



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:29 AM UTC

PDB ID : 9OAE / pdb_00009oae
EMDB ID : EMD-70281
Title : Composite reconstruction of the thermophilic bacteriophage P74-26 Neck and Portal Vertex
Authors : Sedivy, E.L.; Agnello, E.; Song, K.; Xu, C.; Kelch, B.A.
Deposited on : 2025-04-21
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

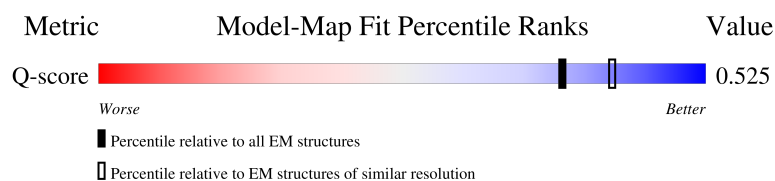
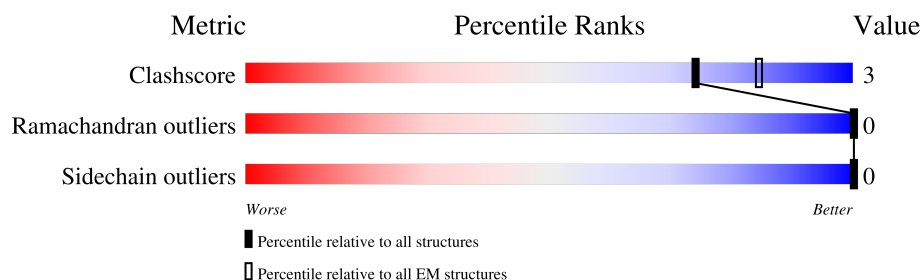
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.



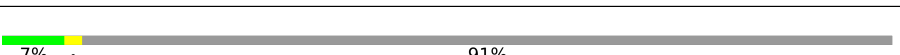
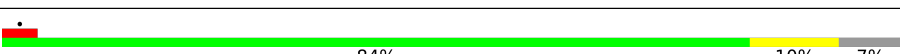
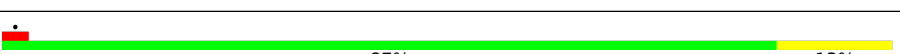
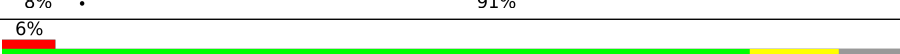
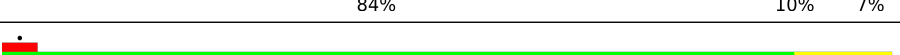
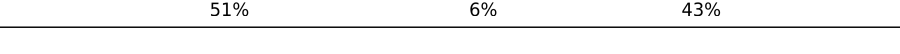
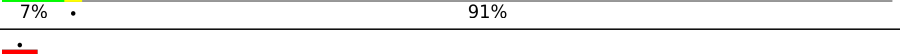
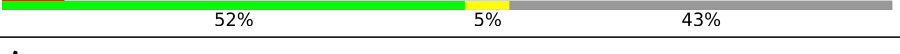
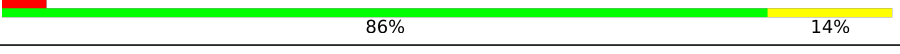
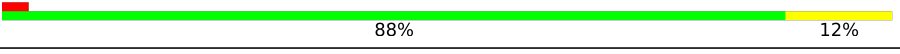
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	Aa	409	
1	Ab	409	
1	Ac	409	
1	Ad	409	

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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	

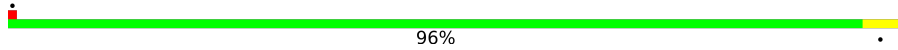
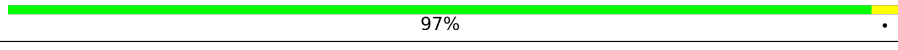
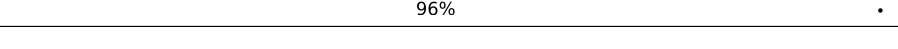
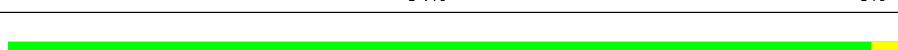
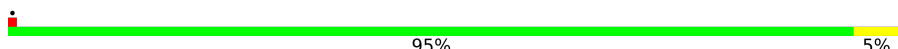
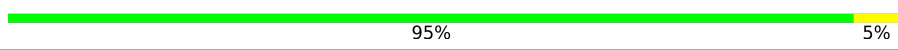
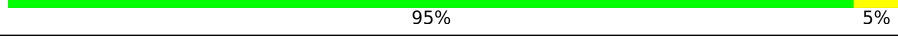
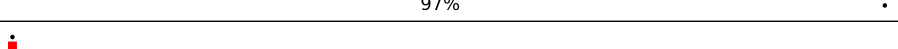
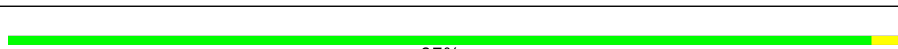
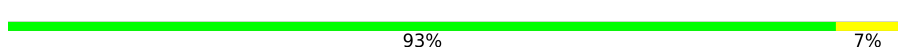
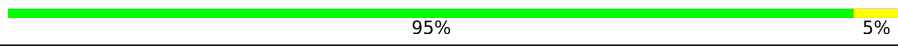
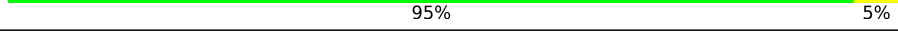
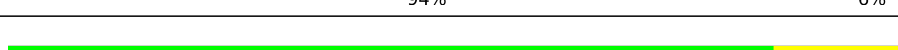
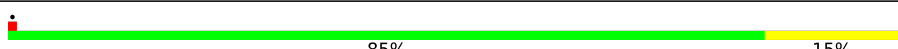
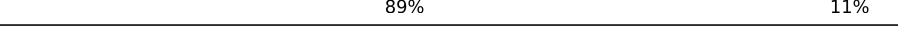
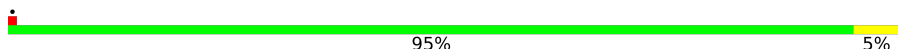
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Mol	Chain	Length	Quality of chain
2	Bj	146	
2	Bk	146	
2	Bl	146	
2	Bm	146	
2	Bn	146	
2	Bo	146	
2	Bp	146	
2	Bq	146	
2	Br	146	
2	Bs	146	
2	Bt	146	
3	Ca	73	
3	Cb	73	
3	Cc	73	
3	Cd	73	
3	Ce	73	
4	Da	423	
4	Db	423	
4	Dc	423	
4	Dd	423	
4	De	423	
4	Df	423	
4	Dg	423	
4	Dh	423	
4	Di	423	

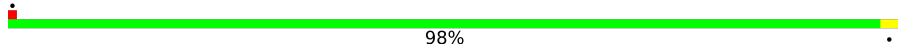
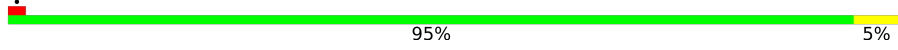
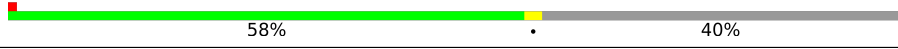
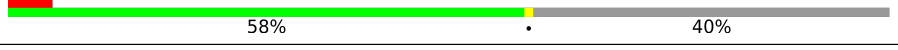
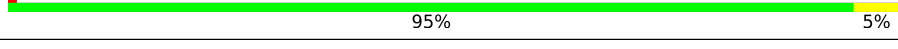
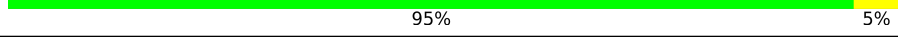
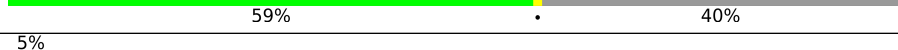
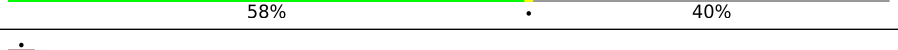
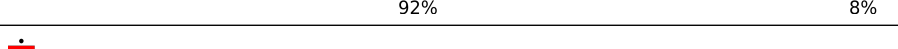
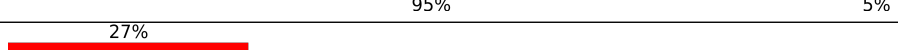
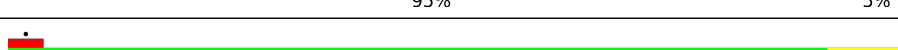
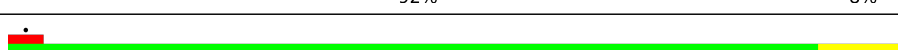
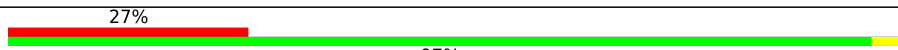
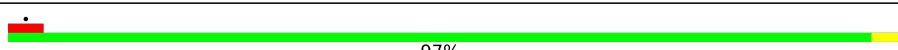
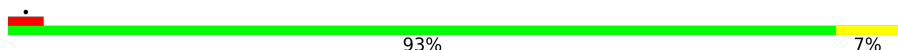
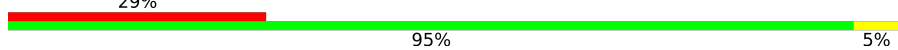
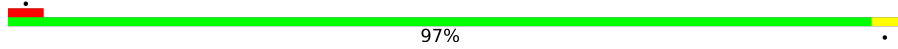
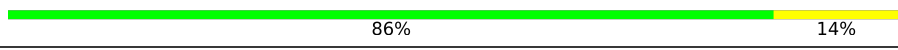
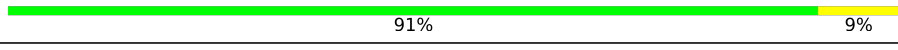
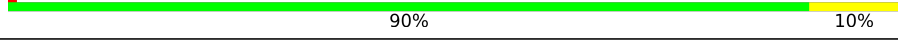
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Mol	Chain	Length	Quality of chain
4	Dj	423	
4	Dk	423	
4	Dl	423	
5	Ea	130	
5	Eb	130	
5	Ec	130	
5	Ed	130	
5	Ee	130	
5	Ef	130	
5	Eg	130	
5	Eh	130	
5	Ei	130	
5	Ej	130	
5	Ek	130	
5	El	130	
6	Fa	155	
6	Fb	155	
6	Fc	155	
6	Fd	155	
6	Fe	155	
6	Ff	155	
7	Ga	146	
7	Gb	146	
7	Gc	146	
7	Gd	146	

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Mol	Chain	Length	Quality of chain
7	Ge	146	
7	Gf	146	
7	Gg	146	
7	Gh	146	
7	Gi	146	
7	Gj	146	
7	Gk	146	
7	Gl	146	
7	Ha	146	
7	Hb	146	
7	Hc	146	
7	Hd	146	
7	He	146	
7	Hf	146	
7	Hg	146	
7	Hh	146	
7	Hi	146	
7	Hj	146	
7	Hk	146	
7	Hi	146	
8	Ia	348	
8	Ib	348	
8	Ic	348	
8	Id	348	
8	Ie	348	

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Mol	Chain	Length	Quality of chain
8	If	348	
9	Ja	31	
9	Jc	31	
9	Je	31	
9	Jg	31	
9	Ji	31	
10	Jb	31	
10	Jd	31	
10	Jf	31	
10	Jh	31	
10	Jj	31	
11	Ka	66	
12	Kb	66	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 173562 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
			3288	2117	551	610	10		
4	Db	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Dc	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Dd	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	De	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Df	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Dg	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Dh	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Di	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Dj	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Dk	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		
4	Dl	423	Total	C	N	O	S	0	0
			3288	2117	551	610	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ea	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Eb	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Ec	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Ed	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Ee	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Ef	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Eg	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Eh	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Ei	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Ej	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	Ek	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
5	El	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		

- Molecule 6 is a protein called Tail terminator.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Fa	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Fb	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
6	Fc	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
6	Fd	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
6	Fe	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
6	Ff	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		

- Molecule 7 is a protein called Collar (P74p112).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ga	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Gb	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Gc	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
7	Gd	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
7	Ge	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Gf	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Gg	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
7	Gh	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
7	Gi	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Gj	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Gk	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
7	Gl	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
7	Ha	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hb	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	Hc	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hd	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	He	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hf	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hg	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hh	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hi	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hj	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hk	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
7	Hl	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		

- Molecule 8 is a protein called Tail Tube Protein gp93.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ia	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
8	Ib	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
8	Ic	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
8	Id	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
8	Ie	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
8	If	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		

- Molecule 9 is a DNA chain called DNA (31-MER).

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

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

- Molecule 10 is a DNA chain called DNA (31-MER).

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

- Molecule 11 is a DNA chain called DNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ka	66	Total	C	N	O	P	0	0
			1334	635	238	395	66		

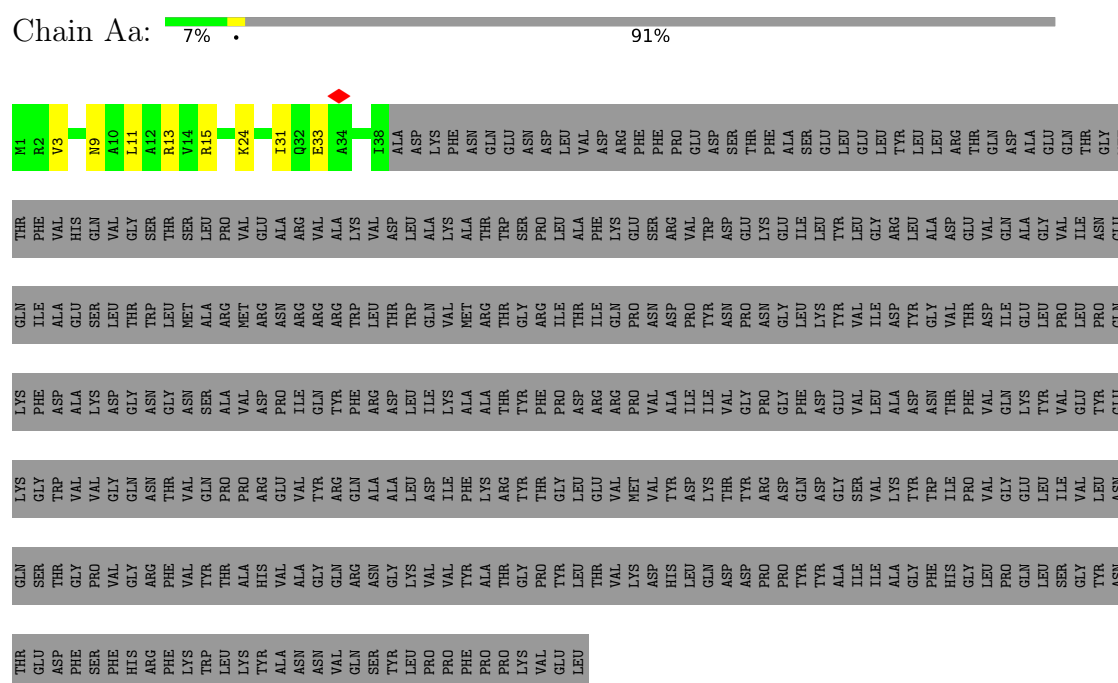
- Molecule 12 is a DNA chain called DNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Kb	66	Total	C	N	O	P	0	0
			1372	648	261	397	66		

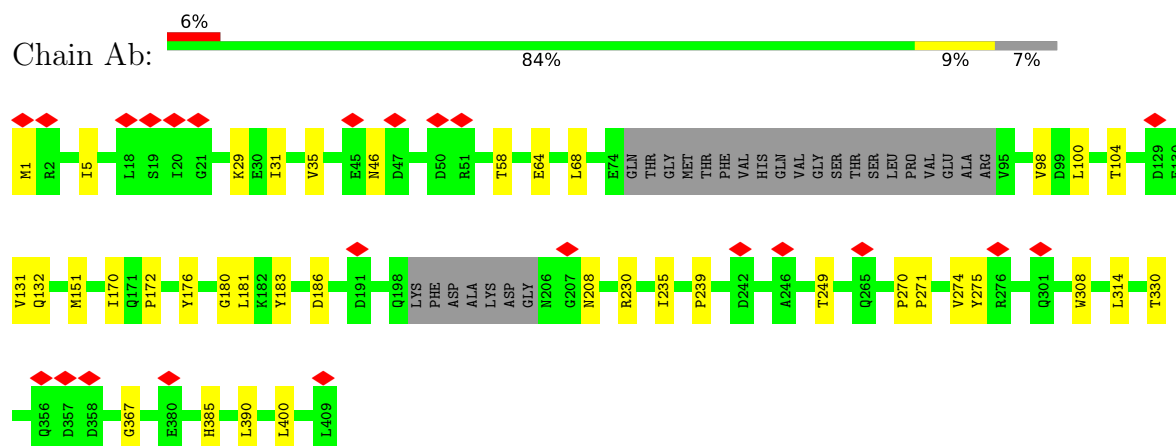
3 Residue-property plots [i](#)

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

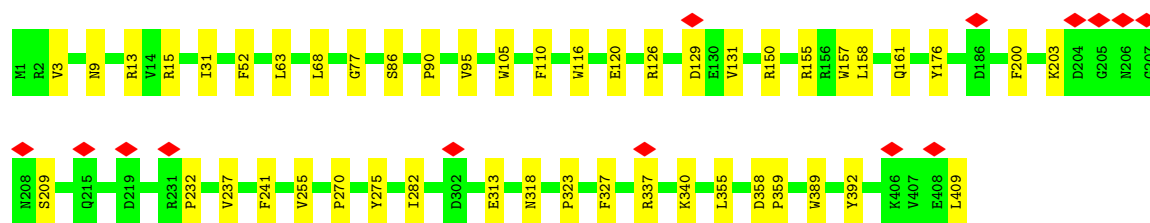
• Molecule 1: Major head protein



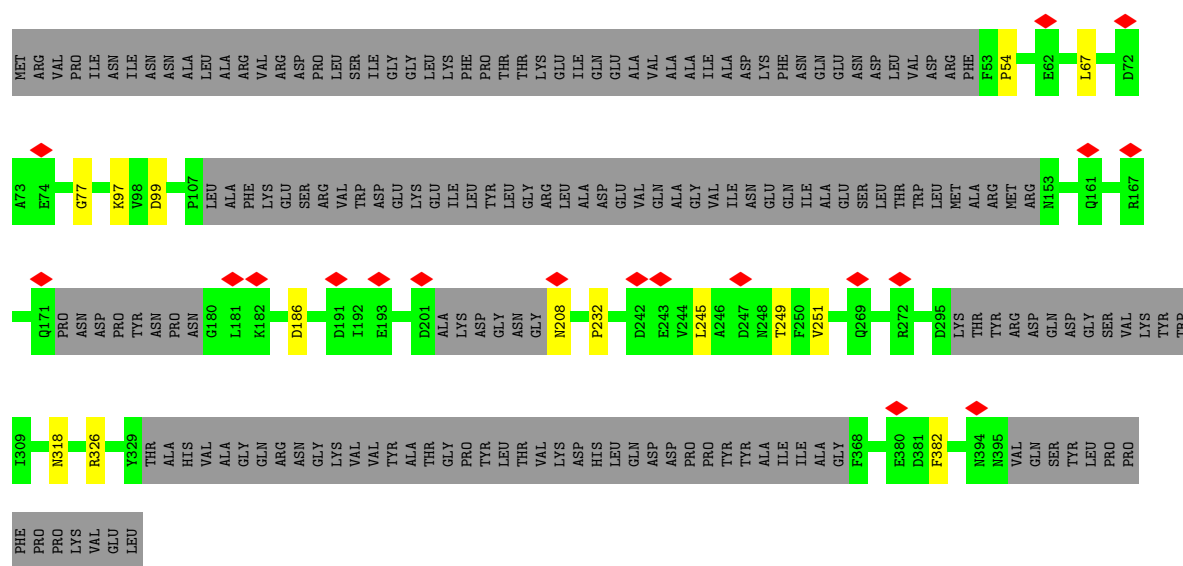
• Molecule 1: Major head protein



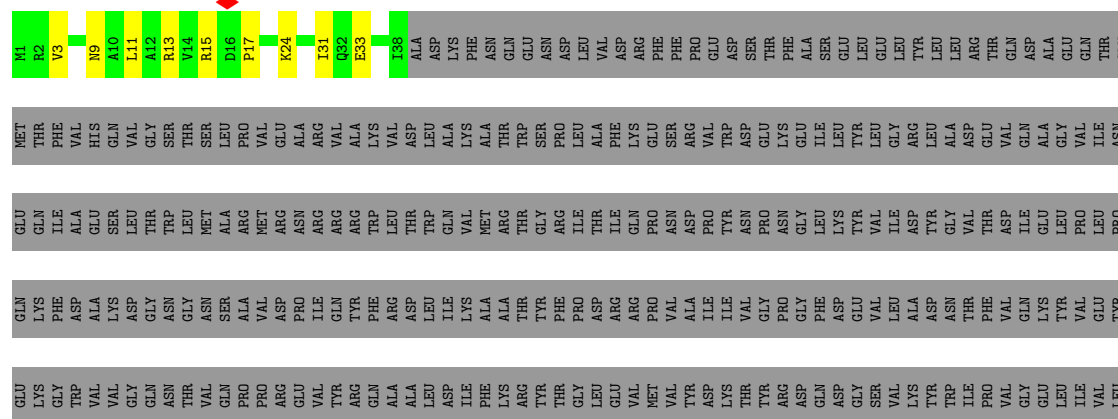
Chain Ac: 89% 11%

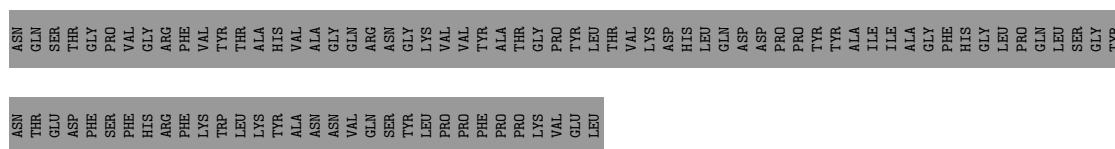


Chain Ad:

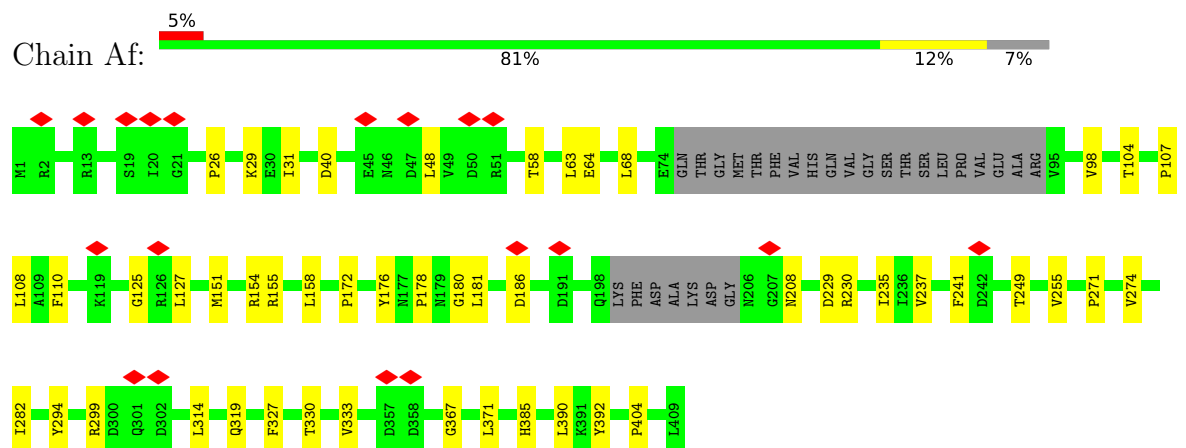


Chain Ae: 7% 91%

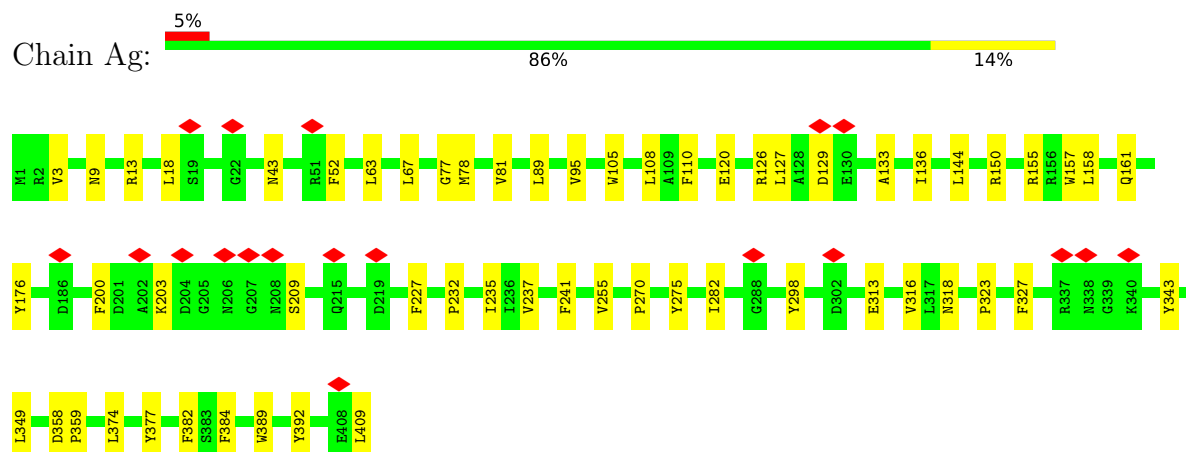




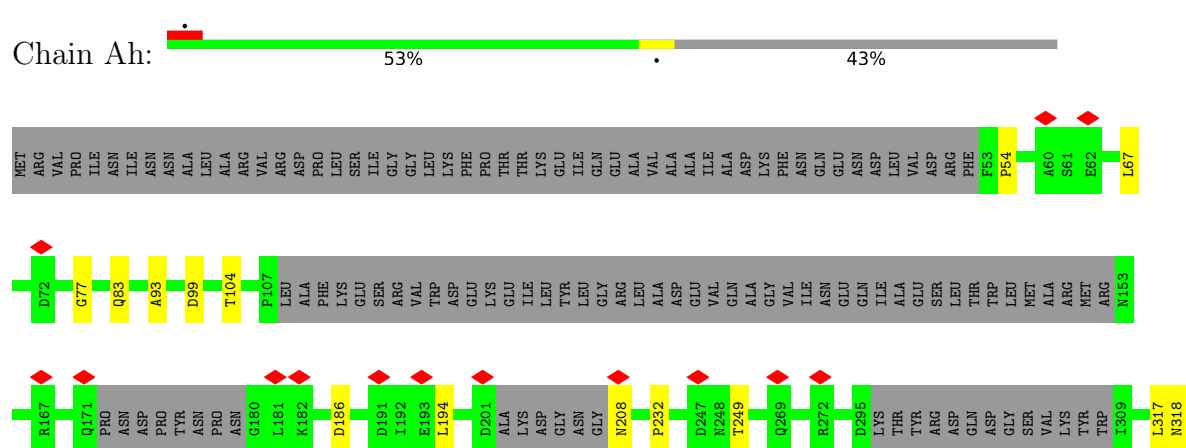
• Molecule 1: Major head protein



• Molecule 1: Major head protein

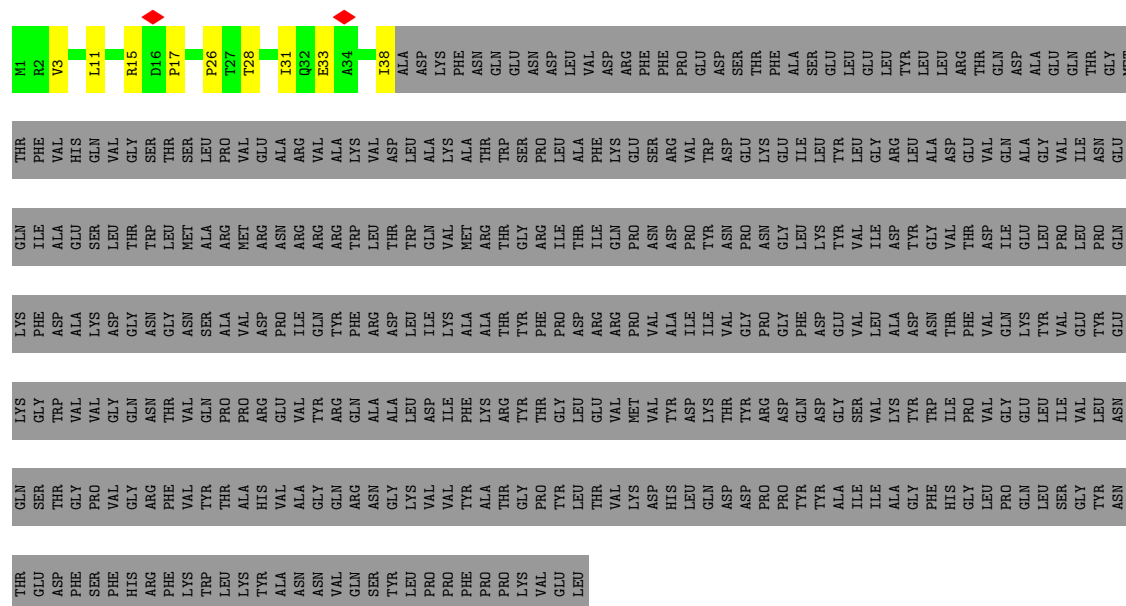


• Molecule 1: Major head protein

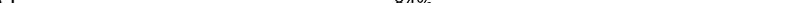


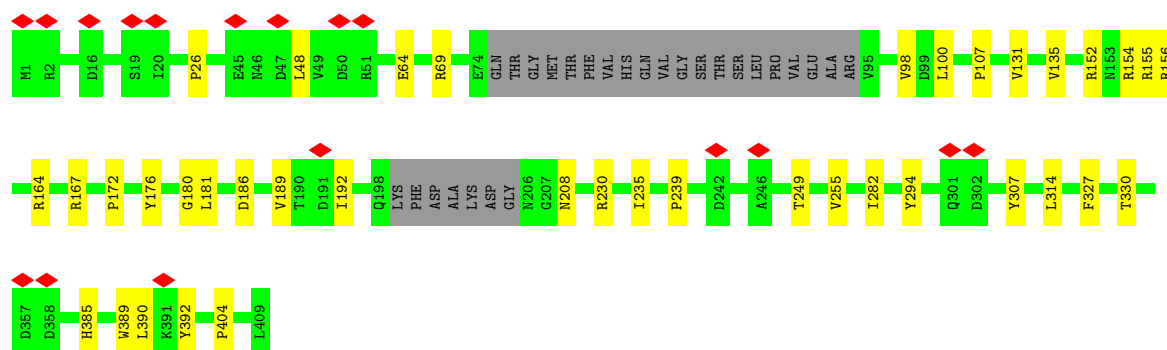
- Molecule 1: Major head protein

Chain Ai: 7% . 91%

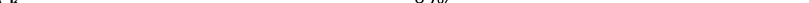


- Molecule 1: Major head protein

Chain A_i: 



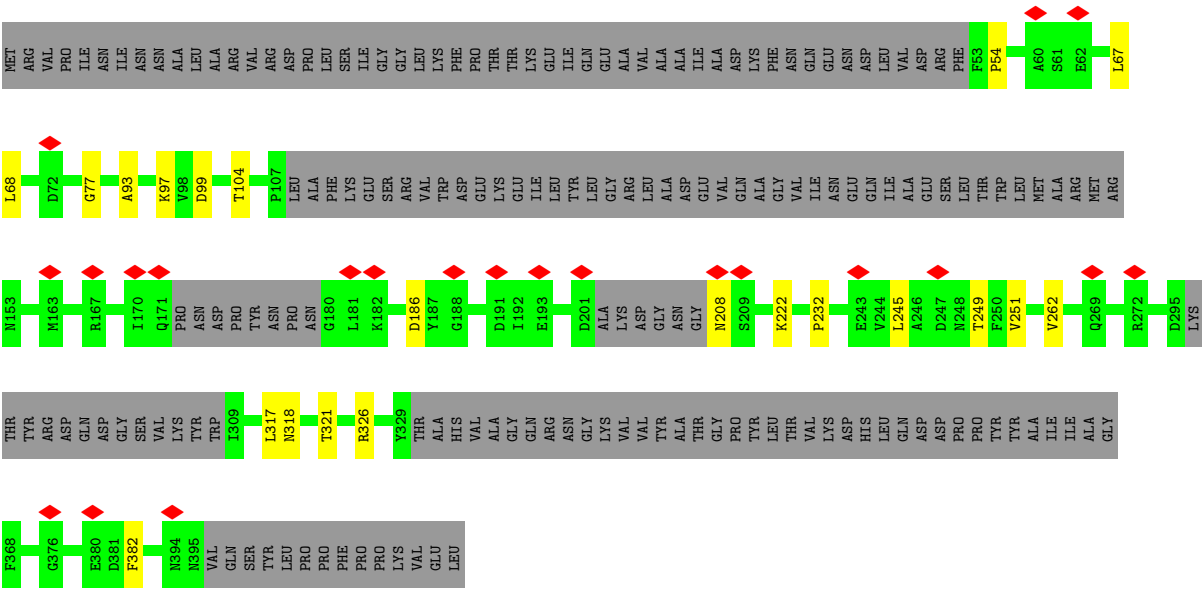
- Molecule 1: Major head protein

Chain Ak:  87% 13%

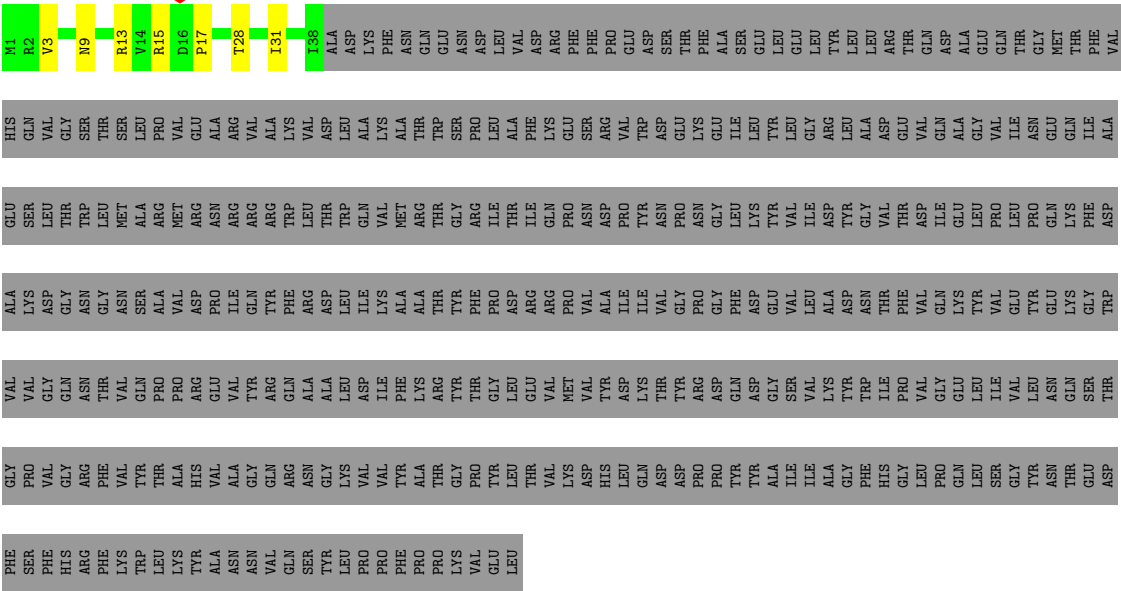




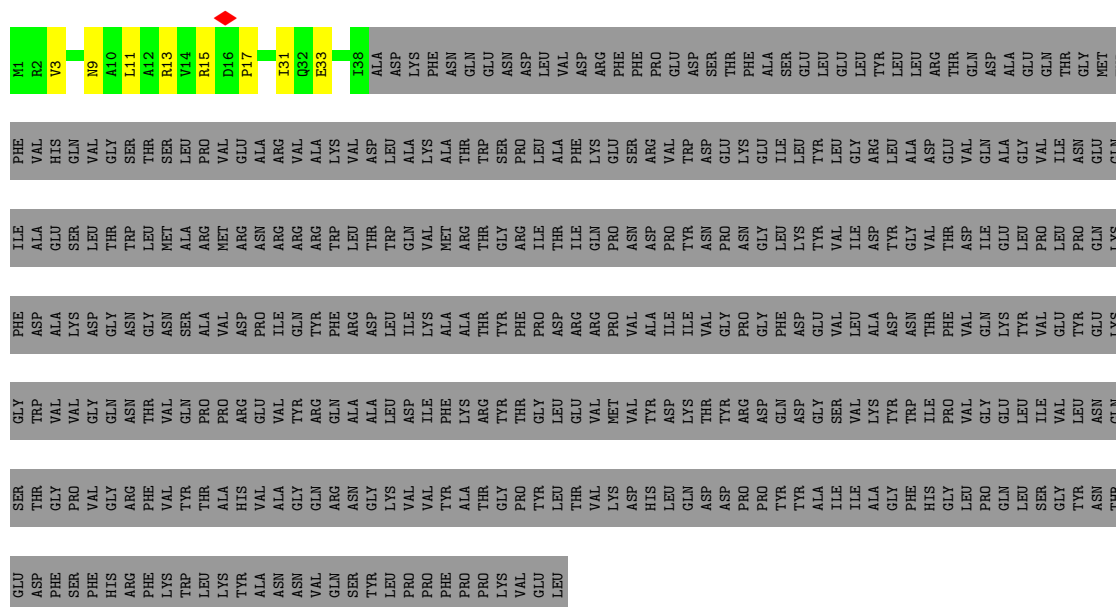
• Molecule 1: Major head protein



• Molecule 1: Major head protein

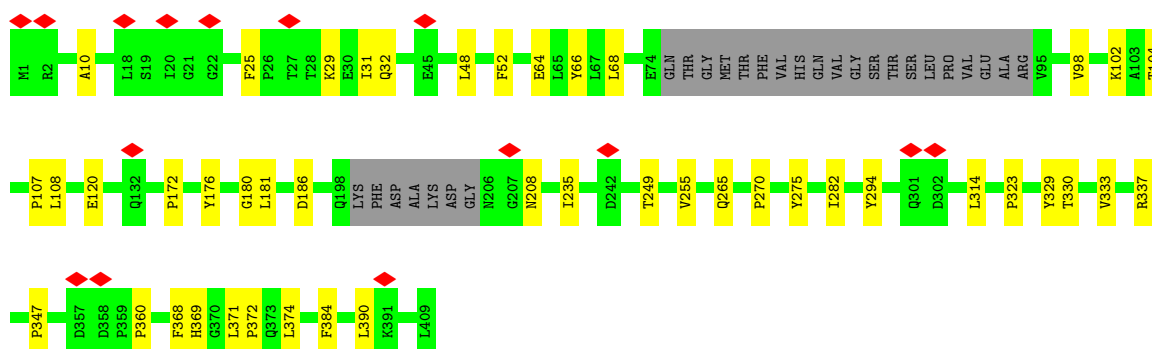


• Molecule 1: Major head protein



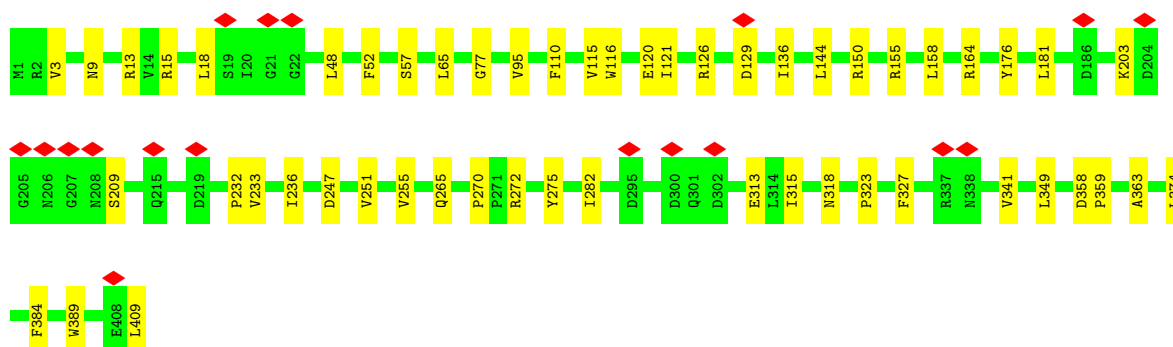
• Molecule 1: Major head protein

Chain Ar: 82% 11% 7%

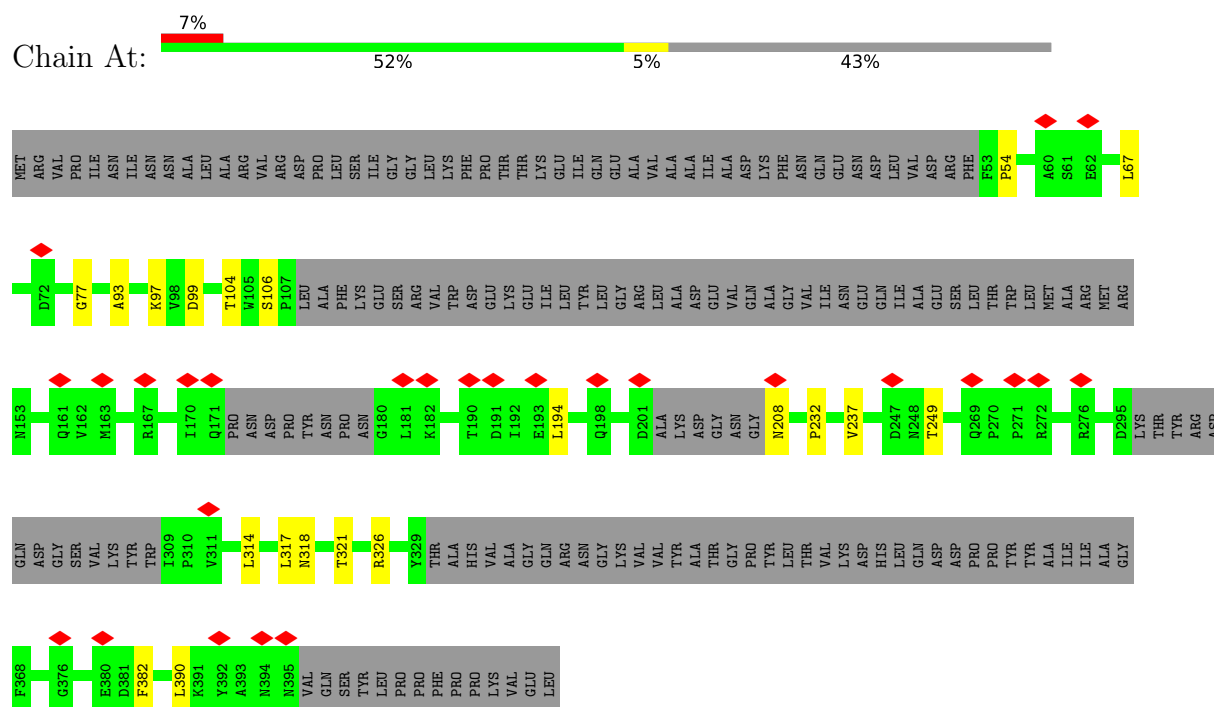


• Molecule 1: Major head protein

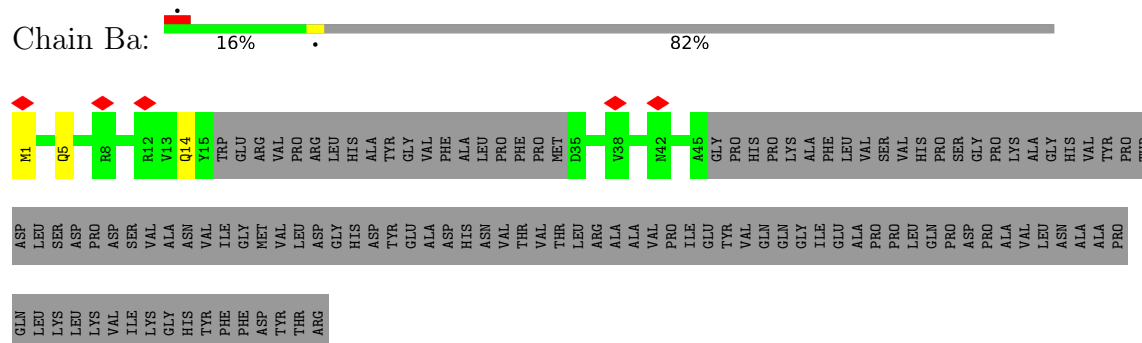
Chain As: 87% 13%



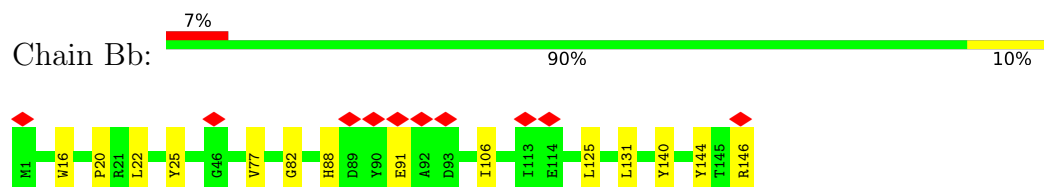
• Molecule 1: Major head protein



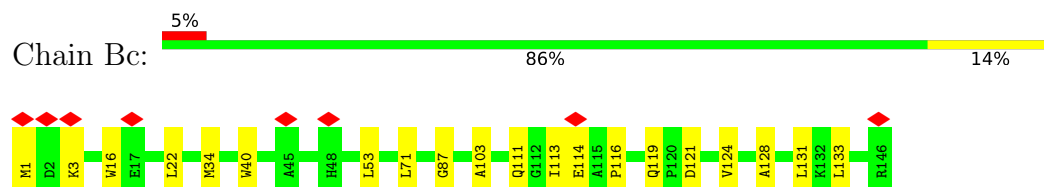
- Molecule 2: P74-26 Head Decoration Protein



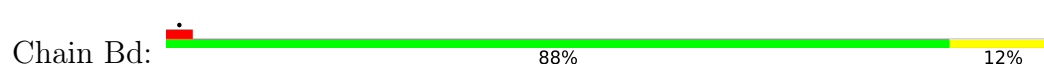
- Molecule 2: P74-26 Head Decoration Protein



- Molecule 2: P74-26 Head Decoration Protein

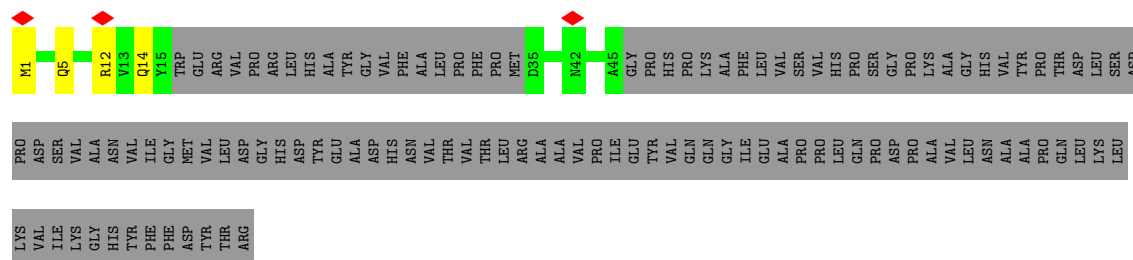


- Molecule 2: P74-26 Head Decoration Protein

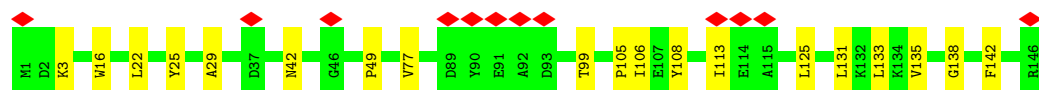




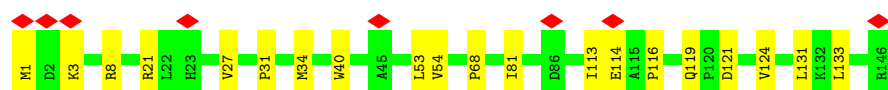
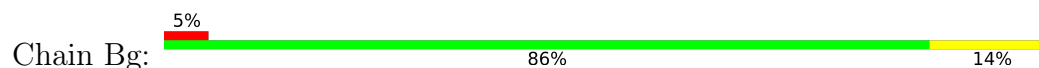
● Molecule 2: P74-26 Head Decoration Protein



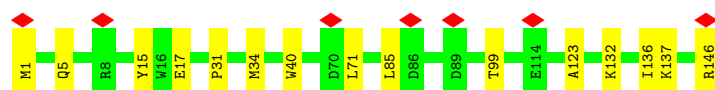
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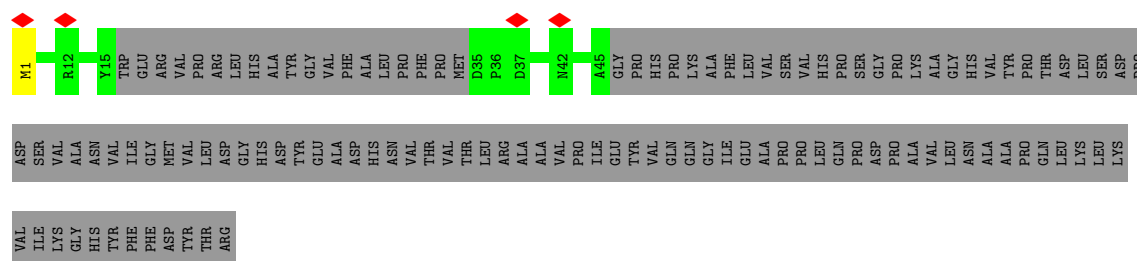
● Molecule 2: P74-26 Head Decoration Protein



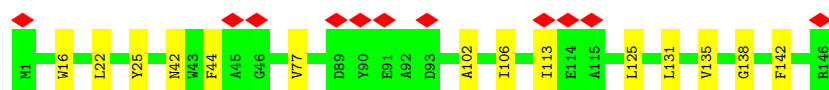
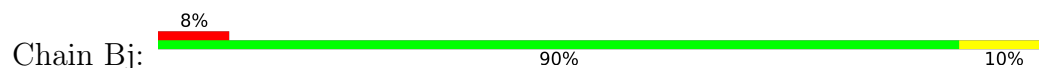
● Molecule 2: P74-26 Head Decoration Protein



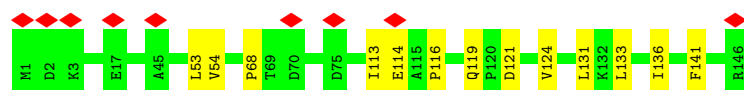
● Molecule 2: P74-26 Head Decoration Protein



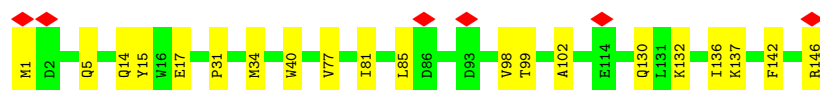
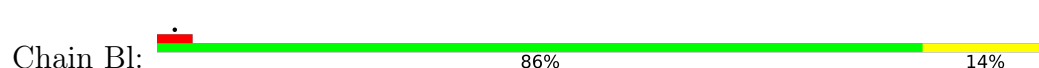
- Molecule 2: P74-26 Head Decoration Protein



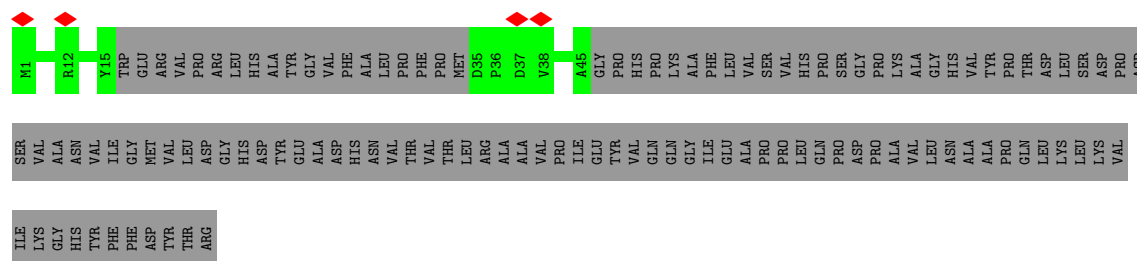
- Molecule 2: P74-26 Head Decoration Protein



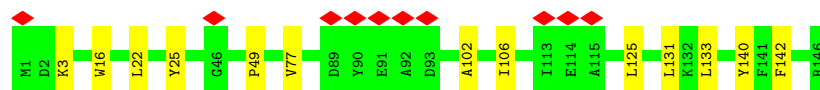
- Molecule 2: P74-26 Head Decoration Protein



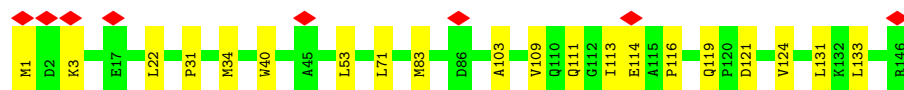
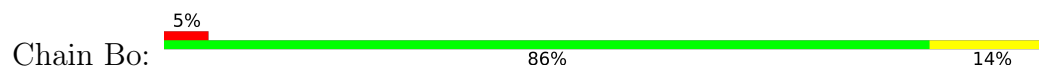
- Molecule 2: P74-26 Head Decoration Protein



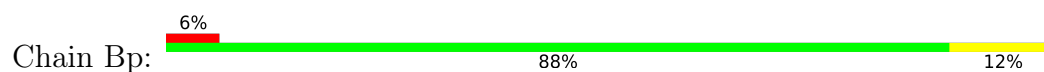
- Molecule 2: P74-26 Head Decoration Protein



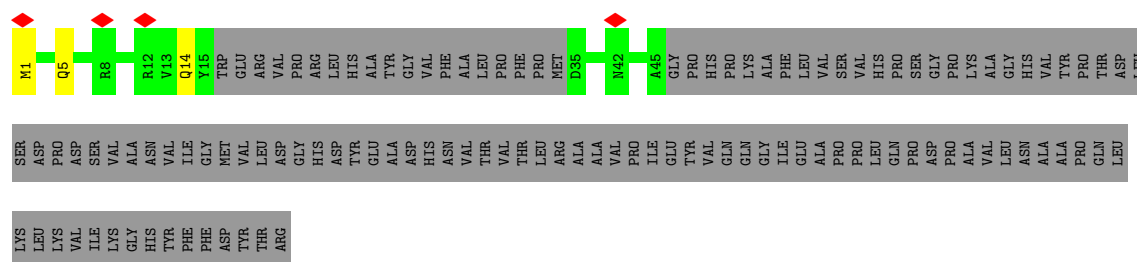
- Molecule 2: P74-26 Head Decoration Protein



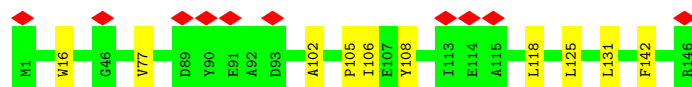
- Molecule 2: P74-26 Head Decoration Protein



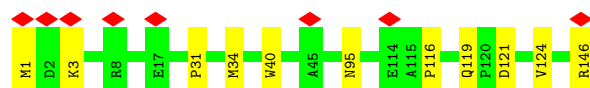
• Molecule 2: P74-26 Head Decoration Protein



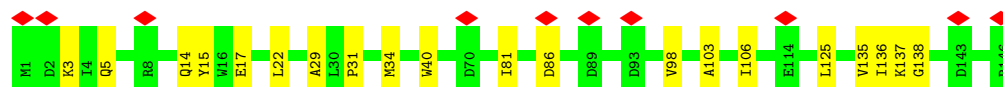
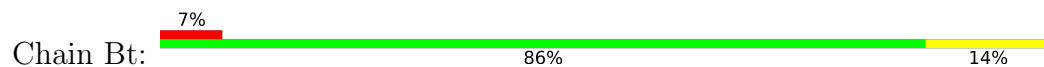
• Molecule 2: P74-26 Head Decoration Protein



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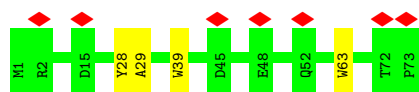
• Molecule 2: P74-26 Head Decoration Protein



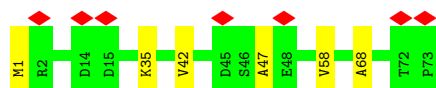
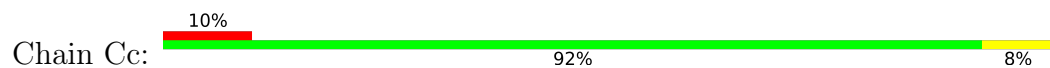
• Molecule 3: Portal Vertex Protein



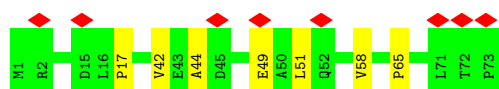
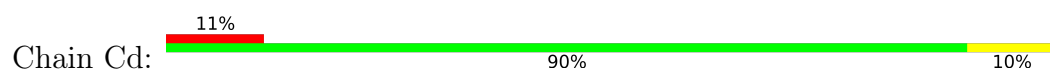
• Molecule 3: Portal Vertex Protein



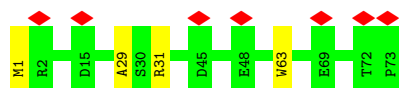
- Molecule 3: Portal Vertex Protein



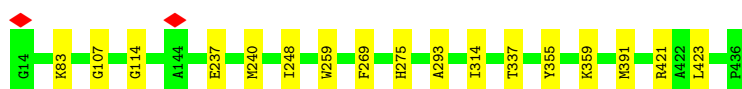
- Molecule 3: Portal Vertex Protein



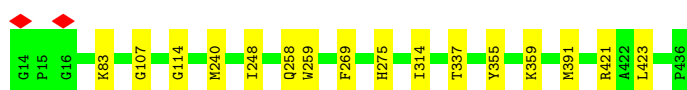
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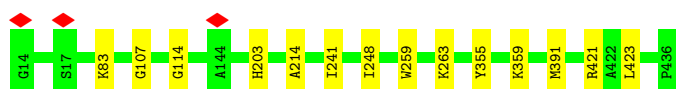
- Molecule 4: Portal protein



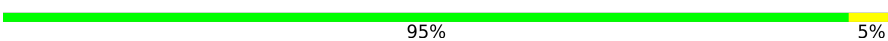
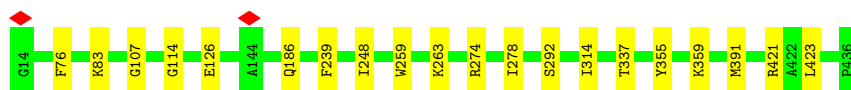
- Molecule 4: Portal protein



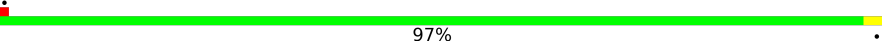
- Molecule 4: Portal protein



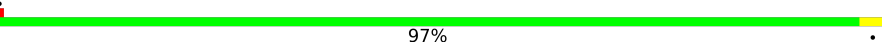
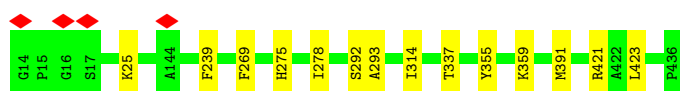
● Molecule 4: Portal protein

Chain Dd:  95% 5%

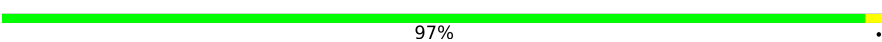
● Molecule 4: Portal protein

Chain De:  97% .

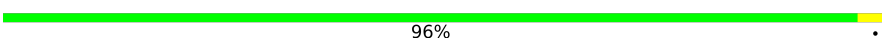
● Molecule 4: Portal protein

Chain Df:  97% .

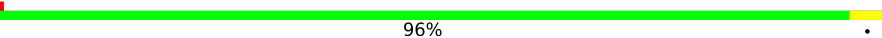
● Molecule 4: Portal protein

Chain Dg:  97% .

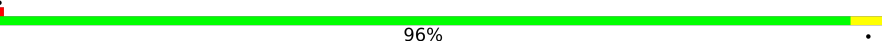
● Molecule 4: Portal protein

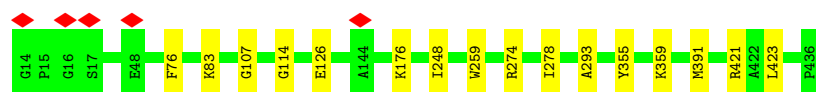
Chain Dh:  96% .

● Molecule 4: Portal protein

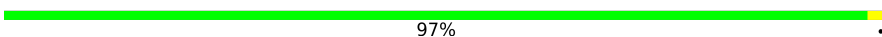
Chain Di:  96% .

● Molecule 4: Portal protein

Chain Dj:  96% .

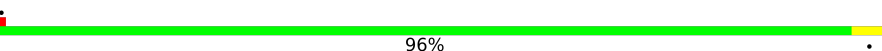


- Molecule 4: Portal protein

Chain Dk:  97%

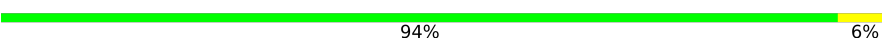


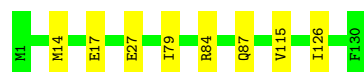
- Molecule 4: Portal protein

Chain Dl:  96%

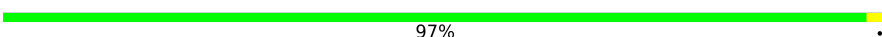


- Molecule 5: Adaptor (P74p90)

Chain Ea:  94%

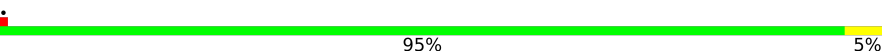


- Molecule 5: Adaptor (P74p90)

Chain Eb:  97%

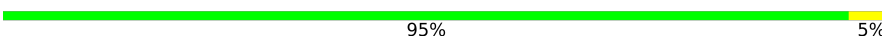


- Molecule 5: Adaptor (P74p90)

Chain Ec:  95%

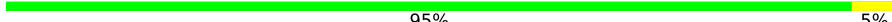


- Molecule 5: Adaptor (P74p90)

Chain Ed:  95%

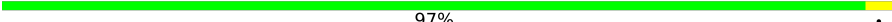


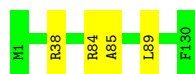
- Molecule 5: Adaptor (P74p90)

Chain Ee:  95% 5%



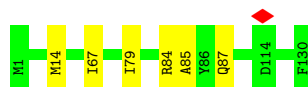
- Molecule 5: Adaptor (P74p90)

Chain Ef:  97% .

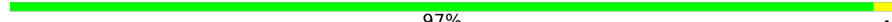


- Molecule 5: Adaptor (P74p90)

Chain Eg:  95% 5%



- Molecule 5: Adaptor (P74p90)

Chain Eh:  97% .



- Molecule 5: Adaptor (P74p90)

Chain Ei:  93% 7%

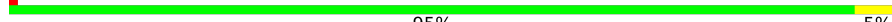


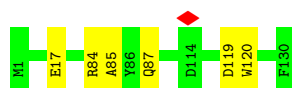
- Molecule 5: Adaptor (P74p90)

Chain Ej:  95% 5%



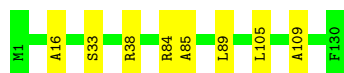
- Molecule 5: Adaptor (P74p90)

Chain Ek:  95% 5%



- Molecule 5: Adaptor (P74p90)

Chain El:  94% 6%



- Molecule 6: Tail terminator

Chain Fa:  86% 14%



- Molecule 6: Tail terminator

Chain Fb:  85% 15%



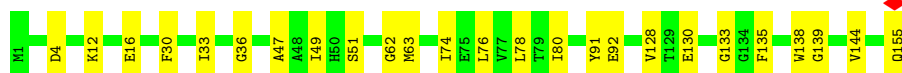
- Molecule 6: Tail terminator

Chain Fc:  81% 19%



- Molecule 6: Tail terminator

Chain Fd:  84% 16%



- Molecule 6: Tail terminator

Chain Fe:  89% 11%



- Molecule 6: Tail terminator

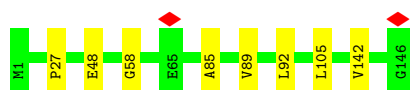
Chain Ff:  87% 13%



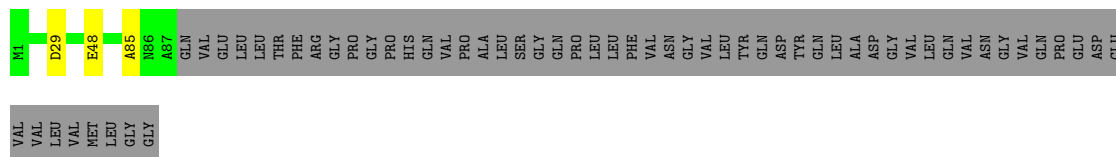
- Molecule 7: Collar (P74p112)



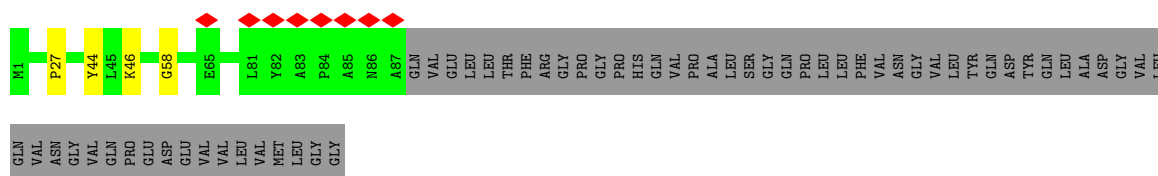
- Molecule 7: Collar (P74p112)



- Molecule 7: Collar (P74p112)



- Molecule 7: Collar (P74p112)



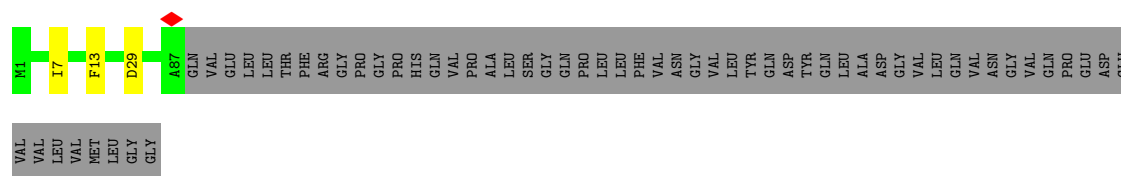
- Molecule 7: Collar (P74p112)



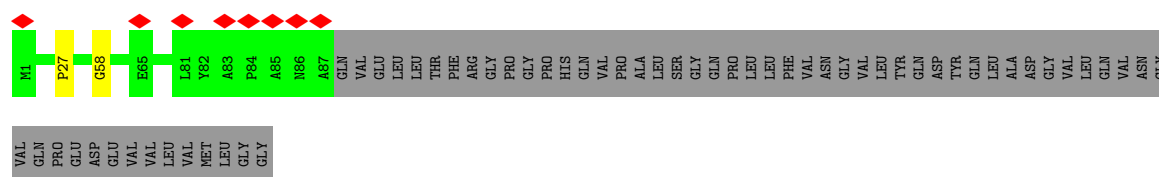
- Molecule 7: Collar (P74p112)



- Molecule 7: Collar (P74p112)



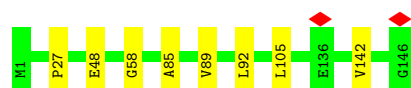
• Molecule 7: Collar (P74p112)



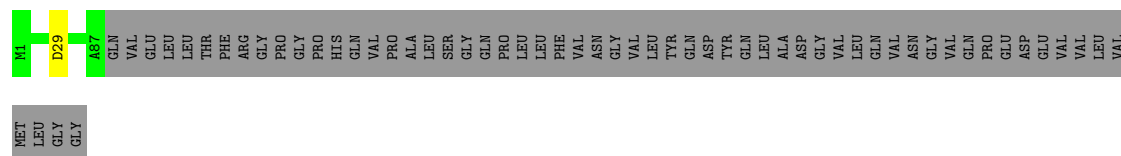
• Molecule 7: Collar (P74p112)



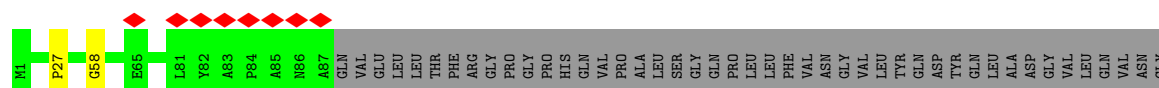
• Molecule 7: Collar (P74p112)



• Molecule 7: Collar (P74p112)

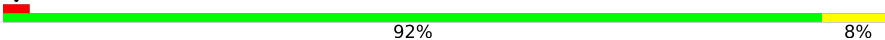


• Molecule 7: Collar (P74p112)



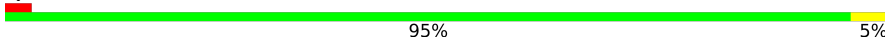
VAL
GLN
PRO
GLU
ASP
GLU
VAL
LEU
VAL
MET
LEU
GLY
GLY

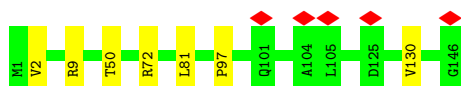
• Molecule 7: Collar (P74p112)

Chain Ha:  92% 8%

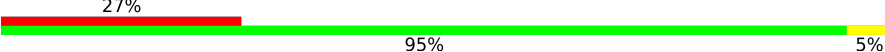


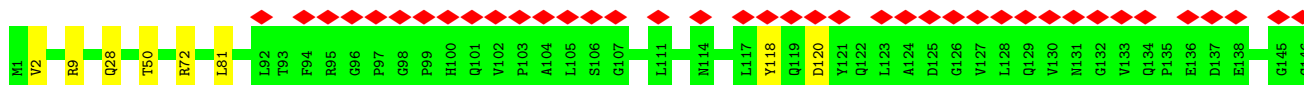
• Molecule 7: Collar (P74p112)

Chain Hb:  95% 5%

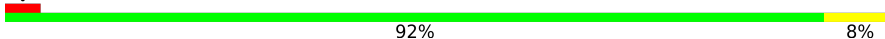


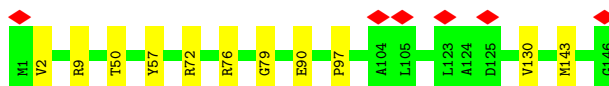
• Molecule 7: Collar (P74p112)

Chain Hc:  27% 95% 5%



• Molecule 7: Collar (P74p112)

Chain Hd:  92% 8%



• Molecule 7: Collar (P74p112)

Chain He:  91% 9%

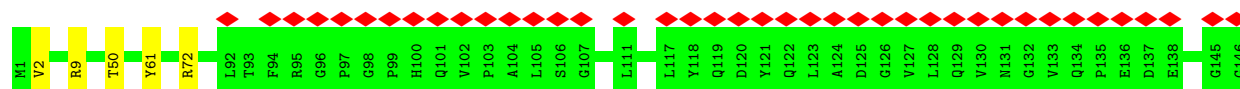


• Molecule 7: Collar (P74p112)

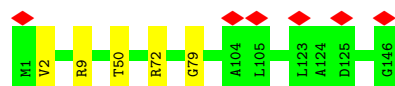
Chain Hf:  91% 9%



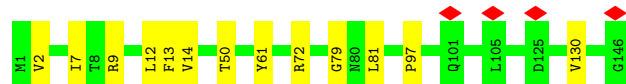
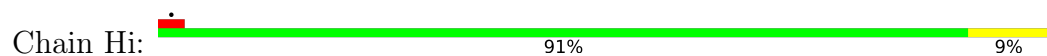
• Molecule 7: Collar (P74p112)



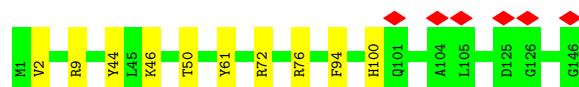
- Molecule 7: Collar (P74p112)



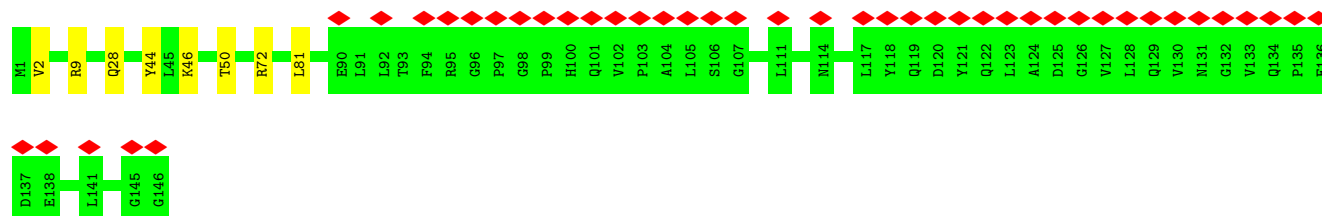
- Molecule 7: Collar (P74p112)



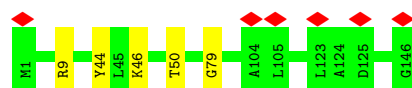
- Molecule 7: Collar (P74p112)



- Molecule 7: Collar (P74p112)

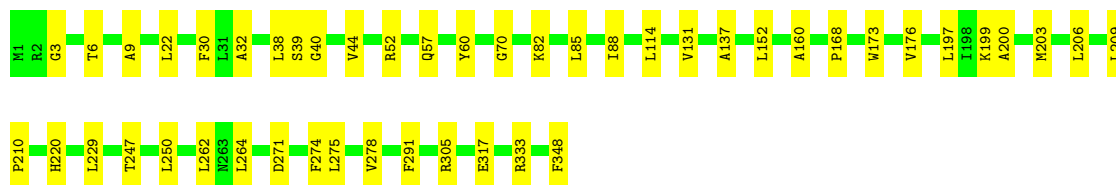


- Molecule 7: Collar (P74p112)



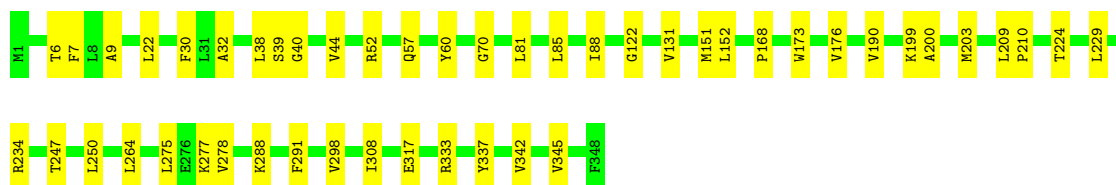
- Molecule 8: Tail Tube Protein gp93

Chain Ia:  86% 14%



- Molecule 8: Tail Tube Protein gp93

Chain Ib:  86% 14%



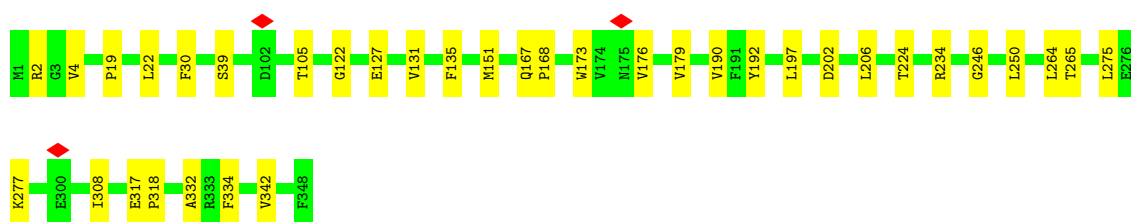
- Molecule 8: Tail Tube Protein gp93

Chain Ic:  91% 9%



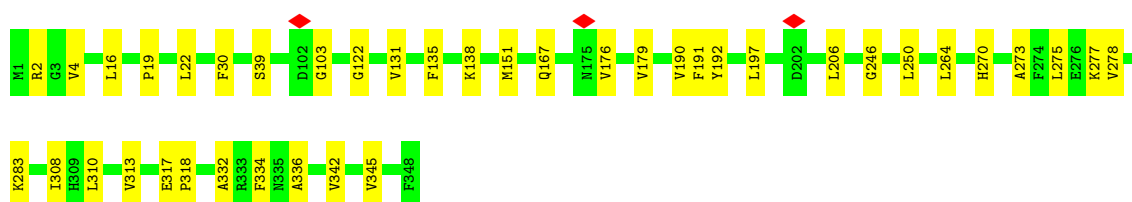
- Molecule 8: Tail Tube Protein gp93

Chain Id:  90% 10%



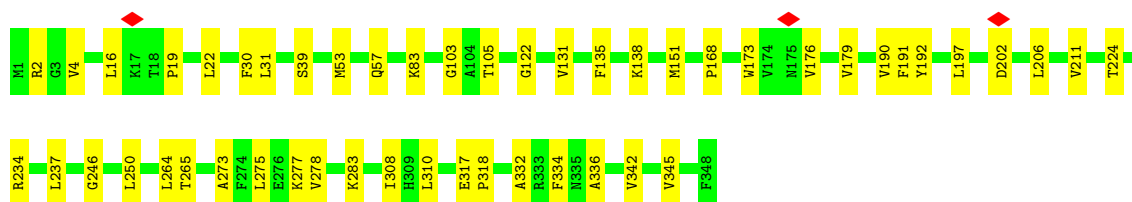
- Molecule 8: Tail Tube Protein gp93

Chain Ie:  89% 11%



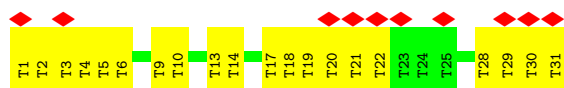
- Molecule 8: Tail Tube Protein gp93

Chain If:  86% 14%



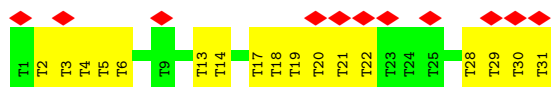
• Molecule 9: DNA (31-MER)

Chain Ja:  32% 35% 65%



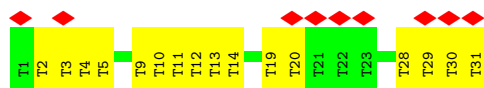
• Molecule 9: DNA (31-MER)

Chain Jc:  35% 45% 55%



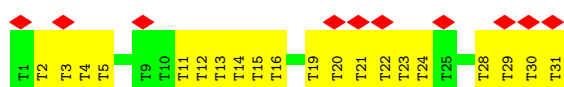
• Molecule 9: DNA (31-MER)

Chain Je:  29% 48% 52%



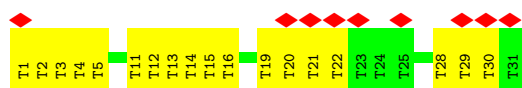
• Molecule 9: DNA (31-MER)

Chain Jg:  32% 35% 65%



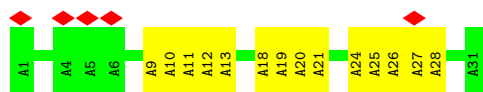
• Molecule 9: DNA (31-MER)

Chain Ji:  29% 42% 58%

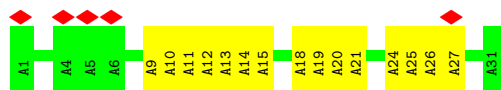


• Molecule 10: DNA (31-MER)

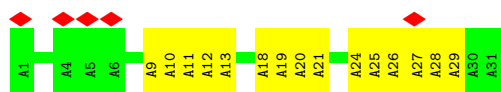
Chain Jb:  16% 55% 45%



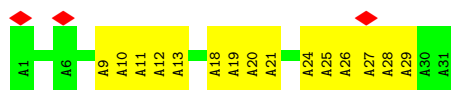
- Molecule 10: DNA (31-MER)



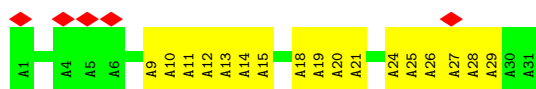
- Molecule 10: DNA (31-MER)



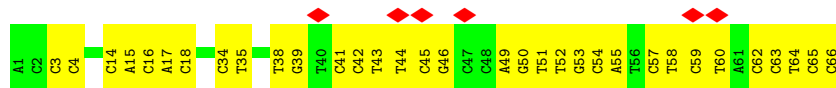
- Molecule 10: DNA (31-MER)



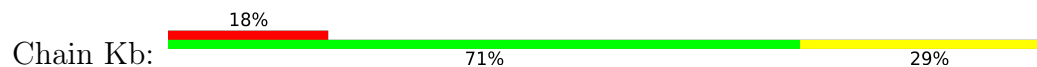
- Molecule 10: DNA (31-MER)



- Molecule 11: DNA (66-MER)



- Molecule 12: DNA (66-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90827	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	1.291	Depositor
Minimum map value	-0.589	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.15	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	0.09	0/291	0.29	0/394
1	Ab	0.10	0/3182	0.31	0/4333
1	Ac	0.10	0/3391	0.31	0/4618
1	Ad	0.08	0/1949	0.24	0/2647
1	Ae	0.10	0/291	0.31	0/394
1	Af	0.10	0/3182	0.29	0/4333
1	Ag	0.10	0/3391	0.31	0/4618
1	Ah	0.07	0/1949	0.24	0/2647
1	Ai	0.09	0/291	0.34	0/394
1	Aj	0.10	0/3182	0.29	0/4333
1	Ak	0.10	0/3391	0.31	0/4618
1	Al	0.07	0/1949	0.25	0/2647
1	Am	0.09	0/291	0.31	0/394
1	An	0.10	0/3182	0.29	0/4333
1	Ao	0.10	0/3391	0.31	0/4618
1	Ap	0.07	0/1949	0.23	0/2647
1	Aq	0.09	0/291	0.32	0/394
1	Ar	0.10	0/3182	0.29	0/4333
1	As	0.11	0/3391	0.32	0/4618
1	At	0.07	0/1949	0.24	0/2647
2	Ba	0.08	0/231	0.20	0/311
2	Bb	0.10	0/1203	0.29	0/1648
2	Bc	0.10	0/1203	0.29	0/1648
2	Bd	0.12	0/1203	0.30	0/1648
2	Be	0.07	0/231	0.19	0/311
2	Bf	0.10	0/1203	0.29	0/1648
2	Bg	0.10	0/1203	0.30	0/1648
2	Bh	0.11	0/1203	0.30	0/1648
2	Bi	0.07	0/231	0.19	0/311
2	Bj	0.10	0/1203	0.29	0/1648
2	Bk	0.11	0/1203	0.30	0/1648
2	Bl	0.10	0/1203	0.28	0/1648
2	Bm	0.07	0/231	0.19	0/311
2	Bn	0.10	0/1203	0.29	0/1648

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Bo	0.10	0/1203	0.28	0/1648
2	Bp	0.09	0/1203	0.29	0/1648
2	Bq	0.07	0/231	0.21	0/311
2	Br	0.10	0/1203	0.34	0/1648
2	Bs	0.10	0/1203	0.29	0/1648
2	Bt	0.10	0/1203	0.29	0/1648
3	Ca	0.12	0/609	0.37	0/826
3	Cb	0.12	0/609	0.32	0/826
3	Cc	0.14	0/609	0.35	0/826
3	Cd	0.12	0/609	0.34	0/826
3	Ce	0.12	0/609	0.33	0/826
4	Da	0.24	0/3362	0.31	0/4567
4	Db	0.24	0/3362	0.31	0/4567
4	Dc	0.24	0/3362	0.32	0/4567
4	Dd	0.24	0/3362	0.30	0/4567
4	De	0.24	0/3362	0.31	0/4567
4	Df	0.24	0/3362	0.31	0/4567
4	Dg	0.24	0/3362	0.31	0/4567
4	Dh	0.24	0/3362	0.31	0/4567
4	Di	0.24	0/3362	0.30	0/4567
4	Dj	0.24	0/3362	0.31	0/4567
4	Dk	0.24	0/3362	0.31	0/4567
4	Dl	0.24	0/3362	0.31	0/4567
5	Ea	0.26	0/1050	0.33	0/1426
5	Eb	0.25	0/1050	0.31	0/1426
5	Ec	0.25	0/1050	0.33	0/1426
5	Ed	0.25	0/1050	0.32	0/1426
5	Ee	0.25	0/1050	0.34	0/1426
5	Ef	0.24	0/1050	0.33	0/1426
5	Eg	0.26	0/1050	0.34	0/1426
5	Eh	0.25	0/1050	0.31	0/1426
5	Ei	0.26	0/1050	0.33	0/1426
5	Ej	0.25	0/1050	0.30	0/1426
5	Ek	0.26	0/1050	0.33	0/1426
5	El	0.25	0/1050	0.30	0/1426
6	Fa	0.21	0/1279	0.36	0/1739
6	Fb	0.21	0/1279	0.38	0/1739
6	Fc	0.21	0/1279	0.36	0/1739
6	Fd	0.21	0/1279	0.38	0/1739
6	Fe	0.21	0/1279	0.36	0/1739
6	Ff	0.21	0/1279	0.36	0/1739
7	Ga	0.19	0/1168	0.28	0/1591
7	Gb	0.19	0/1168	0.28	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	Gc	0.22	0/712	0.28	0/967
7	Gd	0.23	0/712	0.30	0/967
7	Ge	0.19	0/1168	0.28	0/1591
7	Gf	0.19	0/1168	0.28	0/1591
7	Gg	0.21	0/712	0.29	0/967
7	Gh	0.22	0/712	0.29	0/967
7	Gi	0.20	0/1168	0.29	0/1591
7	Gj	0.19	0/1168	0.27	0/1591
7	Gk	0.22	0/712	0.29	0/967
7	Gl	0.23	0/712	0.30	0/967
7	Ha	0.22	0/1168	0.32	0/1591
7	Hb	0.23	0/1168	0.31	0/1591
7	Hc	0.23	0/1168	0.33	0/1591
7	Hd	0.24	0/1168	0.32	0/1591
7	He	0.23	0/1168	0.32	0/1591
7	Hf	0.23	0/1168	0.32	0/1591
7	Hg	0.23	0/1168	0.32	0/1591
7	Hh	0.24	0/1168	0.33	0/1591
7	Hi	0.22	0/1168	0.31	0/1591
7	Hj	0.23	0/1168	0.32	0/1591
7	Hk	0.24	0/1168	0.35	0/1591
7	Hl	0.25	0/1168	0.32	0/1591
8	Ia	0.14	0/2737	0.34	0/3719
8	Ib	0.14	0/2737	0.34	0/3719
8	Ic	0.15	0/2737	0.33	0/3719
8	Id	0.11	0/2737	0.28	0/3719
8	Ie	0.11	0/2737	0.28	0/3719
8	If	0.11	0/2737	0.29	0/3719
9	Ja	0.24	0/681	0.58	0/1050
9	Jc	0.23	0/681	0.59	0/1050
9	Je	0.23	0/681	0.58	0/1050
9	Jg	0.23	0/681	0.58	0/1050
9	Ji	0.23	0/681	0.59	0/1050
10	Jb	0.21	0/743	0.43	0/1143
10	Jd	0.22	0/743	0.43	0/1143
10	Jf	0.21	0/743	0.43	0/1143
10	Jh	0.21	0/743	0.44	0/1143
10	Jj	0.21	0/743	0.44	0/1143
11	Ka	0.33	0/1492	0.82	0/2295
12	Kb	0.31	0/1542	0.72	0/2383
All	All	0.19	0/178800	0.33	0/245112

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

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	27	0
1	Ac	3303	0	3255	34	0
1	Ad	1901	0	1862	10	0
1	Ae	288	0	313	9	0
1	Af	3100	0	3055	35	0
1	Ag	3303	0	3255	40	0
1	Ah	1901	0	1862	13	0
1	Ai	288	0	313	8	0
1	Aj	3100	0	3055	29	0
1	Ak	3303	0	3255	42	0
1	Al	1901	0	1862	15	0
1	Am	288	0	313	7	0
1	An	3100	0	3055	29	0
1	Ao	3303	0	3255	36	0
1	Ap	1901	0	1862	17	0
1	Aq	288	0	313	7	0
1	Ar	3100	0	3055	34	0
1	As	3303	0	3255	40	0
1	At	1901	0	1862	14	0
2	Ba	225	0	212	3	0
2	Bb	1161	0	1129	10	0
2	Bc	1161	0	1129	11	0
2	Bd	1161	0	1129	11	0
2	Be	225	0	212	3	0
2	Bf	1161	0	1129	12	0
2	Bg	1161	0	1129	12	0
2	Bh	1161	0	1129	10	0
2	Bi	225	0	212	2	0
2	Bj	1161	0	1129	10	0
2	Bk	1161	0	1129	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bl	1161	0	1129	13	0
2	Bm	225	0	212	0	0
2	Bn	1161	0	1129	9	0
2	Bo	1161	0	1129	11	0
2	Bp	1161	0	1129	12	0
2	Bq	225	0	212	4	0
2	Br	1161	0	1129	7	0
2	Bs	1161	0	1129	7	0
2	Bt	1161	0	1129	14	0
3	Ca	595	0	584	1	0
3	Cb	595	0	584	2	0
3	Cc	595	0	584	4	0
3	Cd	595	0	584	4	0
3	Ce	595	0	584	4	0
4	Da	3288	0	3319	11	0
4	Db	3288	0	3319	10	0
4	Dc	3288	0	3319	10	0
4	Dd	3288	0	3319	13	0
4	De	3288	0	3319	8	0
4	Df	3288	0	3319	10	0
4	Dg	3288	0	3319	9	0
4	Dh	3288	0	3319	10	0
4	Di	3288	0	3319	11	0
4	Dj	3288	0	3319	11	0
4	Dk	3288	0	3319	10	0
4	Dl	3288	0	3319	10	0
5	Ea	1027	0	1017	7	0
5	Eb	1027	0	1017	4	0
5	Ec	1027	0	1017	6	0
5	Ed	1027	0	1017	6	0
5	Ee	1027	0	1017	6	0
5	Ef	1027	0	1017	4	0
5	Eg	1027	0	1017	6	0
5	Eh	1027	0	1017	4	0
5	Ei	1027	0	1017	7	0
5	Ej	1027	0	1017	5	0
5	Ek	1027	0	1017	6	0
5	El	1027	0	1017	7	0
6	Fa	1244	0	1200	16	0
6	Fb	1244	0	1200	18	0
6	Fc	1244	0	1200	21	0
6	Fd	1244	0	1200	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Fe	1244	0	1200	14	0
6	Ff	1244	0	1200	16	0
7	Ga	1141	0	1140	3	0
7	Gb	1141	0	1140	4	0
7	Gc	695	0	696	2	0
7	Gd	695	0	696	2	0
7	Ge	1141	0	1140	2	0
7	Gf	1141	0	1140	4	0
7	Gg	695	0	696	2	0
7	Gh	695	0	696	1	0
7	Gi	1141	0	1140	4	0
7	Gj	1141	0	1140	4	0
7	Gk	695	0	696	1	0
7	Gl	695	0	696	1	0
7	Ha	1141	0	1140	7	0
7	Hb	1141	0	1140	4	0
7	Hc	1141	0	1140	5	0
7	Hd	1141	0	1140	6	0
7	He	1141	0	1140	8	0
7	Hf	1141	0	1140	7	0
7	Hg	1141	0	1140	3	0
7	Hh	1141	0	1140	3	0
7	Hi	1141	0	1140	8	0
7	Hj	1141	0	1140	6	0
7	Hk	1141	0	1140	5	0
7	Hl	1141	0	1140	3	0
8	Ia	2679	0	2643	34	0
8	Ib	2679	0	2643	35	0
8	Ic	2679	0	2643	20	0
8	Id	2679	0	2643	22	0
8	Ie	2679	0	2643	26	0
8	If	2679	0	2643	31	0
9	Ja	620	0	373	12	0
9	Jc	620	0	373	10	0
9	Je	620	0	373	9	0
9	Jg	620	0	373	11	0
9	Ji	620	0	373	10	0
10	Jb	651	0	342	9	0
10	Jd	651	0	342	10	0
10	Jf	651	0	342	14	0
10	Jh	651	0	342	13	0
10	Jj	651	0	342	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Ka	1334	0	741	27	0
12	Kb	1372	0	742	13	0
All	All	173562	0	168184	1081	0

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

All (1081) 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)
6:Fb:33:ILE:HG12	6:Fb:47:ALA:HB3	1.58	0.86
6:Fc:33:ILE:HG12	6:Fc:47:ALA:HB3	1.58	0.85
6:Fe:33:ILE:HG12	6:Fe:47:ALA:HB3	1.61	0.83
6:Fa:33:ILE:HG12	6:Fa:47:ALA:HB3	1.60	0.83
5:Ek:87:GLN:HG3	6:Ff:135:PHE:HB3	1.61	0.82
6:Ff:33:ILE:HG12	6:Ff:47:ALA:HB3	1.61	0.82
5:Ec:87:GLN:HG3	6:Fb:135:PHE:HB3	1.62	0.81
6:Fd:33:ILE:HG12	6:Fd:47:ALA:HB3	1.63	0.80
5:Ei:87:GLN:HG3	6:Fe:135:PHE:HB3	1.66	0.78
5:Eg:87:GLN:HG3	6:Fd:135:PHE:HB3	1.66	0.77
5:Ea:87:GLN:HG3	6:Fa:135:PHE:HB3	1.67	0.76
5:Ee:87:GLN:HG3	6:Fc:135:PHE:HB3	1.68	0.76
1:Aj:181:LEU:HD21	2:Bh:31:PRO:HB2	1.70	0.74
11:Ka:54:DC:H2'	11:Ka:55:DA:C8	2.25	0.72
1:As:48:LEU:HD21	1:As:236:ILE:HD12	1.71	0.71
1:Af:29:LYS:HE3	1:Af:31:ILE:HD11	1.70	0.71
1:Af:181:LEU:HD21	2:Bd:31:PRO:HB2	1.74	0.69
8:Id:197:LEU:HB3	8:Id:206:LEU:HB3	1.76	0.68
10:Jf:10:DA:H2'	10:Jf:11:DA:C8	2.28	0.68
1:Ak:232:PRO:HA	1:Ak:318:ASN:HA	1.76	0.68
2:Bh:85:LEU:HG	2:Bh:99:THR:HG21	1.76	0.68
7:Hl:9:ARG:HA	7:Hl:50:THR:HG22	1.76	0.67
7:Hh:9:ARG:HA	7:Hh:50:THR:HG22	1.78	0.66
7:Hk:9:ARG:HA	7:Hk:50:THR:HG22	1.77	0.66
2:Bg:53:LEU:HD11	2:Bg:133:LEU:HD11	1.77	0.66
1:Al:208:ASN:HA	1:Al:249:THR:HG21	1.78	0.66
1:Ad:186:ASP:H	2:Bd:1:MET:HG3	1.59	0.66
1:Ar:181:LEU:HD21	2:Bp:31:PRO:HB2	1.78	0.66
12:Kb:32:DA:H2'	12:Kb:33:DG:C8	2.31	0.66
10:Jj:10:DA:H2'	10:Jj:11:DA:C8	2.31	0.66
7:Hb:9:ARG:HA	7:Hb:50:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bo:116:PRO:HB2	2:Bo:119:GLN:HB2	1.79	0.65
7:Hj:9:ARG:HA	7:Hj:50:THR:HG22	1.78	0.65
7:Hc:9:ARG:HA	7:Hc:50:THR:HG22	1.78	0.65
7:Hf:9:ARG:HA	7:Hf:50:THR:HG22	1.79	0.65
7:Hg:9:ARG:HA	7:Hg:50:THR:HG22	1.79	0.65
6:Fb:63:MET:HE3	8:Ia:32:ALA:HB2	1.78	0.65
1:Ac:313:GLU:HG2	1:Ac:389:TRP:CE3	2.32	0.65
10:Jb:10:DA:H2'	10:Jb:11:DA:C8	2.32	0.65
2:Bs:116:PRO:HB2	2:Bs:119:GLN:HB2	1.79	0.64
8:If:264:LEU:HD12	8:If:277:LYS:HE3	1.78	0.64
1:Ab:181:LEU:HD21	2:Bt:31:PRO:HB2	1.79	0.64
1:An:181:LEU:HD21	2:Bl:31:PRO:HB2	1.79	0.64
5:Ef:38:ARG:HH12	7:Ge:29:ASP:HA	1.63	0.64
10:Jh:10:DA:H2'	10:Jh:11:DA:C8	2.34	0.63
1:Ab:29:LYS:HE3	1:Ab:31:ILE:HD11	1.81	0.63
1:As:3:VAL:HG22	2:Bt:15:TYR:HB3	1.81	0.63
9:Jg:11:DT:H2'	9:Jg:12:DT:H71	1.78	0.63
6:Fb:4:ASP:HB3	6:Fb:74:ILE:HD13	1.80	0.63
7:He:9:ARG:HA	7:He:50:THR:HG22	1.81	0.63
1:Ar:29:LYS:HE3	1:Ar:31:ILE:HD11	1.80	0.63
8:Ie:264:LEU:HD12	8:Ie:277:LYS:HE3	1.81	0.63
8:Ia:317:GLU:OE1	8:Ic:39:SER:HB2	1.99	0.62
7:Hi:9:ARG:HA	7:Hi:50:THR:HG22	1.81	0.62
1:Ag:232:PRO:HA	1:Ag:318:ASN:HA	1.82	0.62
8:If:197:LEU:HB3	8:If:206:LEU:HB3	1.80	0.62
9:Je:11:DT:H2'	9:Je:12:DT:H71	1.81	0.62
8:Ie:197:LEU:HB3	8:Ie:206:LEU:HB3	1.80	0.62
9:Jg:15:DT:H2'	9:Jg:16:DT:H71	1.81	0.62
5:Ef:89:LEU:HD11	5:Eg:84:ARG:HG2	1.82	0.62
7:Hd:9:ARG:HA	7:Hd:50:THR:HG22	1.81	0.62
8:Ia:264:LEU:HD21	8:Ia:278:VAL:HG22	1.82	0.62
8:Ie:16:LEU:HD13	8:Ie:138:LYS:HE3	1.82	0.62
6:Fa:60:ARG:HD3	8:Ia:210:PRO:HB2	1.82	0.61
1:Ac:232:PRO:HA	1:Ac:318:ASN:HA	1.81	0.61
10:Jd:10:DA:H2'	10:Jd:11:DA:C8	2.35	0.61
11:Ka:51:DT:H2'	11:Ka:52:DT:H72	1.83	0.61
11:Ka:44:DT:H2'	11:Ka:45:DC:C5	2.36	0.61
5:Eh:89:LEU:HD11	5:Ei:84:ARG:HG2	1.81	0.60
12:Kb:59:DA:H2''	12:Kb:60:DT:C6	2.35	0.60
2:Bk:116:PRO:HB2	2:Bk:119:GLN:HB2	1.83	0.60
8:Ic:22:LEU:HD22	8:Ic:176:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bo:121:ASP:HB3	2:Bo:124:VAL:HG12	1.82	0.60
9:Ja:21:DT:H2'	9:Ja:22:DT:H71	1.83	0.60
11:Ka:41:DC:H2''	11:Ka:42:DC:C5	2.36	0.60
1:Ap:208:ASN:HA	1:Ap:249:THR:HG21	1.83	0.60
7:Ha:9:ARG:HA	7:Ha:50:THR:HG22	1.83	0.60
2:Bl:85:LEU:HG	2:Bl:99:THR:HG21	1.82	0.60
1:Ah:54:PRO:HD2	1:Ah:326:ARG:HA	1.84	0.59
9:Ji:11:DT:H2'	9:Ji:12:DT:H71	1.83	0.59
8:Ib:39:SER:HB2	8:Ic:317:GLU:OE1	2.02	0.59
5:Ej:38:ARG:HH12	7:Gi:29:ASP:HA	1.68	0.59
6:Fd:63:MET:HE3	8:Ib:32:ALA:HB2	1.82	0.59
1:Ap:232:PRO:HA	1:Ap:318:ASN:HA	1.85	0.59
5:Ed:89:LEU:HD11	5:Ee:84:ARG:HG2	1.83	0.59
6:Ff:4:ASP:HB3	6:Ff:74:ILE:HD13	1.85	0.59
1:Ak:121:ILE:HG12	1:Ak:136:ILE:HG12	1.84	0.59
9:Jc:21:DT:H2'	9:Jc:22:DT:H71	1.85	0.59
9:Ji:21:DT:H2'	9:Ji:22:DT:H71	1.85	0.59
11:Ka:44:DT:H2'	11:Ka:45:DC:C6	2.38	0.59
11:Ka:43:DT:H2'	11:Ka:44:DT:H71	1.85	0.59
1:Ak:313:GLU:HG2	1:Ak:389:TRP:CE3	2.38	0.58
8:Ia:22:LEU:HD22	8:Ia:176:VAL:HG21	1.86	0.58
9:Ji:15:DT:H2'	9:Ji:16:DT:H71	1.84	0.58
12:Kb:59:DA:H2''	12:Kb:60:DT:H6	1.68	0.58
1:Ao:126:ARG:HB3	1:Ao:129:ASP:HB2	1.85	0.58
1:Aq:31:ILE:HG12	1:Ar:64:GLU:HB2	1.84	0.58
8:Id:264:LEU:HD12	8:Id:277:LYS:HE3	1.83	0.58
1:Ad:208:ASN:HA	1:Ad:249:THR:HG21	1.85	0.58
9:Jg:23:DT:H2'	9:Jg:24:DT:H71	1.86	0.58
6:Ff:63:MET:HE3	8:Ic:32:ALA:HB2	1.85	0.58
1:Al:232:PRO:HA	1:Al:318:ASN:HA	1.86	0.58
2:Bg:116:PRO:HB2	2:Bg:119:GLN:HB2	1.86	0.58
8:Ic:264:LEU:HD21	8:Ic:278:VAL:HG22	1.85	0.58
5:El:38:ARG:HH12	7:Gk:29:ASP:HA	1.69	0.58
2:Bl:132:LYS:HB3	2:Bl:146:ARG:HH21	1.68	0.57
6:Fa:4:ASP:HB3	6:Fa:74:ILE:HD13	1.86	0.57
8:Id:22:LEU:HD22	8:Id:176:VAL:HG21	1.86	0.57
2:Bs:121:ASP:HB3	2:Bs:124:VAL:HG12	1.86	0.57
1:As:52:PHE:HA	1:As:323:PRO:HA	1.86	0.57
1:As:126:ARG:HB3	1:As:129:ASP:HB2	1.85	0.57
2:Bc:121:ASP:HB3	2:Bc:124:VAL:HG12	1.86	0.57
2:Bk:121:ASP:HB3	2:Bk:124:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Ka:65:DC:H2'	11:Ka:66:DC:C6	2.39	0.57
1:At:93:ALA:HB1	2:Bt:17:GLU:HB2	1.86	0.57
4:Dh:269:PHE:HA	4:Dh:275:HIS:CE1	2.40	0.57
8:Id:167:GLN:NE2	8:Ie:273:ALA:HB3	2.20	0.57
1:As:57:SER:HB3	3:Ce:1:MET:HE1	1.87	0.57
1:Ag:313:GLU:HG2	1:Ag:389:TRP:CE3	2.40	0.56
6:Ff:80:ILE:HB	6:Ff:144:VAL:HB	1.86	0.56
8:Ic:199:LYS:HA	8:Ic:203:MET:HE2	1.87	0.56
1:Am:31:ILE:HG12	1:An:64:GLU:HB2	1.88	0.56
1:At:208:ASN:HA	1:At:249:THR:HG21	1.87	0.56
11:Ka:57:DC:H2''	11:Ka:58:DT:C6	2.41	0.56
1:Ad:54:PRO:HD2	1:Ad:326:ARG:HA	1.86	0.56
1:Ai:31:ILE:HG12	1:Aj:64:GLU:HB2	1.87	0.56
1:Al:97:LYS:HB3	2:Bl:14:GLN:HG2	1.87	0.56
1:Ao:203:LYS:HA	1:Ao:209:SER:HA	1.87	0.56
5:Ed:38:ARG:HH12	7:Gc:29:ASP:HA	1.70	0.56
2:Bh:71:LEU:HD11	2:Bh:123:ALA:HB1	1.87	0.56
8:Ia:137:ALA:HA	8:Ia:160:ALA:HA	1.87	0.56
2:Bn:106:ILE:HD13	2:Bn:125:LEU:HD21	1.86	0.56
5:Eh:38:ARG:HH12	7:Gg:29:ASP:HA	1.71	0.56
1:Ag:144:LEU:HD22	1:Ag:349:LEU:HD21	1.87	0.56
6:Fd:155:GLN:HG3	6:Fe:99:TRP:HH2	1.71	0.56
1:Ao:176:TYR:CZ	1:Ap:77:GLY:HA2	2.41	0.56
1:Ak:313:GLU:HG2	1:Ak:389:TRP:HE3	1.71	0.55
1:At:67:LEU:HD23	1:At:382:PHE:HE1	1.71	0.55
8:Ie:308:ILE:HG12	8:Ie:342:VAL:HG22	1.88	0.55
1:Ah:186:ASP:H	2:Bh:1:MET:HG3	1.71	0.55
2:Bp:85:LEU:HG	2:Bp:99:THR:HG21	1.88	0.55
1:At:54:PRO:HD2	1:At:326:ARG:HA	1.87	0.55
8:Ib:264:LEU:HD21	8:Ib:278:VAL:HG22	1.87	0.55
1:Ac:52:PHE:HA	1:Ac:323:PRO:HA	1.88	0.55
6:Fb:155:GLN:HG3	6:Fc:99:TRP:HH2	1.71	0.55
1:Ap:54:PRO:HD2	1:Ap:326:ARG:HA	1.88	0.55
1:An:208:ASN:HA	1:An:249:THR:HG21	1.89	0.55
1:At:232:PRO:HA	1:At:318:ASN:HA	1.89	0.55
5:Eb:89:LEU:HD11	5:Ec:84:ARG:HG2	1.88	0.55
6:Fb:80:ILE:HB	6:Fb:144:VAL:HB	1.89	0.55
7:Hf:94:PHE:HB3	7:Hf:100:HIS:CD2	2.42	0.55
10:Jd:18:DA:H2''	10:Jd:19:DA:C8	2.42	0.55
12:Kb:1:DG:H2'	12:Kb:2:DG:C8	2.42	0.55
7:Gb:89:VAL:HG13	7:Gb:142:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ib:22:LEU:HD22	8:Ib:176:VAL:HG21	1.89	0.54
5:Ej:89:LEU:HD11	5:Ek:84:ARG:HG2	1.89	0.54
8:Ia:85:LEU:HD23	8:Ia:88:ILE:HD12	1.89	0.54
1:Ac:337:ARG:O	1:Ac:340:LYS:HE2	2.08	0.54
4:Da:391:MET:HE2	4:Da:423:LEU:HD22	1.90	0.54
4:Dd:421:ARG:NH2	4:De:83:LYS:HG3	2.22	0.54
4:Dk:269:PHE:HA	4:Dk:275:HIS:CE1	2.42	0.54
1:Ag:409:LEU:HD21	1:Ah:99:ASP:HB2	1.89	0.54
1:Al:186:ASP:H	2:Bl:1:MET:HG3	1.72	0.54
7:Gi:48:GLU:HG2	7:Gi:85:ALA:HA	1.88	0.54
8:If:19:PRO:HB3	8:If:135:PHE:HB3	1.89	0.54
11:Ka:63:DC:C6	11:Ka:64:DT:H72	2.42	0.54
1:Af:404:PRO:HB3	1:Ag:227:PHE:CE1	2.42	0.54
1:Ak:214:ILE:HG22	1:Ak:218:ARG:HH12	1.73	0.54
8:Ia:39:SER:HB2	8:Ib:317:GLU:OE1	2.07	0.54
2:Bk:53:LEU:HD11	2:Bk:133:LEU:HD11	1.89	0.54
4:Di:241:ILE:HG13	4:Dj:274:ARG:HD3	1.89	0.54
8:Ib:199:LYS:HA	8:Ib:203:MET:HE2	1.88	0.54
1:Ai:3:VAL:HG11	1:Aj:98:VAL:HG23	1.89	0.54
1:Ak:255:VAL:HA	1:Ak:282:ILE:HD13	1.89	0.54
2:Bo:53:LEU:HD11	2:Bo:133:LEU:HD11	1.89	0.54
4:Da:269:PHE:HA	4:Da:275:HIS:CE1	2.43	0.54
8:If:190:VAL:HG21	8:If:192:TYR:CZ	2.43	0.54
1:Ak:95:VAL:HB	2:Bj:16:TRP:CD2	2.43	0.54
1:Ar:172:PRO:HA	1:Ar:180:GLY:HA2	1.90	0.54
1:As:313:GLU:HG2	1:As:389:TRP:HE3	1.73	0.53
8:Ia:247:THR:HG22	8:Ia:333:ARG:HG2	1.89	0.53
10:Jh:18:DA:H2''	10:Jh:19:DA:C8	2.43	0.53
1:Ap:186:ASP:H	2:Bp:1:MET:HG3	1.72	0.53
1:Ar:120:GLU:HB2	3:Ce:31:ARG:NH2	2.23	0.53
11:Ka:15:DA:H2'	11:Ka:16:DC:C6	2.43	0.53
6:Fe:60:ARG:HD3	8:Ic:210:PRO:HB2	1.90	0.53
8:Id:318:PRO:HA	8:Id:332:ALA:HA	1.91	0.53
1:As:232:PRO:HA	1:As:318:ASN:HA	1.89	0.53
1:Aj:230:ARG:HG2	1:Aj:385:HIS:CG	2.43	0.53
11:Ka:3:DC:H1'	11:Ka:4:DC:C5	2.44	0.53
1:Ag:95:VAL:HB	2:Bf:16:TRP:CD2	2.44	0.53
1:Aq:3:VAL:HG11	1:Ar:98:VAL:HG23	1.91	0.53
2:Bb:146:ARG:HD2	2:Bs:146:ARG:HH12	1.74	0.53
1:Al:54:PRO:HD2	1:Al:326:ARG:HA	1.89	0.53
6:Fc:60:ARG:HD3	8:Ib:210:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ah:208:ASN:HA	1:Ah:249:THR:HG21	1.91	0.53
1:Aq:11:LEU:HD21	1:Ar:68:LEU:HB2	1.91	0.53
1:Ac:126:ARG:HB3	1:Ac:129:ASP:HB2	1.90	0.53
1:Aj:186:ASP:HB2	2:Bi:1:MET:HG3	1.90	0.53
11:Ka:64:DT:H2'	11:Ka:65:DC:C5	2.43	0.52
2:Bs:1:MET:HG2	2:Bs:3:LYS:H	1.74	0.52
11:Ka:62:DC:H2'	11:Ka:63:DC:C6	2.45	0.52
1:Ao:313:GLU:HG2	1:Ao:389:TRP:CE3	2.45	0.52
6:Fe:4:ASP:HB3	6:Fe:74:ILE:HD13	1.90	0.52
4:Dj:248:ILE:HD11	4:Dj:259:TRP:CZ3	2.44	0.52
7:Gj:27:PRO:HD3	7:Gj:58:GLY:HA2	1.92	0.52
7:Gb:27:PRO:HD3	7:Gb:58:GLY:HA2	1.92	0.52
7:Ge:48:GLU:HG2	7:Ge:85:ALA:HA	1.91	0.52
1:Ar:32:GLN:HB2	1:As:65:LEU:HD23	1.91	0.52
8:Ia:199:LYS:HA	8:Ia:203:MET:HE2	1.91	0.52
1:Ad:232:PRO:HA	1:Ad:318:ASN:HA	1.92	0.52
6:Fc:4:ASP:HB3	6:Fc:74:ILE:HD13	1.91	0.52
9:Jg:21:DT:H2'	9:Jg:22:DT:H71	1.92	0.52
8:Id:190:VAL:HG21	8:Id:192:TYR:CZ	2.45	0.52
1:Aa:11:LEU:HD21	1:Ab:68:LEU:HB2	1.91	0.52
1:Ab:172:PRO:HA	1:Ab:180:GLY:HA2	1.92	0.52
1:Ah:93:ALA:HB1	2:Bh:17:GLU:HB2	1.92	0.52
1:As:176:TYR:CZ	1:At:77:GLY:HA2	2.44	0.52
1:Ao:110:PHE:CZ	1:Ao:158:LEU:HD11	2.45	0.51
1:Ao:255:VAL:HA	1:Ao:282:ILE:HD13	1.92	0.51
1:At:97:LYS:HB3	2:Bt:14:GLN:HG2	1.92	0.51
8:If:2:ARG:HB2	8:If:4:VAL:HG22	1.92	0.51
1:Ae:3:VAL:HG11	1:Af:98:VAL:HG23	1.92	0.51
1:Ah:232:PRO:HA	1:Ah:318:ASN:HA	1.91	0.51
8:If:103:GLY:H	8:If:345:VAL:HG22	1.75	0.51
4:Db:258:GLN:HE22	5:Ea:115:VAL:HB	1.74	0.51
8:Ib:9:ALA:HB2	8:Ib:30:PHE:CD1	2.45	0.51
1:Aj:176:TYR:CZ	1:Ak:77:GLY:HA2	2.46	0.51
10:Jf:9:DA:H2'	10:Jf:10:DA:H8	1.76	0.51
1:Aa:31:ILE:HG12	1:Ab:64:GLU:HB2	1.92	0.51
2:Bg:121:ASP:HB3	2:Bg:124:VAL:HG12	1.92	0.51
4:Da:83:LYS:HG3	4:Dl:421:ARG:NH2	2.25	0.51
1:Af:48:LEU:HB2	1:Af:294:TYR:CE1	2.46	0.51
1:Ag:176:TYR:CZ	1:Ah:77:GLY:HA2	2.46	0.51
1:Ah:67:LEU:HD23	1:Ah:382:PHE:HE1	1.75	0.51
7:Ga:48:GLU:HG2	7:Ga:85:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:18:LEU:HD11	1:Aj:100:LEU:HD21	1.92	0.51
4:Db:355:TYR:O	4:Db:359:LYS:HG2	2.11	0.51
8:Ic:247:THR:HG22	8:Ic:333:ARG:HG2	1.93	0.51
9:Je:28:DT:H2'	9:Je:29:DT:H72	1.92	0.51
11:Ka:51:DT:H2'	11:Ka:52:DT:C7	2.40	0.51
1:Ac:13:ARG:HB2	1:Ae:17:PRO:HB3	1.93	0.51
1:An:48:LEU:HB2	1:An:294:TYR:CE1	2.46	0.51
3:Ce:29:ALA:HB1	3:Ce:63:TRP:HB3	1.93	0.51
4:Dg:391:MET:HE2	4:Dg:423:LEU:HD22	1.93	0.51
7:Hf:79:GLY:HA2	7:Hg:61:TYR:OH	2.11	0.51
1:Ac:255:VAL:HA	1:Ac:282:ILE:HD13	1.93	0.50
1:Aj:48:LEU:HB2	1:Aj:294:TYR:CE1	2.45	0.50
1:Ak:126:ARG:HB3	1:Ak:129:ASP:HB2	1.93	0.50
1:Ak:270:PRO:HG2	1:Ak:275:TYR:CE2	2.45	0.50
6:Fd:4:ASP:HB3	6:Fd:74:ILE:HD13	1.92	0.50
10:Jd:26:DA:H2''	10:Jd:27:DA:C8	2.47	0.50
1:Aj:208:ASN:HA	1:Aj:249:THR:HG21	1.92	0.50
1:As:144:LEU:HD22	1:As:349:LEU:HD21	1.93	0.50
2:Bt:34:MET:HE3	2:Bt:40:TRP:CG	2.46	0.50
9:Je:29:DT:H2'	9:Je:30:DT:H71	1.92	0.50
1:Aa:3:VAL:HG11	1:Ab:98:VAL:HG23	1.94	0.50
7:Gd:27:PRO:HD3	7:Gd:58:GLY:HA2	1.94	0.50
1:Ab:235:ILE:HG23	1:Ab:314:LEU:HD13	1.93	0.50
1:Ad:67:LEU:HD23	1:Ad:382:PHE:HE1	1.76	0.50
1:Ag:270:PRO:HG2	1:Ag:275:TYR:CE2	2.46	0.50
1:Ak:18:LEU:HD11	1:An:100:LEU:HD21	1.93	0.50
7:Ha:61:TYR:OH	7:Hi:79:GLY:HA2	2.12	0.50
8:Ia:40:GLY:H	8:Ib:317:GLU:CD	2.18	0.50
2:Bd:136:ILE:HG22	2:Bd:137:LYS:HG3	1.93	0.50
1:As:95:VAL:HB	2:Br:16:TRP:CD2	2.46	0.50
4:Dk:355:TYR:O	4:Dk:359:LYS:HG2	2.12	0.50
5:El:33:SER:HB2	7:Hk:28:GLN:OE1	2.12	0.50
8:Ib:168:PRO:HA	8:Ib:173:TRP:CD1	2.47	0.50
8:Ie:310:LEU:HD13	8:Ie:336:ALA:HB2	1.93	0.50
1:Ag:133:ALA:HA	1:Ai:28:THR:HG21	1.94	0.50
2:Bg:34:MET:HE2	2:Bg:40:TRP:CD2	2.46	0.50
4:De:391:MET:HE2	4:De:423:LEU:HD22	1.94	0.50
6:Fd:62:GLY:HA2	8:Ib:6:THR:O	2.12	0.50
4:Di:355:TYR:O	4:Di:359:LYS:HG2	2.11	0.50
4:Dk:258:GLN:HE22	5:Ej:112:ALA:HB3	1.77	0.50
8:Ie:190:VAL:HG21	8:Ie:192:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:313:GLU:HG2	1:Ac:389:TRP:HE3	1.72	0.50
1:Af:104:THR:OG1	2:Be:5:GLN:HB3	2.12	0.50
2:Bg:53:LEU:HD13	2:Bg:131:LEU:HD23	1.94	0.50
4:Dc:421:ARG:NH2	4:Dd:83:LYS:HG3	2.26	0.50
6:Fa:53:LYS:HG3	6:Fb:124:THR:HG22	1.94	0.50
8:If:318:PRO:HA	8:If:332:ALA:HA	1.93	0.50
1:Ak:3:VAL:HG22	2:Bl:15:TYR:HB3	1.93	0.49
1:Ab:104:THR:OG1	2:Ba:5:GLN:HB3	2.12	0.49
1:Ag:126:ARG:HB3	1:Ag:129:ASP:HB2	1.94	0.49
1:As:203:LYS:HA	1:As:209:SER:HA	1.93	0.49
2:Br:77:VAL:HG13	2:Br:131:LEU:HD23	1.93	0.49
6:Fd:80:ILE:HB	6:Fd:144:VAL:HB	1.94	0.49
8:Ib:85:LEU:HD23	8:Ib:88:ILE:HD12	1.93	0.49
8:If:16:LEU:HD13	8:If:138:LYS:HE3	1.93	0.49
10:Jb:26:DA:H2''	10:Jb:27:DA:C8	2.46	0.49
10:Jh:24:DA:H2''	10:Jh:25:DA:C8	2.47	0.49
1:Ac:9:ASN:O	1:Ac:13:ARG:HG2	2.12	0.49
1:Ar:314:LEU:HD21	1:Ar:390:LEU:HD23	1.94	0.49
2:Bh:34:MET:HE3	2:Bh:40:TRP:CG	2.47	0.49
5:Ek:85:ALA:HB1	6:Ff:139:GLY:HA2	1.94	0.49
8:If:22:LEU:HD22	8:If:176:VAL:HG21	1.94	0.49
9:Jc:29:DT:H2'	9:Jc:30:DT:H71	1.94	0.49
10:Jh:26:DA:H2''	10:Jh:27:DA:C8	2.47	0.49
11:Ka:17:DA:H2''	11:Ka:18:DC:C5	2.48	0.49
11:Ka:43:DT:H2'	11:Ka:44:DT:C7	2.43	0.49
12:Kb:55:DG:H2''	12:Kb:56:DC:C5	2.47	0.49
1:Ag:255:VAL:HA	1:Ag:282:ILE:HD13	1.94	0.49
8:Ia:229:LEU:HD22	8:Ie:191:PHE:HB2	1.95	0.49
1:Ah:83:GLN:HB3	2:Bg:31:PRO:HB3	1.95	0.49
1:Ak:203:LYS:HA	1:Ak:209:SER:HA	1.93	0.49
1:Ao:232:PRO:HA	1:Ao:318:ASN:HA	1.95	0.49
1:Ar:270:PRO:HG2	1:Ar:275:TYR:CE2	2.46	0.49
1:As:313:GLU:HG2	1:As:389:TRP:CE3	2.47	0.49
8:If:30:PHE:HB2	8:If:179:VAL:O	2.12	0.49
1:Ai:38:ILE:HD11	1:Aj:69:ARG:HD2	1.93	0.49
10:Jb:24:DA:H2''	10:Jb:25:DA:C8	2.48	0.49
9:Jg:29:DT:H2'	9:Jg:30:DT:H71	1.94	0.49
1:Ac:270:PRO:HG2	1:Ac:275:TYR:CE2	2.48	0.49
1:An:29:LYS:HE3	1:An:31:ILE:HD11	1.95	0.49
2:Bo:53:LEU:HD13	2:Bo:131:LEU:HD23	1.94	0.49
4:Dj:355:TYR:O	4:Dj:359:LYS:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Gc:48:GLU:HG2	7:Gc:85:ALA:HA	1.94	0.49
8:Ia:250:LEU:HD11	8:Ia:275:LEU:HD11	1.94	0.49
8:Ie:318:PRO:HA	8:Ie:332:ALA:HA	1.95	0.49
2:Bo:1:MET:HG2	2:Bo:3:LYS:H	1.77	0.49
4:Dc:355:TYR:O	4:Dc:359:LYS:HG2	2.13	0.49
8:If:202:ASP:HB2	8:If:265:THR:C	2.38	0.49
9:Je:9:DT:H2'	9:Je:10:DT:H71	1.93	0.49
10:Jj:24:DA:H2''	10:Jj:25:DA:C8	2.48	0.49
1:Af:154:ARG:HB2	1:Ag:78:MET:HB3	1.94	0.49
1:Ao:409:LEU:HD21	1:Ap:99:ASP:HB2	1.95	0.49
1:Aq:9:ASN:O	1:Aq:13:ARG:HG2	2.12	0.49
2:Bb:22:LEU:HD22	2:Bb:25:TYR:H	1.76	0.49
7:Hd:90:GLU:HB2	7:Hd:143:MET:HB2	1.95	0.49
8:Id:151:MET:SD	8:Id:190:VAL:HG12	2.53	0.49
1:Ao:9:ASN:O	1:Ao:13:ARG:HG2	2.13	0.49
2:Bb:106:ILE:HD13	2:Bb:125:LEU:HD21	1.94	0.49
6:Fa:99:TRP:HH2	6:Ff:155:GLN:HG3	1.78	0.49
9:Ja:29:DT:H2'	9:Ja:30:DT:H71	1.95	0.49
10:Jb:18:DA:H2''	10:Jb:19:DA:C8	2.48	0.49
1:Ae:24:LYS:HE3	2:Bd:86:ASP:HB2	1.95	0.48
1:Ak:121:ILE:HG23	1:Ak:136:ILE:HG21	1.95	0.48
7:Gf:89:VAL:HG13	7:Gf:142:VAL:HG13	1.94	0.48
1:Ac:95:VAL:HB	2:Bb:16:TRP:CD2	2.48	0.48
1:Al:67:LEU:HD23	1:Al:382:PHE:HE1	1.78	0.48
1:Ar:107:PRO:HG3	1:Ar:330:THR:HG21	1.94	0.48
8:Ia:317:GLU:CD	8:Ic:40:GLY:H	2.21	0.48
11:Ka:17:DA:H2''	11:Ka:18:DC:C6	2.48	0.48
1:Ac:110:PHE:CZ	1:Ac:158:LEU:HD11	2.48	0.48
2:Bt:136:ILE:HG22	2:Bt:137:LYS:HG3	1.95	0.48
7:Hh:79:GLY:HA2	7:Hi:61:TYR:OH	2.13	0.48
7:Hi:44:TYR:HE2	7:Hi:46:LYS:HG2	1.79	0.48
8:Ia:197:LEU:HB3	8:Ia:206:LEU:HB3	1.94	0.48
2:Bn:16:TRP:HB3	2:Bn:49:PRO:HD3	1.95	0.48
4:De:248:ILE:HD11	4:De:259:TRP:CZ3	2.48	0.48
1:Ak:57:SER:HB3	3:Cc:1:MET:HE1	1.95	0.48
1:Ar:48:LEU:HB2	1:Ar:294:TYR:CE1	2.48	0.48
4:Dg:263:LYS:HA	4:Dh:278:ILE:HD11	1.95	0.48
8:Ie:167:GLN:NE2	8:If:273:ALA:HB3	2.29	0.48
10:Jj:26:DA:H2''	10:Jj:27:DA:C8	2.48	0.48
1:Ak:9:ASN:O	1:Ak:13:ARG:HG2	2.14	0.48
1:Ao:121:ILE:HG23	1:Ao:136:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:208:ASN:HA	1:Ar:249:THR:HG21	1.95	0.48
2:Bj:106:ILE:HD12	2:Bj:138:GLY:HA2	1.95	0.48
4:Dj:421:ARG:NH2	4:Dk:83:LYS:HG3	2.28	0.48
1:Ag:110:PHE:CZ	1:Ag:158:LEU:HD11	2.49	0.48
1:At:317:LEU:HD13	1:At:321:THR:HA	1.96	0.48
3:Cb:29:ALA:HB1	3:Cb:63:TRP:HB3	1.96	0.48
4:Df:421:ARG:NH2	4:Dg:83:LYS:HG3	2.29	0.48
7:Gb:92:LEU:HD12	7:Gb:105:LEU:HD11	1.95	0.48
11:Ka:59:DC:H1'	11:Ka:60:DT:C6	2.48	0.48
1:Af:208:ASN:HA	1:Af:249:THR:HG21	1.95	0.48
1:Ag:203:LYS:HA	1:Ag:209:SER:HA	1.95	0.48
1:Ak:342:VAL:HG21	4:Dg:187:PHE:CD1	2.48	0.48
1:Ar:235:ILE:HG23	1:Ar:314:LEU:HD13	1.95	0.48
2:Bn:106:ILE:HG12	2:Bn:140:TYR:CZ	2.48	0.48
4:De:355:TYR:O	4:De:359:LYS:HG2	2.14	0.48
9:Ja:9:DT:H2'	9:Ja:10:DT:H71	1.95	0.48
10:Jj:18:DA:H2''	10:Jj:19:DA:C8	2.47	0.48
1:Ak:157:TRP:O	1:Ak:161:GLN:HG2	2.13	0.48
1:Ao:95:VAL:HB	2:Bn:16:TRP:CD2	2.49	0.48
1:As:9:ASN:O	1:As:13:ARG:HG2	2.14	0.48
4:Db:421:ARG:NH2	4:Dc:83:LYS:HG3	2.29	0.48
4:Dh:355:TYR:O	4:Dh:359:LYS:HG2	2.13	0.48
9:Jc:28:DT:H2'	9:Jc:29:DT:H72	1.96	0.48
10:Jd:20:DA:H2''	10:Jd:21:DA:H8	1.77	0.48
1:Ag:120:GLU:HG2	1:Ag:136:ILE:HD13	1.96	0.48
4:Db:248:ILE:HD11	4:Db:259:TRP:CZ3	2.49	0.48
4:Dh:248:ILE:HD11	4:Dh:259:TRP:CZ3	2.49	0.48
5:Ej:84:ARG:HD3	6:Fe:138:TRP:CD1	2.49	0.47
10:Jj:14:DA:H2''	10:Jj:15:DA:C8	2.49	0.47
4:Df:355:TYR:O	4:Df:359:LYS:HG2	2.15	0.47
4:Dl:391:MET:HE2	4:Dl:423:LEU:HD22	1.97	0.47
7:Hi:97:PRO:HA	7:Hi:130:VAL:HB	1.96	0.47
8:Ib:40:GLY:H	8:Ic:317:GLU:CD	2.22	0.47
8:Ie:2:ARG:HB2	8:Ie:4:VAL:HG22	1.96	0.47
8:Ie:103:GLY:H	8:Ie:345:VAL:HG22	1.79	0.47
1:Af:107:PRO:HG3	1:Af:330:THR:HG21	1.96	0.47
1:Af:176:TYR:CZ	1:Ag:77:GLY:HA2	2.50	0.47
1:At:106:SER:HB3	2:Bt:3:LYS:HB3	1.95	0.47
2:Br:106:ILE:HD13	2:Br:125:LEU:HD21	1.96	0.47
6:Fd:155:GLN:HG3	6:Fe:99:TRP:CH2	2.49	0.47
8:Ia:9:ALA:HB2	8:Ia:30:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Id:308:ILE:HG12	8:Id:342:VAL:HG22	1.97	0.47
10:Jf:26:DA:H2''	10:Jf:27:DA:C8	2.49	0.47
1:Ab:132:GLN:H	1:Ab:132:GLN:CD	2.23	0.47
1:Af:186:ASP:HB2	2:Be:1:MET:HG3	1.95	0.47
1:As:164:ARG:HA	1:As:389:TRP:HE1	1.79	0.47
2:Bd:22:LEU:HB3	2:Bd:103:ALA:HB3	1.97	0.47
1:An:151:MET:HE3	1:An:367:GLY:N	2.29	0.47
12:Kb:31:DC:H2'	12:Kb:32:DA:C8	2.49	0.47
1:Ac:150:ARG:NH1	1:Ad:77:GLY:HA3	2.30	0.47
4:Dg:421:ARG:NH2	4:Dh:83:LYS:HG3	2.30	0.47
4:Di:248:ILE:HD11	4:Di:259:TRP:CZ3	2.50	0.47
1:Ac:409:LEU:HD21	1:Ad:99:ASP:HB2	1.97	0.47
1:Ae:11:LEU:HD13	1:Ae:33:GLU:HB3	1.96	0.47
1:Ag:235:ILE:HG12	1:Ag:316:VAL:HG12	1.96	0.47
1:Aj:255:VAL:HA	1:Aj:282:ILE:HD13	1.96	0.47
1:Ak:57:SER:HB2	1:Ak:345:THR:HG21	1.95	0.47
1:Ak:409:LEU:HD21	1:Al:99:ASP:HB2	1.96	0.47
1:Ao:120:GLU:HG2	1:Ao:136:ILE:HD13	1.97	0.47
2:Bo:71:LEU:HD21	2:Bo:111:GLN:HG2	1.96	0.47
2:Br:102:ALA:HB3	2:Br:142:PHE:CZ	2.50	0.47
4:Dk:248:ILE:HD11	4:Dk:259:TRP:CZ3	2.49	0.47
4:Dl:248:ILE:HD11	4:Dl:259:TRP:CZ3	2.49	0.47
6:Fb:5:LEU:HD11	6:Fc:92:GLU:HG2	1.96	0.47
6:Fc:94:LEU:HD11	6:Fc:142:GLY:HA3	1.96	0.47
8:Id:317:GLU:OE1	8:If:39:SER:HB2	2.14	0.47
9:Ja:19:DT:H2'	9:Ja:20:DT:H71	1.96	0.47
10:Jj:20:DA:H2''	10:Jj:21:DA:H8	1.80	0.47
1:Aa:11:LEU:HD13	1:Aa:33:GLU:HB3	1.97	0.47
1:Af:235:ILE:HG23	1:Af:314:LEU:HD13	1.95	0.47
4:Dg:248:ILE:HD11	4:Dg:259:TRP:CZ3	2.50	0.47
8:Ie:122:GLY:HA2	8:Ie:131:VAL:HA	1.95	0.47
8:Ie:151:MET:SD	8:Ie:190:VAL:HG12	2.55	0.47
10:Jd:12:DA:H4'	10:Jd:13:DA:OP1	2.14	0.47
10:Jd:14:DA:H2''	10:Jd:15:DA:C8	2.48	0.47
10:Jh:12:DA:H4'	10:Jh:13:DA:OP1	2.14	0.47
10:Jj:12:DA:H4'	10:Jj:13:DA:OP1	2.15	0.47
1:Ao:108:LEU:HD23	2:Bn:3:LYS:HE3	1.97	0.47
7:Gj:89:VAL:HG13	7:Gj:142:VAL:HG13	1.97	0.47
10:Jd:24:DA:H2''	10:Jd:25:DA:C8	2.50	0.47
1:Ab:170:ILE:HB	1:Ab:183:TYR:HB2	1.97	0.47
1:As:181:LEU:HD22	2:Bs:95:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Da:355:TYR:O	4:Da:359:LYS:HG2	2.14	0.47
8:Ib:52:ARG:HA	8:If:4:VAL:HB	1.96	0.47
8:Ic:57:GLN:HB2	8:Ic:60:TYR:CD2	2.50	0.47
1:Ab:35:VAL:HG13	1:Ac:68:LEU:HD23	1.97	0.46
1:Ao:121:ILE:HG12	1:Ao:136:ILE:HG12	1.97	0.46
1:Ao:270:PRO:HG2	1:Ao:275:TYR:CE2	2.50	0.46
4:Di:269:PHE:HA	4:Di:275:HIS:CE1	2.49	0.46
8:Ib:247:THR:HG22	8:Ib:333:ARG:HG2	1.97	0.46
8:Ie:22:LEU:HD22	8:Ie:176:VAL:HG21	1.96	0.46
10:Jb:12:DA:H4'	10:Jb:13:DA:OP1	2.14	0.46
1:Ab:208:ASN:HA	1:Ab:249:THR:HG21	1.97	0.46
1:Aj:167:ARG:HH22	2:Bi:1:MET:HE3	1.80	0.46
1:Ak:15:ARG:HH21	1:Am:13:ARG:NH2	2.13	0.46
1:Ar:265:GLN:HA	1:As:265:GLN:HG3	1.97	0.46
7:Ha:97:PRO:HA	7:Ha:130:VAL:HB	1.97	0.46
1:Ae:11:LEU:HD21	1:Af:68:LEU:HB2	1.98	0.46
5:Ea:27:GLU:O	5:El:16:ALA:HB2	2.15	0.46
10:Jb:20:DA:H2''	10:Jb:21:DA:H8	1.79	0.46
9:Je:2:DT:H4'	9:Je:3:DT:OP1	2.16	0.46
10:Jf:18:DA:H2''	10:Jf:19:DA:C8	2.51	0.46
1:Ak:13:ARG:HB3	1:Am:15:ARG:O	2.15	0.46
3:Cd:44:ALA:HB1	3:Cd:49:GLU:HB3	1.96	0.46
8:Id:2:ARG:HB2	8:Id:4:VAL:HG22	1.96	0.46
8:Id:168:PRO:HA	8:Id:173:TRP:CD1	2.50	0.46
10:Jf:24:DA:H2''	10:Jf:25:DA:C8	2.50	0.46
12:Kb:58:DG:H2'	12:Kb:59:DA:C8	2.51	0.46
2:Bf:42:ASN:HB3	2:Bf:113:ILE:HG12	1.97	0.46
2:Bh:132:LYS:HB3	2:Bh:146:ARG:HH21	1.79	0.46
6:Fc:98:ARG:NH1	6:Fc:125:ILE:HG13	2.29	0.46
9:Ja:28:DT:H2'	9:Ja:29:DT:H72	1.97	0.46
1:Ag:52:PHE:HA	1:Ag:323:PRO:HA	1.97	0.46
2:Bh:136:ILE:HG22	2:Bh:137:LYS:HG3	1.97	0.46
2:Bj:106:ILE:HD13	2:Bj:125:LEU:HD21	1.96	0.46
10:Jj:9:DA:H2'	10:Jj:10:DA:H8	1.80	0.46
11:Ka:14:DC:H2'	11:Ka:15:DA:C8	2.50	0.46
4:Db:269:PHE:HA	4:Db:275:HIS:CE1	2.51	0.46
8:Id:127:GLU:HB3	8:Ie:270:HIS:CE1	2.50	0.46
9:Jc:13:DT:H2'	9:Jc:14:DT:H71	1.97	0.46
1:Af:271:PRO:HG2	1:Af:274:VAL:HG23	1.98	0.46
1:An:176:TYR:CZ	1:Ao:77:GLY:HA2	2.50	0.46
1:An:255:VAL:HA	1:An:282:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bl:136:ILE:HG22	2:Bl:137:LYS:HG3	1.98	0.46
2:Br:16:TRP:CH2	2:Br:118:LEU:HD11	2.51	0.46
5:Ec:14:MET:HE1	5:Ec:79:ILE:HB	1.96	0.46
6:Fc:36:GLY:HA2	6:Fd:91:TYR:CG	2.51	0.46
8:Ic:137:ALA:HA	8:Ic:160:ALA:HA	1.98	0.46
11:Ka:49:DA:H2''	11:Ka:50:DG:C8	2.51	0.46
1:Ag:200:PHE:CD2	1:Ag:392:TYR:HB2	2.51	0.46
1:An:107:PRO:HG3	1:An:330:THR:HG21	1.97	0.46
1:Ao:52:PHE:HA	1:Ao:323:PRO:HA	1.98	0.46
1:Ao:59:PHE:CE1	4:Di:189:SER:HB3	2.51	0.46
4:Di:107:GLY:O	4:Di:114:GLY:HA2	2.15	0.46
7:Gd:44:TYR:HE1	7:Gd:46:LYS:HG2	1.80	0.46
9:Jc:4:DT:H2'	9:Jc:5:DT:H71	1.98	0.46
10:Jd:9:DA:H2'	10:Jd:10:DA:H8	1.80	0.46
10:Jh:9:DA:H2'	10:Jh:10:DA:H8	1.81	0.46
5:Ea:17:GLU:HB2	6:Fa:85:PRO:HD2	1.97	0.46
7:Hd:79:GLY:HA2	7:He:61:TYR:OH	2.15	0.46
8:Id:19:PRO:HB3	8:Id:135:PHE:HB3	1.97	0.46
8:Id:167:GLN:HE22	8:Ie:273:ALA:HB3	1.80	0.46
1:Ac:15:ARG:HD2	1:Ac:31:ILE:HD13	1.98	0.45
1:Af:314:LEU:HD21	1:Af:390:LEU:HD23	1.98	0.45
1:Ag:108:LEU:HD23	2:Bf:3:LYS:HE3	1.98	0.45
1:As:110:PHE:CZ	1:As:158:LEU:HD11	2.51	0.45
2:Bf:106:ILE:HD13	2:Bf:125:LEU:HD21	1.98	0.45
4:Dh:391:MET:HE2	4:Dh:423:LEU:HD22	1.98	0.45
7:Hf:44:TYR:HE1	7:Hf:46:LYS:HG2	1.81	0.45
8:If:308:ILE:HG12	8:If:342:VAL:HG22	1.96	0.45
9:Je:30:DT:H2'	9:Je:31:DT:C6	2.51	0.45
9:Jg:28:DT:H2'	9:Jg:29:DT:H72	1.97	0.45
1:Ag:150:ARG:NH1	1:Ah:77:GLY:HA3	2.31	0.45
1:Am:3:VAL:HG11	1:An:98:VAL:HG23	1.98	0.45
1:Ar:25:PHE:CD1	1:As:341:VAL:HG21	2.51	0.45
2:Bj:22:LEU:HD22	2:Bj:25:TYR:H	1.81	0.45
2:Bt:81:ILE:HG23	2:Bt:98:VAL:HG11	1.98	0.45
4:Di:263:LYS:HA	4:Dj:278:ILE:HD11	1.96	0.45
4:Dk:107:GLY:O	4:Dk:114:GLY:HA2	2.16	0.45
8:Ib:200:ALA:O	8:Ib:203:MET:HG3	2.16	0.45
10:Jf:9:DA:H2'	10:Jf:10:DA:C8	2.51	0.45
1:Ab:186:ASP:HB2	2:Ba:1:MET:HG3	1.98	0.45
1:An:40:ASP:OD2	1:An:299:ARG:HG3	2.16	0.45
1:As:181:LEU:HD21	2:Bs:31:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bp:136:ILE:HG22	2:Bp:137:LYS:HG3	1.98	0.45
4:Da:240:MET:HG2	4:Dl:293:ALA:HB3	1.98	0.45
8:Ia:131:VAL:HG23	8:Ia:173:TRP:HZ3	1.81	0.45
11:Ka:45:DC:H2''	11:Ka:46:DG:C8	2.51	0.45
2:Bj:44:PHE:O	3:Cc:35:LYS:HA	2.17	0.45
4:Dl:355:TYR:O	4:Dl:359:LYS:HG2	2.17	0.45
5:Eb:38:ARG:HH12	7:Ga:29:ASP:HA	1.81	0.45
5:Ed:84:ARG:HD3	6:Fb:138:TRP:CG	2.51	0.45
1:Ac:176:TYR:CZ	1:Ad:77:GLY:HA2	2.52	0.45
1:Aj:152:ARG:NH2	1:Aj:156:ARG:HH12	2.14	0.45
5:Ec:87:GLN:CG	6:Fb:135:PHE:HB3	2.40	0.45
6:Fe:53:LYS:HG3	6:Ff:124:THR:HG22	1.99	0.45
1:Ao:115:VAL:HG11	2:Bp:21:ARG:HB3	1.99	0.45
4:Df:269:PHE:HA	4:Df:275:HIS:CE1	2.51	0.45
4:Dk:421:ARG:NH2	4:Dl:83:LYS:HG3	2.31	0.45
5:Eh:16:ALA:HB2	5:Ei:27:GLU:O	2.17	0.45
6:Fd:51:SER:HB3	6:Fd:76:LEU:HD23	1.98	0.45
6:Fe:5:LEU:HD11	6:Ff:92:GLU:HG2	1.99	0.45
8:Ia:57:GLN:HB2	8:Ia:60:TYR:CD2	2.51	0.45
8:Ib:250:LEU:HD11	8:Ib:275:LEU:HD11	1.99	0.45
8:Ie:246:GLY:HA3	8:Ie:334:PHE:CZ	2.52	0.45
9:Ja:2:DT:H4'	9:Ja:3:DT:OP1	2.16	0.45
1:Ae:31:ILE:HG12	1:Af:64:GLU:HB2	1.99	0.45
1:Ag:155:ARG:HG3	1:Ag:327:PHE:CE2	2.52	0.45
1:Al:317:LEU:HD13	1:Al:321:THR:HA	1.99	0.45
2:Bf:22:LEU:HD22	2:Bf:25:TYR:H	1.81	0.45
4:De:263:LYS:HA	4:Df:278:ILE:HD11	1.99	0.45
8:If:151:MET:SD	8:If:190:VAL:HG12	2.56	0.45
9:Jc:30:DT:H2'	9:Jc:31:DT:C6	2.52	0.45
9:Jg:2:DT:H4'	9:Jg:3:DT:OP1	2.15	0.45
1:Ac:157:TRP:O	1:Ac:161:GLN:HG2	2.16	0.45
1:Ak:237:VAL:O	1:Ak:293:VAL:HA	2.16	0.45
1:At:104:THR:HG22	2:Bt:5:GLN:HB3	1.99	0.45
5:Ed:16:ALA:HB2	5:Ee:27:GLU:O	2.16	0.45
5:Ed:33:SER:HB2	7:Hc:28:GLN:OE1	2.17	0.45
11:Ka:38:DT:H1'	11:Ka:39:DG:N7	2.31	0.45
1:Ao:181:LEU:HD21	2:Bo:31:PRO:HB2	1.99	0.45
2:Bp:43:TRP:CD2	2:Bp:113:ILE:HD11	2.52	0.45
7:Gl:27:PRO:HD3	7:Gl:58:GLY:HA2	1.98	0.45
7:Hk:2:VAL:HA	7:Hk:72:ARG:O	2.17	0.45
9:Ji:28:DT:H2'	9:Ji:29:DT:H72	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:15:ARG:HH21	1:Ae:13:ARG:NH2	2.15	0.45
1:Ac:63:LEU:HB2	1:Ac:105:TRP:CE3	2.52	0.45
2:Bf:16:TRP:HB3	2:Bf:49:PRO:HD3	1.99	0.45
2:Bo:113:ILE:HG22	2:Bo:114:GLU:HG2	1.98	0.45
4:Dj:391:MET:HE2	4:Dj:423:LEU:HD22	1.99	0.45
8:Id:30:PHE:HB2	8:Id:179:VAL:O	2.17	0.45
1:Ab:5:ILE:HG23	1:Af:125:GLY:HA2	1.99	0.44
1:Aj:189:VAL:HG11	1:Aj:192:ILE:HD13	1.99	0.44
4:Dc:107:GLY:O	4:Dc:114:GLY:HA2	2.17	0.44
4:Df:25:LYS:HE2	10:Jf:9:DA:H5"	1.99	0.44
4:Dl:268:ASN:ND2	5:Ek:120:TRP:CD2	2.85	0.44
10:Jj:28:DA:H2"	10:Jj:29:DA:H8	1.83	0.44
1:Af:237:VAL:HG21	1:Af:241:PHE:HB2	2.00	0.44
1:Af:255:VAL:HA	1:Af:282:ILE:HD13	1.99	0.44
1:As:121:ILE:HG12	1:As:136:ILE:HG12	1.99	0.44
2:Bn:77:VAL:HG13	2:Bn:131:LEU:HD23	1.98	0.44
5:Eh:84:ARG:HD3	6:Fd:138:TRP:CG	2.52	0.44
8:Ia:82:LYS:HD2	8:Ia:348:PHE:CZ	2.51	0.44
8:Ib:224:THR:HB	8:Ib:234:ARG:NH2	2.32	0.44
8:If:53:MET:SD	8:If:57:GLN:HG3	2.57	0.44
1:Ab:100:LEU:HD21	1:As:18:LEU:HD11	1.99	0.44
1:Ac:63:LEU:HB2	1:Ac:105:TRP:HE3	1.82	0.44
1:Ac:129:ASP:HB3	1:Ac:131:VAL:HG13	1.98	0.44
1:Af:26:PRO:HG2	1:Ag:343:TYR:CD2	2.51	0.44
2:Bp:71:LEU:HD11	2:Bp:123:ALA:HB1	1.98	0.44
8:Ia:291:PHE:O	8:Ia:305:ARG:HA	2.18	0.44
8:Ib:81:LEU:HD22	8:Ib:85:LEU:HD11	1.99	0.44
9:Jg:13:DT:H2'	9:Jg:14:DT:H71	1.98	0.44
9:Ji:2:DT:H4'	9:Ji:3:DT:OP1	2.17	0.44
1:Aa:15:ARG:O	1:As:13:ARG:HB3	2.18	0.44
1:Ae:9:ASN:O	1:Ae:13:ARG:HG2	2.16	0.44
1:Aj:172:PRO:HA	1:Aj:180:GLY:HA2	1.99	0.44
1:An:15:ARG:HH21	1:Ar:360:PRO:HB3	1.82	0.44
2:Bc:34:MET:HE2	2:Bc:40:TRP:CD2	2.53	0.44
2:Bj:106:ILE:HD11	2:Bj:135:VAL:HG13	1.99	0.44
4:De:239:PHE:CZ	4:De:292:SER:HB2	2.52	0.44
5:Ef:85:ALA:HB1	6:Fd:133:GLY:HA3	1.99	0.44
7:Ha:2:VAL:HA	7:Ha:72:ARG:O	2.18	0.44
7:He:113:VAL:HG22	7:He:139:VAL:HG22	1.98	0.44
8:If:105:THR:HA	8:If:342:VAL:O	2.18	0.44
9:Jc:2:DT:H4'	9:Jc:3:DT:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Jf:12:DA:H4'	10:Jf:13:DA:OP1	2.16	0.44
10:Jh:20:DA:H2''	10:Jh:21:DA:H8	1.83	0.44
1:Af:172:PRO:HA	1:Af:180:GLY:HA2	1.99	0.44
1:Ap:67:LEU:HD23	1:Ap:382:PHE:HE1	1.82	0.44
3:Ca:29:ALA:HB1	3:Ca:63:TRP:HB3	2.00	0.44
4:Da:314:ILE:HA	4:Da:337:THR:HG23	1.99	0.44
6:Fb:62:GLY:HA2	8:Ia:6:THR:O	2.17	0.44
7:He:2:VAL:HA	7:He:72:ARG:O	2.18	0.44
1:Ab:131:VAL:HG13	1:Ar:10:ALA:HB1	2.00	0.44
1:Ag:13:ARG:HB2	1:Ai:17:PRO:HB3	1.99	0.44
1:Ag:157:TRP:O	1:Ag:161:GLN:HG2	2.17	0.44
1:Aj:131:VAL:HB	1:Aj:135:VAL:HG21	1.99	0.44
1:Ao:355:LEU:HD22	1:Ar:333:VAL:HG11	1.99	0.44
2:Bb:106:ILE:HG12	2:Bb:140:TYR:CZ	2.53	0.44
2:Bc:128:ALA:HB1	2:Bc:133:LEU:HB2	1.98	0.44
2:Bk:136:ILE:HB	2:Bk:141:PHE:CE1	2.53	0.44
4:Dc:263:LYS:HA	4:Dd:278:ILE:HD11	1.99	0.44
4:Dd:76:PHE:CG	4:Dd:126:GLU:HG2	2.53	0.44
4:Dd:107:GLY:O	4:Dd:114:GLY:HA2	2.17	0.44
4:Dd:355:TYR:O	4:Dd:359:LYS:HG2	2.18	0.44
4:De:107:GLY:O	4:De:114:GLY:HA2	2.18	0.44
4:Dk:391:MET:HE2	4:Dk:423:LEU:HD22	1.98	0.44
8:Ic:131:VAL:HG23	8:Ic:173:TRP:HZ3	1.83	0.44
8:If:211:VAL:HG12	8:If:250:LEU:HB3	1.98	0.44
1:Aa:9:ASN:O	1:Aa:13:ARG:HG2	2.18	0.44
1:Ac:355:LEU:HD22	1:Af:333:VAL:HG11	1.99	0.44
1:Af:108:LEU:N	1:Af:371:LEU:HD23	2.33	0.44
1:Ag:9:ASN:O	1:Ag:13:ARG:HG2	2.17	0.44
1:Aj:404:PRO:HB3	1:Ak:227:PHE:CE1	2.52	0.44
1:Ak:196:LEU:HD23	1:Ak:196:LEU:HA	1.87	0.44
1:An:151:MET:HE3	1:An:367:GLY:H	1.83	0.44
2:Bo:34:MET:HE2	2:Bo:40:TRP:CD2	2.52	0.44
3:Cc:47:ALA:HB1	3:Cc:68:ALA:HB3	2.00	0.44
7:Gf:3:ILE:HD12	7:Gf:71:GLN:NE2	2.33	0.44
7:Hc:2:VAL:HA	7:Hc:72:ARG:O	2.17	0.44
8:Ic:9:ALA:HB2	8:Ic:30:PHE:CD1	2.52	0.44
1:Ag:63:LEU:HB2	1:Ag:105:TRP:CE3	2.52	0.44
1:Am:9:ASN:O	1:Am:13:ARG:HG2	2.18	0.44
1:Ap:104:THR:HG22	2:Bp:5:GLN:HB3	2.00	0.44
2:Bc:22:LEU:HB2	2:Bc:103:ALA:HB3	1.98	0.44
8:Ib:131:VAL:HG23	8:Ib:173:TRP:HZ3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ja:4:DT:H2'	9:Ja:5:DT:H71	1.99	0.44
10:Jf:28:DA:H2''	10:Jf:29:DA:H8	1.82	0.44
10:Jj:28:DA:H2''	10:Jj:29:DA:C8	2.53	0.44
1:Ac:155:ARG:HG3	1:Ac:327:PHE:CE2	2.53	0.44
1:Af:314:LEU:HD23	1:Af:392:TYR:CD1	2.52	0.44
1:Ah:194:LEU:HD12	1:Ah:390:LEU:HB2	1.99	0.44
1:Ao:150:ARG:NH1	1:Ap:77:GLY:HA3	2.33	0.44
1:Ar:371:LEU:HD12	1:Ar:372:PRO:O	2.18	0.44
1:As:236:ILE:HD11	1:As:315:ILE:HD12	2.00	0.44
4:Dg:269:PHE:HA	4:Dg:275:HIS:NE2	2.33	0.44
4:Dl:107:GLY:O	4:Dl:114:GLY:HA2	2.17	0.44
6:Fb:34:ASP:O	6:Fb:48:ALA:HA	2.18	0.44
6:Fb:51:SER:HB3	6:Fb:76:LEU:HD23	2.00	0.44
6:Fc:80:ILE:HB	6:Fc:144:VAL:HB	2.00	0.44
7:Hj:94:PHE:HB3	7:Hj:100:HIS:CD2	2.53	0.44
8:Ie:313:VAL:HG12	8:Ie:336:ALA:HA	2.00	0.44
1:Af:110:PHE:CZ	1:Af:158:LEU:HD11	2.53	0.43
1:Ao:200:PHE:CD2	1:Ao:392:TYR:HB2	2.52	0.43
1:Ap:245:LEU:HD22	1:Ap:251:VAL:HG21	1.99	0.43
1:Aq:11:LEU:HD13	1:Aq:33:GLU:HB3	1.99	0.43
2:Bc:113:ILE:HG22	2:Bc:114:GLU:HG2	1.99	0.43
2:Bd:81:ILE:HG23	2:Bd:98:VAL:HG11	2.00	0.43
2:Bf:106:ILE:HD12	2:Bf:138:GLY:HA2	1.98	0.43
4:Da:421:ARG:NH2	4:Db:83:LYS:HG3	2.31	0.43
4:Dd:314:ILE:HA	4:Dd:337:THR:HG23	2.00	0.43
4:Dk:259:TRP:HZ2	5:Ek:119:ASP:HB2	1.83	0.43
8:If:31:LEU:HD11	8:If:83:LYS:HG2	2.00	0.43
1:Af:40:ASP:OD2	1:Af:299:ARG:HG3	2.18	0.43
1:An:155:ARG:HG3	1:An:327:PHE:CZ	2.54	0.43
1:Ao:7:ILE:HG23	1:Ap:68:LEU:HD23	2.00	0.43
1:Ao:116:TRP:HD1	1:Ao:120:GLU:OE1	2.00	0.43
2:Bl:77:VAL:HG11	2:Bl:130:GLN:HB3	2.01	0.43
4:Dc:241:ILE:HG13	4:Dd:274:ARG:HG2	1.99	0.43
6:Fb:83:GLU:HA	6:Fb:140:PHE:O	2.19	0.43
6:Fd:49:ILE:HG12	6:Fd:78:LEU:HD13	2.00	0.43
7:Gj:48:GLU:HG2	7:Gj:85:ALA:HA	2.00	0.43
7:Hi:2:VAL:HA	7:Hi:72:ARG:O	2.18	0.43
8:Id:250:LEU:HD11	8:Id:275:LEU:HD11	2.00	0.43
10:Jf:20:DA:H2''	10:Jf:21:DA:H8	1.82	0.43
12:Kb:33:DG:H2''	12:Kb:34:DA:C8	2.53	0.43
1:Ac:200:PHE:CD2	1:Ac:392:TYR:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:104:THR:HG22	2:Bl:5:GLN:HB3	1.99	0.43
2:Bd:71:LEU:HD11	2:Bd:123:ALA:HB1	1.99	0.43
2:Bl:34:MET:HE3	2:Bl:40:TRP:CG	2.54	0.43
4:Da:107:GLY:O	4:Da:114:GLY:HA2	2.18	0.43
4:Dc:248:ILE:HD11	4:Dc:259:TRP:CZ3	2.53	0.43
4:Df:391:MET:HE2	4:Df:423:LEU:HD22	1.99	0.43
4:Dh:421:ARG:NH2	4:Di:83:LYS:HG3	2.32	0.43
5:Ea:84:ARG:HG2	5:El:89:LEU:HD11	1.99	0.43
7:He:97:PRO:HA	7:He:130:VAL:HB	1.98	0.43
1:Af:230:ARG:HG2	1:Af:385:HIS:CG	2.54	0.43
1:Aj:154:ARG:HB2	1:Ak:78:MET:HB3	1.99	0.43
1:As:164:ARG:HD2	1:As:389:TRP:CZ2	2.53	0.43
2:Bg:1:MET:HG2	2:Bg:3:LYS:H	1.84	0.43
4:Dg:107:GLY:O	4:Dg:114:GLY:HA2	2.17	0.43
7:Gi:92:LEU:HD12	7:Gi:105:LEU:HD11	2.00	0.43
7:Hb:2:VAL:HA	7:Hb:72:ARG:O	2.18	0.43
8:Ib:38:LEU:HA	8:Ib:70:GLY:HA3	1.99	0.43
8:Ib:264:LEU:HD21	8:Ib:278:VAL:CG2	2.49	0.43
8:Id:122:GLY:HA2	8:Id:131:VAL:HA	2.01	0.43
8:Ie:30:PHE:HB2	8:Ie:179:VAL:O	2.19	0.43
8:If:168:PRO:HA	8:If:173:TRP:CD1	2.54	0.43
1:Ab:270:PRO:HG2	1:Ab:275:TYR:CE2	2.54	0.43
1:Ac:116:TRP:HD1	1:Ac:120:GLU:OE1	2.02	0.43
1:Ak:155:ARG:HG3	1:Ak:327:PHE:CE2	2.53	0.43
1:Ao:13:ARG:HB3	1:Aq:15:ARG:O	2.19	0.43
1:Ar:374:LEU:HD13	1:Ar:384:PHE:CE2	2.54	0.43
1:As:155:ARG:HG3	1:As:327:PHE:CE2	2.53	0.43
2:Bb:82:GLY:HA2	2:Bb:144:TYR:CD2	2.53	0.43
2:Bl:102:ALA:HB3	2:Bl:142:PHE:CZ	2.54	0.43
4:Dc:391:MET:HE2	4:Dc:423:LEU:HD22	2.01	0.43
6:Fa:80:ILE:HB	6:Fa:144:VAL:HB	1.99	0.43
7:Hj:44:TYR:HE1	7:Hj:46:LYS:HG2	1.83	0.43
8:Ia:38:LEU:HA	8:Ia:70:GLY:HA3	2.01	0.43
8:Ib:57:GLN:HB2	8:Ib:60:TYR:CD2	2.54	0.43
1:Ab:239:PRO:HG2	1:Ab:400:LEU:HD11	2.01	0.43
1:Ac:3:VAL:HG22	2:Bd:15:TYR:HB3	2.00	0.43
1:Ar:347:PRO:HA	1:Ar:368:PHE:HB3	2.01	0.43
2:Bc:71:LEU:HD21	2:Bc:111:GLN:HG2	2.01	0.43
5:Eg:85:ALA:HB1	6:Fd:139:GLY:HA2	1.99	0.43
9:Ji:29:DT:H2'	9:Ji:30:DT:H71	2.00	0.43
1:Ag:127:LEU:HD23	1:Ai:26:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:239:PRO:HG3	1:An:307:TYR:CE1	2.54	0.43
2:Bk:53:LEU:HD13	2:Bk:131:LEU:HD23	2.00	0.43
2:Bt:125:LEU:HD12	2:Bt:135:VAL:HG21	2.01	0.43
4:Db:391:MET:HE2	4:Db:423:LEU:HD22	2.01	0.43
5:Di:26:ARG:HE	5:Di:29:GLN:NE2	2.16	0.43
6:Fd:36:GLY:HA2	6:Fe:91:TYR:CG	2.54	0.43
7:He:90:GLU:HB2	7:He:143:MET:HB2	2.01	0.43
10:Jf:28:DA:H2''	10:Jf:29:DA:C8	2.54	0.43
12:Kb:27:DA:H2''	12:Kb:28:DC:C5	2.53	0.43
1:Ak:110:PHE:CZ	1:Ak:158:LEU:HD11	2.53	0.43
1:An:181:LEU:HD12	1:Ao:81:VAL:HG12	2.01	0.43
1:Ao:157:TRP:O	1:Ao:161:GLN:HG2	2.18	0.43
2:Bb:106:ILE:HG12	2:Bb:140:TYR:CE2	2.53	0.43
2:Bo:83:MET:HE1	2:Bo:109:VAL:HG22	2.00	0.43
4:Dd:391:MET:HE2	4:Dd:423:LEU:HD22	2.00	0.43
4:Dj:107:GLY:O	4:Dj:114:GLY:HA2	2.18	0.43
5:Ef:84:ARG:HD3	6:Fc:138:TRP:CD1	2.53	0.43
6:Fc:5:LEU:HD11	6:Fd:92:GLU:HG2	2.00	0.43
8:Ia:271:ASP:HB3	8:Ia:274:PHE:HB2	2.01	0.43
8:If:246:GLY:HA3	8:If:334:PHE:CZ	2.54	0.43
9:Jg:19:DT:H2'	9:Jg:20:DT:H71	2.01	0.43
1:Ak:7:ILE:HG23	1:Al:68:LEU:HD23	2.00	0.43
1:Al:93:ALA:HB1	2:Bl:17:GLU:HB2	2.01	0.43
2:Bg:113:ILE:HG22	2:Bg:114:GLU:HG2	2.00	0.43
2:Bl:81:ILE:HG23	2:Bl:98:VAL:HG11	2.00	0.43
4:Dd:239:PHE:CZ	4:Dd:292:SER:HB2	2.54	0.43
6:Fc:115:VAL:HG13	6:Fc:150:VAL:HG13	2.00	0.43
7:Hd:97:PRO:HA	7:Hd:130:VAL:HB	2.01	0.43
7:Hg:2:VAL:HA	7:Hg:72:ARG:O	2.19	0.43
10:Jh:11:DA:H2''	10:Jh:12:DA:C8	2.54	0.43
1:Ab:151:MET:HE3	1:Ab:367:GLY:N	2.33	0.43
1:Ab:176:TYR:CZ	1:Ac:77:GLY:HA2	2.54	0.43
1:Ac:237:VAL:HG21	1:Ac:241:PHE:HB2	2.01	0.43
1:Ao:237:VAL:HG21	1:Ao:241:PHE:HB2	2.00	0.43
1:As:251:VAL:O	1:As:255:VAL:HG23	2.19	0.43
1:As:270:PRO:HG2	1:As:275:TYR:CE2	2.53	0.43
5:Eg:14:MET:HE1	5:Eg:79:ILE:HB	2.01	0.43
8:Ic:200:ALA:O	8:Ic:203:MET:HG3	2.18	0.43
1:Ap:93:ALA:HB1	2:Bp:17:GLU:HB2	2.01	0.42
1:Ar:120:GLU:HB2	3:Ce:31:ARG:HH21	1.82	0.42
1:Ar:255:VAL:HA	1:Ar:282:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ee:17:GLU:HB2	6:Fc:85:PRO:HD2	2.01	0.42
6:Ff:24:ASP:HA	7:Hj:76:ARG:NH1	2.34	0.42
8:Ia:44:VAL:HG11	8:Ib:337:TYR:OH	2.19	0.42
8:Ia:57:GLN:HB2	8:Ia:60:TYR:HD2	1.84	0.42
8:Ic:7:PHE:CZ	8:Ic:122:GLY:HA3	2.54	0.42
9:Je:4:DT:H2'	9:Je:5:DT:H71	2.01	0.42
1:Ag:43:ASN:HA	1:Ag:298:TYR:HA	2.01	0.42
1:An:371:LEU:HD12	1:An:372:PRO:O	2.19	0.42
1:As:150:ARG:NH1	1:At:77:GLY:HA3	2.34	0.42
2:Bk:54:VAL:HG12	2:Bk:68:PRO:HA	2.00	0.42
6:Fa:130:GLU:OE2	6:Ff:39:SER:HB2	2.19	0.42
7:Gf:48:GLU:HG2	7:Gf:85:ALA:HA	2.00	0.42
7:Hf:97:PRO:HA	7:Hf:130:VAL:HB	2.00	0.42
8:Ie:250:LEU:HD11	8:Ie:275:LEU:HD11	2.01	0.42
8:If:122:GLY:HA2	8:If:131:VAL:HA	2.00	0.42
9:Jc:17:DT:H2''	9:Jc:18:DT:H71	2.01	0.42
12:Kb:50:DT:C2	12:Kb:51:DG:N7	2.87	0.42
1:Aj:155:ARG:HG3	1:Aj:327:PHE:CZ	2.54	0.42
1:Aj:164:ARG:HA	1:Aj:389:TRP:HE1	1.84	0.42
1:Ak:150:ARG:NH1	1:Al:77:GLY:HA3	2.34	0.42
1:As:120:GLU:HG2	1:As:136:ILE:HD13	2.01	0.42
2:Bc:53:LEU:HD13	2:Bc:131:LEU:HD23	2.00	0.42
2:Bg:8:ARG:NH2	4:Dd:186:GLN:HG3	2.34	0.42
6:Fc:49:ILE:HG12	6:Fc:78:LEU:HD13	2.01	0.42
7:Hj:2:VAL:HA	7:Hj:72:ARG:O	2.19	0.42
8:Id:39:SER:HB2	8:Ie:317:GLU:OE1	2.19	0.42
1:Ag:63:LEU:HB2	1:Ag:105:TRP:HE3	1.85	0.42
1:As:115:VAL:HG23	1:As:363:ALA:HB2	2.02	0.42
2:Bp:81:ILE:HG23	2:Bp:98:VAL:HG11	2.00	0.42
3:Cd:42:VAL:HG11	3:Cd:58:VAL:HG11	2.01	0.42
4:Dj:76:PHE:CG	4:Dj:126:GLU:HG2	2.54	0.42
7:Gh:27:PRO:HD3	7:Gh:58:GLY:HA2	2.02	0.42
8:Ie:19:PRO:HB3	8:Ie:135:PHE:HB3	2.01	0.42
9:Ja:30:DT:H2'	9:Ja:31:DT:C6	2.54	0.42
11:Ka:53:DG:H2''	11:Ka:54:DC:C5	2.54	0.42
1:Aj:181:LEU:HD12	1:Ak:81:VAL:HG12	2.01	0.42
1:As:247:ASP:OD1	1:As:272:ARG:HD2	2.18	0.42
2:Ba:14:GLN:HE21	2:Ba:14:GLN:HB3	1.63	0.42
2:Bc:1:MET:HG2	2:Bc:3:LYS:H	1.83	0.42
4:Dh:314:ILE:HA	4:Dh:337:THR:HG23	2.02	0.42
4:Di:421:ARG:NH2	4:Dj:83:LYS:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:El:84:ARG:HD3	6:Ff:138:TRP:CG	2.55	0.42
8:Ia:168:PRO:HA	8:Ia:173:TRP:CD1	2.54	0.42
10:Jf:27:DA:C6	10:Jf:28:DA:C6	3.08	0.42
1:Aa:13:ARG:NH2	1:As:15:ARG:HH21	2.18	0.42
1:Aj:239:PRO:HG3	1:Aj:307:TYR:CE1	2.54	0.42
1:Aj:314:LEU:HD23	1:Aj:392:TYR:CD1	2.55	0.42
1:Ao:110:PHE:CD2	1:Ap:81:VAL:HA	2.55	0.42
1:Ar:329:TYR:HD1	1:Ar:369:HIS:O	2.02	0.42
2:Bo:22:LEU:HB2	2:Bo:103:ALA:HB3	2.02	0.42
5:Ej:11:TRP:CH2	5:Ej:21:PRO:HD3	2.54	0.42
6:Fa:106:VAL:HG13	6:Ff:70:ARG:HE	1.85	0.42
7:Gf:27:PRO:HD3	7:Gf:58:GLY:HA2	2.02	0.42
8:Ib:7:PHE:CZ	8:Ib:122:GLY:HA3	2.55	0.42
9:Ji:4:DT:H2'	9:Ji:5:DT:H71	2.01	0.42
1:Ac:13:ARG:HB3	1:Ae:15:ARG:O	2.20	0.42
1:Af:178:PRO:HG2	1:Ag:89:LEU:HD12	2.01	0.42
1:Af:181:LEU:HD12	1:Ag:81:VAL:HG12	2.01	0.42
1:Ak:13:ARG:HB2	1:Am:17:PRO:HB3	2.02	0.42
2:Bj:77:VAL:HG13	2:Bj:131:LEU:HD23	2.00	0.42
4:Db:107:GLY:O	4:Db:114:GLY:HA2	2.19	0.42
5:EI:11:TRP:CH2	5:EI:21:PRO:HD3	2.55	0.42
6:Fb:70:ARG:HE	6:Fc:106:VAL:HG13	1.83	0.42
7:Gb:48:GLU:HG2	7:Gb:85:ALA:HA	2.00	0.42
7:Gg:7:ILE:HG12	7:Gg:13:PHE:CD1	2.55	0.42
8:Ia:52:ARG:HA	8:Ie:4:VAL:HB	2.01	0.42
8:Ib:152:LEU:HD13	8:Ib:291:PHE:CZ	2.55	0.42
1:Ab:151:MET:HE3	1:Ab:367:GLY:H	1.85	0.42
1:An:25:PHE:CD2	3:Cd:17:PRO:HD3	2.55	0.42
1:An:134:GLY:C	4:Dh:187:PHE:HB3	2.44	0.42
1:Ao:3:VAL:HG22	2:Bp:15:TYR:HB3	2.02	0.42
1:As:116:TRP:HD1	1:As:120:GLU:OE1	2.03	0.42
2:Be:12:ARG:HH21	2:Be:14:GLN:NE2	2.18	0.42
5:Ec:11:TRP:CH2	5:Ec:21:PRO:HD3	2.54	0.42
5:EI:15:PRO:HD2	5:EI:18:VAL:HG21	2.02	0.42
7:Ha:59:HIS:HE1	7:Ha:61:TYR:CZ	2.38	0.42
8:Ia:114:LEU:HD11	8:Ia:220:HIS:CG	2.55	0.42
8:If:250:LEU:HD11	8:If:275:LEU:HD11	2.01	0.42
1:Aj:48:LEU:HB2	1:Aj:294:TYR:CZ	2.55	0.42
1:An:25:PHE:CE2	1:Ao:341:VAL:HG21	2.55	0.42
1:An:397:GLN:HA	1:An:400:LEU:HD23	2.02	0.42
5:Ek:17:GLU:HB2	6:Ff:85:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Fa:5:LEU:HD11	6:Fb:92:GLU:HG2	2.02	0.42
6:Fa:91:TYR:CG	6:Ff:36:GLY:HA2	2.54	0.42
6:Fa:98:ARG:NH1	6:Fa:125:ILE:HG13	2.34	0.42
6:Fa:119:ASP:HB3	6:Fa:149:LYS:HB3	2.01	0.42
8:Ib:264:LEU:HD12	8:Ib:277:LYS:HE3	2.01	0.42
8:Ic:151:MET:HE1	8:Ic:190:VAL:HG23	2.02	0.42
8:Id:105:THR:HA	8:Id:342:VAL:O	2.20	0.42
11:Ka:64:DT:H2'	11:Ka:65:DC:C6	2.55	0.42
1:Ac:86:SER:HA	2:Bt:29:ALA:HB3	2.02	0.42
1:Ak:115:VAL:HG23	1:Ak:363:ALA:HB2	2.02	0.42
1:Al:245:LEU:HD22	1:Al:251:VAL:HG21	2.01	0.42
2:Bj:42:ASN:HB3	2:Bj:113:ILE:HG12	2.02	0.42
3:Cc:42:VAL:HG11	3:Cc:58:VAL:HG11	2.02	0.42
7:Ga:92:LEU:HD12	7:Ga:105:LEU:HD11	2.02	0.42
7:Gi:3:ILE:HD12	7:Gi:71:GLN:NE2	2.35	0.42
7:Hb:9:ARG:O	7:Hb:81:LEU:HB2	2.20	0.42
8:Id:246:GLY:HA3	8:Id:334:PHE:CZ	2.54	0.42
8:If:22:LEU:HD12	8:If:173:TRP:HA	2.01	0.42
9:Ja:1:DT:H6	9:Ja:1:DT:H2'	1.69	0.42
9:Ja:17:DT:H2''	9:Ja:18:DT:H71	2.02	0.42
10:Jb:9:DA:H2'	10:Jb:10:DA:H8	1.84	0.42
9:Ji:13:DT:H2'	9:Ji:14:DT:H71	2.00	0.42
12:Kb:57:DT:H1'	12:Kb:58:DG:C8	2.55	0.42
1:Af:151:MET:HE3	1:Af:367:GLY:N	2.35	0.41
1:Aj:26:PRO:HG2	1:Ak:343:TYR:CD2	2.55	0.41
1:Ak:133:ALA:HA	1:Am:28:THR:HG21	2.01	0.41
1:Ak:251:VAL:O	1:Ak:255:VAL:HG23	2.19	0.41
2:Bf:105:PRO:HB2	2:Bf:108:TYR:CD2	2.55	0.41
2:Bf:106:ILE:HD11	2:Bf:135:VAL:HG13	2.02	0.41
2:Bt:22:LEU:HB3	2:Bt:103:ALA:HB3	2.01	0.41
4:Di:168:GLU:HG2	4:Di:169:GLU:HG2	2.02	0.41
5:El:105:LEU:HA	5:El:109:ALA:HB3	2.01	0.41
6:Fd:30:PHE:CE1	6:Fd:47:ALA:HB2	2.55	0.41
7:Hk:44:TYR:HE1	7:Hk:46:LYS:HG2	1.85	0.41
8:Id:202:ASP:HB2	8:Id:265:THR:C	2.45	0.41
10:Jh:12:DA:H2''	10:Jh:13:DA:H8	1.85	0.41
1:Ab:314:LEU:HD21	1:Ab:390:LEU:HD23	2.02	0.41
1:Ad:245:LEU:HD22	1:Ad:251:VAL:HG21	2.01	0.41
1:Ag:67:LEU:HD23	1:Ag:382:PHE:HE1	1.84	0.41
1:Aj:107:PRO:HG3	1:Aj:330:THR:HG21	2.02	0.41
1:Ao:46:ASN:HB2	1:Ao:308:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:108:LEU:N	1:Ar:371:LEU:HD23	2.36	0.41
2:Bg:54:VAL:HG12	2:Bg:68:PRO:HA	2.02	0.41
2:Bs:34:MET:HE2	2:Bs:40:TRP:CD2	2.55	0.41
3:Cd:51:LEU:HG	3:Cd:65:PRO:HB2	2.03	0.41
4:Da:248:ILE:HD11	4:Da:259:TRP:CZ3	2.55	0.41
4:Da:293:ALA:HB3	4:Db:240:MET:HG2	2.02	0.41
4:Df:293:ALA:HB3	4:Dg:240:MET:HG2	2.02	0.41
4:Dj:176:LYS:HE3	4:Dj:176:LYS:HB2	1.91	0.41
4:Dl:314:ILE:HA	4:Dl:337:THR:HG23	2.02	0.41
5:Ee:67:ILE:HD13	5:Ee:67:ILE:HA	1.91	0.41
6:Fe:98:ARG:NH1	6:Fe:125:ILE:HG13	2.36	0.41
6:Ff:94:LEU:HD11	6:Ff:142:GLY:HA3	2.02	0.41
8:Ia:152:LEU:HD13	8:Ia:291:PHE:CZ	2.56	0.41
9:Ja:5:DT:H2'	9:Ja:6:DT:H71	2.02	0.41
10:Jd:26:DA:H2''	10:Jd:27:DA:H8	1.85	0.41
9:Jg:30:DT:H2'	9:Jg:31:DT:C6	2.56	0.41
11:Ka:52:DT:H2'	11:Ka:53:DG:C8	2.54	0.41
1:Ai:11:LEU:HD13	1:Ai:33:GLU:HB3	2.02	0.41
1:Ar:104:THR:HG1	2:Bq:5:GLN:HB3	1.85	0.41
1:As:409:LEU:HD21	1:At:99:ASP:HB2	2.03	0.41
4:Dd:248:ILE:HD11	4:Dd:259:TRP:CZ3	2.55	0.41
6:Fa:34:ASP:O	6:Fa:48:ALA:HA	2.20	0.41
7:Ha:88:GLN:HG3	7:Ha:146:GLY:HA3	2.02	0.41
7:He:9:ARG:O	7:He:81:LEU:HB2	2.20	0.41
7:Hf:2:VAL:HA	7:Hf:72:ARG:O	2.20	0.41
7:Hh:2:VAL:HA	7:Hh:72:ARG:O	2.21	0.41
7:Hk:9:ARG:O	7:Hk:81:LEU:HB2	2.21	0.41
8:Ib:22:LEU:HD21	8:Ib:131:VAL:HG11	2.02	0.41
8:Ib:298:VAL:HG21	8:Ib:345:VAL:HG12	2.02	0.41
9:Ja:13:DT:H2'	9:Ja:14:DT:H71	2.01	0.41
1:Ab:230:ARG:HG2	1:Ab:385:HIS:CG	2.55	0.41
1:Ap:97:LYS:HB3	2:Bp:14:GLN:HG2	2.03	0.41
1:As:374:LEU:HD13	1:As:384:PHE:CG	2.55	0.41
2:Bb:77:VAL:HG13	2:Bb:131:LEU:HD23	2.02	0.41
2:Bc:116:PRO:HB2	2:Bc:119:GLN:HB2	2.02	0.41
2:Bj:102:ALA:HB3	2:Bj:142:PHE:CZ	2.55	0.41
2:Bq:14:GLN:HE21	2:Bq:14:GLN:HB3	1.63	0.41
7:Hd:2:VAL:HA	7:Hd:72:ARG:O	2.19	0.41
8:Ia:200:ALA:O	8:Ia:203:MET:HG3	2.21	0.41
1:Ac:203:LYS:HA	1:Ac:209:SER:HA	2.02	0.41
1:Ag:13:ARG:HB3	1:Ai:15:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:377:TYR:CD2	1:Ag:384:PHE:HB2	2.55	0.41
1:Ak:116:TRP:CZ2	1:Ak:140:ILE:HA	2.56	0.41
2:Bc:53:LEU:HD11	2:Bc:133:LEU:HD11	2.03	0.41
2:Bg:21:ARG:HD2	2:Bg:27:VAL:HG11	2.01	0.41
5:Eb:85:ALA:HB1	6:Fb:133:GLY:HA3	2.02	0.41
5:Eg:87:GLN:CG	6:Fd:135:PHE:HB3	2.44	0.41
6:Fc:34:ASP:O	6:Fc:48:ALA:HA	2.20	0.41
7:Hi:12:LEU:HG	7:Hi:14:VAL:HG23	2.02	0.41
8:Ib:229:LEU:HD22	8:If:191:PHE:HB2	2.01	0.41
8:If:224:THR:HB	8:If:234:ARG:NH2	2.36	0.41
9:Jg:4:DT:H2'	9:Jg:5:DT:H71	2.02	0.41
9:Ji:19:DT:H2'	9:Ji:20:DT:H71	2.03	0.41
11:Ka:34:DC:H2'	11:Ka:35:DT:H71	2.01	0.41
1:Ab:46:ASN:HB2	1:Ab:308:TRP:CZ2	2.56	0.41
1:Ah:104:THR:HG22	2:Bh:5:GLN:HB3	2.03	0.41
1:Ak:401:PRO:HB3	1:Al:222:LYS:O	2.21	0.41
1:An:270:PRO:HG2	1:An:275:TYR:CE2	2.55	0.41
1:At:237:VAL:HG23	1:At:314:LEU:HB3	2.02	0.41
2:Bf:133:LEU:HD22	2:Bf:142:PHE:HB3	2.02	0.41
2:Br:105:PRO:HB2	2:Br:108:TYR:HD2	1.86	0.41
5:Ea:14:MET:HE1	5:Ea:79:ILE:HB	2.03	0.41
8:Ie:39:SER:HB2	8:If:317:GLU:OE1	2.20	0.41
10:Jb:27:DA:C6	10:Jb:28:DA:C6	3.09	0.41
10:Jf:11:DA:H2''	10:Jf:12:DA:C8	2.56	0.41
1:Ab:271:PRO:HG2	1:Ab:274:VAL:HG23	2.02	0.41
1:An:172:PRO:HA	1:An:180:GLY:HA2	2.01	0.41
1:An:189:VAL:HG11	1:An:192:ILE:HD13	2.02	0.41
1:Ar:186:ASP:HB2	2:Bq:1:MET:HG3	2.02	0.41
1:As:233:VAL:HG22	1:As:318:ASN:O	2.21	0.41
1:As:358:ASP:HB3	1:As:359:PRO:HD3	2.02	0.41
2:Bt:106:ILE:HG23	2:Bt:138:GLY:C	2.45	0.41
4:Dh:263:LYS:HA	4:Di:278:ILE:HD11	2.03	0.41
7:Hc:118:TYR:CE2	7:Hc:120:ASP:HB3	2.56	0.41
7:Hd:57:TYR:CE2	7:Hd:76:ARG:HG2	2.55	0.41
8:Ia:209:LEU:HD21	8:Ia:262:LEU:HD11	2.03	0.41
8:Ib:209:LEU:HD23	8:Ib:209:LEU:HA	1.94	0.41
10:Jh:26:DA:H2''	10:Jh:27:DA:H8	1.85	0.41
12:Kb:52:DT:H1'	12:Kb:53:DG:C8	2.55	0.41
1:Af:108:LEU:H	1:Af:371:LEU:HD23	1.86	0.41
1:Af:155:ARG:HG3	1:Af:327:PHE:CZ	2.56	0.41
1:Ak:200:PHE:CD2	1:Ak:392:TYR:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:At:194:LEU:HD12	1:At:390:LEU:HB2	2.02	0.41
2:Bk:113:ILE:HG22	2:Bk:114:GLU:HG2	2.03	0.41
4:Dc:248:ILE:HD11	4:Dc:259:TRP:CE3	2.56	0.41
4:Df:314:ILE:HA	4:Df:337:THR:HG23	2.03	0.41
4:Dj:293:ALA:HB3	4:Dk:240:MET:HG2	2.01	0.41
6:Fc:29:ARG:HD3	7:He:4:ASP:OD2	2.21	0.41
8:Id:224:THR:HB	8:Id:234:ARG:NH2	2.36	0.41
1:Ac:90:PRO:HB2	2:Bb:20:PRO:HB2	2.03	0.41
1:Af:58:THR:HG21	1:Af:63:LEU:HD11	2.02	0.41
1:Ag:358:ASP:HB3	1:Ag:359:PRO:HD3	2.02	0.41
1:An:164:ARG:HA	1:An:389:TRP:HE1	1.85	0.41
1:Ao:13:ARG:HB2	1:Aq:17:PRO:HB3	2.03	0.41
1:Ar:66:TYR:CZ	1:Ar:102:LYS:HE2	2.56	0.41
1:Ar:176:TYR:CZ	1:As:77:GLY:HA2	2.56	0.41
2:Bf:29:ALA:HB2	2:Bf:99:THR:HG22	2.03	0.41
4:Df:25:LYS:NZ	10:Jf:9:DA:H5''	2.35	0.41
6:Fc:37:TYR:CD1	6:Fd:128:VAL:HG11	2.56	0.41
7:Gj:92:LEU:HD12	7:Gj:105:LEU:HD11	2.03	0.41
7:Hf:12:LEU:HG	7:Hf:14:VAL:HG23	2.03	0.41
8:Ib:44:VAL:HG11	8:Ic:337:TYR:OH	2.21	0.41
8:Ib:151:MET:HE1	8:Ib:190:VAL:HG23	2.03	0.41
8:If:278:VAL:HG13	8:If:283:LYS:HB2	2.01	0.41
10:Jd:9:DA:H2'	10:Jd:10:DA:C8	2.55	0.41
9:Je:13:DT:H2'	9:Je:14:DT:H71	2.03	0.41
10:Jj:9:DA:H2'	10:Jj:10:DA:C8	2.56	0.41
1:Ad:97:LYS:HB3	2:Bd:14:GLN:HG2	2.03	0.41
1:Ah:317:LEU:HD13	1:Ah:321:THR:HA	2.03	0.41
1:Ak:95:VAL:HB	2:Bj:16:TRP:CE3	2.56	0.41
1:Ak:268:VAL:HG13	1:Al:262:VAL:HG12	2.03	0.41
1:Ao:251:VAL:O	1:Ao:255:VAL:HG23	2.22	0.41
1:Ap:317:LEU:HD13	1:Ap:321:THR:HA	2.03	0.41
1:Ar:337:ARG:HB2	1:Ar:337:ARG:CZ	2.51	0.41
1:As:255:VAL:HA	1:As:282:ILE:HD13	2.01	0.41
2:Bb:88:HIS:ND1	2:Bb:91:GLU:HB2	2.36	0.41
2:Bd:43:TRP:CD2	2:Bd:113:ILE:HD11	2.56	0.41
2:Bf:77:VAL:HG13	2:Bf:131:LEU:HD23	2.02	0.41
2:Bn:22:LEU:HD22	2:Bn:25:TYR:H	1.85	0.41
4:Db:314:ILE:HA	4:Db:337:THR:HG23	2.03	0.41
4:Dd:263:LYS:HA	4:De:278:ILE:HD11	2.02	0.41
7:Hb:97:PRO:HA	7:Hb:130:VAL:HB	2.03	0.41
11:Ka:14:DC:C2'	11:Ka:15:DA:C8	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:24:LYS:HE3	2:Bt:86:ASP:HB2	2.03	0.40
1:Ab:1:MET:HE2	1:Af:127:LEU:HD11	2.03	0.40
1:Aj:314:LEU:HD21	1:Aj:390:LEU:HD23	2.02	0.40
1:Ak:236:ILE:HG22	1:Ak:315:ILE:HB	2.03	0.40
1:An:48:LEU:HB2	1:An:294:TYR:CZ	2.57	0.40
2:Bd:34:MET:SD	2:Bd:96:VAL:HG13	2.62	0.40
2:Bg:81:ILE:HD12	2:Bg:81:ILE:HA	1.95	0.40
2:Bn:133:LEU:HD22	2:Bn:142:PHE:HB3	2.03	0.40
3:Cb:28:TYR:CD1	3:Cb:39:TRP:HB3	2.57	0.40
4:Da:237:GLU:CD	5:Ea:126:ILE:HG22	2.46	0.40
5:Eg:67:ILE:HD13	5:Eg:67:ILE:HA	1.89	0.40
6:Fb:61:LEU:HD22	8:Ia:3:GLY:O	2.21	0.40
6:Fc:39:SER:HB2	6:Fd:130:GLU:OE2	2.21	0.40
6:Fd:12:LYS:HE2	6:Fd:16:GLU:OE2	2.22	0.40
8:Ia:85:LEU:HD23	8:Ia:85:LEU:HA	1.95	0.40
8:Ia:85:LEU:HA	8:Ia:88:ILE:HD12	2.03	0.40
8:Ic:246:GLY:HA3	8:Ic:334:PHE:CZ	2.56	0.40
10:Jb:26:DA:H2''	10:Jb:27:DA:H8	1.86	0.40
9:Jc:19:DT:H2'	9:Jc:20:DT:H71	2.03	0.40
10:Jh:28:DA:H2''	10:Jh:29:DA:H8	1.85	0.40
10:Jh:28:DA:H2''	10:Jh:29:DA:C8	2.56	0.40
9:Ji:1:DT:H6	9:Ji:1:DT:H2'	1.70	0.40
1:Aj:235:ILE:HG23	1:Aj:314:LEU:HD13	2.03	0.40
1:An:164:ARG:HA	1:An:389:TRP:NE1	2.37	0.40
1:An:271:PRO:HG2	1:An:274:VAL:HG23	2.03	0.40
1:Ao:268:VAL:HG13	1:Ap:262:VAL:HG12	2.02	0.40
7:Hc:9:ARG:O	7:Hc:81:LEU:HB2	2.21	0.40
7:Hi:7:ILE:HG12	7:Hi:13:PHE:CD1	2.56	0.40
7:Hi:79:GLY:HA2	7:Hj:61:TYR:OH	2.21	0.40
8:If:224:THR:HG22	8:If:237:LEU:HD22	2.02	0.40
10:Jh:9:DA:H2'	10:Jh:10:DA:C8	2.56	0.40
1:Ac:358:ASP:HB3	1:Ac:359:PRO:HD3	2.02	0.40
1:Ag:237:VAL:HG21	1:Ag:241:PHE:HB2	2.02	0.40
1:Ag:374:LEU:HD13	1:Ag:384:PHE:CD2	2.57	0.40
1:Ar:108:LEU:H	1:Ar:371:LEU:HD23	1.86	0.40
2:Bn:102:ALA:HB3	2:Bn:142:PHE:CZ	2.56	0.40
2:Br:105:PRO:HB2	2:Br:108:TYR:CD2	2.56	0.40
4:Dc:203:HIS:NE2	4:Dc:214:ALA:HB2	2.36	0.40
4:Df:239:PHE:CZ	4:Df:292:SER:HB2	2.57	0.40
4:Dl:203:HIS:NE2	4:Dl:214:ALA:HB2	2.37	0.40
5:Ed:85:ALA:HB1	6:Fc:133:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ee:15:PRO:HD2	5:Ee:18:VAL:HG21	2.03	0.40
5:El:85:ALA:HB1	6:Fa:133:GLY:HA3	2.03	0.40
6:Fe:82:TYR:CE2	6:Fe:84:ASP:HB2	2.57	0.40
8:Ib:308:ILE:HG12	8:Ib:342:VAL:HG22	2.03	0.40
8:Ic:317:GLU:HA	8:Ic:318:PRO:HD3	1.92	0.40
8:If:310:LEU:HD13	8:If:336:ALA:HB2	2.03	0.40
9:Jc:5:DT:H2'	9:Jc:6:DT:H71	2.03	0.40
9:Je:19:DT:H2'	9:Je:20:DT:H71	2.02	0.40
10:Jj:25:DA:C6	10:Jj:26:DA:C6	3.09	0.40
1:Ab:58:THR:O	1:Ab:330:THR:HA	2.22	0.40
1:Af:229:ASP:HA	1:Af:319:GLN:HG3	2.04	0.40
1:Ag:3:VAL:HG22	2:Bh:15:TYR:HB3	2.02	0.40
1:Ap:374:LEU:HD13	1:Ap:384:PHE:CE2	2.57	0.40
1:Ar:52:PHE:HA	1:Ar:323:PRO:HA	2.03	0.40
1:Ar:104:THR:OG1	2:Bq:5:GLN:HB3	2.22	0.40
6:Fe:34:ASP:O	6:Fe:48:ALA:HA	2.22	0.40
7:Ha:12:LEU:HG	7:Ha:14:VAL:HG23	2.03	0.40
7:Hi:9:ARG:O	7:Hi:81:LEU:HB2	2.21	0.40
8:Ie:278:VAL:HG13	8:Ie:283:LYS:HB2	2.03	0.40
12:Kb:10:DG:OP2	12:Kb:10:DG:H8	2.05	0.40
1:Aj:164:ARG:HA	1:Aj:389:TRP:NE1	2.36	0.40
2:Bc:16:TRP:CD2	2:Bc:87:GLY:HA3	2.57	0.40
5:Eb:16:ALA:HB2	5:Ec:27:GLU:O	2.21	0.40
5: Ei:87:GLN:CG	6:Fe:135:PHE:HB3	2.45	0.40
8:Ib:288:LYS:HA	8:Ib:308:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	36/409 (9%)	33 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	376/409 (92%)	365 (97%)	11 (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%)	361 (96%)	15 (4%)	0	100	100
1	Ag	407/409 (100%)	397 (98%)	10 (2%)	0	100	100
1	Ah	221/409 (54%)	219 (99%)	2 (1%)	0	100	100
1	Ai	36/409 (9%)	33 (92%)	3 (8%)	0	100	100
1	Aj	376/409 (92%)	361 (96%)	15 (4%)	0	100	100
1	Ak	407/409 (100%)	399 (98%)	8 (2%)	0	100	100
1	Al	221/409 (54%)	216 (98%)	5 (2%)	0	100	100
1	Am	36/409 (9%)	33 (92%)	3 (8%)	0	100	100
1	An	376/409 (92%)	359 (96%)	17 (4%)	0	100	100
1	Ao	407/409 (100%)	398 (98%)	9 (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%)	358 (95%)	18 (5%)	0	100	100
1	As	407/409 (100%)	397 (98%)	10 (2%)	0	100	100
1	At	221/409 (54%)	216 (98%)	5 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	143 (99%)	1 (1%)	0	100	100
3	Ca	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
3	Cb	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
3	Cc	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
3	Cd	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
3	Ce	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
4	Da	421/423 (100%)	417 (99%)	4 (1%)	0	100	100
4	Db	421/423 (100%)	419 (100%)	2 (0%)	0	100	100
4	Dc	421/423 (100%)	418 (99%)	3 (1%)	0	100	100
4	Dd	421/423 (100%)	417 (99%)	4 (1%)	0	100	100
4	De	421/423 (100%)	416 (99%)	5 (1%)	0	100	100
4	Df	421/423 (100%)	416 (99%)	5 (1%)	0	100	100
4	Dg	421/423 (100%)	417 (99%)	4 (1%)	0	100	100
4	Dh	421/423 (100%)	419 (100%)	2 (0%)	0	100	100
4	Di	421/423 (100%)	417 (99%)	4 (1%)	0	100	100
4	Dj	421/423 (100%)	417 (99%)	4 (1%)	0	100	100
4	Dk	421/423 (100%)	419 (100%)	2 (0%)	0	100	100
4	Dl	421/423 (100%)	416 (99%)	5 (1%)	0	100	100
5	Ea	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
5	Eb	128/130 (98%)	128 (100%)	0	0	100	100
5	Ec	128/130 (98%)	126 (98%)	2 (2%)	0	100	100
5	Ed	128/130 (98%)	128 (100%)	0	0	100	100
5	Ee	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
5	Ef	128/130 (98%)	128 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Eg	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
5	Eh	128/130 (98%)	128 (100%)	0	0	100	100
5	Ei	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
5	Ej	128/130 (98%)	128 (100%)	0	0	100	100
5	Ek	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
5	El	128/130 (98%)	128 (100%)	0	0	100	100
6	Fa	153/155 (99%)	153 (100%)	0	0	100	100
6	Fb	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
6	Fc	153/155 (99%)	153 (100%)	0	0	100	100
6	Fd	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
6	Fe	153/155 (99%)	153 (100%)	0	0	100	100
6	Ff	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
7	Ga	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
7	Gb	144/146 (99%)	144 (100%)	0	0	100	100
7	Gc	85/146 (58%)	84 (99%)	1 (1%)	0	100	100
7	Gd	85/146 (58%)	84 (99%)	1 (1%)	0	100	100
7	Ge	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
7	Gf	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
7	Gg	85/146 (58%)	85 (100%)	0	0	100	100
7	Gh	85/146 (58%)	84 (99%)	1 (1%)	0	100	100
7	Gi	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
7	Gj	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
7	Gk	85/146 (58%)	85 (100%)	0	0	100	100
7	Gl	85/146 (58%)	84 (99%)	1 (1%)	0	100	100
7	Ha	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
7	Hb	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
7	Hc	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
7	Hd	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
7	He	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
7	Hf	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
7	Hg	144/146 (99%)	139 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Hh	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
7	Hi	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
7	Hj	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
7	Hk	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
7	Hl	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
8	Ia	346/348 (99%)	341 (99%)	5 (1%)	0	100	100
8	Ib	346/348 (99%)	341 (99%)	5 (1%)	0	100	100
8	Ic	346/348 (99%)	341 (99%)	5 (1%)	0	100	100
8	Id	346/348 (99%)	342 (99%)	4 (1%)	0	100	100
8	Ie	346/348 (99%)	342 (99%)	4 (1%)	0	100	100
8	If	346/348 (99%)	343 (99%)	3 (1%)	0	100	100
All	All	20509/24623 (83%)	20162 (98%)	347 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	352/352 (100%)	352 (100%)	0	100	100
4	Db	352/352 (100%)	352 (100%)	0	100	100
4	Dc	352/352 (100%)	352 (100%)	0	100	100
4	Dd	352/352 (100%)	352 (100%)	0	100	100
4	De	352/352 (100%)	352 (100%)	0	100	100
4	Df	352/352 (100%)	352 (100%)	0	100	100
4	Dg	352/352 (100%)	352 (100%)	0	100	100
4	Dh	352/352 (100%)	352 (100%)	0	100	100
4	Di	352/352 (100%)	352 (100%)	0	100	100
4	Dj	352/352 (100%)	352 (100%)	0	100	100
4	Dk	352/352 (100%)	352 (100%)	0	100	100
4	Dl	352/352 (100%)	352 (100%)	0	100	100
5	Ea	105/105 (100%)	105 (100%)	0	100	100
5	Eb	105/105 (100%)	105 (100%)	0	100	100
5	Ec	105/105 (100%)	105 (100%)	0	100	100
5	Ed	105/105 (100%)	105 (100%)	0	100	100
5	Ee	105/105 (100%)	105 (100%)	0	100	100
5	Ef	105/105 (100%)	105 (100%)	0	100	100
5	Eg	105/105 (100%)	105 (100%)	0	100	100
5	Eh	105/105 (100%)	105 (100%)	0	100	100
5	Ei	105/105 (100%)	105 (100%)	0	100	100
5	Ej	105/105 (100%)	105 (100%)	0	100	100
5	Ek	105/105 (100%)	105 (100%)	0	100	100
5	El	105/105 (100%)	105 (100%)	0	100	100
6	Fa	129/129 (100%)	129 (100%)	0	100	100
6	Fb	129/129 (100%)	129 (100%)	0	100	100
6	Fc	129/129 (100%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Fd	129/129 (100%)	129 (100%)	0	100	100
6	Fe	129/129 (100%)	129 (100%)	0	100	100
6	Ff	129/129 (100%)	129 (100%)	0	100	100
7	Ga	124/124 (100%)	124 (100%)	0	100	100
7	Gb	124/124 (100%)	124 (100%)	0	100	100
7	Gc	75/124 (60%)	75 (100%)	0	100	100
7	Gd	75/124 (60%)	75 (100%)	0	100	100
7	Ge	124/124 (100%)	124 (100%)	0	100	100
7	Gf	124/124 (100%)	124 (100%)	0	100	100
7	Gg	75/124 (60%)	75 (100%)	0	100	100
7	Gh	75/124 (60%)	75 (100%)	0	100	100
7	Gi	124/124 (100%)	124 (100%)	0	100	100
7	Gj	124/124 (100%)	124 (100%)	0	100	100
7	Gk	75/124 (60%)	75 (100%)	0	100	100
7	Gl	75/124 (60%)	75 (100%)	0	100	100
7	Ha	124/124 (100%)	124 (100%)	0	100	100
7	Hb	124/124 (100%)	124 (100%)	0	100	100
7	Hc	124/124 (100%)	124 (100%)	0	100	100
7	Hd	124/124 (100%)	124 (100%)	0	100	100
7	He	124/124 (100%)	124 (100%)	0	100	100
7	Hf	124/124 (100%)	124 (100%)	0	100	100
7	Hg	124/124 (100%)	124 (100%)	0	100	100
7	Hh	124/124 (100%)	124 (100%)	0	100	100
7	Hi	124/124 (100%)	124 (100%)	0	100	100
7	Hj	124/124 (100%)	124 (100%)	0	100	100
7	Hk	124/124 (100%)	124 (100%)	0	100	100
7	Hl	124/124 (100%)	124 (100%)	0	100	100
8	Ia	282/282 (100%)	282 (100%)	0	100	100
8	Ib	282/282 (100%)	282 (100%)	0	100	100
8	Ic	282/282 (100%)	282 (100%)	0	100	100
8	Id	282/282 (100%)	282 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ie	282/282 (100%)	282 (100%)	0	100	100
8	If	282/282 (100%)	282 (100%)	0	100	100
All	All	17487/20736 (84%)	17487 (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 (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ab	9	ASN
1	Ab	248	ASN
1	Ac	82	HIS
1	Ac	139	GLN
1	Ac	179	ASN
1	Ac	319	GLN
1	Ad	198	GLN
1	Af	132	GLN
1	Af	208	ASN
1	Af	248	ASN
1	Ag	71	GLN
1	Ag	139	GLN
1	Ag	179	ASN
1	Ag	319	GLN
1	Ah	198	GLN
1	Ah	319	GLN
1	Aj	137	ASN
1	Aj	208	ASN
1	Aj	248	ASN
1	Ak	71	GLN
1	Ak	139	GLN
1	Ak	179	ASN
1	Ak	369	HIS
1	Al	198	GLN
1	An	6	ASN
1	An	208	ASN
1	An	248	ASN
1	Ao	71	GLN
1	Ao	82	HIS
1	Ao	139	GLN
1	Ao	179	ASN
1	Ao	319	GLN

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Mol	Chain	Res	Type
1	Ao	338	ASN
1	Ap	198	GLN
1	Ap	319	GLN
1	Ar	177	ASN
1	Ar	208	ASN
1	Ar	248	ASN
1	As	71	GLN
1	As	139	GLN
1	As	179	ASN
1	At	198	GLN
1	At	319	GLN
2	Ba	14	GLN
2	Bc	139	HIS
2	Bg	65	HIS
2	Bg	139	HIS
2	Bh	23	HIS
2	Bj	14	GLN
2	Bj	95	ASN
2	Bk	88	HIS
2	Bk	139	HIS
2	Bl	95	ASN
2	Bn	5	GLN
2	Bo	88	HIS
2	Bo	139	HIS
2	Bq	14	GLN
2	Br	23	HIS
2	Bt	14	GLN
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
3	Ce	52	GLN
3	Ce	56	GLN
4	Db	396	ASN
4	Dd	345	GLN
4	Dd	396	ASN
4	De	268	ASN
4	De	345	GLN

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Mol	Chain	Res	Type
4	Dg	51	GLN
4	Dh	234	HIS
4	Dh	271	GLN
4	Dh	396	ASN
4	Di	275	HIS
4	Dk	268	ASN
4	Dl	254	GLN
5	Ef	87	GLN
5	Eg	55	ASN
5	Ek	55	ASN
5	El	87	GLN
6	Fa	104	HIS
6	Fb	10	HIS
6	Fb	88	GLN
6	Fd	10	HIS
6	Fd	88	GLN
6	Fe	153	ASN
6	Ff	10	HIS
6	Ff	88	GLN
7	Ga	108	GLN
7	Gb	129	GLN
7	Gb	134	GLN
7	Ge	71	GLN
7	Gf	129	GLN
7	Gj	129	GLN
7	Ha	38	GLN
7	Hb	66	ASN
7	Hc	38	GLN
7	Hd	38	GLN
7	He	38	GLN
7	Hg	38	GLN
7	Hh	38	GLN
7	Hi	38	GLN
7	Hk	38	GLN
7	Hl	38	GLN
8	Ia	149	ASN
8	Ia	155	ASN
8	Ia	167	GLN
8	Ib	155	ASN
8	Ic	149	ASN
8	Ic	155	ASN
8	Id	57	GLN

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Mol	Chain	Res	Type
8	Ie	57	GLN
8	If	149	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

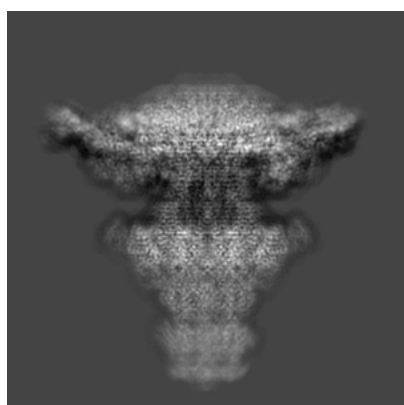
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70281. These allow visual inspection of the internal detail of the map and identification of artifacts.

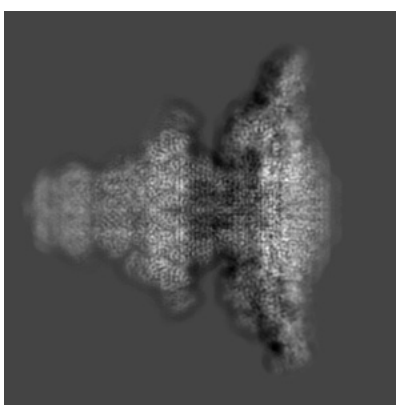
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

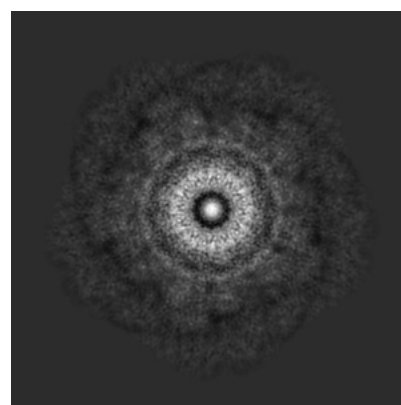
6.1.1 Primary map



X



Y

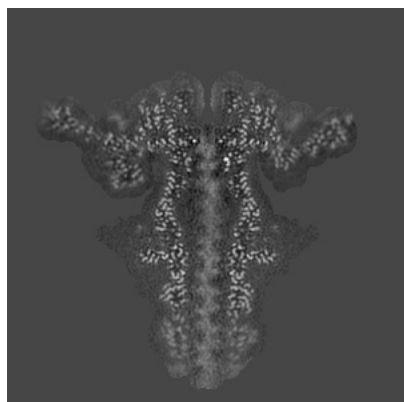


Z

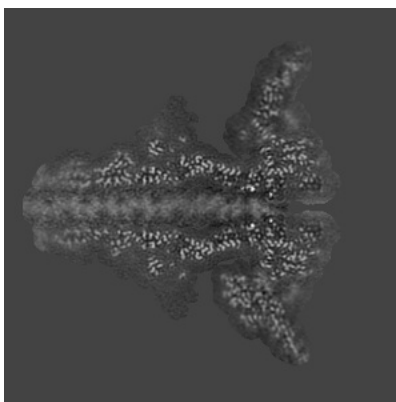
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

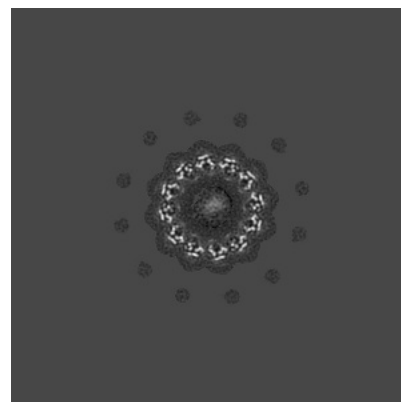
6.2.1 Primary map



X Index: 180



Y Index: 180

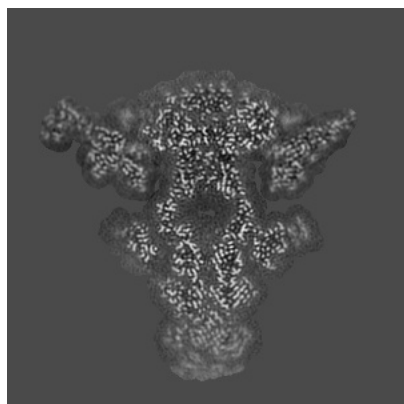


Z Index: 180

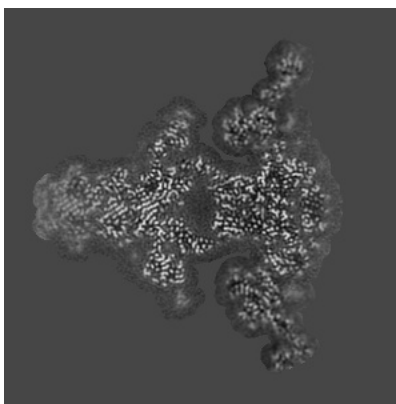
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

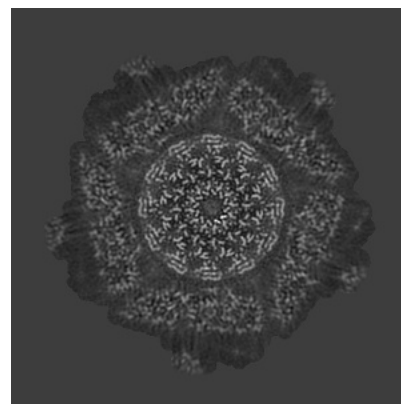
6.3.1 Primary map



X Index: 160



Y Index: 158

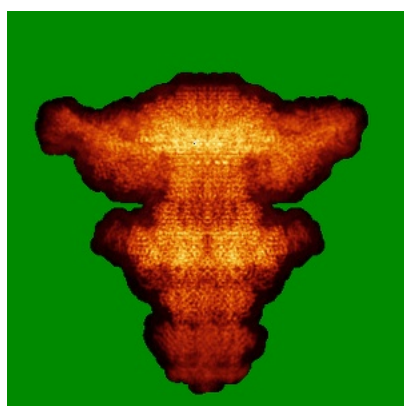


Z Index: 243

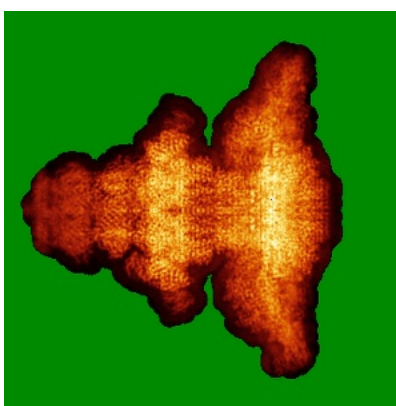
The images above show the largest variance slices of the map in three orthogonal directions.

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

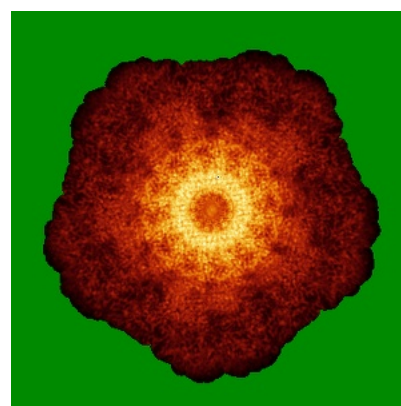
6.4.1 Primary map



X



Y

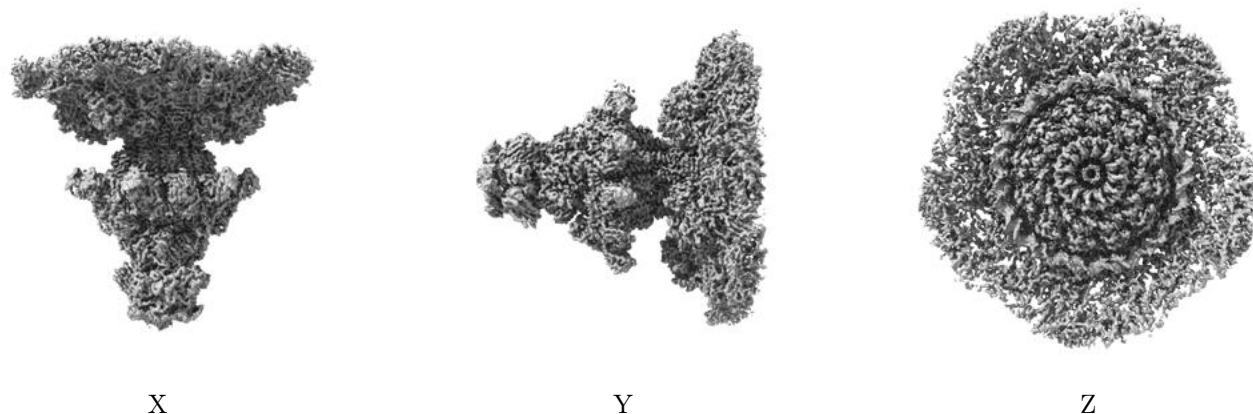


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

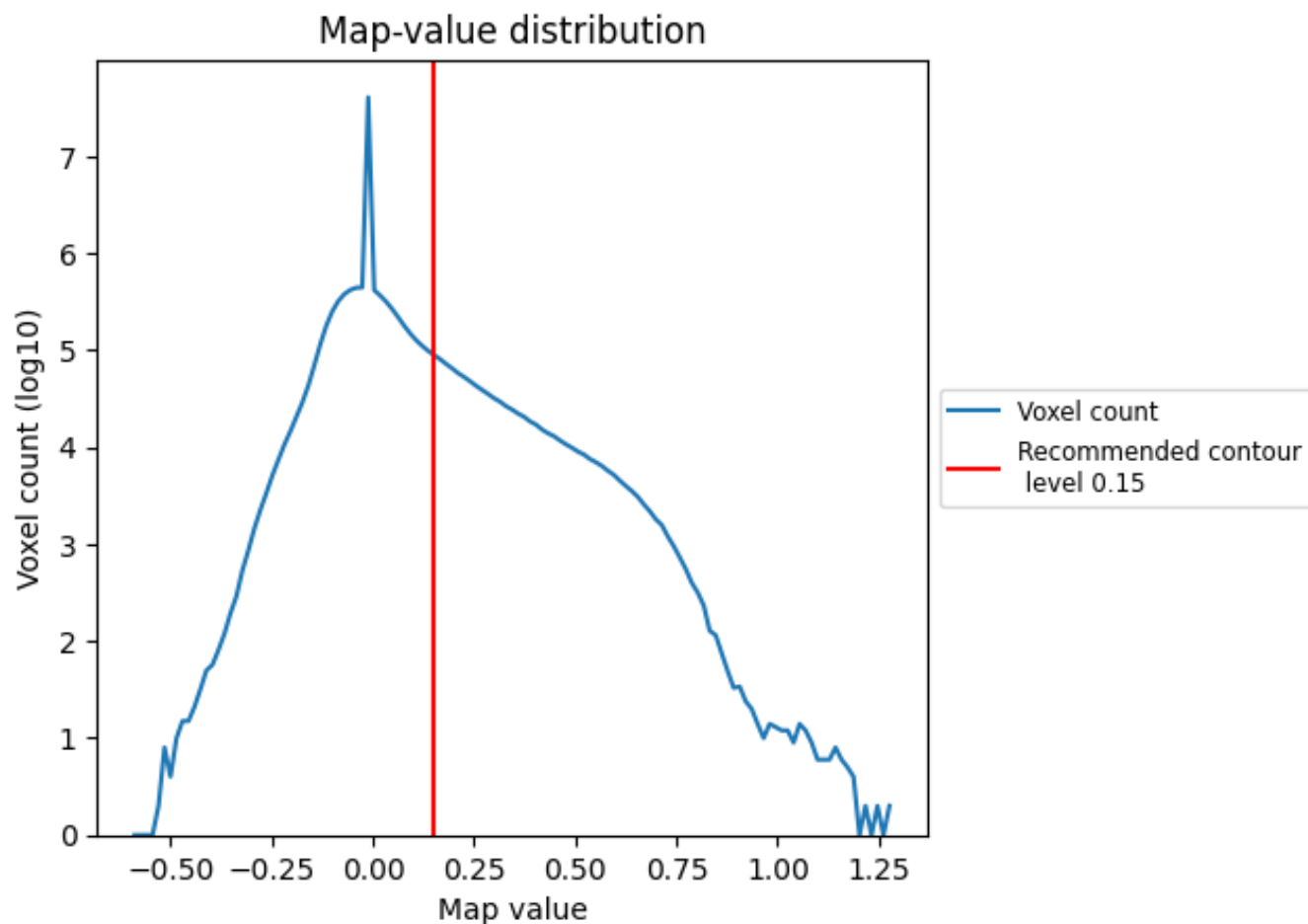
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

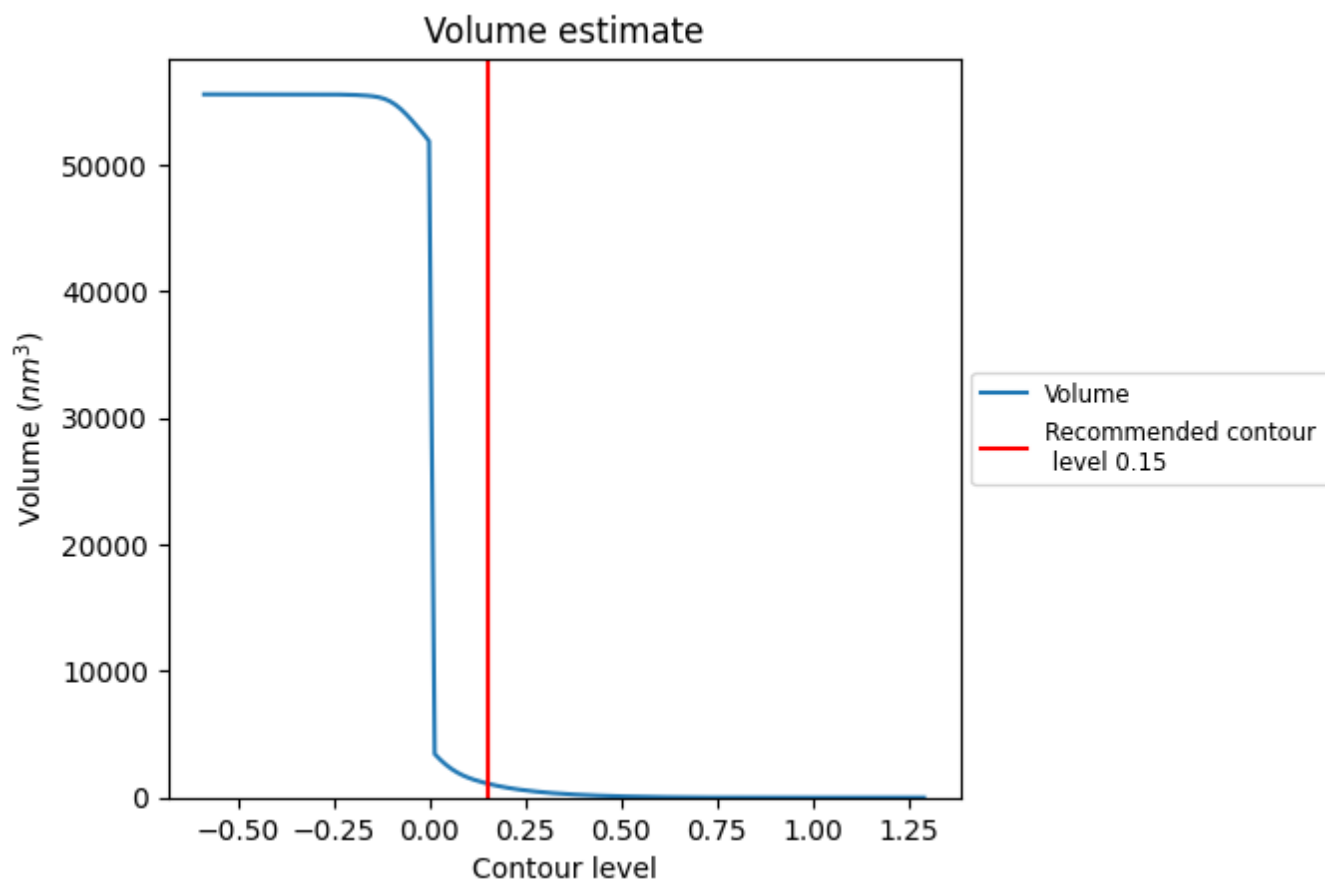
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

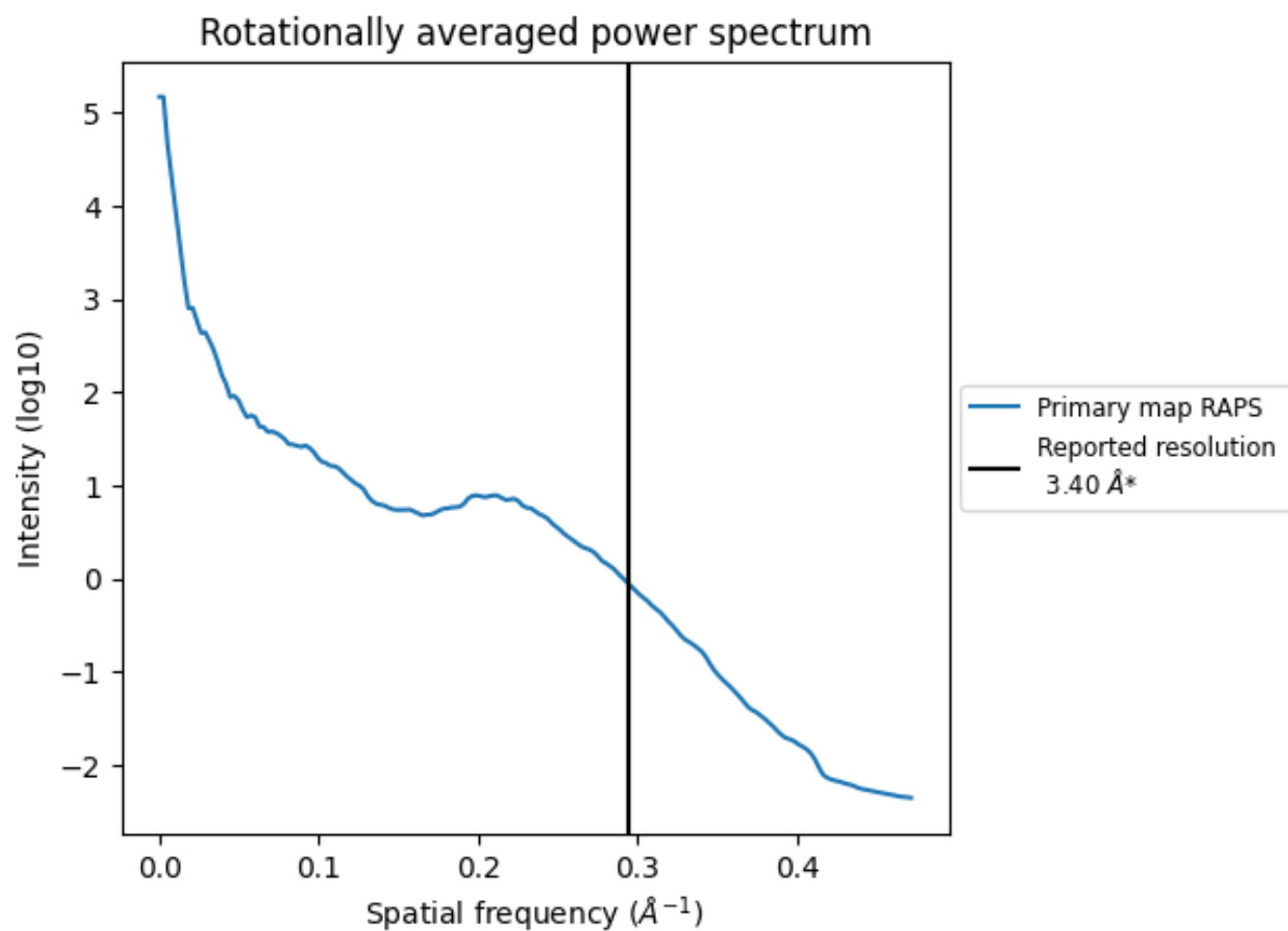
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1114 nm³; this corresponds to an approximate mass of 1006 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 0.294 Å⁻¹

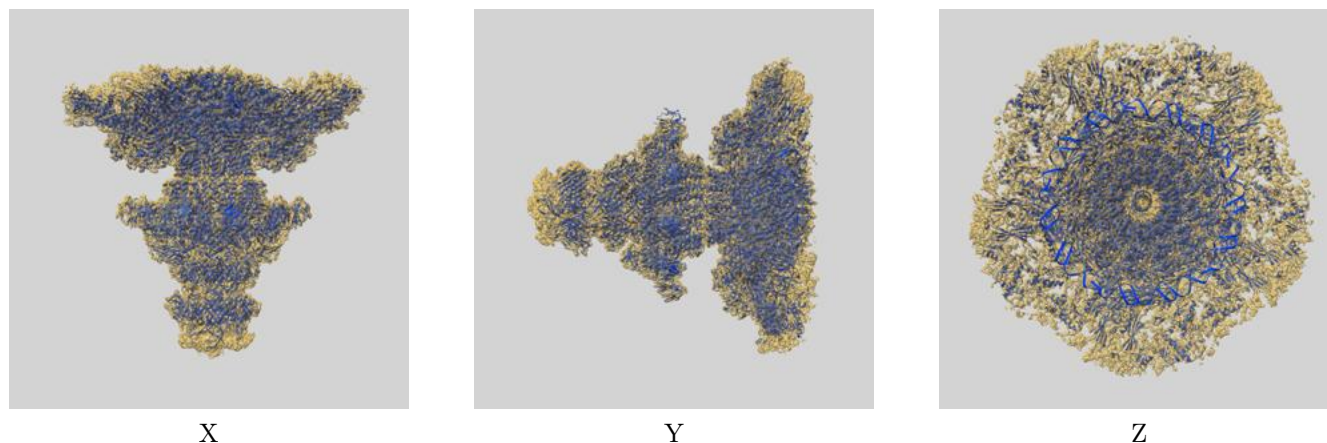
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

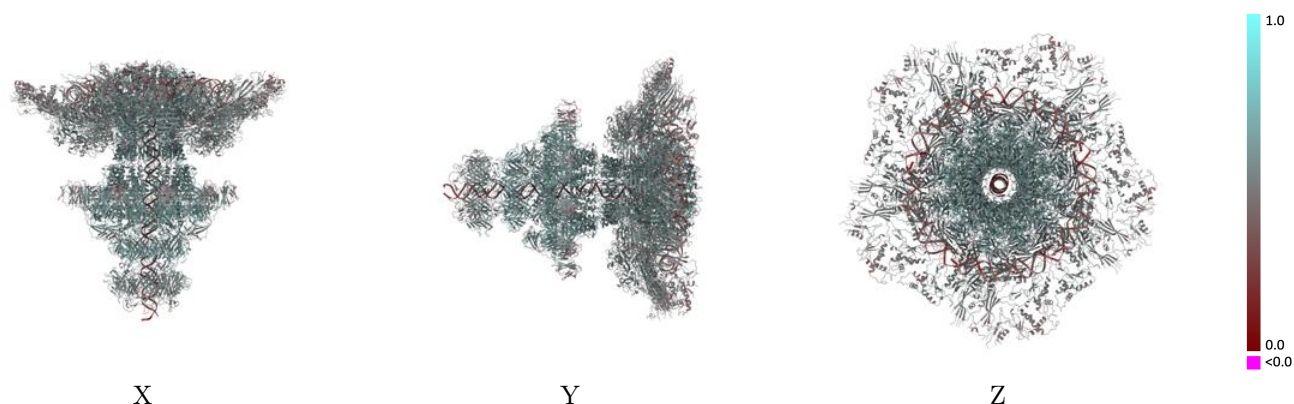
This section contains information regarding the fit between EMDB map EMD-70281 and PDB model 9OAE. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



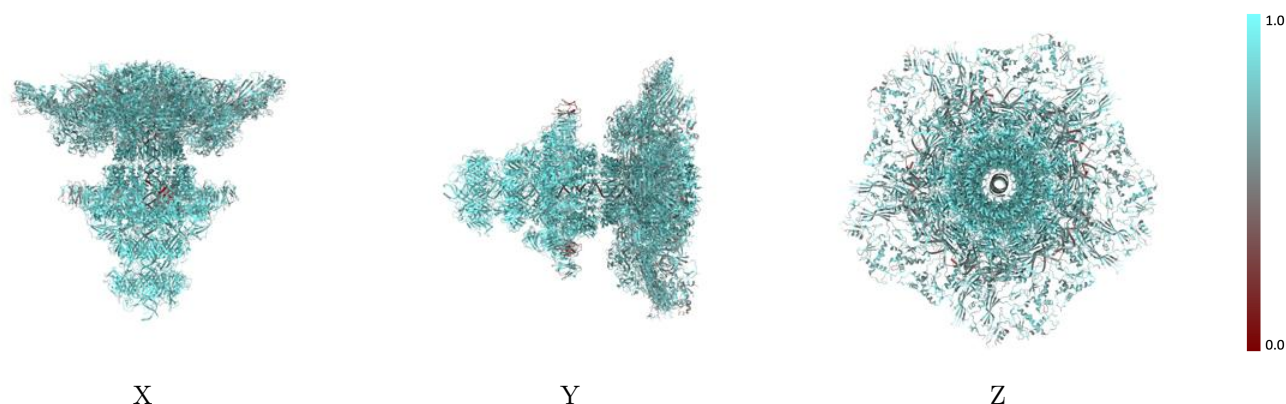
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



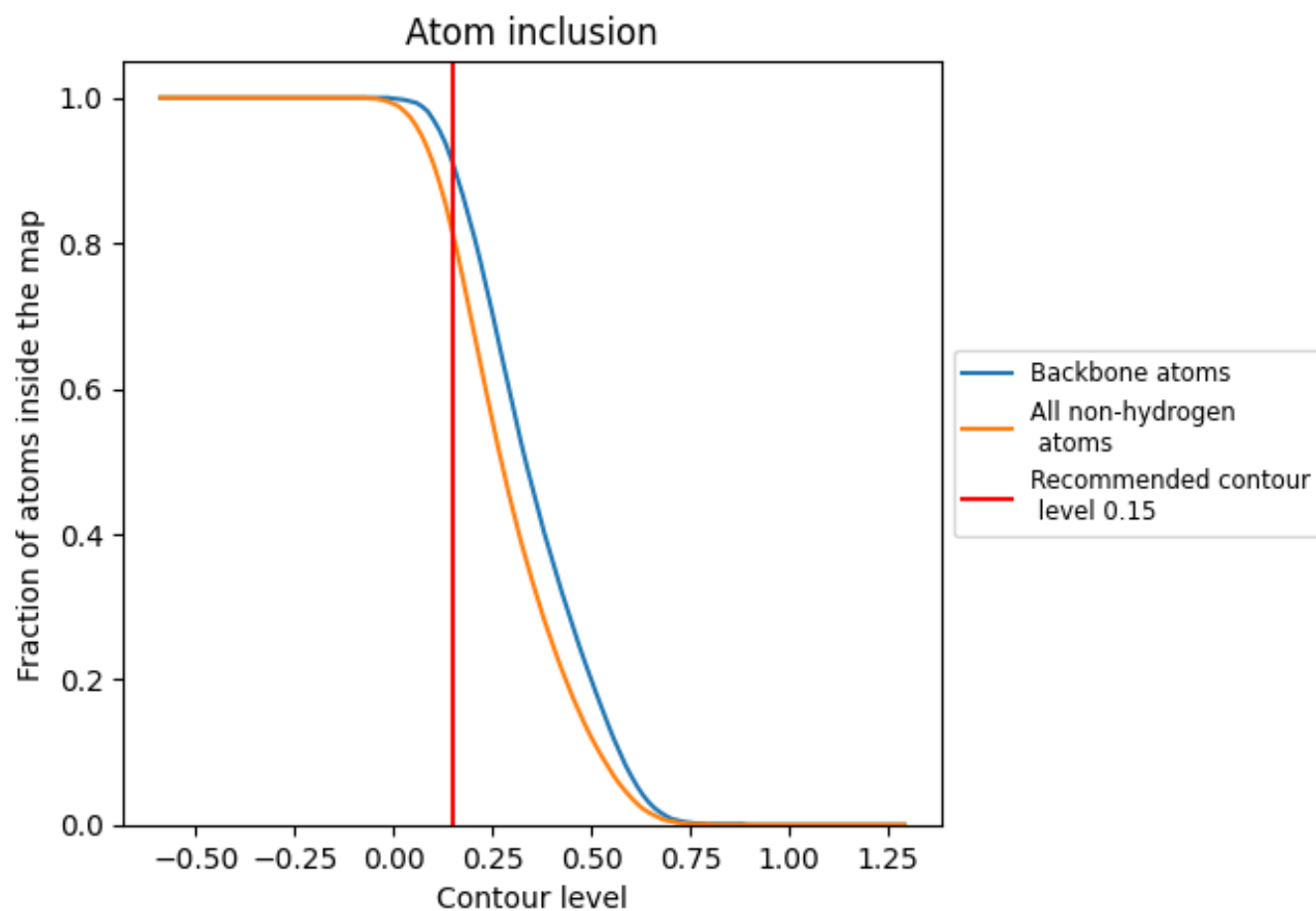
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.5250
Aa	 0.7090	 0.4700
Ab	 0.7230	 0.4800
Ac	 0.7450	 0.4950
Ad	 0.6810	 0.4520
Ae	 0.7380	 0.4730
Af	 0.7360	 0.4850
Ag	 0.7230	 0.4950
Ah	 0.7100	 0.4590
Ai	 0.6950	 0.4750
Aj	 0.7390	 0.4820
Ak	 0.7370	 0.4940
Al	 0.6730	 0.4540
Am	 0.7090	 0.4700
An	 0.7310	 0.4860
Ao	 0.7260	 0.4960
Ap	 0.6700	 0.4540
Aq	 0.7200	 0.4790
Ar	 0.7350	 0.4810
As	 0.7260	 0.4940
At	 0.6590	 0.4580
Ba	 0.6420	 0.4830
Bb	 0.7500	 0.5000
Bc	 0.7240	 0.5030
Bd	 0.7720	 0.5010
Be	 0.6740	 0.4810
Bf	 0.7400	 0.4940
Bg	 0.7090	 0.5010
Bh	 0.7550	 0.4990
Bi	 0.6420	 0.4740
Bj	 0.7520	 0.4980
Bk	 0.7230	 0.4930
Bl	 0.7660	 0.5020
Bm	 0.6240	 0.4770
Bn	 0.7710	 0.5070



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Chain	Atom inclusion	Q-score
Bo	 0.7110	 0.5010
Bp	 0.7460	 0.5030
Bq	 0.6610	 0.4900
Br	 0.7370	 0.4940
Bs	 0.7250	 0.5020
Bt	 0.7610	 0.5010
Ca	 0.6700	 0.4840
Cb	 0.6670	 0.4940
Cc	 0.6680	 0.4890
Cd	 0.6530	 0.4830
Ce	 0.6790	 0.4870
Da	 0.9100	 0.5890
Db	 0.9180	 0.5910
Dc	 0.9070	 0.5890
Dd	 0.9050	 0.5900
De	 0.9110	 0.5900
Df	 0.9070	 0.5860
Dg	 0.9080	 0.5890
Dh	 0.9110	 0.5920
Di	 0.9120	 0.5910
Dj	 0.9120	 0.5890
Dk	 0.9090	 0.5910
Dl	 0.9110	 0.5900
Ea	 0.9040	 0.5890
Eb	 0.9070	 0.5940
Ec	 0.9020	 0.5840
Ed	 0.9020	 0.5890
Ee	 0.9090	 0.5870
Ef	 0.9040	 0.5940
Eg	 0.9020	 0.5860
Eh	 0.8980	 0.5910
Ei	 0.9070	 0.5880
Ej	 0.9070	 0.5930
Ek	 0.9010	 0.5870
El	 0.8990	 0.5930
Fa	 0.9490	 0.6140
Fb	 0.9410	 0.6050
Fc	 0.9460	 0.6110
Fd	 0.9400	 0.6060
Fe	 0.9480	 0.6110
Ff	 0.9410	 0.6080
Ga	 0.8750	 0.5550

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Chain	Atom inclusion	Q-score
Gb	 0.8830	 0.5540
Gc	 0.9040	 0.5800
Gd	 0.8360	 0.5430
Ge	 0.8720	 0.5550
Gf	 0.8780	 0.5550
Gg	 0.9070	 0.5770
Gh	 0.8320	 0.5470
Gi	 0.8740	 0.5570
Gj	 0.8790	 0.5540
Gk	 0.9030	 0.5780
Gl	 0.8350	 0.5520
Ha	 0.8510	 0.5520
Hb	 0.8530	 0.5440
Hc	 0.6960	 0.5290
Hd	 0.8230	 0.5260
He	 0.8490	 0.5540
Hf	 0.8490	 0.5430
Hg	 0.6940	 0.5310
Hh	 0.8100	 0.5250
Hi	 0.8470	 0.5540
Hj	 0.8520	 0.5410
Hk	 0.6910	 0.5270
Hl	 0.8230	 0.5290
Ia	 0.9220	 0.5820
Ib	 0.9210	 0.5830
Ic	 0.9240	 0.5830
Id	 0.8400	 0.4870
Ie	 0.8330	 0.4850
If	 0.8370	 0.4880
Ja	 0.5390	 0.2900
Jb	 0.6140	 0.3190
Jc	 0.5530	 0.2840
Jd	 0.5850	 0.3090
Je	 0.5450	 0.2810
Jf	 0.6180	 0.3090
Jg	 0.5310	 0.2890
Jh	 0.5960	 0.3220
Ji	 0.5690	 0.2920
Jj	 0.6210	 0.3170
Ka	 0.7440	 0.2390
Kb	 0.6650	 0.2380