ed	113	0	98	1	0
5	Ee	113	0	98	2	0
5	Ef	113	0	98	1	0
5	Eg	113	0	98	0	0
5	Eh	113	0	98	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Ei	113	0	98	0	0
5	Ej	113	0	98	1	0
5	Ek	113	0	98	1	0
5	El	113	0	98	0	0
6	Ja	620	0	373	10	0
6	Jc	620	0	373	9	0
6	Je	620	0	373	9	0
6	Jg	620	0	373	9	0
6	Ji	620	0	373	11	0
7	Jb	651	0	342	11	0
7	Jd	651	0	342	12	0
7	Jf	651	0	342	11	0
7	Jh	651	0	342	12	0
7	Jj	651	0	342	12	0
All	All	111630	0	107919	971	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (971) 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:As:232:PRO:HA	1:As:318:ASN:HA	1.59	0.83
1:Ad:186:ASP:H	2:Bd:1:MET:HG3	1.43	0.81
1:Ac:232:PRO:HA	1:Ac:318:ASN:HA	1.63	0.79
2:Bh:85:LEU:HG	2:Bh:99:THR:HG21	1.66	0.78
2:Bl:85:LEU:HG	2:Bl:99:THR:HG21	1.65	0.77
1:Al:232:PRO:HA	1:Al:318:ASN:HA	1.67	0.76
1:At:232:PRO:HA	1:At:318:ASN:HA	1.68	0.75
2:Bk:116:PRO:HB2	2:Bk:119:GLN:HB2	1.70	0.73
1:Ap:54:PRO:HD2	1:Ap:326:ARG:HA	1.70	0.73
1:Ah:54:PRO:HD2	1:Ah:326:ARG:HA	1.71	0.72
1:Ao:232:PRO:HA	1:Ao:318:ASN:HA	1.72	0.72
1:Ap:232:PRO:HA	1:Ap:318:ASN:HA	1.73	0.71
1:Af:181:LEU:HD21	2:Bd:31:PRO:HB2	1.72	0.70
1:Ac:409:LEU:HD21	1:Ad:99:ASP:HB2	1.74	0.70
1:Ah:232:PRO:HA	1:Ah:318:ASN:HA	1.72	0.70
1:Ag:232:PRO:HA	1:Ag:318:ASN:HA	1.74	0.69
1:Ad:54:PRO:HD2	1:Ad:326:ARG:HA	1.75	0.69
1:Ad:232:PRO:HA	1:Ad:318:ASN:HA	1.75	0.69
1:As:48:LEU:HD21	1:As:236:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bs:116:PRO:HB2	2:Bs:119:GLN:HB2	1.76	0.68
1:Ag:57:SER:HB3	3:Cb:1:MET:HE1	1.75	0.68
1:Ak:232:PRO:HA	1:Ak:318:ASN:HA	1.76	0.68
1:Af:29:LYS:HE3	1:Af:31:ILE:HD11	1.75	0.68
2:Bo:116:PRO:HB2	2:Bo:119:GLN:HB2	1.76	0.68
2:Bp:85:LEU:HG	2:Bp:99:THR:HG21	1.74	0.68
2:Bl:146:ARG:HB2	2:Bn:134:LYS:HD2	1.76	0.67
2:Bo:121:ASP:HB3	2:Bo:124:VAL:HG12	1.76	0.67
2:Bk:121:ASP:HB3	2:Bk:124:VAL:HG12	1.75	0.67
2:Bg:116:PRO:HB2	2:Bg:119:GLN:HB2	1.76	0.67
4:Dk:269:PHE:HA	4:Dk:275:HIS:CE1	2.30	0.66
1:Ag:203:LYS:HA	1:Ag:209:SER:HA	1.77	0.66
1:Ab:29:LYS:HE3	1:Ab:31:ILE:HD11	1.77	0.66
2:Bg:121:ASP:HB3	2:Bg:124:VAL:HG12	1.77	0.66
6:Ji:11:DT:H2'	6:Ji:12:DT:H71	1.78	0.65
6:Je:11:DT:H2'	6:Je:12:DT:H71	1.78	0.65
2:Bs:121:ASP:HB3	2:Bs:124:VAL:HG12	1.80	0.64
4:Dd:269:PHE:HA	4:Dd:275:HIS:CE1	2.32	0.64
1:As:203:LYS:HA	1:As:209:SER:HA	1.77	0.64
1:Aj:181:LEU:HD21	2:Bh:31:PRO:HB2	1.80	0.64
2:Bc:116:PRO:HB2	2:Bc:119:GLN:HB2	1.79	0.64
6:Jg:11:DT:H2'	6:Jg:12:DT:H71	1.78	0.64
2:Bc:121:ASP:HB3	2:Bc:124:VAL:HG12	1.80	0.64
6:Jc:11:DT:H2'	6:Jc:12:DT:H71	1.78	0.64
1:Ak:409:LEU:HD21	1:Al:99:ASP:HB2	1.79	0.64
6:Ja:11:DT:H2'	6:Ja:12:DT:H71	1.78	0.63
1:Ac:57:SER:HB3	3:Ca:1:MET:HE1	1.81	0.63
7:Jh:10:DA:H2'	7:Jh:11:DA:C8	2.34	0.63
4:De:269:PHE:HA	4:De:275:HIS:CE1	2.33	0.63
7:Jf:10:DA:H2'	7:Jf:11:DA:C8	2.34	0.63
1:Ag:409:LEU:HD21	1:Ah:99:ASP:HB2	1.81	0.63
1:Al:208:ASN:HA	1:Al:249:THR:HG21	1.81	0.62
7:Jd:10:DA:H2'	7:Jd:11:DA:C8	2.34	0.62
1:Ao:57:SER:HB3	3:Cd:1:MET:HE1	1.80	0.62
7:Jj:10:DA:H2'	7:Jj:11:DA:C8	2.34	0.62
1:Ar:181:LEU:HD21	2:Bp:31:PRO:HB2	1.82	0.62
1:An:181:LEU:HD21	2:Bl:31:PRO:HB2	1.82	0.62
1:Am:31:ILE:HG12	1:An:64:GLU:HB2	1.82	0.62
7:Jb:10:DA:H2'	7:Jb:11:DA:C8	2.34	0.62
1:As:9:ASN:O	1:As:13:ARG:HG2	2.00	0.61
1:Ac:313:GLU:HG2	1:Ac:389:TRP:CE3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dh:269:PHE:HA	4:Dh:275:HIS:CE1	2.36	0.61
1:Al:54:PRO:HD2	1:Al:326:ARG:HA	1.82	0.61
2:Bj:106:ILE:HD13	2:Bj:125:LEU:HD21	1.80	0.61
3:Cb:1:MET:HA	7:Jd:17:DA:OP1	2.00	0.61
1:Ak:236:ILE:HG22	1:Ak:315:ILE:HB	1.83	0.60
4:Da:63:LEU:HD11	4:Da:130:ILE:HG21	1.82	0.60
1:At:106:SER:HB3	2:Bt:3:LYS:HB3	1.83	0.60
1:Ao:203:LYS:HA	1:Ao:209:SER:HA	1.84	0.60
1:At:54:PRO:HD2	1:At:326:ARG:HA	1.84	0.60
1:Ab:100:LEU:HD21	1:As:18:LEU:HD11	1.84	0.60
4:Di:269:PHE:HA	4:Di:275:HIS:CE1	2.37	0.60
1:Ad:208:ASN:HA	1:Ad:249:THR:HG21	1.84	0.59
1:Aq:3:VAL:HG11	1:Ar:98:VAL:HG23	1.83	0.59
1:Ak:150:ARG:NH1	1:Al:77:GLY:HA3	2.17	0.59
1:As:236:ILE:HD11	1:As:315:ILE:HD12	1.85	0.59
2:Bl:71:LEU:HD11	2:Bl:123:ALA:HB1	1.85	0.59
6:Je:21:DT:H2'	6:Je:22:DT:H71	1.85	0.59
6:Ji:21:DT:H2'	6:Ji:22:DT:H71	1.85	0.59
1:Ac:9:ASN:O	1:Ac:13:ARG:HG2	2.02	0.59
4:Dl:225:LYS:HE2	4:Dl:229:ILE:HD11	1.85	0.59
1:Ab:208:ASN:HA	1:Ab:249:THR:HG21	1.85	0.59
6:Jc:21:DT:H2'	6:Jc:22:DT:H71	1.85	0.59
1:Ae:31:ILE:HG12	1:Af:64:GLU:HB2	1.84	0.59
2:Bg:22:LEU:HB2	2:Bg:103:ALA:HB3	1.85	0.59
6:Ja:21:DT:H2'	6:Ja:22:DT:H71	1.85	0.59
1:Ah:93:ALA:HB1	2:Bh:17:GLU:HB2	1.85	0.58
1:Ar:29:LYS:HE3	1:Ar:31:ILE:HD11	1.83	0.58
6:Jg:21:DT:H2'	6:Jg:22:DT:H71	1.85	0.58
4:Df:269:PHE:HA	4:Df:275:HIS:CE1	2.38	0.58
1:Ac:108:LEU:HD23	2:Bb:3:LYS:HE3	1.86	0.58
1:Ao:236:ILE:HD11	1:Ao:317:LEU:HD11	1.86	0.58
1:As:236:ILE:HG12	1:As:315:ILE:HB	1.85	0.58
4:Df:25:LYS:HE2	7:Jf:9:DA:H5''	1.85	0.58
1:Ag:9:ASN:O	1:Ag:13:ARG:HG2	2.03	0.58
1:Ag:150:ARG:NH1	1:Ah:77:GLY:HA3	2.19	0.57
4:Dj:63:LEU:HD11	4:Dj:130:ILE:HG21	1.85	0.57
1:Ai:9:ASN:O	1:Ai:13:ARG:HG2	2.03	0.57
4:De:63:LEU:HD11	4:De:130:ILE:HG21	1.86	0.57
1:An:48:LEU:HB2	1:An:294:TYR:CZ	2.39	0.57
1:Ap:186:ASP:H	2:Bp:1:MET:HG3	1.69	0.57
1:Ap:208:ASN:HA	1:Ap:249:THR:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dg:269:PHE:HA	4:Dg:275:HIS:CE1	2.40	0.57
1:Ak:95:VAL:HB	2:Bj:16:TRP:CD2	2.40	0.57
2:Bg:53:LEU:HD11	2:Bg:133:LEU:HD11	1.86	0.57
1:Ak:9:ASN:O	1:Ak:13:ARG:HG2	2.05	0.56
1:Ak:57:SER:HB3	3:Cc:1:MET:HE1	1.86	0.56
1:Ai:3:VAL:HG11	1:Aj:98:VAL:HG23	1.86	0.56
1:Aq:9:ASN:O	1:Aq:13:ARG:HG2	2.04	0.56
1:Af:155:ARG:HG3	1:Af:327:PHE:CZ	2.40	0.56
1:Ak:57:SER:HB2	1:Ak:345:THR:HG21	1.86	0.56
1:Ar:208:ASN:HA	1:Ar:249:THR:HG21	1.87	0.56
1:As:95:VAL:HB	2:Br:16:TRP:CD2	2.41	0.56
1:As:105:TRP:CZ2	1:As:371:LEU:HB3	2.40	0.56
1:Aa:9:ASN:O	1:Aa:13:ARG:HG2	2.06	0.56
1:Ak:3:VAL:HG22	2:Bl:15:TYR:HB3	1.88	0.56
1:Aa:11:LEU:HD13	1:Aa:33:GLU:HB3	1.88	0.56
1:Ac:355:LEU:HD22	1:Af:333:VAL:HG11	1.87	0.56
4:Dc:63:LEU:HD11	4:Dc:130:ILE:HG21	1.88	0.56
7:Jf:26:DA:H2''	7:Jf:27:DA:C8	2.41	0.55
2:Bd:71:LEU:HD11	2:Bd:123:ALA:HB1	1.87	0.55
7:Jd:26:DA:H2''	7:Jd:27:DA:C8	2.41	0.55
1:Ag:18:LEU:HD11	1:Aj:100:LEU:HD21	1.88	0.55
1:Am:9:ASN:O	1:Am:13:ARG:HG2	2.06	0.55
1:Ad:55:GLU:HA	1:Ad:327:PHE:HB3	1.89	0.55
1:Ae:3:VAL:HG11	1:Af:98:VAL:HG23	1.87	0.55
1:Ao:409:LEU:HD21	1:Ap:99:ASP:HB2	1.89	0.55
1:Ar:265:GLN:HA	1:As:265:GLN:HG3	1.88	0.55
2:Bh:71:LEU:HD11	2:Bh:123:ALA:HB1	1.87	0.55
7:Jb:26:DA:H2''	7:Jb:27:DA:C8	2.41	0.55
7:Jh:26:DA:H2''	7:Jh:27:DA:C8	2.41	0.55
7:Jj:26:DA:H2''	7:Jj:27:DA:C8	2.42	0.55
1:Ar:314:LEU:HD21	1:Ar:390:LEU:HD23	1.88	0.55
2:Bn:106:ILE:HD13	2:Bn:125:LEU:HD21	1.89	0.55
1:Ag:237:VAL:HG21	1:Ag:241:PHE:HB2	1.89	0.54
1:Ac:176:TYR:CZ	1:Ad:77:GLY:HA2	2.41	0.54
3:Cc:42:VAL:HG11	3:Cc:58:VAL:HG11	1.89	0.54
1:Ak:157:TRP:O	1:Ak:161:GLN:HG2	2.06	0.54
1:Al:186:ASP:H	2:Bl:1:MET:HG3	1.71	0.54
1:Ar:120:GLU:HB2	3:Cc:31:ARG:HH21	1.72	0.54
2:Br:106:ILE:HD13	2:Br:125:LEU:HD21	1.89	0.54
1:Ao:157:TRP:O	1:Ao:161:GLN:HG2	2.06	0.54
1:Ad:237:VAL:O	1:Ad:293:VAL:HA	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:146:ARG:HB2	2:Bf:134:LYS:HD2	1.90	0.54
2:Bl:146:ARG:H	2:Bn:134:LYS:HD3	1.72	0.54
1:Ap:55:GLU:HA	1:Ap:327:PHE:HB3	1.89	0.54
1:Ao:255:VAL:HA	1:Ao:282:ILE:HD13	1.89	0.53
1:At:55:GLU:HA	1:At:327:PHE:HB3	1.89	0.53
4:De:225:LYS:HE2	4:De:229:ILE:HD11	1.91	0.53
6:Jg:29:DT:H2'	6:Jg:30:DT:H71	1.90	0.53
2:Bb:134:LYS:HD3	2:Bt:146:ARG:H	1.73	0.53
1:Af:38:ILE:HG13	1:Af:409:LEU:HD11	1.90	0.53
1:As:351:VAL:HG22	1:As:364:ILE:HG22	1.90	0.53
1:Ac:164:ARG:HD2	1:Ac:389:TRP:CZ2	2.44	0.53
1:An:155:ARG:HG3	1:An:327:PHE:CZ	2.44	0.53
2:Bl:22:LEU:HB3	2:Bl:103:ALA:HB3	1.89	0.53
4:Da:269:PHE:HA	4:Da:275:HIS:CE1	2.43	0.53
6:Je:29:DT:H2'	6:Je:30:DT:H71	1.90	0.53
1:Ak:203:LYS:HA	1:Ak:209:SER:HA	1.89	0.53
1:Ao:150:ARG:NH1	1:Ap:77:GLY:HA3	2.23	0.53
1:Ag:157:TRP:O	1:Ag:161:GLN:HG2	2.08	0.53
1:Ap:258:GLU:HG3	1:Ap:285:ARG:HH12	1.73	0.53
6:Ji:29:DT:H2'	6:Ji:30:DT:H71	1.90	0.53
1:An:229:ASP:HA	1:An:319:GLN:HG3	1.91	0.53
1:Ab:170:ILE:HB	1:Ab:183:TYR:HB2	1.91	0.53
1:Ak:313:GLU:HG2	1:Ak:389:TRP:CE3	2.44	0.53
1:Ao:9:ASN:O	1:Ao:13:ARG:HG2	2.09	0.53
2:Bf:29:ALA:HB2	2:Bf:99:THR:HG22	1.91	0.53
1:As:150:ARG:NH1	1:At:77:GLY:HA3	2.24	0.53
4:Db:293:ALA:HB3	4:Dc:240:MET:HE3	1.90	0.52
6:Jc:29:DT:H2'	6:Jc:30:DT:H71	1.90	0.52
1:Ag:13:ARG:HB2	1:Ai:17:PRO:HB3	1.91	0.52
1:Al:318:ASN:HD21	1:Al:388:LYS:HE2	1.74	0.52
1:Ab:318:ASN:HD21	1:Ab:388:LYS:HD2	1.75	0.52
1:Ac:170:ILE:HD12	1:Ac:183:TYR:HB2	1.91	0.52
1:Ag:116:TRP:HD1	1:Ag:120:GLU:OE1	1.93	0.52
1:As:157:TRP:O	1:As:161:GLN:HG2	2.08	0.52
2:Bh:132:LYS:HB3	2:Bh:146:ARG:HH21	1.72	0.52
1:Ah:186:ASP:H	2:Bh:1:MET:HG3	1.75	0.52
1:Ab:314:LEU:HD21	1:Ab:390:LEU:HD23	1.91	0.52
1:Al:258:GLU:HG2	1:Al:285:ARG:HH22	1.73	0.52
2:Bo:41:GLY:O	2:Bo:45:ALA:HB2	2.08	0.52
6:Ja:29:DT:H2'	6:Ja:30:DT:H71	1.90	0.52
1:Ak:69:ARG:HB2	1:Ak:99:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:105:TRP:CZ2	1:Ak:371:LEU:HB3	2.44	0.52
1:At:93:ALA:HB1	2:Bt:17:GLU:HB2	1.92	0.52
2:Bf:106:ILE:HD12	2:Bf:138:GLY:HA2	1.91	0.52
4:Dl:269:PHE:HA	4:Dl:275:HIS:CE1	2.44	0.52
1:Ab:229:ASP:HA	1:Ab:319:GLN:HG3	1.91	0.52
1:Ad:245:LEU:HD22	1:Ad:251:VAL:HG21	1.91	0.52
1:Ao:313:GLU:HG2	1:Ao:389:TRP:CE3	2.45	0.52
2:Bb:106:ILE:HD13	2:Bb:125:LEU:HD21	1.91	0.52
4:Dg:56:LEU:HB3	4:Dg:159:PHE:HE1	1.74	0.52
1:Ao:18:LEU:HD11	1:Ar:100:LEU:HD21	1.92	0.52
1:As:57:SER:HB3	3:Ce:1:MET:HE1	1.91	0.52
1:At:104:THR:HG22	2:Bt:5:GLN:HB3	1.92	0.52
2:Bp:136:ILE:HG22	2:Bp:137:LYS:HG3	1.91	0.52
4:Df:86:VAL:HG23	4:Df:108:ILE:HG13	1.90	0.52
1:Ar:110:PHE:CZ	1:Ar:158:LEU:HD11	2.45	0.52
2:Bj:133:LEU:HD22	2:Bj:142:PHE:HB3	1.91	0.52
1:Ae:9:ASN:O	1:Ae:13:ARG:HG2	2.10	0.52
2:Bg:41:GLY:O	2:Bg:45:ALA:HB2	2.10	0.52
1:Ag:313:GLU:HG2	1:Ag:389:TRP:CE3	2.46	0.51
1:Ao:69:ARG:HB2	1:Ao:99:ASP:OD1	2.11	0.51
4:Dc:241:ILE:HG13	4:Dd:274:ARG:HG2	1.92	0.51
4:Df:241:ILE:HG13	4:Dg:274:ARG:HG2	1.93	0.51
1:Ah:55:GLU:HA	1:Ah:327:PHE:HB3	1.91	0.51
1:An:208:ASN:HA	1:An:249:THR:HG21	1.90	0.51
1:Af:255:VAL:HA	1:Af:282:ILE:HD13	1.91	0.51
1:Ak:18:LEU:HD11	1:An:100:LEU:HD21	1.91	0.51
1:Ao:270:PRO:HG2	1:Ao:275:TYR:CE2	2.45	0.51
2:Bd:136:ILE:HG22	2:Bd:137:LYS:HG3	1.93	0.51
1:Ac:67:LEU:HD23	1:Ac:382:PHE:HE1	1.76	0.51
1:Ao:67:LEU:HD23	1:Ao:382:PHE:HE1	1.76	0.51
1:Ac:157:TRP:O	1:Ac:161:GLN:HG2	2.11	0.51
1:Ag:115:VAL:HG23	1:Ag:363:ALA:HB2	1.93	0.51
1:Ar:104:THR:OG1	2:Bq:5:GLN:HB3	2.11	0.51
1:Al:104:THR:HG22	2:Bl:5:GLN:HB3	1.91	0.51
1:As:46:ASN:HB2	1:As:308:TRP:CE2	2.46	0.51
1:Aa:17:PRO:HB3	1:As:13:ARG:HB2	1.93	0.51
1:At:258:GLU:HG3	1:At:285:ARG:HH12	1.75	0.51
2:Br:88:HIS:HD1	2:Br:91:GLU:HB2	1.75	0.51
1:Ap:258:GLU:HG2	1:Ap:285:ARG:HH22	1.74	0.51
2:Bp:56:VAL:HG21	2:Bp:81:ILE:HD13	1.93	0.51
1:Ac:13:ARG:HB2	1:Ae:17:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:218:ARG:HH22	1:Ag:286:TYR:HB3	1.75	0.51
2:Bf:133:LEU:HD22	2:Bf:142:PHE:HB3	1.93	0.51
4:Dd:259:TRP:HZ2	5:Ed:119:ASP:HB2	1.76	0.51
1:Af:32:GLN:HB3	2:Bg:6:LEU:HD11	1.93	0.50
1:Ao:110:PHE:CZ	1:Ao:158:LEU:HD11	2.46	0.50
1:Ao:268:VAL:HG13	1:Ap:262:VAL:HG12	1.93	0.50
6:Jc:28:DT:H2'	6:Jc:29:DT:H72	1.93	0.50
6:Ji:28:DT:H2'	6:Ji:29:DT:H72	1.93	0.50
1:Af:48:LEU:HB2	1:Af:294:TYR:CZ	2.46	0.50
1:Ag:126:ARG:HB3	1:Ag:129:ASP:HB2	1.93	0.50
7:Jb:24:DA:H2''	7:Jb:25:DA:C8	2.47	0.50
7:Jd:18:DA:H2''	7:Jd:19:DA:C8	2.47	0.50
2:Bg:1:MET:HG2	2:Bg:3:LYS:H	1.76	0.50
2:Bl:56:VAL:HG21	2:Bl:81:ILE:HD13	1.93	0.50
7:Jh:20:DA:H2''	7:Jh:21:DA:H8	1.77	0.50
1:Aj:104:THR:OG1	2:Bi:5:GLN:HB3	2.12	0.50
7:Jb:18:DA:H2''	7:Jb:19:DA:C8	2.47	0.50
7:Jd:24:DA:H2''	7:Jd:25:DA:C8	2.46	0.50
1:Af:270:PRO:HG2	1:Af:275:TYR:CE2	2.46	0.50
1:Ao:13:ARG:HB2	1:Aq:17:PRO:HB3	1.94	0.50
1:As:69:ARG:HB2	1:As:99:ASP:OD1	2.10	0.50
1:Ad:93:ALA:HB1	2:Bd:17:GLU:HB2	1.92	0.50
1:Af:229:ASP:HA	1:Af:319:GLN:HG3	1.92	0.50
1:Ap:93:ALA:HB1	2:Bp:17:GLU:HB2	1.93	0.50
2:Bg:21:ARG:HD2	2:Bg:27:VAL:HG11	1.94	0.50
1:Ab:181:LEU:HD21	2:Bt:31:PRO:HB2	1.94	0.50
7:Jf:24:DA:H2''	7:Jf:25:DA:C8	2.47	0.50
6:Jg:28:DT:H2'	6:Jg:29:DT:H72	1.93	0.50
7:Jj:20:DA:H2''	7:Jj:21:DA:H8	1.77	0.50
7:Jj:24:DA:H2''	7:Jj:25:DA:C8	2.46	0.50
1:Aj:314:LEU:HD21	1:Aj:390:LEU:HD23	1.94	0.50
1:Ak:268:VAL:HG13	1:Al:262:VAL:HG12	1.92	0.50
1:An:48:LEU:HD12	1:An:294:TYR:CD2	2.47	0.50
1:Ao:251:VAL:O	1:Ao:255:VAL:HG23	2.12	0.50
1:Ap:104:THR:HG22	2:Bp:5:GLN:HB3	1.94	0.50
2:Bf:22:LEU:HD22	2:Bf:25:TYR:H	1.75	0.50
1:Ab:116:TRP:CZ2	1:Ab:118:GLU:HB2	2.47	0.50
1:Ae:24:LYS:HE3	2:Bd:86:ASP:HB2	1.94	0.50
1:Ag:69:ARG:HB2	1:Ag:99:ASP:OD1	2.11	0.50
1:Ak:218:ARG:HH22	1:Ak:286:TYR:HB3	1.77	0.50
7:Jh:24:DA:H2''	7:Jh:25:DA:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:268:VAL:HG13	1:Ad:262:VAL:HG12	1.94	0.49
1:Ao:127:LEU:HD23	1:Aq:26:PRO:HB3	1.94	0.49
2:Bp:146:ARG:HB2	2:Br:134:LYS:HD2	1.93	0.49
1:Ar:164:ARG:HA	1:Ar:389:TRP:HE1	1.78	0.49
6:Je:28:DT:H2'	6:Je:29:DT:H72	1.93	0.49
7:Jf:20:DA:H2''	7:Jf:21:DA:H8	1.77	0.49
1:Ab:151:MET:HE3	1:Ab:367:GLY:N	2.27	0.49
1:Ac:218:ARG:HH22	1:Ac:286:TYR:HB3	1.78	0.49
1:Ar:38:ILE:HG13	1:Ar:409:LEU:HD11	1.95	0.49
1:Ar:120:GLU:HB2	3:Ce:31:ARG:NH2	2.26	0.49
2:Bb:134:LYS:HD2	2:Bt:146:ARG:HB2	1.94	0.49
6:Ja:28:DT:H2'	6:Ja:29:DT:H72	1.93	0.49
1:Al:93:ALA:HB1	2:Bl:17:GLU:HB2	1.94	0.49
2:Bj:102:ALA:HB3	2:Bj:142:PHE:CZ	2.47	0.49
4:Da:239:PHE:CZ	4:Da:292:SER:HB2	2.47	0.49
4:Dk:259:TRP:HZ2	5:Ek:119:ASP:HB2	1.78	0.49
7:Jf:18:DA:H2''	7:Jf:19:DA:C8	2.47	0.49
1:Ab:104:THR:OG1	2:Ba:5:GLN:HB3	2.13	0.49
1:Ao:126:ARG:HB3	1:Ao:129:ASP:HB2	1.94	0.49
1:Ac:129:ASP:HB3	1:Ac:131:VAL:HG13	1.93	0.49
1:Ah:237:VAL:O	1:Ah:293:VAL:HA	2.12	0.49
1:As:251:VAL:O	1:As:255:VAL:HG23	2.12	0.49
1:Ap:245:LEU:HD22	1:Ap:251:VAL:HG21	1.94	0.49
4:Db:199:VAL:HG13	4:Db:355:TYR:HB2	1.93	0.49
7:Jh:18:DA:H2''	7:Jh:19:DA:C8	2.47	0.49
1:Ab:132:GLN:H	1:Ab:132:GLN:CD	2.20	0.49
1:Ac:203:LYS:HA	1:Ac:209:SER:HA	1.95	0.49
1:Ak:236:ILE:CG2	1:Ak:315:ILE:HB	2.42	0.49
2:Bt:34:MET:HE3	2:Bt:40:TRP:CG	2.48	0.49
4:Dg:248:ILE:HD11	4:Dg:259:TRP:CZ3	2.48	0.49
7:Jb:20:DA:H2''	7:Jb:21:DA:H8	1.77	0.49
1:An:108:LEU:N	1:An:371:LEU:HD23	2.28	0.49
7:Jd:20:DA:H2''	7:Jd:21:DA:H8	1.77	0.49
4:Dj:76:PHE:CG	4:Dj:126:GLU:HG2	2.48	0.49
1:Ac:69:ARG:HB2	1:Ac:99:ASP:OD1	2.13	0.48
1:Ag:155:ARG:HG3	1:Ag:327:PHE:CE2	2.48	0.48
2:Bh:146:ARG:H	2:Bj:134:LYS:HD3	1.78	0.48
2:Bj:106:ILE:HD12	2:Bj:138:GLY:HA2	1.93	0.48
3:Cb:29:ALA:HB1	3:Cb:63:TRP:HB3	1.93	0.48
4:Dd:217:ALA:HB1	4:De:66:GLY:HA2	1.95	0.48
2:Bh:146:ARG:HB2	2:Bj:134:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bl:30:LEU:HD12	2:Bl:100:LEU:HD11	1.95	0.48
4:Da:199:VAL:HG13	4:Da:355:TYR:HB2	1.94	0.48
7:Jj:18:DA:H2"	7:Jj:19:DA:C8	2.47	0.48
1:Ak:127:LEU:HD23	1:Am:26:PRO:HB3	1.94	0.48
1:Al:237:VAL:O	1:Al:293:VAL:HA	2.13	0.48
1:Ao:233:VAL:HG22	1:Ao:318:ASN:O	2.13	0.48
2:Bf:106:ILE:HD13	2:Bf:125:LEU:HD21	1.93	0.48
4:Dg:199:VAL:HG13	4:Dg:355:TYR:HB2	1.94	0.48
4:Di:241:ILE:HG13	4:Dj:274:ARG:HD3	1.95	0.48
1:Ag:351:VAL:HG22	1:Ag:364:ILE:HG22	1.95	0.48
1:Am:15:ARG:HD3	1:Am:31:ILE:HD12	1.95	0.48
1:An:48:LEU:HB2	1:An:294:TYR:CE1	2.48	0.48
1:Ao:222:LYS:HA	1:Ao:225:THR:HG23	1.95	0.48
1:Aq:31:ILE:HG12	1:Ar:64:GLU:HB2	1.95	0.48
1:As:270:PRO:HG2	1:As:275:TYR:CE2	2.49	0.48
3:Cd:42:VAL:HG11	3:Cd:58:VAL:HG11	1.95	0.48
1:Ac:222:LYS:HA	1:Ac:225:THR:HG23	1.95	0.48
1:Ak:110:PHE:CZ	1:Ak:158:LEU:HD11	2.49	0.48
1:An:377:TYR:HB2	2:Bm:7:PHE:HE2	1.78	0.48
4:Dg:346:ARG:NH2	4:Dh:81:SER:HA	2.29	0.48
4:Dk:199:VAL:HG13	4:Dk:355:TYR:HB2	1.94	0.48
1:Ac:150:ARG:NH1	1:Ad:77:GLY:HA3	2.29	0.48
1:Ak:222:LYS:HA	1:Ak:225:THR:HG23	1.96	0.48
2:Bp:34:MET:HE3	2:Bp:40:TRP:CG	2.49	0.48
4:Db:241:ILE:HG13	4:Dc:274:ARG:HG2	1.94	0.48
4:Di:76:PHE:CG	4:Di:126:GLU:HG2	2.48	0.48
1:Aa:12:ALA:HB1	1:As:13:ARG:NH1	2.28	0.48
1:Ag:46:ASN:HB2	1:Ag:308:TRP:CE2	2.48	0.48
1:Ag:235:ILE:HG12	1:Ag:316:VAL:HG12	1.94	0.48
1:As:63:LEU:HD13	1:As:105:TRP:CZ3	2.48	0.48
1:As:313:GLU:HG2	1:As:389:TRP:HE3	1.77	0.48
4:Dj:259:TRP:HZ2	5:Ej:119:ASP:HB2	1.78	0.48
1:Ab:300:ASP:HB3	1:Ab:302:ASP:OD1	2.14	0.48
1:Aj:255:VAL:HA	1:Aj:282:ILE:HD13	1.95	0.48
6:Ji:17:DT:H2"	6:Ji:18:DT:H71	1.96	0.48
1:Ab:108:LEU:N	1:Ab:371:LEU:HD23	2.28	0.48
1:Ad:104:THR:HG22	2:Bd:5:GLN:HE21	1.79	0.48
1:Ag:251:VAL:O	1:Ag:255:VAL:HG23	2.14	0.48
2:Bn:102:ALA:HB3	2:Bn:142:PHE:CZ	2.48	0.48
4:De:421:ARG:NH2	4:Df:83:LYS:HG3	2.28	0.48
1:An:29:LYS:HE3	1:An:31:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:107:PRO:HG3	1:Ar:330:THR:HG21	1.96	0.48
1:As:409:LEU:HD21	1:At:99:ASP:HB2	1.96	0.48
1:At:237:VAL:O	1:At:293:VAL:HA	2.14	0.48
2:Bb:133:LEU:HD22	2:Bb:142:PHE:HB3	1.94	0.48
2:Bd:146:ARG:H	2:Bf:134:LYS:HD3	1.79	0.48
2:Bo:113:ILE:HG22	2:Bo:114:GLU:HG2	1.96	0.48
1:Ag:299:ARG:CZ	1:Ag:406:LYS:HB3	2.44	0.47
1:Ai:31:ILE:HG12	1:Aj:64:GLU:HB2	1.96	0.47
1:Ao:95:VAL:HB	2:Bn:16:TRP:CD2	2.49	0.47
1:Ao:105:TRP:CZ2	1:Ao:371:LEU:HB3	2.49	0.47
4:Dj:346:ARG:NH2	4:Dk:81:SER:HA	2.28	0.47
4:Dk:86:VAL:HG23	4:Dk:108:ILE:HG13	1.96	0.47
7:Jj:12:DA:H4'	7:Jj:13:DA:OP1	2.14	0.47
1:Ac:15:ARG:HH21	1:Ae:13:ARG:NH2	2.12	0.47
1:Aj:208:ASN:HA	1:Aj:249:THR:HG21	1.95	0.47
2:Bh:136:ILE:HG22	2:Bh:137:LYS:HG3	1.95	0.47
1:Ag:110:PHE:CZ	1:Ag:158:LEU:HD11	2.49	0.47
1:Ak:126:ARG:HB3	1:Ak:129:ASP:HB2	1.95	0.47
1:An:73:ALA:HB2	1:An:95:VAL:HG12	1.97	0.47
1:As:116:TRP:HD1	1:As:120:GLU:OE1	1.96	0.47
1:As:233:VAL:HG22	1:As:318:ASN:O	2.14	0.47
4:Dc:269:PHE:HA	4:Dc:275:HIS:CE1	2.48	0.47
4:De:254:GLN:HA	4:De:259:TRP:CG	2.50	0.47
4:Dg:86:VAL:HG23	4:Dg:108:ILE:HG13	1.97	0.47
7:Jh:12:DA:H4'	7:Jh:13:DA:OP1	2.14	0.47
1:Ab:48:LEU:HB2	1:Ab:294:TYR:CE1	2.50	0.47
1:Ac:110:PHE:CZ	1:Ac:158:LEU:HD11	2.49	0.47
1:Af:108:LEU:N	1:Af:371:LEU:HD23	2.29	0.47
1:Ak:255:VAL:HA	1:Ak:282:ILE:HD13	1.95	0.47
2:Bg:53:LEU:HD13	2:Bg:131:LEU:HD23	1.95	0.47
1:Aj:48:LEU:HB2	1:Aj:294:TYR:CE1	2.49	0.47
7:Jd:12:DA:H4'	7:Jd:13:DA:OP1	2.14	0.47
7:Jf:12:DA:H4'	7:Jf:13:DA:OP1	2.14	0.47
1:Ab:172:PRO:HA	1:Ab:180:GLY:HA2	1.97	0.47
1:Ac:95:VAL:HB	2:Bb:16:TRP:CD2	2.50	0.47
1:Af:48:LEU:HD12	1:Af:294:TYR:CD2	2.49	0.47
1:Ao:355:LEU:HD22	1:Ar:333:VAL:HG11	1.96	0.47
1:Aq:15:ARG:HD3	1:Aq:31:ILE:HD12	1.96	0.47
1:Ar:154:ARG:HB2	1:As:78:MET:HB3	1.97	0.47
2:Bt:71:LEU:HD11	2:Bt:123:ALA:HB1	1.96	0.47
1:Ac:261:TRP:CD1	1:Ac:267:THR:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:251:VAL:O	1:Ak:255:VAL:HG23	2.15	0.47
1:Ao:176:TYR:CZ	1:Ap:77:GLY:HA2	2.50	0.47
1:Ar:374:LEU:HD13	1:Ar:384:PHE:CE2	2.49	0.47
2:Bt:136:ILE:HG22	2:Bt:137:LYS:HG3	1.96	0.47
4:Df:268:ASN:ND2	5:Ee:120:TRP:CD2	2.83	0.47
4:Dl:76:PHE:CG	4:Dl:126:GLU:HG2	2.49	0.47
7:Jb:12:DA:H4'	7:Jb:13:DA:OP1	2.14	0.47
1:Ab:110:PHE:CE2	1:Ab:158:LEU:HD11	2.50	0.47
1:Af:104:THR:OG1	2:Be:5:GLN:HB3	2.15	0.47
1:Ao:129:ASP:HB3	1:Ao:131:VAL:HG13	1.96	0.47
1:Ac:18:LEU:HD11	1:Af:100:LEU:HD21	1.97	0.47
1:Ah:258:GLU:HG2	1:Ah:285:ARG:HH22	1.80	0.47
1:Ar:73:ALA:HB2	1:Ar:95:VAL:HG12	1.97	0.47
2:Bc:1:MET:HG2	2:Bc:3:LYS:H	1.79	0.47
2:Bt:22:LEU:HB3	2:Bt:103:ALA:HB3	1.97	0.47
1:Ab:270:PRO:HG2	1:Ab:275:TYR:CE2	2.50	0.47
1:Ac:116:TRP:HD1	1:Ac:120:GLU:OE1	1.98	0.47
1:Al:245:LEU:HD22	1:Al:251:VAL:HG21	1.96	0.47
1:An:49:VAL:HG23	1:An:163:MET:SD	2.55	0.47
2:Bl:136:ILE:HG22	2:Bl:137:LYS:HG3	1.97	0.47
2:Bs:1:MET:HG2	2:Bs:3:LYS:H	1.80	0.47
1:Ac:105:TRP:NE1	1:Ac:371:LEU:HD23	2.31	0.46
1:Ac:200:PHE:CE2	1:Ac:213:PRO:HB3	2.51	0.46
1:Af:151:MET:HE3	1:Af:367:GLY:N	2.30	0.46
1:An:164:ARG:HA	1:An:389:TRP:HE1	1.80	0.46
1:Aq:11:LEU:HD13	1:Aq:33:GLU:HB3	1.96	0.46
1:As:313:GLU:HG2	1:As:389:TRP:CE3	2.50	0.46
2:Br:133:LEU:HD22	2:Br:142:PHE:HB3	1.97	0.46
4:Dk:54:ASP:O	4:Dk:58:VAL:HG23	2.16	0.46
1:Ac:251:VAL:O	1:Ac:255:VAL:HG23	2.15	0.46
1:At:168:ILE:HG12	1:At:185:ILE:HB	1.97	0.46
1:At:194:LEU:HD12	1:At:390:LEU:HB2	1.98	0.46
6:Jc:2:DT:H4'	6:Jc:3:DT:OP1	2.16	0.46
1:Ac:105:TRP:CZ2	1:Ac:371:LEU:HB3	2.50	0.46
1:Ac:313:GLU:HG2	1:Ac:389:TRP:HE3	1.80	0.46
1:Ak:108:LEU:HD23	2:Bj:3:LYS:HE3	1.98	0.46
1:An:154:ARG:HB2	1:Ao:78:MET:HB3	1.97	0.46
4:Dg:391:MET:HA	4:Dg:394:LEU:HD12	1.98	0.46
4:Dl:248:ILE:HD11	4:Dl:259:TRP:CZ3	2.51	0.46
6:Je:2:DT:H4'	6:Je:3:DT:OP1	2.16	0.46
6:Ji:19:DT:H2'	6:Ji:20:DT:H71	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ab:407:VAL:HG21	1:Ac:380:GLU:HG2	1.96	0.46
1:Ag:311:VAL:HG22	1:Ag:396:VAL:HB	1.97	0.46
1:Ap:55:GLU:HG2	1:Ap:155:ARG:HD2	1.98	0.46
4:Dh:239:PHE:CZ	4:Dh:292:SER:HB2	2.50	0.46
1:Ag:105:TRP:CZ2	1:Ag:371:LEU:HB3	2.51	0.46
1:Aj:48:LEU:HB2	1:Aj:294:TYR:CZ	2.51	0.46
1:Al:55:GLU:HA	1:Al:327:PHE:HB3	1.98	0.46
1:Ac:316:VAL:O	1:Ac:387:PHE:HA	2.16	0.46
1:Ak:313:GLU:HG2	1:Ak:389:TRP:HE3	1.78	0.46
4:De:215:LEU:O	4:De:219:VAL:HG23	2.15	0.46
4:Di:217:ALA:HB1	4:Dj:66:GLY:HA2	1.98	0.46
1:Af:40:ASP:OD2	1:Af:299:ARG:HG3	2.14	0.46
1:Ag:200:PHE:CE2	1:Ag:213:PRO:HB3	2.51	0.46
1:Aj:132:GLN:CD	1:Aj:134:GLY:H	2.24	0.46
1:Ak:116:TRP:HD1	1:Ak:120:GLU:OE1	1.99	0.46
1:Ap:261:TRP:CZ3	1:Ap:270:PRO:HG3	2.49	0.46
4:Db:391:MET:HE2	4:Db:423:LEU:HD22	1.98	0.46
4:Df:203:HIS:NE2	4:Df:214:ALA:HB2	2.31	0.46
4:Di:225:LYS:HE2	4:Di:229:ILE:HD11	1.97	0.46
6:Jg:19:DT:H2'	6:Jg:20:DT:H71	1.98	0.46
1:Ac:126:ARG:HB3	1:Ac:129:ASP:HB2	1.96	0.46
1:Ag:63:LEU:HD13	1:Ag:105:TRP:CZ3	2.51	0.46
1:Ag:127:LEU:HD23	1:Ai:26:PRO:HB3	1.97	0.46
1:An:151:MET:HE3	1:An:367:GLY:N	2.31	0.46
1:As:126:ARG:HB3	1:As:129:ASP:HB2	1.98	0.46
4:Df:427:ASP:HB3	4:Df:430:ARG:HB3	1.98	0.46
1:Ab:58:THR:O	1:Ab:330:THR:HA	2.16	0.46
1:Ar:270:PRO:HG2	1:Ar:275:TYR:CE2	2.51	0.46
2:Bc:22:LEU:HB2	2:Bc:103:ALA:HB3	1.97	0.46
4:Dc:391:MET:HA	4:Dc:394:LEU:HD12	1.98	0.46
7:Jh:1:DA:N7	7:Jj:31:DA:H1'	2.31	0.46
1:Ah:86:SER:HB3	2:Bg:31:PRO:HD3	1.97	0.45
1:Aj:49:VAL:HG23	1:Aj:163:MET:SD	2.56	0.45
1:Ad:168:ILE:HG12	1:Ad:185:ILE:HB	1.98	0.45
1:At:312:GLY:HA2	1:At:393:ALA:HB3	1.98	0.45
2:Br:29:ALA:HB2	2:Br:99:THR:HG22	1.98	0.45
2:Br:106:ILE:HD12	2:Br:138:GLY:HA2	1.98	0.45
4:Dh:394:LEU:O	4:Dh:398:VAL:HG22	2.16	0.45
4:Di:76:PHE:CD1	4:Di:126:GLU:HG2	2.51	0.45
6:Jc:19:DT:H2'	6:Jc:20:DT:H71	1.98	0.45
6:Ji:2:DT:H4'	6:Ji:3:DT:OP1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:3:VAL:HG11	1:Ab:98:VAL:HG23	1.97	0.45
1:Ab:170:ILE:HD12	1:Ab:183:TYR:HB2	1.99	0.45
1:Af:108:LEU:H	1:Af:371:LEU:HD23	1.82	0.45
1:Ak:270:PRO:HG2	1:Ak:275:TYR:CE2	2.50	0.45
1:Ap:237:VAL:O	1:Ap:293:VAL:HA	2.16	0.45
4:Di:346:ARG:NH2	4:Dj:81:SER:HA	2.32	0.45
6:Ja:2:DT:H4'	6:Ja:3:DT:OP1	2.16	0.45
6:Je:13:DT:H2'	6:Je:14:DT:H71	1.98	0.45
1:Ab:151:MET:HE3	1:Ab:367:GLY:H	1.81	0.45
1:Ac:63:LEU:HD13	1:Ac:105:TRP:CZ3	2.51	0.45
1:Af:235:ILE:HG23	1:Af:314:LEU:HD13	1.98	0.45
1:Ag:95:VAL:HB	2:Bf:16:TRP:CD2	2.51	0.45
1:As:315:ILE:HD11	1:As:389:TRP:CZ2	2.52	0.45
2:Bc:113:ILE:HG22	2:Bc:114:GLU:HG2	1.98	0.45
2:Bg:128:ALA:HB1	2:Bg:133:LEU:HB2	1.98	0.45
4:Dk:346:ARG:NH2	4:Dl:81:SER:HA	2.31	0.45
7:Jb:9:DA:H2'	7:Jb:10:DA:H8	1.82	0.45
6:Jc:13:DT:H2'	6:Jc:14:DT:H71	1.99	0.45
1:Aj:56:ASP:O	1:Aj:328:VAL:HA	2.17	0.45
1:At:258:GLU:HG2	1:At:285:ARG:HH22	1.82	0.45
2:Bn:133:LEU:HD22	2:Bn:142:PHE:HB3	1.97	0.45
4:Df:76:PHE:CD1	4:Df:126:GLU:HG2	2.51	0.45
4:Dk:248:ILE:HD11	4:Dk:259:TRP:CZ3	2.52	0.45
7:Jj:9:DA:H2'	7:Jj:10:DA:H8	1.82	0.45
1:Ag:270:PRO:HG2	1:Ag:275:TYR:CE2	2.51	0.45
1:Aj:404:PRO:HB3	1:Ak:227:PHE:CE1	2.52	0.45
1:Ak:115:VAL:HG23	1:Ak:363:ALA:HB2	1.99	0.45
1:Am:3:VAL:HG11	1:An:98:VAL:HG23	1.99	0.45
1:An:110:PHE:CZ	1:An:158:LEU:HD11	2.51	0.45
2:Bt:34:MET:SD	2:Bt:94:HIS:HA	2.56	0.45
4:Df:199:VAL:HG13	4:Df:355:TYR:HB2	1.98	0.45
6:Ja:13:DT:H2'	6:Ja:14:DT:H71	1.98	0.45
1:Af:110:PHE:CE2	1:Af:158:LEU:HD11	2.52	0.45
1:At:318:ASN:HD21	1:At:388:LYS:HE2	1.81	0.45
4:Da:411:LEU:O	4:Da:415:LEU:HG	2.17	0.45
4:Di:427:ASP:HB3	4:Di:430:ARG:HB3	1.99	0.45
6:Ja:19:DT:H2'	6:Ja:20:DT:H71	1.98	0.45
7:Jf:9:DA:H2'	7:Jf:10:DA:H8	1.82	0.45
1:Ab:49:VAL:HG23	1:Ab:163:MET:SD	2.56	0.45
1:Af:110:PHE:CZ	1:Af:158:LEU:HD11	2.52	0.45
1:Ag:129:ASP:HB3	1:Ag:131:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:255:VAL:HA	1:Ag:282:ILE:HD13	1.98	0.45
1:Aj:407:VAL:HG21	1:Ak:380:GLU:HG2	1.99	0.45
1:At:86:SER:HB3	2:Bs:31:PRO:HD3	1.99	0.45
2:Bc:41:GLY:O	2:Bc:45:ALA:HB2	2.15	0.45
1:Aa:11:LEU:HD21	1:Ab:68:LEU:HB2	1.99	0.45
1:Ah:168:ILE:HG12	1:Ah:185:ILE:HB	1.99	0.45
1:Aj:66:TYR:CZ	1:Aj:102:LYS:HE2	2.52	0.45
1:Ak:299:ARG:CZ	1:Ak:406:LYS:HB3	2.46	0.45
1:An:150:ARG:HG2	1:Ao:77:GLY:C	2.42	0.45
1:An:248:ASN:O	1:An:252:GLN:HG3	2.16	0.45
1:Ar:172:PRO:HA	1:Ar:180:GLY:HA2	1.99	0.45
1:As:110:PHE:CZ	1:As:158:LEU:HD11	2.52	0.45
2:Bc:34:MET:HE2	2:Bc:40:TRP:CD2	2.51	0.45
2:Bj:42:ASN:HB3	2:Bj:113:ILE:HG12	1.99	0.45
2:Bl:34:MET:SD	2:Bl:94:HIS:HA	2.57	0.45
1:Ac:337:ARG:O	1:Ac:340:LYS:HE2	2.17	0.45
1:Ag:13:ARG:HB3	1:Ai:15:ARG:O	2.17	0.45
1:Aj:48:LEU:HD12	1:Aj:294:TYR:CD2	2.51	0.45
1:An:255:VAL:HA	1:An:282:ILE:HD13	1.98	0.45
1:Ao:261:TRP:CD1	1:Ao:267:THR:HG21	2.52	0.45
1:Ar:229:ASP:HA	1:Ar:319:GLN:HG3	1.99	0.45
2:Bn:106:ILE:HD12	2:Bn:138:GLY:HA2	1.97	0.45
4:Da:21:SER:O	4:Da:25:LYS:HE3	2.17	0.45
4:Da:78:ARG:CG	4:Da:341:ILE:HG21	2.46	0.45
6:Je:19:DT:H2'	6:Je:20:DT:H71	1.98	0.45
1:Af:48:LEU:HB2	1:Af:294:TYR:CE1	2.52	0.44
1:Ah:259:LYS:HB3	1:Ah:261:TRP:CE2	2.52	0.44
1:An:270:PRO:HG2	1:An:275:TYR:CE2	2.51	0.44
1:Aq:24:LYS:HE3	2:Bp:86:ASP:HB2	1.98	0.44
2:Bp:146:ARG:H	2:Br:134:LYS:HD3	1.82	0.44
4:De:259:TRP:HZ2	5:Ee:119:ASP:HB2	1.82	0.44
4:Df:230:LEU:HD21	5:Ef:130:PHE:H	1.82	0.44
6:Jg:2:DT:H4'	6:Jg:3:DT:OP1	2.16	0.44
7:Jh:9:DA:H2'	7:Jh:10:DA:H8	1.82	0.44
1:Aa:31:ILE:HG12	1:Ab:64:GLU:HB2	1.99	0.44
1:Ac:235:ILE:HG12	1:Ac:316:VAL:HG12	1.99	0.44
1:Ag:13:ARG:NH1	1:Ai:12:ALA:HB1	2.33	0.44
1:Aj:55:GLU:HG3	1:Aj:329:TYR:CE2	2.52	0.44
1:Aj:58:THR:O	1:Aj:330:THR:HA	2.16	0.44
1:Ap:53:PHE:HA	1:Ap:325:GLY:O	2.17	0.44
1:At:245:LEU:HD22	1:At:251:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bk:22:LEU:HB2	2:Bk:103:ALA:HB3	2.00	0.44
4:Da:172:PRO:HG3	4:Da:209:PHE:CZ	2.52	0.44
4:Dd:63:LEU:HD11	4:Dd:130:ILE:HG21	1.98	0.44
4:Df:225:LYS:HE2	4:Df:229:ILE:HD11	1.99	0.44
7:Jd:9:DA:H2'	7:Jd:10:DA:H8	1.82	0.44
1:Af:49:VAL:HG23	1:Af:163:MET:SD	2.57	0.44
1:An:189:VAL:HG11	1:An:192:ILE:HD13	1.98	0.44
1:As:150:ARG:HD2	1:At:77:GLY:C	2.41	0.44
4:Dh:76:PHE:CG	4:Dh:126:GLU:HG2	2.52	0.44
1:Ac:270:PRO:HG2	1:Ac:275:TYR:CE2	2.52	0.44
1:Aj:222:LYS:HA	1:Aj:225:THR:HG23	2.00	0.44
1:An:164:ARG:HA	1:An:389:TRP:NE1	2.33	0.44
1:Ao:218:ARG:HH22	1:Ao:286:TYR:HB3	1.81	0.44
2:Bc:53:LEU:HD13	2:Bc:131:LEU:HD23	1.99	0.44
2:Bd:56:VAL:HG21	2:Bd:81:ILE:HD13	1.98	0.44
2:Bp:71:LEU:HD11	2:Bp:123:ALA:HB1	2.00	0.44
4:Dd:346:ARG:NH2	4:De:81:SER:HA	2.33	0.44
4:Df:26:LEU:HA	4:Dg:197:LYS:HE2	1.99	0.44
4:Dg:391:MET:HE2	4:Dg:423:LEU:HD22	1.98	0.44
6:Jg:13:DT:H2'	6:Jg:14:DT:H71	1.98	0.44
1:Aj:189:VAL:HG11	1:Aj:192:ILE:HD13	1.99	0.44
1:Am:24:LYS:HE3	2:Bl:86:ASP:HB2	2.00	0.44
2:Bc:54:VAL:HG12	2:Bc:68:PRO:HA	2.00	0.44
2:Bd:34:MET:SD	2:Bd:94:HIS:HA	2.58	0.44
2:Bh:81:ILE:HG23	2:Bh:98:VAL:HG11	1.98	0.44
1:Ab:222:LYS:HA	1:Ab:225:THR:HG23	1.98	0.44
1:Ao:116:TRP:HD1	1:Ao:120:GLU:OE1	2.01	0.44
1:Ar:337:ARG:HB2	1:Ar:337:ARG:CZ	2.48	0.44
2:Bl:12:ARG:HH12	2:Bl:14:GLN:HE21	1.65	0.44
3:Cb:27:VAL:HG11	3:Cb:54:VAL:HG21	1.99	0.44
1:Ad:258:GLU:HG2	1:Ad:285:ARG:HH22	1.82	0.44
1:Ag:236:ILE:HD11	1:Ag:317:LEU:HD11	1.99	0.44
1:Ah:104:THR:HG22	2:Bh:5:GLN:HB3	1.99	0.44
1:An:56:ASP:O	1:An:328:VAL:HA	2.17	0.44
1:Ar:68:LEU:HD13	1:Ar:100:LEU:HB3	1.99	0.44
2:Bb:22:LEU:HD22	2:Bb:25:TYR:H	1.82	0.44
3:Cd:1:MET:HA	7:Jh:17:DA:OP1	2.18	0.44
1:Ah:53:PHE:HA	1:Ah:325:GLY:O	2.18	0.44
1:At:234:ALA:HB3	1:At:317:LEU:HD12	2.00	0.44
2:Bb:16:TRP:HB3	2:Bb:49:PRO:HD3	2.00	0.44
2:Bo:53:LEU:HD13	2:Bo:131:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dd:329:ASN:ND2	4:Dd:332:GLU:HB2	2.33	0.44
4:Dj:394:LEU:O	4:Dj:398:VAL:HG22	2.17	0.44
7:Jb:1:DA:N7	7:Jd:31:DA:H1'	2.33	0.44
2:Bb:53:LEU:HD22	2:Bb:80:VAL:HG11	2.00	0.44
2:Bd:22:LEU:HB3	2:Bd:103:ALA:HB3	2.00	0.44
3:Ce:42:VAL:HG11	3:Ce:58:VAL:HG11	1.98	0.44
4:Dc:248:ILE:HD11	4:Dc:259:TRP:CZ3	2.53	0.44
4:Dk:15:PRO:HD2	4:Dl:354:LEU:HD11	1.99	0.44
1:Ab:230:ARG:HG2	1:Ab:385:HIS:CG	2.53	0.43
1:Ac:237:VAL:HG21	1:Ac:241:PHE:HB2	2.00	0.43
1:An:194:LEU:HD21	1:An:388:LYS:HD3	2.00	0.43
1:As:105:TRP:NE1	1:As:371:LEU:HD23	2.33	0.43
2:Bs:22:LEU:HB2	2:Bs:103:ALA:HB3	1.99	0.43
2:Bs:40:TRP:CH2	2:Bs:68:PRO:HD3	2.53	0.43
4:Df:25:LYS:CE	7:Jf:9:DA:H5''	2.46	0.43
4:Dk:394:LEU:O	4:Dk:398:VAL:HG22	2.17	0.43
6:Ji:4:DT:H2'	6:Ji:5:DT:H71	2.00	0.43
1:Ab:255:VAL:HA	1:Ab:282:ILE:HD13	2.00	0.43
1:Ac:15:ARG:HD2	1:Ac:31:ILE:HD13	2.00	0.43
1:Ae:15:ARG:HD3	1:Ae:31:ILE:HD12	2.00	0.43
1:Af:222:LYS:HA	1:Af:225:THR:HG23	2.00	0.43
1:Ah:222:LYS:HA	1:Ah:225:THR:HG23	2.00	0.43
1:Ao:108:LEU:HD23	2:Bn:3:LYS:HE3	2.00	0.43
1:Ap:259:LYS:HB3	1:Ap:261:TRP:CE2	2.53	0.43
2:Bd:30:LEU:HD12	2:Bd:100:LEU:HD11	2.00	0.43
2:Bl:77:VAL:HG11	2:Bl:130:GLN:HB3	2.00	0.43
2:Bn:103:ALA:HA	2:Bn:140:TYR:O	2.19	0.43
4:Di:394:LEU:O	4:Di:398:VAL:HG22	2.18	0.43
7:Jb:26:DA:H2''	7:Jb:27:DA:H8	1.83	0.43
1:Ab:66:TYR:CZ	1:Ab:102:LYS:HE2	2.53	0.43
1:Ak:317:LEU:C	1:Ak:386:ARG:O	2.61	0.43
1:As:181:LEU:HD22	2:Bs:95:ASN:HB3	1.99	0.43
2:Bc:40:TRP:CH2	2:Bc:68:PRO:HD3	2.53	0.43
2:Bs:34:MET:HE2	2:Bs:40:TRP:CE2	2.53	0.43
4:Da:66:GLY:HA2	4:Dl:217:ALA:HB1	2.00	0.43
4:De:76:PHE:CG	4:De:126:GLU:HG2	2.53	0.43
4:Df:364:ASN:HB2	4:Df:365:TRP:CE3	2.53	0.43
6:Ji:13:DT:H2'	6:Ji:14:DT:H71	1.99	0.43
1:Ak:63:LEU:HD13	1:Ak:105:TRP:CZ3	2.54	0.43
1:Ar:116:TRP:CZ2	1:Ar:118:GLU:HB2	2.53	0.43
1:Ar:300:ASP:HB3	1:Ar:302:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:371:LEU:HD12	1:Ar:372:PRO:O	2.19	0.43
4:Dc:293:ALA:HB3	4:Dd:240:MET:HG2	2.01	0.43
4:Df:391:MET:HE2	4:Df:423:LEU:HD22	2.00	0.43
4:Dj:355:TYR:O	4:Dj:359:LYS:HG2	2.18	0.43
1:Ac:115:VAL:HG23	1:Ac:363:ALA:HB2	2.00	0.43
1:Af:59:PHE:HA	1:Af:331:ALA:HB2	2.00	0.43
1:Ah:170:ILE:O	1:Ah:182:LYS:HB2	2.18	0.43
1:Aj:230:ARG:HG2	1:Aj:385:HIS:CG	2.54	0.43
1:Ar:58:THR:O	1:Ar:330:THR:HA	2.19	0.43
1:Ar:177:ASN:HD21	1:Ar:181:LEU:N	2.17	0.43
1:As:255:VAL:HA	1:As:282:ILE:HD13	1.99	0.43
1:As:268:VAL:HG13	1:At:262:VAL:HG12	2.01	0.43
2:Bk:83:MET:HE1	2:Bk:109:VAL:HG22	1.99	0.43
4:Dl:394:LEU:O	4:Dl:398:VAL:HG22	2.18	0.43
1:Ab:108:LEU:H	1:Ab:371:LEU:HD23	1.83	0.43
1:Aj:177:ASN:HD21	1:Aj:181:LEU:N	2.17	0.43
1:Ak:235:ILE:HG23	1:Ak:314:LEU:HD13	2.00	0.43
2:Bc:34:MET:HE2	2:Bc:40:TRP:CE2	2.54	0.43
4:Da:427:ASP:HB3	4:Da:430:ARG:HB3	2.00	0.43
7:Jd:26:DA:H2''	7:Jd:27:DA:H8	1.84	0.43
7:Jj:26:DA:H2''	7:Jj:27:DA:H8	1.84	0.43
1:Ag:256:GLU:HG2	1:Ag:261:TRP:O	2.18	0.43
1:Ak:200:PHE:CD2	1:Ak:392:TYR:HB2	2.53	0.43
1:An:146:TRP:CD1	1:Ao:75:GLN:HA	2.53	0.43
2:Bh:56:VAL:HG21	2:Bh:81:ILE:HD13	2.01	0.43
4:De:346:ARG:NH2	4:Df:81:SER:HA	2.34	0.43
4:Db:427:ASP:HB3	4:Db:430:ARG:HB3	2.00	0.43
1:Aj:73:ALA:HB2	1:Aj:95:VAL:HG12	2.01	0.43
1:An:32:GLN:HB3	2:Bo:6:LEU:HD11	1.99	0.43
1:Ao:63:LEU:HD13	1:Ao:105:TRP:CZ3	2.53	0.43
1:Ar:222:LYS:HA	1:Ar:225:THR:HG23	1.99	0.43
1:As:261:TRP:CD1	1:As:267:THR:HG21	2.54	0.43
2:Bt:30:LEU:HD12	2:Bt:100:LEU:HD11	2.01	0.43
4:Df:411:LEU:O	4:Df:415:LEU:HG	2.18	0.43
4:Dg:421:ARG:NH2	4:Dh:83:LYS:HG3	2.33	0.43
4:Di:15:PRO:HD2	4:Dj:354:LEU:HD11	2.00	0.43
4:Di:279:LEU:HD11	4:Di:285:PHE:HB2	2.01	0.43
6:Ja:4:DT:H2'	6:Ja:5:DT:H71	2.00	0.43
6:Jg:4:DT:H2'	6:Jg:5:DT:H71	2.00	0.43
1:Af:146:TRP:CD1	1:Ag:75:GLN:HA	2.53	0.43
1:Ag:105:TRP:NE1	1:Ag:371:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:222:LYS:HA	1:An:225:THR:HG23	2.00	0.43
1:Ap:105:TRP:CZ2	1:Ap:328:VAL:HB	2.54	0.43
1:Ar:48:LEU:HD12	1:Ar:294:TYR:CD2	2.54	0.43
1:As:164:ARG:HD2	1:As:389:TRP:CZ2	2.54	0.43
2:Bt:85:LEU:HG	2:Bt:99:THR:OG1	2.19	0.43
3:Ca:39:TRP:HZ3	3:Ca:41:VAL:HG23	1.84	0.43
4:Db:217:ALA:HB1	4:Dc:66:GLY:HA2	2.01	0.43
4:Dc:199:VAL:HG13	4:Dc:355:TYR:HB2	2.00	0.43
4:Dg:394:LEU:O	4:Dg:398:VAL:HG22	2.19	0.43
6:Je:4:DT:H2'	6:Je:5:DT:H71	2.00	0.43
7:Jh:1:DA:C8	7:Jj:31:DA:H1'	2.54	0.43
1:Af:189:VAL:HG11	1:Af:192:ILE:HD13	2.01	0.42
1:An:300:ASP:HB3	1:An:302:ASP:OD1	2.19	0.42
1:Ap:234:ALA:HB3	1:Ap:317:LEU:HD12	2.00	0.42
1:Ar:151:MET:HE3	1:Ar:367:GLY:N	2.34	0.42
1:As:67:LEU:HD23	1:As:382:PHE:HE1	1.84	0.42
1:As:95:VAL:HB	2:Br:16:TRP:CE3	2.54	0.42
1:At:258:GLU:CG	1:At:285:ARG:HH22	2.32	0.42
2:Bs:113:ILE:HG22	2:Bs:114:GLU:HG2	2.00	0.42
3:Ca:26:ARG:HB2	3:Ca:71:LEU:HD21	2.01	0.42
3:Ce:1:MET:HA	7:Jj:17:DA:OP1	2.19	0.42
4:Dc:86:VAL:HG23	4:Dc:108:ILE:HG13	2.01	0.42
4:Dc:394:LEU:O	4:Dc:398:VAL:HG22	2.19	0.42
4:Di:168:GLU:HG2	4:Di:169:GLU:HG2	2.01	0.42
4:Dl:215:LEU:O	4:Dl:219:VAL:HG23	2.19	0.42
1:Aa:15:ARG:HD3	1:Aa:31:ILE:HD12	2.00	0.42
1:Ae:10:ALA:O	1:Ae:14:VAL:HG23	2.19	0.42
1:Ah:234:ALA:HB3	1:Ah:317:LEU:HD12	2.00	0.42
1:Ah:249:THR:HA	1:Ah:252:GLN:OE1	2.19	0.42
1:Ak:241:PHE:CZ	1:Ak:245:LEU:HD11	2.54	0.42
1:Ap:222:LYS:HA	1:Ap:225:THR:HG23	2.01	0.42
1:As:218:ARG:HH22	1:As:286:TYR:HB3	1.84	0.42
2:Bb:106:ILE:HG12	2:Bb:140:TYR:CE2	2.54	0.42
2:Bc:83:MET:HE1	2:Bc:109:VAL:HG22	2.01	0.42
2:Bk:113:ILE:HG22	2:Bk:114:GLU:HG2	2.02	0.42
4:Dg:54:ASP:O	4:Dg:58:VAL:HG23	2.19	0.42
4:Dk:76:PHE:CG	4:Dk:126:GLU:HG2	2.55	0.42
1:Ab:48:LEU:HD12	1:Ab:294:TYR:CD2	2.55	0.42
1:An:25:PHE:CE2	1:Ao:341:VAL:HG21	2.54	0.42
1:As:48:LEU:HG	1:As:52:PHE:HE2	1.84	0.42
4:De:306:ALA:O	4:De:310:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dg:196:TRP:CZ3	4:Dg:197:LYS:HD3	2.54	0.42
1:Af:271:PRO:HG2	1:Af:274:VAL:HG23	2.02	0.42
1:Ah:245:LEU:HD22	1:Ah:251:VAL:HG21	2.02	0.42
1:Ao:196:LEU:HD23	1:Ao:196:LEU:HA	1.78	0.42
2:Bh:34:MET:HE3	2:Bh:40:TRP:CG	2.53	0.42
2:Bk:136:ILE:HB	2:Bk:141:PHE:CE1	2.55	0.42
2:Bo:21:ARG:HD2	2:Bo:27:VAL:HG11	2.00	0.42
4:Dd:76:PHE:CD1	4:Dd:126:GLU:HG2	2.55	0.42
1:Ac:146:TRP:O	1:Ac:150:ARG:HG2	2.18	0.42
1:Ad:262:VAL:HG23	1:Ad:266:ASN:H	1.84	0.42
1:Af:107:PRO:HG3	1:Af:330:THR:HG21	2.02	0.42
1:Ai:10:ALA:O	1:Ai:14:VAL:HG23	2.19	0.42
1:Ak:15:ARG:HD2	1:Ak:31:ILE:HD13	2.00	0.42
1:Ak:155:ARG:HG3	1:Ak:327:PHE:CZ	2.55	0.42
1:Ak:233:VAL:HG22	1:Ak:318:ASN:O	2.20	0.42
1:An:113:SER:HB2	1:Ao:88:SER:OG	2.19	0.42
1:Ao:237:VAL:HG21	1:Ao:241:PHE:HB2	2.01	0.42
2:Bc:83:MET:HG3	2:Bc:142:PHE:CZ	2.54	0.42
4:Dd:258:GLN:HG2	5:Ec:117:THR:OG1	2.19	0.42
4:De:76:PHE:CD1	4:De:126:GLU:HG2	2.55	0.42
4:De:340:THR:O	4:De:344:LEU:HG	2.20	0.42
4:Di:355:TYR:O	4:Di:359:LYS:HG2	2.19	0.42
1:Ag:164:ARG:HD2	1:Ag:389:TRP:CZ2	2.54	0.42
1:Al:222:LYS:HA	1:Al:225:THR:HG23	2.02	0.42
1:An:58:THR:HG21	1:An:63:LEU:HD11	2.02	0.42
1:Ao:146:TRP:O	1:Ao:150:ARG:HG2	2.19	0.42
1:Ao:358:ASP:HB3	1:Ao:359:PRO:HD3	2.02	0.42
1:Ar:248:ASN:O	1:Ar:252:GLN:HG3	2.19	0.42
4:Db:46:PHE:CZ	4:Dc:61:LYS:HG2	2.54	0.42
4:Dd:103:HIS:CE1	4:Dd:108:ILE:HB	2.55	0.42
4:Df:394:LEU:O	4:Df:398:VAL:HG22	2.19	0.42
1:Ag:58:THR:N	1:Ag:345:THR:HG21	2.35	0.42
1:Ah:83:GLN:HB3	2:Bg:31:PRO:HB3	2.01	0.42
1:An:104:THR:OG1	2:Bm:5:GLN:HB3	2.19	0.42
1:Ao:155:ARG:HG3	1:Ao:327:PHE:CZ	2.54	0.42
1:As:176:TYR:CZ	1:At:77:GLY:HA2	2.54	0.42
2:Br:22:LEU:HD22	2:Br:25:TYR:H	1.83	0.42
4:Dc:76:PHE:CG	4:Dc:126:GLU:HG2	2.55	0.42
4:De:364:ASN:HB2	4:De:365:TRP:CE3	2.54	0.42
6:Jc:4:DT:H2'	6:Jc:5:DT:H71	2.01	0.42
1:Ac:336:GLN:HG2	3:Ca:11:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:68:LEU:HD13	1:An:100:LEU:HB3	2.01	0.42
1:As:146:TRP:O	1:As:150:ARG:HG2	2.20	0.42
1:As:255:VAL:HG22	1:As:282:ILE:HD12	2.01	0.42
2:Bp:81:ILE:HG23	2:Bp:98:VAL:HG11	2.02	0.42
2:Bs:41:GLY:O	2:Bs:45:ALA:HB2	2.20	0.42
4:Dc:203:HIS:NE2	4:Dc:214:ALA:HB2	2.35	0.42
4:Dg:85:TYR:HA	4:Dg:108:ILE:HG21	2.00	0.42
1:Ac:118:GLU:HB2	1:Ac:360:PRO:HG2	2.02	0.42
1:An:66:TYR:CZ	1:An:102:LYS:HE2	2.55	0.42
1:Ao:348:TYR:CD1	3:Cd:13:GLN:HG2	2.55	0.42
1:Ar:40:ASP:OD2	1:Ar:299:ARG:HG3	2.20	0.42
2:Bf:102:ALA:HB3	2:Bf:142:PHE:CZ	2.55	0.42
2:Bh:22:LEU:HB3	2:Bh:103:ALA:HB3	2.00	0.42
2:Bh:34:MET:SD	2:Bh:94:HIS:HA	2.60	0.42
2:Bn:136:ILE:HB	2:Bn:141:PHE:CE1	2.55	0.42
2:Bo:22:LEU:HB2	2:Bo:103:ALA:HB3	2.01	0.42
4:De:62:MET:SD	4:De:219:VAL:HG22	2.59	0.42
4:Dh:355:TYR:O	4:Dh:359:LYS:HG2	2.20	0.42
4:Dj:176:LYS:HE3	4:Dj:176:LYS:HB2	1.90	0.42
1:Ab:56:ASP:O	1:Ab:328:VAL:HA	2.19	0.42
1:Ac:13:ARG:NH1	1:Ae:12:ALA:HB1	2.35	0.42
1:Af:371:LEU:HD12	1:Af:372:PRO:O	2.20	0.42
1:Ag:146:TRP:O	1:Ag:150:ARG:HG2	2.20	0.42
1:Ak:146:TRP:O	1:Ak:150:ARG:HG2	2.19	0.42
1:Ak:255:VAL:HG22	1:Ak:282:ILE:HD12	2.01	0.42
1:An:371:LEU:HD12	1:An:372:PRO:O	2.20	0.42
1:Ar:49:VAL:HG23	1:Ar:163:MET:SD	2.59	0.42
1:Ar:377:TYR:HB2	2:Bq:7:PHE:HE2	1.85	0.42
1:As:256:GLU:HG3	1:As:261:TRP:HB2	2.01	0.42
2:Bs:54:VAL:HG12	2:Bs:68:PRO:HA	2.02	0.42
4:Di:215:LEU:O	4:Di:219:VAL:HG23	2.19	0.42
4:Dk:364:ASN:HB2	4:Dk:365:TRP:CE3	2.55	0.42
7:Jf:26:DA:H2"	7:Jf:27:DA:H8	1.84	0.42
1:Am:10:ALA:O	1:Am:14:VAL:HG23	2.19	0.41
4:Da:81:SER:HA	4:Dl:346:ARG:NH2	2.35	0.41
4:Db:254:GLN:HG2	4:Db:259:TRP:CE2	2.55	0.41
4:Di:419:MET:O	4:Di:423:LEU:HG	2.20	0.41
4:Dk:355:TYR:O	4:Dk:359:LYS:HG2	2.19	0.41
6:Je:23:DT:C6	6:Je:24:DT:H72	2.55	0.41
1:Af:177:ASN:HD21	1:Af:181:LEU:N	2.17	0.41
1:Aj:120:GLU:HB2	3:Cc:31:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:235:ILE:HA	1:Ao:315:ILE:O	2.20	0.41
2:Bb:29:ALA:HB2	2:Bb:99:THR:HG22	2.02	0.41
2:Bt:81:ILE:HG23	2:Bt:98:VAL:HG11	2.02	0.41
4:Da:178:SER:HA	4:Da:189:SER:HA	2.01	0.41
4:Dd:103:HIS:NE2	4:Dd:108:ILE:HB	2.35	0.41
4:Dg:427:ASP:HB3	4:Dg:430:ARG:HB3	2.02	0.41
6:Jg:23:DT:C6	6:Jg:24:DT:H72	2.55	0.41
1:Ab:110:PHE:CZ	1:Ab:158:LEU:HD11	2.55	0.41
1:Ac:59:PHE:CE2	1:Ac:344:ALA:HA	2.56	0.41
1:Ae:11:LEU:HD21	1:Af:68:LEU:HB2	2.02	0.41
1:Ah:196:LEU:HD21	1:Ah:199:LYS:HA	2.01	0.41
1:Aj:146:TRP:CD1	1:Ak:75:GLN:HA	2.55	0.41
1:Aj:270:PRO:HG2	1:Aj:275:TYR:CE2	2.55	0.41
1:Ao:115:VAL:HG23	1:Ao:363:ALA:HB2	2.02	0.41
1:Ap:314:LEU:HD23	1:Ap:392:TYR:CD1	2.56	0.41
2:Bc:30:LEU:HD23	2:Bc:30:LEU:HA	1.90	0.41
2:Bf:132:LYS:HE2	2:Bf:132:LYS:HB2	1.88	0.41
2:Bg:81:ILE:HD12	2:Bg:81:ILE:HA	1.93	0.41
2:Bk:40:TRP:CH2	2:Bk:68:PRO:HD3	2.55	0.41
2:Bo:1:MET:HG2	2:Bo:3:LYS:H	1.84	0.41
4:Db:355:TYR:O	4:Db:359:LYS:HG2	2.20	0.41
4:Dh:411:LEU:O	4:Dh:415:LEU:HG	2.19	0.41
7:Jj:28:DA:H2''	7:Jj:29:DA:H8	1.85	0.41
1:Af:113:SER:HB2	1:Ag:88:SER:OG	2.20	0.41
1:Af:248:ASN:O	1:Af:252:GLN:HG3	2.21	0.41
1:Ak:237:VAL:O	1:Ak:293:VAL:HA	2.21	0.41
1:Al:170:ILE:O	1:Al:182:LYS:HB2	2.20	0.41
2:Bl:34:MET:HE3	2:Bl:40:TRP:CG	2.56	0.41
2:Bq:14:GLN:HE21	2:Bq:14:GLN:HB3	1.63	0.41
4:Da:310:ARG:HG2	4:Db:321:LEU:HD11	2.01	0.41
4:Di:62:MET:SD	4:Di:219:VAL:HG22	2.60	0.41
7:Jb:1:DA:C8	7:Jd:31:DA:H1'	2.55	0.41
1:Ab:177:ASN:HD21	1:Ab:181:LEU:N	2.18	0.41
1:Al:82:HIS:CG	1:Al:83:GLN:N	2.89	0.41
1:As:115:VAL:HG23	1:As:363:ALA:HB2	2.02	0.41
2:Bg:54:VAL:HG12	2:Bg:68:PRO:HA	2.02	0.41
2:Bk:54:VAL:HG12	2:Bk:68:PRO:HA	2.01	0.41
2:Br:136:ILE:HB	2:Br:141:PHE:CE1	2.56	0.41
2:Bs:128:ALA:HB1	2:Bs:133:LEU:HB2	2.02	0.41
4:De:394:LEU:O	4:De:398:VAL:HG22	2.20	0.41
1:Ab:107:PRO:HG3	1:Ab:330:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:13:ARG:NH1	1:Aq:12:ALA:HB1	2.36	0.41
1:Ao:106:SER:O	2:Bn:3:LYS:HB3	2.20	0.41
1:Ao:214:ILE:HG22	1:Ao:218:ARG:HH12	1.84	0.41
1:At:196:LEU:HD23	1:At:199:LYS:HG2	2.02	0.41
2:Bh:82:GLY:HA2	2:Bh:144:TYR:CE2	2.56	0.41
3:Ce:27:VAL:HG11	3:Ce:54:VAL:HG21	2.02	0.41
4:Da:157:HIS:CE1	4:Da:159:PHE:CD2	3.09	0.41
4:Da:394:LEU:O	4:Da:398:VAL:HG22	2.21	0.41
4:De:234:HIS:ND1	4:Df:273:PRO:HG3	2.36	0.41
4:Dh:346:ARG:NH2	4:Di:81:SER:HA	2.34	0.41
7:Jf:28:DA:H2''	7:Jf:29:DA:H8	1.85	0.41
1:Ag:222:LYS:HA	1:Ag:225:THR:HG23	2.03	0.41
1:Al:258:GLU:CG	1:Al:285:ARG:HH22	2.34	0.41
1:An:181:LEU:HD12	1:Ao:81:VAL:HG12	2.02	0.41
1:Ao:235:ILE:HG23	1:Ao:314:LEU:HD13	2.02	0.41
1:Ap:262:VAL:HG23	1:Ap:266:ASN:H	1.86	0.41
1:Aq:3:VAL:HG21	1:Ar:98:VAL:HG21	2.01	0.41
1:Ar:318:ASN:HD21	1:Ar:388:LYS:HD2	1.86	0.41
1:As:241:PHE:CZ	1:As:245:LEU:HD11	2.55	0.41
2:Bh:43:TRP:CD2	2:Bh:113:ILE:HD11	2.55	0.41
2:Bj:103:ALA:HA	2:Bj:140:TYR:O	2.20	0.41
2:Bm:12:ARG:HH21	2:Bm:14:GLN:NE2	2.18	0.41
2:Bo:40:TRP:CH2	2:Bo:68:PRO:HD3	2.55	0.41
3:Ca:29:ALA:HB1	3:Ca:63:TRP:HB3	2.02	0.41
3:Cd:27:VAL:HG11	3:Cd:54:VAL:HG21	2.03	0.41
4:Dk:90:SER:HB2	4:Dk:95:ASP:OD2	2.20	0.41
6:Ja:23:DT:C6	6:Ja:24:DT:H72	2.55	0.41
1:Al:68:LEU:HD12	1:Al:99:ASP:O	2.20	0.41
1:Ao:200:PHE:CE2	1:Ao:213:PRO:HB3	2.56	0.41
1:Ar:352:LYS:HB3	1:Ar:352:LYS:HE3	1.92	0.41
1:As:235:ILE:HA	1:As:315:ILE:O	2.21	0.41
2:Bc:128:ALA:HB1	2:Bc:133:LEU:HB2	2.02	0.41
2:Bg:34:MET:HE2	2:Bg:40:TRP:CD2	2.55	0.41
3:Cd:26:ARG:HB2	3:Cd:71:LEU:HD21	2.02	0.41
4:Dc:411:LEU:O	4:Dc:415:LEU:HG	2.21	0.41
4:Dl:199:VAL:HG13	4:Dl:355:TYR:HB2	2.01	0.41
4:Dl:279:LEU:HD11	4:Dl:285:PHE:HB2	2.03	0.41
7:Jb:28:DA:H2''	7:Jb:29:DA:H8	1.85	0.41
6:Jc:23:DT:C6	6:Jc:24:DT:H72	2.55	0.41
1:Af:300:ASP:HB3	1:Af:302:ASP:OD1	2.21	0.41
1:Ai:5:ILE:HD12	1:Ai:5:ILE:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:15:ARG:HD3	1:Ai:31:ILE:HD12	2.03	0.41
1:Aj:116:TRP:CZ2	1:Aj:118:GLU:HB2	2.56	0.41
1:Ak:13:ARG:HB2	1:Am:17:PRO:HB3	2.02	0.41
1:Ak:113:SER:O	1:Al:90:PRO:HA	2.21	0.41
1:Ak:237:VAL:HG21	1:Ak:241:PHE:HB2	2.02	0.41
1:Al:262:VAL:HG23	1:Al:266:ASN:H	1.86	0.41
1:Ao:59:PHE:CE1	4:Di:189:SER:HB3	2.56	0.41
1:Ar:235:ILE:HG23	1:Ar:314:LEU:HD13	2.02	0.41
1:As:222:LYS:HA	1:As:225:THR:HG23	2.03	0.41
2:Bl:102:ALA:HB3	2:Bl:142:PHE:CZ	2.56	0.41
3:Cc:26:ARG:HB2	3:Cc:71:LEU:HD21	2.03	0.41
4:Db:54:ASP:O	4:Db:58:VAL:HG23	2.21	0.41
4:Dc:76:PHE:CD1	4:Dc:126:GLU:HG2	2.55	0.41
4:De:254:GLN:HG2	4:De:259:TRP:CZ2	2.56	0.41
4:Dj:76:PHE:CD1	4:Dj:126:GLU:HG2	2.56	0.41
7:Jh:28:DA:H2"	7:Jh:29:DA:H8	1.85	0.41
6:Ji:23:DT:C6	6:Ji:24:DT:H72	2.55	0.41
1:Ab:371:LEU:HD12	1:Ab:372:PRO:O	2.21	0.41
1:Ac:246:ALA:HB2	1:Ac:276:ARG:HA	2.01	0.41
1:Aj:176:TYR:CZ	1:Ak:77:GLY:HA2	2.55	0.41
1:Al:68:LEU:HD12	1:Al:100:LEU:HB3	2.03	0.41
1:Ar:58:THR:HG21	1:Ar:63:LEU:HD11	2.03	0.41
4:Dc:427:ASP:HB3	4:Dc:430:ARG:HB3	2.03	0.41
4:De:103:HIS:NE2	4:De:108:ILE:HB	2.36	0.41
4:De:310:ARG:HG2	4:Df:321:LEU:HD11	2.02	0.41
1:Ab:164:ARG:HA	1:Ab:389:TRP:CZ2	2.56	0.40
1:Ab:271:PRO:HG2	1:Ab:274:VAL:HG23	2.02	0.40
1:Ak:13:ARG:HB3	1:Am:15:ARG:O	2.21	0.40
1:Al:249:THR:HA	1:Al:252:GLN:OE1	2.21	0.40
1:An:108:LEU:H	1:An:371:LEU:HD23	1.85	0.40
1:Ao:256:GLU:HG2	1:Ao:261:TRP:O	2.21	0.40
1:As:290:GLU:OE2	1:As:292:MET:HB2	2.21	0.40
1:At:68:LEU:HD12	1:At:100:LEU:HB3	2.03	0.40
1:At:222:LYS:HA	1:At:225:THR:HG23	2.03	0.40
2:Bb:146:ARG:HD2	2:Bs:146:ARG:HH12	1.86	0.40
2:Bd:14:GLN:HE21	2:Bd:14:GLN:HB3	1.75	0.40
2:Bg:40:TRP:CH2	2:Bg:68:PRO:HD3	2.56	0.40
2:Bt:106:ILE:HG23	2:Bt:138:GLY:C	2.46	0.40
4:Dc:346:ARG:NH2	4:Dd:81:SER:HA	2.36	0.40
4:Dj:427:ASP:HB3	4:Dj:430:ARG:HB3	2.02	0.40
1:Ah:208:ASN:HA	1:Ah:249:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:271:PRO:HG2	1:Aj:274:VAL:HG23	2.02	0.40
1:An:107:PRO:HG3	1:An:330:THR:HG21	2.04	0.40
1:Ao:13:ARG:HB3	1:Aq:15:ARG:O	2.22	0.40
2:Bl:106:ILE:HG23	2:Bl:138:GLY:C	2.46	0.40
4:Dl:364:ASN:HB2	4:Dl:365:TRP:CE3	2.56	0.40
4:Dl:411:LEU:O	4:Dl:415:LEU:HG	2.21	0.40
7:Jd:28:DA:H2"	7:Jd:29:DA:H8	1.85	0.40
1:Ab:333:VAL:HG11	1:As:355:LEU:HD22	2.04	0.40
1:Ad:170:ILE:O	1:Ad:182:LYS:HB2	2.21	0.40
1:Ag:196:LEU:HD23	1:Ag:196:LEU:HA	1.80	0.40
1:Ag:337:ARG:HG3	1:Ag:337:ARG:HH11	1.86	0.40
1:Ak:95:VAL:HB	2:Bj:16:TRP:CE3	2.56	0.40
1:Ak:318:ASN:ND2	1:Ak:385:HIS:O	2.54	0.40
1:Al:238:GLY:HA2	1:Al:294:TYR:O	2.21	0.40
1:Al:259:LYS:HB3	1:Al:261:TRP:CE2	2.57	0.40
1:Ao:46:ASN:HB2	1:Ao:308:TRP:CE2	2.56	0.40
1:As:10:ALA:O	1:As:14:VAL:HG23	2.21	0.40
1:At:99:ASP:OD1	2:Bt:9:THR:HG23	2.22	0.40
2:Bc:71:LEU:HD21	2:Bc:111:GLN:HG2	2.03	0.40
2:Bj:105:PRO:HB2	2:Bj:108:TYR:CD2	2.55	0.40
2:Bo:34:MET:HE2	2:Bo:40:TRP:CD2	2.56	0.40
4:De:411:LEU:O	4:De:415:LEU:HG	2.21	0.40
1:Ab:235:ILE:HG23	1:Ab:314:LEU:HD13	2.03	0.40
1:Ad:183:TYR:HB3	2:Bd:2:ASP:OD2	2.22	0.40
1:Ag:45:GLU:HG2	1:Ag:156:ARG:NH1	2.36	0.40
1:Ak:155:ARG:HG3	1:Ak:327:PHE:CE2	2.56	0.40
1:Ao:229:ASP:HA	1:Ao:319:GLN:CD	2.47	0.40
2:Bn:22:LEU:HD22	2:Bn:25:TYR:H	1.86	0.40
2:Bo:54:VAL:HG12	2:Bo:68:PRO:HA	2.02	0.40
3:Cb:42:VAL:HG11	3:Cb:58:VAL:HG11	2.02	0.40
4:Dc:62:MET:HG2	4:Dc:222:TRP:CD2	2.56	0.40
4:Dc:391:MET:HE2	4:Dc:423:LEU:HD22	2.04	0.40
4:Dh:263:LYS:HA	4:Di:278:ILE:HD11	2.03	0.40
4:Dk:203:HIS:NE2	4:Dk:214:ALA:HB2	2.36	0.40
7:Jh:26:DA:H2"	7:Jh:27:DA:H8	1.83	0.40
1:Ab:113:SER:HB2	1:Ac:88:SER:OG	2.22	0.40
1:Ab:155:ARG:HG3	1:Ab:327:PHE:CZ	2.56	0.40
1:Ac:67:LEU:HD23	1:Ac:382:PHE:CE1	2.56	0.40
1:Aj:400:LEU:HD13	1:Aj:400:LEU:HA	1.87	0.40
1:Ak:218:ARG:NH2	1:Ak:286:TYR:HB3	2.36	0.40
1:Ak:256:GLU:HG2	1:Ak:261:TRP:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:168:ILE:HG12	1:Al:185:ILE:HB	2.04	0.40
1:An:40:ASP:OD2	1:An:299:ARG:HG3	2.21	0.40
1:An:55:GLU:HG3	1:An:329:TYR:CE2	2.57	0.40
1:Ao:150:ARG:HD2	1:Ap:77:GLY:C	2.46	0.40
1:As:200:PHE:CD2	1:As:392:TYR:HB2	2.56	0.40
2:Ba:14:GLN:HE21	2:Ba:14:GLN:HB3	1.64	0.40
4:Dd:364:ASN:HB2	4:Dd:365:TRP:CE3	2.57	0.40
6:Ja:1:DT:H6	6:Ja:1:DT:H2'	1.71	0.40
6:Ji:5:DT:H2'	6:Ji:6:DT:H71	2.03	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	Aa	36/409 (9%)	33 (92%)	3 (8%)	0	100	100
1	Ab	376/409 (92%)	364 (97%)	12 (3%)	0	100	100
1	Ac	407/409 (100%)	396 (97%)	11 (3%)	0	100	100
1	Ad	221/409 (54%)	217 (98%)	4 (2%)	0	100	100
1	Ae	36/409 (9%)	33 (92%)	3 (8%)	0	100	100
1	Af	376/409 (92%)	360 (96%)	16 (4%)	0	100	100
1	Ag	407/409 (100%)	397 (98%)	10 (2%)	0	100	100
1	Ah	221/409 (54%)	218 (99%)	3 (1%)	0	100	100
1	Ai	36/409 (9%)	33 (92%)	3 (8%)	0	100	100
1	Aj	376/409 (92%)	360 (96%)	16 (4%)	0	100	100
1	Ak	407/409 (100%)	400 (98%)	7 (2%)	0	100	100
1	Al	221/409 (54%)	217 (98%)	4 (2%)	0	100	100
1	Am	36/409 (9%)	33 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	An	376/409 (92%)	360 (96%)	16 (4%)	0	100	100
1	Ao	407/409 (100%)	397 (98%)	10 (2%)	0	100	100
1	Ap	221/409 (54%)	218 (99%)	3 (1%)	0	100	100
1	Aq	36/409 (9%)	33 (92%)	3 (8%)	0	100	100
1	Ar	376/409 (92%)	359 (96%)	17 (4%)	0	100	100
1	As	407/409 (100%)	396 (97%)	11 (3%)	0	100	100
1	At	221/409 (54%)	215 (97%)	6 (3%)	0	100	100
2	Ba	22/146 (15%)	21 (96%)	1 (4%)	0	100	100
2	Bb	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	Bc	144/146 (99%)	144 (100%)	0	0	100	100
2	Bd	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	Be	22/146 (15%)	21 (96%)	1 (4%)	0	100	100
2	Bf	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	Bg	144/146 (99%)	144 (100%)	0	0	100	100
2	Bh	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	Bi	22/146 (15%)	21 (96%)	1 (4%)	0	100	100
2	Bj	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	Bk	144/146 (99%)	144 (100%)	0	0	100	100
2	Bl	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	Bm	22/146 (15%)	21 (96%)	1 (4%)	0	100	100
2	Bn	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	Bo	144/146 (99%)	144 (100%)	0	0	100	100
2	Bp	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	Bq	22/146 (15%)	21 (96%)	1 (4%)	0	100	100
2	Br	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	Bs	144/146 (99%)	144 (100%)	0	0	100	100
2	Bt	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
3	Ca	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
3	Cb	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
3	Cc	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
3	Cd	71/73 (97%)	67 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ce	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
4	Da	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
4	Db	421/448 (94%)	419 (100%)	2 (0%)	0	100	100
4	Dc	421/448 (94%)	418 (99%)	3 (1%)	0	100	100
4	Dd	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
4	De	421/448 (94%)	416 (99%)	5 (1%)	0	100	100
4	Df	421/448 (94%)	416 (99%)	5 (1%)	0	100	100
4	Dg	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
4	Dh	421/448 (94%)	420 (100%)	1 (0%)	0	100	100
4	Di	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
4	Dj	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
4	Dk	421/448 (94%)	419 (100%)	2 (0%)	0	100	100
4	Dl	421/448 (94%)	416 (99%)	5 (1%)	0	100	100
5	Ea	12/130 (9%)	12 (100%)	0	0	100	100
5	Eb	12/130 (9%)	12 (100%)	0	0	100	100
5	Ec	12/130 (9%)	11 (92%)	1 (8%)	0	100	100
5	Ed	12/130 (9%)	12 (100%)	0	0	100	100
5	Ee	12/130 (9%)	12 (100%)	0	0	100	100
5	Ef	12/130 (9%)	12 (100%)	0	0	100	100
5	Eg	12/130 (9%)	12 (100%)	0	0	100	100
5	Eh	12/130 (9%)	12 (100%)	0	0	100	100
5	Ei	12/130 (9%)	12 (100%)	0	0	100	100
5	Ej	12/130 (9%)	12 (100%)	0	0	100	100
5	Ek	12/130 (9%)	12 (100%)	0	0	100	100
5	El	12/130 (9%)	12 (100%)	0	0	100	100
All	All	13021/18401 (71%)	12770 (98%)	251 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	31/352 (9%)	31 (100%)	0	100	100
1	Ab	330/352 (94%)	330 (100%)	0	100	100
1	Ac	352/352 (100%)	352 (100%)	0	100	100
1	Ad	204/352 (58%)	204 (100%)	0	100	100
1	Ae	31/352 (9%)	31 (100%)	0	100	100
1	Af	330/352 (94%)	330 (100%)	0	100	100
1	Ag	352/352 (100%)	352 (100%)	0	100	100
1	Ah	204/352 (58%)	204 (100%)	0	100	100
1	Ai	31/352 (9%)	31 (100%)	0	100	100
1	Aj	330/352 (94%)	330 (100%)	0	100	100
1	Ak	352/352 (100%)	352 (100%)	0	100	100
1	Al	204/352 (58%)	204 (100%)	0	100	100
1	Am	31/352 (9%)	31 (100%)	0	100	100
1	An	330/352 (94%)	330 (100%)	0	100	100
1	Ao	352/352 (100%)	352 (100%)	0	100	100
1	Ap	204/352 (58%)	204 (100%)	0	100	100
1	Aq	31/352 (9%)	31 (100%)	0	100	100
1	Ar	330/352 (94%)	330 (100%)	0	100	100
1	As	352/352 (100%)	352 (100%)	0	100	100
1	At	204/352 (58%)	204 (100%)	0	100	100
2	Ba	23/123 (19%)	23 (100%)	0	100	100
2	Bb	123/123 (100%)	123 (100%)	0	100	100
2	Bc	123/123 (100%)	123 (100%)	0	100	100
2	Bd	123/123 (100%)	123 (100%)	0	100	100
2	Be	23/123 (19%)	23 (100%)	0	100	100
2	Bf	123/123 (100%)	123 (100%)	0	100	100
2	Bg	123/123 (100%)	123 (100%)	0	100	100
2	Bh	123/123 (100%)	123 (100%)	0	100	100
2	Bi	23/123 (19%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bj	123/123 (100%)	123 (100%)	0	100	100
2	Bk	123/123 (100%)	123 (100%)	0	100	100
2	Bl	123/123 (100%)	123 (100%)	0	100	100
2	Bm	23/123 (19%)	23 (100%)	0	100	100
2	Bn	123/123 (100%)	123 (100%)	0	100	100
2	Bo	123/123 (100%)	123 (100%)	0	100	100
2	Bp	123/123 (100%)	123 (100%)	0	100	100
2	Bq	23/123 (19%)	23 (100%)	0	100	100
2	Br	123/123 (100%)	123 (100%)	0	100	100
2	Bs	123/123 (100%)	123 (100%)	0	100	100
2	Bt	123/123 (100%)	123 (100%)	0	100	100
3	Ca	62/62 (100%)	62 (100%)	0	100	100
3	Cb	62/62 (100%)	62 (100%)	0	100	100
3	Cc	62/62 (100%)	62 (100%)	0	100	100
3	Cd	62/62 (100%)	62 (100%)	0	100	100
3	Ce	62/62 (100%)	62 (100%)	0	100	100
4	Da	352/374 (94%)	352 (100%)	0	100	100
4	Db	352/374 (94%)	352 (100%)	0	100	100
4	Dc	352/374 (94%)	352 (100%)	0	100	100
4	Dd	352/374 (94%)	352 (100%)	0	100	100
4	De	352/374 (94%)	352 (100%)	0	100	100
4	Df	352/374 (94%)	352 (100%)	0	100	100
4	Dg	352/374 (94%)	352 (100%)	0	100	100
4	Dh	352/374 (94%)	352 (100%)	0	100	100
4	Di	352/374 (94%)	352 (100%)	0	100	100
4	Dj	352/374 (94%)	352 (100%)	0	100	100
4	Dk	352/374 (94%)	352 (100%)	0	100	100
4	Dl	352/374 (94%)	352 (100%)	0	100	100
5	Ea	12/105 (11%)	12 (100%)	0	100	100
5	Eb	12/105 (11%)	12 (100%)	0	100	100
5	Ec	12/105 (11%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Ed	12/105 (11%)	12 (100%)	0	100	100
5	Ee	12/105 (11%)	12 (100%)	0	100	100
5	Ef	12/105 (11%)	12 (100%)	0	100	100
5	Eg	12/105 (11%)	12 (100%)	0	100	100
5	Eh	12/105 (11%)	12 (100%)	0	100	100
5	Ei	12/105 (11%)	12 (100%)	0	100	100
5	Ej	12/105 (11%)	12 (100%)	0	100	100
5	Ek	12/105 (11%)	12 (100%)	0	100	100
5	El	12/105 (11%)	12 (100%)	0	100	100
All	All	11223/15558 (72%)	11223 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ab	177	ASN
1	Ab	208	ASN
1	Ab	248	ASN
1	Ab	318	ASN
1	Ac	71	GLN
1	Ac	179	ASN
1	Ac	319	GLN
1	Ad	198	GLN
1	Af	208	ASN
1	Af	248	ASN
1	Ag	71	GLN
1	Ag	265	GLN
1	Ah	198	GLN
1	Aj	6	ASN
1	Aj	208	ASN
1	Aj	248	ASN
1	Aj	354	HIS
1	Ak	139	GLN
1	Ak	179	ASN
1	Ak	265	GLN
1	Al	198	GLN
1	Al	318	ASN
1	Al	319	GLN

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Mol	Chain	Res	Type
1	An	208	ASN
1	An	248	ASN
1	Ao	139	GLN
1	Ao	179	ASN
1	Ao	265	GLN
1	Ao	338	ASN
1	Ap	198	GLN
1	Ar	137	ASN
1	Ar	208	ASN
1	Ar	248	ASN
1	As	179	ASN
1	As	338	ASN
1	At	318	ASN
2	Ba	14	GLN
2	Bb	126	ASN
2	Bf	126	ASN
2	Bg	139	HIS
2	Bh	23	HIS
2	Bh	48	HIS
2	Bh	79	ASN
2	Bj	14	GLN
2	Bj	126	ASN
2	Bk	88	HIS
2	Bl	14	GLN
2	Bl	48	HIS
2	Bl	79	ASN
2	Bn	126	ASN
2	Bo	88	HIS
2	Bp	23	HIS
2	Bq	14	GLN
2	Br	126	ASN
2	Bs	139	HIS
3	Ca	52	GLN
3	Ca	56	GLN
3	Cb	52	GLN
3	Cb	56	GLN
3	Cc	52	GLN
3	Cc	56	GLN
3	Cd	52	GLN
3	Cd	56	GLN
4	Da	268	ASN
4	Db	271	GLN

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Mol	Chain	Res	Type
4	Dc	271	GLN
4	Dd	212	GLN
4	Dd	234	HIS
4	Dd	268	ASN
4	Dd	345	GLN
4	De	275	HIS
4	Df	234	HIS
4	Dg	186	GLN
4	Dg	258	GLN
4	Dg	275	HIS
4	Di	234	HIS
4	Di	345	GLN
4	Dj	234	HIS
4	Dj	268	ASN
4	Dj	271	GLN
4	Dk	271	GLN
4	Dl	275	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

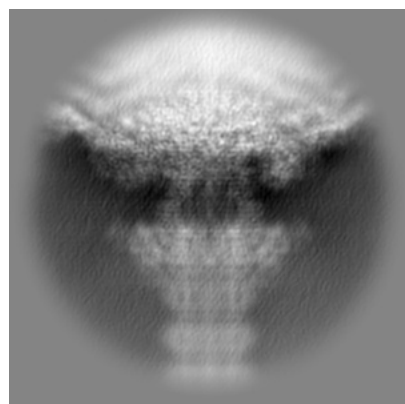
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70280. These allow visual inspection of the internal detail of the map and identification of artifacts.

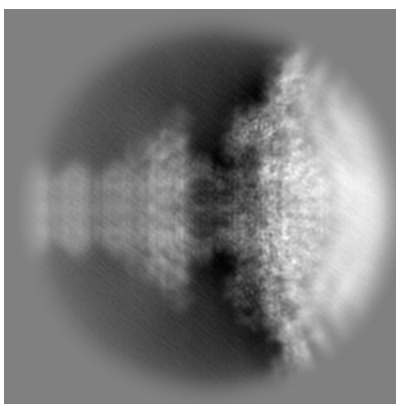
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

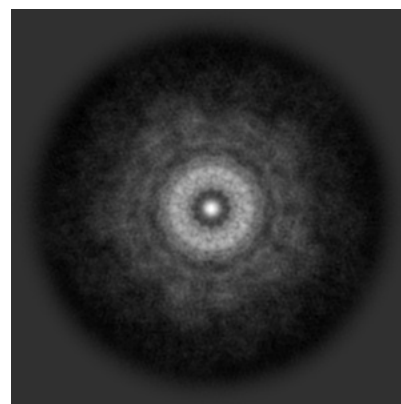
#### 6.1.1 Primary map



X

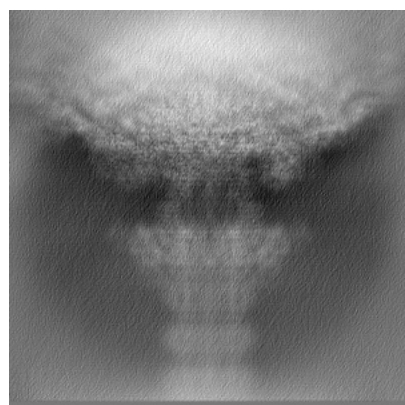


Y

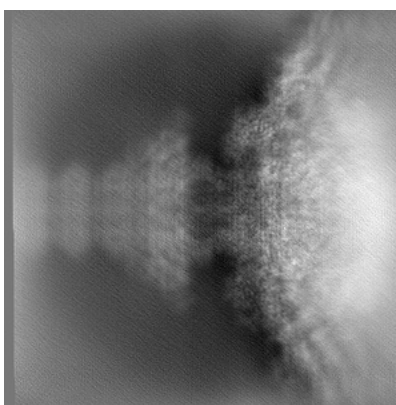


Z

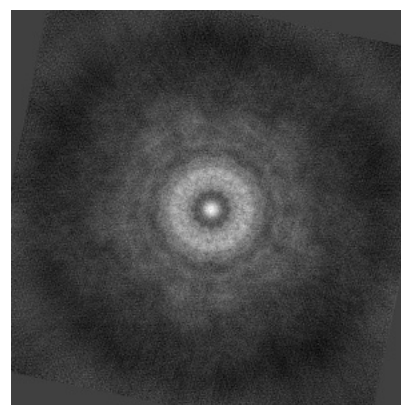
#### 6.1.2 Raw map



X



Y

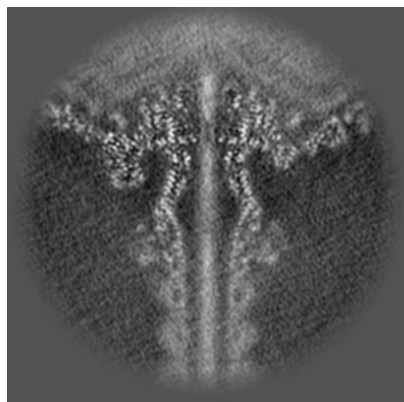


Z

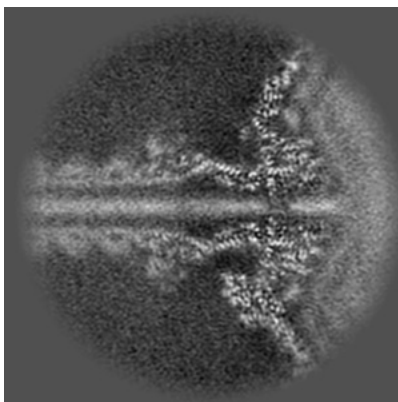
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

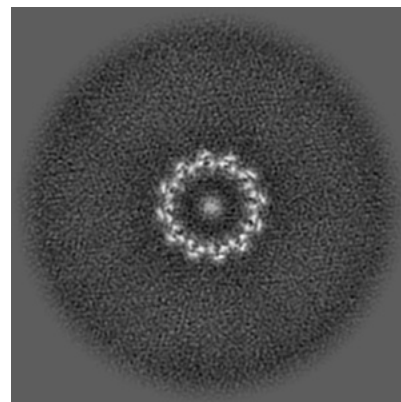
### 6.2.1 Primary map



X Index: 180



Y Index: 180

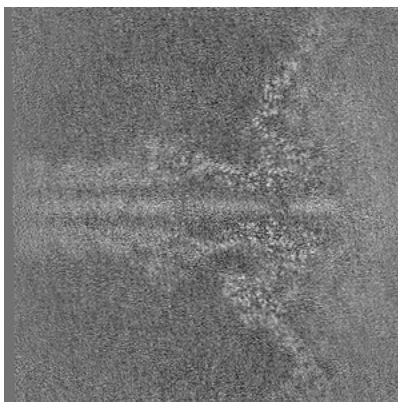


Z Index: 180

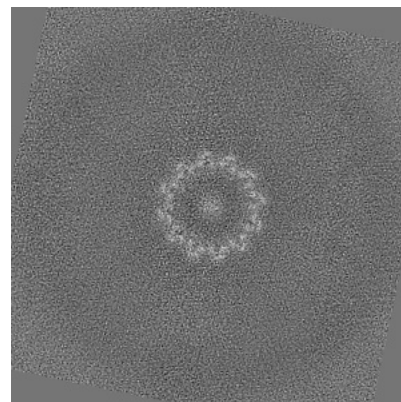
### 6.2.2 Raw map



X Index: 180



Y Index: 180

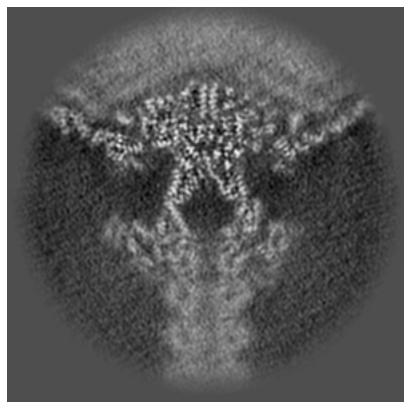


Z Index: 180

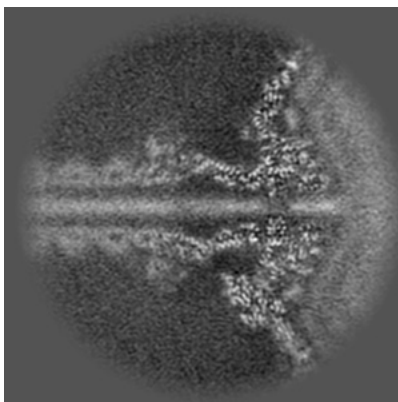
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

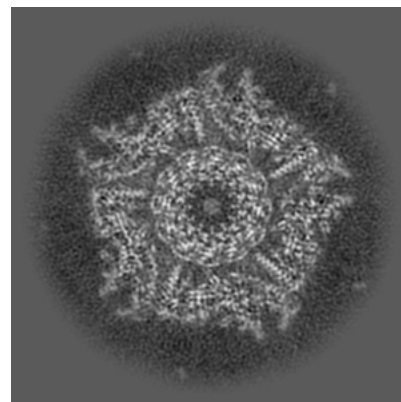
### 6.3.1 Primary map



X Index: 198

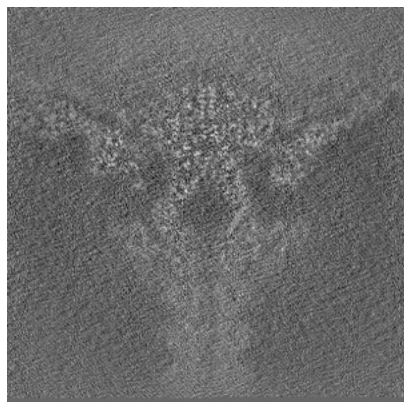


Y Index: 179

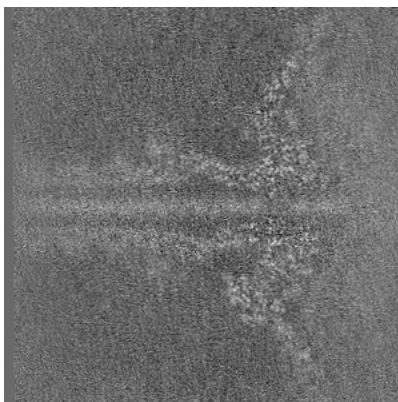


Z Index: 237

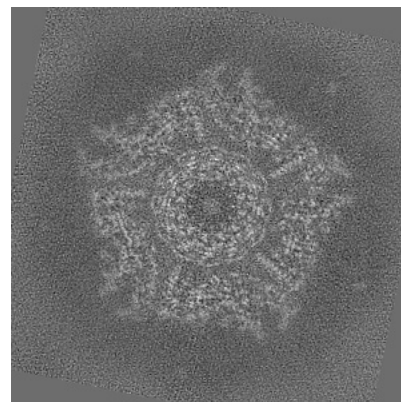
### 6.3.2 Raw map



X Index: 162



Y Index: 179



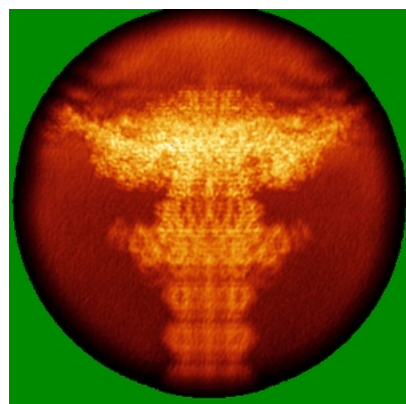
Z Index: 237

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

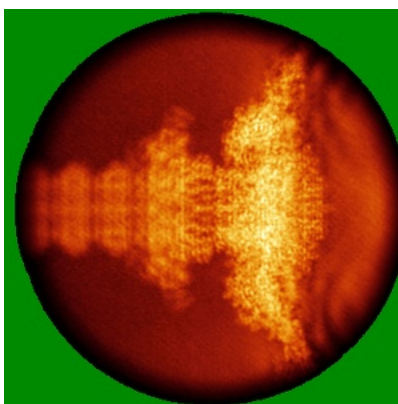


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

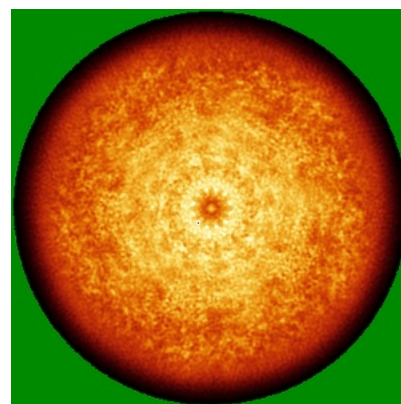
### 6.4.1 Primary map



X

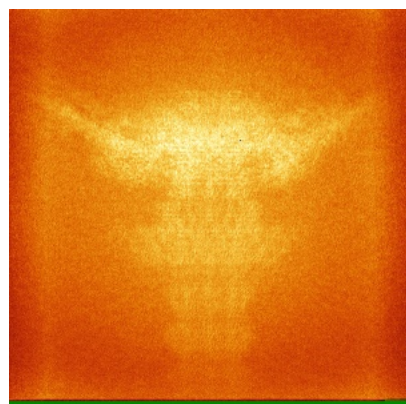


Y

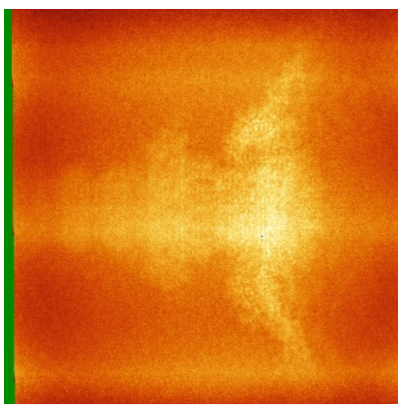


Z

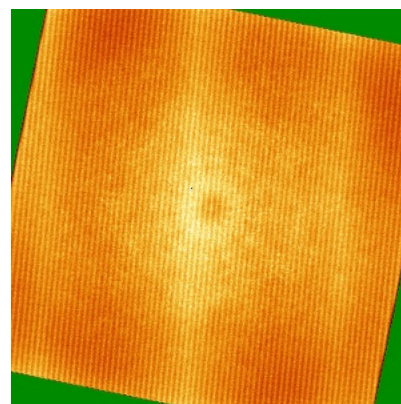
### 6.4.2 Raw map



X



Y



Z

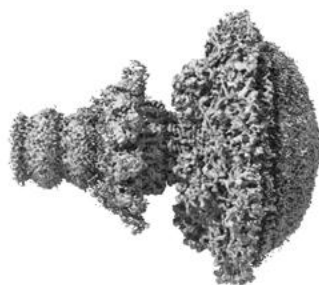
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



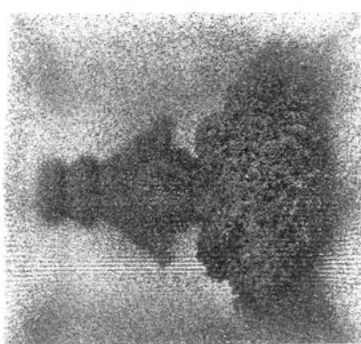
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

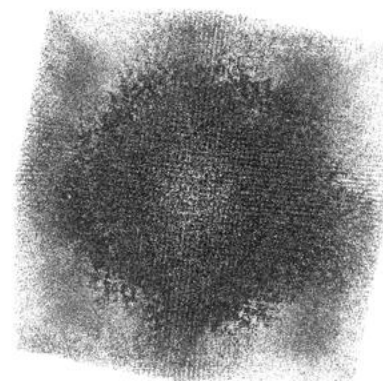
### 6.5.2 Raw map



X



Y



Z

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



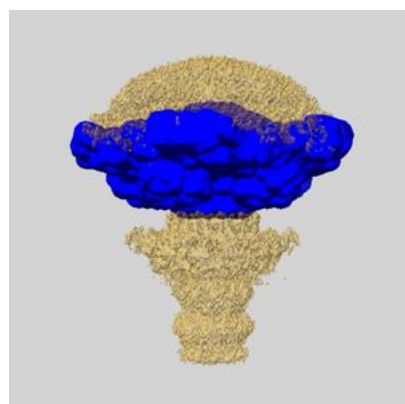
## 6.6 Mask visualisation [i](#)

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

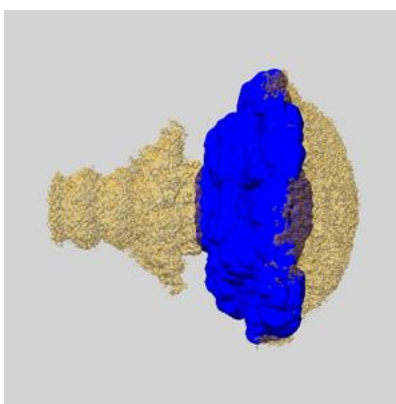
A mask typically either:

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

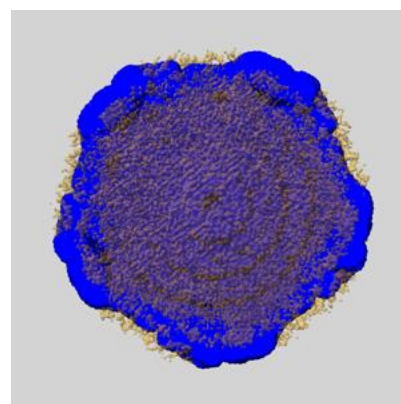
### 6.6.1 emd\_70280\_msk\_1.map [i](#)



X



Y

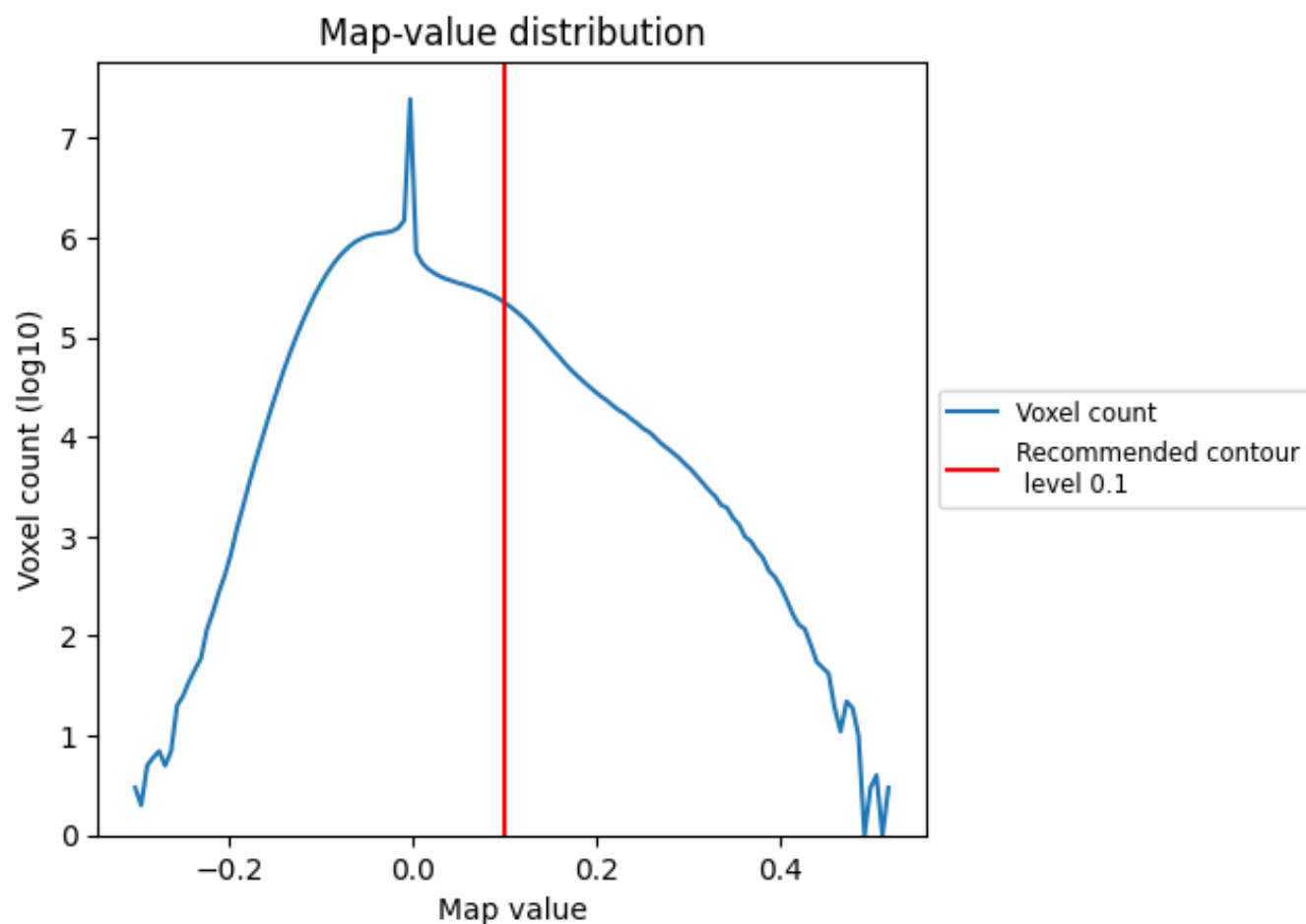


Z

## 7 Map analysis [i](#)

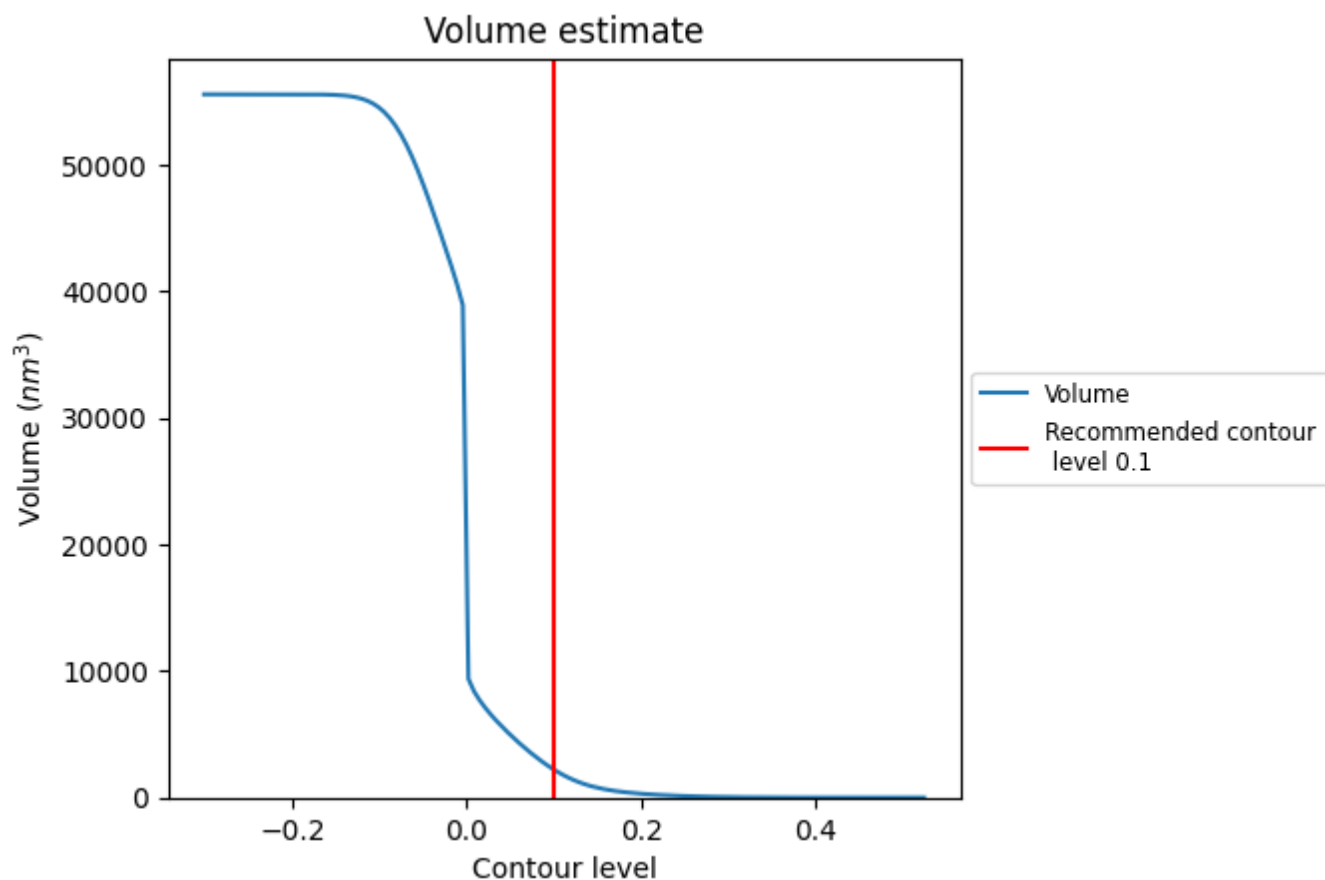
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

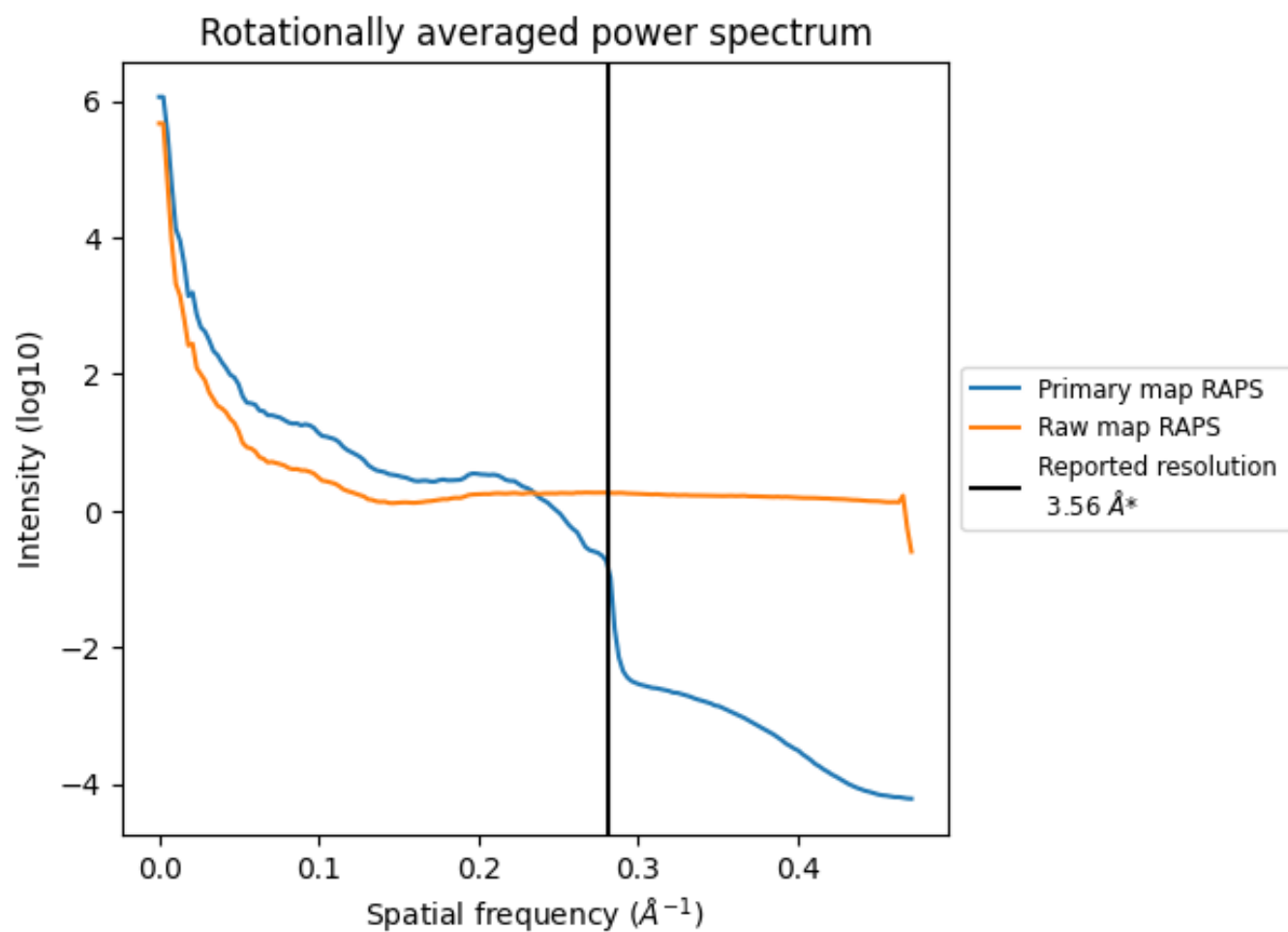
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2210  $\text{nm}^3$ ; this corresponds to an approximate mass of 1997 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

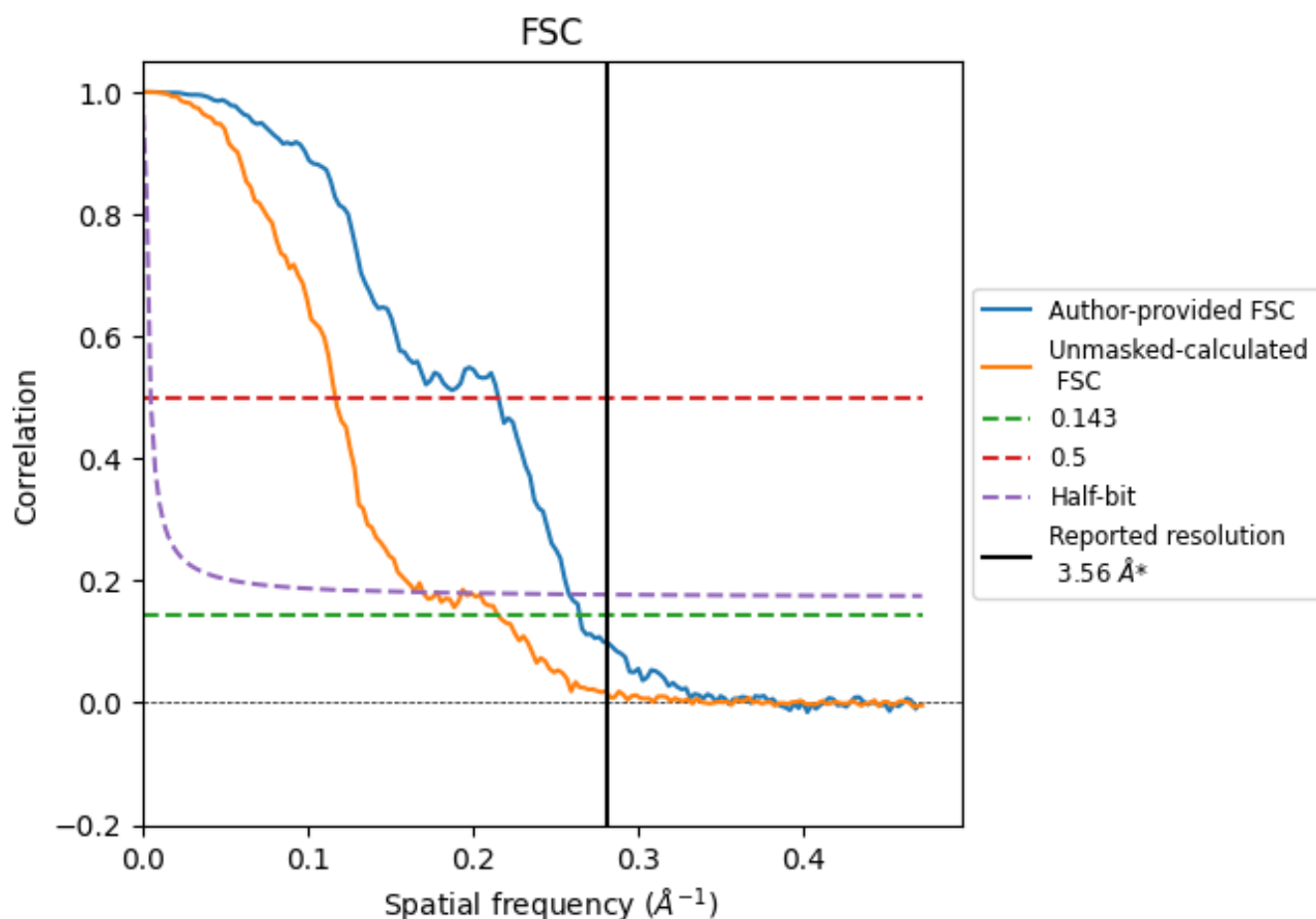


\*Reported resolution corresponds to spatial frequency of 0.281  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.281  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

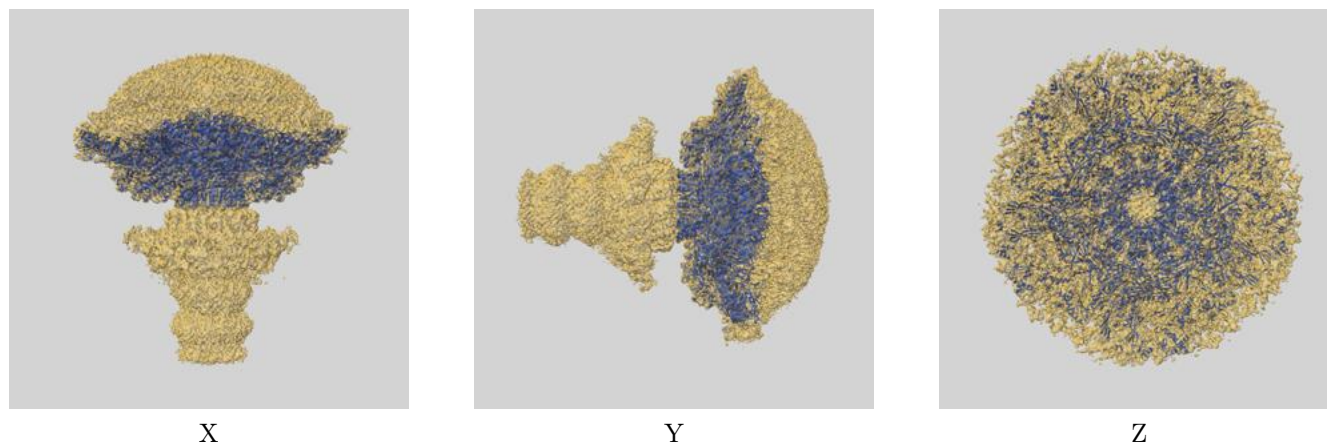
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.78	4.64	3.87
Unmasked-calculated*	4.65	8.56	5.88

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.65 differs from the reported value 3.56 by more than 10 %

## 9 Map-model fit [i](#)

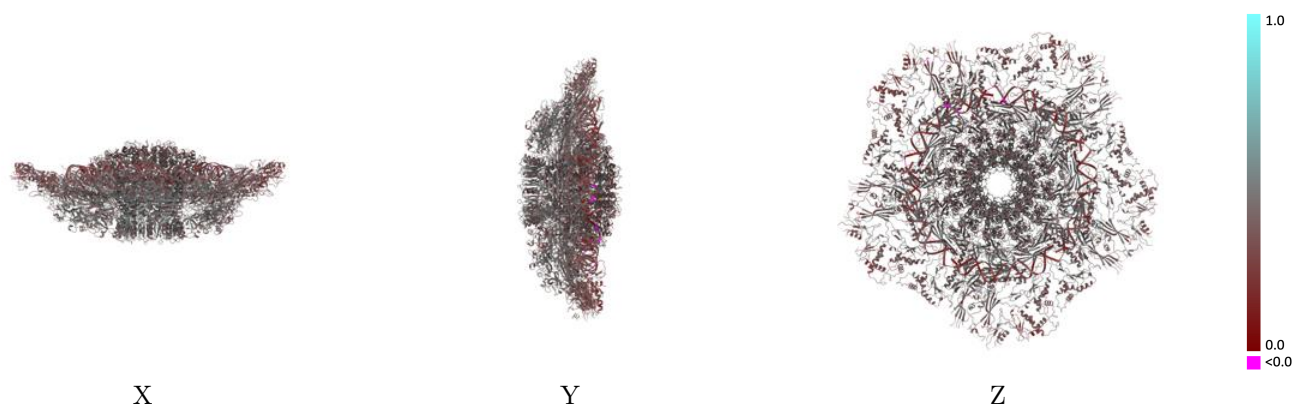
This section contains information regarding the fit between EMDB map EMD-70280 and PDB model 9OAD. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [i](#)



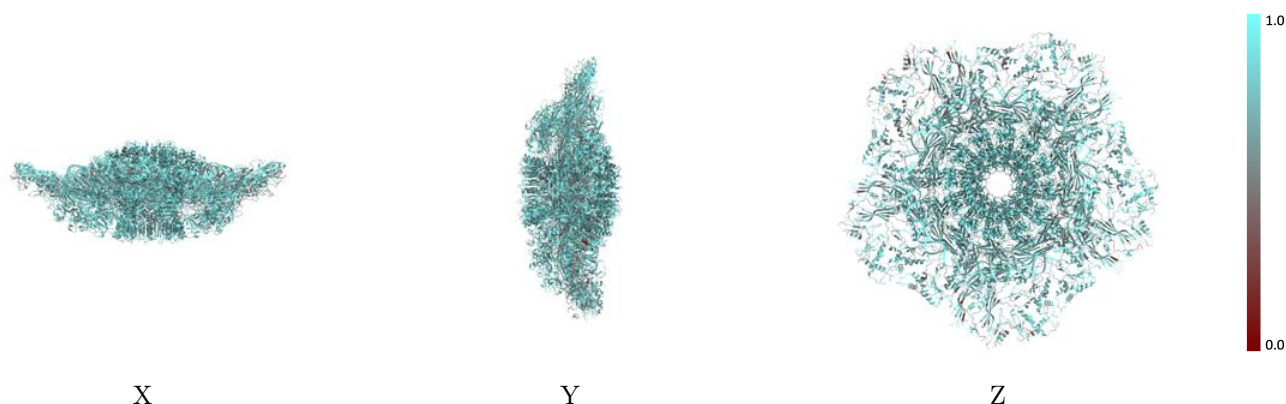
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

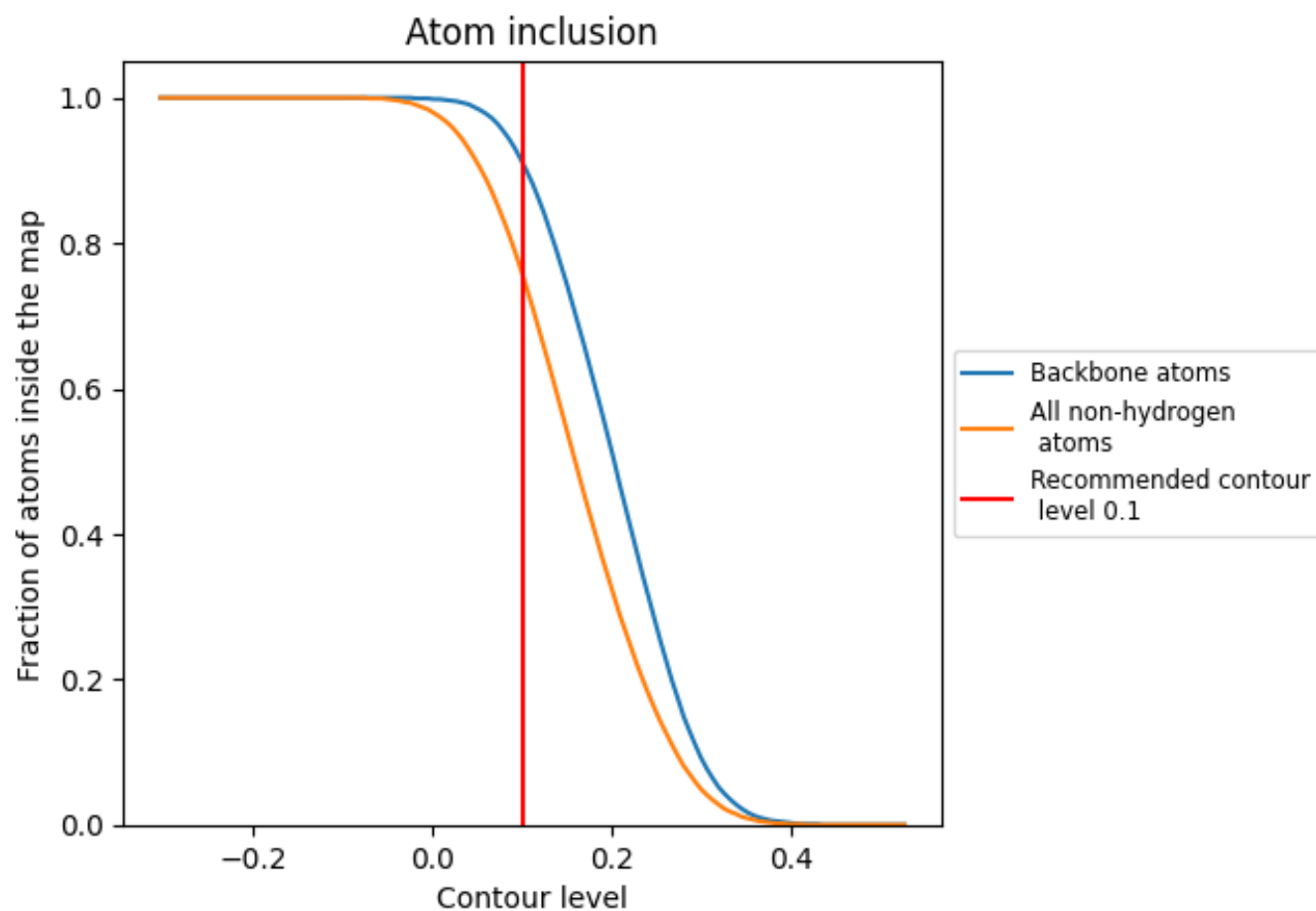
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.4010
Aa	 0.6990	 0.3600
Ab	 0.7020	 0.3750
Ac	 0.7440	 0.3980
Ad	 0.7020	 0.3450
Ae	 0.7450	 0.3940
Af	 0.7790	 0.4190
Ag	 0.7660	 0.4260
Ah	 0.7560	 0.3740
Ai	 0.7690	 0.4000
Aj	 0.7550	 0.4010
Ak	 0.7460	 0.4060
Al	 0.6950	 0.3490
Am	 0.7340	 0.3960
An	 0.7470	 0.4070
Ao	 0.7470	 0.4150
Ap	 0.7150	 0.3640
Aq	 0.7620	 0.3970
Ar	 0.7360	 0.3980
As	 0.7090	 0.3910
At	 0.6210	 0.3160
Ba	 0.4910	 0.3460
Bb	 0.7680	 0.4100
Bc	 0.7170	 0.4150
Bd	 0.7720	 0.4170
Be	 0.6380	 0.3810
Bf	 0.7670	 0.4360
Bg	 0.7640	 0.4390
Bh	 0.7780	 0.4220
Bi	 0.5830	 0.3700
Bj	 0.7900	 0.4230
Bk	 0.7750	 0.4360
Bl	 0.7960	 0.4210
Bm	 0.5870	 0.3770
Bn	 0.7800	 0.4300









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Chain	Atom inclusion	Q-score
Bo	 0.7360	 0.4240
Bp	 0.7750	 0.4170
Bq	 0.5960	 0.3760
Br	 0.7670	 0.4200
Bs	 0.7010	 0.4010
Bt	 0.7330	 0.3890
Ca	 0.6630	 0.4230
Cb	 0.7330	 0.4470
Cc	 0.7520	 0.4360
Cd	 0.5970	 0.3920
Ce	 0.6790	 0.4120
Da	 0.7970	 0.4210
Db	 0.7830	 0.4220
Dc	 0.7970	 0.4280
Dd	 0.7870	 0.4320
De	 0.7970	 0.4310
Df	 0.7970	 0.4330
Dg	 0.8080	 0.4340
Dh	 0.8130	 0.4360
Di	 0.7980	 0.4240
Dj	 0.8010	 0.4200
Dk	 0.7870	 0.4210
Dl	 0.7860	 0.4160
Ea	 0.7770	 0.4430
Eb	 0.7230	 0.4470
Ec	 0.7050	 0.4370
Ed	 0.7320	 0.4270
Ee	 0.7680	 0.4580
Ef	 0.8120	 0.4600
Eg	 0.8120	 0.4700
Eh	 0.7590	 0.4630
Ei	 0.7590	 0.4300
Ej	 0.7680	 0.4570
Ek	 0.7770	 0.4630
El	 0.8210	 0.4670
Ja	 0.7560	 0.2350
Jb	 0.7910	 0.2480
Jc	 0.7260	 0.2530
Jd	 0.7560	 0.2520
Je	 0.7360	 0.2160
Jf	 0.7570	 0.2390
Jg	 0.7770	 0.2400

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Chain	Atom inclusion	Q-score
Jh	 0.7990	 0.2610
Ji	 0.6870	 0.2200
Jj	 0.7360	 0.2060