



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:07 PM UTC

PDB ID : 8B3Q / pdb_00008b3q
EMDB ID : EMD-15833
Title : CryoEM structure of the central filamentous region of the f1 filamentous bacteriophage, consisting of the major capsid protein pVIII
Authors : Conners, R.; McLaren, M.; Gold, V.A.M.
Deposited on : 2022-09-16
Resolution : 2.58 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

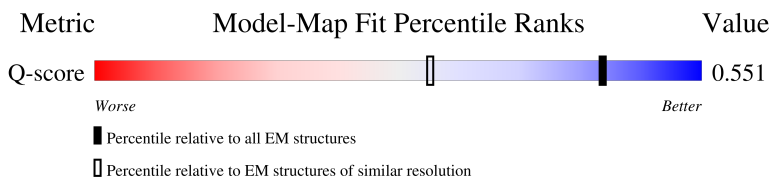
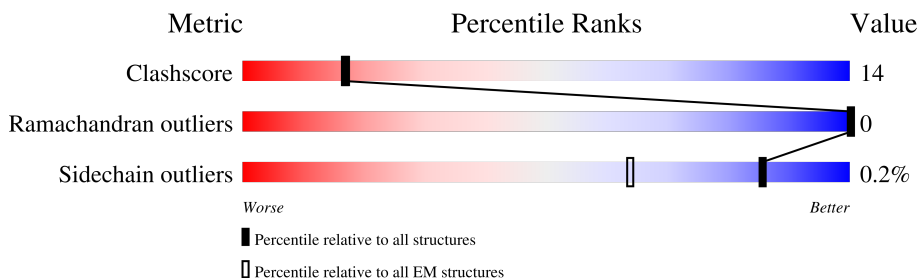
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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.



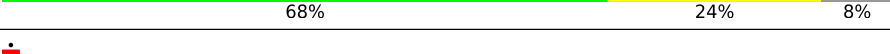
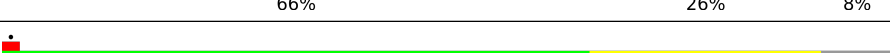
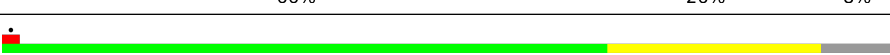
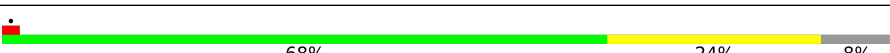
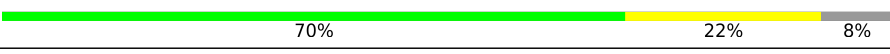
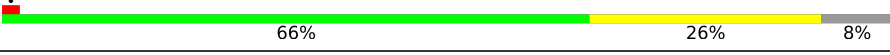
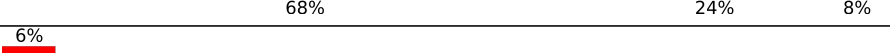
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7675 (2.08 - 3.08)

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	AAA	50	 72% 20% 8%
1	AaA	50	 70% 22% 8%
1	AbA	50	 68% 24% 8%
1	AcA	50	 66% 26% 8%

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Mol	Chain	Length	Quality of chain
1	AdA	50	
1	AeA	50	
1	AfA	50	
1	AgA	50	
1	AhA	50	
1	AiA	50	
1	AjA	50	
1	AkA	50	
1	AlA	50	
1	AmA	50	
1	AnA	50	
1	BBB	50	
1	BaB	50	
1	BbB	50	
1	BcB	50	
1	BdB	50	
1	BeB	50	
1	BfB	50	
1	BgB	50	
1	BhB	50	
1	BiB	50	
1	BjB	50	
1	BkB	50	
1	BlB	50	
1	BmB	50	

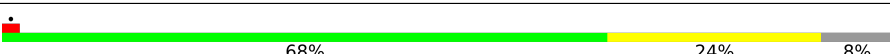
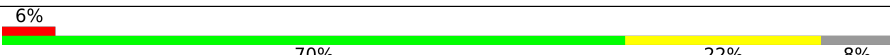
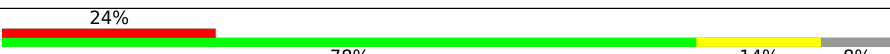
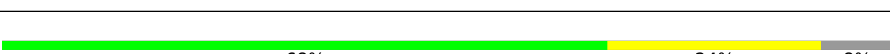
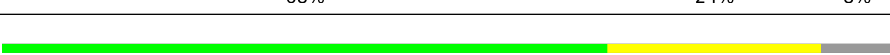
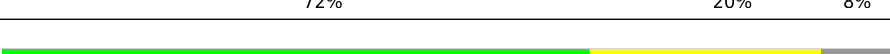
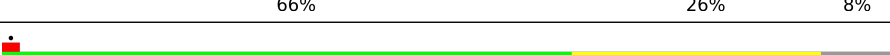
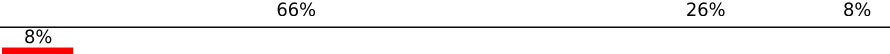
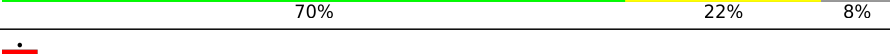
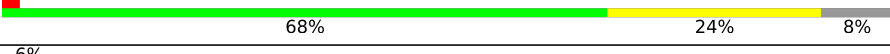
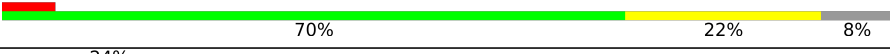
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Mol	Chain	Length	Quality of chain
1	BnB	50	
1	CCC	50	
1	CaC	50	
1	CbC	50	
1	CcC	50	
1	CdC	50	
1	CeC	50	
1	CfC	50	
1	CgC	50	
1	ChC	50	
1	CiC	50	
1	CjC	50	
1	CkC	50	
1	ClC	50	
1	CmC	50	
1	CnC	50	
1	DDD	50	
1	DaD	50	
1	DbD	50	
1	DcD	50	
1	DdD	50	
1	DeD	50	
1	DfD	50	
1	DgD	50	
1	DhD	50	

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Mol	Chain	Length	Quality of chain
1	DiD	50	
1	DjD	50	
1	DkD	50	
1	DlD	50	
1	DmD	50	
1	DnD	50	
1	EEE	50	
1	EaE	50	
1	EbE	50	
1	EcE	50	
1	EdE	50	
1	EeE	50	
1	EfE	50	
1	EgE	50	
1	EhE	50	
1	EiE	50	
1	EjE	50	
1	EkE	50	
1	ElE	50	
1	EmE	50	
1	EnE	50	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25095 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 Capsid protein G8P.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AAA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BBB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CCC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DDD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EEE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AaA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BaB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CaC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DaD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EaE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AbA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BbB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CbC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DbD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EbE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AcA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BcB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CcC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DcD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EcE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AdA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BdB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CdC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DdD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EdE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AeA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BeB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CeC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DeD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EeE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AfA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BfB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CfC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DfD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EfE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AgA	35	Total	C	N	O	S	0	0
			259	172	40	45	2		
1	BgB	35	Total	C	N	O	S	0	0
			259	172	40	45	2		
1	CgC	35	Total	C	N	O	S	0	0
			259	172	40	45	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DgD	35	Total	C	N	O	S	0	0
			259	172	40	45	2		
1	EgE	35	Total	C	N	O	S	0	0
			259	172	40	45	2		
1	AhA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BhB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	ChC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DhD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EhE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AiA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BiB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CiC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DiD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EiE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AjA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BjB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CjC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DjD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EjE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AkA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BkB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CkC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DkD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EkE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AlA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BlB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	ClC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DiD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	ElE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AmA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BmB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CmC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DmD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EmE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	AnA	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	BnB	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	CnC	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	DnD	46	Total	C	N	O	S	0	0
			340	223	53	62	2		
1	EnE	46	Total	C	N	O	S	0	0
			340	223	53	62	2		

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	21	MET	TYR	engineered mutation	UNP P69540
BBB	21	MET	TYR	engineered mutation	UNP P69540
CCC	21	MET	TYR	engineered mutation	UNP P69540
DDD	21	MET	TYR	engineered mutation	UNP P69540
EEE	21	MET	TYR	engineered mutation	UNP P69540
AaA	21	MET	TYR	engineered mutation	UNP P69540
BaB	21	MET	TYR	engineered mutation	UNP P69540

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Chain	Residue	Modelled	Actual	Comment	Reference
CaC	21	MET	TYR	engineered mutation	UNP P69540
DaD	21	MET	TYR	engineered mutation	UNP P69540
EaE	21	MET	TYR	engineered mutation	UNP P69540
AbA	21	MET	TYR	engineered mutation	UNP P69540
BbB	21	MET	TYR	engineered mutation	UNP P69540
CbC	21	MET	TYR	engineered mutation	UNP P69540
DbD	21	MET	TYR	engineered mutation	UNP P69540
EbE	21	MET	TYR	engineered mutation	UNP P69540
AcA	21	MET	TYR	engineered mutation	UNP P69540
BcB	21	MET	TYR	engineered mutation	UNP P69540
CcC	21	MET	TYR	engineered mutation	UNP P69540
DcD	21	MET	TYR	engineered mutation	UNP P69540
EcE	21	MET	TYR	engineered mutation	UNP P69540
AdA	21	MET	TYR	engineered mutation	UNP P69540
BdB	21	MET	TYR	engineered mutation	UNP P69540
CdC	21	MET	TYR	engineered mutation	UNP P69540
DdD	21	MET	TYR	engineered mutation	UNP P69540
EdE	21	MET	TYR	engineered mutation	UNP P69540
AeA	21	MET	TYR	engineered mutation	UNP P69540
BeB	21	MET	TYR	engineered mutation	UNP P69540
CeC	21	MET	TYR	engineered mutation	UNP P69540
DeD	21	MET	TYR	engineered mutation	UNP P69540
EeE	21	MET	TYR	engineered mutation	UNP P69540
AfA	21	MET	TYR	engineered mutation	UNP P69540
BfB	21	MET	TYR	engineered mutation	UNP P69540
CfC	21	MET	TYR	engineered mutation	UNP P69540
DfD	21	MET	TYR	engineered mutation	UNP P69540
EfE	21	MET	TYR	engineered mutation	UNP P69540
AgA	21	MET	TYR	engineered mutation	UNP P69540
BgB	21	MET	TYR	engineered mutation	UNP P69540
CgC	21	MET	TYR	engineered mutation	UNP P69540
DgD	21	MET	TYR	engineered mutation	UNP P69540
EgE	21	MET	TYR	engineered mutation	UNP P69540
AhA	21	MET	TYR	engineered mutation	UNP P69540
BhB	21	MET	TYR	engineered mutation	UNP P69540
ChC	21	MET	TYR	engineered mutation	UNP P69540
DhD	21	MET	TYR	engineered mutation	UNP P69540
EhE	21	MET	TYR	engineered mutation	UNP P69540
AiA	21	MET	TYR	engineered mutation	UNP P69540
BiB	21	MET	TYR	engineered mutation	UNP P69540
CiC	21	MET	TYR	engineered mutation	UNP P69540
DiD	21	MET	TYR	engineered mutation	UNP P69540

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Chain	Residue	Modelled	Actual	Comment	Reference
EiE	21	MET	TYR	engineered mutation	UNP P69540
AjA	21	MET	TYR	engineered mutation	UNP P69540
BjB	21	MET	TYR	engineered mutation	UNP P69540
CjC	21	MET	TYR	engineered mutation	UNP P69540
DjD	21	MET	TYR	engineered mutation	UNP P69540
EjE	21	MET	TYR	engineered mutation	UNP P69540
AkA	21	MET	TYR	engineered mutation	UNP P69540
BkB	21	MET	TYR	engineered mutation	UNP P69540
CkC	21	MET	TYR	engineered mutation	UNP P69540
DkD	21	MET	TYR	engineered mutation	UNP P69540
EkE	21	MET	TYR	engineered mutation	UNP P69540
AlA	21	MET	TYR	engineered mutation	UNP P69540
BlB	21	MET	TYR	engineered mutation	UNP P69540
ClC	21	MET	TYR	engineered mutation	UNP P69540
DlD	21	MET	TYR	engineered mutation	UNP P69540
ElE	21	MET	TYR	engineered mutation	UNP P69540
AmA	21	MET	TYR	engineered mutation	UNP P69540
BmB	21	MET	TYR	engineered mutation	UNP P69540
CmC	21	MET	TYR	engineered mutation	UNP P69540
DmD	21	MET	TYR	engineered mutation	UNP P69540
EmE	21	MET	TYR	engineered mutation	UNP P69540
AnA	21	MET	TYR	engineered mutation	UNP P69540
BnB	21	MET	TYR	engineered mutation	UNP P69540
CnC	21	MET	TYR	engineered mutation	UNP P69540
DnD	21	MET	TYR	engineered mutation	UNP P69540
EnE	21	MET	TYR	engineered mutation	UNP P69540

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: Capsid protein G8P

Chain AAA:  72% 20% 8%



- Molecule 1: Capsid protein G8P

Chain BBB:  70% 22% 8%



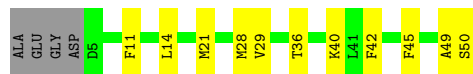
- Molecule 1: Capsid protein G8P

Chain CCC:  70% 22% 8%



- Molecule 1: Capsid protein G8P

Chain DDD:  70% 22% 8%



- Molecule 1: Capsid protein G8P

Chain EEE:  68% 24% 8%



- Molecule 1: Capsid protein G8P

Chain AaA:  70% 22% 8%



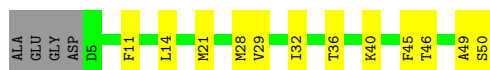
- Molecule 1: Capsid protein G8P

Chain BaB:  72% 20% 8%



- Molecule 1: Capsid protein G8P

Chain CaC:  68% 24% 8%



- Molecule 1: Capsid protein G8P

Chain DaD:  68% 24% 8%



- Molecule 1: Capsid protein G8P

Chain EaE:  68% 24% 8%



- Molecule 1: Capsid protein G8P

Chain AbA:  68% 24% 8%



- Molecule 1: Capsid protein G8P

Chain BbB:  70% 22% 8%



- Molecule 1: Capsid protein G8P

Chain CbC:  70% 22% 8%



- Molecule 1: Capsid protein G8P

Chain DbD:  66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain EbE:  72% 20% 8%



- Molecule 1: Capsid protein G8P

Chain AcA:  66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain BcB:  66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain CcC:  70% 22% 8%



- Molecule 1: Capsid protein G8P

Chain DcD:  66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain EcE:  66% 26% 8%



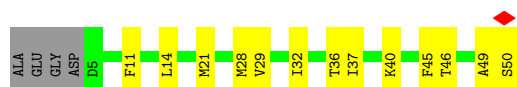
- Molecule 1: Capsid protein G8P

Chain AdA:  64% 28% 8%



- Molecule 1: Capsid protein G8P

Chain BdB:  66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain CdC:  66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain DdD:  66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain EdE:  64% 28% 8%

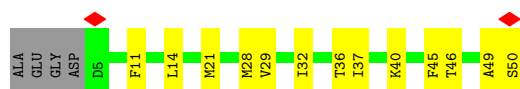


- Molecule 1: Capsid protein G8P

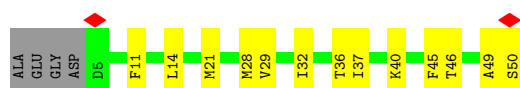
Chain AeA:  66% 26% 8%



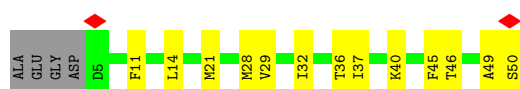
- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



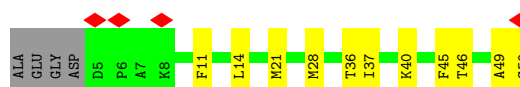
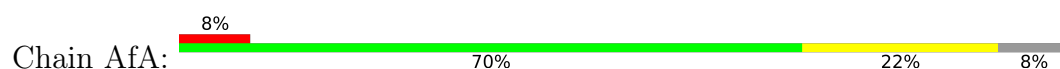
- Molecule 1: Capsid protein G8P



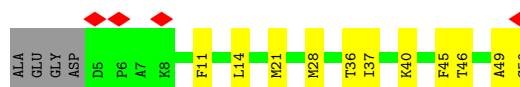
- Molecule 1: Capsid protein G8P



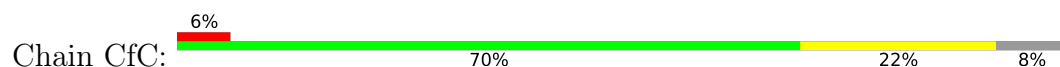
- Molecule 1: Capsid protein G8P



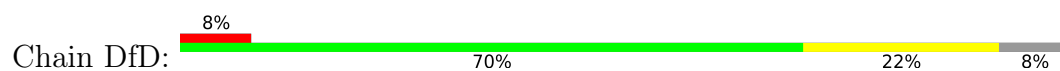
- Molecule 1: Capsid protein G8P



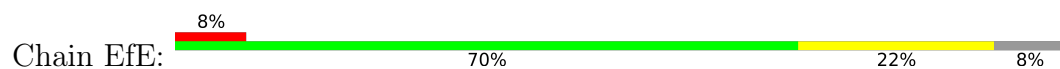
- Molecule 1: Capsid protein G8P



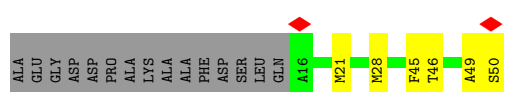
- Molecule 1: Capsid protein G8P



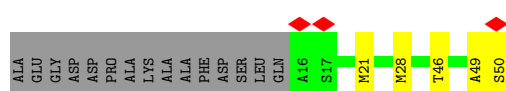
- Molecule 1: Capsid protein G8P



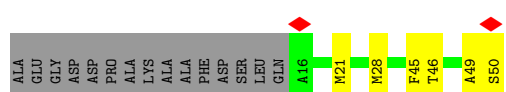
- Molecule 1: Capsid protein G8P



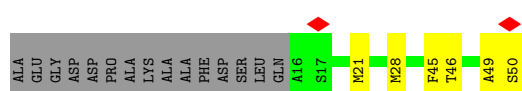
- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P





- Molecule 1: Capsid protein G8P

Chain AhA: 68% 24% 8%



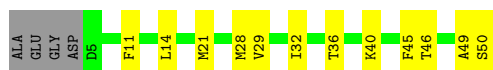
- Molecule 1: Capsid protein G8P

Chain BhB: 66% 26% 8%



- Molecule 1: Capsid protein G8P

Chain ChC: 68% 24% 8%



- Molecule 1: Capsid protein G8P

Chain DhD: 70% 22% 8%



- Molecule 1: Capsid protein G8P

Chain EhE: 68% 24% 8%



- Molecule 1: Capsid protein G8P

Chain AiA: 66% 26% 8%



- Molecule 1: Capsid protein G8P

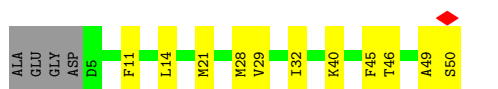
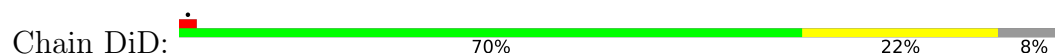
Chain BiB: 66% 26% 8%



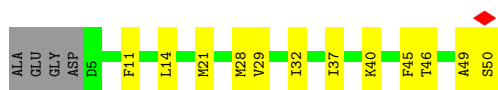
- Molecule 1: Capsid protein G8P



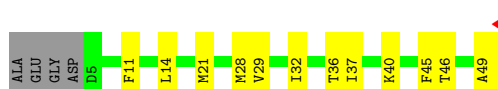
- Molecule 1: Capsid protein G8P



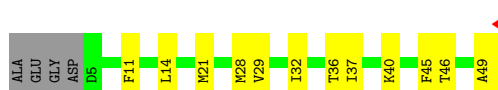
- Molecule 1: Capsid protein G8P



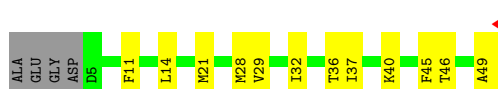
- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



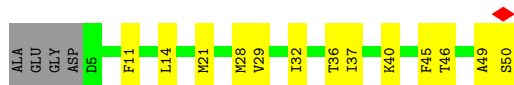
- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P

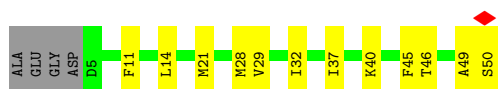




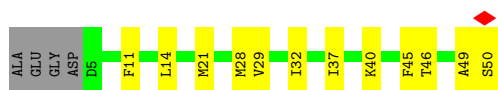
- Molecule 1: Capsid protein G8P



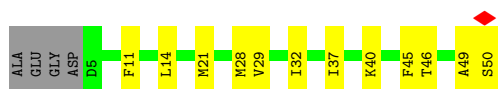
- Molecule 1: Capsid protein G8P



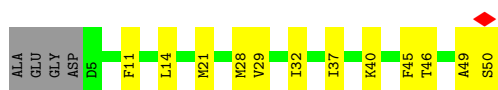
- Molecule 1: Capsid protein G8P



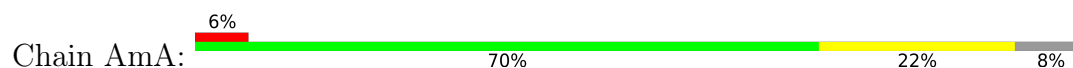
- Molecule 1: Capsid protein G8P



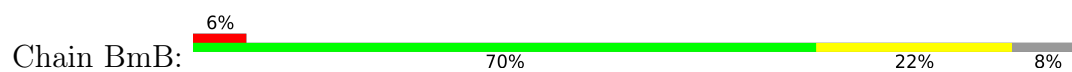
- Molecule 1: Capsid protein G8P



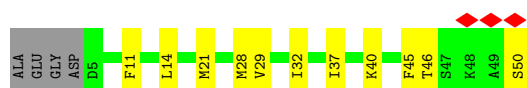
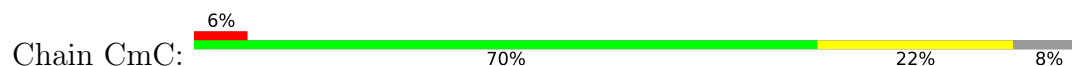
- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



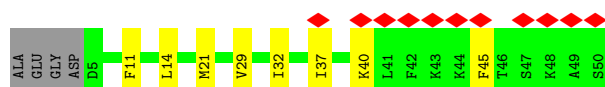
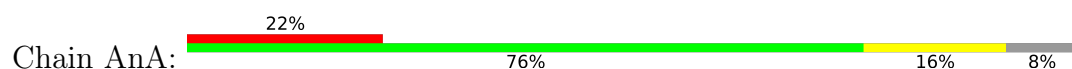
- Molecule 1: Capsid protein G8P



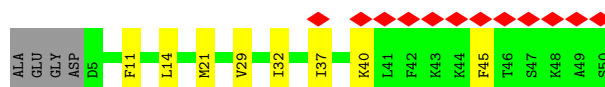
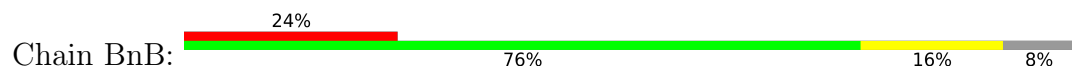
- Molecule 1: Capsid protein G8P



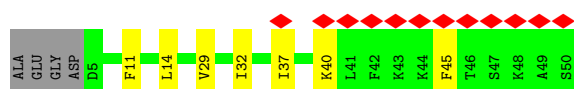
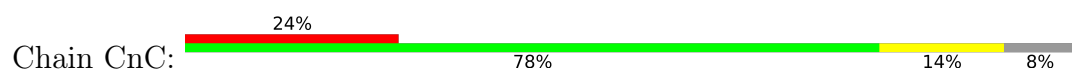
- Molecule 1: Capsid protein G8P



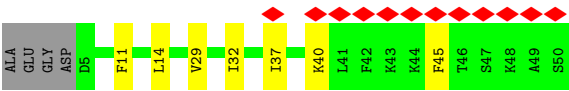
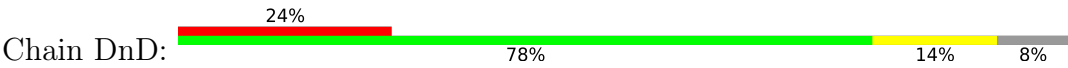
- Molecule 1: Capsid protein G8P



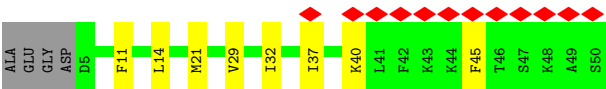
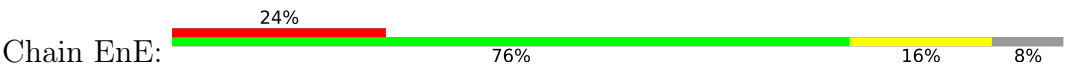
- Molecule 1: Capsid protein G8P



● Molecule 1: Capsid protein G8P



● Molecule 1: Capsid protein G8P



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=37.437°, rise=16.599 Å, axial sym=C5	Depositor
Number of segments used	1139813	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 ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.696	Depositor
Minimum map value	-0.218	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	330.36, 330.36, 330.36	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1012, 1.1012, 1.1012	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	0.74	0/346	1.15	2/465 (0.4%)
1	AaA	0.74	0/346	1.13	2/465 (0.4%)
1	AbA	0.72	0/346	1.13	2/465 (0.4%)
1	AcA	0.71	0/346	1.12	2/465 (0.4%)
1	AdA	0.68	0/346	1.10	2/465 (0.4%)
1	AeA	0.65	0/346	1.09	2/465 (0.4%)
1	AfA	0.62	0/346	1.10	2/465 (0.4%)
1	AgA	0.66	0/263	1.12	1/352 (0.3%)
1	AhA	0.75	0/346	1.14	2/465 (0.4%)
1	AiA	0.72	0/346	1.15	2/465 (0.4%)
1	AjA	0.72	0/346	1.15	2/465 (0.4%)
1	AkA	0.68	0/346	1.12	1/465 (0.2%)
1	AlA	0.65	0/346	1.12	0/465
1	AmA	0.62	0/346	1.10	1/465 (0.2%)
1	AnA	0.58	0/346	1.11	1/465 (0.2%)
1	BBB	0.74	0/346	1.13	2/465 (0.4%)
1	BaB	0.74	0/346	1.16	2/465 (0.4%)
1	BbB	0.72	0/346	1.13	2/465 (0.4%)
1	BcB	0.71	0/346	1.11	2/465 (0.4%)
1	BdB	0.67	0/346	1.11	2/465 (0.4%)
1	BeB	0.64	0/346	1.08	2/465 (0.4%)
1	BfB	0.62	0/346	1.10	2/465 (0.4%)
1	BgB	0.64	0/263	1.11	0/352
1	BhB	0.74	0/346	1.15	2/465 (0.4%)
1	BiB	0.73	0/346	1.15	2/465 (0.4%)
1	BjB	0.71	0/346	1.14	2/465 (0.4%)
1	BkB	0.68	0/346	1.14	2/465 (0.4%)
1	BlB	0.65	0/346	1.11	1/465 (0.2%)
1	BmB	0.62	0/346	1.10	1/465 (0.2%)
1	BnB	0.59	0/346	1.11	1/465 (0.2%)
1	CCC	0.75	0/346	1.14	2/465 (0.4%)
1	CaC	0.73	0/346	1.14	2/465 (0.4%)
1	CbC	0.72	0/346	1.13	2/465 (0.4%)
1	CcC	0.70	0/346	1.12	2/465 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CdC	0.68	0/346	1.11	2/465 (0.4%)
1	CeC	0.65	0/346	1.09	2/465 (0.4%)
1	CfC	0.62	0/346	1.10	2/465 (0.4%)
1	CgC	0.64	0/263	1.12	1/352 (0.3%)
1	ChC	0.75	0/346	1.15	2/465 (0.4%)
1	CiC	0.73	0/346	1.14	1/465 (0.2%)
1	CjC	0.71	0/346	1.13	2/465 (0.4%)
1	CkC	0.68	0/346	1.14	1/465 (0.2%)
1	ClC	0.66	0/346	1.12	1/465 (0.2%)
1	CmC	0.62	0/346	1.10	1/465 (0.2%)
1	CnC	0.59	0/346	1.11	1/465 (0.2%)
1	DDD	0.75	0/346	1.14	2/465 (0.4%)
1	DaD	0.74	0/346	1.14	2/465 (0.4%)
1	DbD	0.72	0/346	1.14	2/465 (0.4%)
1	DcD	0.70	0/346	1.11	2/465 (0.4%)
1	DdD	0.67	0/346	1.11	2/465 (0.4%)
1	DeD	0.64	0/346	1.10	2/465 (0.4%)
1	DfD	0.62	0/346	1.10	2/465 (0.4%)
1	DgD	0.66	0/263	1.11	1/352 (0.3%)
1	DhD	0.74	0/346	1.13	2/465 (0.4%)
1	DiD	0.72	0/346	1.14	1/465 (0.2%)
1	DjD	0.72	0/346	1.14	2/465 (0.4%)
1	DkD	0.68	0/346	1.12	2/465 (0.4%)
1	DlD	0.66	0/346	1.11	1/465 (0.2%)
1	DmD	0.62	0/346	1.11	1/465 (0.2%)
1	DnD	0.59	0/346	1.11	1/465 (0.2%)
1	EEE	0.74	0/346	1.13	2/465 (0.4%)
1	EaE	0.74	0/346	1.15	2/465 (0.4%)
1	EbE	0.73	0/346	1.14	2/465 (0.4%)
1	EcE	0.70	0/346	1.11	2/465 (0.4%)
1	EdE	0.68	0/346	1.11	2/465 (0.4%)
1	EeE	0.64	0/346	1.08	2/465 (0.4%)
1	EfE	0.62	0/346	1.11	2/465 (0.4%)
1	EgE	0.66	0/263	1.12	1/352 (0.3%)
1	UhE	0.75	0/346	1.14	2/465 (0.4%)
1	EiE	0.73	0/346	1.14	1/465 (0.2%)
1	EjE	0.71	0/346	1.13	2/465 (0.4%)
1	EkE	0.68	0/346	1.12	2/465 (0.4%)
1	ElE	0.66	0/346	1.12	1/465 (0.2%)
1	EmE	0.62	0/346	1.09	1/465 (0.2%)
1	EnE	0.59	0/346	1.11	1/465 (0.2%)
All	All	0.68	0/25535	1.12	123/34310 (0.4%)

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AcA	45	PHE	CA-CB-CG	-6.24	107.56	113.80
1	AbA	45	PHE	CA-CB-CG	-6.23	107.57	113.80
1	CaC	45	PHE	CA-CB-CG	-6.17	107.64	113.80
1	EbE	45	PHE	CA-CB-CG	-6.14	107.66	113.80
1	DcD	45	PHE	CA-CB-CG	-6.12	107.68	113.80
1	BdB	45	PHE	CA-CB-CG	-6.09	107.71	113.80
1	EEE	45	PHE	CA-CB-CG	-6.08	107.72	113.80
1	CbC	45	PHE	CA-CB-CG	-6.02	107.78	113.80
1	CcC	45	PHE	CA-CB-CG	-5.99	107.81	113.80
1	BhB	45	PHE	CA-CB-CG	-5.97	107.83	113.80
1	DbD	45	PHE	CA-CB-CG	-5.95	107.85	113.80
1	DaD	45	PHE	CA-CB-CG	-5.93	107.87	113.80
1	DdD	45	PHE	CA-CB-CG	-5.92	107.88	113.80
1	AaA	45	PHE	CA-CB-CG	-5.91	107.89	113.80
1	EaE	45	PHE	CA-CB-CG	-5.90	107.90	113.80
1	BbB	45	PHE	CA-CB-CG	-5.87	107.93	113.80
1	BaB	45	PHE	CA-CB-CG	-5.85	107.95	113.80
1	BcB	45	PHE	CA-CB-CG	-5.82	107.98	113.80
1	AnA	45	PHE	CA-CB-CG	-5.81	107.99	113.80
1	BeB	45	PHE	CA-CB-CG	-5.80	108.00	113.80
1	AAA	45	PHE	CA-CB-CG	-5.79	108.02	113.80
1	CCC	45	PHE	CA-CB-CG	-5.78	108.02	113.80
1	EeE	45	PHE	CA-CB-CG	-5.78	108.02	113.80
1	ChC	45	PHE	CA-CB-CG	-5.78	108.02	113.80
1	EcE	45	PHE	CA-CB-CG	-5.78	108.02	113.80
1	BBB	45	PHE	CA-CB-CG	-5.78	108.02	113.80
1	EaE	36	THR	CA-CB-OG1	-5.76	100.96	109.60
1	CnC	45	PHE	CA-CB-CG	-5.75	108.05	113.80
1	AdA	45	PHE	CA-CB-CG	-5.74	108.06	113.80
1	DnD	45	PHE	CA-CB-CG	-5.74	108.06	113.80
1	AbA	36	THR	CA-CB-OG1	-5.71	101.03	109.60
1	AhA	45	PHE	CA-CB-CG	-5.70	108.10	113.80
1	DhD	45	PHE	CA-CB-CG	-5.70	108.10	113.80
1	EdE	45	PHE	CA-CB-CG	-5.69	108.11	113.80
1	CaC	36	THR	CA-CB-OG1	-5.66	101.10	109.60
1	CiC	45	PHE	CA-CB-CG	-5.66	108.14	113.80
1	BnB	45	PHE	CA-CB-CG	-5.65	108.15	113.80
1	CbC	36	THR	CA-CB-OG1	-5.65	101.13	109.60
1	DDD	45	PHE	CA-CB-CG	-5.64	108.16	113.80
1	EbE	36	THR	CA-CB-OG1	-5.64	101.14	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EnE	45	PHE	CA-CB-CG	-5.64	108.16	113.80
1	CdC	45	PHE	CA-CB-CG	-5.63	108.17	113.80
1	DbD	36	THR	CA-CB-OG1	-5.62	101.16	109.60
1	EhE	45	PHE	CA-CB-CG	-5.62	108.18	113.80
1	AaA	36	THR	CA-CB-OG1	-5.61	101.18	109.60
1	EiE	45	PHE	CA-CB-CG	-5.61	108.19	113.80
1	AiA	45	PHE	CA-CB-CG	-5.60	108.20	113.80
1	DeD	45	PHE	CA-CB-CG	-5.60	108.20	113.80
1	BmB	45	PHE	CA-CB-CG	-5.59	108.21	113.80
1	DmD	45	PHE	CA-CB-CG	-5.59	108.21	113.80
1	AeA	45	PHE	CA-CB-CG	-5.59	108.21	113.80
1	CeC	45	PHE	CA-CB-CG	-5.56	108.24	113.80
1	DiD	45	PHE	CA-CB-CG	-5.55	108.25	113.80
1	BBB	36	THR	CA-CB-OG1	-5.54	101.29	109.60
1	CfC	45	PHE	CA-CB-CG	-5.53	108.27	113.80
1	DcD	36	THR	CA-CB-OG1	-5.51	101.33	109.60
1	CCC	36	THR	CA-CB-OG1	-5.51	101.34	109.60
1	EfE	45	PHE	CA-CB-CG	-5.51	108.29	113.80
1	DaD	36	THR	CA-CB-OG1	-5.50	101.34	109.60
1	BiB	45	PHE	CA-CB-CG	-5.50	108.30	113.80
1	AjA	45	PHE	CA-CB-CG	-5.49	108.31	113.80
1	AAA	36	THR	CA-CB-OG1	-5.49	101.36	109.60
1	BbB	36	THR	CA-CB-OG1	-5.48	101.38	109.60
1	BaB	36	THR	CA-CB-OG1	-5.47	101.39	109.60
1	CmC	45	PHE	CA-CB-CG	-5.44	108.36	113.80
1	DeD	36	THR	CA-CB-OG1	-5.42	101.47	109.60
1	EcE	36	THR	CA-CB-OG1	-5.40	101.49	109.60
1	AfA	45	PHE	CA-CB-CG	-5.40	108.40	113.80
1	AmA	45	PHE	CA-CB-CG	-5.39	108.41	113.80
1	EEE	36	THR	CA-CB-OG1	-5.39	101.51	109.60
1	BfB	45	PHE	CA-CB-CG	-5.38	108.42	113.80
1	AhA	36	THR	CA-CB-OG1	-5.37	101.54	109.60
1	BdB	36	THR	CA-CB-OG1	-5.34	101.58	109.60
1	CcC	36	THR	CA-CB-OG1	-5.34	101.60	109.60
1	EmE	45	PHE	CA-CB-CG	-5.32	108.48	113.80
1	CjC	45	PHE	CA-CB-CG	-5.32	108.48	113.80
1	DDD	36	THR	CA-CB-OG1	-5.30	101.65	109.60
1	CkC	45	PHE	CA-CB-CG	-5.30	108.50	113.80
1	EkE	45	PHE	CA-CB-CG	-5.29	108.51	113.80
1	AeA	36	THR	CA-CB-OG1	-5.28	101.69	109.60
1	DdD	36	THR	CA-CB-OG1	-5.27	101.70	109.60
1	AgA	45	PHE	CA-CB-CG	-5.26	108.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ChC	36	THR	CA-CB-OG1	-5.26	101.71	109.60
1	DjD	45	PHE	CA-CB-CG	-5.25	108.55	113.80
1	BhB	36	THR	CA-CB-OG1	-5.24	101.75	109.60
1	BkB	45	PHE	CA-CB-CG	-5.24	108.56	113.80
1	DfD	36	THR	CA-CB-OG1	-5.23	101.76	109.60
1	DfD	45	PHE	CA-CB-CG	-5.22	108.58	113.80
1	CeC	36	THR	CA-CB-OG1	-5.21	101.78	109.60
1	EjE	45	PHE	CA-CB-CG	-5.20	108.60	113.80
1	AcA	36	THR	CA-CB-OG1	-5.20	101.80	109.60
1	BeB	36	THR	CA-CB-OG1	-5.19	101.81	109.60
1	EdE	36	THR	CA-CB-OG1	-5.19	101.81	109.60
1	BfB	36	THR	CA-CB-OG1	-5.19	101.82	109.60
1	EeE	36	THR	CA-CB-OG1	-5.18	101.83	109.60
1	EfE	36	THR	CA-CB-OG1	-5.18	101.83	109.60
1	CgC	45	PHE	CA-CB-CG	-5.18	108.62	113.80
1	CdC	36	THR	CA-CB-OG1	-5.17	101.84	109.60
1	BjB	45	PHE	CA-CB-CG	-5.16	108.64	113.80
1	AfA	36	THR	CA-CB-OG1	-5.14	101.88	109.60
1	CfC	36	THR	CA-CB-OG1	-5.14	101.88	109.60
1	EhE	36	THR	CA-CB-OG1	-5.14	101.89	109.60
1	BcB	36	THR	CA-CB-OG1	-5.13	101.91	109.60
1	BkB	36	THR	CA-CB-OG1	-5.13	101.91	109.60
1	DgD	45	PHE	CA-CB-CG	-5.13	108.67	113.80
1	BlB	45	PHE	CA-CB-CG	-5.12	108.68	113.80
1	AkA	45	PHE	CA-CB-CG	-5.10	108.70	113.80
1	DkD	45	PHE	CA-CB-CG	-5.10	108.70	113.80
1	DhD	36	THR	CA-CB-OG1	-5.09	101.96	109.60
1	ElE	45	PHE	CA-CB-CG	-5.09	108.71	113.80
1	EgE	45	PHE	CA-CB-CG	-5.09	108.71	113.80
1	DkD	36	THR	CA-CB-OG1	-5.08	101.98	109.60
1	DjD	36	THR	CA-CB-OG1	-5.07	101.99	109.60
1	BjB	36	THR	CA-CB-OG1	-5.07	102.00	109.60
1	AiA	36	THR	CA-CB-OG1	-5.07	102.00	109.60
1	CjC	36	THR	CA-CB-OG1	-5.05	102.02	109.60
1	EkE	36	THR	CA-CB-OG1	-5.05	102.02	109.60
1	EjE	36	THR	CA-CB-OG1	-5.04	102.04	109.60
1	AjA	36	THR	CA-CB-OG1	-5.04	102.04	109.60
1	DiD	45	PHE	CA-CB-CG	-5.02	108.78	113.80
1	BiB	36	THR	CA-CB-OG1	-5.01	102.08	109.60
1	ClC	45	PHE	CA-CB-CG	-5.01	108.79	113.80
1	AdA	36	THR	CA-CB-OG1	-5.00	102.09	109.60

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	AAA	340	0	354	18	0
1	AaA	340	0	354	19	0
1	AbA	340	0	354	19	0
1	AcA	340	0	354	20	0
1	AdA	340	0	354	19	0
1	AeA	340	0	354	20	0
1	AfA	340	0	354	17	0
1	AgA	259	0	278	10	0
1	AhA	340	0	354	20	0
1	AiA	340	0	354	20	0
1	AjA	340	0	354	20	0
1	AkA	340	0	354	19	0
1	AlA	340	0	354	21	0
1	AmA	340	0	354	18	0
1	AnA	340	0	354	12	0
1	BBB	340	0	354	19	0
1	BaB	340	0	354	18	0
1	BbB	340	0	354	18	0
1	BcB	340	0	354	19	0
1	BdB	340	0	354	20	0
1	BeB	340	0	354	20	0
1	BfB	340	0	354	17	0
1	BgB	259	0	278	10	0
1	BhB	340	0	354	20	0
1	BiB	340	0	354	19	0
1	BjB	340	0	354	21	0
1	BkB	340	0	354	20	0
1	BlB	340	0	354	21	0
1	BmB	340	0	354	17	0
1	BnB	340	0	354	11	0
1	CCC	340	0	354	20	0
1	CaC	340	0	354	19	0
1	CbC	340	0	354	16	0
1	CcC	340	0	354	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CdC	340	0	354	19	0
1	CeC	340	0	354	19	0
1	CfC	340	0	354	17	0
1	CgC	259	0	278	10	0
1	ChC	340	0	354	20	0
1	CiC	340	0	354	22	0
1	CjC	340	0	354	21	0
1	CkC	340	0	354	21	0
1	ClC	340	0	354	21	0
1	CmC	340	0	354	17	0
1	CnC	340	0	354	10	0
1	DDD	340	0	354	19	0
1	DaD	340	0	354	20	0
1	DbD	340	0	354	20	0
1	DcD	340	0	354	19	0
1	DdD	340	0	354	19	0
1	DeD	340	0	354	19	0
1	DfD	340	0	354	17	0
1	DgD	259	0	278	10	0
1	DhD	340	0	354	19	0
1	DiD	340	0	354	20	0
1	DjD	340	0	354	19	0
1	DkD	340	0	354	20	0
1	DlD	340	0	354	20	0
1	DmD	340	0	354	18	0
1	DnD	340	0	354	11	0
1	EEE	340	0	354	20	0
1	EaE	340	0	354	21	0
1	EbE	340	0	354	17	0
1	EcE	340	0	354	20	0
1	EdE	340	0	354	19	0
1	EeE	340	0	354	20	0
1	EfE	340	0	354	18	0
1	EgE	259	0	278	10	0
1	EhE	340	0	354	20	0
1	EiE	340	0	354	21	0
1	EjE	340	0	354	20	0
1	EkE	340	0	354	19	0
1	ElE	340	0	354	20	0
1	EmE	340	0	354	17	0
1	EnE	340	0	354	11	0
All	All	25095	0	26170	711	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 14.

All (711) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AeA:11:PHE:HE2	1:AfA:21:MET:CE	1.84	0.90
1:CeC:11:PHE:HE2	1:CfC:21:MET:CE	1.85	0.90
1:DeD:11:PHE:HE2	1:DfD:21:MET:CE	1.85	0.90
1:CfC:11:PHE:HE2	1:CgC:21:MET:CE	1.85	0.90
1:EdE:11:PHE:HE2	1:EeE:21:MET:CE	1.86	0.89
1:BfB:11:PHE:HE2	1:BgB:21:MET:CE	1.86	0.89
1:AdA:11:PHE:HE2	1:AeA:21:MET:CE	1.86	0.88
1:EfE:11:PHE:HE2	1:EgE:21:MET:CE	1.86	0.88
1:DdD:11:PHE:HE2	1:DeD:21:MET:CE	1.86	0.88
1:BeB:11:PHE:HE2	1:BfB:21:MET:CE	1.87	0.88
1:BdB:11:PHE:HE2	1:BeB:21:MET:CE	1.86	0.88
1:CdC:11:PHE:HE2	1:CeC:21:MET:CE	1.86	0.87
1:CmC:21:MET:CE	1:CnC:11:PHE:HE2	1.87	0.87
1:BmB:21:MET:CE	1:BnB:11:PHE:HE2	1.87	0.87
1:DcD:11:PHE:HE2	1:DdD:21:MET:CE	1.88	0.86
1:EmE:21:MET:CE	1:EnE:11:PHE:HE2	1.88	0.86
1:DmD:21:MET:CE	1:DnD:11:PHE:HE2	1.87	0.86
1:DfD:11:PHE:HE2	1:DgD:21:MET:CE	1.87	0.86
1:CcC:11:PHE:HE2	1:CdC:21:MET:CE	1.89	0.86
1:AmA:21:MET:CE	1:AnA:11:PHE:HE2	1.87	0.86
1:BcB:11:PHE:HE2	1:BdB:21:MET:CE	1.88	0.86
1:EcE:11:PHE:HE2	1:EdE:21:MET:CE	1.88	0.85
1:AfA:11:PHE:HE2	1:AgA:21:MET:CE	1.87	0.85
1:EbE:11:PHE:HE2	1:EcE:21:MET:CE	1.89	0.85
1:AlA:21:MET:CE	1:AmA:11:PHE:HE2	1.89	0.85
1:AcA:11:PHE:HE2	1:AdA:21:MET:CE	1.88	0.85
1:AbA:11:PHE:HE2	1:AcA:21:MET:CE	1.90	0.84
1:EeE:11:PHE:HE2	1:EfE:21:MET:CE	1.89	0.84
1:BiB:21:MET:CE	1:BmB:11:PHE:HE2	1.89	0.84
1:CiC:21:MET:CE	1:CmC:11:PHE:HE2	1.90	0.84
1:ElE:21:MET:CE	1:EmE:11:PHE:HE2	1.90	0.84
1:BbB:11:PHE:HE2	1:BcB:21:MET:CE	1.90	0.84
1:DiD:21:MET:CE	1:DmD:11:PHE:HE2	1.89	0.83
1:CiC:21:MET:CE	1:CjC:11:PHE:HE2	1.91	0.83
1:CbC:11:PHE:HE2	1:CcC:21:MET:CE	1.90	0.83
1:DbD:11:PHE:HE2	1:DcD:21:MET:CE	1.91	0.83
1:BjB:21:MET:CE	1:BkB:11:PHE:HE2	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DkD:21:MET:CE	1:DiD:11:PHE:HE2	1.92	0.82
1:AhA:21:MET:CE	1:AiA:11:PHE:HE2	1.92	0.82
1:DiD:21:MET:CE	1:DjD:11:PHE:HE2	1.92	0.82
1:BiB:21:MET:CE	1:BjB:11:PHE:HE2	1.92	0.82
1:CkC:21:MET:CE	1:ClC:11:PHE:HE2	1.92	0.82
1:EhE:21:MET:CE	1:EiE:11:PHE:HE2	1.93	0.82
1:AjA:21:MET:CE	1:AkA:11:PHE:HE2	1.93	0.82
1:BkB:21:MET:CE	1:BiB:11:PHE:HE2	1.91	0.82
1:AiA:21:MET:CE	1:AjA:11:PHE:HE2	1.91	0.81
1:DjD:21:MET:CE	1:DkD:11:PHE:HE2	1.93	0.81
1:AkA:21:MET:CE	1:AlA:11:PHE:HE2	1.93	0.81
1:DDD:21:MET:CE	1:DhD:11:PHE:HE2	1.93	0.81
1:DaD:11:PHE:HE2	1:DbD:21:MET:CE	1.92	0.81
1:EkE:21:MET:CE	1:ElE:11:PHE:HE2	1.92	0.81
1:EiE:21:MET:CE	1:EjE:11:PHE:HE2	1.92	0.81
1:CjC:21:MET:CE	1:CkC:11:PHE:HE2	1.92	0.81
1:EaE:11:PHE:HE2	1:EbE:21:MET:CE	1.93	0.81
1:BhB:21:MET:CE	1:BiB:11:PHE:HE2	1.92	0.81
1:CCC:11:PHE:HE2	1:CaC:21:MET:CE	1.93	0.81
1:CaC:11:PHE:HE2	1:CbC:21:MET:CE	1.93	0.81
1:ChC:21:MET:CE	1:CiC:11:PHE:HE2	1.94	0.81
1:AAA:11:PHE:HE2	1:AaA:21:MET:CE	1.94	0.81
1:DDD:11:PHE:HE2	1:DaD:21:MET:CE	1.94	0.81
1:BaB:11:PHE:HE2	1:BbB:21:MET:CE	1.93	0.81
1:EjE:21:MET:CE	1:EkE:11:PHE:HE2	1.93	0.81
1:AAA:21:MET:CE	1:AhA:11:PHE:HE2	1.94	0.80
1:BBB:11:PHE:HE2	1:BaB:21:MET:CE	1.95	0.80
1:DhD:21:MET:CE	1:DiD:11:PHE:HE2	1.93	0.80
1:CCC:21:MET:CE	1:ChC:11:PHE:HE2	1.94	0.80
1:EEE:11:PHE:HE2	1:EaE:21:MET:CE	1.94	0.80
1:EEE:21:MET:CE	1:EhE:11:PHE:HE2	1.94	0.80
1:AaA:11:PHE:HE2	1:AbA:21:MET:CE	1.93	0.79
1:BBB:21:MET:CE	1:BhB:11:PHE:HE2	1.94	0.79
1:AAA:28:MET:HE1	1:AhA:14:LEU:HB3	1.69	0.74
1:EEE:28:MET:HE1	1:EhE:14:LEU:HB3	1.70	0.73
1:BjB:28:MET:HE1	1:BkB:14:LEU:HB3	1.70	0.73
1:EjE:28:MET:HE1	1:EkE:14:LEU:HB3	1.69	0.73
1:DDD:28:MET:HE1	1:DhD:14:LEU:HB3	1.69	0.73
1:DjD:28:MET:HE1	1:DkD:14:LEU:HB3	1.69	0.72
1:EfE:11:PHE:HE2	1:EgE:21:MET:HE3	1.54	0.72
1:AiA:28:MET:HE1	1:AjA:14:LEU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CkC:28:MET:HE1	1:ClC:14:LEU:HB3	1.71	0.72
1:BBB:14:LEU:HB3	1:BaB:28:MET:HE1	1.71	0.72
1:ChC:28:MET:HE1	1:CiC:14:LEU:HB3	1.72	0.72
1:EhE:28:MET:HE1	1:EiE:14:LEU:HB3	1.71	0.72
1:BiB:28:MET:HE1	1:BjB:14:LEU:HB3	1.70	0.72
1:AkA:28:MET:HE1	1:AlA:14:LEU:HB3	1.71	0.72
1:CCC:28:MET:HE1	1:ChC:14:LEU:HB3	1.70	0.71
1:BBB:28:MET:HE1	1:BhB:14:LEU:HB3	1.71	0.71
1:CcC:14:LEU:HB3	1:CdC:28:MET:HE1	1.72	0.71
1:CiC:28:MET:HE1	1:CjC:14:LEU:HB3	1.71	0.71
1:CCC:14:LEU:HB3	1:CaC:28:MET:HE1	1.71	0.71
1:DiD:28:MET:HE1	1:DjD:14:LEU:HB3	1.71	0.71
1:BkB:28:MET:HE1	1:BlB:14:LEU:HB3	1.71	0.71
1:BaB:14:LEU:HB3	1:BbB:28:MET:HE1	1.72	0.71
1:CbC:14:LEU:HB3	1:CcC:28:MET:HE1	1.73	0.71
1:BdB:14:LEU:HB3	1:BeB:28:MET:HE1	1.73	0.71
1:BhB:28:MET:HE1	1:BiB:14:LEU:HB3	1.71	0.71
1:EEE:14:LEU:HB3	1:EaE:28:MET:HE1	1.72	0.70
1:BcB:14:LEU:HB3	1:BdB:28:MET:HE1	1.73	0.70
1:CjC:28:MET:HE1	1:CkC:14:LEU:HB3	1.72	0.70
1:AbA:14:LEU:HB3	1:AcA:28:MET:HE1	1.73	0.70
1:DdD:14:LEU:HB3	1:DeD:28:MET:HE1	1.73	0.70
1:AhA:28:MET:HE1	1:AiA:14:LEU:HB3	1.71	0.70
1:AjA:28:MET:HE1	1:AkA:14:LEU:HB3	1.71	0.70
1:DkD:28:MET:HE1	1:DiD:14:LEU:HB3	1.73	0.70
1:DcD:14:LEU:HB3	1:DdD:28:MET:HE1	1.72	0.70
1:EdE:14:LEU:HB3	1:EeE:28:MET:HE1	1.72	0.70
1:EcE:14:LEU:HB3	1:EdE:28:MET:HE1	1.72	0.70
1:CdC:14:LEU:HB3	1:CeC:28:MET:HE1	1.74	0.70
1:DhD:28:MET:HE1	1:DiD:14:LEU:HB3	1.72	0.70
1:AaA:14:LEU:HB3	1:AbA:28:MET:HE1	1.74	0.70
1:BbB:14:LEU:HB3	1:BcB:28:MET:HE1	1.74	0.70
1:CaC:14:LEU:HB3	1:CbC:28:MET:HE1	1.73	0.69
1:EaE:14:LEU:HB3	1:EbE:28:MET:HE1	1.72	0.69
1:AlA:28:MET:HE1	1:AmA:14:LEU:HB3	1.72	0.69
1:AcA:14:LEU:HB3	1:AdA:28:MET:HE1	1.72	0.69
1:ClC:28:MET:HE1	1:CmC:14:LEU:HB3	1.74	0.69
1:BmB:28:MET:HE1	1:BnB:14:LEU:HB3	1.75	0.69
1:DbD:14:LEU:HB3	1:DcD:28:MET:HE1	1.73	0.69
1:AdA:14:LEU:HB3	1:AeA:28:MET:HE1	1.74	0.69
1:BlB:28:MET:HE1	1:BmB:14:LEU:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DiD:28:MET:HE1	1:DmD:14:LEU:HB3	1.74	0.69
1:AAA:14:LEU:HB3	1:AaA:28:MET:HE1	1.75	0.69
1:EkE:28:MET:HE1	1:ElE:14:LEU:HB3	1.73	0.68
1:DDD:14:LEU:HB3	1:DaD:28:MET:HE1	1.73	0.68
1:EmE:28:MET:HE1	1:EnE:14:LEU:HB3	1.75	0.68
1:ElE:28:MET:HE1	1:EjE:14:LEU:HB3	1.74	0.68
1:ElE:28:MET:HE1	1:EmE:14:LEU:HB3	1.74	0.68
1:DaD:14:LEU:HB3	1:DbD:28:MET:HE1	1.74	0.68
1:AmA:28:MET:HE1	1:AnA:14:LEU:HB3	1.77	0.67
1:CeC:14:LEU:HB3	1:CfC:28:MET:HE1	1.77	0.67
1:DmD:28:MET:HE1	1:DnD:14:LEU:HB3	1.77	0.67
1:DeD:11:PHE:HE2	1:DfD:21:MET:HE3	1.58	0.67
1:CmC:28:MET:HE1	1:CnC:14:LEU:HB3	1.77	0.67
1:DmD:21:MET:HE3	1:DnD:11:PHE:HE2	1.60	0.66
1:EbE:14:LEU:HB3	1:EcE:28:MET:HE1	1.75	0.66
1:AdA:11:PHE:CE2	1:AeA:21:MET:CE	2.75	0.66
1:BeB:14:LEU:HB3	1:BfB:28:MET:HE1	1.77	0.66
1:CfC:11:PHE:HE2	1:CgC:21:MET:HE3	1.60	0.66
1:DcD:11:PHE:CE2	1:DdD:21:MET:CE	2.77	0.66
1:CmC:21:MET:HE3	1:CnC:11:PHE:HE2	1.61	0.66
1:EeE:14:LEU:HB3	1:EfE:28:MET:HE1	1.78	0.65
1:DeD:14:LEU:HB3	1:DfD:28:MET:HE1	1.79	0.65
1:CcC:11:PHE:CE2	1:CdC:21:MET:CE	2.78	0.65
1:EcE:11:PHE:CE2	1:EdE:21:MET:CE	2.77	0.65
1:BcB:11:PHE:CE2	1:BdB:21:MET:CE	2.77	0.65
1:BdB:11:PHE:CE2	1:BeB:21:MET:CE	2.76	0.65
1:BiB:21:MET:CE	1:BmB:11:PHE:CE2	2.78	0.64
1:DiD:49:ALA:HA	1:CnC:29:VAL:HG22	1.80	0.64
1:AmA:21:MET:HE3	1:AnA:11:PHE:HE2	1.62	0.64
1:AeA:11:PHE:HE2	1:AfA:21:MET:HE3	1.61	0.64
1:CbC:11:PHE:CE2	1:CcC:21:MET:CE	2.79	0.63
1:AeA:14:LEU:HB3	1:AfA:28:MET:HE1	1.80	0.63
1:EfE:11:PHE:CE2	1:EgE:21:MET:HE3	2.33	0.63
1:EmE:21:MET:CE	1:EnE:11:PHE:CE2	2.77	0.63
1:BmB:21:MET:HE3	1:BnB:11:PHE:HE2	1.61	0.63
1:CkC:21:MET:CE	1:ClC:11:PHE:CE2	2.81	0.63
1:BkB:49:ALA:HA	1:AmA:29:VAL:HG22	1.80	0.63
1:AmA:21:MET:CE	1:AnA:11:PHE:CE2	2.77	0.63
1:CcC:11:PHE:HE2	1:CfC:21:MET:HE3	1.60	0.63
1:DaD:11:PHE:HE2	1:DbD:21:MET:HE3	1.64	0.63
1:BbB:11:PHE:CE2	1:BcB:21:MET:CE	2.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CiC:21:MET:HE3	1:CjC:11:PHE:HE2	1.62	0.63
1:BfB:11:PHE:HE2	1:BgB:21:MET:HE3	1.62	0.63
1:AiA:21:MET:HE3	1:AjA:11:PHE:HE2	1.64	0.63
1:ElE:21:MET:HE3	1:EmE:11:PHE:HE2	1.63	0.63
1:CfC:11:PHE:CE2	1:CgC:21:MET:CE	2.76	0.62
1:AkA:49:ALA:HA	1:EmE:29:VAL:HG22	1.81	0.62
1:EmE:21:MET:HE3	1:EnE:11:PHE:HE2	1.62	0.62
1:AfA:11:PHE:CE2	1:AgA:21:MET:CE	2.78	0.62
1:DeD:11:PHE:CE2	1:DfD:21:MET:CE	2.76	0.62
1:EfE:11:PHE:CE2	1:EgE:21:MET:CE	2.77	0.62
1:ElE:49:ALA:HA	1:DnD:29:VAL:HG22	1.82	0.62
1:BiB:21:MET:HE3	1:BjB:11:PHE:HE2	1.65	0.62
1:DkD:49:ALA:HA	1:CmC:29:VAL:HG22	1.81	0.62
1:EbE:11:PHE:CE2	1:EcE:21:MET:CE	2.79	0.62
1:EdE:11:PHE:CE2	1:EeE:21:MET:CE	2.76	0.62
1:DfD:11:PHE:CE2	1:DgD:21:MET:CE	2.78	0.62
1:CdC:11:PHE:CE2	1:CeC:21:MET:CE	2.76	0.62
1:DdD:11:PHE:CE2	1:DeD:21:MET:CE	2.76	0.62
1:BeB:11:PHE:CE2	1:BfB:21:MET:CE	2.78	0.62
1:AbA:11:PHE:HE2	1:AcA:21:MET:HE3	1.64	0.61
1:EbE:11:PHE:HE2	1:EcE:21:MET:HE3	1.62	0.61
1:AcA:11:PHE:CE2	1:AdA:21:MET:CE	2.78	0.61
1:EkE:49:ALA:HA	1:DmD:29:VAL:HG22	1.80	0.61
1:DmD:21:MET:CE	1:DnD:11:PHE:CE2	2.77	0.61
1:CbC:11:PHE:HE2	1:CcC:21:MET:HE3	1.65	0.61
1:AiA:49:ALA:HA	1:EkE:29:VAL:HG22	1.82	0.61
1:AlA:49:ALA:HA	1:EnE:29:VAL:HG22	1.82	0.61
1:BcB:11:PHE:HE2	1:BdB:21:MET:HE3	1.63	0.61
1:CiC:21:MET:CE	1:CjC:11:PHE:CE2	2.80	0.61
1:BiB:49:ALA:HA	1:AnA:29:VAL:HG22	1.81	0.61
1:ElE:21:MET:CE	1:EmE:11:PHE:CE2	2.79	0.61
1:AlA:21:MET:HE3	1:AmA:11:PHE:HE2	1.65	0.61
1:DbD:11:PHE:HE2	1:DcD:21:MET:HE3	1.66	0.61
1:DeD:11:PHE:CE2	1:DfD:21:MET:HE3	2.36	0.61
1:DfD:11:PHE:HE2	1:DgD:21:MET:HE3	1.63	0.61
1:CaC:11:PHE:CE2	1:CbC:21:MET:CE	2.81	0.61
1:DaD:11:PHE:CE2	1:DbD:21:MET:CE	2.80	0.61
1:BkB:21:MET:CE	1:BiB:11:PHE:CE2	2.80	0.61
1:AkA:21:MET:CE	1:AlA:11:PHE:CE2	2.81	0.60
1:EaE:11:PHE:CE2	1:EbE:21:MET:CE	2.81	0.60
1:BaB:11:PHE:CE2	1:BbB:21:MET:CE	2.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BbB:11:PHE:HE2	1:BcB:21:MET:HE3	1.64	0.60
1:CmC:21:MET:CE	1:CnC:11:PHE:CE2	2.77	0.60
1:EbE:40:LYS:NZ	1:EcE:50:SER:OXT	2.35	0.60
1:DdD:40:LYS:NZ	1:DeD:50:SER:OXT	2.35	0.60
1:AhA:21:MET:HE3	1:AiA:11:PHE:HE2	1.66	0.60
1:BhB:49:ALA:HA	1:AjA:29:VAL:HG22	1.84	0.60
1:AiA:21:MET:CE	1:AjA:11:PHE:CE2	2.81	0.60
1:ClC:49:ALA:HA	1:BnB:29:VAL:HG22	1.83	0.60
1:CCC:11:PHE:CE2	1:CaC:21:MET:CE	2.82	0.60
1:DDD:21:MET:CE	1:DhD:11:PHE:CE2	2.83	0.60
1:BaB:11:PHE:HE2	1:BbB:21:MET:HE3	1.66	0.60
1:AjA:49:ALA:HA	1:ElE:29:VAL:HG22	1.83	0.60
1:EaE:11:PHE:HE2	1:EbE:21:MET:HE3	1.66	0.60
1:ChC:49:ALA:HA	1:BjB:29:VAL:HG22	1.84	0.60
1:BiB:49:ALA:HA	1:AkA:29:VAL:HG22	1.83	0.60
1:CkC:49:ALA:HA	1:BmB:29:VAL:HG22	1.82	0.60
1:EcE:11:PHE:HE2	1:EdE:21:MET:HE3	1.67	0.59
1:DdD:11:PHE:HE2	1:DeD:21:MET:HE3	1.67	0.59
1:AhA:49:ALA:HA	1:EjE:29:VAL:HG22	1.84	0.59
1:BlB:21:MET:HE3	1:BmB:11:PHE:HE2	1.64	0.59
1:CdC:40:LYS:NZ	1:CeC:50:SER:OXT	2.35	0.59
1:AjA:21:MET:CE	1:AkA:11:PHE:CE2	2.82	0.59
1:AAA:49:ALA:HA	1:ElE:29:VAL:HG22	1.84	0.59
1:CaC:11:PHE:HE2	1:CbC:21:MET:HE3	1.66	0.59
1:BdB:40:LYS:NZ	1:BeB:50:SER:OXT	2.35	0.59
1:EdE:40:LYS:NZ	1:EeE:50:SER:OXT	2.35	0.59
1:EeE:11:PHE:HE2	1:EfE:21:MET:HE3	1.66	0.59
1:DDD:11:PHE:HE2	1:DaD:21:MET:HE3	1.66	0.59
1:ElE:49:ALA:HA	1:DkD:29:VAL:HG22	1.84	0.59
1:EeE:40:LYS:NZ	1:EfE:50:SER:OXT	2.36	0.59
1:EfE:14:LEU:HB3	1:EgE:28:MET:HE1	1.85	0.59
1:AhA:21:MET:CE	1:AiA:11:PHE:CE2	2.82	0.59
1:ClC:21:MET:CE	1:CmC:11:PHE:CE2	2.80	0.59
1:BmB:21:MET:CE	1:BnB:11:PHE:CE2	2.77	0.59
1:AeA:11:PHE:CE2	1:AfA:21:MET:CE	2.75	0.59
1:EeE:29:VAL:HG22	1:AgA:49:ALA:HA	1.84	0.59
1:DiD:49:ALA:HA	1:CkC:29:VAL:HG22	1.83	0.59
1:AbA:11:PHE:CE2	1:AcA:21:MET:CE	2.80	0.59
1:BbB:40:LYS:NZ	1:BcB:50:SER:OXT	2.36	0.59
1:CbC:40:LYS:NZ	1:CcC:50:SER:OXT	2.36	0.59
1:BcB:40:LYS:NZ	1:BdB:50:SER:OXT	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DcD:11:PHE:HE2	1:DdD:21:MET:HE3	1.66	0.59
1:CiC:49:ALA:HA	1:BkB:29:VAL:HG22	1.83	0.59
1:BaB:40:LYS:NZ	1:BbB:50:SER:OXT	2.36	0.59
1:EaE:40:LYS:NZ	1:EbE:50:SER:OXT	2.36	0.59
1:DiD:21:MET:HE3	1:DjD:11:PHE:HE2	1.66	0.59
1:DjD:49:ALA:HA	1:ClC:29:VAL:HG22	1.83	0.59
1:EjE:49:ALA:HA	1:DiD:29:VAL:HG22	1.83	0.59
1:CcC:40:LYS:NZ	1:CdC:50:SER:OXT	2.36	0.59
1:AdA:40:LYS:NZ	1:AeA:50:SER:OXT	2.35	0.59
1:BfB:14:LEU:HB3	1:BgB:28:MET:HE1	1.85	0.59
1:DiD:21:MET:HE3	1:DmD:11:PHE:HE2	1.66	0.59
1:DcD:40:LYS:NZ	1:DdD:50:SER:OXT	2.36	0.59
1:DeD:40:LYS:NZ	1:DfD:50:SER:OXT	2.36	0.59
1:DfD:14:LEU:HB3	1:DgD:28:MET:HE1	1.85	0.59
1:EfE:40:LYS:NZ	1:EgE:50:SER:OXT	2.36	0.59
1:CjC:49:ALA:HA	1:BiB:29:VAL:HG22	1.83	0.59
1:AlA:21:MET:CE	1:AmA:11:PHE:CE2	2.78	0.59
1:DiD:21:MET:CE	1:DmD:11:PHE:CE2	2.79	0.59
1:CCC:49:ALA:HA	1:BiB:29:VAL:HG22	1.85	0.58
1:AaA:11:PHE:CE2	1:AbA:21:MET:CE	2.82	0.58
1:DbD:40:LYS:NZ	1:DcD:50:SER:OXT	2.35	0.58
1:CeC:40:LYS:NZ	1:CfC:50:SER:OXT	2.36	0.58
1:DeD:29:VAL:HG22	1:EgE:49:ALA:HA	1.85	0.58
1:AfA:40:LYS:NZ	1:AgA:50:SER:OXT	2.36	0.58
1:DhD:49:ALA:HA	1:CjC:29:VAL:HG22	1.84	0.58
1:EhE:49:ALA:HA	1:DjD:29:VAL:HG22	1.84	0.58
1:BBB:21:MET:CE	1:BhB:11:PHE:CE2	2.83	0.58
1:DDD:50:SER:OXT	1:DhD:40:LYS:NZ	2.36	0.58
1:BdB:11:PHE:HE2	1:BeB:21:MET:HE3	1.66	0.58
1:AAA:11:PHE:CE2	1:AaA:21:MET:CE	2.82	0.58
1:BBB:49:ALA:HA	1:AiA:29:VAL:HG22	1.86	0.58
1:AeA:40:LYS:NZ	1:AfA:50:SER:OXT	2.36	0.58
1:BeB:29:VAL:HG22	1:CgC:49:ALA:HA	1.84	0.58
1:BfB:40:LYS:NZ	1:BgB:50:SER:OXT	2.36	0.58
1:EiE:21:MET:HE3	1:EjE:11:PHE:HE2	1.67	0.58
1:BmB:21:MET:HE3	1:BnB:11:PHE:CE2	2.39	0.58
1:BfB:11:PHE:CE2	1:BgB:21:MET:CE	2.77	0.58
1:DmD:21:MET:HE3	1:DnD:11:PHE:CE2	2.38	0.58
1:DDD:40:LYS:NZ	1:DaD:50:SER:OXT	2.37	0.58
1:AaA:40:LYS:NZ	1:AbA:50:SER:OXT	2.36	0.58
1:DaD:40:LYS:NZ	1:DbD:50:SER:OXT	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AcA:40:LYS:NZ	1:AdA:50:SER:OXT	2.36	0.58
1:AeA:29:VAL:HG22	1:BgB:49:ALA:HA	1.84	0.58
1:CeC:11:PHE:CE2	1:CfC:21:MET:CE	2.76	0.58
1: EiE:21:MET:CE	1:EjE:11:PHE:CE2	2.81	0.58
1:EEE:49:ALA:HA	1:DiD:29:VAL:HG22	1.85	0.58
1:BeB:40:LYS:NZ	1:BfB:50:SER:OXT	2.36	0.58
1:BBB:11:PHE:CE2	1:BaB:21:MET:CE	2.84	0.58
1:CCC:50:SER:OXT	1:ChC:40:LYS:NZ	2.37	0.58
1:AaA:11:PHE:HE2	1:AbA:21:MET:HE3	1.67	0.58
1:AbA:40:LYS:NZ	1:AcA:50:SER:OXT	2.37	0.58
1:CcC:29:VAL:HG22	1:DeD:49:ALA:HA	1.86	0.58
1:EcE:40:LYS:NZ	1:EdE:50:SER:OXT	2.36	0.58
1:CiC:21:MET:HE3	1:CjC:11:PHE:CE2	2.38	0.58
1:AdA:11:PHE:HE2	1:AeA:21:MET:HE3	1.66	0.58
1:BjB:49:ALA:HA	1:AlA:29:VAL:HG22	1.85	0.58
1:EkE:21:MET:CE	1:ElE:11:PHE:CE2	2.81	0.58
1:AfA:14:LEU:HB3	1:AgA:28:MET:HE1	1.86	0.58
1:CfC:11:PHE:CE2	1:CgC:21:MET:HE3	2.39	0.58
1:CaC:40:LYS:NZ	1:CbC:50:SER:OXT	2.36	0.58
1:DfD:40:LYS:NZ	1:DgD:50:SER:OXT	2.36	0.58
1:AbA:29:VAL:HG22	1:BdB:49:ALA:HA	1.86	0.57
1:CfC:40:LYS:NZ	1:CgC:50:SER:OXT	2.36	0.57
1:AAA:11:PHE:HE2	1:AaA:21:MET:HE3	1.67	0.57
1:BBB:40:LYS:NZ	1:BaB:50:SER:OXT	2.37	0.57
1:AAA:21:MET:CE	1:AhA:11:PHE:CE2	2.83	0.57
1:EEE:40:LYS:NZ	1:EaE:50:SER:OXT	2.37	0.57
1:BhB:21:MET:CE	1:BiB:11:PHE:CE2	2.82	0.57
1:CjC:21:MET:CE	1:CkC:11:PHE:CE2	2.82	0.57
1:DkD:21:MET:CE	1:DiD:11:PHE:CE2	2.80	0.57
1:ClC:21:MET:HE3	1:CmC:11:PHE:HE2	1.69	0.57
1:EmE:21:MET:HE3	1:EnE:11:PHE:CE2	2.38	0.57
1:DDD:11:PHE:CE2	1:DaD:21:MET:CE	2.82	0.57
1:CeC:29:VAL:HG22	1:DgD:49:ALA:HA	1.84	0.57
1:AAA:40:LYS:NZ	1:AaA:50:SER:OXT	2.37	0.57
1:DdD:29:VAL:HG22	1:EfE:49:ALA:HA	1.87	0.57
1:EjE:21:MET:CE	1:EkE:11:PHE:CE2	2.82	0.57
1:EEE:50:SER:OXT	1:EhE:40:LYS:NZ	2.37	0.57
1:EcE:29:VAL:HG22	1:AeA:49:ALA:HA	1.86	0.57
1:BjB:21:MET:CE	1:BkB:11:PHE:CE2	2.81	0.57
1:EbE:11:PHE:CE2	1:EcE:21:MET:HE3	2.39	0.57
1:DiD:21:MET:CE	1:DjD:11:PHE:CE2	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BaB:49:ALA:HA	1:AhA:29:VAL:HG22	1.87	0.57
1:CaC:49:ALA:HA	1:BhB:29:VAL:HG22	1.87	0.57
1:DcD:29:VAL:HG22	1:EeE:49:ALA:HA	1.85	0.57
1:EeE:11:PHE:CE2	1:EfE:21:MET:CE	2.80	0.57
1:EhE:21:MET:CE	1: EiE:11:PHE:CE2	2.83	0.57
1:BiB:21:MET:CE	1:BjB:11:PHE:CE2	2.81	0.57
1:DDD:49:ALA:HA	1:CiC:29:VAL:HG22	1.86	0.57
1:DaD:49:ALA:HA	1:ChC:29:VAL:HG22	1.87	0.57
1:BlB:50:SER:OXT	1:BmB:40:LYS:NZ	2.38	0.57
1:ClC:50:SER:OXT	1:CmC:40:LYS:NZ	2.38	0.57
1:AAA:50:SER:OXT	1:AhA:40:LYS:NZ	2.37	0.57
1:BbB:29:VAL:HG22	1:CdC:49:ALA:HA	1.86	0.57
1:CdC:11:PHE:HE2	1:CeC:21:MET:HE3	1.68	0.57
1:CkC:50:SER:OXT	1:ClC:40:LYS:NZ	2.38	0.57
1:BbB:11:PHE:CE2	1:BcB:21:MET:HE3	2.40	0.56
1:CbC:29:VAL:HG22	1:DdD:49:ALA:HA	1.86	0.56
1:CdC:29:VAL:HG22	1:DfD:49:ALA:HA	1.86	0.56
1:EdE:29:VAL:HG22	1:AfA:49:ALA:HA	1.87	0.56
1:CfC:14:LEU:HB3	1:CgC:28:MET:HE1	1.87	0.56
1:EbE:29:VAL:HG22	1:AdA:49:ALA:HA	1.87	0.56
1:AcA:29:VAL:HG22	1:BeB:49:ALA:HA	1.86	0.56
1:BcB:29:VAL:HG22	1:CeC:49:ALA:HA	1.86	0.56
1:BdB:29:VAL:HG22	1:CfC:49:ALA:HA	1.86	0.56
1:ElE:21:MET:HE3	1:EmE:11:PHE:CE2	2.39	0.56
1:CCC:21:MET:CE	1:ChC:11:PHE:CE2	2.83	0.56
1:CCC:21:MET:HE3	1:ChC:11:PHE:HE2	1.70	0.56
1:EaE:49:ALA:HA	1:DhD:29:VAL:HG22	1.87	0.56
1:ChC:21:MET:CE	1:CiC:11:PHE:CE2	2.84	0.56
1:DhD:50:SER:OXT	1:DiD:40:LYS:NZ	2.37	0.56
1:CjC:50:SER:OXT	1:CkC:40:LYS:NZ	2.38	0.56
1:CmC:21:MET:HE3	1:CnC:11:PHE:CE2	2.38	0.56
1:BBB:29:VAL:HG22	1:CbC:49:ALA:HA	1.88	0.56
1:DaD:11:PHE:CE2	1:DbD:21:MET:HE3	2.39	0.56
1:AaA:49:ALA:HA	1:EhE:29:VAL:HG22	1.87	0.56
1:AmA:21:MET:HE3	1:AnA:11:PHE:CE2	2.39	0.56
1:CmC:50:SER:OXT	1:CnC:40:LYS:NZ	2.39	0.56
1:EEE:11:PHE:HE2	1:EaE:21:MET:HE3	1.70	0.56
1:AbA:11:PHE:CE2	1:AcA:21:MET:HE3	2.41	0.56
1:AAA:29:VAL:HG22	1:BbB:49:ALA:HA	1.87	0.56
1:AaA:29:VAL:HG22	1:BcB:49:ALA:HA	1.87	0.56
1:CaC:29:VAL:HG22	1:DcD:49:ALA:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EdE:11:PHE:HE2	1:EeE:21:MET:HE3	1.66	0.56
1:EEE:21:MET:CE	1:EhE:11:PHE:CE2	2.84	0.56
1:DaD:29:VAL:HG22	1:EcE:49:ALA:HA	1.88	0.56
1:DbD:11:PHE:CE2	1:DcD:21:MET:CE	2.80	0.56
1:CcC:11:PHE:CE2	1:CfC:21:MET:HE3	2.39	0.56
1:BhB:21:MET:HE3	1:BiB:11:PHE:HE2	1.70	0.56
1:AdA:29:VAL:HG22	1:BfB:49:ALA:HA	1.86	0.55
1:BjB:50:SER:OXT	1:BkB:40:LYS:NZ	2.38	0.55
1:AkA:50:SER:OXT	1:AlA:40:LYS:NZ	2.38	0.55
1:DkD:21:MET:HE3	1:DlD:11:PHE:HE2	1.71	0.55
1:BlB:21:MET:HE3	1:BmB:11:PHE:CE2	2.41	0.55
1:DbD:29:VAL:HG22	1:EdE:49:ALA:HA	1.87	0.55
1:DiD:50:SER:OXT	1:DjD:40:LYS:NZ	2.38	0.55
1:DjD:21:MET:CE	1:DkD:11:PHE:CE2	2.82	0.55
1:CiC:50:SER:OXT	1:CjC:40:LYS:NZ	2.38	0.55
1:CCC:29:VAL:HG22	1:DbD:49:ALA:HA	1.89	0.55
1:CCC:40:LYS:NZ	1:CaC:50:SER:OXT	2.37	0.55
1:EhE:50:SER:OXT	1:EiE:40:LYS:NZ	2.38	0.55
1:BjB:21:MET:HE3	1:BkB:11:PHE:HE2	1.71	0.55
1:BkB:21:MET:HE3	1:BlB:11:PHE:HE2	1.71	0.55
1:BaB:11:PHE:CE2	1:BbB:21:MET:HE3	2.42	0.55
1:BaB:29:VAL:HG22	1:CcC:49:ALA:HA	1.89	0.55
1:AiA:21:MET:HE3	1:AjA:11:PHE:CE2	2.41	0.55
1:BBB:50:SER:OXT	1:BhB:40:LYS:NZ	2.37	0.55
1:DDD:11:PHE:CE2	1:DaD:21:MET:HE3	2.41	0.55
1:EEE:11:PHE:CE2	1:EaE:21:MET:CE	2.82	0.55
1:BeB:11:PHE:HE2	1:BfB:21:MET:HE3	1.66	0.55
1:BmB:50:SER:OXT	1:BnB:40:LYS:NZ	2.39	0.55
1:EEE:29:VAL:HG22	1:AbA:49:ALA:HA	1.88	0.55
1:EaE:11:PHE:CE2	1:EbE:21:MET:HE3	2.42	0.55
1:BcB:11:PHE:CE2	1:BdD:21:MET:HE3	2.40	0.55
1:AhA:50:SER:OXT	1:AiA:40:LYS:NZ	2.38	0.55
1:BiB:21:MET:HE3	1:BjB:11:PHE:CE2	2.41	0.55
1:DiD:21:MET:HE3	1:DjD:11:PHE:CE2	2.43	0.54
1:AAA:11:PHE:CE2	1:AaA:21:MET:HE3	2.43	0.54
1:DhD:21:MET:CE	1:DiD:11:PHE:CE2	2.83	0.54
1:CCC:11:PHE:HE2	1:CaC:21:MET:HE3	1.69	0.54
1:EiE:50:SER:OXT	1:EjE:40:LYS:NZ	2.38	0.54
1:EaE:29:VAL:HG22	1:AcA:49:ALA:HA	1.88	0.54
1:CaC:11:PHE:CE2	1:CbC:21:MET:HE3	2.41	0.54
1:AlA:21:MET:HE3	1:AmA:11:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AcA:11:PHE:HE2	1:AdA:21:MET:HE3	1.68	0.53
1:BkB:50:SER:OXT	1:BIB:40:LYS:NZ	2.38	0.53
1:DDD:29:VAL:HG22	1:EbE:49:ALA:HA	1.89	0.53
1:CbC:11:PHE:CE2	1:CcC:21:MET:HE3	2.42	0.53
1:AjA:50:SER:OXT	1:AkA:40:LYS:NZ	2.37	0.53
1:CcC:11:PHE:HE2	1:CdC:21:MET:HE3	1.70	0.53
1:DjD:50:SER:OXT	1:DkD:40:LYS:NZ	2.38	0.53
1:AlA:50:SER:OXT	1:AmA:40:LYS:NZ	2.38	0.53
1:AiA:50:SER:OXT	1:AjA:40:LYS:NZ	2.37	0.53
1:EiE:21:MET:HE3	1:EjE:11:PHE:CE2	2.42	0.53
1:BhB:50:SER:OXT	1:BiB:40:LYS:NZ	2.38	0.53
1:EhE:21:MET:HE3	1:EiE:11:PHE:HE2	1.72	0.53
1:CjC:21:MET:HE3	1:CkC:11:PHE:HE2	1.71	0.53
1:BdB:11:PHE:CE2	1:BeB:21:MET:HE3	2.44	0.53
1:DlD:21:MET:HE3	1:DmD:11:PHE:CE2	2.42	0.53
1:BfB:11:PHE:CE2	1:BgB:21:MET:HE3	2.41	0.53
1:EkE:50:SER:OXT	1:ElE:40:LYS:NZ	2.37	0.53
1:AeA:11:PHE:CE2	1:AfA:21:MET:HE3	2.41	0.52
1:AjA:21:MET:HE3	1:AkA:11:PHE:HE2	1.74	0.52
1:EjE:50:SER:OXT	1:EkE:40:LYS:NZ	2.38	0.52
1:AAA:21:MET:HE3	1:AhA:11:PHE:HE2	1.73	0.52
1:ElE:50:SER:OXT	1:EmE:40:LYS:NZ	2.38	0.52
1:BeB:11:PHE:CE2	1:BfB:21:MET:HE3	2.45	0.52
1:EjE:21:MET:HE3	1:EkE:11:PHE:HE2	1.72	0.52
1:AhA:21:MET:HE3	1:AiA:11:PHE:CE2	2.42	0.52
1:ClC:21:MET:HE3	1:CmC:11:PHE:CE2	2.44	0.52
1:AaA:11:PHE:CE2	1:AbA:21:MET:HE3	2.43	0.52
1:DkD:50:SER:OXT	1:DlD:40:LYS:NZ	2.38	0.52
1:EEE:21:MET:HE3	1:EhE:11:PHE:HE2	1.74	0.51
1:DlD:50:SER:OXT	1:DmD:40:LYS:NZ	2.38	0.51
1:BBB:21:MET:HE3	1:BhB:11:PHE:HE2	1.75	0.51
1:DdD:11:PHE:CE2	1:DeD:21:MET:HE3	2.45	0.51
1:DhD:21:MET:HE3	1:DiD:11:PHE:HE2	1.71	0.51
1:EEE:11:PHE:CE2	1:EaE:21:MET:HE3	2.45	0.51
1:DcD:11:PHE:CE2	1:DdD:21:MET:HE3	2.43	0.51
1:DDD:21:MET:HE3	1:DhD:11:PHE:HE2	1.73	0.51
1:BhB:50:SER:HA	1:AjA:32:ILE:HD13	1.92	0.51
1:BiB:50:SER:OXT	1:BjB:40:LYS:NZ	2.38	0.51
1:DfD:11:PHE:CE2	1:DgD:21:MET:HE3	2.42	0.51
1:CkC:21:MET:HE3	1:ClC:11:PHE:CE2	2.46	0.51
1:DbD:11:PHE:CE2	1:DcD:21:MET:HE3	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BkB:21:MET:HE3	1:BiB:11:PHE:CE2	2.46	0.51
1:CkC:21:MET:HE3	1:ClC:11:PHE:HE2	1.72	0.51
1:EcE:11:PHE:CE2	1:EdE:21:MET:HE3	2.44	0.51
1:AdA:11:PHE:CE2	1:AeA:21:MET:HE3	2.43	0.50
1:CCC:21:MET:HE3	1:ChC:11:PHE:CE2	2.46	0.50
1:CcC:11:PHE:CE2	1:CdC:21:MET:HE3	2.46	0.50
1:AkA:21:MET:HE3	1:AlA:11:PHE:HE2	1.73	0.50
1:EEE:50:SER:HA	1:DiD:32:ILE:HD13	1.93	0.50
1:BhB:21:MET:HE3	1:BiB:11:PHE:CE2	2.46	0.50
1:AmA:50:SER:OXT	1:AnA:40:LYS:NZ	2.40	0.50
1:EmE:50:SER:OXT	1:EnE:40:LYS:NZ	2.39	0.50
1:EeE:11:PHE:CE2	1:EfE:21:MET:HE3	2.44	0.50
1:ChC:21:MET:HE3	1:CiC:11:PHE:HE2	1.76	0.50
1:EkE:21:MET:HE3	1:ElE:11:PHE:CE2	2.46	0.50
1:EkE:21:MET:HE3	1:ElE:11:PHE:HE2	1.71	0.50
1:EdE:11:PHE:CE2	1:EeE:21:MET:HE3	2.44	0.50
1:CCC:11:PHE:CE2	1:CaC:21:MET:HE3	2.45	0.49
1:AfA:11:PHE:HE2	1:AgA:21:MET:HE3	1.72	0.49
1:ChC:50:SER:OXT	1:CiC:40:LYS:NZ	2.39	0.49
1:BjB:21:MET:HE3	1:BkB:11:PHE:CE2	2.46	0.49
1:CjC:21:MET:HE3	1:CkC:11:PHE:CE2	2.46	0.49
1:BiB:50:SER:HA	1:AnA:32:ILE:HD13	1.94	0.49
1:DmD:50:SER:OXT	1:DnD:40:LYS:NZ	2.40	0.49
1:DiD:46:THR:CG2	1:DmD:37:ILE:HG13	2.43	0.49
1:ChC:50:SER:HA	1:BjB:32:ILE:HD13	1.94	0.49
1:DhD:50:SER:HA	1:CjC:32:ILE:HD13	1.95	0.49
1:DkD:21:MET:HE3	1:DiD:11:PHE:CE2	2.45	0.49
1:CmC:46:THR:CG2	1:CnC:37:ILE:HG13	2.42	0.49
1:BBB:11:PHE:HE2	1:BaB:21:MET:HE3	1.73	0.48
1:AhA:50:SER:HA	1:EjE:32:ILE:HD13	1.93	0.48
1:AlA:46:THR:CG2	1:AmA:37:ILE:HG13	2.43	0.48
1:EhE:21:MET:HE3	1:EiE:11:PHE:CE2	2.48	0.48
1:DDD:21:MET:HE3	1:DhD:11:PHE:CE2	2.48	0.48
1:EhE:50:SER:HA	1:DjD:32:ILE:HD13	1.95	0.48
1:EfE:21:MET:HE2	1:EfE:21:MET:HB3	1.78	0.48
1:ElE:50:SER:HA	1:DnD:32:ILE:HD13	1.95	0.48
1:AlA:50:SER:HA	1:EnE:32:ILE:HD13	1.95	0.48
1:AAA:50:SER:HA	1:EiE:32:ILE:HD13	1.95	0.48
1:AkA:21:MET:HE3	1:AlA:11:PHE:CE2	2.48	0.48
1:DmD:46:THR:CG2	1:DnD:37:ILE:HG13	2.43	0.48
1:DhD:21:MET:HE3	1:DiD:11:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ElE:46:THR:CG2	1:EmE:37:ILE:HG13	2.44	0.48
1:AAA:21:MET:HE3	1:AhA:11:PHE:CE2	2.48	0.47
1:AcA:11:PHE:CE2	1:AdA:21:MET:HE3	2.45	0.47
1:BBB:50:SER:HA	1:AiA:32:ILE:HD13	1.95	0.47
1:ClC:46:THR:CG2	1:CmC:37:ILE:HG13	2.44	0.47
1:DID:50:SER:HA	1:CnC:32:ILE:HD13	1.96	0.47
1:AjA:21:MET:HE3	1:AkA:11:PHE:CE2	2.49	0.47
1:DID:49:ALA:HA	1:CnC:29:VAL:CG2	2.44	0.47
1:AbA:21:MET:HE2	1:AbA:21:MET:HB3	1.74	0.47
1:AiA:50:SER:HA	1:EkE:32:ILE:HD13	1.96	0.47
1:BIB:49:ALA:HA	1:AnA:29:VAL:CG2	2.45	0.47
1:AmA:46:THR:CG2	1:AnA:37:ILE:HG13	2.45	0.47
1:BBB:11:PHE:CE2	1:BaB:21:MET:HE3	2.48	0.47
1:AaA:21:MET:HE2	1:AaA:21:MET:HB3	1.73	0.47
1:CdC:11:PHE:CE2	1:CeC:21:MET:HE3	2.46	0.47
1:BIB:21:MET:HE2	1:BIB:21:MET:HB3	1.79	0.47
1:BIB:46:THR:CG2	1:BmB:37:ILE:HG13	2.45	0.47
1:DjD:21:MET:HE3	1:DkD:11:PHE:CE2	2.50	0.47
1:CiC:21:MET:HE2	1:CiC:21:MET:HB3	1.76	0.46
1:DiD:50:SER:HA	1:CkC:32:ILE:HD13	1.98	0.46
1:DmD:21:MET:HE2	1:DmD:21:MET:HB3	1.79	0.46
1:DjD:21:MET:HE3	1:DkD:11:PHE:HE2	1.74	0.46
1:BmB:21:MET:HE2	1:BmB:21:MET:HB3	1.79	0.46
1:EmE:46:THR:CG2	1:EnE:37:ILE:HG13	2.45	0.46
1:EcE:21:MET:HB3	1:EcE:21:MET:HE2	1.75	0.46
1:CiC:50:SER:HA	1:BkB:32:ILE:HD13	1.98	0.46
1:ClC:50:SER:HA	1:BnB:32:ILE:HD13	1.98	0.46
1:BBB:21:MET:HE2	1:BBB:21:MET:HB3	1.81	0.46
1:DDD:50:SER:HA	1:CiC:32:ILE:HD13	1.97	0.46
1:EiE:50:SER:HA	1:DkD:32:ILE:HD13	1.96	0.46
1:DfD:21:MET:HE2	1:DfD:21:MET:HB3	1.80	0.46
1:AlA:49:ALA:HA	1:EnE:29:VAL:CG2	2.46	0.46
1:EjE:21:MET:HE3	1:EkE:11:PHE:CE2	2.47	0.46
1:CCC:50:SER:HA	1:BiB:32:ILE:HD13	1.98	0.45
1:AeA:21:MET:HE2	1:AeA:21:MET:HB3	1.79	0.45
1:EbE:21:MET:HE2	1:EbE:21:MET:HB3	1.72	0.45
1:BaB:21:MET:HB3	1:BaB:21:MET:HE2	1.76	0.45
1:AkA:21:MET:HE2	1:AkA:21:MET:HB3	1.80	0.45
1:BmB:46:THR:CG2	1:BnB:37:ILE:HG13	2.46	0.45
1:CcC:21:MET:HE2	1:CcC:21:MET:HB3	1.76	0.45
1:EdE:21:MET:HE2	1:EdE:21:MET:HB3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DiD:21:MET:HE2	1:DiD:21:MET:HB3	1.79	0.45
1:EjE:21:MET:HB3	1:EjE:21:MET:HE2	1.80	0.45
1:DaD:21:MET:HE2	1:DaD:21:MET:HB3	1.73	0.45
1:ChC:21:MET:HE3	1:CiC:11:PHE:CE2	2.52	0.45
1:AjA:21:MET:HE2	1:AjA:21:MET:HB3	1.82	0.45
1:EEE:21:MET:HE3	1:EhE:11:PHE:CE2	2.49	0.45
1:DiD:49:ALA:HA	1:CkC:29:VAL:CG2	2.47	0.45
1:ClC:49:ALA:HA	1:BnB:29:VAL:CG2	2.47	0.45
1:ElE:49:ALA:HA	1:DnD:29:VAL:CG2	2.47	0.45
1:AiA:21:MET:HE2	1:AiA:21:MET:HB3	1.79	0.45
1:AAA:49:ALA:HA	1:EiE:29:VAL:CG2	2.47	0.44
1:ChC:49:ALA:HA	1:BjB:29:VAL:CG2	2.47	0.44
1:DdD:21:MET:HE2	1:DdD:21:MET:HB3	1.78	0.44
1:EeE:21:MET:HE2	1:EeE:21:MET:HB3	1.80	0.44
1:EEE:49:ALA:HA	1:DiD:29:VAL:CG2	2.48	0.44
1:AcA:21:MET:HE2	1:AcA:21:MET:HB3	1.73	0.44
1:DcD:21:MET:HE2	1:DcD:21:MET:HB3	1.74	0.44
1:DeD:21:MET:HB3	1:DeD:21:MET:HE2	1.81	0.44
1:EgE:21:MET:HB3	1:EgE:21:MET:HE2	1.75	0.44
1:BiB:50:SER:HA	1:AkA:32:ILE:HD13	1.99	0.44
1:AlA:21:MET:HE2	1:AlA:21:MET:HB3	1.79	0.44
1:DbD:21:MET:HE2	1:DbD:21:MET:HB3	1.73	0.44
1:AdA:21:MET:HE2	1:AdA:21:MET:HB3	1.78	0.44
1:DhD:49:ALA:HA	1:CjC:29:VAL:CG2	2.47	0.44
1:ElE:49:ALA:HA	1:DkD:29:VAL:CG2	2.48	0.44
1:BkB:46:THR:CG2	1:BlB:37:ILE:HG13	2.48	0.44
1:AmA:21:MET:HE2	1:AmA:21:MET:HB3	1.80	0.44
1:DaD:32:ILE:HD13	1:EcE:50:SER:HA	1.99	0.44
1:BdB:32:ILE:HD13	1:CfC:50:SER:HA	1.99	0.44
1:BjB:50:SER:HA	1:AlA:32:ILE:HD13	2.00	0.44
1:AkA:46:THR:CG2	1:AlA:37:ILE:HG13	2.48	0.44
1:CkC:46:THR:CG2	1:ClC:37:ILE:HG13	2.47	0.44
1:AAA:21:MET:HE2	1:AAA:21:MET:HB3	1.78	0.44
1:BjB:21:MET:HB3	1:BjB:21:MET:HE2	1.82	0.44
1:EkE:46:THR:CG2	1:ElE:37:ILE:HG13	2.48	0.44
1:AfA:37:ILE:HG13	1:AgA:46:THR:CG2	2.48	0.44
1:AeA:32:ILE:HD13	1:BgB:50:SER:HA	2.00	0.44
1:ClC:49:ALA:HA	1:BkB:29:VAL:CG2	2.48	0.44
1:ElE:21:MET:HE2	1:ElE:21:MET:HB3	1.80	0.44
1:EcE:32:ILE:HD13	1:AeA:50:SER:HA	2.00	0.44
1:BeB:32:ILE:HD13	1:CgC:50:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DeD:32:ILE:HD13	1:EgE:50:SER:HA	2.00	0.44
1:BhB:49:ALA:HA	1:AjA:29:VAL:CG2	2.47	0.44
1:EkE:21:MET:HE2	1:EkE:21:MET:HB3	1.80	0.44
1:EaE:21:MET:HE2	1:EaE:21:MET:HB3	1.76	0.43
1:BfB:37:ILE:HG13	1:BgB:46:THR:CG2	2.48	0.43
1:CCC:49:ALA:HA	1:BiB:29:VAL:CG2	2.48	0.43
1:BgB:21:MET:HB3	1:BgB:21:MET:HE2	1.77	0.43
1:EEE:21:MET:HE2	1:EEE:21:MET:HB3	1.79	0.43
1:AaA:21:MET:HE1	1:BcB:42:PHE:HA	2.00	0.43
1:EhE:49:ALA:HA	1:DjD:29:VAL:CG2	2.48	0.43
1:DkD:46:THR:CG2	1:DiD:37:ILE:HG13	2.48	0.43
1:EaE:49:ALA:HA	1:DhD:29:VAL:CG2	2.48	0.43
1:EhE:21:MET:HE2	1:EhE:21:MET:HB3	1.79	0.43
1:DDD:49:ALA:HA	1:CiC:29:VAL:CG2	2.49	0.43
1:AjA:50:SER:HA	1:EiE:32:ILE:HD13	2.00	0.43
1:BBB:49:ALA:HA	1:AiA:29:VAL:CG2	2.49	0.43
1:CgC:21:MET:HE2	1:CgC:21:MET:HB3	1.77	0.43
1:EiE:21:MET:HB3	1:EiE:21:MET:HE2	1.78	0.43
1:CaC:50:SER:HA	1:BhB:32:ILE:HD13	2.00	0.43
1:BcB:21:MET:HE2	1:BcB:21:MET:HB3	1.74	0.43
1:EjE:50:SER:HA	1:DiD:32:ILE:HD13	2.01	0.43
1:DDD:21:MET:HE2	1:DDD:21:MET:HB3	1.80	0.43
1:EeE:37:ILE:HG13	1:EfE:46:THR:CG2	2.49	0.43
1:DgD:21:MET:HE2	1:DgD:21:MET:HB3	1.78	0.43
1:AhA:49:ALA:HA	1:EjE:29:VAL:CG2	2.48	0.43
1:DjD:50:SER:HA	1:ClC:32:ILE:HD13	2.00	0.43
1:DkD:50:SER:HA	1:CmC:32:ILE:HD13	2.01	0.43
1:CmC:21:MET:HB3	1:CmC:21:MET:HE2	1.79	0.43
1:DaD:21:MET:HE1	1:EcE:42:PHE:HA	2.01	0.42
1:BcB:29:VAL:CG2	1:CeC:49:ALA:HA	2.49	0.42
1:CdC:32:ILE:HD13	1:DfD:50:SER:HA	2.01	0.42
1:BkB:21:MET:HE2	1:BkB:21:MET:HB3	1.80	0.42
1:CcC:29:VAL:CG2	1:DeD:49:ALA:HA	2.49	0.42
1:EcE:29:VAL:CG2	1:AeA:49:ALA:HA	2.49	0.42
1:CfC:37:ILE:HG13	1:CgC:46:THR:CG2	2.48	0.42
1:DcD:32:ILE:HD13	1:EeE:50:SER:HA	2.01	0.42
1:BdB:21:MET:HE2	1:BdB:21:MET:HB3	1.75	0.42
1:CdC:37:ILE:HG13	1:CeC:46:THR:CG2	2.48	0.42
1:AhA:21:MET:HB3	1:AhA:21:MET:HE2	1.78	0.42
1:AeA:37:ILE:HG13	1:AfA:46:THR:CG2	2.50	0.42
1:CeC:32:ILE:HD13	1:DgD:50:SER:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DfD:37:ILE:HG13	1:DgD:46:THR:CG2	2.48	0.42
1:BjB:49:ALA:HA	1:AlA:29:VAL:CG2	2.50	0.42
1:DkD:21:MET:HE2	1:DkD:21:MET:HB3	1.79	0.42
1:BnB:21:MET:HE2	1:BnB:21:MET:HB3	1.90	0.42
1:CCC:21:MET:HE2	1:CCC:21:MET:HB3	1.76	0.42
1:CaC:32:ILE:HD13	1:DcD:50:SER:HA	2.02	0.42
1:BeB:37:ILE:HG13	1:BfB:46:THR:CG2	2.50	0.42
1:CeC:37:ILE:HG13	1:CfC:46:THR:CG2	2.49	0.42
1:AfA:11:PHE:CE2	1:AgA:21:MET:HE3	2.52	0.42
1:EmE:21:MET:HB3	1:EmE:21:MET:HE2	1.79	0.42
1:BBB:21:MET:HE3	1:BhB:11:PHE:CE2	2.51	0.42
1:DhD:21:MET:HE2	1:DhD:21:MET:HB3	1.79	0.42
1:AiA:46:THR:CG2	1:AjA:37:ILE:HG13	2.50	0.42
1:AbA:32:ILE:HD13	1:BdB:50:SER:HA	2.01	0.42
1:EbE:21:MET:HE1	1:AdA:42:PHE:HA	2.01	0.42
1:EdE:37:ILE:HG13	1:EeE:46:THR:CG2	2.49	0.42
1:EfE:37:ILE:HG13	1:EgE:46:THR:CG2	2.50	0.42
1:CiC:46:THR:CG2	1:CjC:37:ILE:HG13	2.50	0.42
1:EjE:46:THR:CG2	1:EkE:37:ILE:HG13	2.49	0.42
1:CkC:21:MET:HB3	1:CkC:21:MET:HE2	1.81	0.42
1:AcA:32:ILE:HD13	1:BeB:50:SER:HA	2.01	0.42
1:BhB:46:THR:CG2	1:BiB:37:ILE:HG13	2.50	0.42
1:DiD:21:MET:HE2	1:DiD:21:MET:HB3	1.78	0.42
1:CjC:21:MET:HB3	1:CjC:21:MET:HE2	1.81	0.42
1:BBB:29:VAL:CG2	1:CbC:49:ALA:HA	2.49	0.42
1:BaB:49:ALA:HA	1:AhA:29:VAL:CG2	2.49	0.42
1:AdA:32:ILE:HD13	1:BfB:50:SER:HA	2.02	0.42
1:AaA:49:ALA:HA	1:EhE:29:VAL:CG2	2.50	0.42
1:EaE:21:MET:HE1	1:AcA:42:PHE:HA	2.02	0.42
1:BbB:21:MET:HE2	1:BbB:21:MET:HB3	1.74	0.42
1:AjA:46:THR:CG2	1:AkA:37:ILE:HG13	2.49	0.42
1:CjC:50:SER:HA	1:BlB:32:ILE:HD13	2.02	0.42
1:EkE:50:SER:HA	1:DmD:32:ILE:HD13	2.01	0.42
1:EcE:37:ILE:HG13	1:EdE:46:THR:CG2	2.51	0.41
1:AcA:37:ILE:HG13	1:AdA:46:THR:CG2	2.50	0.41
1:CdC:21:MET:HE2	1:CdC:21:MET:HB3	1.78	0.41
1:ChC:46:THR:CG2	1:CiC:37:ILE:HG13	2.50	0.41
1:BiB:46:THR:CG2	1:BjB:37:ILE:HG13	2.51	0.41
1:DiD:46:THR:CG2	1:DjD:37:ILE:HG13	2.50	0.41
1:CjC:46:THR:CG2	1:CkC:37:ILE:HG13	2.50	0.41
1:EhE:46:THR:CG2	1:EiE:37:ILE:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: EiE:46:THR:CG2	1: EjE:37:ILE:HG13	2.50	0.41
1: BjB:46:THR:CG2	1: BkB:37:ILE:HG13	2.50	0.41
1: EEE:32:ILE:HD13	1: AbA:50:SER:HA	2.03	0.41
1: AdA:37:ILE:HG13	1: AeA:46:THR:CG2	2.50	0.41
1: CkC:50:SER:HA	1: BmB:32:ILE:HD13	2.02	0.41
1: DmD:28:MET:HE1	1: DnD:14:LEU:CB	2.48	0.41
1: DDD:42:PHE:HA	1: CiC:21:MET:HE1	2.02	0.41
1: DdD:37:ILE:HG13	1: DeD:46:THR:CG2	2.50	0.41
1: EdE:32:ILE:HD13	1: AfA:50:SER:HA	2.03	0.41
1: EeE:32:ILE:HD13	1: AgA:50:SER:HA	2.01	0.41
1: BfB:21:MET:HE2	1: BfB:21:MET:HB3	1.83	0.41
1: AgA:21:MET:HB3	1: AgA:21:MET:HE2	1.82	0.41
1: BdB:14:LEU:CB	1: BeB:28:MET:HE1	2.47	0.41
1: DeD:37:ILE:HG13	1: DfD:46:THR:CG2	2.51	0.41
1: BkB:50:SER:HA	1: AmA:32:ILE:HD13	2.03	0.41
1: AaA:37:ILE:HG13	1: AbA:46:THR:CG2	2.50	0.41
1: DaD:49:ALA:HA	1: ChC:29:VAL:CG2	2.50	0.41
1: DbD:21:MET:HE1	1: EdE:42:PHE:HA	2.02	0.41
1: EaE:32:ILE:HD13	1: AcA:50:SER:HA	2.03	0.41
1: DcD:37:ILE:HG13	1: DdD:46:THR:CG2	2.51	0.41
1: BeB:21:MET:HE2	1: BeB:21:MET:HB3	1.80	0.41
1: AhA:46:THR:CG2	1: AiA:37:ILE:HG13	2.51	0.41
1: EnE:21:MET:HE2	1: EnE:21:MET:HB3	1.92	0.41
1: AAA:29:VAL:CG2	1: BbB:49:ALA:HA	2.51	0.41
1: BaB:21:MET:HE1	1: CcC:42:PHE:HA	2.02	0.41
1: CaC:49:ALA:HA	1: BhB:29:VAL:CG2	2.49	0.41
1: BcB:37:ILE:HG13	1: BdB:46:THR:CG2	2.50	0.41
1: BdB:37:ILE:HG13	1: BeB:46:THR:CG2	2.50	0.41
1: ChC:21:MET:HE2	1: ChC:21:MET:HB3	1.83	0.41
1: CjC:49:ALA:HA	1: BlB:29:VAL:CG2	2.48	0.41
1: DjD:46:THR:CG2	1: DkD:37:ILE:HG13	2.50	0.41
1: AmA:28:MET:HE1	1: AnA:14:LEU:CB	2.49	0.41
1: AnA:21:MET:HE2	1: AnA:21:MET:HB3	1.91	0.41
1: CCC:29:VAL:CG2	1: DbD:49:ALA:HA	2.51	0.41
1: BcB:32:ILE:HD13	1: CeC:50:SER:HA	2.03	0.41
1: AfA:21:MET:HB3	1: AfA:21:MET:HE2	1.82	0.41
1: BBB:46:THR:CG2	1: BhB:37:ILE:HG13	2.51	0.40
1: CCC:21:MET:HE1	1: DbD:42:PHE:HA	2.03	0.40
1: DDD:29:VAL:CG2	1: EbE:49:ALA:HA	2.52	0.40
1: EEE:37:ILE:HG13	1: EaE:46:THR:CG2	2.51	0.40
1: BbB:32:ILE:HD13	1: CdC:50:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CfC:21:MET:HE2	1:CfC:21:MET:HB3	1.81	0.40
1:AkA:50:SER:HA	1:EmE:32:ILE:HD13	2.03	0.40
1:CkC:21:MET:HE1	1:ClC:11:PHE:HE2	1.82	0.40
1:EEE:29:VAL:CG2	1:AbA:49:ALA:HA	2.51	0.40
1:CaC:21:MET:HE2	1:CaC:21:MET:HB3	1.76	0.40
1:EaE:29:VAL:CG2	1:AcA:49:ALA:HA	2.51	0.40
1:EaE:50:SER:HA	1:DhD:32:ILE:HD13	2.04	0.40
1:CbC:32:ILE:HD13	1:DdD:50:SER:HA	2.03	0.40
1:DdD:32:ILE:HD13	1:EfE:50:SER:HA	2.02	0.40
1:AaA:50:SER:HA	1:EhE:32:ILE:HD13	2.03	0.40
1:BbB:21:MET:HE1	1:CdC:42:PHE:HA	2.02	0.40
1:CCC:37:ILE:HG13	1:CaC:46:THR:CG2	2.52	0.40
1:BaB:50:SER:HA	1:AhA:32:ILE:HD13	2.03	0.40
1:DaD:37:ILE:HG13	1:DbD:46:THR:CG2	2.51	0.40
1:EeE:14:LEU:CB	1:EfE:28:MET:HE1	2.50	0.40
1:ClC:21:MET:HB3	1:ClC:21:MET:HE2	1.81	0.40
1:DaD:50:SER:HA	1:ChC:32:ILE:HD13	2.03	0.40
1:DbD:37:ILE:HG13	1:DcD:46:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	44/50 (88%)	44 (100%)	0	0	100	100
1	AaA	44/50 (88%)	44 (100%)	0	0	100	100
1	AbA	44/50 (88%)	44 (100%)	0	0	100	100
1	AcA	44/50 (88%)	44 (100%)	0	0	100	100
1	AdA	44/50 (88%)	44 (100%)	0	0	100	100
1	AeA	44/50 (88%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AfA	44/50 (88%)	44 (100%)	0	0	100	100
1	AgA	33/50 (66%)	33 (100%)	0	0	100	100
1	AhA	44/50 (88%)	44 (100%)	0	0	100	100
1	AiA	44/50 (88%)	44 (100%)	0	0	100	100
1	AjA	44/50 (88%)	44 (100%)	0	0	100	100
1	AkA	44/50 (88%)	44 (100%)	0	0	100	100
1	AlA	44/50 (88%)	44 (100%)	0	0	100	100
1	AmA	44/50 (88%)	44 (100%)	0	0	100	100
1	AnA	44/50 (88%)	44 (100%)	0	0	100	100
1	BBB	44/50 (88%)	44 (100%)	0	0	100	100
1	BaB	44/50 (88%)	44 (100%)	0	0	100	100
1	BbB	44/50 (88%)	44 (100%)	0	0	100	100
1	BcB	44/50 (88%)	44 (100%)	0	0	100	100
1	BdB	44/50 (88%)	44 (100%)	0	0	100	100
1	BeB	44/50 (88%)	44 (100%)	0	0	100	100
1	BfB	44/50 (88%)	44 (100%)	0	0	100	100
1	BgB	33/50 (66%)	33 (100%)	0	0	100	100
1	BhB	44/50 (88%)	44 (100%)	0	0	100	100
1	BiB	44/50 (88%)	44 (100%)	0	0	100	100
1	BjB	44/50 (88%)	44 (100%)	0	0	100	100
1	BkB	44/50 (88%)	44 (100%)	0	0	100	100
1	BlB	44/50 (88%)	44 (100%)	0	0	100	100
1	BmB	44/50 (88%)	44 (100%)	0	0	100	100
1	BnB	44/50 (88%)	44 (100%)	0	0	100	100
1	CCC	44/50 (88%)	44 (100%)	0	0	100	100
1	CaC	44/50 (88%)	44 (100%)	0	0	100	100
1	CbC	44/50 (88%)	44 (100%)	0	0	100	100
1	CcC	44/50 (88%)	44 (100%)	0	0	100	100
1	CdC	44/50 (88%)	44 (100%)	0	0	100	100
1	CeC	44/50 (88%)	44 (100%)	0	0	100	100
1	CfC	44/50 (88%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CgC	33/50 (66%)	33 (100%)	0	0	100	100
1	ChC	44/50 (88%)	44 (100%)	0	0	100	100
1	CiC	44/50 (88%)	44 (100%)	0	0	100	100
1	CjC	44/50 (88%)	44 (100%)	0	0	100	100
1	CkC	44/50 (88%)	44 (100%)	0	0	100	100
1	ClC	44/50 (88%)	44 (100%)	0	0	100	100
1	CmC	44/50 (88%)	44 (100%)	0	0	100	100
1	CnC	44/50 (88%)	44 (100%)	0	0	100	100
1	DDD	44/50 (88%)	44 (100%)	0	0	100	100
1	DaD	44/50 (88%)	44 (100%)	0	0	100	100
1	DbD	44/50 (88%)	44 (100%)	0	0	100	100
1	DcD	44/50 (88%)	44 (100%)	0	0	100	100
1	DdD	44/50 (88%)	44 (100%)	0	0	100	100
1	DeD	44/50 (88%)	44 (100%)	0	0	100	100
1	DfD	44/50 (88%)	44 (100%)	0	0	100	100
1	DgD	33/50 (66%)	33 (100%)	0	0	100	100
1	DhD	44/50 (88%)	44 (100%)	0	0	100	100
1	DiD	44/50 (88%)	44 (100%)	0	0	100	100
1	DjD	44/50 (88%)	44 (100%)	0	0	100	100
1	DkD	44/50 (88%)	44 (100%)	0	0	100	100
1	DlD	44/50 (88%)	44 (100%)	0	0	100	100
1	DmD	44/50 (88%)	44 (100%)	0	0	100	100
1	DnD	44/50 (88%)	44 (100%)	0	0	100	100
1	EEE	44/50 (88%)	44 (100%)	0	0	100	100
1	EaE	44/50 (88%)	44 (100%)	0	0	100	100
1	EbE	44/50 (88%)	44 (100%)	0	0	100	100
1	EcE	44/50 (88%)	44 (100%)	0	0	100	100
1	EdE	44/50 (88%)	44 (100%)	0	0	100	100
1	EeE	44/50 (88%)	44 (100%)	0	0	100	100
1	EfE	44/50 (88%)	44 (100%)	0	0	100	100
1	EgE	33/50 (66%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EhE	44/50 (88%)	44 (100%)	0	0	100	100
1	EiE	44/50 (88%)	44 (100%)	0	0	100	100
1	EjE	44/50 (88%)	44 (100%)	0	0	100	100
1	EkE	44/50 (88%)	44 (100%)	0	0	100	100
1	ElE	44/50 (88%)	44 (100%)	0	0	100	100
1	EmE	44/50 (88%)	44 (100%)	0	0	100	100
1	EnE	44/50 (88%)	44 (100%)	0	0	100	100
All	All	3245/3750 (86%)	3245 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	34/36 (94%)	34 (100%)	0	100	100
1	AaA	34/36 (94%)	34 (100%)	0	100	100
1	AbA	34/36 (94%)	34 (100%)	0	100	100
1	AcA	34/36 (94%)	34 (100%)	0	100	100
1	AdA	34/36 (94%)	34 (100%)	0	100	100
1	AeA	34/36 (94%)	34 (100%)	0	100	100
1	AfA	34/36 (94%)	34 (100%)	0	100	100
1	AgA	26/36 (72%)	26 (100%)	0	100	100
1	AhA	34/36 (94%)	34 (100%)	0	100	100
1	AiA	34/36 (94%)	34 (100%)	0	100	100
1	AjA	34/36 (94%)	34 (100%)	0	100	100
1	AkA	34/36 (94%)	34 (100%)	0	100	100
1	AlA	34/36 (94%)	33 (97%)	1 (3%)	37	63
1	AmA	34/36 (94%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AnA	34/36 (94%)	34 (100%)	0	100	100
1	BBB	34/36 (94%)	34 (100%)	0	100	100
1	BaB	34/36 (94%)	34 (100%)	0	100	100
1	BbB	34/36 (94%)	34 (100%)	0	100	100
1	BcB	34/36 (94%)	34 (100%)	0	100	100
1	BdB	34/36 (94%)	34 (100%)	0	100	100
1	BeB	34/36 (94%)	34 (100%)	0	100	100
1	BfB	34/36 (94%)	34 (100%)	0	100	100
1	BgB	26/36 (72%)	26 (100%)	0	100	100
1	BhB	34/36 (94%)	34 (100%)	0	100	100
1	BiB	34/36 (94%)	34 (100%)	0	100	100
1	BjB	34/36 (94%)	34 (100%)	0	100	100
1	BkB	34/36 (94%)	33 (97%)	1 (3%)	37	63
1	BlB	34/36 (94%)	34 (100%)	0	100	100
1	BmB	34/36 (94%)	34 (100%)	0	100	100
1	BnB	34/36 (94%)	34 (100%)	0	100	100
1	CCC	34/36 (94%)	34 (100%)	0	100	100
1	CaC	34/36 (94%)	34 (100%)	0	100	100
1	CbC	34/36 (94%)	34 (100%)	0	100	100
1	CcC	34/36 (94%)	34 (100%)	0	100	100
1	CdC	34/36 (94%)	34 (100%)	0	100	100
1	CeC	34/36 (94%)	34 (100%)	0	100	100
1	CfC	34/36 (94%)	34 (100%)	0	100	100
1	CgC	26/36 (72%)	26 (100%)	0	100	100
1	ChC	34/36 (94%)	34 (100%)	0	100	100
1	CiC	34/36 (94%)	34 (100%)	0	100	100
1	CjC	34/36 (94%)	34 (100%)	0	100	100
1	CkC	34/36 (94%)	33 (97%)	1 (3%)	37	63
1	ClC	34/36 (94%)	34 (100%)	0	100	100
1	CmC	34/36 (94%)	34 (100%)	0	100	100
1	CnC	34/36 (94%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DDD	34/36 (94%)	34 (100%)	0	100	100
1	DaD	34/36 (94%)	34 (100%)	0	100	100
1	DbD	34/36 (94%)	34 (100%)	0	100	100
1	DcD	34/36 (94%)	34 (100%)	0	100	100
1	DdD	34/36 (94%)	34 (100%)	0	100	100
1	DeD	34/36 (94%)	34 (100%)	0	100	100
1	DfD	34/36 (94%)	34 (100%)	0	100	100
1	DgD	26/36 (72%)	26 (100%)	0	100	100
1	DhD	34/36 (94%)	34 (100%)	0	100	100
1	DiD	34/36 (94%)	34 (100%)	0	100	100
1	DjD	34/36 (94%)	34 (100%)	0	100	100
1	DkD	34/36 (94%)	33 (97%)	1 (3%)	37	63
1	DlD	34/36 (94%)	34 (100%)	0	100	100
1	DmD	34/36 (94%)	34 (100%)	0	100	100
1	DnD	34/36 (94%)	34 (100%)	0	100	100
1	EEE	34/36 (94%)	34 (100%)	0	100	100
1	EaE	34/36 (94%)	34 (100%)	0	100	100
1	EbE	34/36 (94%)	34 (100%)	0	100	100
1	EcE	34/36 (94%)	34 (100%)	0	100	100
1	EdE	34/36 (94%)	34 (100%)	0	100	100
1	EeE	34/36 (94%)	34 (100%)	0	100	100
1	EfE	34/36 (94%)	34 (100%)	0	100	100
1	EgE	26/36 (72%)	26 (100%)	0	100	100
1	EhE	34/36 (94%)	34 (100%)	0	100	100
1	EiE	34/36 (94%)	34 (100%)	0	100	100
1	EjE	34/36 (94%)	34 (100%)	0	100	100
1	EkE	34/36 (94%)	33 (97%)	1 (3%)	37	63
1	ElE	34/36 (94%)	34 (100%)	0	100	100
1	EmE	34/36 (94%)	34 (100%)	0	100	100
1	EnE	34/36 (94%)	34 (100%)	0	100	100
All	All	2510/2700 (93%)	2505 (100%)	5 (0%)	85	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BkB	13	SER
1	CkC	13	SER
1	DkD	13	SER
1	EkE	13	SER
1	AlA	13	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

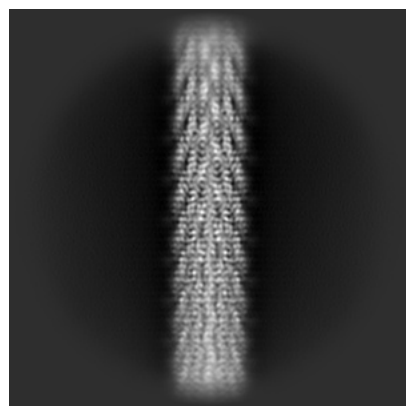
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15833. These allow visual inspection of the internal detail of the map and identification of artifacts.

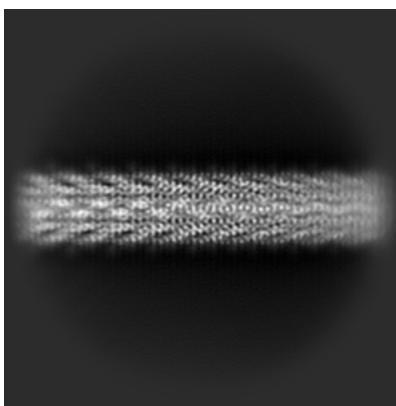
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

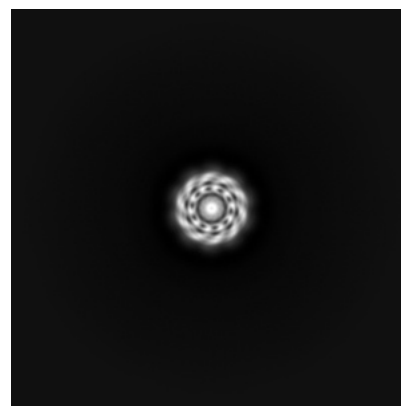
6.1.1 Primary map



X

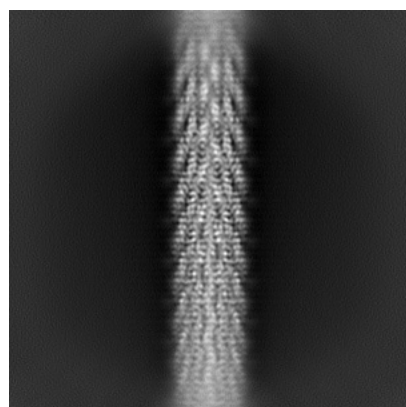


Y

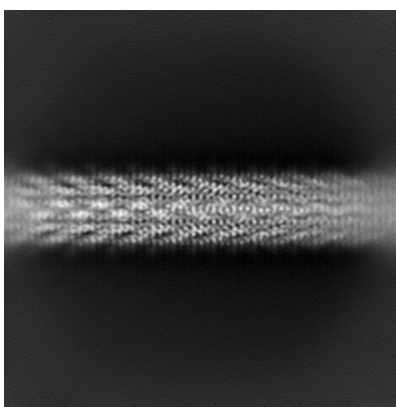


Z

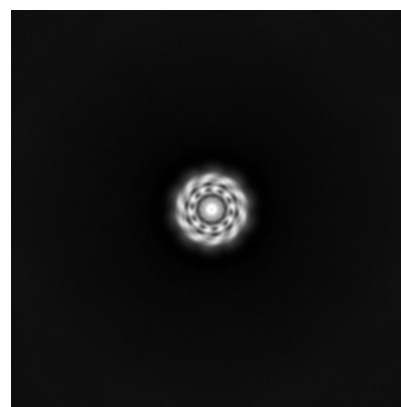
6.1.2 Raw map



X



Y

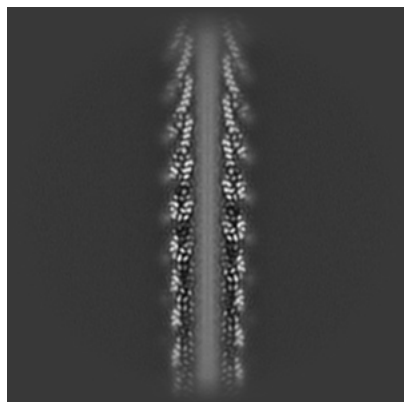


Z

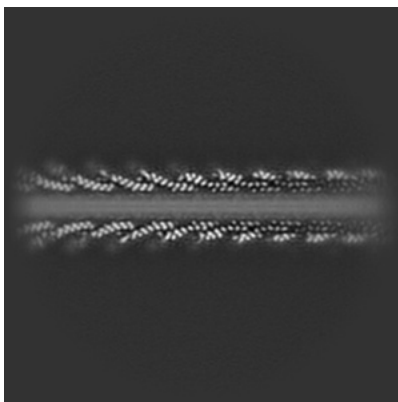
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

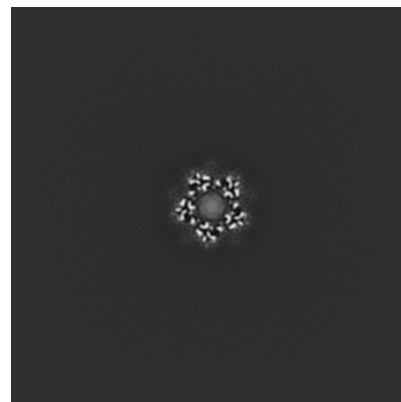
6.2.1 Primary map



X Index: 150

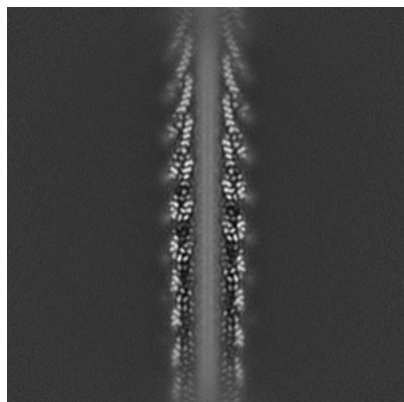


Y Index: 150

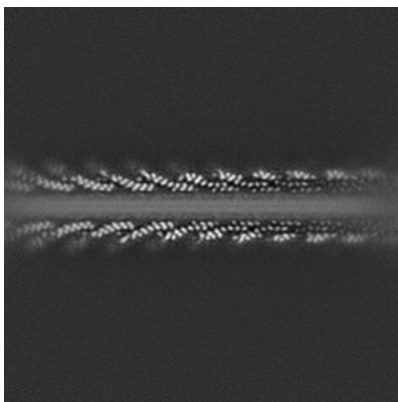


Z Index: 150

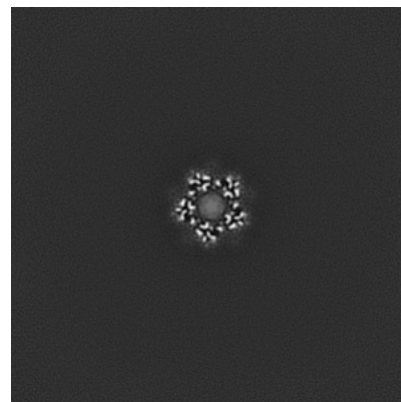
6.2.2 Raw map



X Index: 150



Y Index: 150

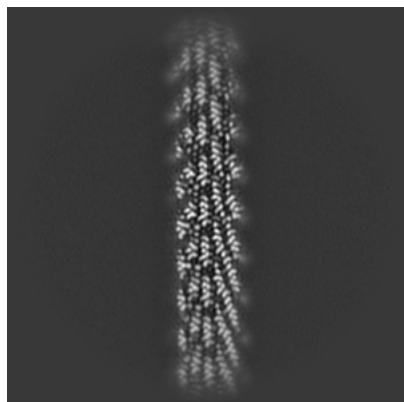


Z Index: 150

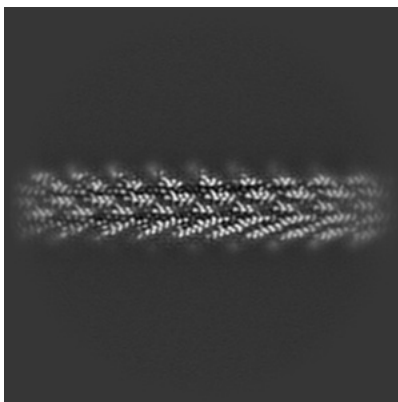
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

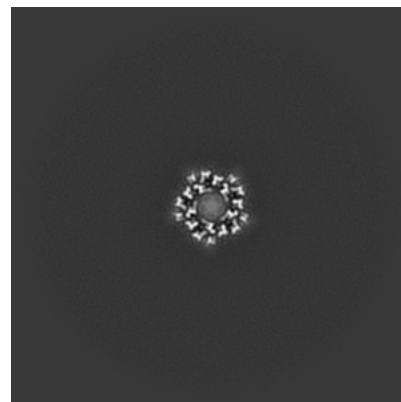
6.3.1 Primary map



X Index: 135

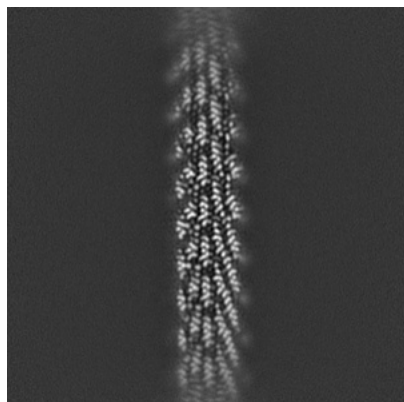


Y Index: 137

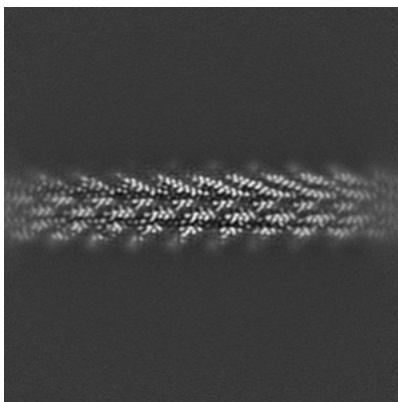


Z Index: 147

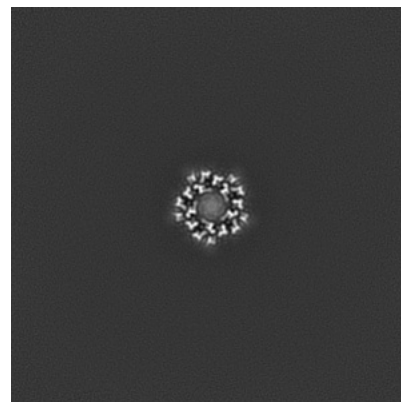
6.3.2 Raw map



X Index: 135



Y Index: 163

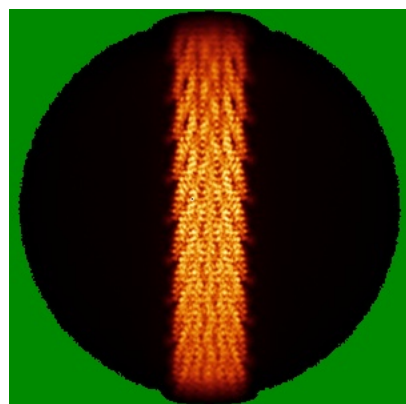


Z Index: 147

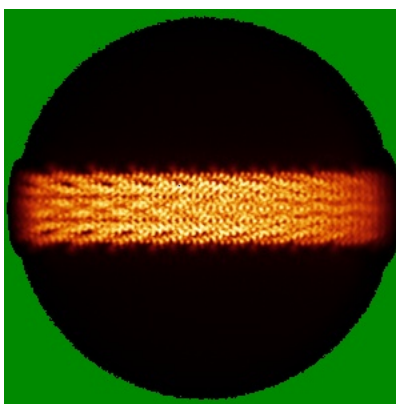
The images above show the largest variance slices of the map in three orthogonal directions.

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

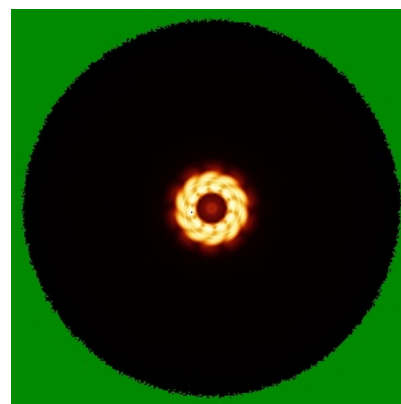
6.4.1 Primary map



X

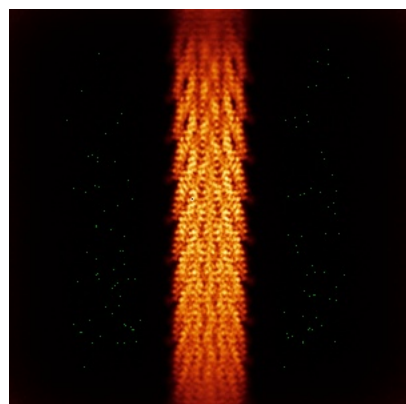


Y

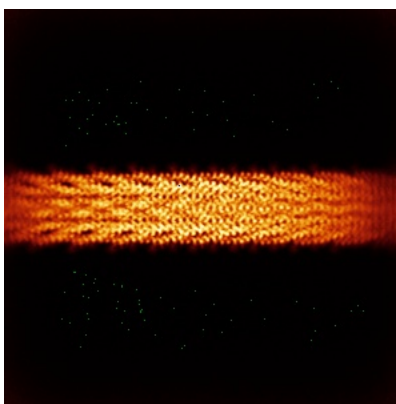


Z

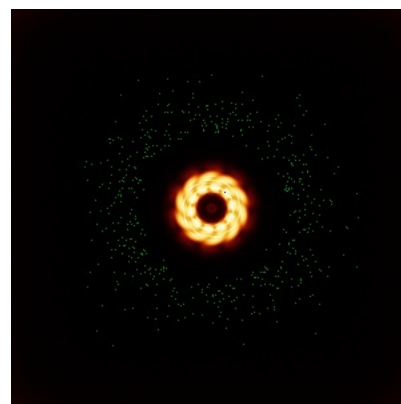
6.4.2 Raw map



X



Y

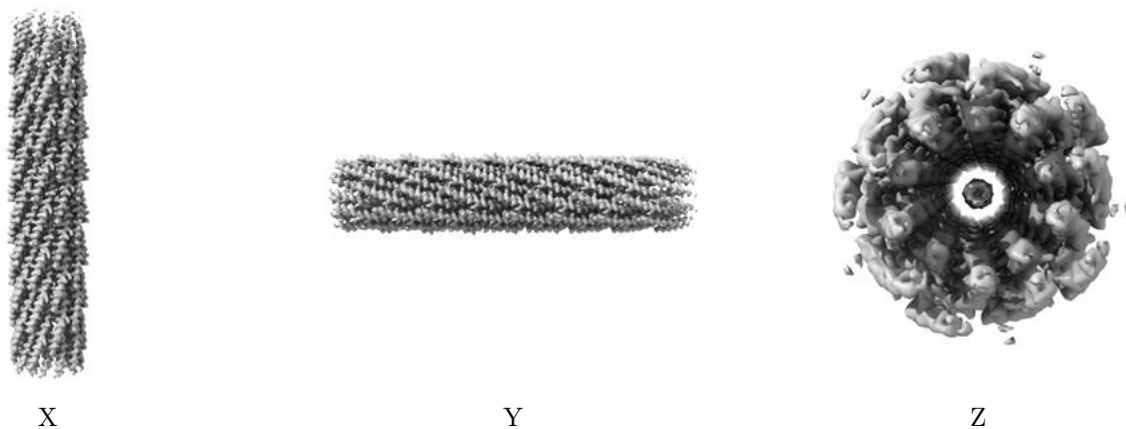


Z

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

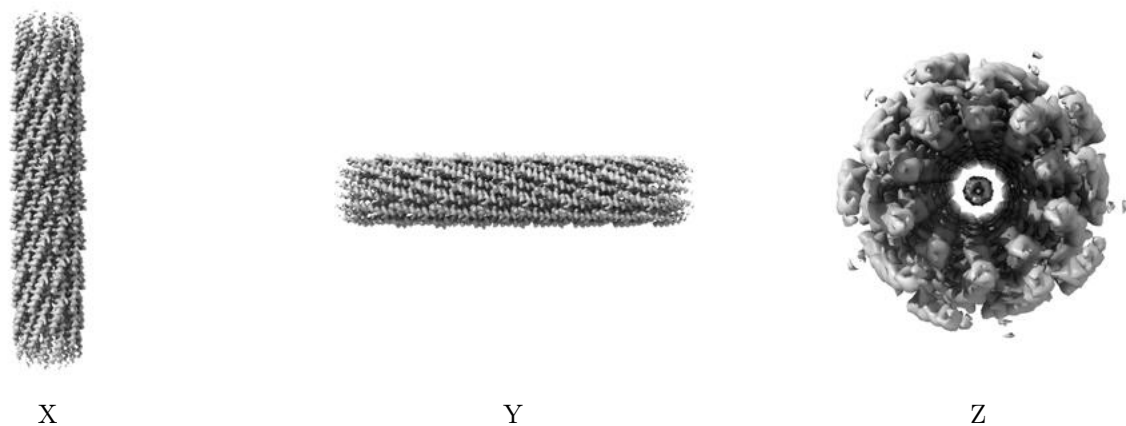
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

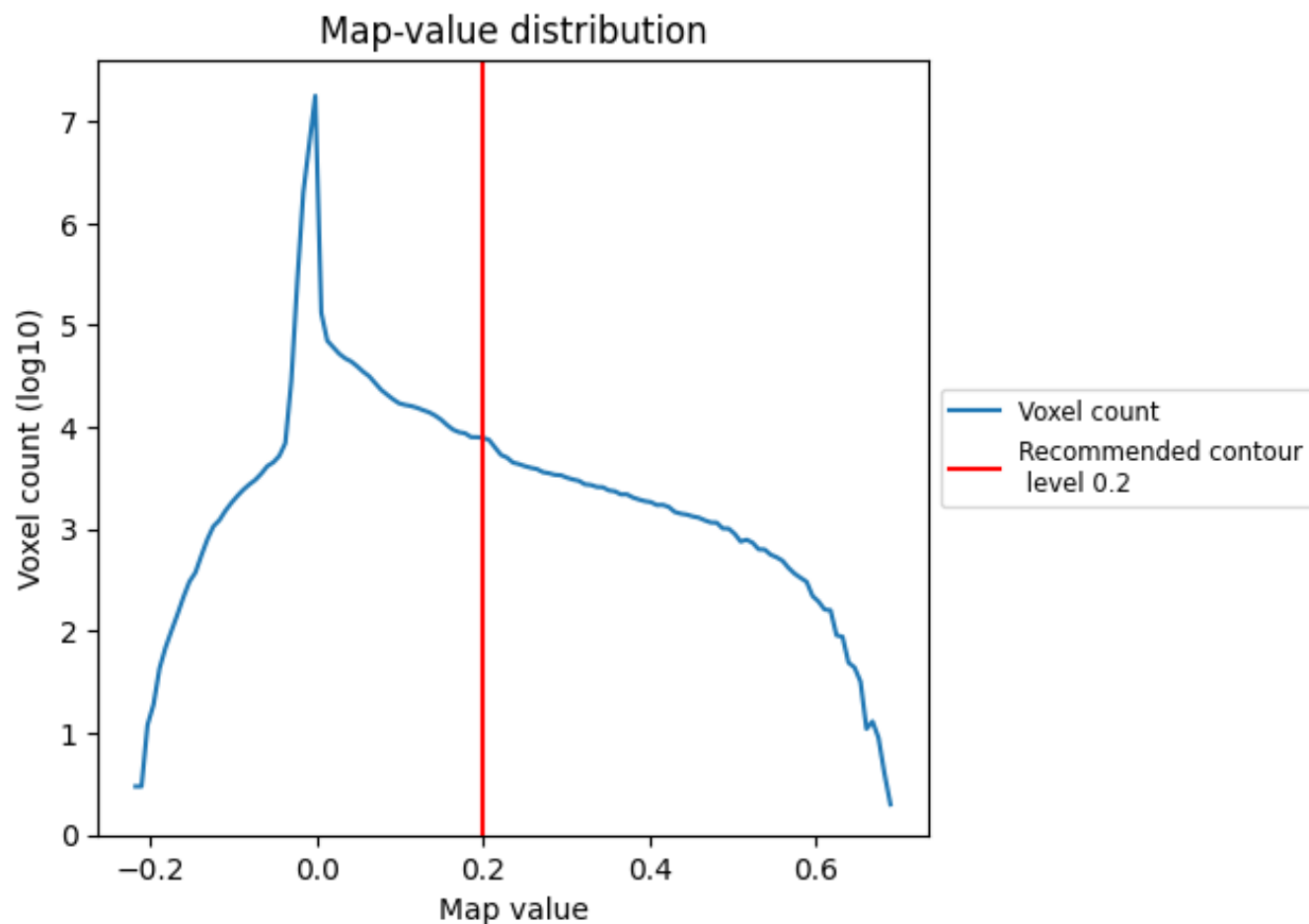
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

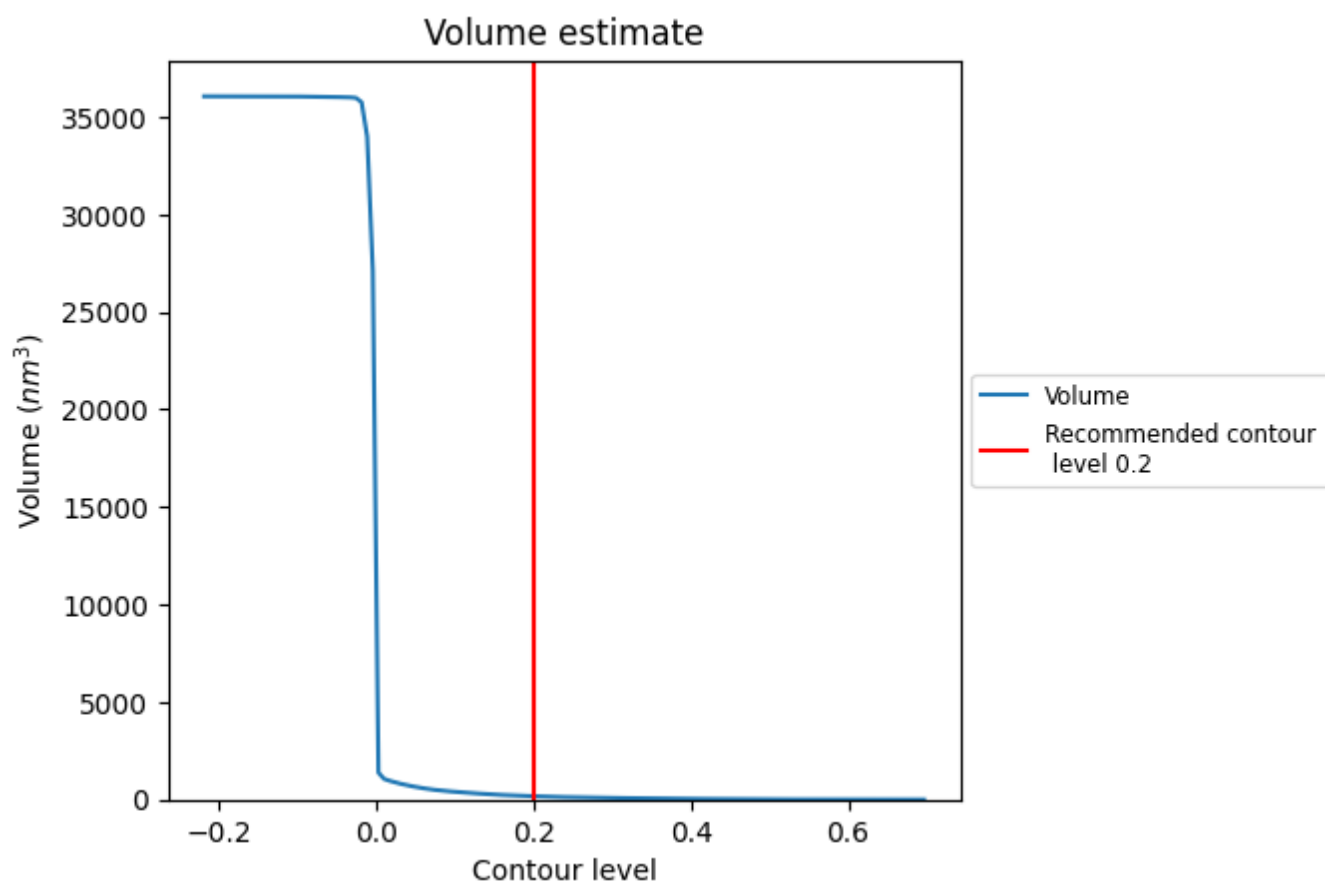
This section contains the results of statistical analysis of the map.

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.

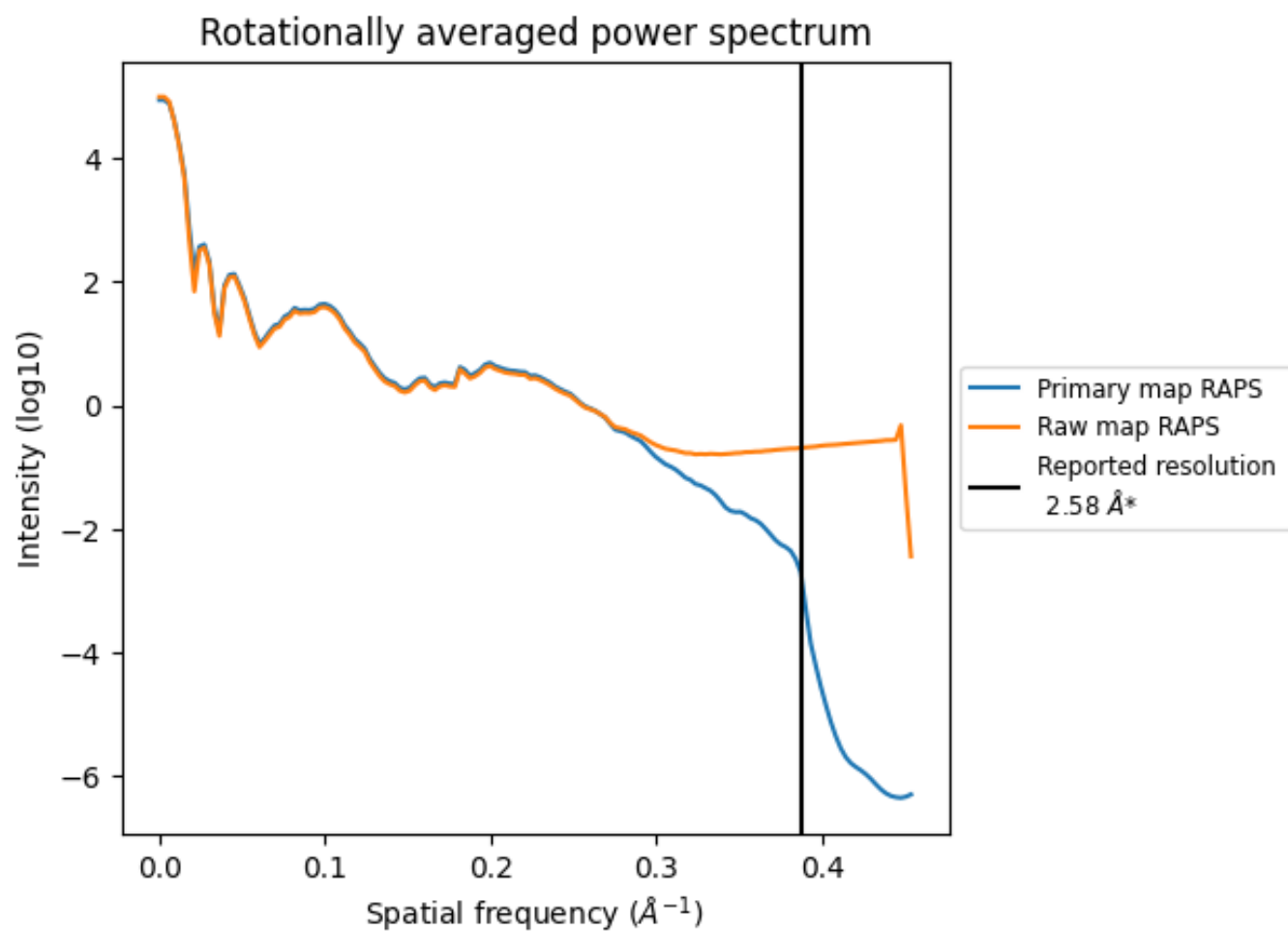
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 156 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 ⓘ

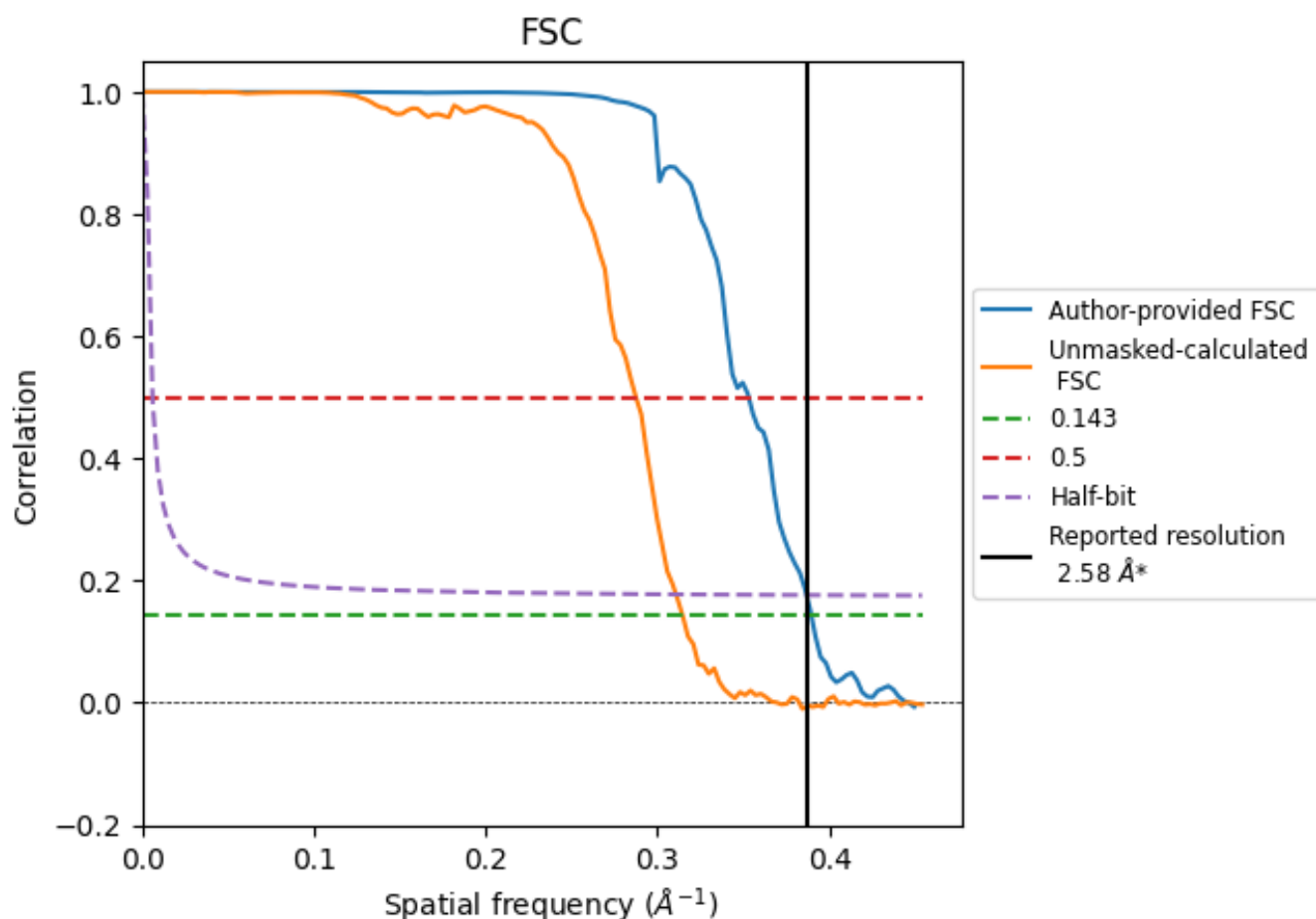


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

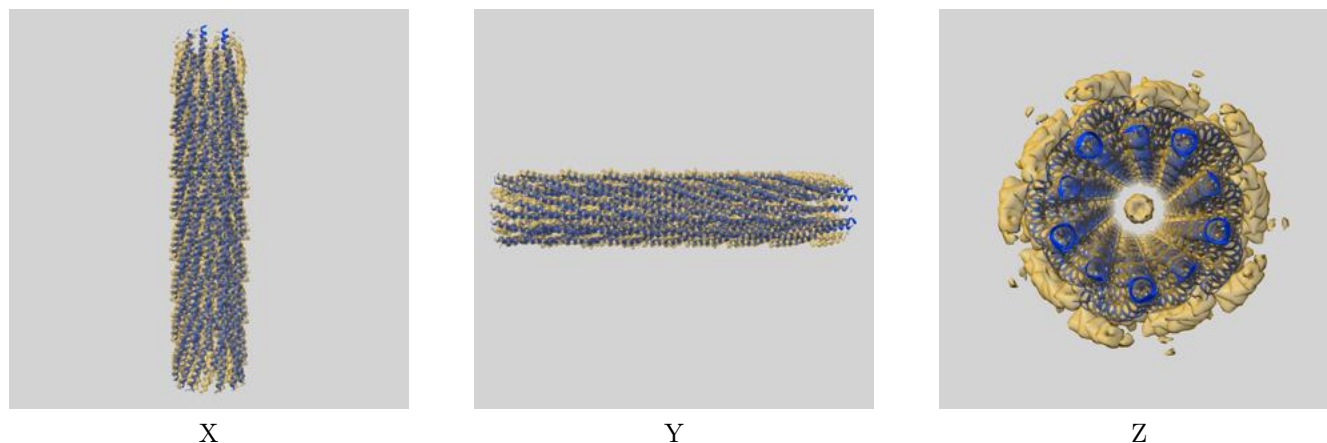
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.83	2.59
Unmasked-calculated*	3.18	3.48	3.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.58 by more than 10 %

9 Map-model fit [i](#)

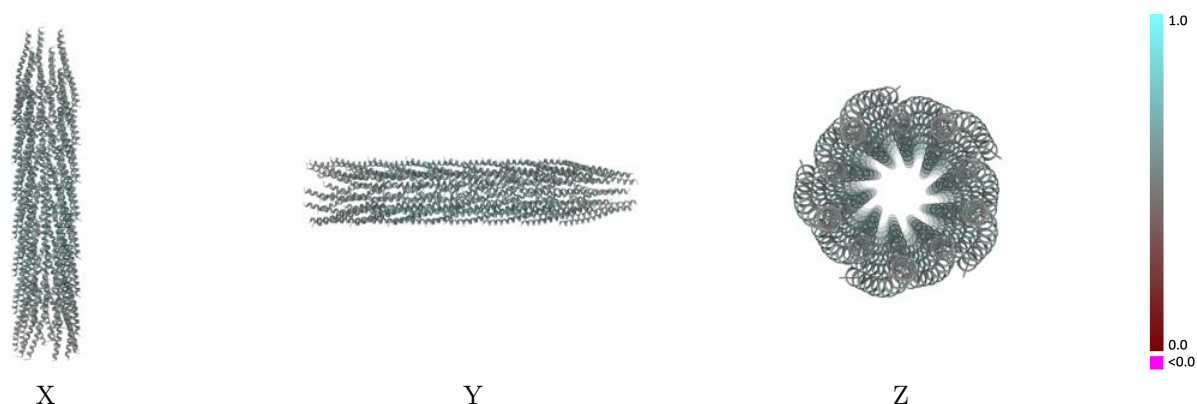
This section contains information regarding the fit between EMDB map EMD-15833 and PDB model 8B3Q. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



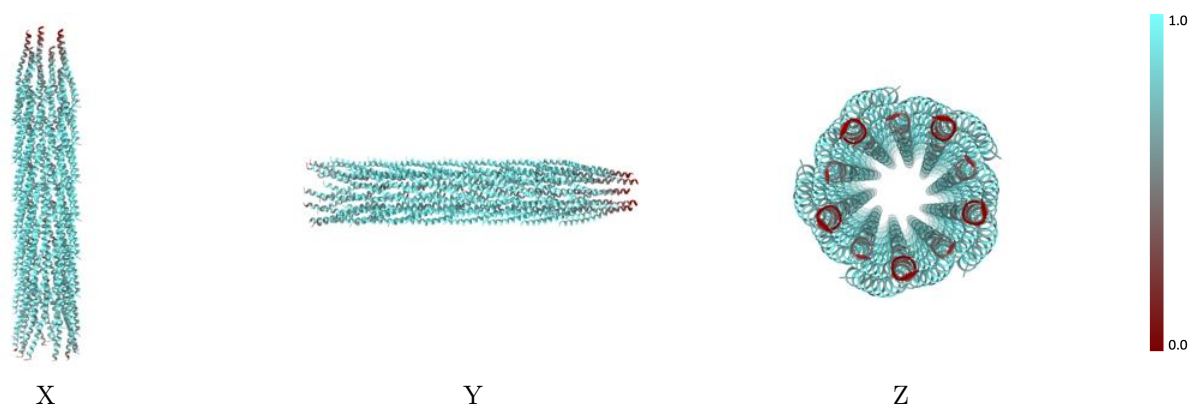
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



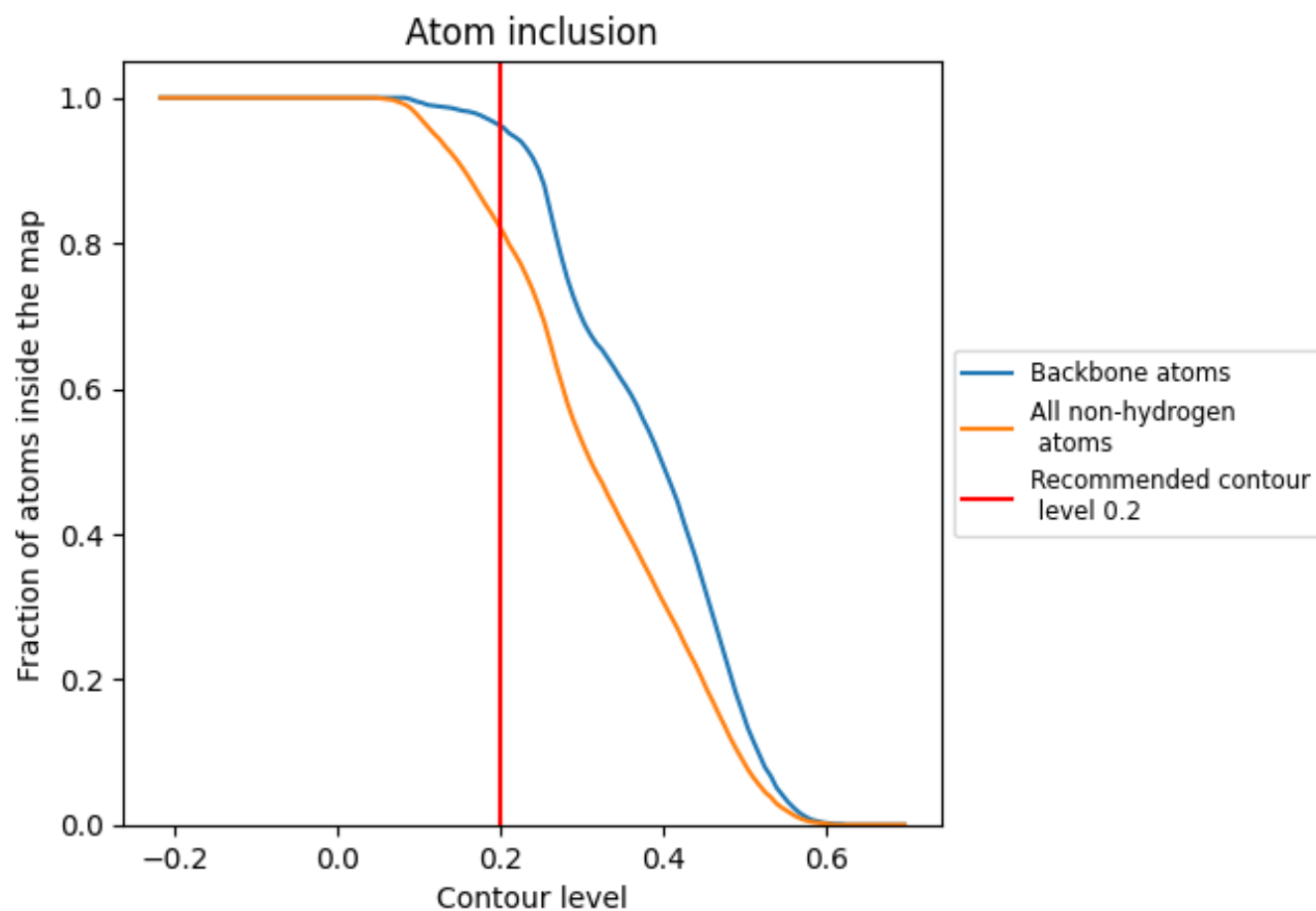
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 82% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5510
AAA	 0.8990	 0.5740
AaA	 0.8900	 0.5750
AbA	 0.8880	 0.5660
AcA	 0.8790	 0.5620
AdA	 0.8550	 0.5530
AeA	 0.8110	 0.5420
AfA	 0.7130	 0.5280
AgA	 0.7040	 0.5220
AhA	 0.8990	 0.5710
AiA	 0.8930	 0.5710
AjA	 0.8700	 0.5610
AkA	 0.8520	 0.5570
AlA	 0.7930	 0.5420
AmA	 0.7280	 0.5280
AnA	 0.6040	 0.5100
BBB	 0.8930	 0.5730
BaB	 0.8930	 0.5720
BbB	 0.8900	 0.5690
BcB	 0.8820	 0.5630
BdB	 0.8550	 0.5540
BeB	 0.8110	 0.5400
BfB	 0.7130	 0.5230
BgB	 0.7040	 0.5220
BhB	 0.8990	 0.5690
BiB	 0.8900	 0.5700
BjB	 0.8760	 0.5640
BkB	 0.8490	 0.5550
BlB	 0.7870	 0.5400
BmB	 0.7190	 0.5310
BnB	 0.5950	 0.5120
CCC	 0.8930	 0.5720
CaC	 0.8900	 0.5700
CbC	 0.8930	 0.5700
CcC	 0.8880	 0.5640



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Chain	Atom inclusion	Q-score
CdC	 0.8670	 0.5540
CeC	 0.8080	 0.5410
CfC	 0.7220	 0.5240
CgC	 0.7120	 0.5200
ChC	 0.8990	 0.5690
CiC	 0.8900	 0.5670
CjC	 0.8730	 0.5620
CkC	 0.8520	 0.5560
ClC	 0.7930	 0.5440
CmC	 0.7250	 0.5310
CnC	 0.5950	 0.5140
DDD	 0.8960	 0.5710
DaD	 0.8900	 0.5690
DbD	 0.8900	 0.5680
DcD	 0.8850	 0.5610
DdD	 0.8730	 0.5540
DeD	 0.8110	 0.5450
DfD	 0.7190	 0.5260
DgD	 0.7200	 0.5230
DhD	 0.8900	 0.5690
DiD	 0.8900	 0.5680
DjD	 0.8670	 0.5630
DkD	 0.8520	 0.5570
DlD	 0.7900	 0.5460
DmD	 0.7160	 0.5310
DnD	 0.6010	 0.5110
EEE	 0.8960	 0.5720
EaE	 0.8960	 0.5700
EbE	 0.8850	 0.5670
EcE	 0.8820	 0.5630
EdE	 0.8610	 0.5550
EeE	 0.7990	 0.5410
EfE	 0.7250	 0.5260
EgE	 0.7040	 0.5250
EhE	 0.8930	 0.5720
EiE	 0.8880	 0.5670
EjE	 0.8760	 0.5640
EkE	 0.8460	 0.5570
ElE	 0.7840	 0.5430
EmE	 0.7190	 0.5290
EnE	 0.5950	 0.5100