Full wwPDB EM Validation Report (i)

Mar 9, 2024 – 06:52 AM EST

PDB ID	:	6NM5
EMDB ID	:	EMD-9397
Title	:	F-pilus/MS2 Maturation protein complex
Authors	:	Meng, R.; Chang, J.; Zhang, J.
Deposited on	:	2019-01-10
Resolution	:	6.20 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 (i) 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 (i)) were used in the production of this report:

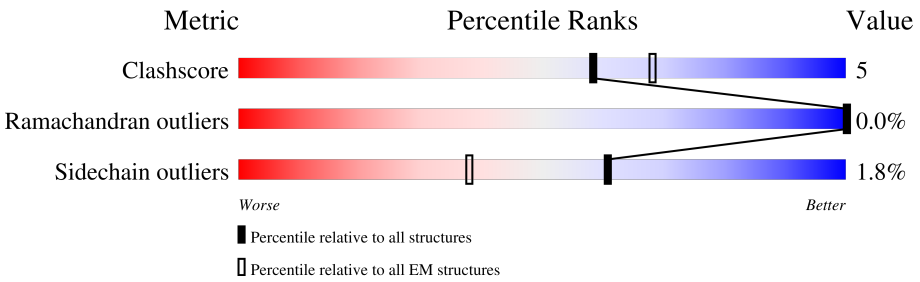
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1A	65	40% 83% 15% •
1	1B	65	34% 86% 12% •
1	1C	65	31% 85% 15%
1	1D	65	20% 86% 14%
1	1E	65	22% 88% 12%
1	1F	65	20% 86% 14%
1	1G	65	17% 86% 12% •
1	1H	65	23% 89% 11%

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Mol	Chain	Length	Quality of chain
1	1I	65	12% 83% 15%
1	1J	65	22% 86% 14%
1	1K	65	28% 83% 17%
1	1L	65	32% 83% 17%
1	1M	65	29% 82% 17%
1	1N	65	31% 82% 17%
1	1O	65	37% 85% 14%
1	2A	65	40% 86% 12%
1	2B	65	29% 85% 14%
1	2C	65	26% 82% 18%
1	2D	65	17% 86% 14%
1	2E	65	17% 85% 15%
1	2F	65	18% 85% 15%
1	2G	65	22% 85% 14%
1	2H	65	25% 85% 15%
1	2I	65	28% 83% 17%
1	2J	65	28% 83% 17%
1	2K	65	26% 88% 12%
1	2L	65	31% 86% 14%
1	2M	65	38% 80% 18%
1	2N	65	31% 83% 15%
1	2O	65	34% 85% 14%
1	3A	65	29% 88% 11%
1	3B	65	20% 86% 14%
1	3C	65	18% 83% 17%

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Mol	Chain	Length	Quality of chain
1	3D	65	23% 82% 17%
1	3E	65	25% 85% 14%
1	3F	65	23% 86% 14%
1	3G	65	23% 82% 18%
1	3H	65	22% 85% 15%
1	3I	65	23% 80% 20%
1	3J	65	28% 88% 12%
1	3K	65	18% 86% 14%
1	3L	65	23% 83% 17%
1	3M	65	25% 83% 15%
1	3N	65	34% 85% 14%
1	3O	65	34% 88% 11%
1	4A	65	34% 88% 11%
1	4B	65	26% 86% 12%
1	4C	65	23% 83% 17%
1	4D	65	25% 82% 18%
1	4E	65	26% 82% 17%
1	4F	65	22% 88% 12%
1	4G	65	25% 85% 15%
1	4H	65	22% 86% 14%
1	4I	65	20% 83% 17%
1	4J	65	22% 80% 18%
1	4K	65	26% 82% 18%
1	4L	65	25% 82% 17%
1	4M	65	29% 83% 15%

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Mol	Chain	Length	Quality of chain
1	4N	65	35% 89% 11%
1	4O	65	31% 88% 11%
1	5A	65	35% 89% 9%
1	5B	65	37% 82% 17%
1	5C	65	29% 83% 15%
1	5D	65	23% 85% 15%
1	5E	65	26% 83% 15%
1	5F	65	17% 82% 17%
1	5G	65	18% 91% 9%
1	5H	65	18% 91% 9%
1	5I	65	20% 86% 14%
1	5J	65	18% 83% 17%
1	5K	65	22% 85% 15%
1	5L	65	26% 85% 14%
1	5M	65	31% 86% 14%
1	5N	65	34% 91% 9%
1	5O	65	37% 88% 11%
2	M	393	88% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 39224 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Type IV conjugative transfer system pilin TraA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	65	476	314	74	83	5	0	0
1	1B	65	476	314	74	83	5	0	0
1	1C	65	476	314	74	83	5	0	0
1	1D	65	476	314	74	83	5	0	0
1	1E	65	476	314	74	83	5	0	0
1	1F	65	476	314	74	83	5	0	0
1	1G	65	476	314	74	83	5	0	0
1	1H	65	476	314	74	83	5	0	0
1	1I	65	476	314	74	83	5	0	0
1	1J	65	476	314	74	83	5	0	0
1	1K	65	476	314	74	83	5	0	0
1	1L	65	476	314	74	83	5	0	0
1	1M	65	476	314	74	83	5	0	0
1	1N	65	476	314	74	83	5	0	0
1	1O	65	476	314	74	83	5	0	0
1	2A	65	476	314	74	83	5	0	0
1	2B	65	476	314	74	83	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2C	65	476	314	74	83	5	0	0
1	2D	65	476	314	74	83	5	0	0
1	2E	65	476	314	74	83	5	0	0
1	2F	65	476	314	74	83	5	0	0
1	2G	65	476	314	74	83	5	0	0
1	2H	65	476	314	74	83	5	0	0
1	2I	65	476	314	74	83	5	0	0
1	2J	65	476	314	74	83	5	0	0
1	2K	65	476	314	74	83	5	0	0
1	2L	65	476	314	74	83	5	0	0
1	2M	65	476	314	74	83	5	0	0
1	2N	65	476	314	74	83	5	0	0
1	2O	65	476	314	74	83	5	0	0
1	3A	65	476	314	74	83	5	0	0
1	3B	65	476	314	74	83	5	0	0
1	3C	65	476	314	74	83	5	0	0
1	3D	65	476	314	74	83	5	0	0
1	3E	65	476	314	74	83	5	0	0
1	3F	65	476	314	74	83	5	0	0
1	3G	65	476	314	74	83	5	0	0
1	3H	65	476	314	74	83	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3I	65	476	314	74	83	5	0	0
1	3J	65	476	314	74	83	5	0	0
1	3K	65	476	314	74	83	5	0	0
1	3L	65	476	314	74	83	5	0	0
1	3M	65	476	314	74	83	5	0	0
1	3N	65	476	314	74	83	5	0	0
1	3O	65	476	314	74	83	5	0	0
1	4A	65	476	314	74	83	5	0	0
1	4B	65	476	314	74	83	5	0	0
1	4C	65	476	314	74	83	5	0	0
1	4D	65	476	314	74	83	5	0	0
1	4E	65	476	314	74	83	5	0	0
1	4F	65	476	314	74	83	5	0	0
1	4G	65	476	314	74	83	5	0	0
1	4H	65	476	314	74	83	5	0	0
1	4I	65	476	314	74	83	5	0	0
1	4J	65	476	314	74	83	5	0	0
1	4K	65	476	314	74	83	5	0	0
1	4L	65	476	314	74	83	5	0	0
1	4M	65	476	314	74	83	5	0	0
1	4N	65	476	314	74	83	5	0	0

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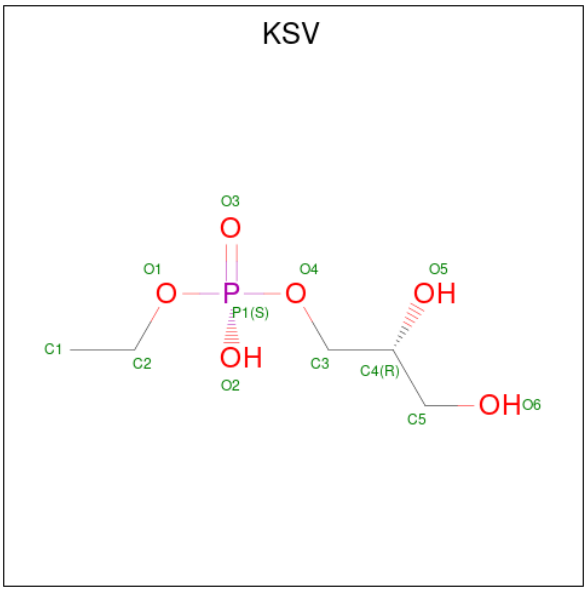
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4O	65	476	314	74	83	5	0	0
1	5A	65	476	314	74	83	5	0	0
1	5B	65	476	314	74	83	5	0	0
1	5C	65	476	314	74	83	5	0	0
1	5D	65	476	314	74	83	5	0	0
1	5E	65	476	314	74	83	5	0	0
1	5F	65	476	314	74	83	5	0	0
1	5G	65	476	314	74	83	5	0	0
1	5H	65	476	314	74	83	5	0	0
1	5I	65	476	314	74	83	5	0	0
1	5J	65	476	314	74	83	5	0	0
1	5K	65	476	314	74	83	5	0	0
1	5L	65	476	314	74	83	5	0	0
1	5M	65	476	314	74	83	5	0	0
1	5N	65	476	314	74	83	5	0	0
1	5O	65	476	314	74	83	5	0	0

- Molecule 2 is a protein called Maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	393	2684	1736	467	470	11	0	61

- Molecule 3 is (2R)-2,3-dihydroxypropyl ethyl hydrogen (S)-phosphate (three-letter code: KSV) (formula: $C_5H_{13}O_6P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	1A	1	12	5	6	1	0
3	1B	1	12	5	6	1	0
3	1B	1	12	5	6	1	0
3	1C	1	12	5	6	1	0
3	1D	1	12	5	6	1	0
3	1F	1	12	5	6	1	0
3	1F	1	12	5	6	1	0
3	1G	1	12	5	6	1	0
3	1H	1	12	5	6	1	0
3	1I	1	12	5	6	1	0
3	1J	1	12	5	6	1	0
3	1J	1	12	5	6	1	0
3	1K	1	12	5	6	1	0
3	1K	1	12	5	6	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	1L	1	12	5	6	1	0
3	1M	1	12	5	6	1	0
3	1N	1	12	5	6	1	0
3	2B	1	12	5	6	1	0
3	2C	1	12	5	6	1	0
3	2D	1	12	5	6	1	0
3	2E	1	12	5	6	1	0
3	2E	1	12	5	6	1	0
3	2F	1	12	5	6	1	0
3	2G	1	12	5	6	1	0
3	2H	1	12	5	6	1	0
3	2I	1	12	5	6	1	0
3	2J	1	12	5	6	1	0
3	2L	1	12	5	6	1	0
3	2M	1	12	5	6	1	0
3	2N	1	12	5	6	1	0
3	3A	1	12	5	6	1	0
3	3A	1	12	5	6	1	0
3	3B	1	12	5	6	1	0
3	3C	1	12	5	6	1	0
3	3D	1	12	5	6	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	3E	1	12	5	6	1	0
3	3G	1	12	5	6	1	0
3	3H	1	12	5	6	1	0
3	3I	1	12	5	6	1	0
3	3J	1	12	5	6	1	0
3	3K	1	12	5	6	1	0
3	3K	1	12	5	6	1	0
3	3L	1	12	5	6	1	0
3	3M	1	12	5	6	1	0
3	3N	1	12	5	6	1	0
3	4A	1	12	5	6	1	0
3	4B	1	12	5	6	1	0
3	4C	1	12	5	6	1	0
3	4D	1	12	5	6	1	0
3	4E	1	12	5	6	1	0
3	4F	1	12	5	6	1	0
3	4F	1	12	5	6	1	0
3	4G	1	12	5	6	1	0
3	4H	1	12	5	6	1	0
3	4L	1	12	5	6	1	0
3	4M	1	12	5	6	1	0

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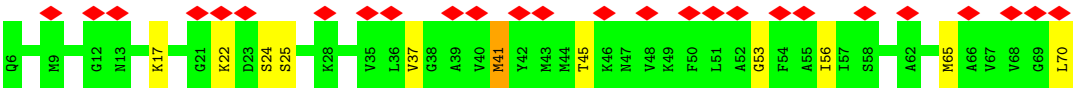
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	4N	1	12	5	6	1	0
3	5A	1	12	5	6	1	0
3	5C	1	12	5	6	1	0
3	5D	1	12	5	6	1	0
3	5E	1	12	5	6	1	0
3	5G	1	12	5	6	1	0
3	5H	1	12	5	6	1	0
3	5I	1	12	5	6	1	0
3	5I	1	12	5	6	1	0
3	5J	1	12	5	6	1	0
3	5K	1	12	5	6	1	0
3	5L	1	12	5	6	1	0
3	5M	1	12	5	6	1	0
3	5N	1	12	5	6	1	0

3 Residue-property plots (i)

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

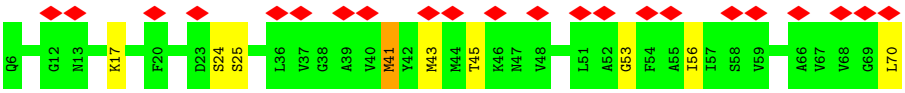
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1A:



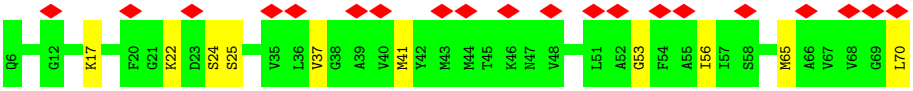
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1B:



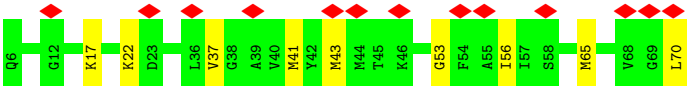
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1C:



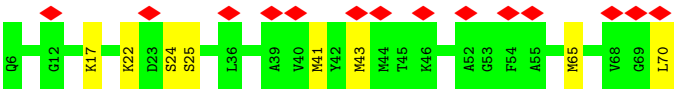
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1D:



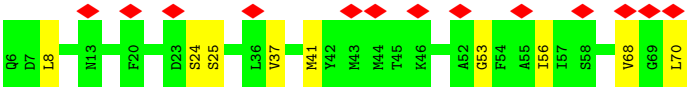
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1E:



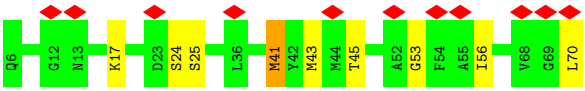
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1F:



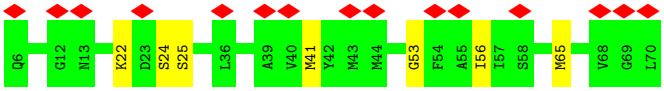
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1G:



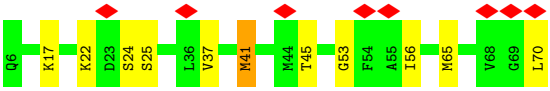
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1H:



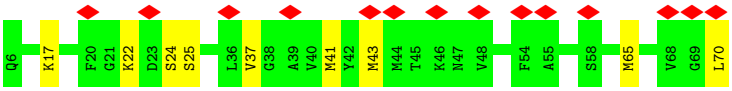
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1I:



• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1J:

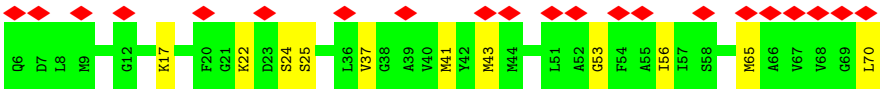


• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1K:

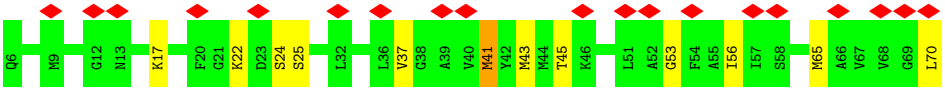
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1L:



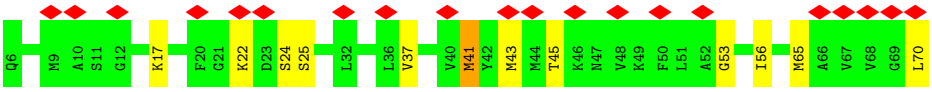
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1M:



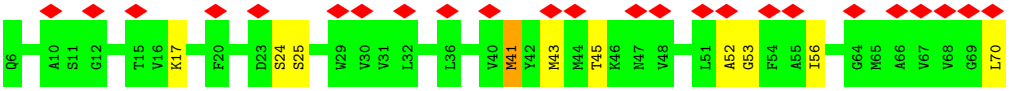
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1N:



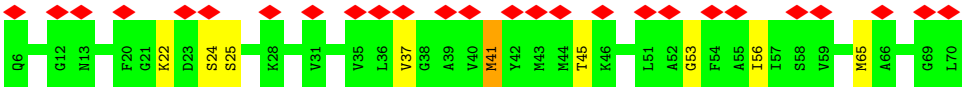
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 1O:



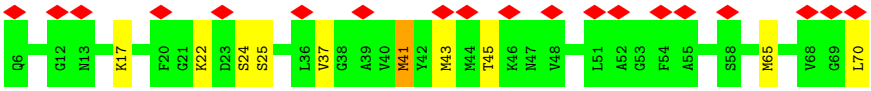
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2A:



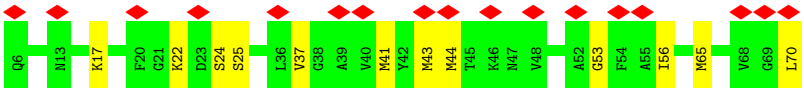
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2B:



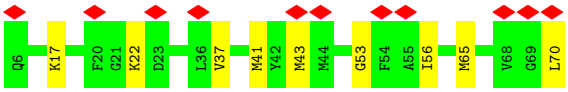
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2C:



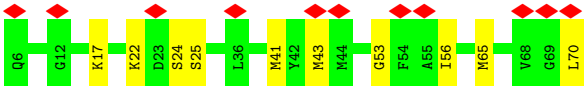
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2D:



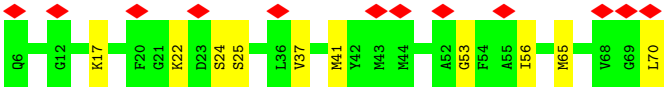
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2E:



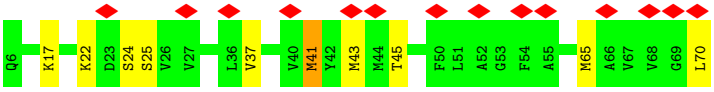
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2F:



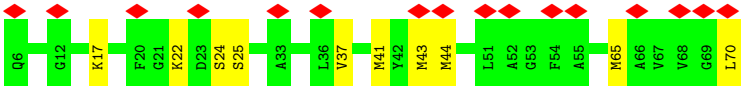
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2G:



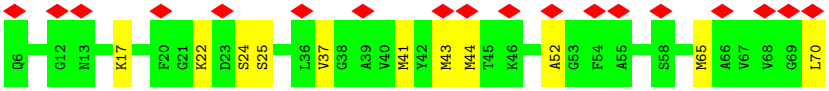
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2H:



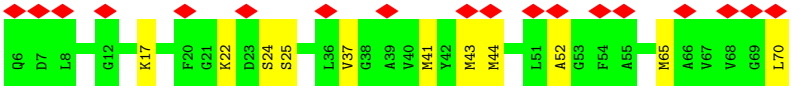
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2I:



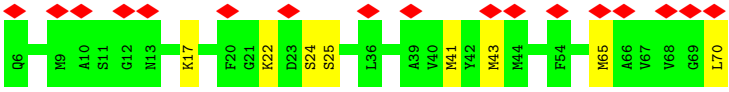
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2J:



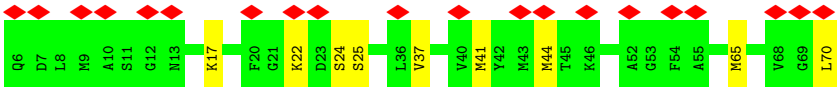
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2K:



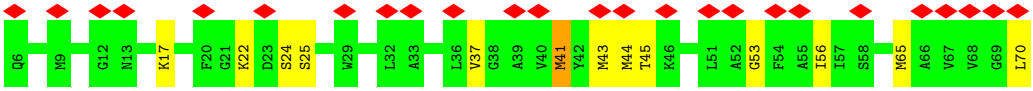
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2L:



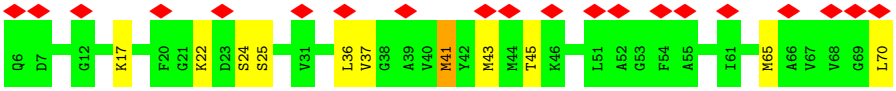
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2M:



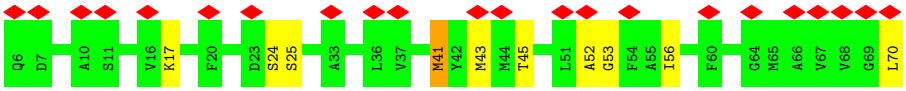
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2N:



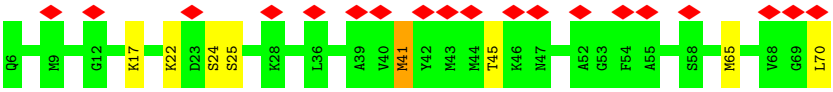
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 2O:



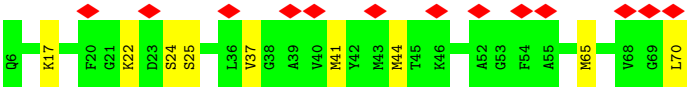
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3A:



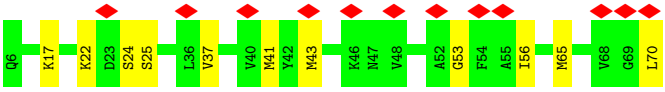
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3B:



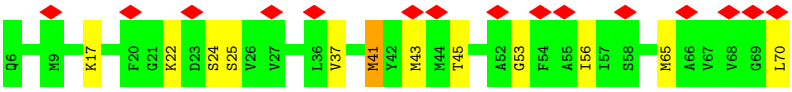
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3C:



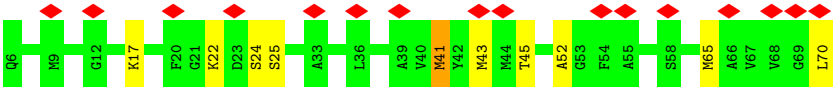
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3D:



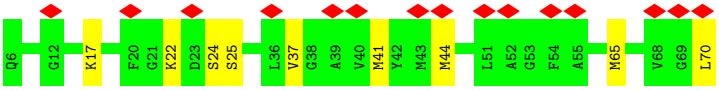
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3E:



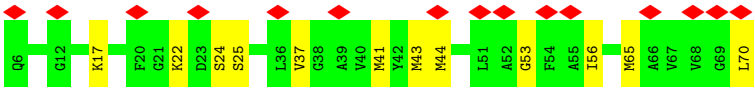
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3F:



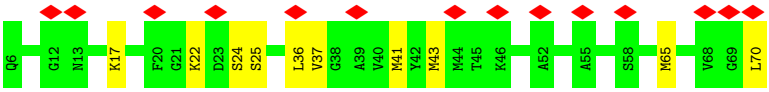
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3G:



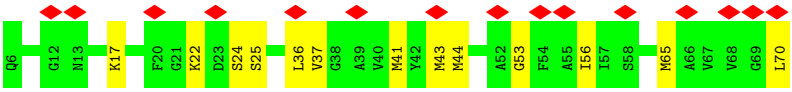
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3H:



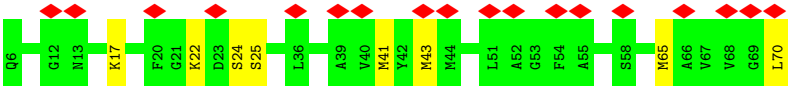
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3I:



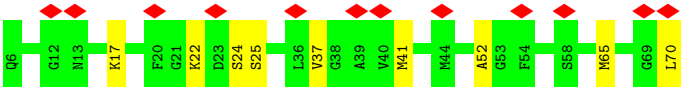
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3J:



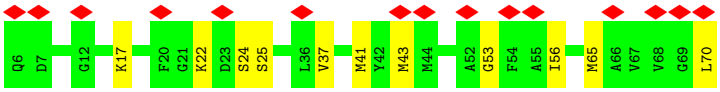
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3K:



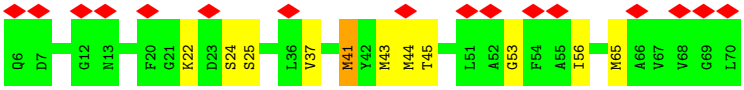
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3L:



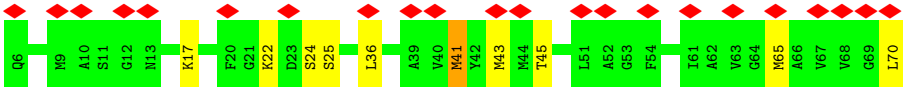
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3M:



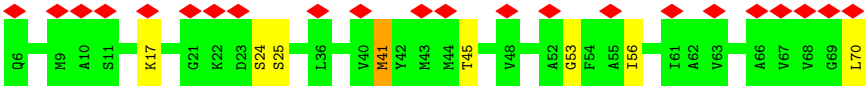
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3N:



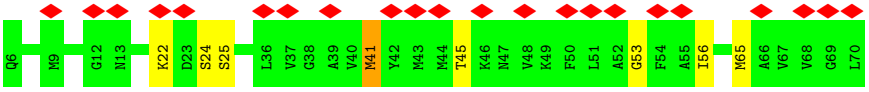
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 3O:



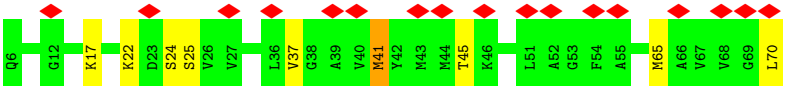
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4A:



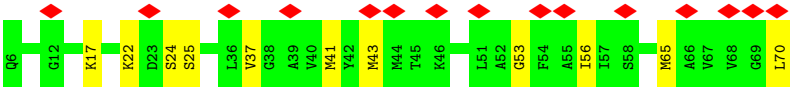
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4B:



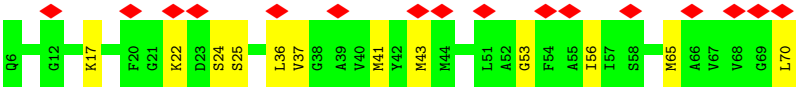
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4C:



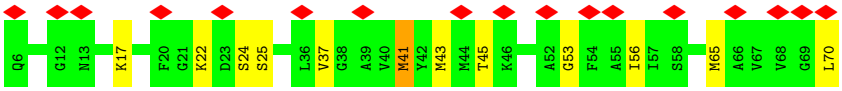
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4D:



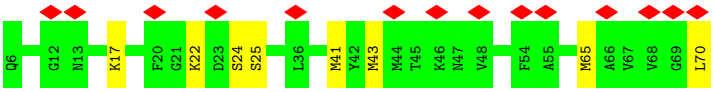
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4E:



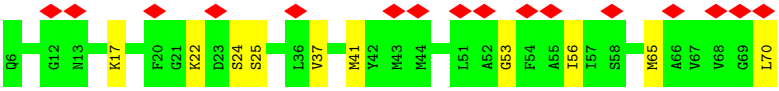
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4F:



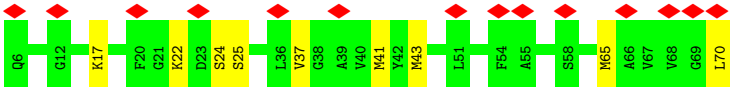
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4G:



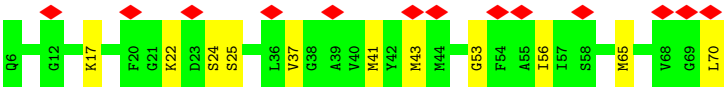
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4H:



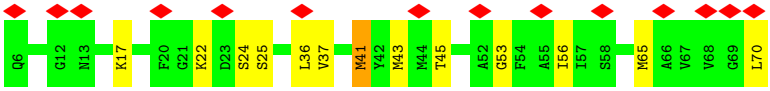
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4I:



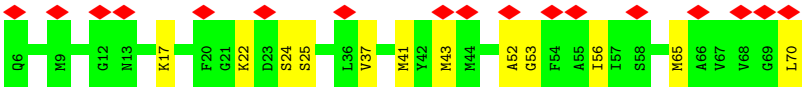
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4J:



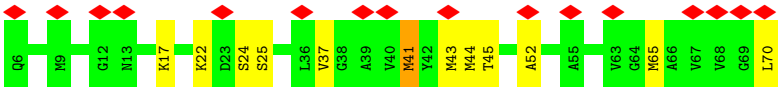
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4K:



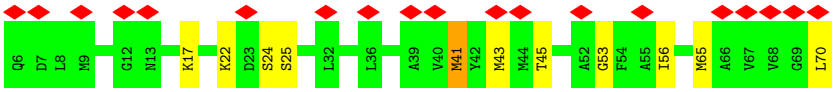
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4L:



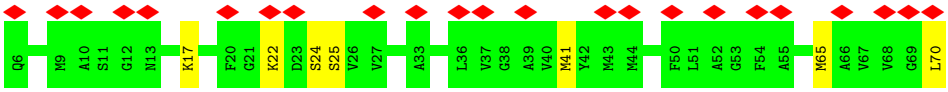
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4M:



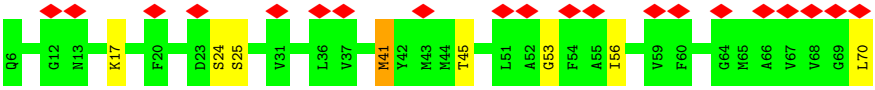
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4N:



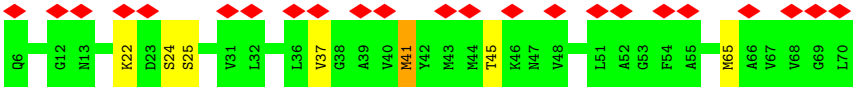
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 4O:



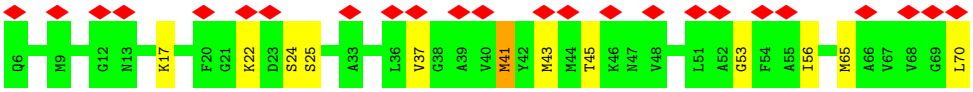
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5A:



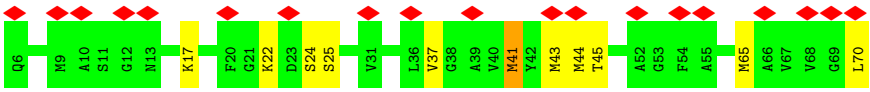
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5B:



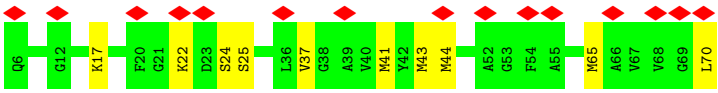
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5C:



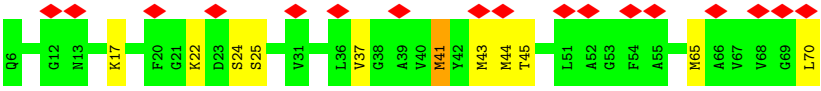
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5D:



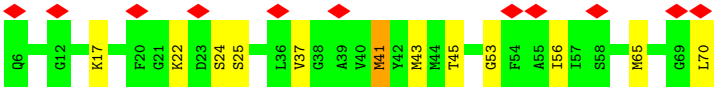
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5E:



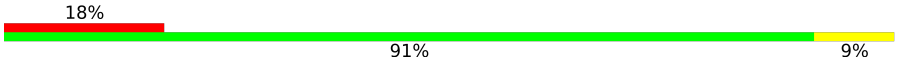
• Molecule 1: Type IV conjugative transfer system pilin TraA

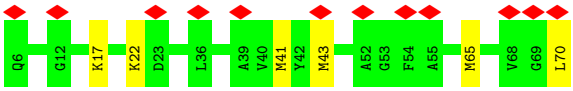
Chain 5F:



• Molecule 1: Type IV conjugative transfer system pilin TraA

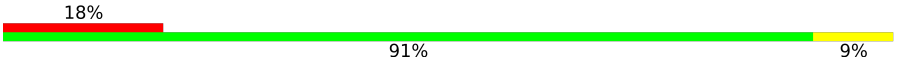
Chain 5G:

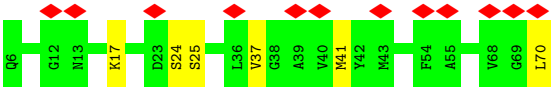




• Molecule 1: Type IV conjugative transfer system pilin TraA

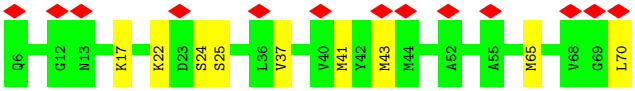
Chain 5H:





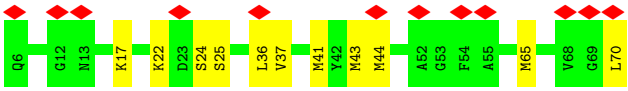
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5I:



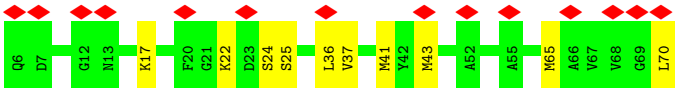
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5J:



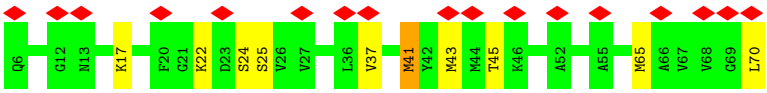
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5K:



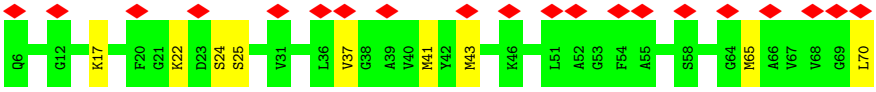
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5L:



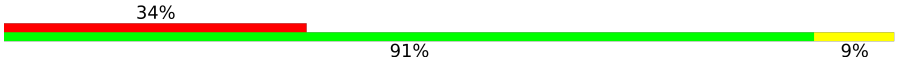
• Molecule 1: Type IV conjugative transfer system pilin TraA

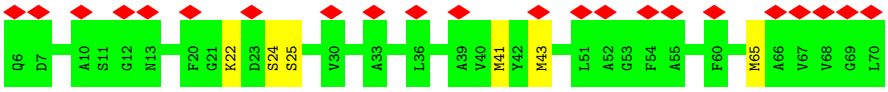
Chain 5M:



• Molecule 1: Type IV conjugative transfer system pilin TraA

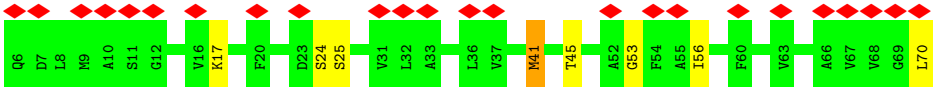
Chain 5N:





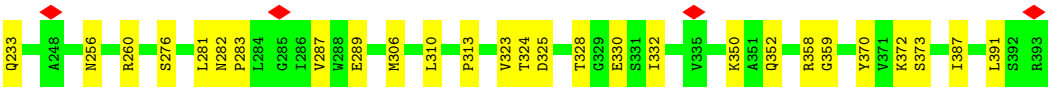
• Molecule 1: Type IV conjugative transfer system pilin TraA

Chain 5O:



• Molecule 2: Maturation protein

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	168989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.313	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	531.36, 531.36, 531.36	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.46, 2.46, 2.46	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KSV

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	1A	0.25	0/482	0.40	0/651
1	1B	0.24	0/482	0.41	0/651
1	1C	0.25	0/482	0.41	0/651
1	1D	0.25	0/482	0.42	0/651
1	1E	0.25	0/482	0.41	0/651
1	1F	0.25	0/482	0.42	0/651
1	1G	0.25	0/482	0.41	0/651
1	1H	0.25	0/482	0.41	0/651
1	1I	0.25	0/482	0.41	0/651
1	1J	0.25	0/482	0.41	0/651
1	1K	0.25	0/482	0.41	0/651
1	1L	0.25	0/482	0.41	0/651
1	1M	0.25	0/482	0.40	0/651
1	1N	0.25	0/482	0.41	0/651
1	1O	0.25	0/482	0.41	0/651
1	2A	0.25	0/482	0.40	0/651
1	2B	0.25	0/482	0.41	0/651
1	2C	0.25	0/482	0.41	0/651
1	2D	0.25	0/482	0.42	0/651
1	2E	0.25	0/482	0.42	0/651
1	2F	0.25	0/482	0.42	0/651
1	2G	0.25	0/482	0.41	0/651
1	2H	0.25	0/482	0.42	0/651
1	2I	0.25	0/482	0.41	0/651
1	2J	0.24	0/482	0.40	0/651
1	2K	0.24	0/482	0.40	0/651
1	2L	0.25	0/482	0.42	0/651
1	2M	0.25	0/482	0.40	0/651
1	2N	0.25	0/482	0.41	0/651
1	2O	0.25	0/482	0.40	0/651
1	3A	0.25	0/482	0.41	0/651
1	3B	0.25	0/482	0.41	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	3C	0.25	0/482	0.41	0/651
1	3D	0.25	0/482	0.41	0/651
1	3E	0.25	0/482	0.42	0/651
1	3F	0.24	0/482	0.41	0/651
1	3G	0.24	0/482	0.41	0/651
1	3H	0.25	0/482	0.41	0/651
1	3I	0.25	0/482	0.41	0/651
1	3J	0.25	0/482	0.40	0/651
1	3K	0.25	0/482	0.42	0/651
1	3L	0.25	0/482	0.41	0/651
1	3M	0.24	0/482	0.40	0/651
1	3N	0.25	0/482	0.42	0/651
1	3O	0.25	0/482	0.41	0/651
1	4A	0.25	0/482	0.41	0/651
1	4B	0.24	0/482	0.41	0/651
1	4C	0.24	0/482	0.40	0/651
1	4D	0.25	0/482	0.41	0/651
1	4E	0.24	0/482	0.40	0/651
1	4F	0.24	0/482	0.40	0/651
1	4G	0.24	0/482	0.40	0/651
1	4H	0.24	0/482	0.41	0/651
1	4I	0.25	0/482	0.41	0/651
1	4J	0.24	0/482	0.41	0/651
1	4K	0.25	0/482	0.39	0/651
1	4L	0.25	0/482	0.41	0/651
1	4M	0.25	0/482	0.41	0/651
1	4N	0.24	0/482	0.41	0/651
1	4O	0.24	0/482	0.41	0/651
1	5A	0.24	0/482	0.40	0/651
1	5B	0.24	0/482	0.40	0/651
1	5C	0.25	0/482	0.41	0/651
1	5D	0.24	0/482	0.40	0/651
1	5E	0.24	0/482	0.40	0/651
1	5F	0.25	0/482	0.42	0/651
1	5G	0.25	0/482	0.40	0/651
1	5H	0.24	0/482	0.41	0/651
1	5I	0.25	0/482	0.41	0/651
1	5J	0.25	0/482	0.41	0/651
1	5K	0.24	0/482	0.41	0/651
1	5L	0.25	0/482	0.42	0/651
1	5M	0.25	0/482	0.43	0/651
1	5N	0.25	0/482	0.41	0/651
1	5O	0.25	0/482	0.41	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	M	0.23	0/2681	0.39	0/3638
All	All	0.25	0/38831	0.41	0/52463

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	476	0	509	6	0
1	1B	476	0	509	5	0
1	1C	476	0	509	5	0
1	1D	476	0	509	5	0
1	1E	476	0	509	4	0
1	1F	476	0	509	5	0
1	1G	476	0	509	5	0
1	1H	476	0	509	3	0
1	1I	476	0	509	6	0
1	1J	476	0	509	5	0
1	1K	476	0	509	6	0
1	1L	476	0	509	6	0
1	1M	476	0	509	7	0
1	1N	476	0	509	7	0
1	1O	476	0	509	6	0
1	2A	476	0	509	6	0
1	2B	476	0	509	7	0
1	2C	476	0	509	7	0
1	2D	476	0	509	5	0
1	2E	476	0	509	5	0
1	2F	476	0	509	5	0
1	2G	476	0	509	7	0
1	2H	476	0	509	7	0
1	2I	476	0	509	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2J	476	0	509	7	0
1	2K	476	0	509	4	0
1	2L	476	0	509	5	0
1	2M	476	0	509	8	0
1	2N	476	0	509	7	0
1	2O	476	0	509	6	0
1	3A	476	0	509	4	0
1	3B	476	0	509	5	0
1	3C	476	0	509	6	0
1	3D	476	0	509	7	0
1	3E	476	0	509	6	0
1	3F	476	0	509	5	0
1	3G	476	0	509	7	0
1	3H	476	0	509	6	0
1	3I	476	0	509	8	0
1	3J	476	0	509	4	0
1	3K	476	0	509	5	0
1	3L	476	0	509	6	0
1	3M	476	0	509	7	0
1	3N	476	0	509	6	0
1	3O	476	0	509	4	0
1	4A	476	0	509	4	0
1	4B	476	0	509	5	0
1	4C	476	0	509	6	0
1	4D	476	0	509	7	0
1	4E	476	0	509	7	0
1	4F	476	0	509	4	0
1	4G	476	0	509	5	0
1	4H	476	0	509	5	0
1	4I	476	0	509	6	0
1	4J	476	0	509	8	0
1	4K	476	0	509	7	0
1	4L	476	0	509	8	0
1	4M	476	0	509	6	0
1	4N	476	0	509	3	0
1	4O	476	0	509	4	0
1	5A	476	0	509	5	0
1	5B	476	0	509	8	0
1	5C	476	0	509	7	0
1	5D	476	0	509	6	0
1	5E	476	0	509	7	0
1	5F	476	0	509	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5G	476	0	509	3	0
1	5H	476	0	509	3	0
1	5I	476	0	509	5	0
1	5J	476	0	509	7	0
1	5K	476	0	509	6	0
1	5L	476	0	509	6	0
1	5M	476	0	509	6	0
1	5N	476	0	509	4	0
1	5O	476	0	509	4	0
2	M	2684	0	2635	26	0
3	1A	12	0	0	0	0
3	1B	24	0	0	0	0
3	1C	12	0	0	1	0
3	1D	12	0	0	0	0
3	1F	24	0	0	0	0
3	1G	12	0	0	0	0
3	1H	12	0	0	1	0
3	1I	12	0	0	1	0
3	1J	24	0	0	1	0
3	1K	24	0	0	0	0
3	1L	12	0	0	1	0
3	1M	12	0	0	1	0
3	1N	12	0	0	0	0
3	2B	12	0	0	1	0
3	2C	12	0	0	0	0
3	2D	12	0	0	0	0
3	2E	24	0	0	0	0
3	2F	12	0	0	1	0
3	2G	12	0	0	1	0
3	2H	12	0	0	0	0
3	2I	12	0	0	1	0
3	2J	12	0	0	0	0
3	2L	12	0	0	0	0
3	2M	12	0	0	1	0
3	2N	12	0	0	0	0
3	3A	24	0	0	0	0
3	3B	12	0	0	0	0
3	3C	12	0	0	0	0
3	3D	12	0	0	0	0
3	3E	12	0	0	0	0
3	3G	12	0	0	0	0
3	3H	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3I	12	0	0	0	0
3	3J	12	0	0	0	0
3	3K	24	0	0	0	0
3	3L	12	0	0	1	0
3	3M	12	0	0	0	0
3	3N	12	0	0	0	0
3	4A	12	0	0	0	0
3	4B	12	0	0	0	0
3	4C	12	0	0	1	0
3	4D	12	0	0	1	0
3	4E	12	0	0	1	0
3	4F	24	0	0	0	0
3	4G	12	0	0	0	0
3	4H	12	0	0	0	0
3	4L	12	0	0	0	0
3	4M	12	0	0	0	0
3	4N	12	0	0	0	0
3	5A	12	0	0	0	0
3	5C	12	0	0	0	0
3	5D	12	0	0	0	0
3	5E	12	0	0	0	0
3	5G	12	0	0	0	0
3	5H	12	0	0	0	0
3	5I	24	0	0	0	0
3	5J	12	0	0	1	0
3	5K	12	0	0	0	0
3	5L	12	0	0	0	0
3	5M	12	0	0	0	0
3	5N	12	0	0	0	0
All	All	39224	0	40810	388	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 5.

All (388) 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)
1:1F:8:LEU:HD22	2:M:110:ASN:HD22	1.64	0.63
1:1I:37:VAL:HG11	1:1J:43:MET:HG2	1.84	0.60
1:5I:37:VAL:HG11	1:5J:43:MET:HG2	1.85	0.59
1:5A:37:VAL:HG11	1:5B:43:MET:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2B:37:VAL:HG11	1:2C:43:MET:HG2	1.87	0.57
1:1D:37:VAL:HG11	1:1E:43:MET:HA	1.86	0.57
1:2A:37:VAL:HG11	1:2B:43:MET:HG2	1.86	0.57
1:2C:37:VAL:HG11	1:2D:43:MET:HG2	1.87	0.57
1:2I:37:VAL:HG11	1:2J:43:MET:HG2	1.86	0.56
1:2H:37:VAL:HG11	1:2I:43:MET:HG2	1.88	0.55
1:5O:41:MET:SD	1:5O:45:THR:OG1	2.64	0.55
1:1J:37:VAL:HG11	1:1K:43:MET:HG2	1.88	0.55
2:M:102:TYR:OH	2:M:109:GLN:NE2	2.39	0.55
1:3B:37:VAL:HG11	1:3C:43:MET:HG2	1.88	0.55
1:3F:37:VAL:HG11	1:3G:43:MET:HG2	1.89	0.55
1:2J:37:VAL:HG11	1:2K:43:MET:HG2	1.88	0.55
1:4B:41:MET:SD	1:4B:45:THR:OG1	2.65	0.55
1:3D:37:VAL:HG11	1:3E:43:MET:HA	1.89	0.54
1:4H:37:VAL:HG11	1:4I:43:MET:HG2	1.90	0.54
2:M:330:GLU:HG2	2:M:352:GLN:HG2	1.88	0.54
1:1F:53:GLY:HA2	1:1F:56:ILE:HG12	1.88	0.54
1:1C:37:VAL:HG11	1:1D:43:MET:HG2	1.89	0.54
1:1O:41:MET:SD	1:1O:45:THR:OG1	2.66	0.54
1:1A:37:VAL:HG11	1:1B:43:MET:HG2	1.90	0.54
1:1K:37:VAL:HG11	1:1L:43:MET:HG2	1.90	0.54
1:1I:41:MET:SD	1:1I:45:THR:OG1	2.66	0.53
2:M:287:VAL:HG12	2:M:289:GLU:H	1.74	0.53
2:M:324:THR:HG22	2:M:358:ARG:HG2	1.91	0.53
1:5B:37:VAL:HG11	1:5C:43:MET:HG2	1.91	0.53
1:4O:41:MET:SD	1:4O:45:THR:OG1	2.67	0.52
1:3O:41:MET:SD	1:3O:45:THR:OG1	2.68	0.52
3:4D:101:KSV:O5	1:5D:44:MET:SD	2.67	0.52
1:4I:37:VAL:HG11	1:4J:43:MET:HG2	1.93	0.51
3:1I:101:KSV:O5	1:2I:44:MET:SD	2.68	0.51
2:M:387:ILE:HG12	2:M:391:LEU:HD12	1.93	0.51
3:4E:101:KSV:O5	1:5E:44:MET:SD	2.68	0.51
1:3G:37:VAL:HG11	1:3H:43:MET:HG2	1.92	0.51
1:4G:37:VAL:HG11	1:4H:43:MET:HG2	1.93	0.51
1:2D:22:LYS:HE3	1:2D:65:MET:HB3	1.93	0.51
2:M:118:GLN:O	2:M:122:ASN:ND2	2.43	0.51
1:2O:41:MET:SD	1:2O:45:THR:OG1	2.69	0.50
1:2M:37:VAL:HG11	1:2N:43:MET:HG2	1.92	0.50
1:4M:22:LYS:HE3	1:4M:65:MET:HB3	1.94	0.50
3:1M:101:KSV:O5	1:2M:44:MET:SD	2.69	0.50
2:M:211:GLN:NE2	2:M:281:LEU:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:41:MET:SD	1:2A:45:THR:OG1	2.70	0.50
1:2B:22:LYS:HE3	1:2B:65:MET:HB3	1.94	0.50
1:1N:22:LYS:HE3	1:1N:65:MET:HB3	1.94	0.50
1:1L:37:VAL:HG11	1:1M:43:MET:HG2	1.93	0.49
1:5F:37:VAL:HG11	1:5G:43:MET:HG2	1.94	0.49
1:1A:41:MET:SD	1:1A:45:THR:OG1	2.69	0.49
1:4D:37:VAL:HG11	1:4E:43:MET:HG2	1.94	0.49
1:2N:22:LYS:HE3	1:2N:65:MET:HB3	1.95	0.49
1:3F:22:LYS:HE3	1:3F:65:MET:HB3	1.94	0.49
2:M:332:ILE:HG12	2:M:350:LYS:HG2	1.94	0.49
1:4E:37:VAL:HG11	1:4F:43:MET:HG2	1.93	0.49
1:4I:53:GLY:HA2	1:4I:56:ILE:HG12	1.94	0.49
1:4K:37:VAL:HG11	1:4L:43:MET:HG2	1.93	0.49
1:5E:22:LYS:HE3	1:5E:65:MET:HB3	1.95	0.49
1:5G:22:LYS:HE3	1:5G:65:MET:HB3	1.95	0.49
3:3L:101:KSV:O5	1:4L:44:MET:SD	2.71	0.49
1:1M:37:VAL:HG11	1:1N:43:MET:HG2	1.95	0.49
2:M:211:GLN:HE22	2:M:282:ASN:HA	1.77	0.49
1:5J:44:MET:SD	3:5J:101:KSV:O5	2.70	0.49
1:2J:22:LYS:HE3	1:2J:65:MET:HB3	1.95	0.48
1:2L:24:SER:OG	1:2L:25:SER:N	2.46	0.48
1:4L:22:LYS:HE3	1:4L:65:MET:HB3	1.94	0.48
1:2I:22:LYS:HE3	1:2I:65:MET:HB3	1.94	0.48
2:M:135:GLY:HA3	2:M:372:LYS:HE3	1.96	0.48
1:1E:22:LYS:HE3	1:1E:65:MET:HB3	1.96	0.48
1:3E:41:MET:SD	1:3E:45:THR:OG1	2.66	0.48
1:2F:37:VAL:HG11	1:2G:43:MET:HG2	1.95	0.48
1:2K:22:LYS:HE3	1:2K:65:MET:HB3	1.94	0.48
1:3C:37:VAL:HG11	1:3D:43:MET:HG2	1.95	0.48
1:5A:22:LYS:HE3	1:5A:65:MET:HB3	1.96	0.48
2:M:214:TYR:HE1	2:M:306:MET:HG3	1.78	0.48
2:M:313:PRO:HB2	2:M:370:TYR:HB3	1.95	0.48
1:4H:22:LYS:HE3	1:4H:65:MET:HB3	1.95	0.48
1:5F:24:SER:OG	1:5F:25:SER:N	2.46	0.48
1:4N:22:LYS:HE3	1:4N:65:MET:HB3	1.96	0.48
2:M:11:ASN:ND2	2:M:37:SER:OG	2.47	0.48
3:1L:101:KSV:O5	1:2L:44:MET:SD	2.72	0.48
1:3E:22:LYS:HE3	1:3E:65:MET:HB3	1.96	0.48
1:4L:52:ALA:HB2	1:5K:36:LEU:HD21	1.95	0.48
1:5D:37:VAL:HG11	1:5E:43:MET:HG2	1.96	0.48
1:2H:22:LYS:HE3	1:2H:65:MET:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3G:17:LYS:HG3	1:3G:70:LEU:HD21	1.96	0.48
1:4B:22:LYS:HE3	1:4B:65:MET:HB3	1.95	0.48
1:1I:53:GLY:HA2	1:1I:56:ILE:HG12	1.96	0.48
1:4I:22:LYS:HE3	1:4I:65:MET:HB3	1.96	0.48
1:4L:37:VAL:HG11	1:4M:43:MET:HG2	1.96	0.48
2:M:310:LEU:O	2:M:373:SER:OG	2.28	0.48
1:2F:22:LYS:HE3	1:2F:65:MET:HB3	1.96	0.47
1:5A:37:VAL:HG21	1:5B:43:MET:HA	1.96	0.47
2:M:131:LYS:HB3	2:M:136:ASN:HB3	1.96	0.47
1:4D:24:SER:OG	1:4D:25:SER:N	2.47	0.47
1:4F:22:LYS:HE3	1:4F:65:MET:HB3	1.95	0.47
1:5B:41:MET:SD	1:5B:45:THR:OG1	2.68	0.47
2:M:218:THR:HB	2:M:276:SER:HA	1.96	0.47
1:2A:22:LYS:HE3	1:2A:65:MET:HB3	1.96	0.47
1:4J:37:VAL:HG11	1:4K:43:MET:HG2	1.96	0.47
3:2M:101:KSV:O5	1:3M:44:MET:SD	2.73	0.47
1:3L:22:LYS:HE3	1:3L:65:MET:HB3	1.96	0.47
1:3N:24:SER:OG	1:3N:25:SER:N	2.47	0.47
1:4E:17:LYS:HG3	1:4E:70:LEU:HD21	1.96	0.47
1:5D:17:LYS:HG3	1:5D:70:LEU:HD21	1.96	0.47
1:5N:22:LYS:HE3	1:5N:65:MET:HB3	1.95	0.47
1:3H:17:LYS:HG3	1:3H:70:LEU:HD21	1.96	0.47
1:3K:37:VAL:HG11	1:3L:43:MET:HG2	1.96	0.47
1:4K:52:ALA:HB2	1:5J:36:LEU:HD21	1.96	0.47
1:1G:24:SER:OG	1:1G:25:SER:N	2.47	0.47
1:1G:53:GLY:HA2	1:1G:56:ILE:HG12	1.97	0.47
1:2I:24:SER:OG	1:2I:25:SER:N	2.47	0.47
1:4C:24:SER:OG	1:4C:25:SER:N	2.47	0.47
1:4G:24:SER:OG	1:4G:25:SER:N	2.48	0.47
1:5F:53:GLY:HA2	1:5F:56:ILE:HG12	1.97	0.47
1:1H:24:SER:OG	1:1H:25:SER:N	2.48	0.47
1:2C:22:LYS:HE3	1:2C:65:MET:HB3	1.97	0.47
1:5N:24:SER:OG	1:5N:25:SER:N	2.48	0.47
2:M:106:PRO:HB2	2:M:115:GLU:HB2	1.95	0.47
1:1B:41:MET:O	1:1B:45:THR:OG1	2.32	0.47
1:4M:24:SER:OG	1:4M:25:SER:N	2.47	0.47
1:4M:41:MET:O	1:4M:45:THR:OG1	2.31	0.47
1:2H:24:SER:OG	1:2H:25:SER:N	2.47	0.47
1:2J:17:LYS:HG3	1:2J:70:LEU:HD21	1.97	0.47
1:2L:37:VAL:HG11	1:2M:43:MET:HG2	1.97	0.47
1:4A:41:MET:SD	1:4A:45:THR:OG1	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2C:24:SER:OG	1:2C:25:SER:N	2.48	0.46
1:3I:24:SER:OG	1:3I:25:SER:N	2.47	0.46
1:3O:24:SER:OG	1:3O:25:SER:N	2.47	0.46
1:4C:17:LYS:HG3	1:4C:70:LEU:HD21	1.97	0.46
1:5M:37:VAL:HG11	1:5N:43:MET:HG2	1.97	0.46
1:1A:22:LYS:HE3	1:1A:65:MET:HB3	1.96	0.46
1:1H:53:GLY:HA2	1:1H:56:ILE:HG12	1.98	0.46
1:2F:17:LYS:HG3	1:2F:70:LEU:HD21	1.98	0.46
1:3B:22:LYS:HE3	1:3B:65:MET:HB3	1.97	0.46
1:3L:37:VAL:HG11	1:3M:43:MET:HG2	1.97	0.46
1:4D:17:LYS:HG3	1:4D:70:LEU:HD21	1.97	0.46
1:2O:24:SER:OG	1:2O:25:SER:N	2.47	0.46
1:3K:24:SER:OG	1:3K:25:SER:N	2.48	0.46
1:4K:22:LYS:HE3	1:4K:65:MET:HB3	1.97	0.46
1:5F:17:LYS:HG3	1:5F:70:LEU:HD21	1.97	0.46
1:1C:17:LYS:HG3	1:1C:70:LEU:HD21	1.96	0.46
3:1J:101:KSV:O5	1:2J:44:MET:SD	2.74	0.46
1:1O:53:GLY:HA2	1:1O:56:ILE:HG12	1.98	0.46
1:2E:22:LYS:HE3	1:2E:65:MET:HB3	1.97	0.46
1:3J:24:SER:OG	1:3J:25:SER:N	2.46	0.46
1:3M:24:SER:OG	1:3M:25:SER:N	2.48	0.46
1:5A:24:SER:OG	1:5A:25:SER:N	2.49	0.46
1:1M:22:LYS:HE3	1:1M:65:MET:HB3	1.98	0.46
1:2A:37:VAL:HG21	1:2B:43:MET:HA	1.98	0.46
1:3D:24:SER:OG	1:3D:25:SER:N	2.47	0.46
1:4F:24:SER:OG	1:4F:25:SER:N	2.47	0.46
1:4J:17:LYS:HG3	1:4J:70:LEU:HD21	1.97	0.46
1:5D:22:LYS:HE3	1:5D:65:MET:HB3	1.98	0.46
2:M:233:GLN:HB2	2:M:260:ARG:HE	1.81	0.46
1:1K:22:LYS:HE3	1:1K:65:MET:HB3	1.96	0.46
1:2H:17:LYS:HG3	1:2H:70:LEU:HD21	1.98	0.46
1:2K:17:LYS:HG3	1:2K:70:LEU:HD21	1.98	0.46
1:4A:22:LYS:HE3	1:4A:65:MET:HB3	1.98	0.46
1:5C:17:LYS:HG3	1:5C:70:LEU:HD21	1.97	0.46
1:5E:24:SER:OG	1:5E:25:SER:N	2.47	0.46
1:3C:53:GLY:HA2	1:3C:56:ILE:HG12	1.97	0.46
3:4C:101:KSV:O5	1:5C:44:MET:SD	2.74	0.46
1:5M:22:LYS:HE3	1:5M:65:MET:HB3	1.97	0.46
1:5M:24:SER:OG	1:5M:25:SER:N	2.48	0.46
1:2B:24:SER:OG	1:2B:25:SER:N	2.48	0.46
3:2I:101:KSV:O5	1:3I:44:MET:SD	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3C:17:LYS:HG3	1:3C:70:LEU:HD21	1.97	0.46
1:3E:24:SER:OG	1:3E:25:SER:N	2.48	0.46
1:3L:24:SER:OG	1:3L:25:SER:N	2.47	0.46
1:4O:24:SER:OG	1:4O:25:SER:N	2.47	0.46
1:5I:22:LYS:HE3	1:5I:65:MET:HB3	1.97	0.46
1:5L:17:LYS:HG3	1:5L:70:LEU:HD21	1.98	0.46
1:1L:22:LYS:HE3	1:1L:65:MET:HB3	1.98	0.46
1:3L:17:LYS:HG3	1:3L:70:LEU:HD21	1.98	0.46
1:4H:24:SER:OG	1:4H:25:SER:N	2.47	0.46
3:1H:101:KSV:O5	1:2H:44:MET:SD	2.74	0.46
1:3C:22:LYS:HE3	1:3C:65:MET:HB3	1.98	0.46
1:3N:41:MET:O	1:3N:45:THR:OG1	2.32	0.46
1:5H:37:VAL:HG11	1:5I:43:MET:HG2	1.98	0.46
1:2G:17:LYS:HG3	1:2G:70:LEU:HD21	1.98	0.45
1:5K:17:LYS:HG3	1:5K:70:LEU:HD21	1.97	0.45
1:5K:24:SER:OG	1:5K:25:SER:N	2.48	0.45
1:3H:22:LYS:HE3	1:3H:65:MET:HB3	1.98	0.45
1:3K:22:LYS:HE3	1:3K:65:MET:HB3	1.99	0.45
1:4A:24:SER:OG	1:4A:25:SER:N	2.48	0.45
1:4E:53:GLY:HA2	1:4E:56:ILE:HG12	1.99	0.45
1:1E:24:SER:OG	1:1E:25:SER:N	2.48	0.45
1:2K:24:SER:OG	1:2K:25:SER:N	2.47	0.45
1:3I:22:LYS:HE3	1:3I:65:MET:HB3	1.98	0.45
1:4J:53:GLY:HA2	1:4J:56:ILE:HG12	1.98	0.45
1:5C:24:SER:OG	1:5C:25:SER:N	2.47	0.45
1:5E:17:LYS:HG3	1:5E:70:LEU:HD21	1.98	0.45
1:5E:37:VAL:HG11	1:5F:43:MET:HG2	1.99	0.45
1:5J:17:LYS:HG3	1:5J:70:LEU:HD21	1.98	0.45
3:2B:101:KSV:O5	1:3B:44:MET:SD	2.74	0.45
1:2M:24:SER:OG	1:2M:25:SER:N	2.48	0.45
1:3A:22:LYS:HE3	1:3A:65:MET:HB3	1.98	0.45
1:3C:24:SER:OG	1:3C:25:SER:N	2.46	0.45
1:3H:37:VAL:HG11	1:3I:43:MET:HG2	1.99	0.45
1:3J:22:LYS:HE3	1:3J:65:MET:HB3	1.97	0.45
1:4F:17:LYS:HG3	1:4F:70:LEU:HD21	1.98	0.45
1:4G:17:LYS:HG3	1:4G:70:LEU:HD21	1.98	0.45
1:4G:53:GLY:HA2	1:4G:56:ILE:HG12	1.98	0.45
1:5C:37:VAL:HG11	1:5D:43:MET:HG2	1.99	0.45
1:5J:22:LYS:HE3	1:5J:65:MET:HB3	1.97	0.45
1:1C:53:GLY:HA2	1:1C:56:ILE:HG12	1.99	0.45
1:1I:17:LYS:HG3	1:1I:70:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1I:24:SER:OG	1:1I:25:SER:N	2.48	0.45
1:1O:24:SER:OG	1:1O:25:SER:N	2.48	0.45
1:2M:41:MET:O	1:2M:45:THR:OG1	2.34	0.45
1:3H:24:SER:OG	1:3H:25:SER:N	2.47	0.45
1:3J:17:LYS:HG3	1:3J:70:LEU:HD21	1.98	0.45
1:5D:24:SER:OG	1:5D:25:SER:N	2.47	0.45
1:5I:17:LYS:HG3	1:5I:70:LEU:HD21	1.98	0.45
1:1G:17:LYS:HG3	1:1G:70:LEU:HD21	1.98	0.45
1:2E:24:SER:OG	1:2E:25:SER:N	2.49	0.45
1:1C:24:SER:OG	1:1C:25:SER:N	2.47	0.45
1:1J:22:LYS:HE3	1:1J:65:MET:HB3	1.99	0.45
1:1L:17:LYS:HG3	1:1L:70:LEU:HD21	1.99	0.45
1:1M:24:SER:OG	1:1M:25:SER:N	2.48	0.45
1:4C:53:GLY:HA2	1:4C:56:ILE:HG12	1.98	0.45
1:4L:24:SER:OG	1:4L:25:SER:N	2.47	0.45
1:5G:17:LYS:HG3	1:5G:70:LEU:HD21	1.98	0.45
1:5L:22:LYS:HE3	1:5L:65:MET:HB3	1.99	0.45
1:1I:22:LYS:HE3	1:1I:65:MET:HB3	1.98	0.45
1:1J:24:SER:OG	1:1J:25:SER:N	2.47	0.45
1:1M:17:LYS:HG3	1:1M:70:LEU:HD21	1.98	0.45
1:2C:53:GLY:HA2	1:2C:56:ILE:HG12	1.98	0.45
1:2J:24:SER:OG	1:2J:25:SER:N	2.49	0.45
1:5B:22:LYS:HE3	1:5B:65:MET:HB3	1.97	0.45
1:5B:24:SER:OG	1:5B:25:SER:N	2.49	0.45
1:1B:53:GLY:HA2	1:1B:56:ILE:HG12	2.00	0.45
1:2N:24:SER:OG	1:2N:25:SER:N	2.47	0.45
1:3E:17:LYS:HG3	1:3E:70:LEU:HD21	1.99	0.45
1:3I:17:LYS:HG3	1:3I:70:LEU:HD21	1.97	0.45
1:3N:22:LYS:HE3	1:3N:65:MET:HB3	1.99	0.45
1:3O:53:GLY:HA2	1:3O:56:ILE:HG12	1.98	0.45
1:4N:24:SER:OG	1:4N:25:SER:N	2.47	0.45
2:M:218:THR:HA	2:M:222:LEU:HD12	1.98	0.45
1:1L:53:GLY:HA2	1:1L:56:ILE:HG12	2.00	0.44
1:1N:37:VAL:HG11	1:1O:43:MET:HG2	1.98	0.44
1:3B:24:SER:OG	1:3B:25:SER:N	2.49	0.44
1:4E:24:SER:OG	1:4E:25:SER:N	2.48	0.44
1:5E:41:MET:O	1:5E:45:THR:OG1	2.33	0.44
1:5K:22:LYS:HE3	1:5K:65:MET:HB3	1.98	0.44
1:2G:37:VAL:HG21	1:2H:43:MET:HA	2.00	0.44
1:2O:53:GLY:HA2	1:2O:56:ILE:HG12	1.99	0.44
1:3D:17:LYS:HG3	1:3D:70:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5C:22:LYS:HE3	1:5C:65:MET:HB3	1.98	0.44
1:5M:17:LYS:HG3	1:5M:70:LEU:HD21	1.98	0.44
1:4B:17:LYS:HG3	1:4B:70:LEU:HD21	1.99	0.44
1:4I:24:SER:OG	1:4I:25:SER:N	2.47	0.44
1:4J:24:SER:OG	1:4J:25:SER:N	2.49	0.44
1:5J:24:SER:OG	1:5J:25:SER:N	2.48	0.44
1:2G:22:LYS:HE3	1:2G:65:MET:HB3	1.99	0.44
1:2M:17:LYS:HG3	1:2M:70:LEU:HD21	1.98	0.44
1:4C:22:LYS:HE3	1:4C:65:MET:HB3	1.99	0.44
1:1H:22:LYS:HE3	1:1H:65:MET:HB3	2.00	0.44
1:2L:22:LYS:HE3	1:2L:65:MET:HB3	1.99	0.44
1:4B:24:SER:OG	1:4B:25:SER:N	2.48	0.44
1:5L:24:SER:OG	1:5L:25:SER:N	2.47	0.44
1:5O:53:GLY:HA2	1:5O:56:ILE:HG12	2.00	0.44
1:1K:53:GLY:HA2	1:1K:56:ILE:HG12	2.00	0.44
1:2E:17:LYS:HG3	1:2E:70:LEU:HD21	1.99	0.44
1:1B:17:LYS:HG3	1:1B:70:LEU:HD21	2.00	0.44
1:2G:24:SER:OG	1:2G:25:SER:N	2.48	0.44
1:3F:17:LYS:HG3	1:3F:70:LEU:HD21	1.99	0.44
1:1L:24:SER:OG	1:1L:25:SER:N	2.47	0.44
1:2F:24:SER:OG	1:2F:25:SER:N	2.47	0.44
1:2F:53:GLY:HA2	1:2F:56:ILE:HG12	1.99	0.44
1:3D:41:MET:O	1:3D:45:THR:OG1	2.31	0.44
1:3G:24:SER:OG	1:3G:25:SER:N	2.48	0.44
1:4C:37:VAL:HG11	1:4D:43:MET:HG2	1.99	0.44
1:4D:22:LYS:HE3	1:4D:65:MET:HB3	2.00	0.44
1:4D:53:GLY:HA2	1:4D:56:ILE:HG12	1.99	0.44
1:4E:22:LYS:HE3	1:4E:65:MET:HB3	1.99	0.44
1:4I:17:LYS:HG3	1:4I:70:LEU:HD21	1.99	0.44
1:2N:17:LYS:HG3	1:2N:70:LEU:HD21	2.00	0.44
1:1G:41:MET:O	1:1G:45:THR:OG1	2.34	0.43
1:2B:17:LYS:HG3	1:2B:70:LEU:HD21	1.99	0.43
1:3E:52:ALA:HB2	1:4D:36:LEU:HD21	1.99	0.43
1:4A:53:GLY:HA2	1:4A:56:ILE:HG12	2.00	0.43
1:1O:52:ALA:HB2	1:2N:36:LEU:HD21	1.99	0.43
1:4H:17:LYS:HG3	1:4H:70:LEU:HD21	2.00	0.43
1:2L:17:LYS:HG3	1:2L:70:LEU:HD21	1.99	0.43
1:2N:41:MET:O	1:2N:45:THR:OG1	2.32	0.43
1:3K:52:ALA:HB2	1:4J:36:LEU:HD21	2.00	0.43
1:4K:24:SER:OG	1:4K:25:SER:N	2.48	0.43
1:5F:41:MET:O	1:5F:45:THR:OG1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3F:24:SER:OG	1:3F:25:SER:N	2.48	0.43
1:4B:37:VAL:HG11	1:4C:43:MET:HG2	2.00	0.43
1:4L:41:MET:O	1:4L:45:THR:OG1	2.33	0.43
1:4M:17:LYS:HG3	1:4M:70:LEU:HD21	2.00	0.43
1:2M:22:LYS:HE3	1:2M:65:MET:HB3	2.00	0.43
1:5J:37:VAL:HG11	1:5K:43:MET:HG2	1.99	0.43
2:M:207:MET:HB3	2:M:283:PRO:HG3	2.00	0.43
1:2A:24:SER:OG	1:2A:25:SER:N	2.49	0.43
1:4G:22:LYS:HE3	1:4G:65:MET:HB3	2.00	0.43
1:5H:24:SER:OG	1:5H:25:SER:N	2.49	0.43
1:5I:24:SER:OG	1:5I:25:SER:N	2.47	0.43
1:1K:17:LYS:HG3	1:1K:70:LEU:HD21	2.01	0.43
1:1M:41:MET:O	1:1M:45:THR:OG1	2.33	0.43
1:3D:22:LYS:HE3	1:3D:65:MET:HB3	1.99	0.43
1:3A:24:SER:OG	1:3A:25:SER:N	2.47	0.43
1:5O:17:LYS:HE2	1:5O:70:LEU:HG	2.01	0.43
1:1N:53:GLY:HA2	1:1N:56:ILE:HG12	2.01	0.43
1:3D:53:GLY:HA2	1:3D:56:ILE:HG12	2.01	0.43
1:5F:22:LYS:HE3	1:5F:65:MET:HB3	2.00	0.43
1:5O:24:SER:OG	1:5O:25:SER:N	2.48	0.43
1:1C:22:LYS:HE3	1:1C:65:MET:HB3	2.01	0.43
1:1N:24:SER:OG	1:1N:25:SER:N	2.47	0.43
1:2I:17:LYS:HG3	1:2I:70:LEU:HD21	2.00	0.43
1:4L:17:LYS:HG3	1:4L:70:LEU:HD21	2.00	0.43
2:M:233:GLN:OE1	2:M:260:ARG:NH1	2.45	0.43
1:1A:24:SER:OG	1:1A:25:SER:N	2.48	0.42
1:2D:53:GLY:HA2	1:2D:56:ILE:HG12	2.00	0.42
1:3G:22:LYS:HE3	1:3G:65:MET:HB3	2.00	0.42
1:3M:22:LYS:HE3	1:3M:65:MET:HB3	2.00	0.42
1:5L:41:MET:SD	1:5L:45:THR:OG1	2.76	0.42
1:1K:24:SER:OG	1:1K:25:SER:N	2.48	0.42
1:1D:53:GLY:HA2	1:1D:56:ILE:HG12	2.00	0.42
1:1B:24:SER:OG	1:1B:25:SER:N	2.48	0.42
1:1D:22:LYS:HE3	1:1D:65:MET:HB3	2.01	0.42
1:5B:17:LYS:HG3	1:5B:70:LEU:HD21	2.00	0.42
1:3A:41:MET:SD	1:3A:45:THR:OG1	2.76	0.42
1:3O:17:LYS:HE2	1:3O:70:LEU:HG	2.02	0.42
1:1F:24:SER:OG	1:1F:25:SER:N	2.49	0.42
1:3K:17:LYS:HG3	1:3K:70:LEU:HD21	2.01	0.42
1:1N:17:LYS:HG3	1:1N:70:LEU:HD21	2.01	0.42
3:2G:101:KSV:O5	1:3G:44:MET:SD	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5K:37:VAL:HG11	1:5L:43:MET:HG2	2.01	0.42
1:5M:37:VAL:HG21	1:5N:43:MET:HA	2.01	0.42
1:4K:17:LYS:HG3	1:4K:70:LEU:HD21	2.02	0.42
1:4M:53:GLY:HA2	1:4M:56:ILE:HG12	2.02	0.42
1:4J:22:LYS:HE3	1:4J:65:MET:HB3	2.00	0.42
1:5A:41:MET:SD	1:5A:45:THR:OG1	2.78	0.42
1:5L:37:VAL:HG11	1:5M:43:MET:HG2	2.01	0.42
1:1J:17:LYS:HG3	1:1J:70:LEU:HD21	2.02	0.41
1:2D:17:LYS:HG3	1:2D:70:LEU:HD21	2.02	0.41
1:2G:41:MET:SD	1:2G:45:THR:OG1	2.77	0.41
1:5C:41:MET:O	1:5C:45:THR:OG1	2.33	0.41
1:3L:53:GLY:HA2	1:3L:56:ILE:HG12	2.01	0.41
1:3M:41:MET:O	1:3M:45:THR:OG1	2.38	0.41
1:3M:53:GLY:HA2	1:3M:56:ILE:HG12	2.01	0.41
1:4O:53:GLY:HA2	1:4O:56:ILE:HG12	2.01	0.41
1:5B:53:GLY:HA2	1:5B:56:ILE:HG12	2.01	0.41
1:1A:17:LYS:HG3	1:1A:70:LEU:HD21	2.02	0.41
1:2D:37:VAL:HG11	1:2E:43:MET:HG2	2.02	0.41
1:3N:17:LYS:HG3	1:3N:70:LEU:HD21	2.02	0.41
1:4O:17:LYS:HE2	1:4O:70:LEU:HG	2.02	0.41
2:M:156:GLN:HE22	2:M:209:ASP:HB3	1.86	0.41
1:1A:53:GLY:HA2	1:1A:56:ILE:HG12	2.03	0.41
1:1D:17:LYS:HG3	1:1D:70:LEU:HD21	2.03	0.41
1:2J:52:ALA:HB2	1:3I:36:LEU:HD21	2.03	0.41
2:M:323:VAL:O	2:M:359:GLY:N	2.43	0.41
1:1F:68:VAL:HG12	1:1F:70:LEU:H	1.85	0.41
3:2F:101:KSV:O5	1:3F:44:MET:SD	2.79	0.41
1:2I:52:ALA:HB2	1:3H:36:LEU:HD21	2.03	0.41
1:2M:53:GLY:HA2	1:2M:56:ILE:HG12	2.02	0.41
1:3A:17:LYS:HG3	1:3A:70:LEU:HD21	2.02	0.41
1:4N:17:LYS:HG3	1:4N:70:LEU:HD21	2.01	0.41
3:1C:101:KSV:O5	1:2C:44:MET:SD	2.79	0.41
1:1F:37:VAL:HG11	1:1G:43:MET:HG2	2.02	0.41
1:1M:53:GLY:HA2	1:1M:56:ILE:HG12	2.01	0.41
1:1N:41:MET:O	1:1N:45:THR:OG1	2.35	0.41
1:1O:17:LYS:HE2	1:1O:70:LEU:HG	2.03	0.41
1:2C:17:LYS:HG3	1:2C:70:LEU:HD21	2.02	0.41
1:2O:17:LYS:HE2	1:2O:70:LEU:HG	2.01	0.41
1:3B:17:LYS:HG3	1:3B:70:LEU:HD21	2.03	0.41
1:4E:41:MET:O	1:4E:45:THR:OG1	2.36	0.41
1:2N:37:VAL:HG11	1:2O:43:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2O:52:ALA:HB2	1:3N:36:LEU:HD21	2.03	0.41
1:4J:41:MET:O	1:4J:45:THR:OG1	2.34	0.41
1:4K:53:GLY:HA2	1:4K:56:ILE:HG12	2.02	0.41
1:5H:17:LYS:HG3	1:5H:70:LEU:HD21	2.02	0.41
1:2E:53:GLY:HA2	1:2E:56:ILE:HG12	2.02	0.40
1:2G:37:VAL:HG11	1:2H:43:MET:HG2	2.03	0.40
1:3G:53:GLY:HA2	1:3G:56:ILE:HG12	2.03	0.40
1:3I:37:VAL:HG11	1:3J:43:MET:HG2	2.04	0.40
1:2A:53:GLY:HA2	1:2A:56:ILE:HG12	2.03	0.40
1:2B:41:MET:O	1:2B:45:THR:OG1	2.33	0.40
1:3M:37:VAL:HG11	1:3N:43:MET:HG2	2.04	0.40
2:M:114:ILE:HD12	2:M:325:ASP:HB3	2.03	0.40
2:M:256:ASN:N	2:M:328:THR:O	2.47	0.40
1:1E:17:LYS:HG3	1:1E:70:LEU:HD21	2.04	0.40
1:3I:53:GLY:HA2	1:3I:56:ILE:HG12	2.02	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	1A	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	1B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1C	63/65 (97%)	54 (86%)	9 (14%)	0	100	100
1	1D	63/65 (97%)	54 (86%)	9 (14%)	0	100	100
1	1E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1F	63/65 (97%)	55 (87%)	8 (13%)	0	100	100
1	1G	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	1H	63/65 (97%)	53 (84%)	10 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1I	63/65 (97%)	54 (86%)	9 (14%)	0	100	100
1	1J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1K	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1L	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	1M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1N	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1O	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2A	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	2B	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2D	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2F	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2G	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	2H	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2I	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	2J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2O	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	3A	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3D	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	3E	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	3F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3G	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	3H	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	3I	63/65 (97%)	50 (79%)	13 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3J	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3M	63/65 (97%)	49 (78%)	14 (22%)	0	100	100
1	3N	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3O	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	4A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4B	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	4C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4G	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	4H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4I	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	4J	63/65 (97%)	49 (78%)	14 (22%)	0	100	100
1	4K	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4M	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	4N	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4O	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5A	63/65 (97%)	49 (78%)	14 (22%)	0	100	100
1	5B	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5D	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	5E	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	5F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5G	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	5H	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	5I	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
1	5J	63/65 (97%)	50 (79%)	13 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5K	63/65 (97%)	49 (78%)	14 (22%)	0	100	100
1	5L	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	5M	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
1	5N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5O	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
2	M	322/393 (82%)	304 (94%)	17 (5%)	1 (0%)	41	76
All	All	5047/5268 (96%)	4167 (83%)	879 (17%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	68	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1B	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1C	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1D	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1E	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1F	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1G	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1H	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1I	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1J	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1K	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1L	51/51 (100%)	50 (98%)	1 (2%)	55	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1M	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1N	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	1O	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2A	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2B	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2C	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2D	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2E	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2F	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2G	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2H	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2I	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2J	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2K	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2L	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2M	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2N	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	2O	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3A	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3B	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3C	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3D	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3E	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3F	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3G	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3H	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3I	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3J	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3K	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3L	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3M	51/51 (100%)	50 (98%)	1 (2%)	55	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3N	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	3O	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4A	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4B	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4C	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4D	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4E	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4F	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4G	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4H	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4I	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4J	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4K	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4L	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4M	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4N	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	4O	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5A	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5B	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5C	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5D	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5E	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5F	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5G	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5H	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5I	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5J	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5K	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5L	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5M	51/51 (100%)	50 (98%)	1 (2%)	55	74
1	5N	51/51 (100%)	50 (98%)	1 (2%)	55	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5O	51/51 (100%)	50 (98%)	1 (2%)	55	74
2	M	281/330 (85%)	281 (100%)	0	100	100
All	All	4106/4155 (99%)	4031 (98%)	75 (2%)	61	77

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	41	MET
1	1B	41	MET
1	1C	41	MET
1	1D	41	MET
1	1E	41	MET
1	1F	41	MET
1	1G	41	MET
1	1H	41	MET
1	1I	41	MET
1	1J	41	MET
1	1K	41	MET
1	1L	41	MET
1	1M	41	MET
1	1N	41	MET
1	1O	41	MET
1	2A	41	MET
1	2B	41	MET
1	2C	41	MET
1	2D	41	MET
1	2E	41	MET
1	2F	41	MET
1	2G	41	MET
1	2H	41	MET
1	2I	41	MET
1	2J	41	MET
1	2K	41	MET
1	2L	41	MET
1	2M	41	MET
1	2N	41	MET
1	2O	41	MET
1	3A	41	MET
1	3B	41	MET
1	3C	41	MET
1	3D	41	MET

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Mol	Chain	Res	Type
1	3E	41	MET
1	3F	41	MET
1	3G	41	MET
1	3H	41	MET
1	3I	41	MET
1	3J	41	MET
1	3K	41	MET
1	3L	41	MET
1	3M	41	MET
1	3N	41	MET
1	3O	41	MET
1	4A	41	MET
1	4B	41	MET
1	4C	41	MET
1	4D	41	MET
1	4E	41	MET
1	4F	41	MET
1	4G	41	MET
1	4H	41	MET
1	4I	41	MET
1	4J	41	MET
1	4K	41	MET
1	4L	41	MET
1	4M	41	MET
1	4N	41	MET
1	4O	41	MET
1	5A	41	MET
1	5B	41	MET
1	5C	41	MET
1	5D	41	MET
1	5E	41	MET
1	5F	41	MET
1	5G	41	MET
1	5H	41	MET
1	5I	41	MET
1	5J	41	MET
1	5K	41	MET
1	5L	41	MET
1	5M	41	MET
1	5N	41	MET
1	5O	41	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	2E	13	ASN
2	M	11	ASN
2	M	109	GLN
2	M	110	ASN
2	M	156	GLN
2	M	211	GLN
2	M	305	ASN
2	M	357	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

70 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	KSV	2L	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	5I	102	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1A	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	1J	102	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	KSV	4C	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5G	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1D	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	4F	102	-	11,11,11	1.42	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	5N	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5J	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	4B	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1H	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	3H	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	4L	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.92	1 (8%)
3	KSV	3K	102	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	3B	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.92	1 (8%)
3	KSV	4D	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5D	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1K	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2I	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5M	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1C	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	3D	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2B	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.92	1 (8%)
3	KSV	3I	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	3M	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	3C	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	4M	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2J	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2N	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	3A	102	-	11,11,11	1.42	2 (18%)	12,14,14	0.92	1 (8%)
3	KSV	1F	102	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	3J	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	5I	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1I	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	4E	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	5H	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1B	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	1K	102	-	11,11,11	1.42	2 (18%)	12,14,14	0.91	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	KSV	2C	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	4H	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1J	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	3A	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	4A	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	3L	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	1F	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1M	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.93	1 (8%)
3	KSV	3K	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	4G	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	5K	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1B	102	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2E	102	-	11,11,11	1.40	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	2D	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5A	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5C	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	4N	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	4F	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2M	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	1G	101	-	11,11,11	1.44	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	1N	101	-	11,11,11	1.42	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	3N	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.92	1 (8%)
3	KSV	2E	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2F	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5L	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2G	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	5E	101	-	11,11,11	1.40	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	1L	101	-	11,11,11	1.41	2 (18%)	12,14,14	0.94	1 (8%)
3	KSV	3G	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	2H	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)
3	KSV	3E	101	-	11,11,11	1.43	2 (18%)	12,14,14	0.91	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KSV	2L	101	-	-	8/12/12/12	-
3	KSV	5I	102	-	-	6/12/12/12	-
3	KSV	1A	101	-	-	5/12/12/12	-
3	KSV	1J	102	-	-	4/12/12/12	-
3	KSV	4C	101	-	-	3/12/12/12	-
3	KSV	5G	101	-	-	2/12/12/12	-
3	KSV	1D	101	-	-	3/12/12/12	-
3	KSV	4F	102	-	-	1/12/12/12	-
3	KSV	5N	101	-	-	8/12/12/12	-
3	KSV	5J	101	-	-	5/12/12/12	-
3	KSV	4B	101	-	-	3/12/12/12	-
3	KSV	1H	101	-	-	3/12/12/12	-
3	KSV	3H	101	-	-	2/12/12/12	-
3	KSV	4L	101	-	-	3/12/12/12	-
3	KSV	3K	102	-	-	6/12/12/12	-
3	KSV	3B	101	-	-	4/12/12/12	-
3	KSV	4D	101	-	-	3/12/12/12	-
3	KSV	5D	101	-	-	6/12/12/12	-
3	KSV	1K	101	-	-	4/12/12/12	-
3	KSV	2I	101	-	-	5/12/12/12	-
3	KSV	5M	101	-	-	7/12/12/12	-
3	KSV	1C	101	-	-	4/12/12/12	-
3	KSV	3D	101	-	-	3/12/12/12	-
3	KSV	2B	101	-	-	5/12/12/12	-
3	KSV	3I	101	-	-	6/12/12/12	-
3	KSV	3M	101	-	-	6/12/12/12	-
3	KSV	3C	101	-	-	5/12/12/12	-
3	KSV	4M	101	-	-	2/12/12/12	-
3	KSV	2J	101	-	-	7/12/12/12	-
3	KSV	2N	101	-	-	5/12/12/12	-
3	KSV	3A	102	-	-	6/12/12/12	-
3	KSV	1F	102	-	-	5/12/12/12	-
3	KSV	3J	101	-	-	3/12/12/12	-
3	KSV	5I	101	-	-	4/12/12/12	-
3	KSV	1I	101	-	-	5/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KSV	4E	101	-	-	3/12/12/12	-
3	KSV	5H	101	-	-	3/12/12/12	-
3	KSV	1B	101	-	-	5/12/12/12	-
3	KSV	1K	102	-	-	2/12/12/12	-
3	KSV	2C	101	-	-	7/12/12/12	-
3	KSV	4H	101	-	-	4/12/12/12	-
3	KSV	1J	101	-	-	3/12/12/12	-
3	KSV	3A	101	-	-	6/12/12/12	-
3	KSV	4A	101	-	-	4/12/12/12	-
3	KSV	3L	101	-	-	5/12/12/12	-
3	KSV	1F	101	-	-	5/12/12/12	-
3	KSV	1M	101	-	-	4/12/12/12	-
3	KSV	3K	101	-	-	4/12/12/12	-
3	KSV	4G	101	-	-	5/12/12/12	-
3	KSV	5K	101	-	-	4/12/12/12	-
3	KSV	1B	102	-	-	5/12/12/12	-
3	KSV	2E	102	-	-	6/12/12/12	-
3	KSV	2D	101	-	-	3/12/12/12	-
3	KSV	5A	101	-	-	6/12/12/12	-
3	KSV	5C	101	-	-	5/12/12/12	-
3	KSV	4N	101	-	-	2/12/12/12	-
3	KSV	4F	101	-	-	3/12/12/12	-
3	KSV	2M	101	-	-	2/12/12/12	-
3	KSV	1G	101	-	-	3/12/12/12	-
3	KSV	1N	101	-	-	5/12/12/12	-
3	KSV	3N	101	-	-	5/12/12/12	-
3	KSV	2E	101	-	-	4/12/12/12	-
3	KSV	2F	101	-	-	1/12/12/12	-
3	KSV	5L	101	-	-	6/12/12/12	-
3	KSV	2G	101	-	-	5/12/12/12	-
3	KSV	5E	101	-	-	6/12/12/12	-
3	KSV	1L	101	-	-	4/12/12/12	-
3	KSV	3G	101	-	-	4/12/12/12	-
3	KSV	2H	101	-	-	7/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KSV	3E	101	-	-	7/12/12/12	-

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1D	101	KSV	P1-O4	2.72	1.70	1.59
3	4M	101	KSV	P1-O4	2.67	1.70	1.59
3	2M	101	KSV	P1-O4	2.67	1.70	1.59
3	2C	101	KSV	P1-O4	2.66	1.70	1.59
3	1M	101	KSV	P1-O4	2.66	1.70	1.59
3	1J	101	KSV	P1-O4	2.66	1.70	1.59
3	5D	101	KSV	P1-O4	2.66	1.70	1.59
3	4D	101	KSV	P1-O4	2.66	1.70	1.59
3	5A	101	KSV	P1-O4	2.65	1.70	1.59
3	4A	101	KSV	P1-O4	2.65	1.70	1.59
3	4E	101	KSV	P1-O4	2.65	1.70	1.59
3	1A	101	KSV	P1-O4	2.65	1.70	1.59
3	2F	101	KSV	P1-O4	2.65	1.70	1.59
3	4N	101	KSV	P1-O4	2.65	1.70	1.59
3	4F	101	KSV	P1-O4	2.65	1.70	1.59
3	3I	101	KSV	P1-O4	2.65	1.70	1.59
3	5M	101	KSV	P1-O4	2.65	1.70	1.59
3	3A	101	KSV	P1-O4	2.64	1.70	1.59
3	4F	102	KSV	P1-O4	2.64	1.70	1.59
3	5N	101	KSV	P1-O4	2.64	1.70	1.59
3	4C	101	KSV	P1-O4	2.64	1.70	1.59
3	1B	101	KSV	P1-O4	2.64	1.70	1.59
3	2N	101	KSV	P1-O4	2.64	1.70	1.59
3	1J	102	KSV	P1-O4	2.64	1.70	1.59
3	4B	101	KSV	P1-O4	2.64	1.70	1.59
3	5C	101	KSV	P1-O4	2.64	1.70	1.59
3	2G	101	KSV	P1-O4	2.63	1.70	1.59
3	3M	101	KSV	P1-O4	2.63	1.70	1.59
3	2D	101	KSV	P1-O4	2.63	1.70	1.59
3	1K	101	KSV	P1-O4	2.63	1.69	1.59
3	2L	101	KSV	P1-O4	2.63	1.69	1.59
3	2H	101	KSV	P1-O4	2.63	1.69	1.59
3	1F	102	KSV	P1-O4	2.63	1.69	1.59
3	1B	102	KSV	P1-O4	2.63	1.69	1.59
3	1G	101	KSV	P1-O4	2.63	1.69	1.59
3	5J	101	KSV	P1-O4	2.63	1.69	1.59
3	3E	101	KSV	P1-O4	2.63	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5L	101	KSV	P1-O4	2.63	1.69	1.59
3	3L	101	KSV	P1-O4	2.63	1.69	1.59
3	5I	102	KSV	P1-O4	2.62	1.69	1.59
3	5G	101	KSV	P1-O4	2.62	1.69	1.59
3	4G	101	KSV	P1-O4	2.62	1.69	1.59
3	1F	101	KSV	P1-O4	2.62	1.69	1.59
3	1N	101	KSV	P1-O4	2.62	1.69	1.59
3	3K	102	KSV	P1-O4	2.62	1.69	1.59
3	5I	101	KSV	P1-O4	2.62	1.69	1.59
3	3D	101	KSV	P1-O4	2.62	1.69	1.59
3	3A	102	KSV	P1-O4	2.62	1.69	1.59
3	3C	101	KSV	P1-O4	2.62	1.69	1.59
3	3J	101	KSV	P1-O4	2.62	1.69	1.59
3	1I	101	KSV	P1-O4	2.62	1.69	1.59
3	2E	101	KSV	P1-O4	2.61	1.69	1.59
3	1L	101	KSV	P1-O4	2.61	1.69	1.59
3	2J	101	KSV	P1-O4	2.61	1.69	1.59
3	1C	101	KSV	P1-O4	2.61	1.69	1.59
3	3K	101	KSV	P1-O4	2.61	1.69	1.59
3	3H	101	KSV	P1-O4	2.61	1.69	1.59
3	1K	102	KSV	P1-O4	2.61	1.69	1.59
3	3B	101	KSV	P1-O4	2.61	1.69	1.59
3	4L	101	KSV	P1-O4	2.61	1.69	1.59
3	5H	101	KSV	P1-O4	2.61	1.69	1.59
3	2E	102	KSV	P1-O4	2.60	1.69	1.59
3	3G	101	KSV	P1-O4	2.60	1.69	1.59
3	4H	101	KSV	P1-O4	2.60	1.69	1.59
3	2B	101	KSV	P1-O4	2.60	1.69	1.59
3	5E	101	KSV	P1-O4	2.60	1.69	1.59
3	2I	101	KSV	P1-O4	2.60	1.69	1.59
3	1H	101	KSV	P1-O4	2.60	1.69	1.59
3	5K	101	KSV	P1-O4	2.60	1.69	1.59
3	3N	101	KSV	P1-O4	2.59	1.69	1.59
3	3C	101	KSV	P1-O1	2.22	1.68	1.59
3	1G	101	KSV	P1-O1	2.22	1.68	1.59
3	3K	102	KSV	P1-O1	2.22	1.68	1.59
3	5D	101	KSV	P1-O1	2.22	1.68	1.59
3	2C	101	KSV	P1-O1	2.22	1.68	1.59
3	1N	101	KSV	P1-O1	2.22	1.68	1.59
3	3K	101	KSV	P1-O1	2.22	1.68	1.59
3	2E	101	KSV	P1-O1	2.21	1.68	1.59
3	4F	102	KSV	P1-O1	2.21	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1D	101	KSV	P1-O1	2.21	1.68	1.59
3	1K	101	KSV	P1-O1	2.21	1.68	1.59
3	5A	101	KSV	P1-O1	2.21	1.68	1.59
3	4D	101	KSV	P1-O1	2.21	1.68	1.59
3	3I	101	KSV	P1-O1	2.20	1.68	1.59
3	3L	101	KSV	P1-O1	2.20	1.68	1.59
3	5C	101	KSV	P1-O1	2.20	1.68	1.59
3	4H	101	KSV	P1-O1	2.20	1.68	1.59
3	3J	101	KSV	P1-O1	2.20	1.68	1.59
3	1J	101	KSV	P1-O1	2.20	1.68	1.59
3	2D	101	KSV	P1-O1	2.20	1.68	1.59
3	4B	101	KSV	P1-O1	2.20	1.68	1.59
3	5M	101	KSV	P1-O1	2.20	1.68	1.59
3	2M	101	KSV	P1-O1	2.20	1.68	1.59
3	5I	101	KSV	P1-O1	2.20	1.68	1.59
3	5L	101	KSV	P1-O1	2.20	1.68	1.59
3	3M	101	KSV	P1-O1	2.20	1.68	1.59
3	4C	101	KSV	P1-O1	2.20	1.68	1.59
3	4M	101	KSV	P1-O1	2.19	1.68	1.59
3	3G	101	KSV	P1-O1	2.19	1.68	1.59
3	3E	101	KSV	P1-O1	2.19	1.68	1.59
3	1A	101	KSV	P1-O1	2.19	1.68	1.59
3	3H	101	KSV	P1-O1	2.19	1.68	1.59
3	4F	101	KSV	P1-O1	2.19	1.68	1.59
3	4G	101	KSV	P1-O1	2.19	1.68	1.59
3	2N	101	KSV	P1-O1	2.19	1.68	1.59
3	2J	101	KSV	P1-O1	2.19	1.68	1.59
3	2G	101	KSV	P1-O1	2.19	1.68	1.59
3	1F	102	KSV	P1-O1	2.19	1.68	1.59
3	4N	101	KSV	P1-O1	2.19	1.68	1.59
3	3A	101	KSV	P1-O1	2.19	1.68	1.59
3	1J	102	KSV	P1-O1	2.19	1.68	1.59
3	2F	101	KSV	P1-O1	2.19	1.68	1.59
3	1C	101	KSV	P1-O1	2.19	1.68	1.59
3	2E	102	KSV	P1-O1	2.19	1.68	1.59
3	4E	101	KSV	P1-O1	2.19	1.68	1.59
3	1L	101	KSV	P1-O1	2.19	1.68	1.59
3	1F	101	KSV	P1-O1	2.19	1.68	1.59
3	2H	101	KSV	P1-O1	2.19	1.68	1.59
3	1B	101	KSV	P1-O1	2.19	1.68	1.59
3	1M	101	KSV	P1-O1	2.19	1.68	1.59
3	2B	101	KSV	P1-O1	2.18	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5I	102	KSV	P1-O1	2.18	1.68	1.59
3	1B	102	KSV	P1-O1	2.18	1.68	1.59
3	5J	101	KSV	P1-O1	2.18	1.68	1.59
3	3D	101	KSV	P1-O1	2.18	1.68	1.59
3	4A	101	KSV	P1-O1	2.18	1.68	1.59
3	1I	101	KSV	P1-O1	2.18	1.68	1.59
3	2L	101	KSV	P1-O1	2.18	1.68	1.59
3	5G	101	KSV	P1-O1	2.18	1.68	1.59
3	5N	101	KSV	P1-O1	2.18	1.68	1.59
3	1K	102	KSV	P1-O1	2.17	1.68	1.59
3	3N	101	KSV	P1-O1	2.16	1.68	1.59
3	5K	101	KSV	P1-O1	2.16	1.68	1.59
3	3A	102	KSV	P1-O1	2.16	1.68	1.59
3	4L	101	KSV	P1-O1	2.16	1.68	1.59
3	5E	101	KSV	P1-O1	2.16	1.68	1.59
3	5H	101	KSV	P1-O1	2.16	1.68	1.59
3	2I	101	KSV	P1-O1	2.15	1.68	1.59
3	3B	101	KSV	P1-O1	2.15	1.68	1.59
3	1H	101	KSV	P1-O1	2.15	1.68	1.59

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3A	102	KSV	O2-P1-O3	2.66	125.41	112.24
3	4L	101	KSV	O2-P1-O3	2.66	125.40	112.24
3	2E	102	KSV	O2-P1-O3	2.66	125.40	112.24
3	3B	101	KSV	O2-P1-O3	2.66	125.39	112.24
3	3N	101	KSV	O2-P1-O3	2.66	125.39	112.24
3	2B	101	KSV	O2-P1-O3	2.66	125.38	112.24
3	5H	101	KSV	O2-P1-O3	2.66	125.37	112.24
3	5L	101	KSV	O2-P1-O3	2.66	125.37	112.24
3	2G	101	KSV	O2-P1-O3	2.66	125.37	112.24
3	2H	101	KSV	O2-P1-O3	2.66	125.37	112.24
3	3J	101	KSV	O2-P1-O3	2.66	125.37	112.24
3	1A	101	KSV	O2-P1-O3	2.66	125.37	112.24
3	1B	101	KSV	O2-P1-O3	2.65	125.36	112.24
3	4H	101	KSV	O2-P1-O3	2.65	125.36	112.24
3	2D	101	KSV	O2-P1-O3	2.65	125.36	112.24
3	2I	101	KSV	O2-P1-O3	2.65	125.36	112.24
3	5E	101	KSV	O2-P1-O3	2.65	125.35	112.24
3	1H	101	KSV	O2-P1-O3	2.65	125.35	112.24
3	3L	101	KSV	O2-P1-O3	2.65	125.35	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5C	101	KSV	O2-P1-O3	2.65	125.35	112.24
3	5N	101	KSV	O2-P1-O3	2.65	125.35	112.24
3	3E	101	KSV	O2-P1-O3	2.65	125.35	112.24
3	4E	101	KSV	O2-P1-O3	2.65	125.35	112.24
3	1F	102	KSV	O2-P1-O3	2.65	125.34	112.24
3	4D	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	5A	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	5I	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	1D	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	1B	102	KSV	O2-P1-O3	2.65	125.34	112.24
3	1G	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	1N	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	1L	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	2L	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	3M	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	4A	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	5K	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	1J	101	KSV	O2-P1-O3	2.65	125.34	112.24
3	4B	101	KSV	O2-P1-O3	2.65	125.33	112.24
3	4F	102	KSV	O2-P1-O3	2.65	125.33	112.24
3	2M	101	KSV	O2-P1-O3	2.65	125.33	112.24
3	3C	101	KSV	O2-P1-O3	2.65	125.33	112.24
3	3I	101	KSV	O2-P1-O3	2.65	125.33	112.24
3	1K	101	KSV	O2-P1-O3	2.65	125.33	112.24
3	3K	102	KSV	O2-P1-O3	2.65	125.33	112.24
3	3D	101	KSV	O2-P1-O3	2.65	125.32	112.24
3	3K	101	KSV	O2-P1-O3	2.65	125.32	112.24
3	5J	101	KSV	O2-P1-O3	2.65	125.32	112.24
3	2N	101	KSV	O2-P1-O3	2.64	125.32	112.24
3	3H	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	4M	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	2E	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	4G	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	4N	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	1F	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	5I	102	KSV	O2-P1-O3	2.64	125.31	112.24
3	1C	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	5G	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	3A	101	KSV	O2-P1-O3	2.64	125.31	112.24
3	1M	101	KSV	O2-P1-O3	2.64	125.30	112.24
3	5M	101	KSV	O2-P1-O3	2.64	125.29	112.24
3	1J	102	KSV	O2-P1-O3	2.64	125.29	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	4C	101	KSV	O2-P1-O3	2.64	125.28	112.24
3	1K	102	KSV	O2-P1-O3	2.64	125.28	112.24
3	2C	101	KSV	O2-P1-O3	2.64	125.28	112.24
3	3G	101	KSV	O2-P1-O3	2.64	125.28	112.24
3	4F	101	KSV	O2-P1-O3	2.64	125.28	112.24
3	2F	101	KSV	O2-P1-O3	2.64	125.28	112.24
3	2J	101	KSV	O2-P1-O3	2.64	125.27	112.24
3	1I	101	KSV	O2-P1-O3	2.64	125.27	112.24
3	5D	101	KSV	O2-P1-O3	2.62	125.18	112.24

There are no chirality outliers.

All (310) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1A	101	KSV	C3-O4-P1-O3
3	1B	101	KSV	C3-C4-C5-O6
3	1B	101	KSV	C3-O4-P1-O3
3	1B	102	KSV	C2-O1-P1-O2
3	1C	101	KSV	C3-O4-P1-O3
3	1C	101	KSV	C3-O4-P1-O2
3	1F	101	KSV	C3-C4-C5-O6
3	1F	101	KSV	C2-O1-P1-O2
3	1F	102	KSV	O4-C3-C4-O5
3	1F	102	KSV	C2-O1-P1-O2
3	1G	101	KSV	C2-O1-P1-O2
3	1H	101	KSV	C3-C4-C5-O6
3	1I	101	KSV	C3-C4-C5-O6
3	1I	101	KSV	C3-O4-P1-O2
3	1J	101	KSV	C3-C4-C5-O6
3	1J	101	KSV	C2-O1-P1-O2
3	1J	102	KSV	C3-O4-P1-O2
3	1K	101	KSV	C3-C4-C5-O6
3	1K	101	KSV	C2-O1-P1-O2
3	1K	102	KSV	C2-O1-P1-O2
3	1L	101	KSV	C3-C4-C5-O6
3	1M	101	KSV	C2-O1-P1-O3
3	1N	101	KSV	C3-C4-C5-O6
3	1N	101	KSV	C3-O4-P1-O3
3	2B	101	KSV	O4-C3-C4-C5
3	2B	101	KSV	C3-C4-C5-O6
3	2C	101	KSV	C2-O1-P1-O3
3	2D	101	KSV	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
3	2D	101	KSV	C3-O4-P1-O2
3	2E	101	KSV	O4-C3-C4-C5
3	2E	101	KSV	O4-C3-C4-O5
3	2E	102	KSV	C3-C4-C5-O6
3	2E	102	KSV	C2-O1-P1-O4
3	2F	101	KSV	C2-O1-P1-O2
3	2G	101	KSV	C2-O1-P1-O2
3	2H	101	KSV	C2-O1-P1-O2
3	2I	101	KSV	O4-C3-C4-O5
3	2I	101	KSV	C3-C4-C5-O6
3	2I	101	KSV	O5-C4-C5-O6
3	2J	101	KSV	C3-C4-C5-O6
3	2J	101	KSV	C2-O1-P1-O2
3	2L	101	KSV	C3-C4-C5-O6
3	2L	101	KSV	C3-O4-P1-O3
3	2M	101	KSV	C3-O4-P1-O3
3	2N	101	KSV	C2-O1-P1-O3
3	2N	101	KSV	C3-O4-P1-O3
3	3A	101	KSV	C2-O1-P1-O3
3	3A	102	KSV	O4-C3-C4-C5
3	3A	102	KSV	C3-C4-C5-O6
3	3B	101	KSV	O4-C3-C4-O5
3	3C	101	KSV	C2-O1-P1-O2
3	3D	101	KSV	C3-O4-P1-O3
3	3D	101	KSV	C3-O4-P1-O1
3	3D	101	KSV	C3-O4-P1-O2
3	3E	101	KSV	C3-C4-C5-O6
3	3E	101	KSV	C3-O4-P1-O2
3	3G	101	KSV	C2-O1-P1-O2
3	3H	101	KSV	C2-O1-P1-O2
3	3I	101	KSV	C2-O1-P1-O3
3	3I	101	KSV	C3-O4-P1-O3
3	3I	101	KSV	C3-O4-P1-O1
3	3J	101	KSV	C2-O1-P1-O3
3	3J	101	KSV	C3-O4-P1-O3
3	3K	101	KSV	C3-O4-P1-O3
3	3K	102	KSV	C2-O1-P1-O3
3	3L	101	KSV	C3-C4-C5-O6
3	3L	101	KSV	C3-O4-P1-O3
3	3M	101	KSV	C2-O1-P1-O3
3	3N	101	KSV	O4-C3-C4-O5
3	3N	101	KSV	C3-C4-C5-O6

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Mol	Chain	Res	Type	Atoms
3	4A	101	KSV	C2-O1-P1-O2
3	4B	101	KSV	C3-O4-P1-O2
3	4C	101	KSV	C2-O1-P1-O2
3	4D	101	KSV	C2-O1-P1-O2
3	4E	101	KSV	C2-O1-P1-O3
3	4F	101	KSV	C3-C4-C5-O6
3	4F	101	KSV	C2-O1-P1-O2
3	4F	102	KSV	C3-O4-P1-O3
3	4G	101	KSV	C3-C4-C5-O6
3	4G	101	KSV	C3-O4-P1-O3
3	4H	101	KSV	C2-O1-P1-O3
3	4N	101	KSV	C2-O1-P1-O2
3	5A	101	KSV	O4-C3-C4-O5
3	5A	101	KSV	C3-C4-C5-O6
3	5A	101	KSV	C3-O4-P1-O2
3	5C	101	KSV	C3-C4-C5-O6
3	5C	101	KSV	C2-O1-P1-O2
3	5D	101	KSV	C2-O1-P1-O3
3	5D	101	KSV	C3-O4-P1-O3
3	5E	101	KSV	O4-C3-C4-O5
3	5E	101	KSV	C3-C4-C5-O6
3	5E	101	KSV	C2-O1-P1-O3
3	5G	101	KSV	C2-O1-P1-O2
3	5I	101	KSV	C3-C4-C5-O6
3	5I	101	KSV	C2-O1-P1-O2
3	5I	102	KSV	C3-C4-C5-O6
3	5I	102	KSV	C2-O1-P1-O3
3	5J	101	KSV	C3-C4-C5-O6
3	5J	101	KSV	C3-O4-P1-O2
3	5K	101	KSV	C3-C4-C5-O6
3	5L	101	KSV	C3-C4-C5-O6
3	5L	101	KSV	C2-O1-P1-O2
3	5M	101	KSV	O4-C3-C4-O5
3	5M	101	KSV	C3-O4-P1-O2
3	5N	101	KSV	C3-C4-C5-O6
3	5N	101	KSV	C3-O4-P1-O2
3	1M	101	KSV	O4-C3-C4-O5
3	2B	101	KSV	O4-C3-C4-O5
3	2E	102	KSV	O4-C3-C4-O5
3	2L	101	KSV	O4-C3-C4-O5
3	3A	102	KSV	O4-C3-C4-O5
3	3K	102	KSV	O4-C3-C4-O5

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Mol	Chain	Res	Type	Atoms
3	4H	101	KSV	O4-C3-C4-O5
3	4L	101	KSV	O4-C3-C4-O5
3	5D	101	KSV	O4-C3-C4-O5
3	5K	101	KSV	O4-C3-C4-O5
3	5N	101	KSV	O4-C3-C4-O5
3	2E	102	KSV	O4-C3-C4-C5
3	2L	101	KSV	O4-C3-C4-C5
3	3K	102	KSV	O4-C3-C4-C5
3	4L	101	KSV	O4-C3-C4-C5
3	5E	101	KSV	O4-C3-C4-C5
3	5N	101	KSV	O4-C3-C4-C5
3	1A	101	KSV	O4-C3-C4-O5
3	1J	101	KSV	O5-C4-C5-O6
3	2B	101	KSV	O5-C4-C5-O6
3	5C	101	KSV	O5-C4-C5-O6
3	5E	101	KSV	O5-C4-C5-O6
3	3E	101	KSV	O4-C3-C4-O5
3	1C	101	KSV	C3-O4-P1-O1
3	1I	101	KSV	C3-O4-P1-O1
3	1J	102	KSV	C3-O4-P1-O1
3	1L	101	KSV	C2-O1-P1-O4
3	1N	101	KSV	C3-O4-P1-O1
3	2D	101	KSV	C3-O4-P1-O1
3	3K	101	KSV	C3-O4-P1-O1
3	3L	101	KSV	C3-O4-P1-O1
3	4G	101	KSV	C3-O4-P1-O1
3	5J	101	KSV	C3-O4-P1-O1
3	1F	102	KSV	O4-C3-C4-C5
3	2I	101	KSV	O4-C3-C4-C5
3	3B	101	KSV	O4-C3-C4-C5
3	3N	101	KSV	O4-C3-C4-C5
3	4H	101	KSV	O4-C3-C4-C5
3	5A	101	KSV	O4-C3-C4-C5
3	5K	101	KSV	O4-C3-C4-C5
3	5M	101	KSV	O4-C3-C4-C5
3	3A	101	KSV	O4-C3-C4-O5
3	4E	101	KSV	O4-C3-C4-O5
3	2E	101	KSV	C3-C4-C5-O6
3	2G	101	KSV	C3-C4-C5-O6
3	5M	101	KSV	C3-C4-C5-O6
3	1B	101	KSV	O5-C4-C5-O6
3	1K	101	KSV	O5-C4-C5-O6

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Mol	Chain	Res	Type	Atoms
3	1L	101	KSV	O5-C4-C5-O6
3	1N	101	KSV	O5-C4-C5-O6
3	2J	101	KSV	O5-C4-C5-O6
3	3N	101	KSV	O5-C4-C5-O6
3	4F	101	KSV	O5-C4-C5-O6
3	5A	101	KSV	O5-C4-C5-O6
3	5I	102	KSV	O5-C4-C5-O6
3	5K	101	KSV	O5-C4-C5-O6
3	5N	101	KSV	O5-C4-C5-O6
3	1B	101	KSV	O4-C3-C4-O5
3	5D	101	KSV	O4-C3-C4-C5
3	5N	101	KSV	C3-O4-P1-O1
3	1M	101	KSV	O4-C3-C4-C5
3	1F	101	KSV	O5-C4-C5-O6
3	1H	101	KSV	O5-C4-C5-O6
3	1I	101	KSV	O5-C4-C5-O6
3	2E	102	KSV	O5-C4-C5-O6
3	2G	101	KSV	O5-C4-C5-O6
3	2L	101	KSV	O5-C4-C5-O6
3	3A	102	KSV	O5-C4-C5-O6
3	3E	101	KSV	O5-C4-C5-O6
3	3L	101	KSV	O5-C4-C5-O6
3	4G	101	KSV	O5-C4-C5-O6
3	5I	101	KSV	O5-C4-C5-O6
3	5J	101	KSV	O5-C4-C5-O6
3	5L	101	KSV	O5-C4-C5-O6
3	5M	101	KSV	O5-C4-C5-O6
3	2J	101	KSV	O4-C3-C4-O5
3	2L	101	KSV	C3-O4-P1-O1
3	1B	102	KSV	O5-C4-C5-O6
3	1G	101	KSV	O5-C4-C5-O6
3	3A	101	KSV	O5-C4-C5-O6
3	3K	101	KSV	O5-C4-C5-O6
3	4C	101	KSV	O5-C4-C5-O6
3	1A	101	KSV	O4-C3-C4-C5
3	3E	101	KSV	O4-C3-C4-C5
3	3K	102	KSV	C4-C3-O4-P1
3	5I	102	KSV	C4-C3-O4-P1
3	4E	101	KSV	O4-C3-C4-C5
3	1F	102	KSV	O5-C4-C5-O6
3	1M	101	KSV	O5-C4-C5-O6
3	2C	101	KSV	O5-C4-C5-O6

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Mol	Chain	Res	Type	Atoms
3	2H	101	KSV	O5-C4-C5-O6
3	2N	101	KSV	O5-C4-C5-O6
3	4A	101	KSV	O5-C4-C5-O6
3	4B	101	KSV	O5-C4-C5-O6
3	4D	101	KSV	O5-C4-C5-O6
3	1B	102	KSV	C3-C4-C5-O6
3	3A	101	KSV	C3-C4-C5-O6
3	4C	101	KSV	C3-C4-C5-O6
3	5D	101	KSV	C3-C4-C5-O6
3	3C	101	KSV	C3-O4-P1-O1
3	3E	101	KSV	C3-O4-P1-O1
3	5D	101	KSV	C3-O4-P1-O1
3	5C	101	KSV	C4-C3-O4-P1
3	5M	101	KSV	C4-C3-O4-P1
3	1A	101	KSV	C2-O1-P1-O3
3	1D	101	KSV	C2-O1-P1-O3
3	1I	101	KSV	C3-O4-P1-O3
3	1J	102	KSV	C3-O4-P1-O3
3	1L	101	KSV	C2-O1-P1-O3
3	1N	101	KSV	C3-O4-P1-O2
3	2C	101	KSV	C3-O4-P1-O3
3	2E	102	KSV	C2-O1-P1-O2
3	2L	101	KSV	C3-O4-P1-O2
3	2M	101	KSV	C2-O1-P1-O3
3	3A	101	KSV	C3-O4-P1-O3
3	3K	101	KSV	C3-O4-P1-O2
3	3L	101	KSV	C3-O4-P1-O2
3	4G	101	KSV	C3-O4-P1-O2
3	4M	101	KSV	C3-O4-P1-O2
3	5J	101	KSV	C3-O4-P1-O3
3	5N	101	KSV	C3-O4-P1-O3
3	2J	101	KSV	O4-C3-C4-C5
3	2C	101	KSV	O4-C3-C4-O5
3	2H	101	KSV	O4-C3-C4-O5
3	3I	101	KSV	O4-C3-C4-O5
3	3M	101	KSV	O4-C3-C4-O5
3	2L	101	KSV	C4-C3-O4-P1
3	5N	101	KSV	C4-C3-O4-P1
3	1B	102	KSV	C3-O4-P1-O1
3	1D	101	KSV	C3-O4-P1-O1
3	1F	101	KSV	C3-O4-P1-O1
3	1G	101	KSV	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
3	1H	101	KSV	C2-O1-P1-O4
3	1K	102	KSV	C3-O4-P1-O1
3	2B	101	KSV	C2-O1-P1-O4
3	2C	101	KSV	C3-O4-P1-O1
3	2G	101	KSV	C3-O4-P1-O1
3	2H	101	KSV	C3-O4-P1-O1
3	2I	101	KSV	C2-O1-P1-O4
3	2J	101	KSV	C3-O4-P1-O1
3	2N	101	KSV	C3-O4-P1-O1
3	3A	102	KSV	C2-O1-P1-O4
3	3B	101	KSV	C2-O1-P1-O4
3	3G	101	KSV	C3-O4-P1-O1
3	3H	101	KSV	C3-O4-P1-O1
3	3J	101	KSV	C3-O4-P1-O1
3	3K	102	KSV	C3-O4-P1-O1
3	3M	101	KSV	C3-O4-P1-O1
3	3N	101	KSV	C2-O1-P1-O4
3	4H	101	KSV	C2-O1-P1-O4
3	4L	101	KSV	C2-O1-P1-O4
3	5C	101	KSV	C3-O4-P1-O1
3	5E	101	KSV	C2-O1-P1-O4
3	5G	101	KSV	C3-O4-P1-O1
3	5H	101	KSV	C2-O1-P1-O4
3	5H	101	KSV	C3-O4-P1-O1
3	5I	101	KSV	C3-O4-P1-O1
3	5I	102	KSV	C2-O1-P1-O4
3	5L	101	KSV	C3-O4-P1-O1
3	3A	102	KSV	C4-C3-O4-P1
3	3A	101	KSV	O4-C3-C4-C5
3	1A	101	KSV	O5-C4-C5-O6
3	1C	101	KSV	O5-C4-C5-O6
3	5A	101	KSV	C4-C3-O4-P1
3	1B	101	KSV	O4-C3-C4-C5
3	2H	101	KSV	O4-C3-C4-C5
3	3I	101	KSV	O4-C3-C4-C5
3	3M	101	KSV	O4-C3-C4-C5
3	3I	101	KSV	C4-C3-O4-P1
3	4N	101	KSV	O5-C4-C5-O6
3	2C	101	KSV	O4-C3-C4-C5
3	3C	101	KSV	C4-C3-O4-P1
3	2C	101	KSV	C3-C4-C5-O6
3	2N	101	KSV	C3-C4-C5-O6

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Mol	Chain	Res	Type	Atoms
3	4A	101	KSV	C3-C4-C5-O6
3	4A	101	KSV	O4-C3-C4-O5
3	1J	102	KSV	O5-C4-C5-O6
3	1F	102	KSV	C3-C4-C5-O6
3	2H	101	KSV	C3-C4-C5-O6
3	4B	101	KSV	C3-C4-C5-O6
3	4D	101	KSV	C3-C4-C5-O6
3	1F	101	KSV	O4-C3-C4-C5
3	3G	101	KSV	O4-C3-C4-C5
3	5H	101	KSV	O4-C3-C4-C5
3	5I	102	KSV	O4-C3-C4-C5
3	1B	102	KSV	C3-O4-P1-O3
3	1D	101	KSV	C3-O4-P1-O3
3	1K	101	KSV	C2-O1-P1-O3
3	2G	101	KSV	C3-O4-P1-O3
3	2H	101	KSV	C3-O4-P1-O3
3	2J	101	KSV	C3-O4-P1-O3
3	3B	101	KSV	C2-O1-P1-O3
3	3C	101	KSV	C2-O1-P1-O3
3	3C	101	KSV	C3-O4-P1-O2
3	3E	101	KSV	C3-O4-P1-O3
3	3G	101	KSV	C3-O4-P1-O3
3	3K	102	KSV	C3-O4-P1-O3
3	3M	101	KSV	C3-O4-P1-O3
3	4M	101	KSV	C2-O1-P1-O2
3	5L	101	KSV	C3-O4-P1-O3
3	5M	101	KSV	C3-O4-P1-O3
3	2E	101	KSV	O5-C4-C5-O6
3	3M	101	KSV	O5-C4-C5-O6
3	5L	101	KSV	O4-C3-C4-C5

There are no ring outliers.

16 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4C	101	KSV	1	0
3	5J	101	KSV	1	0
3	1H	101	KSV	1	0
3	4D	101	KSV	1	0
3	2I	101	KSV	1	0
3	1C	101	KSV	1	0
3	2B	101	KSV	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1I	101	KSV	1	0
3	4E	101	KSV	1	0
3	1J	101	KSV	1	0
3	3L	101	KSV	1	0
3	1M	101	KSV	1	0
3	2M	101	KSV	1	0
3	2F	101	KSV	1	0
3	2G	101	KSV	1	0
3	1L	101	KSV	1	0

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)

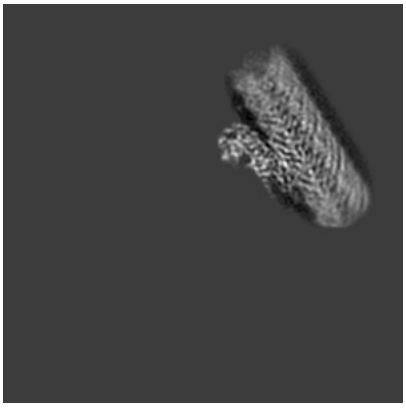
This section contains visualisations of the EMDB entry EMD-9397. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

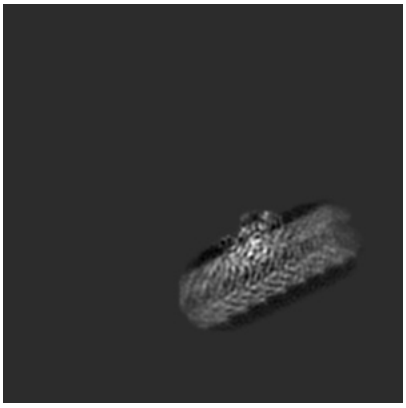
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y



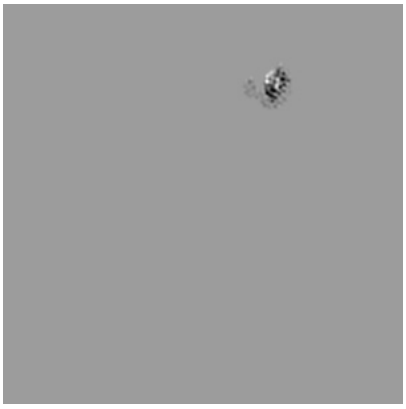
Z

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

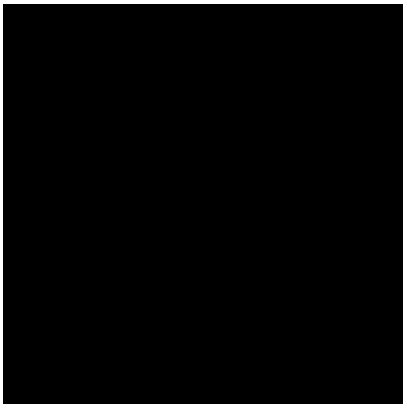
6.2 Central slices (i)

6.2.1 Primary map

X Index: 108



Y Index: 108



Z Index: 108

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: 141

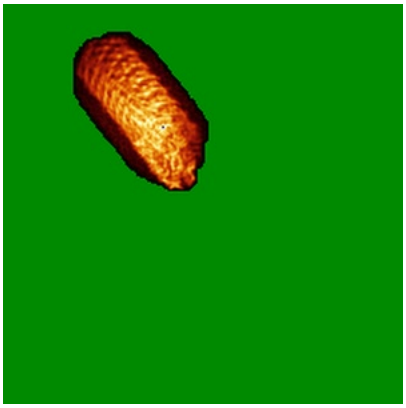
Y Index: 80

Z Index: 150

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

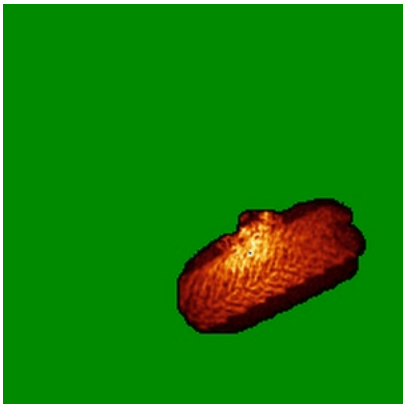
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X

Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

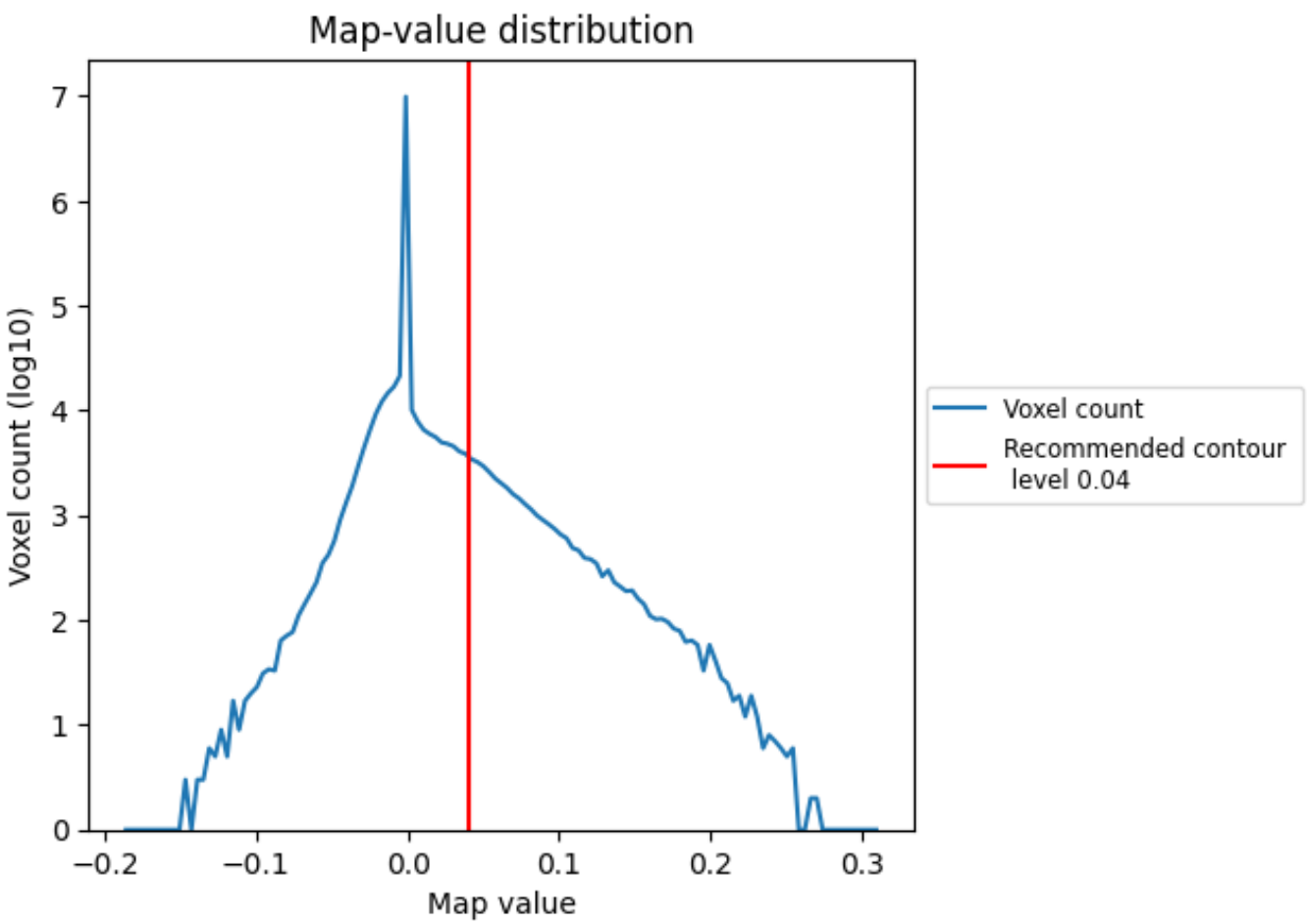
6.6 Mask visualisation (i)

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

7 Map analysis (i)

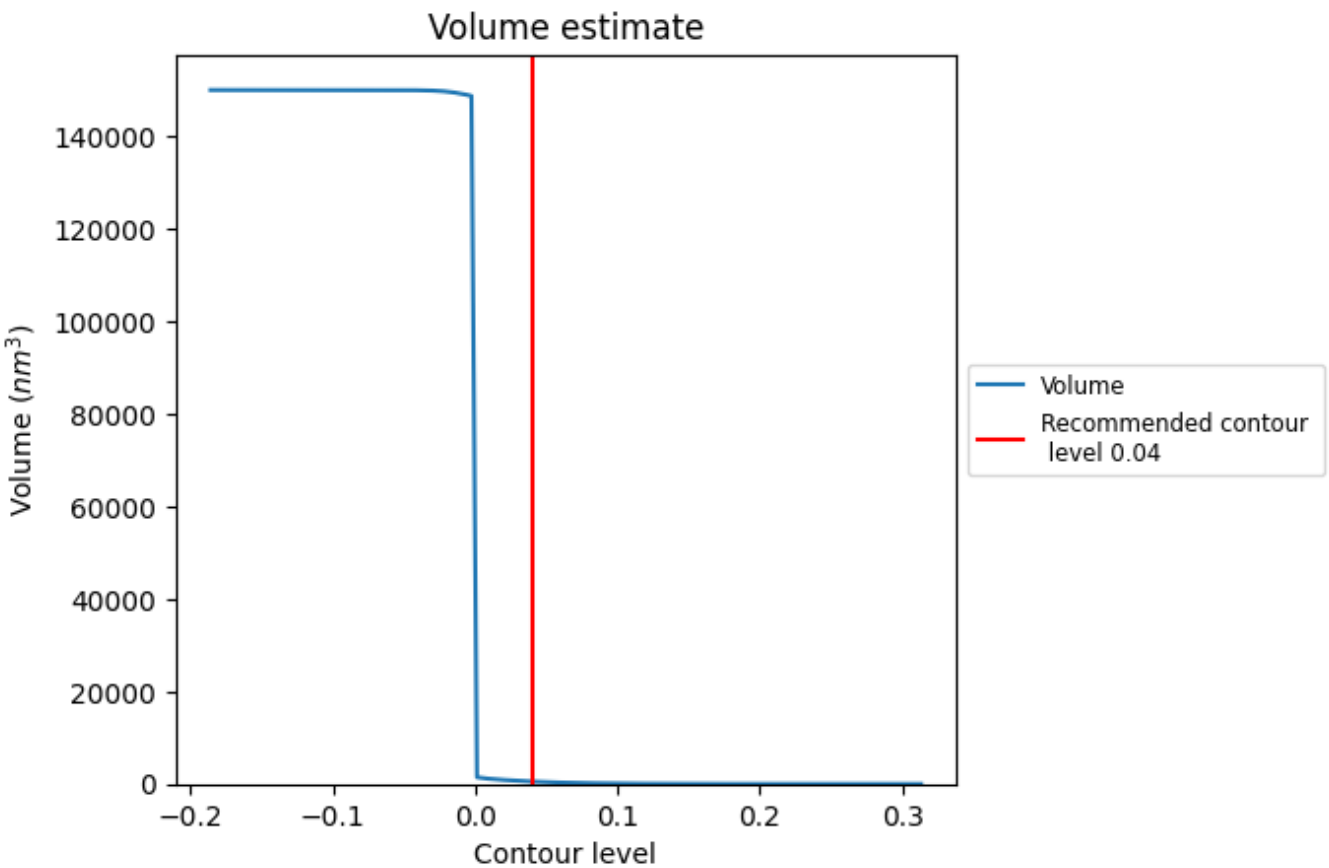
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

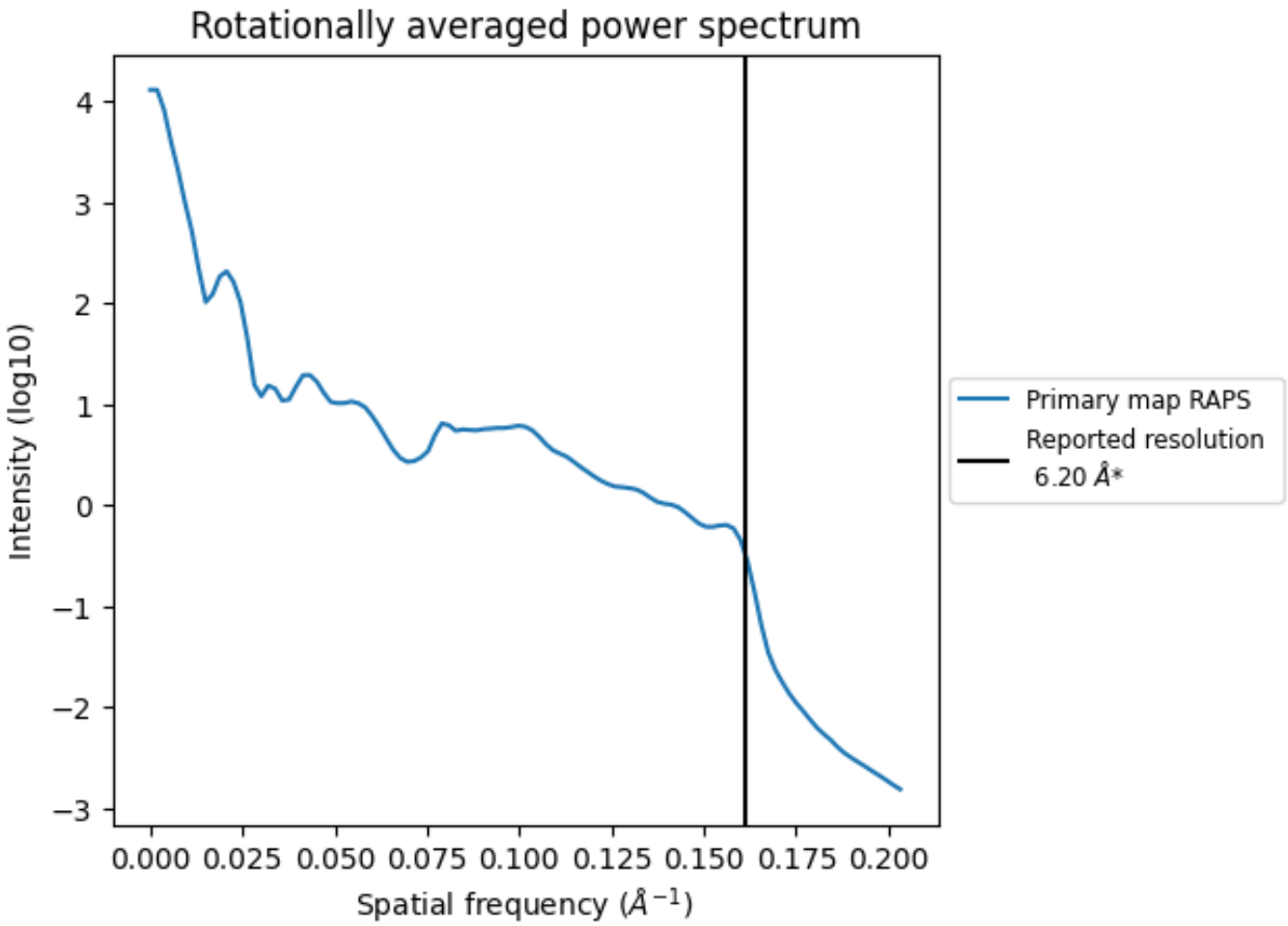
7.2 Volume estimate (i)



The volume at the recommended contour level is 526 nm^3; this corresponds to an approximate mass of 475 kDa.

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

7.3 Rotationally averaged power spectrum (i)

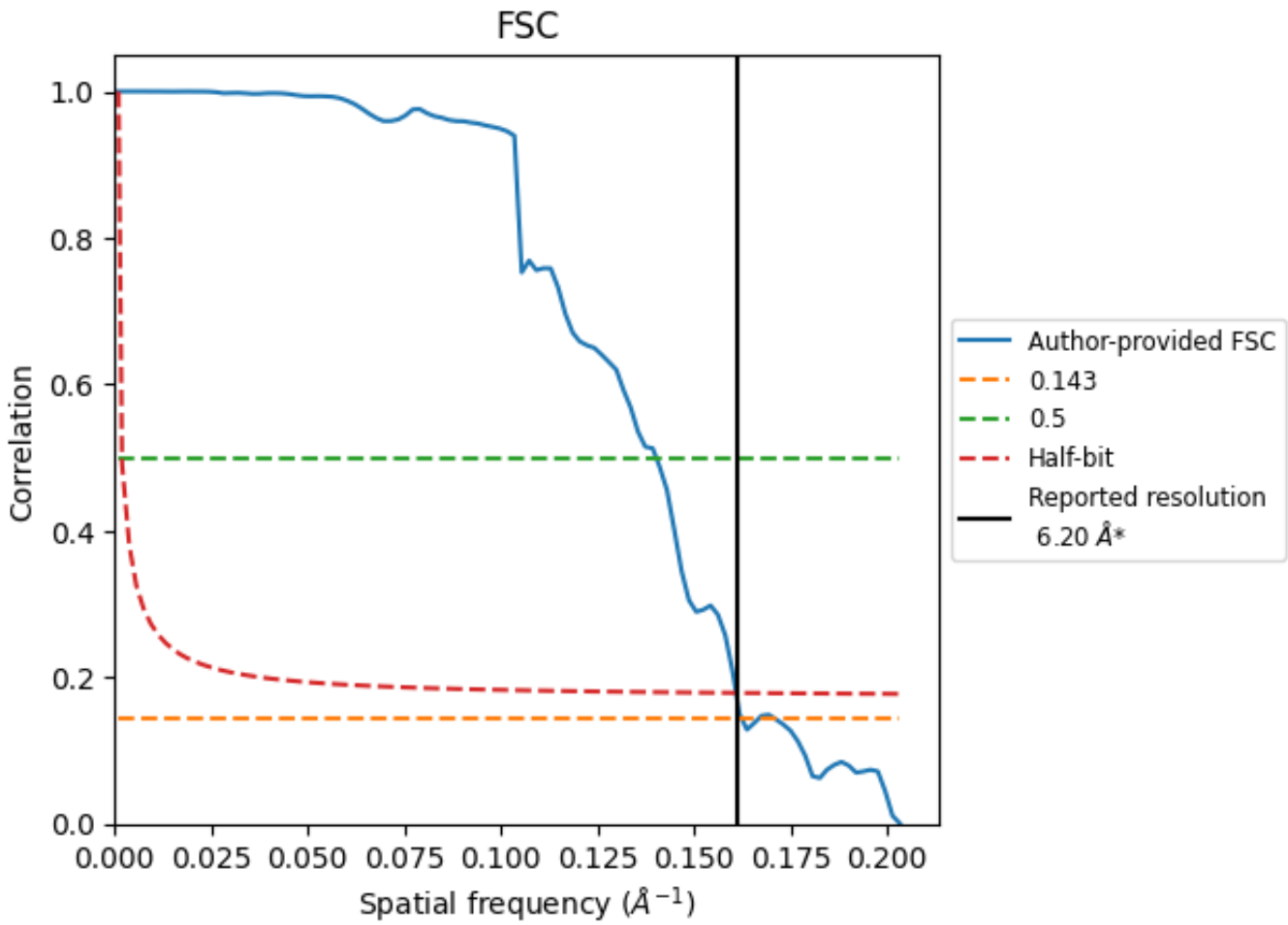


*Reported resolution corresponds to spatial frequency of 0.161 Å^{-1}

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 0.161 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.16	7.13	6.22
Unmasked-calculated*	-	-	-

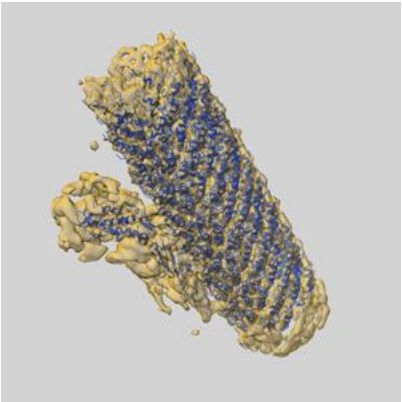
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

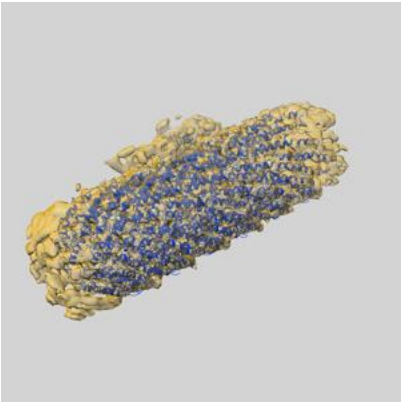
This section contains information regarding the fit between EMDB map EMD-9397 and PDB model 6NM5. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)

X



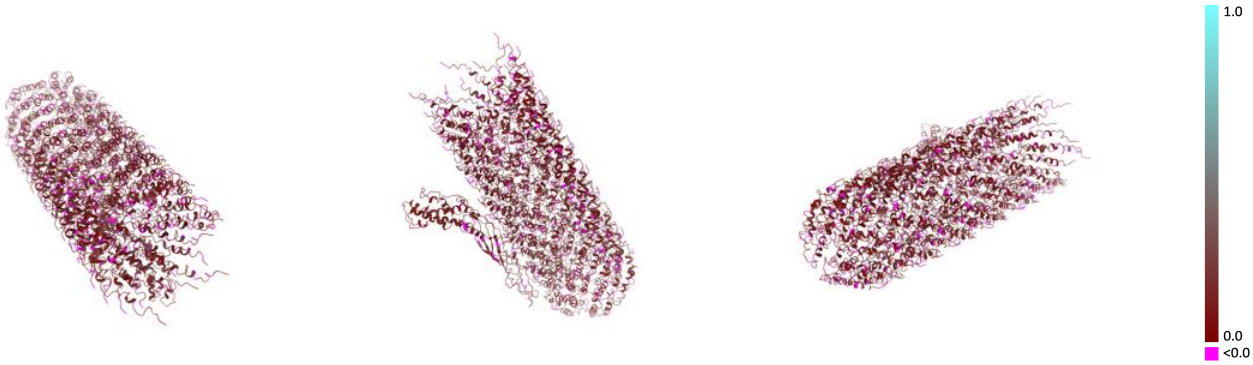
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

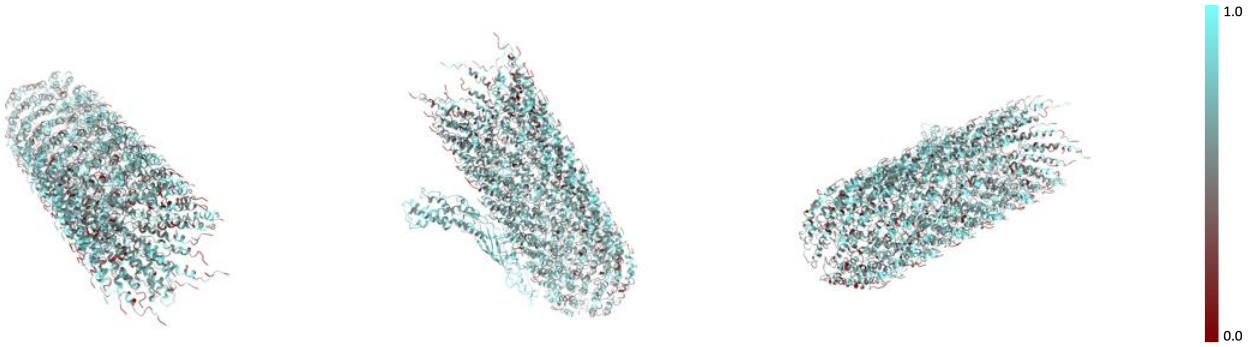
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

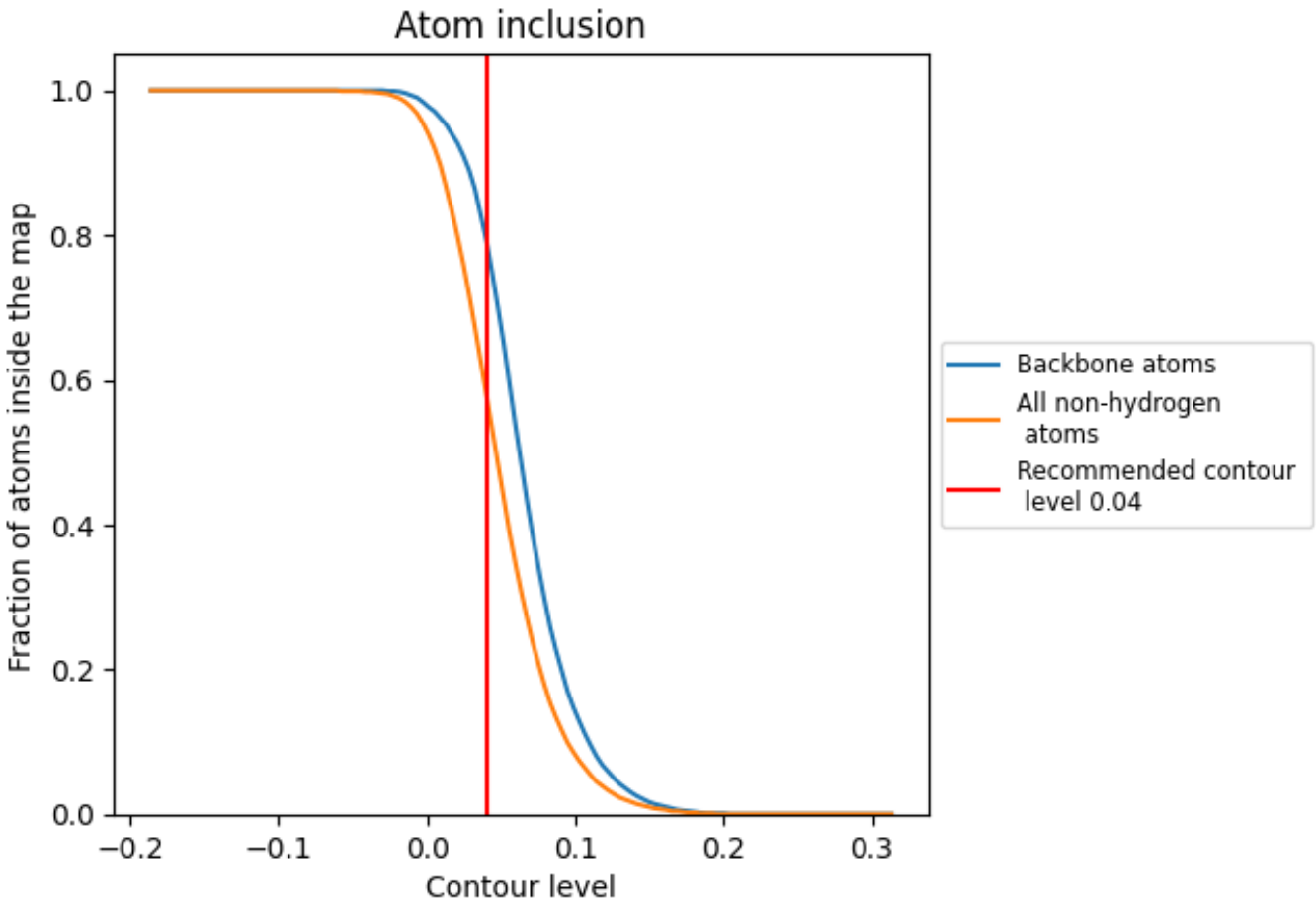
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5820	0.1360
1A	0.4710	0.1330
1B	0.5260	0.1260
1C	0.5530	0.1330
1D	0.6150	0.1330
1E	0.5930	0.1340
1F	0.6190	0.1510
1G	0.5950	0.1440
1H	0.6130	0.1470
1I	0.6380	0.1570
1J	0.6280	0.1590
1K	0.6250	0.1480
1L	0.5230	0.1320
1M	0.5660	0.1430
1N	0.5330	0.1300
1O	0.5130	0.1340
2A	0.5270	0.1280
2B	0.5560	0.1320
2C	0.5820	0.1280
2D	0.6030	0.1500
2E	0.5980	0.1470
2F	0.6090	0.1530
2G	0.6110	0.1410
2H	0.5990	0.1320
2I	0.5760	0.1290
2J	0.5580	0.1230
2K	0.5740	0.1230
2L	0.5450	0.1300
2M	0.5180	0.1200
2N	0.5210	0.1170
2O	0.5020	0.1370
3A	0.5520	0.1380
3B	0.5700	0.1400
3C	0.5970	0.1440
3D	0.5950	0.1370

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Chain	Atom inclusion	Q-score
3E	0.6130	0.1470
3F	0.6200	0.1420
3G	0.5930	0.1300
3H	0.5990	0.1200
3I	0.5990	0.1550
3J	0.5760	0.1280
3K	0.5900	0.1290
3L	0.5740	0.1360
3M	0.5470	0.1360
3N	0.5100	0.1400
3O	0.5250	0.1350
4A	0.5270	0.1380
4B	0.5620	0.1380
4C	0.5840	0.1360
4D	0.5860	0.1400
4E	0.6070	0.1300
4F	0.6060	0.1350
4G	0.6050	0.1360
4H	0.6090	0.1430
4I	0.6120	0.1390
4J	0.5890	0.1260
4K	0.5650	0.1310
4L	0.5640	0.1370
4M	0.5580	0.1230
4N	0.5350	0.1200
4O	0.5530	0.1210
5A	0.5250	0.1290
5B	0.5250	0.1280
5C	0.5530	0.1250
5D	0.5800	0.1240
5E	0.5840	0.1250
5F	0.6140	0.1370
5G	0.5950	0.1470
5H	0.6030	0.1240
5I	0.5860	0.1480
5J	0.5910	0.1380
5K	0.5930	0.1330
5L	0.5990	0.1400
5M	0.5720	0.1260
5N	0.5120	0.1100
5O	0.4730	0.1060
M	0.7210	0.1620