



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 03:54 PM UTC

PDB ID : 7ADZ / pdb_00007adz
EMDB ID : EMD-11734
Title : Cryo-EM structure of an extracellular contractile injection system in marine bacterium *Algoriphagus machipongonensis*, the cap portion in extended state.
Authors : Xu, J.; Ericson, C.; Feldmueller, M.; Lien, Y.W.; Pilhofer, M.
Deposited on : 2020-09-17
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

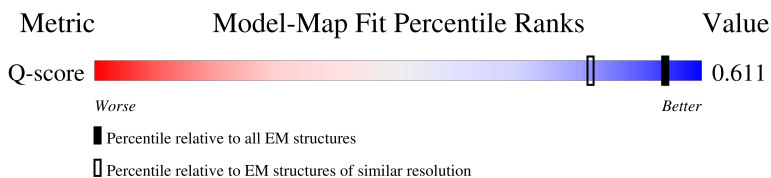
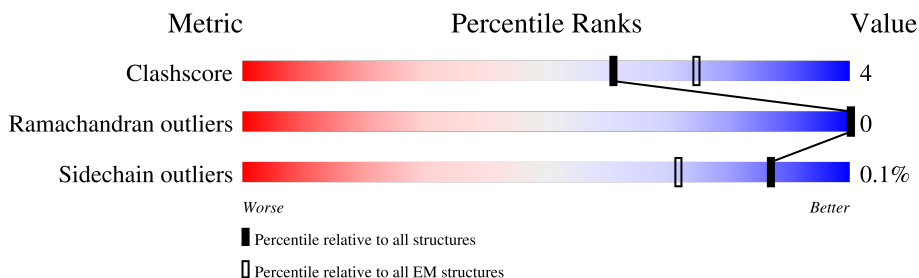
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



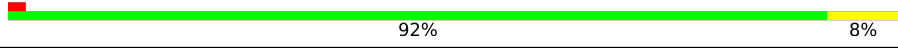
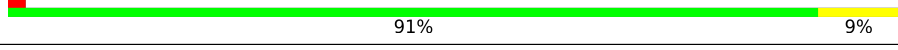
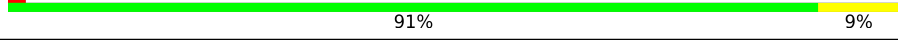
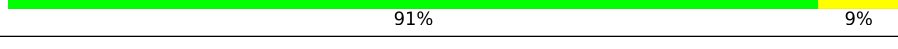
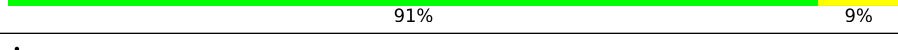
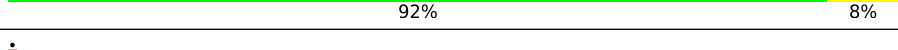
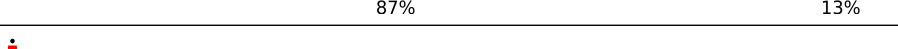
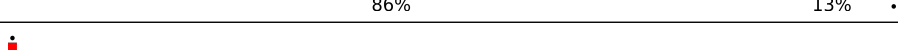
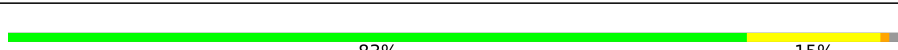
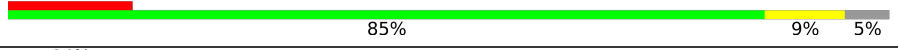
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	0A	197	
1	0B	197	
1	0C	197	
1	0D	197	

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Mol	Chain	Length	Quality of chain
1	0E	197	
1	0F	197	
2	1A	284	
2	1B	284	
2	1C	284	
2	1D	284	
2	1E	284	
2	1F	284	
3	1a	142	
3	1b	142	
3	1c	142	
3	1d	142	
3	1e	142	
3	1f	142	
3	2a	142	
3	2b	142	
3	2c	142	
3	2d	142	
3	2e	142	
3	2f	142	
4	2A	692	
4	2B	692	
4	2C	692	
4	2D	692	
4	2E	692	

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Mol	Chain	Length	Quality of chain
4	2F	692	14% 85% 9% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 67794 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 cap protein (Algo1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0A	197	Total	C	N	O	S	0	0
			1615	1030	265	313	7		
1	0B	197	Total	C	N	O	S	0	0
			1615	1030	265	313	7		
1	0C	197	Total	C	N	O	S	0	0
			1615	1030	265	313	7		
1	0D	197	Total	C	N	O	S	0	0
			1615	1030	265	313	7		
1	0E	197	Total	C	N	O	S	0	0
			1615	1030	265	313	7		
1	0F	197	Total	C	N	O	S	0	0
			1615	1030	265	313	7		

- Molecule 2 is a protein called cap adaptor protein (Algo2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1A	284	Total	C	N	O	S	0	0
			2337	1512	373	446	6		
2	1B	284	Total	C	N	O	S	0	0
			2337	1512	373	446	6		
2	1C	284	Total	C	N	O	S	0	0
			2337	1512	373	446	6		
2	1D	284	Total	C	N	O	S	0	0
			2337	1512	373	446	6		
2	1E	284	Total	C	N	O	S	0	0
			2337	1512	373	446	6		
2	1F	284	Total	C	N	O	S	0	0
			2337	1512	373	446	6		

- Molecule 3 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1a	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	1b	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	1c	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	1d	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	1e	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	1f	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	2a	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	2b	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	2c	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	2d	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	2e	141	Total 1145	C 731	N 190	O 221	S 3	0	0
3	2f	141	Total 1145	C 731	N 190	O 221	S 3	0	0

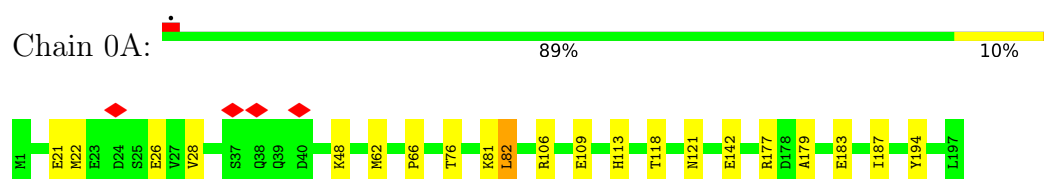
- Molecule 4 is a protein called Putative phage tail sheath protein FI.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2A	655	Total 5057	C 3204	N 832	O 1009	S 12	0	0
4	2B	655	Total 5057	C 3204	N 832	O 1009	S 12	0	0
4	2C	655	Total 5057	C 3204	N 832	O 1009	S 12	0	0
4	2D	655	Total 5057	C 3204	N 832	O 1009	S 12	0	0
4	2E	655	Total 5057	C 3204	N 832	O 1009	S 12	0	0
4	2F	655	Total 5057	C 3204	N 832	O 1009	S 12	0	0

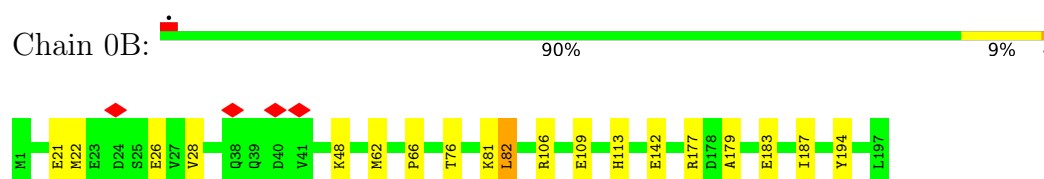
3 Residue-property plots [i](#)

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.

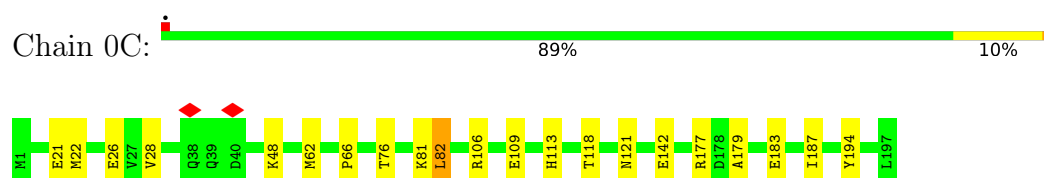
- Molecule 1: cap protein (Algo1)



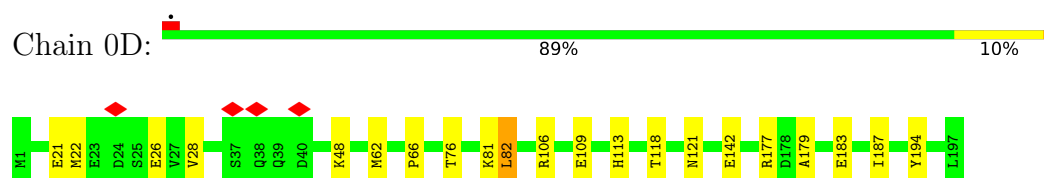
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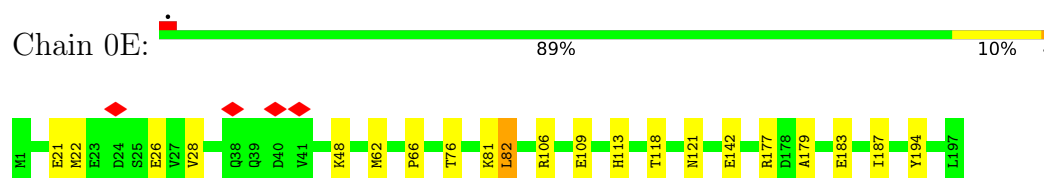
- Molecule 1: cap protein (Algo1)



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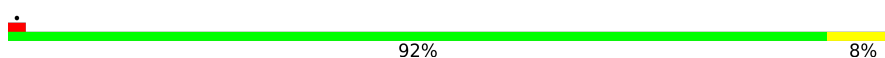


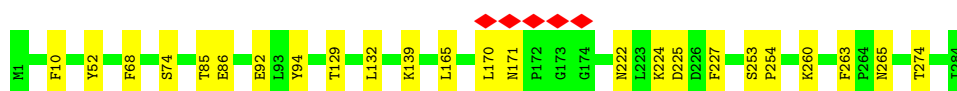
- Molecule 1: cap protein (Algo1)

Chain 0F:  89% 10%

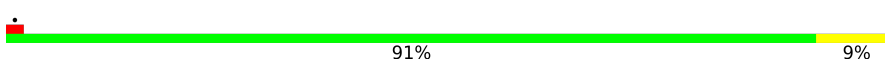


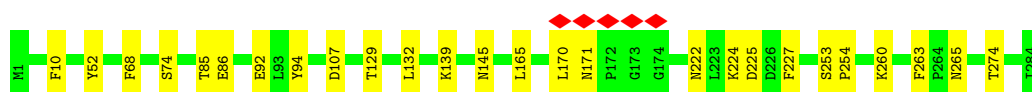
- Molecule 2: cap adaptor protein (Algo2)

Chain 1A:  92% 8%

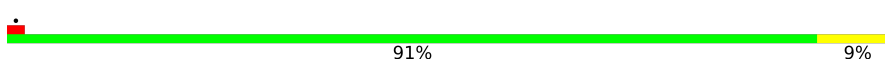


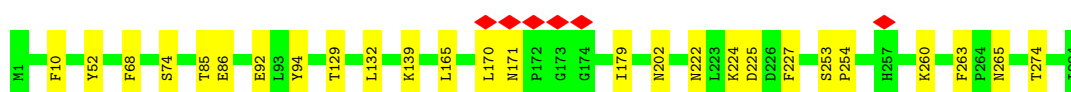
- Molecule 2: cap adaptor protein (Algo2)

Chain 1B:  91% 9%

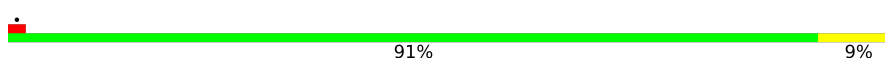


- Molecule 2: cap adaptor protein (Algo2)

Chain 1C:  91% 9%

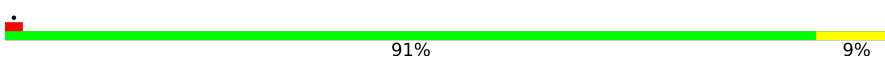


- Molecule 2: cap adaptor protein (Algo2)

Chain 1D:  91% 9%

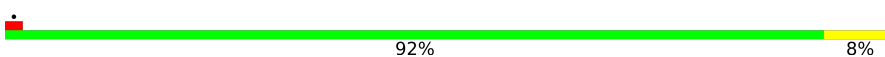


- Molecule 2: cap adaptor protein (Algo2)

Chain 1E:  91% 9%

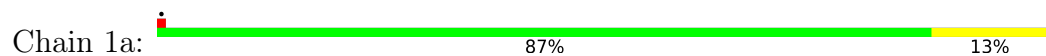


- Molecule 2: cap adaptor protein (Algo2)

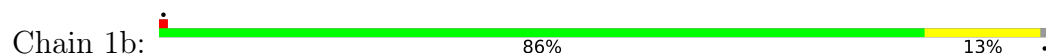
Chain 1F:  92% 8%



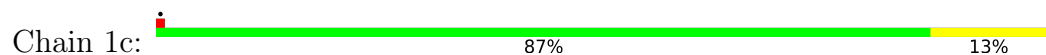
- Molecule 3: Phage tail protein



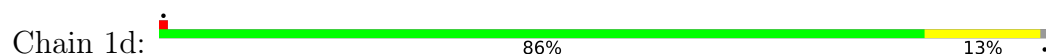
- Molecule 3: Phage tail protein



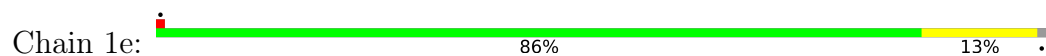
- Molecule 3: Phage tail protein



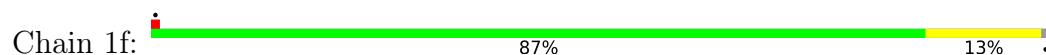
- Molecule 3: Phage tail protein



- Molecule 3: Phage tail protein



- Molecule 3: Phage tail protein



- Molecule 3: Phage tail protein

Chain 2a:  83% 15% ..



• Molecule 3: Phage tail protein

Chain 2b:  83% 15% ..



• Molecule 3: Phage tail protein

Chain 2c:  83% 15% ..



• Molecule 3: Phage tail protein

Chain 2d:  83% 15% ..



• Molecule 3: Phage tail protein

Chain 2e:  84% 15% ..



• Molecule 3: Phage tail protein

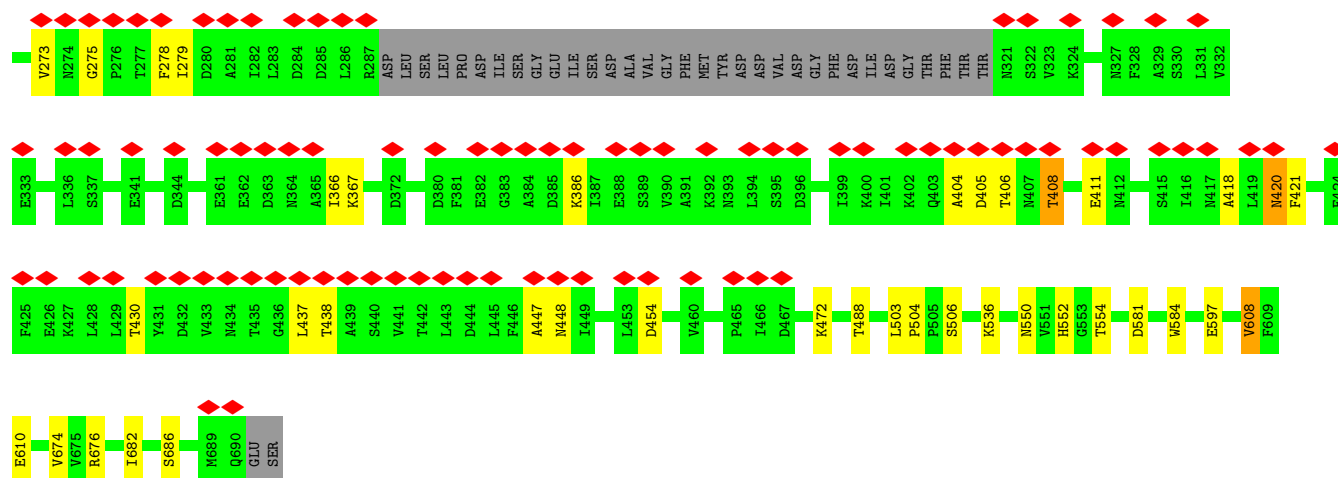
Chain 2f:  83% 15% ..



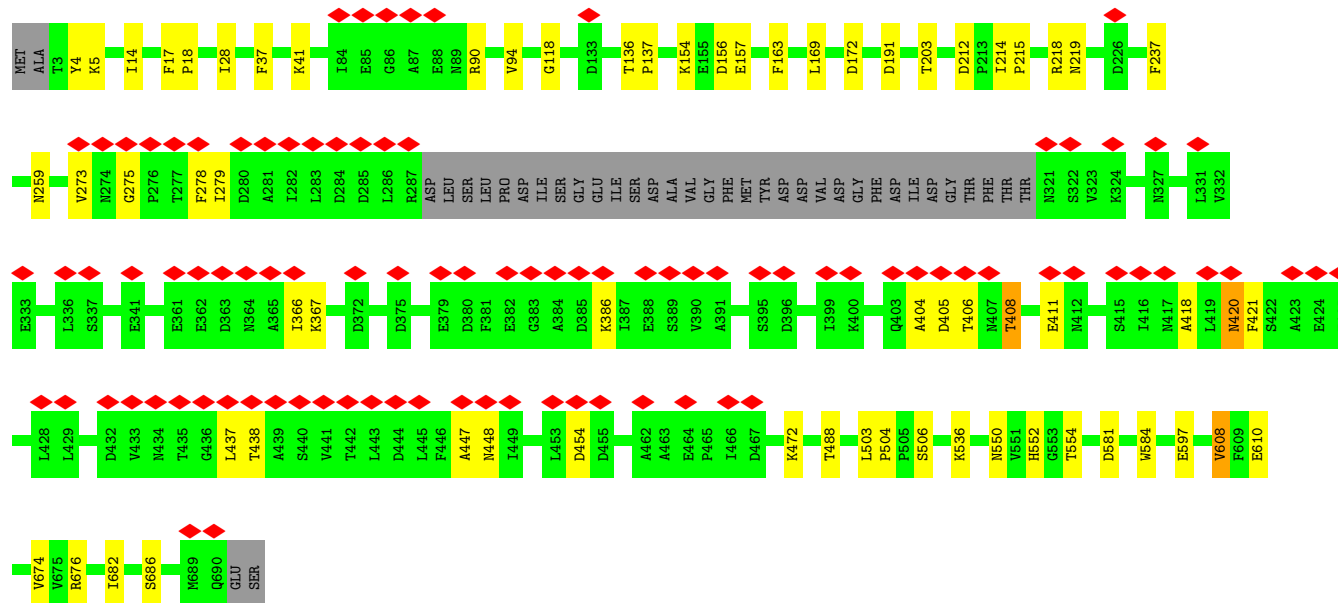
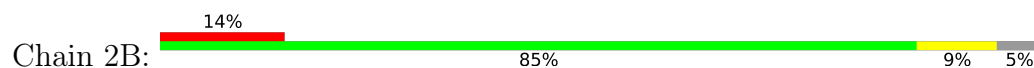
• Molecule 4: Putative phage tail sheath protein FI

Chain 2A:  14% 85% 9% • 5%

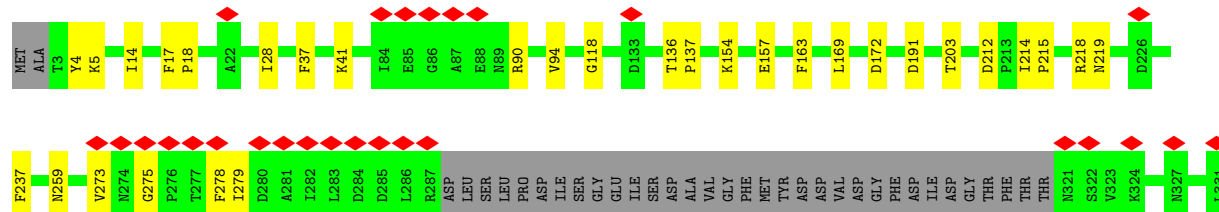
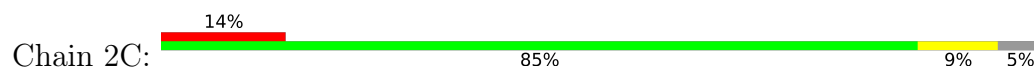


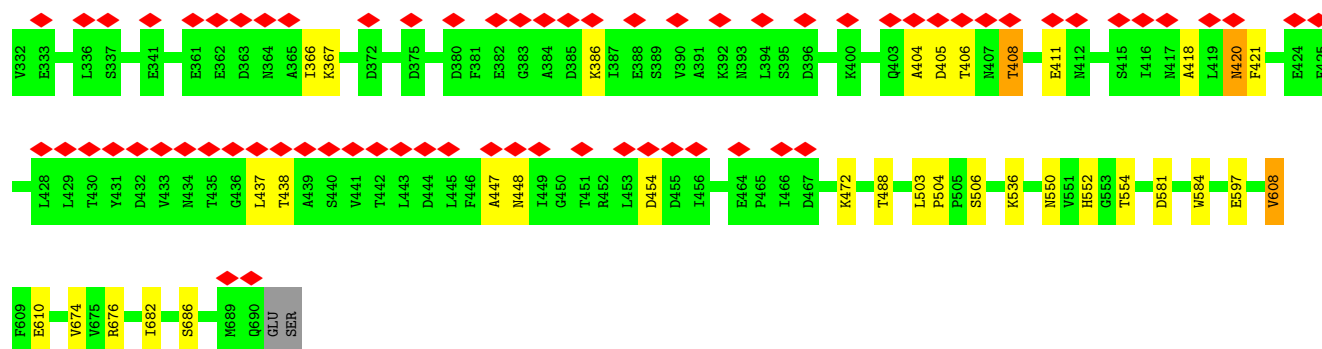


• Molecule 4: Putative phage tail sheath protein FI

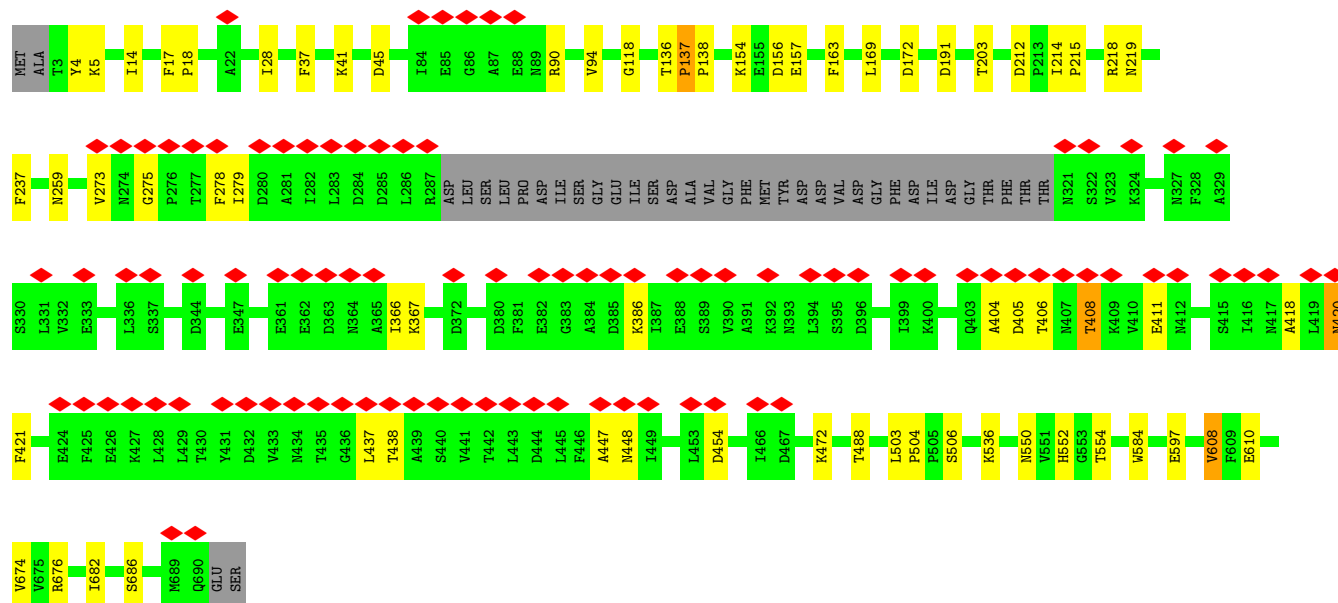
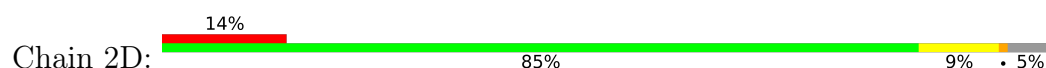


• Molecule 4: Putative phage tail sheath protein FI

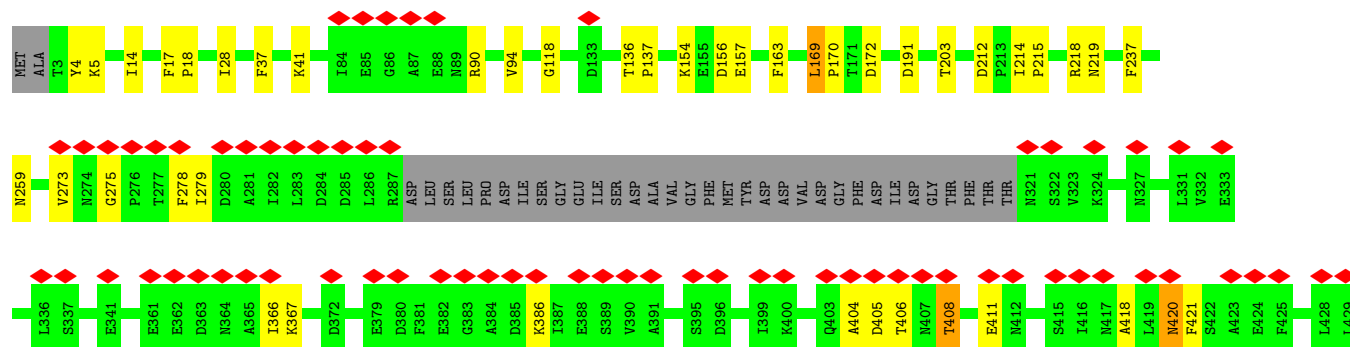
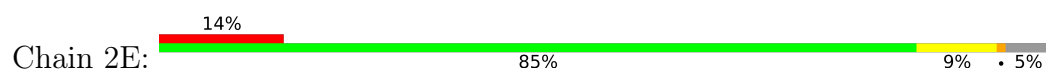


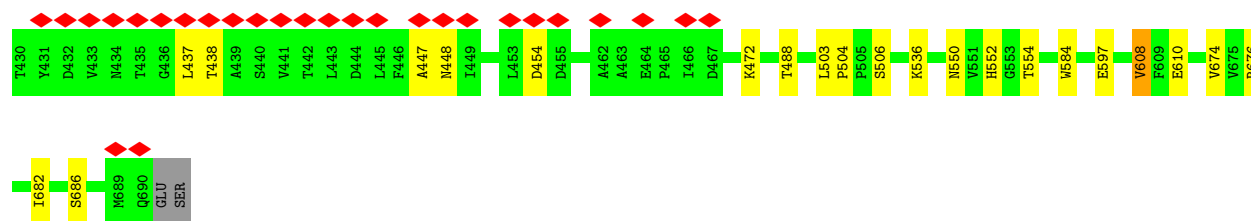


• Molecule 4: Putative phage tail sheath protein FI

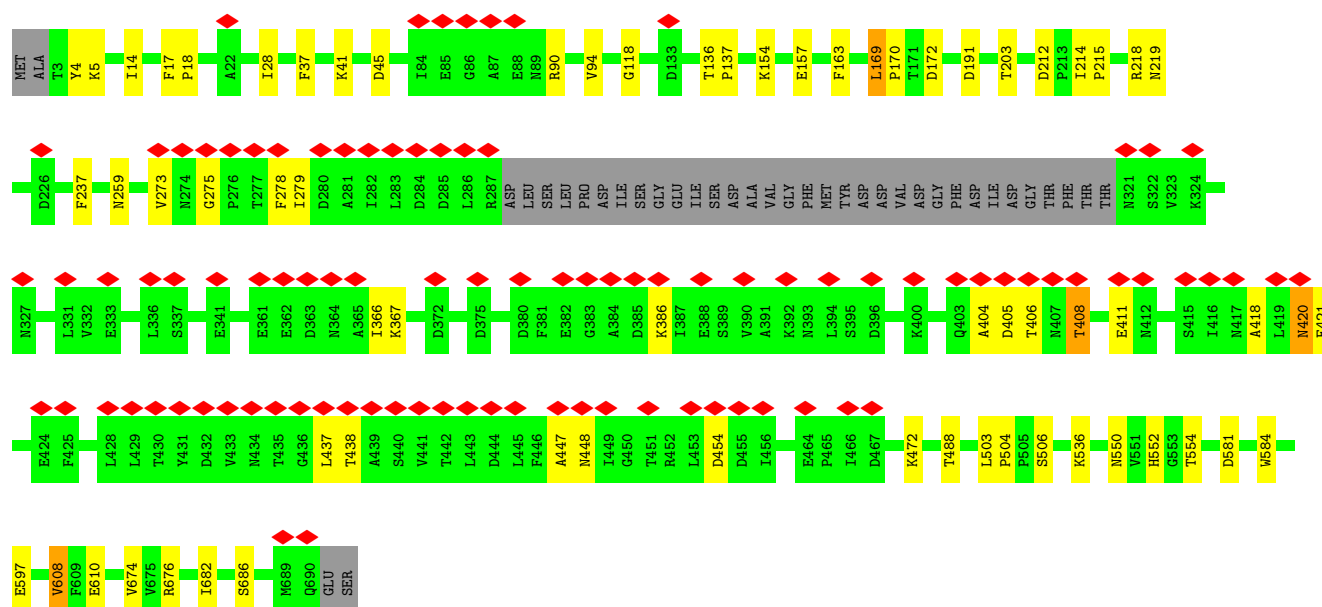
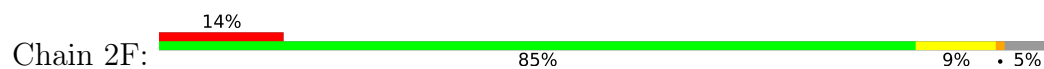


• Molecule 4: Putative phage tail sheath protein FI





• Molecule 4: Putative phage tail sheath protein FI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65059	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0A	0.45	2/1642 (0.1%)	0.83	6/2219 (0.3%)
1	0B	0.45	2/1642 (0.1%)	0.84	6/2219 (0.3%)
1	0C	0.45	2/1642 (0.1%)	0.83	6/2219 (0.3%)
1	0D	0.45	2/1642 (0.1%)	0.83	6/2219 (0.3%)
1	0E	0.45	2/1642 (0.1%)	0.84	6/2219 (0.3%)
1	0F	0.45	2/1642 (0.1%)	0.83	6/2219 (0.3%)
2	1A	0.83	0/2398	1.18	23/3235 (0.7%)
2	1B	0.83	0/2398	1.18	23/3235 (0.7%)
2	1C	0.83	0/2398	1.18	23/3235 (0.7%)
2	1D	0.83	0/2398	1.18	23/3235 (0.7%)
2	1E	0.83	0/2398	1.18	23/3235 (0.7%)
2	1F	0.83	0/2398	1.18	23/3235 (0.7%)
3	1a	0.37	0/1172	0.61	0/1584
3	1b	0.37	0/1172	0.61	0/1584
3	1c	0.37	0/1172	0.61	0/1584
3	1d	0.37	0/1172	0.61	0/1584
3	1e	0.37	0/1172	0.61	0/1584
3	1f	0.37	0/1172	0.61	0/1584
3	2a	0.90	0/1172	1.30	16/1584 (1.0%)
3	2b	0.90	0/1172	1.30	16/1584 (1.0%)
3	2c	0.90	0/1172	1.30	16/1584 (1.0%)
3	2d	0.90	0/1172	1.30	16/1584 (1.0%)
3	2e	0.90	0/1172	1.30	16/1584 (1.0%)
3	2f	0.90	0/1172	1.30	16/1584 (1.0%)
4	2A	0.88	0/5155	1.24	56/7021 (0.8%)
4	2B	0.88	0/5155	1.24	55/7021 (0.8%)
4	2C	0.88	0/5155	1.24	55/7021 (0.8%)
4	2D	0.88	0/5155	1.24	55/7021 (0.8%)
4	2E	0.88	0/5155	1.24	55/7021 (0.8%)
4	2F	0.88	0/5155	1.24	55/7021 (0.8%)
All	All	0.78	12/69234 (0.0%)	1.13	601/93858 (0.6%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0F	82	LEU	C-N	-12.15	1.17	1.33
1	0B	82	LEU	C-N	-12.10	1.17	1.33
1	0E	82	LEU	C-N	-12.10	1.17	1.33
1	0A	82	LEU	C-N	-12.07	1.17	1.33
1	0D	82	LEU	C-N	-12.07	1.17	1.33
1	0C	82	LEU	C-N	-12.05	1.17	1.33
1	0E	81	LYS	C-N	-9.04	1.20	1.33
1	0C	81	LYS	C-N	-9.03	1.20	1.33
1	0F	81	LYS	C-N	-9.01	1.20	1.33
1	0B	81	LYS	C-N	-9.00	1.20	1.33
1	0A	81	LYS	C-N	-8.98	1.20	1.33
1	0D	81	LYS	C-N	-8.96	1.20	1.33

All (601) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0B	82	LEU	O-C-N	-19.60	100.59	123.13
1	0E	82	LEU	O-C-N	-19.59	100.61	123.13
1	0F	82	LEU	O-C-N	-19.57	100.62	123.13
1	0A	82	LEU	O-C-N	-19.55	100.64	123.13
1	0D	82	LEU	O-C-N	-19.55	100.64	123.13
1	0C	82	LEU	O-C-N	-19.54	100.66	123.13
1	0B	81	LYS	CA-C-N	12.27	138.86	122.30
1	0B	81	LYS	C-N-CA	12.27	138.86	122.30
1	0F	81	LYS	CA-C-N	12.25	138.84	122.30
1	0F	81	LYS	C-N-CA	12.25	138.84	122.30
1	0E	81	LYS	CA-C-N	12.23	138.81	122.30
1	0E	81	LYS	C-N-CA	12.23	138.81	122.30
1	0C	81	LYS	CA-C-N	12.23	138.81	122.30
1	0C	81	LYS	C-N-CA	12.23	138.81	122.30
1	0D	81	LYS	CA-C-N	12.19	138.76	122.30
1	0D	81	LYS	C-N-CA	12.19	138.76	122.30
1	0A	81	LYS	CA-C-N	12.18	138.74	122.30
1	0A	81	LYS	C-N-CA	12.18	138.74	122.30
3	2c	109	TRP	CA-C-N	9.63	131.88	119.84
3	2c	109	TRP	C-N-CA	9.63	131.88	119.84
3	2f	109	TRP	CA-C-N	9.63	131.88	119.84
3	2f	109	TRP	C-N-CA	9.63	131.88	119.84
3	2b	109	TRP	CA-C-N	9.63	131.88	119.84
3	2b	109	TRP	C-N-CA	9.63	131.88	119.84
3	2a	109	TRP	CA-C-N	9.63	131.87	119.84
3	2a	109	TRP	C-N-CA	9.63	131.87	119.84
3	2d	109	TRP	CA-C-N	9.61	131.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2d	109	TRP	C-N-CA	9.61	131.85	119.84
3	2e	109	TRP	CA-C-N	9.60	131.84	119.84
3	2e	109	TRP	C-N-CA	9.60	131.84	119.84
1	0B	82	LEU	CA-C-N	9.45	136.31	122.99
1	0B	82	LEU	C-N-CA	9.45	136.31	122.99
1	0E	82	LEU	CA-C-N	9.43	136.28	122.99
1	0E	82	LEU	C-N-CA	9.43	136.28	122.99
1	0F	82	LEU	CA-C-N	9.42	136.28	122.99
1	0F	82	LEU	C-N-CA	9.42	136.28	122.99
1	0D	82	LEU	CA-C-N	9.40	136.24	122.99
1	0D	82	LEU	C-N-CA	9.40	136.24	122.99
1	0A	82	LEU	CA-C-N	9.39	136.24	122.99
1	0A	82	LEU	C-N-CA	9.39	136.24	122.99
1	0C	82	LEU	CA-C-N	9.38	136.21	122.99
1	0C	82	LEU	C-N-CA	9.38	136.21	122.99
4	2D	420	ASN	N-CA-C	9.01	124.00	112.92
4	2C	420	ASN	N-CA-C	9.00	123.98	112.92
4	2A	420	ASN	N-CA-C	8.97	123.96	112.92
4	2B	420	ASN	N-CA-C	8.97	123.96	112.92
4	2E	420	ASN	N-CA-C	8.97	123.96	112.92
4	2F	420	ASN	N-CA-C	8.94	123.92	112.92
2	1C	253	SER	CA-C-N	8.78	126.07	119.66
2	1C	253	SER	C-N-CA	8.78	126.07	119.66
2	1F	253	SER	CA-C-N	8.72	126.03	119.66
2	1F	253	SER	C-N-CA	8.72	126.03	119.66
4	2E	137	PRO	CA-C-N	8.72	129.25	119.92
4	2E	137	PRO	C-N-CA	8.72	129.25	119.92
4	2F	137	PRO	CA-C-N	8.71	129.24	119.92
4	2F	137	PRO	C-N-CA	8.71	129.24	119.92
4	2D	137	PRO	CA-C-N	8.70	129.23	119.92
4	2D	137	PRO	C-N-CA	8.70	129.23	119.92
4	2B	137	PRO	CA-C-N	8.69	129.22	119.92
4	2B	137	PRO	C-N-CA	8.69	129.22	119.92
4	2C	137	PRO	CA-C-N	8.69	129.22	119.92
4	2C	137	PRO	C-N-CA	8.69	129.22	119.92
4	2A	137	PRO	CA-C-N	8.66	129.19	119.92
4	2A	137	PRO	C-N-CA	8.66	129.19	119.92
2	1A	253	SER	CA-C-N	8.65	125.97	119.66
2	1A	253	SER	C-N-CA	8.65	125.97	119.66
2	1B	253	SER	CA-C-N	8.62	125.95	119.66
2	1B	253	SER	C-N-CA	8.62	125.95	119.66
2	1E	253	SER	CA-C-N	8.62	125.95	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1E	253	SER	C-N-CA	8.62	125.95	119.66
2	1D	253	SER	CA-C-N	8.61	125.94	119.66
2	1D	253	SER	C-N-CA	8.61	125.94	119.66
4	2E	503	LEU	CA-C-N	8.25	125.68	119.66
4	2E	503	LEU	C-N-CA	8.25	125.68	119.66
4	2A	503	LEU	CA-C-N	8.19	125.64	119.66
4	2A	503	LEU	C-N-CA	8.19	125.64	119.66
4	2C	503	LEU	CA-C-N	8.16	125.62	119.66
4	2C	503	LEU	C-N-CA	8.16	125.62	119.66
4	2F	503	LEU	CA-C-N	8.16	125.62	119.66
4	2F	503	LEU	C-N-CA	8.16	125.62	119.66
4	2B	503	LEU	CA-C-N	8.15	125.61	119.66
4	2B	503	LEU	C-N-CA	8.15	125.61	119.66
4	2D	503	LEU	CA-C-N	8.15	125.61	119.66
4	2D	503	LEU	C-N-CA	8.15	125.61	119.66
1	0B	81	LYS	O-C-N	-8.03	113.89	122.96
1	0F	81	LYS	O-C-N	-7.99	113.93	122.96
1	0E	81	LYS	O-C-N	-7.96	113.96	122.96
1	0C	81	LYS	O-C-N	-7.96	113.96	122.96
1	0D	81	LYS	O-C-N	-7.94	113.99	122.96
1	0A	81	LYS	O-C-N	-7.94	113.99	122.96
2	1B	263	PHE	CA-C-N	7.76	127.77	119.78
2	1B	263	PHE	C-N-CA	7.76	127.77	119.78
4	2B	676	ARG	CA-C-N	7.75	127.90	120.31
4	2B	676	ARG	C-N-CA	7.75	127.90	120.31
2	1E	263	PHE	CA-C-N	7.74	127.75	119.78
2	1E	263	PHE	C-N-CA	7.74	127.75	119.78
2	1C	263	PHE	CA-C-N	7.73	127.74	119.78
2	1C	263	PHE	C-N-CA	7.73	127.74	119.78
4	2F	676	ARG	CA-C-N	7.72	127.88	120.31
4	2F	676	ARG	C-N-CA	7.72	127.88	120.31
4	2E	676	ARG	CA-C-N	7.71	127.87	120.31
4	2E	676	ARG	C-N-CA	7.71	127.87	120.31
4	2A	676	ARG	CA-C-N	7.71	127.87	120.31
4	2A	676	ARG	C-N-CA	7.71	127.87	120.31
2	1F	263	PHE	CA-C-N	7.71	127.72	119.78
2	1F	263	PHE	C-N-CA	7.71	127.72	119.78
2	1A	263	PHE	CA-C-N	7.71	127.72	119.78
2	1A	263	PHE	C-N-CA	7.71	127.72	119.78
4	2C	676	ARG	CA-C-N	7.70	127.86	120.31
4	2C	676	ARG	C-N-CA	7.70	127.86	120.31
4	2D	676	ARG	CA-C-N	7.70	127.85	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2D	676	ARG	C-N-CA	7.70	127.85	120.31
2	1D	263	PHE	CA-C-N	7.67	127.68	119.78
2	1D	263	PHE	C-N-CA	7.67	127.68	119.78
4	2E	17	PHE	CA-C-N	7.55	125.17	119.66
4	2E	17	PHE	C-N-CA	7.55	125.17	119.66
4	2C	17	PHE	CA-C-N	7.52	125.15	119.66
4	2C	17	PHE	C-N-CA	7.52	125.15	119.66
4	2A	17	PHE	CA-C-N	7.52	125.15	119.66
4	2A	17	PHE	C-N-CA	7.52	125.15	119.66
4	2F	17	PHE	CA-C-N	7.50	125.14	119.66
4	2F	17	PHE	C-N-CA	7.50	125.14	119.66
4	2B	17	PHE	CA-C-N	7.48	125.12	119.66
4	2B	17	PHE	C-N-CA	7.48	125.12	119.66
4	2D	17	PHE	CA-C-N	7.46	125.10	119.66
4	2D	17	PHE	C-N-CA	7.46	125.10	119.66
3	2d	41	SER	CA-C-N	7.32	127.03	119.56
3	2d	41	SER	C-N-CA	7.32	127.03	119.56
3	2b	41	SER	CA-C-N	7.30	127.01	119.56
3	2b	41	SER	C-N-CA	7.30	127.01	119.56
3	2e	41	SER	CA-C-N	7.29	127.00	119.56
3	2e	41	SER	C-N-CA	7.29	127.00	119.56
3	2a	41	SER	CA-C-N	7.29	126.99	119.56
3	2a	41	SER	C-N-CA	7.29	126.99	119.56
3	2c	41	SER	CA-C-N	7.24	126.95	119.56
3	2c	41	SER	C-N-CA	7.24	126.95	119.56
3	2f	41	SER	CA-C-N	7.24	126.95	119.56
3	2f	41	SER	C-N-CA	7.24	126.95	119.56
4	2D	169	LEU	CA-C-N	7.20	127.83	119.47
4	2D	169	LEU	C-N-CA	7.20	127.83	119.47
4	2C	169	LEU	CA-C-N	7.18	127.80	119.47
4	2C	169	LEU	C-N-CA	7.18	127.80	119.47
4	2E	169	LEU	CA-C-N	7.17	127.79	119.47
4	2E	169	LEU	C-N-CA	7.17	127.79	119.47
4	2F	169	LEU	CA-C-N	7.17	127.79	119.47
4	2F	169	LEU	C-N-CA	7.17	127.79	119.47
4	2D	448	ASN	CA-C-N	7.17	130.28	120.46
4	2D	448	ASN	C-N-CA	7.17	130.28	120.46
4	2A	169	LEU	CA-C-N	7.16	127.78	119.47
4	2A	169	LEU	C-N-CA	7.16	127.78	119.47
4	2B	448	ASN	CA-C-N	7.15	130.26	120.46
4	2B	448	ASN	C-N-CA	7.15	130.26	120.46
4	2B	169	LEU	CA-C-N	7.15	127.76	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2B	169	LEU	C-N-CA	7.15	127.76	119.47
4	2E	448	ASN	CA-C-N	7.14	130.24	120.46
4	2E	448	ASN	C-N-CA	7.14	130.24	120.46
4	2A	448	ASN	CA-C-N	7.12	130.21	120.46
4	2A	448	ASN	C-N-CA	7.12	130.21	120.46
4	2F	448	ASN	CA-C-N	7.10	130.19	120.46
4	2F	448	ASN	C-N-CA	7.10	130.19	120.46
4	2C	448	ASN	CA-C-N	7.10	130.19	120.46
4	2C	448	ASN	C-N-CA	7.10	130.19	120.46
4	2D	418	ALA	N-CA-C	-7.10	105.15	113.88
4	2E	418	ALA	N-CA-C	-7.08	105.18	113.88
4	2B	418	ALA	N-CA-C	-7.06	105.19	113.88
4	2A	418	ALA	N-CA-C	-7.06	105.20	113.88
4	2F	418	ALA	N-CA-C	-7.06	105.20	113.88
4	2C	418	ALA	N-CA-C	-7.05	105.21	113.88
3	2d	70	GLU	N-CA-C	7.01	118.92	111.28
3	2a	70	GLU	N-CA-C	7.00	118.91	111.28
3	2b	70	GLU	N-CA-C	6.97	118.88	111.28
3	2e	70	GLU	N-CA-C	6.97	118.88	111.28
3	2f	70	GLU	N-CA-C	6.95	118.86	111.28
3	2c	70	GLU	N-CA-C	6.94	118.84	111.28
4	2D	94	VAL	CA-C-N	6.90	127.07	120.31
4	2D	94	VAL	C-N-CA	6.90	127.07	120.31
4	2B	94	VAL	CA-C-N	6.89	127.07	120.31
4	2B	94	VAL	C-N-CA	6.89	127.07	120.31
4	2E	94	VAL	CA-C-N	6.89	127.06	120.31
4	2E	94	VAL	C-N-CA	6.89	127.06	120.31
4	2A	94	VAL	CA-C-N	6.86	127.03	120.31
4	2A	94	VAL	C-N-CA	6.86	127.03	120.31
4	2C	94	VAL	CA-C-N	6.84	127.02	120.31
4	2C	94	VAL	C-N-CA	6.84	127.02	120.31
4	2F	94	VAL	CA-C-N	6.84	127.02	120.31
4	2F	94	VAL	C-N-CA	6.84	127.02	120.31
4	2B	536	LYS	CA-C-N	6.78	126.77	119.78
4	2B	536	LYS	C-N-CA	6.78	126.77	119.78
4	2A	536	LYS	CA-C-N	6.78	126.76	119.78
4	2A	536	LYS	C-N-CA	6.78	126.76	119.78
4	2D	536	LYS	CA-C-N	6.77	126.76	119.78
4	2D	536	LYS	C-N-CA	6.77	126.76	119.78
4	2C	536	LYS	CA-C-N	6.76	126.74	119.78
4	2C	536	LYS	C-N-CA	6.76	126.74	119.78
3	2f	3	TYR	CA-C-N	6.74	126.70	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2f	3	TYR	C-N-CA	6.74	126.70	120.03
4	2E	536	LYS	CA-C-N	6.74	126.72	119.78
4	2E	536	LYS	C-N-CA	6.74	126.72	119.78
2	1E	52	TYR	CA-C-N	6.73	126.64	119.85
2	1E	52	TYR	C-N-CA	6.73	126.64	119.85
4	2F	536	LYS	CA-C-N	6.71	126.69	119.78
4	2F	536	LYS	C-N-CA	6.71	126.69	119.78
2	1B	52	TYR	CA-C-N	6.71	126.63	119.85
2	1B	52	TYR	C-N-CA	6.71	126.63	119.85
3	2b	3	TYR	CA-C-N	6.68	126.65	120.03
3	2b	3	TYR	C-N-CA	6.68	126.65	120.03
3	2c	3	TYR	CA-C-N	6.68	126.65	120.03
3	2c	3	TYR	C-N-CA	6.68	126.65	120.03
2	1C	52	TYR	CA-C-N	6.68	126.60	119.85
2	1C	52	TYR	C-N-CA	6.68	126.60	119.85
2	1A	52	TYR	CA-C-N	6.68	126.60	119.85
2	1A	52	TYR	C-N-CA	6.68	126.60	119.85
3	2a	3	TYR	CA-C-N	6.68	126.64	120.03
3	2a	3	TYR	C-N-CA	6.68	126.64	120.03
3	2d	3	TYR	CA-C-N	6.68	126.64	120.03
3	2d	3	TYR	C-N-CA	6.68	126.64	120.03
3	2e	3	TYR	CA-C-N	6.68	126.64	120.03
3	2e	3	TYR	C-N-CA	6.68	126.64	120.03
4	2D	408	THR	N-CA-C	6.67	118.66	108.52
4	2C	408	THR	N-CA-C	6.67	118.65	108.52
4	2E	408	THR	N-CA-C	6.66	118.65	108.52
2	1D	52	TYR	CA-C-N	6.66	126.58	119.85
2	1D	52	TYR	C-N-CA	6.66	126.58	119.85
4	2A	408	THR	N-CA-C	6.66	118.64	108.52
4	2B	408	THR	N-CA-C	6.66	118.64	108.52
4	2F	408	THR	N-CA-C	6.65	118.63	108.52
4	2D	118	GLY	CA-C-N	6.65	126.62	119.78
4	2D	118	GLY	C-N-CA	6.65	126.62	119.78
2	1F	52	TYR	CA-C-N	6.64	126.56	119.85
2	1F	52	TYR	C-N-CA	6.64	126.56	119.85
4	2C	118	GLY	CA-C-N	6.64	126.62	119.78
4	2C	118	GLY	C-N-CA	6.64	126.62	119.78
4	2A	118	GLY	CA-C-N	6.63	126.61	119.78
4	2A	118	GLY	C-N-CA	6.63	126.61	119.78
4	2B	118	GLY	CA-C-N	6.61	126.59	119.78
4	2B	118	GLY	C-N-CA	6.61	126.59	119.78
4	2F	118	GLY	CA-C-N	6.60	126.58	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2F	118	GLY	C-N-CA	6.60	126.58	119.78
4	2E	118	GLY	CA-C-N	6.58	126.55	119.78
4	2E	118	GLY	C-N-CA	6.58	126.55	119.78
2	1D	254	PRO	CA-C-N	6.49	126.41	119.85
2	1D	254	PRO	C-N-CA	6.49	126.41	119.85
4	2F	163	PHE	CA-C-N	6.49	127.00	119.47
4	2F	163	PHE	C-N-CA	6.49	127.00	119.47
2	1A	254	PRO	CA-C-N	6.49	126.40	119.85
2	1A	254	PRO	C-N-CA	6.49	126.40	119.85
4	2D	163	PHE	CA-C-N	6.49	127.00	119.47
4	2D	163	PHE	C-N-CA	6.49	127.00	119.47
4	2A	163	PHE	CA-C-N	6.48	126.99	119.47
4	2A	163	PHE	C-N-CA	6.48	126.99	119.47
4	2E	163	PHE	CA-C-N	6.47	126.98	119.47
4	2E	163	PHE	C-N-CA	6.47	126.98	119.47
4	2C	163	PHE	CA-C-N	6.46	126.97	119.47
4	2C	163	PHE	C-N-CA	6.46	126.97	119.47
4	2B	163	PHE	CA-C-N	6.46	126.96	119.47
4	2B	163	PHE	C-N-CA	6.46	126.96	119.47
4	2E	136	THR	CA-C-N	6.45	127.03	120.38
4	2E	136	THR	C-N-CA	6.45	127.03	120.38
2	1E	254	PRO	CA-C-N	6.43	126.35	119.85
2	1E	254	PRO	C-N-CA	6.43	126.35	119.85
2	1B	254	PRO	CA-C-N	6.43	126.34	119.85
2	1B	254	PRO	C-N-CA	6.43	126.34	119.85
4	2B	136	THR	CA-C-N	6.43	127.00	120.38
4	2B	136	THR	C-N-CA	6.43	127.00	120.38
2	1C	254	PRO	CA-C-N	6.42	126.33	119.85
2	1C	254	PRO	C-N-CA	6.42	126.33	119.85
4	2D	136	THR	CA-C-N	6.42	126.99	120.38
4	2D	136	THR	C-N-CA	6.42	126.99	120.38
2	1F	254	PRO	CA-C-N	6.41	126.32	119.85
2	1F	254	PRO	C-N-CA	6.41	126.32	119.85
4	2C	136	THR	CA-C-N	6.40	126.97	120.38
4	2C	136	THR	C-N-CA	6.40	126.97	120.38
4	2A	136	THR	CA-C-N	6.40	126.97	120.38
4	2A	136	THR	C-N-CA	6.40	126.97	120.38
4	2F	136	THR	CA-C-N	6.40	126.97	120.38
4	2F	136	THR	C-N-CA	6.40	126.97	120.38
2	1A	132	LEU	CA-C-N	6.39	126.08	119.56
2	1A	132	LEU	C-N-CA	6.39	126.08	119.56
2	1C	132	LEU	CA-C-N	6.39	126.08	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1C	132	LEU	C-N-CA	6.39	126.08	119.56
2	1D	74	SER	N-CA-C	6.39	117.85	108.14
4	2F	275	GLY	CA-C-N	6.38	126.07	119.56
4	2F	275	GLY	C-N-CA	6.38	126.07	119.56
2	1C	74	SER	N-CA-C	6.37	117.83	108.14
2	1A	74	SER	N-CA-C	6.37	117.82	108.14
4	2E	275	GLY	CA-C-N	6.37	126.06	119.56
4	2E	275	GLY	C-N-CA	6.37	126.06	119.56
2	1B	132	LEU	CA-C-N	6.36	126.05	119.56
2	1B	132	LEU	C-N-CA	6.36	126.05	119.56
2	1E	274	THR	CA-C-N	6.36	126.05	119.56
2	1E	274	THR	C-N-CA	6.36	126.05	119.56
4	2A	275	GLY	CA-C-N	6.36	126.05	119.56
4	2A	275	GLY	C-N-CA	6.36	126.05	119.56
2	1F	74	SER	N-CA-C	6.36	117.81	108.14
4	2B	420	ASN	CA-C-N	-6.36	111.76	120.28
4	2B	420	ASN	C-N-CA	-6.36	111.76	120.28
4	2E	420	ASN	CA-C-N	-6.36	111.76	120.28
4	2E	420	ASN	C-N-CA	-6.36	111.76	120.28
2	1E	74	SER	N-CA-C	6.36	117.80	108.14
2	1B	274	THR	CA-C-N	6.36	126.04	119.56
2	1B	274	THR	C-N-CA	6.36	126.04	119.56
2	1D	132	LEU	CA-C-N	6.35	126.04	119.56
2	1D	132	LEU	C-N-CA	6.35	126.04	119.56
2	1F	132	LEU	CA-C-N	6.35	126.04	119.56
2	1F	132	LEU	C-N-CA	6.35	126.04	119.56
4	2D	275	GLY	CA-C-N	6.35	126.04	119.56
4	2D	275	GLY	C-N-CA	6.35	126.04	119.56
4	2C	275	GLY	CA-C-N	6.35	126.04	119.56
4	2C	275	GLY	C-N-CA	6.35	126.04	119.56
4	2C	420	ASN	CA-C-N	-6.35	111.78	120.28
4	2C	420	ASN	C-N-CA	-6.35	111.78	120.28
4	2A	420	ASN	CA-C-N	-6.34	111.78	120.28
4	2A	420	ASN	C-N-CA	-6.34	111.78	120.28
2	1E	132	LEU	CA-C-N	6.34	126.03	119.56
2	1E	132	LEU	C-N-CA	6.34	126.03	119.56
4	2B	275	GLY	CA-C-N	6.33	126.02	119.56
4	2B	275	GLY	C-N-CA	6.33	126.02	119.56
2	1C	274	THR	CA-C-N	6.33	126.02	119.56
2	1C	274	THR	C-N-CA	6.33	126.02	119.56
2	1F	274	THR	CA-C-N	6.33	126.02	119.56
2	1F	274	THR	C-N-CA	6.33	126.02	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2D	420	ASN	CA-C-N	-6.33	111.80	120.28
4	2D	420	ASN	C-N-CA	-6.33	111.80	120.28
2	1B	74	SER	N-CA-C	6.33	117.75	108.14
2	1A	274	THR	CA-C-N	6.32	126.00	119.56
2	1A	274	THR	C-N-CA	6.32	126.00	119.56
4	2F	420	ASN	CA-C-N	-6.32	111.82	120.28
4	2F	420	ASN	C-N-CA	-6.32	111.82	120.28
2	1D	274	THR	CA-C-N	6.30	125.99	119.56
2	1D	274	THR	C-N-CA	6.30	125.99	119.56
4	2E	584	TRP	N-CA-C	6.29	120.66	112.92
4	2B	584	TRP	N-CA-C	6.29	120.65	112.92
4	2C	584	TRP	N-CA-C	6.29	120.65	112.92
4	2F	584	TRP	N-CA-C	6.29	120.65	112.92
4	2A	584	TRP	N-CA-C	6.27	120.63	112.92
4	2D	584	TRP	N-CA-C	6.27	120.63	112.92
2	1E	129	THR	CA-C-N	6.22	126.68	120.52
2	1E	129	THR	C-N-CA	6.22	126.68	120.52
2	1D	265	ASN	CA-C-N	6.22	126.41	120.31
2	1D	265	ASN	C-N-CA	6.22	126.41	120.31
2	1D	129	THR	CA-C-N	6.20	126.65	120.52
2	1D	129	THR	C-N-CA	6.20	126.65	120.52
2	1B	129	THR	CA-C-N	6.18	126.64	120.52
2	1B	129	THR	C-N-CA	6.18	126.64	120.52
2	1C	265	ASN	CA-C-N	6.18	126.37	120.31
2	1C	265	ASN	C-N-CA	6.18	126.37	120.31
2	1E	265	ASN	CA-C-N	6.18	126.36	120.31
2	1E	265	ASN	C-N-CA	6.18	126.36	120.31
2	1A	129	THR	CA-C-N	6.18	126.63	120.52
2	1A	129	THR	C-N-CA	6.18	126.63	120.52
2	1A	265	ASN	CA-C-N	6.17	126.36	120.31
2	1A	265	ASN	C-N-CA	6.17	126.36	120.31
2	1B	265	ASN	CA-C-N	6.17	126.36	120.31
2	1B	265	ASN	C-N-CA	6.17	126.36	120.31
2	1F	265	ASN	CA-C-N	6.17	126.35	120.31
2	1F	265	ASN	C-N-CA	6.17	126.35	120.31
2	1C	129	THR	CA-C-N	6.14	126.60	120.52
2	1C	129	THR	C-N-CA	6.14	126.60	120.52
3	2e	49	MET	CA-C-N	6.14	126.09	119.76
3	2e	49	MET	C-N-CA	6.14	126.09	119.76
3	2b	49	MET	CA-C-N	6.14	126.09	119.76
3	2b	49	MET	C-N-CA	6.14	126.09	119.76
3	2a	49	MET	CA-C-N	6.12	126.06	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2a	49	MET	C-N-CA	6.12	126.06	119.76
3	2c	49	MET	CA-C-N	6.12	126.06	119.76
3	2c	49	MET	C-N-CA	6.12	126.06	119.76
3	2f	49	MET	CA-C-N	6.12	126.06	119.76
3	2f	49	MET	C-N-CA	6.12	126.06	119.76
4	2D	608	VAL	N-CA-C	6.11	116.78	110.36
4	2B	608	VAL	N-CA-C	6.11	116.77	110.36
3	2d	49	MET	CA-C-N	6.09	126.03	119.76
3	2d	49	MET	C-N-CA	6.09	126.03	119.76
4	2F	608	VAL	N-CA-C	6.08	116.74	110.36
4	2A	608	VAL	N-CA-C	6.07	116.73	110.36
2	1F	129	THR	CA-C-N	6.07	126.53	120.52
2	1F	129	THR	C-N-CA	6.07	126.53	120.52
4	2C	608	VAL	N-CA-C	6.06	116.72	110.36
4	2E	608	VAL	N-CA-C	6.02	116.68	110.36
4	2B	259	ASN	CA-C-N	5.95	125.89	119.76
4	2B	259	ASN	C-N-CA	5.95	125.89	119.76
4	2C	506	SER	N-CA-C	5.95	118.72	111.82
4	2A	506	SER	N-CA-C	5.94	118.72	111.82
4	2F	506	SER	N-CA-C	5.94	118.71	111.82
4	2C	259	ASN	CA-C-N	5.93	125.87	119.76
4	2C	259	ASN	C-N-CA	5.93	125.87	119.76
4	2D	28	ILE	N-CA-C	5.92	114.40	107.77
4	2E	28	ILE	N-CA-C	5.92	114.40	107.77
4	2E	506	SER	N-CA-C	5.92	118.69	111.82
4	2D	506	SER	N-CA-C	5.92	118.68	111.82
4	2B	506	SER	N-CA-C	5.91	118.67	111.82
4	2F	259	ASN	CA-C-N	5.90	125.84	119.76
4	2F	259	ASN	C-N-CA	5.90	125.84	119.76
2	1A	171	ASN	CA-C-N	5.90	126.31	119.47
2	1A	171	ASN	C-N-CA	5.90	126.31	119.47
4	2A	28	ILE	N-CA-C	5.89	114.37	107.77
2	1E	139	LYS	CA-C-N	5.89	126.35	120.52
2	1E	139	LYS	C-N-CA	5.89	126.35	120.52
4	2A	259	ASN	CA-C-N	5.89	125.83	119.76
4	2A	259	ASN	C-N-CA	5.89	125.83	119.76
2	1B	171	ASN	CA-C-N	5.89	126.30	119.47
2	1B	171	ASN	C-N-CA	5.89	126.30	119.47
2	1B	139	LYS	CA-C-N	5.89	126.35	120.52
2	1B	139	LYS	C-N-CA	5.89	126.35	120.52
2	1E	171	ASN	CA-C-N	5.88	126.30	119.47
2	1E	171	ASN	C-N-CA	5.88	126.30	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2E	259	ASN	CA-C-N	5.88	125.81	119.76
4	2E	259	ASN	C-N-CA	5.88	125.81	119.76
2	1C	171	ASN	CA-C-N	5.87	126.28	119.47
2	1C	171	ASN	C-N-CA	5.87	126.28	119.47
2	1F	171	ASN	CA-C-N	5.87	126.28	119.47
2	1F	171	ASN	C-N-CA	5.87	126.28	119.47
4	2F	28	ILE	N-CA-C	5.87	114.34	107.77
2	1F	139	LYS	CA-C-N	5.86	126.33	120.52
2	1F	139	LYS	C-N-CA	5.86	126.33	120.52
4	2B	28	ILE	N-CA-C	5.86	114.33	107.77
4	2D	259	ASN	CA-C-N	5.85	125.79	119.76
4	2D	259	ASN	C-N-CA	5.85	125.79	119.76
4	2C	28	ILE	N-CA-C	5.85	114.33	107.77
2	1A	139	LYS	CA-C-N	5.85	126.31	120.52
2	1A	139	LYS	C-N-CA	5.85	126.31	120.52
2	1D	171	ASN	CA-C-N	5.84	126.24	119.47
2	1D	171	ASN	C-N-CA	5.84	126.24	119.47
2	1C	139	LYS	CA-C-N	5.82	126.28	120.52
2	1C	139	LYS	C-N-CA	5.82	126.28	120.52
2	1B	68	PHE	CA-CB-CG	5.82	119.62	113.80
3	2f	93	LEU	N-CA-C	5.80	119.51	110.17
4	2A	386	LYS	N-CA-C	5.80	118.88	107.98
4	2C	386	LYS	N-CA-C	5.79	118.88	107.98
4	2D	386	LYS	N-CA-C	5.79	118.87	107.98
3	2c	93	LEU	N-CA-C	5.79	119.49	110.17
4	2E	386	LYS	N-CA-C	5.78	118.86	107.98
4	2F	386	LYS	N-CA-C	5.78	118.85	107.98
3	2a	93	LEU	N-CA-C	5.78	119.47	110.17
3	2b	93	LEU	N-CA-C	5.78	119.47	110.17
3	2e	93	LEU	N-CA-C	5.78	119.47	110.17
4	2B	386	LYS	N-CA-C	5.78	118.84	107.98
4	2B	18	PRO	CA-C-N	5.77	125.74	120.03
4	2B	18	PRO	C-N-CA	5.77	125.74	120.03
2	1D	68	PHE	CA-CB-CG	5.76	119.56	113.80
2	1D	139	LYS	CA-C-N	5.76	126.22	120.52
2	1D	139	LYS	C-N-CA	5.76	126.22	120.52
3	2d	93	LEU	N-CA-C	5.75	119.44	110.17
4	2A	18	PRO	CA-C-N	5.75	125.72	120.03
4	2A	18	PRO	C-N-CA	5.75	125.72	120.03
2	1E	68	PHE	CA-CB-CG	5.75	119.55	113.80
4	2F	18	PRO	CA-C-N	5.74	125.72	120.03
4	2F	18	PRO	C-N-CA	5.74	125.72	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1F	68	PHE	CA-CB-CG	5.74	119.54	113.80
2	1C	68	PHE	CA-CB-CG	5.73	119.53	113.80
2	1A	68	PHE	CA-CB-CG	5.73	119.53	113.80
4	2C	18	PRO	CA-C-N	5.72	125.69	120.03
4	2C	18	PRO	C-N-CA	5.72	125.69	120.03
4	2D	157	GLU	N-CA-C	5.72	121.28	113.16
4	2D	18	PRO	CA-C-N	5.71	125.69	120.03
4	2D	18	PRO	C-N-CA	5.71	125.69	120.03
4	2E	157	GLU	N-CA-C	5.71	121.27	113.16
4	2A	157	GLU	N-CA-C	5.71	121.26	113.16
4	2C	157	GLU	N-CA-C	5.70	121.25	113.16
4	2E	18	PRO	CA-C-N	5.70	125.67	120.03
4	2E	18	PRO	C-N-CA	5.70	125.67	120.03
4	2B	157	GLU	N-CA-C	5.69	121.24	113.16
4	2F	157	GLU	N-CA-C	5.68	121.23	113.16
4	2E	504	PRO	N-CA-C	-5.66	105.03	110.47
4	2F	504	PRO	N-CA-C	-5.66	105.03	110.47
4	2B	504	PRO	N-CA-C	-5.64	105.05	110.47
4	2D	504	PRO	N-CA-C	-5.64	105.06	110.47
4	2C	504	PRO	N-CA-C	-5.64	105.06	110.47
3	2a	100	VAL	N-CA-C	-5.62	107.18	111.62
3	2c	100	VAL	N-CA-C	-5.62	107.18	111.62
3	2d	107	ASN	N-CA-C	5.62	119.19	111.54
3	2f	100	VAL	N-CA-C	-5.62	107.18	111.62
3	2f	107	ASN	N-CA-C	5.61	119.17	111.54
4	2A	504	PRO	N-CA-C	-5.61	105.09	110.47
3	2a	107	ASN	N-CA-C	5.60	119.16	111.54
3	2b	100	VAL	N-CA-C	-5.60	107.20	111.62
3	2e	100	VAL	N-CA-C	-5.60	107.20	111.62
3	2b	107	ASN	N-CA-C	5.60	119.15	111.54
3	2c	107	ASN	N-CA-C	5.59	119.14	111.54
3	2d	100	VAL	N-CA-C	-5.58	107.22	111.62
4	2B	37	PHE	CA-CB-CG	5.57	119.37	113.80
3	2e	107	ASN	N-CA-C	5.57	119.12	111.54
4	2B	454	ASP	CA-CB-CG	5.56	118.16	112.60
4	2A	37	PHE	CA-CB-CG	5.55	119.35	113.80
4	2D	37	PHE	CA-CB-CG	5.54	119.34	113.80
4	2D	454	ASP	CA-CB-CG	5.54	118.14	112.60
4	2E	454	ASP	CA-CB-CG	5.53	118.13	112.60
4	2A	454	ASP	CA-CB-CG	5.53	118.13	112.60
4	2F	454	ASP	CA-CB-CG	5.52	118.12	112.60
4	2F	37	PHE	CA-CB-CG	5.52	119.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2C	37	PHE	CA-CB-CG	5.51	119.31	113.80
4	2E	37	PHE	CA-CB-CG	5.51	119.31	113.80
4	2C	674	VAL	CA-C-N	5.50	128.47	120.98
4	2C	674	VAL	C-N-CA	5.50	128.47	120.98
3	2d	98	GLU	CA-C-N	5.50	125.43	119.76
3	2d	98	GLU	C-N-CA	5.50	125.43	119.76
4	2A	472	LYS	N-CA-C	5.50	117.98	111.33
4	2D	472	LYS	N-CA-C	5.50	117.98	111.33
4	2C	454	ASP	CA-CB-CG	5.49	118.09	112.60
4	2B	472	LYS	N-CA-C	5.48	117.96	111.33
4	2A	674	VAL	CA-C-N	5.48	128.44	120.98
4	2A	674	VAL	C-N-CA	5.48	128.44	120.98
4	2E	472	LYS	N-CA-C	5.48	117.96	111.33
4	2C	472	LYS	N-CA-C	5.46	117.94	111.33
4	2E	674	VAL	CA-C-N	5.46	128.40	120.98
4	2E	674	VAL	C-N-CA	5.46	128.40	120.98
4	2F	674	VAL	CA-C-N	5.46	128.40	120.98
4	2F	674	VAL	C-N-CA	5.46	128.40	120.98
4	2C	237	PHE	CA-CB-CG	5.44	119.24	113.80
4	2B	674	VAL	CA-C-N	5.44	128.38	120.98
4	2B	674	VAL	C-N-CA	5.44	128.38	120.98
4	2F	237	PHE	CA-CB-CG	5.44	119.24	113.80
3	2a	98	GLU	CA-C-N	5.44	125.36	119.76
3	2a	98	GLU	C-N-CA	5.44	125.36	119.76
4	2D	674	VAL	CA-C-N	5.43	128.37	120.98
4	2D	674	VAL	C-N-CA	5.43	128.37	120.98
4	2F	472	LYS	N-CA-C	5.42	117.89	111.33
4	2A	237	PHE	CA-CB-CG	5.42	119.22	113.80
4	2B	237	PHE	CA-CB-CG	5.42	119.22	113.80
4	2F	203	THR	N-CA-C	-5.42	102.03	110.10
3	2e	98	GLU	CA-C-N	5.41	125.33	119.76
3	2e	98	GLU	C-N-CA	5.41	125.33	119.76
4	2C	203	THR	N-CA-C	-5.41	102.04	110.10
4	2E	237	PHE	CA-CB-CG	5.41	119.21	113.80
3	2f	98	GLU	CA-C-N	5.40	125.33	119.76
3	2f	98	GLU	C-N-CA	5.40	125.33	119.76
3	2b	98	GLU	CA-C-N	5.40	125.33	119.76
3	2b	98	GLU	C-N-CA	5.40	125.33	119.76
4	2D	237	PHE	CA-CB-CG	5.40	119.20	113.80
4	2D	203	THR	N-CA-C	-5.39	102.06	110.10
3	2d	132	LEU	N-CA-C	5.39	118.27	109.59
4	2B	203	THR	N-CA-C	-5.39	102.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2E	203	THR	N-CA-C	-5.39	102.07	110.10
4	2A	203	THR	N-CA-C	-5.38	102.08	110.10
3	2c	98	GLU	CA-C-N	5.38	125.30	119.76
3	2c	98	GLU	C-N-CA	5.38	125.30	119.76
2	1E	10	PHE	CA-CB-CG	5.38	119.18	113.80
3	2a	132	LEU	N-CA-C	5.37	118.23	109.59
3	2b	132	LEU	N-CA-C	5.36	118.22	109.59
3	2e	132	LEU	N-CA-C	5.36	118.22	109.59
3	2c	132	LEU	N-CA-C	5.36	118.22	109.59
3	2f	132	LEU	N-CA-C	5.36	118.22	109.59
2	1F	10	PHE	CA-CB-CG	5.34	119.14	113.80
2	1C	10	PHE	CA-CB-CG	5.32	119.12	113.80
2	1B	10	PHE	CA-CB-CG	5.31	119.11	113.80
2	1A	10	PHE	CA-CB-CG	5.29	119.09	113.80
2	1D	10	PHE	CA-CB-CG	5.29	119.08	113.80
4	2D	610	GLU	CA-C-N	5.27	125.19	119.76
4	2D	610	GLU	C-N-CA	5.27	125.19	119.76
4	2F	610	GLU	CA-C-N	5.27	125.19	119.76
4	2F	610	GLU	C-N-CA	5.27	125.19	119.76
4	2A	610	GLU	CA-C-N	5.24	125.16	119.76
4	2A	610	GLU	C-N-CA	5.24	125.16	119.76
4	2E	610	GLU	CA-C-N	5.23	125.15	119.76
4	2E	610	GLU	C-N-CA	5.23	125.15	119.76
4	2B	279	ILE	N-CA-C	5.19	120.14	109.34
4	2D	41	LYS	CA-C-N	5.19	125.49	119.47
4	2D	41	LYS	C-N-CA	5.19	125.49	119.47
4	2B	41	LYS	CA-C-N	5.19	125.49	119.47
4	2B	41	LYS	C-N-CA	5.19	125.49	119.47
4	2C	610	GLU	CA-C-N	5.17	125.09	119.76
4	2C	610	GLU	C-N-CA	5.17	125.09	119.76
4	2F	41	LYS	CA-C-N	5.17	125.47	119.47
4	2F	41	LYS	C-N-CA	5.17	125.47	119.47
4	2A	279	ILE	N-CA-C	5.17	120.10	109.34
4	2C	279	ILE	N-CA-C	5.17	120.10	109.34
4	2A	41	LYS	CA-C-N	5.17	125.47	119.47
4	2A	41	LYS	C-N-CA	5.17	125.47	119.47
4	2F	279	ILE	N-CA-C	5.17	120.09	109.34
4	2E	41	LYS	CA-C-N	5.17	125.46	119.47
4	2E	41	LYS	C-N-CA	5.17	125.46	119.47
4	2E	279	ILE	N-CA-C	5.17	120.09	109.34
4	2B	610	GLU	CA-C-N	5.16	125.07	119.76
4	2B	610	GLU	C-N-CA	5.16	125.07	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2C	41	LYS	CA-C-N	5.16	125.46	119.47
4	2C	41	LYS	C-N-CA	5.16	125.46	119.47
4	2D	279	ILE	N-CA-C	5.15	120.06	109.34
4	2F	447	ALA	N-CA-C	5.14	119.13	112.86
4	2A	447	ALA	N-CA-C	5.13	119.12	112.86
4	2C	447	ALA	N-CA-C	5.13	119.11	112.86
4	2E	447	ALA	N-CA-C	5.12	119.11	112.86
4	2D	447	ALA	N-CA-C	5.11	119.09	112.86
4	2B	447	ALA	N-CA-C	5.08	119.06	112.86
4	2E	279	ILE	CA-C-N	-5.07	113.09	120.29
4	2E	279	ILE	C-N-CA	-5.07	113.09	120.29
4	2A	279	ILE	CA-C-N	-5.06	113.10	120.29
4	2A	279	ILE	C-N-CA	-5.06	113.10	120.29
4	2B	279	ILE	CA-C-N	-5.06	113.11	120.29
4	2B	279	ILE	C-N-CA	-5.06	113.11	120.29
4	2C	279	ILE	CA-C-N	-5.05	113.11	120.29
4	2C	279	ILE	C-N-CA	-5.05	113.11	120.29
4	2D	279	ILE	CA-C-N	-5.05	113.12	120.29
4	2D	279	ILE	C-N-CA	-5.05	113.12	120.29
3	2a	12	VAL	N-CA-C	5.05	115.24	107.77
3	2c	12	VAL	N-CA-C	5.05	115.24	107.77
3	2d	12	VAL	N-CA-C	5.05	115.24	107.77
3	2f	12	VAL	N-CA-C	5.05	115.24	107.77
3	2e	12	VAL	N-CA-C	5.04	115.24	107.77
3	2b	12	VAL	N-CA-C	5.04	115.23	107.77
4	2F	279	ILE	CA-C-N	-5.04	113.13	120.29
4	2F	279	ILE	C-N-CA	-5.04	113.13	120.29
4	2A	430	THR	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0A	1615	0	1603	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0B	1615	0	1603	20	0
1	0C	1615	0	1603	21	0
1	0D	1615	0	1603	21	0
1	0E	1615	0	1603	21	0
1	0F	1615	0	1603	21	0
2	1A	2337	0	2288	16	0
2	1B	2337	0	2288	19	0
2	1C	2337	0	2288	19	0
2	1D	2337	0	2288	19	0
2	1E	2337	0	2288	19	0
2	1F	2337	0	2288	17	0
3	1a	1145	0	1118	26	0
3	1b	1145	0	1118	27	0
3	1c	1145	0	1118	26	0
3	1d	1145	0	1118	27	0
3	1e	1145	0	1118	28	0
3	1f	1145	0	1118	27	0
3	2a	1145	0	1117	22	0
3	2b	1145	0	1117	21	0
3	2c	1145	0	1117	21	0
3	2d	1145	0	1117	20	0
3	2e	1145	0	1117	19	0
3	2f	1145	0	1117	22	0
4	2A	5057	0	4910	73	0
4	2B	5057	0	4910	72	0
4	2C	5057	0	4910	71	0
4	2D	5057	0	4910	74	0
4	2E	5057	0	4910	73	0
4	2F	5057	0	4910	74	0
All	All	67794	0	66216	593	0

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

All (593) 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)
4:2D:406:THR:HG21	4:2E:554:THR:CG2	1.26	1.61
4:2E:406:THR:HG21	4:2F:554:THR:CG2	1.24	1.60
4:2A:554:THR:CG2	4:2F:406:THR:HG21	1.22	1.60
4:2B:406:THR:HG21	4:2C:554:THR:CG2	1.24	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2C:406:THR:HG21	4:2D:554:THR:CG2	1.23	1.57
4:2A:406:THR:HG21	4:2B:554:THR:CG2	1.22	1.54
4:2D:406:THR:CG2	4:2E:554:THR:HG21	1.03	1.51
4:2D:406:THR:CG2	4:2E:554:THR:CG2	1.82	1.50
4:2E:406:THR:CG2	4:2F:554:THR:HG21	1.02	1.50
4:2A:554:THR:CG2	4:2F:406:THR:CG2	1.79	1.49
4:2C:406:THR:CG2	4:2D:554:THR:HG21	1.01	1.48
4:2A:554:THR:HG21	4:2F:406:THR:CG2	1.00	1.47
4:2B:406:THR:CG2	4:2C:554:THR:HG21	1.02	1.46
4:2A:406:THR:CG2	4:2B:554:THR:HG21	1.00	1.45
4:2C:406:THR:CG2	4:2D:554:THR:CG2	1.80	1.40
4:2E:406:THR:CG2	4:2F:554:THR:CG2	1.80	1.40
4:2A:406:THR:CG2	4:2B:554:THR:CG2	1.79	1.38
4:2B:406:THR:CG2	4:2C:554:THR:CG2	1.80	1.35
4:2A:406:THR:HG21	4:2B:554:THR:CB	1.72	1.18
4:2C:406:THR:HG21	4:2D:554:THR:CB	1.73	1.18
4:2A:554:THR:CB	4:2F:406:THR:HG21	1.73	1.17
4:2E:406:THR:HG21	4:2F:554:THR:CB	1.72	1.17
4:2B:406:THR:HG21	4:2C:554:THR:CB	1.74	1.16
2:1C:94:TYR:CE1	4:2C:154:LYS:NZ	2.14	1.16
2:1D:94:TYR:CE1	4:2D:154:LYS:NZ	2.14	1.16
4:2D:406:THR:HG21	4:2E:554:THR:CB	1.73	1.15
2:1F:94:TYR:CE1	4:2F:154:LYS:NZ	2.13	1.13
2:1B:94:TYR:CE1	4:2B:154:LYS:NZ	2.15	1.13
4:2D:406:THR:OG1	4:2E:552:HIS:HE1	1.32	1.13
4:2E:406:THR:OG1	4:2F:552:HIS:HE1	1.31	1.13
2:1E:94:TYR:CE1	4:2E:154:LYS:NZ	2.16	1.13
2:1A:94:TYR:CE1	4:2A:154:LYS:NZ	2.14	1.12
1:0C:194:TYR:OH	4:2E:597:GLU:OE1	1.68	1.12
1:0E:194:TYR:OH	4:2C:597:GLU:OE1	1.68	1.12
4:2E:406:THR:CB	4:2F:554:THR:HG21	1.80	1.12
4:2A:552:HIS:HE1	4:2F:406:THR:OG1	1.32	1.11
4:2C:406:THR:OG1	4:2D:552:HIS:HE1	1.32	1.11
1:0D:194:TYR:OH	4:2D:597:GLU:OE1	1.69	1.11
4:2B:406:THR:OG1	4:2C:552:HIS:HE1	1.32	1.11
4:2A:406:THR:CB	4:2B:554:THR:HG21	1.81	1.10
4:2A:406:THR:OG1	4:2B:552:HIS:HE1	1.32	1.09
4:2D:406:THR:CB	4:2E:554:THR:HG21	1.82	1.09
4:2A:554:THR:HG21	4:2F:406:THR:CB	1.83	1.09
4:2C:406:THR:CB	4:2D:554:THR:HG21	1.82	1.08
1:0F:194:TYR:OH	4:2B:597:GLU:OE1	1.70	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2B:406:THR:CB	4:2C:554:THR:HG21	1.83	1.08
1:0B:194:TYR:OH	4:2F:597:GLU:OE1	1.71	1.07
1:0A:194:TYR:OH	4:2A:597:GLU:OE1	1.69	1.06
2:1A:222:ASN:ND2	2:1A:227:PHE:HE2	1.57	1.03
4:2A:554:THR:HG23	4:2F:406:THR:HG21	1.39	1.03
2:1E:222:ASN:ND2	2:1E:227:PHE:HE2	1.57	1.02
4:2C:406:THR:HG21	4:2D:554:THR:HG23	1.41	1.02
2:1C:222:ASN:ND2	2:1C:227:PHE:HE2	1.57	1.01
2:1F:222:ASN:ND2	2:1F:227:PHE:HE2	1.57	1.01
2:1B:222:ASN:ND2	2:1B:227:PHE:HE2	1.57	1.01
2:1D:222:ASN:ND2	2:1D:227:PHE:HE2	1.57	1.01
4:2A:406:THR:HG21	4:2B:554:THR:HG23	1.40	1.01
4:2D:406:THR:HG22	4:2E:554:THR:HG21	1.01	1.00
2:1D:222:ASN:ND2	2:1D:227:PHE:CE2	2.30	1.00
2:1E:222:ASN:ND2	2:1E:227:PHE:CE2	2.30	1.00
4:2D:406:THR:OG1	4:2E:552:HIS:CE1	2.14	1.00
4:2B:406:THR:HG21	4:2C:554:THR:HG23	1.41	1.00
2:1A:222:ASN:ND2	2:1A:227:PHE:CE2	2.30	0.99
4:2E:406:THR:HG21	4:2F:554:THR:HG23	1.43	0.99
4:2C:406:THR:HG22	4:2D:554:THR:HG21	1.00	0.99
4:2E:406:THR:OG1	4:2F:552:HIS:CE1	2.14	0.99
4:2E:406:THR:HG22	4:2F:554:THR:HG21	1.01	0.99
2:1F:222:ASN:ND2	2:1F:227:PHE:CE2	2.30	0.99
4:2B:406:THR:OG1	4:2C:552:HIS:CE1	2.15	0.99
4:2D:406:THR:HG21	4:2E:554:THR:HG23	1.43	0.99
2:1B:222:ASN:ND2	2:1B:227:PHE:CE2	2.30	0.99
2:1C:222:ASN:ND2	2:1C:227:PHE:CE2	2.30	0.99
4:2A:552:HIS:CE1	4:2F:406:THR:OG1	2.16	0.99
4:2B:406:THR:HG22	4:2C:554:THR:HG21	0.99	0.98
4:2A:406:THR:OG1	4:2B:552:HIS:CE1	2.16	0.98
4:2C:406:THR:OG1	4:2D:552:HIS:CE1	2.15	0.98
4:2A:406:THR:HG22	4:2B:554:THR:HG21	0.99	0.97
2:1A:94:TYR:HE1	4:2A:154:LYS:NZ	1.57	0.97
4:2C:408:THR:HG23	4:2C:411:GLU:HG2	1.47	0.96
1:0D:21:GLU:OE2	2:1D:260:LYS:NZ	1.97	0.96
1:0A:21:GLU:OE2	2:1A:260:LYS:NZ	1.99	0.96
4:2A:554:THR:HG21	4:2F:406:THR:HG22	0.99	0.96
4:2B:408:THR:HG23	4:2B:411:GLU:HG2	1.47	0.96
1:0B:21:GLU:OE2	2:1F:260:LYS:NZ	2.00	0.95
4:2E:408:THR:HG23	4:2E:411:GLU:HG2	1.47	0.94
4:2F:408:THR:HG23	4:2F:411:GLU:HG2	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2A:408:THR:HG23	4:2A:411:GLU:HG2	1.47	0.94
4:2D:408:THR:HG23	4:2D:411:GLU:HG2	1.47	0.94
1:0E:194:TYR:CZ	4:2C:597:GLU:OE1	2.20	0.93
1:0C:194:TYR:CZ	4:2E:597:GLU:OE1	2.20	0.93
1:0C:21:GLU:OE2	2:1E:260:LYS:NZ	2.01	0.93
1:0F:194:TYR:CZ	4:2B:597:GLU:OE1	2.21	0.93
1:0A:194:TYR:CZ	4:2A:597:GLU:OE1	2.21	0.93
2:1D:94:TYR:HE1	4:2D:154:LYS:NZ	1.57	0.93
3:2e:111:LEU:CD2	3:2f:33:ILE:HD11	1.99	0.93
1:0B:194:TYR:CZ	4:2F:597:GLU:OE1	2.22	0.92
3:2a:33:ILE:HD11	3:2f:111:LEU:CD2	1.99	0.92
4:2A:406:THR:CB	4:2B:554:THR:CG2	2.45	0.92
3:2c:117:ASP:OD1	3:2d:24:VAL:O	1.87	0.92
1:0D:194:TYR:CZ	4:2D:597:GLU:OE1	2.21	0.92
1:0E:21:GLU:OE2	2:1C:260:LYS:NZ	2.00	0.92
3:2a:111:LEU:CD2	3:2b:33:ILE:HD11	2.01	0.91
3:2b:111:LEU:CD2	3:2c:33:ILE:HD11	1.99	0.91
1:0F:21:GLU:OE2	2:1B:260:LYS:NZ	2.02	0.91
3:2d:117:ASP:OD1	3:2e:24:VAL:O	1.88	0.91
3:2a:24:VAL:O	3:2f:117:ASP:OD1	1.87	0.91
3:2b:117:ASP:OD1	3:2c:24:VAL:O	1.89	0.91
4:2A:554:THR:CG2	4:2F:406:THR:CB	2.46	0.91
3:2c:111:LEU:CD2	3:2d:33:ILE:HD11	2.00	0.91
2:1C:94:TYR:HE1	4:2C:154:LYS:NZ	1.57	0.90
3:2a:117:ASP:OD1	3:2b:24:VAL:O	1.89	0.90
2:1E:94:TYR:HE1	4:2E:154:LYS:NZ	1.58	0.90
2:1F:94:TYR:HE1	4:2F:154:LYS:NZ	1.56	0.90
3:1e:68:ASP:OD1	3:1e:70:GLU:HG2	1.72	0.90
3:1f:68:ASP:OD1	3:1f:70:GLU:HG2	1.72	0.90
3:1d:68:ASP:OD1	3:1d:70:GLU:HG2	1.72	0.89
3:2d:111:LEU:CD2	3:2e:33:ILE:HD11	2.01	0.89
3:2a:33:ILE:HD11	3:2f:111:LEU:HD21	1.55	0.89
3:2e:117:ASP:OD1	3:2f:24:VAL:O	1.89	0.89
4:2E:406:THR:CB	4:2F:554:THR:CG2	2.44	0.89
3:1a:68:ASP:OD1	3:1a:70:GLU:HG2	1.72	0.89
3:1c:68:ASP:OD1	3:1c:70:GLU:HG2	1.72	0.89
2:1B:94:TYR:HE1	4:2B:154:LYS:NZ	1.57	0.88
3:1b:68:ASP:OD1	3:1b:70:GLU:HG2	1.72	0.88
4:2C:406:THR:CB	4:2D:554:THR:CG2	2.45	0.88
3:2e:111:LEU:HD21	3:2f:33:ILE:HD11	1.54	0.88
3:2a:111:LEU:HD21	3:2b:33:ILE:HD11	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:408:THR:CG2	4:2E:411:GLU:HG2	2.06	0.86
3:2b:111:LEU:HD21	3:2c:33:ILE:HD11	1.54	0.86
4:2E:406:THR:HG21	4:2F:554:THR:OG1	1.76	0.86
4:2D:406:THR:CB	4:2E:554:THR:CG2	2.46	0.86
4:2D:408:THR:CG2	4:2D:411:GLU:HG2	2.06	0.86
4:2F:408:THR:CG2	4:2F:411:GLU:HG2	2.06	0.86
3:1d:112:LYS:HE2	3:1e:30:GLU:OE2	1.76	0.86
3:2c:111:LEU:HD21	3:2d:33:ILE:HD11	1.56	0.86
3:1a:112:LYS:HE2	3:1b:30:GLU:OE2	1.74	0.86
4:2C:408:THR:CG2	4:2C:411:GLU:HG2	2.06	0.85
2:1D:94:TYR:HE1	4:2D:154:LYS:HZ2	1.19	0.85
3:1c:112:LYS:HE2	3:1d:30:GLU:OE2	1.75	0.85
4:2D:406:THR:HG21	4:2E:554:THR:OG1	1.77	0.85
3:2d:111:LEU:HD21	3:2e:33:ILE:HD11	1.55	0.85
3:1b:112:LYS:HE2	3:1c:30:GLU:OE2	1.75	0.85
4:2E:405:ASP:O	4:2F:219:ASN:OD1	1.95	0.85
4:2A:408:THR:CG2	4:2A:411:GLU:HG2	2.06	0.85
3:1a:30:GLU:OE2	3:1f:112:LYS:HE2	1.76	0.85
3:1e:112:LYS:HE2	3:1f:30:GLU:OE2	1.75	0.85
4:2B:408:THR:CG2	4:2B:411:GLU:HG2	2.06	0.84
4:2D:405:ASP:O	4:2E:219:ASN:OD1	1.96	0.83
4:2C:406:THR:HG21	4:2D:554:THR:OG1	1.78	0.83
4:2A:405:ASP:O	4:2B:219:ASN:OD1	1.96	0.83
4:2C:405:ASP:O	4:2D:219:ASN:OD1	1.97	0.82
4:2A:219:ASN:OD1	4:2F:405:ASP:O	1.98	0.82
4:2B:406:THR:CB	4:2C:554:THR:CG2	2.46	0.82
4:2A:406:THR:HG21	4:2B:554:THR:OG1	1.78	0.82
4:2B:406:THR:HG21	4:2C:554:THR:OG1	1.79	0.81
4:2A:554:THR:OG1	4:2F:406:THR:HG21	1.80	0.81
4:2B:405:ASP:O	4:2C:219:ASN:OD1	1.98	0.81
1:0F:142:GLU:OE2	3:1a:123:ASN:ND2	2.19	0.76
1:0B:187:ILE:O	4:2F:608:VAL:O	2.05	0.74
1:0E:187:ILE:O	4:2C:608:VAL:O	2.04	0.74
1:0C:187:ILE:O	4:2E:608:VAL:O	2.06	0.74
1:0A:187:ILE:O	4:2A:608:VAL:O	2.04	0.74
4:2B:406:THR:CG2	4:2C:554:THR:CB	2.50	0.74
1:0F:187:ILE:O	4:2B:608:VAL:O	2.05	0.73
1:0B:142:GLU:OE2	3:1e:123:ASN:ND2	2.21	0.73
1:0D:187:ILE:O	4:2D:608:VAL:O	2.06	0.73
4:2D:406:THR:CG2	4:2E:554:THR:CB	2.50	0.73
1:0E:142:GLU:OE2	3:1b:123:ASN:ND2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0C:142:GLU:OE2	3:1d:123:ASN:ND2	2.23	0.72
1:0A:142:GLU:OE2	3:1f:123:ASN:ND2	2.23	0.71
2:1D:94:TYR:CD1	4:2D:154:LYS:NZ	2.58	0.71
2:1F:94:TYR:CD1	4:2F:154:LYS:NZ	2.58	0.71
2:1A:94:TYR:HE1	4:2A:154:LYS:HZ2	1.32	0.71
2:1C:94:TYR:CD1	4:2C:154:LYS:NZ	2.58	0.71
2:1C:94:TYR:HE1	4:2C:154:LYS:HZ2	1.32	0.71
4:2E:406:THR:HB	4:2F:554:THR:CG2	2.21	0.71
1:0D:142:GLU:OE2	3:1c:123:ASN:ND2	2.24	0.70
2:1E:222:ASN:HD22	2:1E:227:PHE:HE2	1.20	0.70
4:2D:4:TYR:CE1	4:2E:682:ILE:HD11	2.26	0.70
2:1B:94:TYR:CD1	4:2B:154:LYS:NZ	2.59	0.70
3:2a:33:ILE:CD1	3:2f:111:LEU:HD21	2.22	0.70
3:2e:111:LEU:HD21	3:2f:33:ILE:CD1	2.22	0.70
2:1E:94:TYR:CD1	4:2E:154:LYS:NZ	2.60	0.70
3:1d:82:LYS:HE2	3:2e:95:GLU:OE2	1.92	0.69
3:1f:82:LYS:HE2	3:2a:95:GLU:OE2	1.92	0.69
4:2C:4:TYR:CE1	4:2D:682:ILE:HD11	2.27	0.69
2:1A:94:TYR:CD1	4:2A:154:LYS:NZ	2.59	0.69
4:2E:4:TYR:CE1	4:2F:682:ILE:HD11	2.26	0.69
2:1F:94:TYR:HE1	4:2F:154:LYS:HZ2	1.37	0.69
3:1a:82:LYS:HE2	3:2b:95:GLU:OE2	1.91	0.69
4:2E:406:THR:CG2	4:2F:554:THR:CB	2.49	0.69
3:2b:111:LEU:HD21	3:2c:33:ILE:CD1	2.22	0.69
4:2B:4:TYR:CE1	4:2C:682:ILE:HD11	2.28	0.69
4:2A:4:TYR:CE1	4:2B:682:ILE:HD11	2.28	0.68
3:1c:82:LYS:HE2	3:2d:95:GLU:OE2	1.93	0.68
4:2D:406:THR:HB	4:2E:554:THR:CG2	2.22	0.68
3:2a:111:LEU:HD21	3:2b:33:ILE:CD1	2.24	0.68
3:2d:111:LEU:HD21	3:2e:33:ILE:CD1	2.23	0.68
3:1e:82:LYS:HE2	3:2f:95:GLU:OE2	1.93	0.68
3:1b:82:LYS:HE2	3:2c:95:GLU:OE2	1.93	0.68
4:2D:406:THR:CG2	4:2E:554:THR:HG23	2.11	0.67
4:2A:406:THR:HB	4:2B:554:THR:CG2	2.23	0.67
4:2B:406:THR:HG23	4:2C:218:ARG:HD3	1.76	0.67
4:2C:406:THR:HB	4:2D:554:THR:CG2	2.23	0.67
4:2A:554:THR:CG2	4:2F:406:THR:HB	2.24	0.67
4:2D:406:THR:HG23	4:2E:218:ARG:HD3	1.74	0.67
4:2E:406:THR:HG23	4:2F:218:ARG:HD3	1.75	0.67
3:2c:111:LEU:HD21	3:2d:33:ILE:CD1	2.23	0.67
4:2A:682:ILE:HD11	4:2F:4:TYR:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2B:406:THR:HB	4:2C:554:THR:CG2	2.24	0.67
3:1a:81:ASN:HB3	3:1b:49:MET:CE	2.25	0.66
3:1c:81:ASN:HB3	3:1d:49:MET:CE	2.26	0.66
4:2A:554:THR:CB	4:2F:406:THR:CG2	2.50	0.66
4:2C:406:THR:HG23	4:2D:218:ARG:HD3	1.77	0.66
4:2C:406:THR:CG2	4:2D:554:THR:CB	2.50	0.66
2:1D:222:ASN:HD22	2:1D:227:PHE:HE2	1.20	0.66
4:2A:406:THR:HG23	4:2B:218:ARG:HD3	1.78	0.66
4:2E:406:THR:CG2	4:2F:554:THR:HG23	2.10	0.65
3:2e:75:TYR:OH	3:2f:31:THR:HG23	1.97	0.65
4:2A:218:ARG:HD3	4:2F:406:THR:HG23	1.78	0.65
3:2a:31:THR:HG23	3:2f:75:TYR:OH	1.96	0.65
1:0F:142:GLU:CD	3:1a:123:ASN:ND2	2.55	0.65
3:2b:75:TYR:OH	3:2c:31:THR:HG23	1.97	0.65
3:1b:81:ASN:HB3	3:1c:49:MET:CE	2.28	0.64
3:2c:75:TYR:OH	3:2d:31:THR:HG23	1.97	0.64
3:1d:81:ASN:HB3	3:1e:49:MET:CE	2.28	0.64
2:1C:222:ASN:HD22	2:1C:227:PHE:HE2	1.20	0.64
4:2A:406:THR:CG2	4:2B:554:THR:CB	2.49	0.64
3:1a:49:MET:CE	3:1f:81:ASN:HB3	2.28	0.63
3:1e:81:ASN:HB3	3:1f:49:MET:CE	2.28	0.63
1:0B:142:GLU:CD	3:1e:123:ASN:ND2	2.57	0.63
4:2A:554:THR:HG23	4:2F:406:THR:CG2	2.08	0.63
1:0C:142:GLU:CD	3:1d:123:ASN:ND2	2.58	0.62
1:0E:142:GLU:CD	3:1b:123:ASN:ND2	2.57	0.62
3:1a:124:GLU:HB2	3:1b:7:LYS:HE2	1.81	0.62
3:2d:75:TYR:OH	3:2e:31:THR:HG23	2.00	0.62
1:0A:142:GLU:CD	3:1f:123:ASN:ND2	2.58	0.62
3:2a:75:TYR:OH	3:2b:31:THR:HG23	1.99	0.62
1:0D:142:GLU:CD	3:1c:123:ASN:ND2	2.59	0.61
4:2A:14:ILE:O	4:2B:686:SER:HB3	2.01	0.61
4:2D:14:ILE:O	4:2E:686:SER:HB3	1.99	0.61
4:2E:14:ILE:O	4:2F:686:SER:HB3	2.00	0.61
4:2C:406:THR:CG2	4:2D:554:THR:OG1	2.49	0.60
4:2E:406:THR:CG2	4:2F:554:THR:OG1	2.47	0.60
4:2D:406:THR:CG2	4:2E:554:THR:OG1	2.48	0.60
1:0B:22:MET:HE1	1:0B:106:ARG:HG2	1.83	0.60
4:2C:14:ILE:O	4:2D:686:SER:HB3	2.00	0.60
1:0E:22:MET:HE1	1:0E:106:ARG:HG2	1.83	0.59
1:0F:22:MET:HE1	1:0F:106:ARG:HG2	1.83	0.59
1:0D:22:MET:HE1	1:0D:106:ARG:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1f:88:LEU:HB3	3:1f:105:VAL:HB	1.85	0.59
3:1e:88:LEU:HB3	3:1e:105:VAL:HB	1.85	0.59
4:2A:406:THR:CG2	4:2B:554:THR:OG1	2.49	0.59
1:0A:22:MET:HE1	1:0A:106:ARG:HG2	1.83	0.59
3:1e:124:GLU:HB2	3:1f:7:LYS:HE2	1.85	0.59
4:2B:14:ILE:O	4:2C:686:SER:HB3	2.02	0.59
3:1d:88:LEU:HB3	3:1d:105:VAL:HB	1.85	0.59
4:2A:686:SER:HB3	4:2F:14:ILE:O	2.03	0.59
1:0C:22:MET:HE1	1:0C:106:ARG:HG2	1.83	0.58
3:1d:124:GLU:HB2	3:1e:7:LYS:HE2	1.84	0.58
3:2a:33:ILE:CD1	3:2f:111:LEU:CD2	2.79	0.58
3:1a:88:LEU:HB3	3:1a:105:VAL:HB	1.85	0.58
4:2A:554:THR:CG2	4:2F:406:THR:HG22	1.89	0.58
3:1d:68:ASP:OD1	3:1d:70:GLU:CG	2.50	0.58
3:1e:68:ASP:OD1	3:1e:70:GLU:CG	2.50	0.58
2:1B:94:TYR:HE1	4:2B:154:LYS:HZ2	0.73	0.58
3:1c:88:LEU:HB3	3:1c:105:VAL:HB	1.85	0.58
3:1a:7:LYS:HE2	3:1f:124:GLU:HB2	1.86	0.58
3:1c:81:ASN:HB3	3:1d:49:MET:HE2	1.86	0.58
3:1b:88:LEU:HB3	3:1b:105:VAL:HB	1.85	0.57
3:1b:124:GLU:HB2	3:1c:7:LYS:HE2	1.85	0.57
3:1c:124:GLU:HB2	3:1d:7:LYS:HE2	1.84	0.57
4:2C:406:THR:HB	4:2D:554:THR:HG21	1.82	0.57
1:0F:194:TYR:CE2	4:2B:597:GLU:OE1	2.58	0.57
4:2B:406:THR:CB	4:2C:554:THR:HG23	2.34	0.57
3:2e:111:LEU:HD22	3:2f:33:ILE:HD11	1.85	0.57
1:0E:194:TYR:CE2	4:2C:597:GLU:OE1	2.56	0.57
4:2A:554:THR:OG1	4:2F:406:THR:CG2	2.50	0.57
1:0D:194:TYR:CE2	4:2D:597:GLU:OE1	2.58	0.56
4:2B:406:THR:CG2	4:2C:554:THR:OG1	2.49	0.56
3:1a:81:ASN:HB3	3:1b:49:MET:HE2	1.86	0.56
4:2E:406:THR:HG22	4:2F:554:THR:CG2	1.91	0.56
4:2D:406:THR:CB	4:2E:554:THR:HG23	2.34	0.56
3:1f:68:ASP:OD1	3:1f:70:GLU:CG	2.50	0.56
1:0A:194:TYR:CE2	4:2A:597:GLU:OE1	2.58	0.56
1:0C:194:TYR:CE2	4:2E:597:GLU:OE1	2.57	0.56
3:2b:111:LEU:HD22	3:2c:33:ILE:HD11	1.85	0.56
3:1c:68:ASP:OD1	3:1c:70:GLU:CG	2.50	0.56
1:0B:194:TYR:CE2	4:2F:597:GLU:OE1	2.59	0.55
4:2D:172:ASP:N	4:2D:172:ASP:OD1	2.38	0.55
1:0F:76:THR:HG22	1:0F:183:GLU:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1a:49:MET:HE2	3:1f:81:ASN:HB3	1.88	0.55
4:2E:5:LYS:O	4:2F:550:ASN:ND2	2.38	0.55
3:2c:111:LEU:HD22	3:2d:33:ILE:HD11	1.86	0.55
1:0E:76:THR:HG22	1:0E:183:GLU:HG2	1.89	0.55
3:1b:68:ASP:OD1	3:1b:70:GLU:CG	2.50	0.55
3:1b:81:ASN:HB3	3:1c:49:MET:HE2	1.88	0.55
4:2C:172:ASP:N	4:2C:172:ASP:OD1	2.38	0.55
3:2a:33:ILE:HD11	3:2f:111:LEU:HD22	1.86	0.55
3:2e:111:LEU:CD2	3:2f:33:ILE:CD1	2.79	0.55
2:1E:94:TYR:HE1	4:2E:154:LYS:HZ2	0.70	0.55
3:1d:81:ASN:HB3	3:1e:49:MET:HE2	1.88	0.55
4:2A:554:THR:HG23	4:2F:406:THR:CB	2.33	0.55
1:0D:76:THR:HG22	1:0D:183:GLU:HG2	1.89	0.54
4:2D:406:THR:HG22	4:2E:554:THR:CG2	1.91	0.54
3:1a:68:ASP:OD1	3:1a:70:GLU:CG	2.50	0.54
3:2d:111:LEU:HD22	3:2e:33:ILE:HD11	1.88	0.54
3:1e:81:ASN:HB3	3:1f:49:MET:HE2	1.88	0.54
4:2A:406:THR:CB	4:2B:554:THR:HG23	2.33	0.54
3:2c:111:LEU:CD2	3:2d:33:ILE:CD1	2.80	0.54
3:2b:111:LEU:CD2	3:2c:33:ILE:CD1	2.79	0.54
1:0A:76:THR:HG22	1:0A:183:GLU:HG2	1.89	0.54
1:0C:76:THR:HG22	1:0C:183:GLU:HG2	1.89	0.54
4:2A:212:ASP:OD1	4:2A:215:PRO:HD2	2.08	0.54
4:2C:406:THR:CB	4:2D:554:THR:HG23	2.33	0.53
4:2E:212:ASP:OD1	4:2E:215:PRO:HD2	2.08	0.53
4:2F:172:ASP:OD1	4:2F:172:ASP:N	2.38	0.53
4:2A:5:LYS:O	4:2B:550:ASN:ND2	2.38	0.53
4:2C:212:ASP:OD1	4:2C:215:PRO:HD2	2.08	0.53
4:2B:212:ASP:OD1	4:2B:215:PRO:HD2	2.08	0.53
4:2D:212:ASP:OD1	4:2D:215:PRO:HD2	2.08	0.53
4:2C:90:ARG:NH1	4:2C:488:THR:OG1	2.42	0.53
1:0B:76:THR:HG22	1:0B:183:GLU:HG2	1.89	0.53
4:2B:90:ARG:NH1	4:2B:488:THR:OG1	2.42	0.53
4:2B:172:ASP:OD1	4:2B:172:ASP:N	2.38	0.53
4:2C:5:LYS:O	4:2D:550:ASN:ND2	2.38	0.53
4:2A:554:THR:HG21	4:2F:406:THR:HB	1.84	0.53
4:2A:550:ASN:ND2	4:2F:5:LYS:O	2.40	0.52
4:2F:212:ASP:OD1	4:2F:215:PRO:HD2	2.08	0.52
2:1E:224:LYS:HG3	2:1E:225:ASP:OD1	2.10	0.52
4:2D:90:ARG:NH1	4:2D:488:THR:OG1	2.42	0.52
4:2E:90:ARG:NH1	4:2E:488:THR:OG1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2A:90:ARG:NH1	4:2A:488:THR:OG1	2.42	0.52
4:2E:406:THR:CB	4:2F:554:THR:HG23	2.33	0.52
4:2F:90:ARG:NH1	4:2F:488:THR:OG1	2.42	0.52
4:2A:406:THR:HG22	4:2B:554:THR:CG2	1.89	0.52
2:1D:224:LYS:HG3	2:1D:225:ASP:OD1	2.10	0.52
4:2D:5:LYS:O	4:2E:550:ASN:ND2	2.38	0.52
2:1B:224:LYS:HG3	2:1B:225:ASP:OD1	2.10	0.52
2:1F:224:LYS:HG3	2:1F:225:ASP:OD1	2.10	0.52
4:2B:5:LYS:O	4:2C:550:ASN:ND2	2.40	0.51
2:1C:92:GLU:O	4:2C:154:LYS:HE2	2.11	0.51
2:1A:224:LYS:HG3	2:1A:225:ASP:OD1	2.10	0.51
2:1F:92:GLU:O	4:2F:154:LYS:HE2	2.10	0.51
2:1C:224:LYS:HG3	2:1C:225:ASP:OD1	2.10	0.51
3:2a:111:LEU:HD22	3:2b:33:ILE:HD11	1.87	0.51
1:0C:62:MET:HE1	3:1e:2:SER:O	2.11	0.51
2:1D:92:GLU:O	4:2D:154:LYS:HE2	2.11	0.51
4:2B:411:GLU:OE1	4:2B:411:GLU:HA	2.11	0.51
3:2d:115:SER:OG	3:2e:27:LEU:HB2	2.11	0.51
1:0E:62:MET:HE1	3:1c:2:SER:O	2.11	0.50
1:0F:142:GLU:CD	3:1a:123:ASN:HD22	2.19	0.50
4:2E:172:ASP:OD1	4:2E:172:ASP:N	2.38	0.50
4:2A:411:GLU:OE1	4:2A:411:GLU:HA	2.11	0.50
1:0B:142:GLU:CD	3:1e:123:ASN:HD22	2.20	0.50
4:2E:4:TYR:CE1	4:2F:682:ILE:CD1	2.95	0.50
4:2E:411:GLU:HA	4:2E:411:GLU:OE1	2.11	0.50
4:2D:411:GLU:HA	4:2D:411:GLU:OE1	2.12	0.50
4:2F:411:GLU:OE1	4:2F:411:GLU:HA	2.11	0.50
4:2C:406:THR:HG22	4:2D:554:THR:CG2	1.90	0.50
4:2C:411:GLU:OE1	4:2C:411:GLU:HA	2.11	0.50
1:0D:62:MET:HE1	3:1d:2:SER:O	2.12	0.50
1:0F:62:MET:HE1	3:1b:2:SER:O	2.11	0.50
4:2A:437:LEU:O	4:2A:438:THR:C	2.55	0.50
1:0B:62:MET:HE1	3:1f:2:SER:O	2.12	0.49
1:0E:142:GLU:CD	3:1b:123:ASN:HD22	2.20	0.49
2:1E:92:GLU:O	4:2E:154:LYS:HE2	2.12	0.49
4:2D:437:LEU:O	4:2D:438:THR:C	2.55	0.49
1:0A:142:GLU:CD	3:1f:123:ASN:HD22	2.20	0.49
2:1A:92:GLU:O	4:2A:154:LYS:HE2	2.12	0.49
2:1B:92:GLU:O	4:2B:154:LYS:HE2	2.12	0.49
3:2a:111:LEU:CD2	3:2b:33:ILE:CD1	2.81	0.49
1:0D:28:VAL:HG21	1:0D:48:LYS:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1C:85:THR:OG1	2:1C:86:GLU:N	2.45	0.49
1:0C:28:VAL:HG21	1:0C:48:LYS:HD3	1.94	0.49
2:1B:85:THR:OG1	2:1B:86:GLU:N	2.45	0.49
2:1D:85:THR:OG1	2:1D:86:GLU:N	2.45	0.49
1:0B:28:VAL:HG21	1:0B:48:LYS:HD3	1.94	0.49
2:1E:85:THR:OG1	2:1E:86:GLU:N	2.45	0.49
3:2e:117:ASP:OD2	3:2e:119:LYS:NZ	2.46	0.49
4:2B:406:THR:HG22	4:2C:554:THR:CG2	1.90	0.49
4:2A:172:ASP:OD1	4:2A:172:ASP:N	2.38	0.48
3:2a:115:SER:OG	3:2b:27:LEU:HB2	2.12	0.48
3:2b:117:ASP:OD2	3:2b:119:LYS:NZ	2.46	0.48
3:2c:117:ASP:OD2	3:2c:119:LYS:NZ	2.46	0.48
1:0C:142:GLU:CD	3:1d:123:ASN:HD22	2.21	0.48
1:0D:142:GLU:OE2	3:1d:8:PHE:CZ	2.66	0.48
1:0E:28:VAL:HG21	1:0E:48:LYS:HD3	1.94	0.48
3:2f:117:ASP:OD2	3:2f:119:LYS:NZ	2.46	0.48
1:0A:62:MET:HE1	3:1a:2:SER:O	2.13	0.48
3:2d:117:ASP:OD2	3:2d:119:LYS:NZ	2.46	0.48
1:0C:142:GLU:OE2	3:1e:8:PHE:CZ	2.65	0.48
3:2a:117:ASP:OD2	3:2a:119:LYS:NZ	2.46	0.48
3:2a:27:LEU:HB2	3:2f:115:SER:OG	2.13	0.48
1:0B:177:ARG:HD2	1:0C:109:GLU:HG2	1.96	0.48
2:1E:165:LEU:HD22	2:1E:170:LEU:HD12	1.96	0.48
1:0A:28:VAL:HG21	1:0A:48:LYS:HD3	1.94	0.48
4:2D:4:TYR:CE1	4:2E:682:ILE:CD1	2.95	0.48
2:1A:165:LEU:HD22	2:1A:170:LEU:HD12	1.96	0.48
2:1D:165:LEU:HD22	2:1D:170:LEU:HD12	1.96	0.48
3:1a:124:GLU:CB	3:1b:7:LYS:HE2	2.44	0.48
2:1F:85:THR:OG1	2:1F:86:GLU:N	2.45	0.48
2:1F:222:ASN:HD22	2:1F:227:PHE:HE2	1.20	0.48
4:2E:437:LEU:O	4:2E:438:THR:C	2.55	0.48
1:0D:142:GLU:CD	3:1c:123:ASN:HD22	2.22	0.47
1:0C:177:ARG:HD2	1:0D:109:GLU:HG2	1.96	0.47
2:1F:165:LEU:HD22	2:1F:170:LEU:HD12	1.96	0.47
4:2B:437:LEU:O	4:2B:438:THR:C	2.55	0.47
3:2c:115:SER:OG	3:2d:27:LEU:HB2	2.14	0.47
3:2d:111:LEU:CD2	3:2e:33:ILE:CD1	2.81	0.47
1:0F:28:VAL:HG21	1:0F:48:LYS:HD3	1.94	0.47
2:1B:165:LEU:HD22	2:1B:170:LEU:HD12	1.96	0.47
2:1C:222:ASN:CB	2:1C:227:PHE:CE2	2.98	0.47
4:2F:420:ASN:O	4:2F:421:PHE:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0A:109:GLU:HG2	1:0F:177:ARG:HD2	1.97	0.47
2:1E:222:ASN:CB	2:1E:227:PHE:CE2	2.98	0.47
3:2e:115:SER:OG	3:2f:27:LEU:HB2	2.14	0.47
1:0A:113:HIS:CD2	1:0F:179:ALA:HB3	2.50	0.47
1:0B:179:ALA:HB3	1:0C:113:HIS:CD2	2.50	0.47
1:0F:142:GLU:OE2	3:1b:8:PHE:CZ	2.67	0.47
2:1B:222:ASN:CB	2:1B:227:PHE:CE2	2.98	0.47
4:2F:437:LEU:O	4:2F:438:THR:C	2.55	0.47
1:0E:142:GLU:OE2	3:1c:8:PHE:CZ	2.68	0.47
2:1C:165:LEU:HD22	2:1C:170:LEU:HD12	1.96	0.47
4:2A:4:TYR:CE1	4:2B:682:ILE:CD1	2.97	0.47
4:2A:682:ILE:CD1	4:2F:4:TYR:CE1	2.98	0.47
3:2b:115:SER:OG	3:2c:27:LEU:HB2	2.14	0.47
1:0A:177:ARG:HD2	1:0B:109:GLU:HG2	1.97	0.47
1:0E:177:ARG:HD2	1:0F:109:GLU:HG2	1.97	0.47
4:2E:420:ASN:O	4:2E:421:PHE:C	2.57	0.47
1:0A:142:GLU:OE2	3:1a:8:PHE:CZ	2.68	0.46
4:2C:4:TYR:CE1	4:2D:682:ILE:CD1	2.96	0.46
2:1D:222:ASN:CB	2:1D:227:PHE:CE2	2.98	0.46
2:1F:222:ASN:CB	2:1F:227:PHE:CE2	2.98	0.46
3:1a:7:LYS:HD2	3:1f:117:ASP:O	2.15	0.46
4:2B:4:TYR:CE1	4:2C:682:ILE:CD1	2.97	0.46
4:2D:420:ASN:O	4:2D:421:PHE:C	2.57	0.46
1:0C:142:GLU:OE2	3:1e:8:PHE:CE2	2.69	0.46
1:0B:142:GLU:OE2	3:1f:8:PHE:CZ	2.68	0.46
2:1A:222:ASN:CB	2:1A:227:PHE:CE2	2.98	0.46
1:0D:177:ARG:HD2	1:0E:109:GLU:HG2	1.98	0.46
4:2B:420:ASN:O	4:2B:421:PHE:C	2.57	0.46
3:2b:109:TRP:HA	3:2b:110:PRO:HD3	1.64	0.46
3:2d:68:ASP:OD1	3:2d:70:GLU:HG2	2.16	0.46
1:0C:179:ALA:HB3	1:0D:113:HIS:CD2	2.51	0.46
4:2B:156:ASP:OD1	4:2B:156:ASP:N	2.47	0.46
4:2E:273:VAL:HG13	4:2E:278:PHE:CE2	2.51	0.46
1:0A:179:ALA:HB3	1:0B:113:HIS:CD2	2.51	0.46
3:2e:68:ASP:OD1	3:2e:70:GLU:HG2	2.16	0.46
2:1A:222:ASN:HD22	2:1A:227:PHE:HE2	1.20	0.45
4:2C:273:VAL:HG13	4:2C:278:PHE:CE2	2.51	0.45
2:1A:85:THR:OG1	2:1A:86:GLU:N	2.45	0.45
4:2B:191:ASP:OD1	4:2B:191:ASP:N	2.48	0.45
4:2C:191:ASP:N	4:2C:191:ASP:OD1	2.48	0.45
4:2F:273:VAL:HG13	4:2F:278:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0E:179:ALA:HB3	1:0F:113:HIS:CD2	2.51	0.45
2:1D:222:ASN:CG	2:1D:227:PHE:CE2	2.94	0.45
3:1c:81:ASN:HB3	3:1d:49:MET:HE3	1.98	0.45
4:2A:273:VAL:HG13	4:2A:278:PHE:CE2	2.51	0.45
4:2D:273:VAL:HG13	4:2D:278:PHE:CE2	2.51	0.45
4:2B:273:VAL:HG13	4:2B:278:PHE:CE2	2.51	0.45
3:2b:68:ASP:OD1	3:2b:70:GLU:HG2	2.16	0.45
1:0D:142:GLU:OE2	3:1d:8:PHE:CE2	2.69	0.45
1:0D:179:ALA:HB3	1:0E:113:HIS:CD2	2.51	0.45
2:1C:222:ASN:CG	2:1C:227:PHE:CE2	2.94	0.45
2:1E:222:ASN:CG	2:1E:227:PHE:CE2	2.94	0.45
1:0A:142:GLU:OE2	3:1a:8:PHE:CE2	2.70	0.44
1:0F:142:GLU:OE2	3:1b:8:PHE:CE2	2.70	0.44
2:1F:222:ASN:CG	2:1F:227:PHE:CE2	2.94	0.44
3:1a:81:ASN:HB3	3:1b:49:MET:HE3	1.98	0.44
3:1d:117:ASP:O	3:1e:7:LYS:HD2	2.17	0.44
3:2c:68:ASP:OD1	3:2c:70:GLU:HG2	2.16	0.44
3:2f:68:ASP:OD1	3:2f:70:GLU:HG2	2.16	0.44
3:1b:124:GLU:CB	3:1c:7:LYS:HE2	2.47	0.44
4:2C:437:LEU:O	4:2C:438:THR:C	2.55	0.44
3:2a:68:ASP:OD1	3:2a:70:GLU:HG2	2.16	0.44
4:2D:137:PRO:HA	4:2D:138:PRO:HD3	1.87	0.44
2:1A:222:ASN:CG	2:1A:227:PHE:CE2	2.94	0.44
3:1b:117:ASP:O	3:1c:7:LYS:HD2	2.18	0.44
4:2E:191:ASP:OD1	4:2E:191:ASP:N	2.48	0.44
3:2f:109:TRP:HA	3:2f:110:PRO:HD3	1.63	0.44
1:0B:142:GLU:OE2	3:1f:8:PHE:CE2	2.71	0.44
3:1e:117:ASP:O	3:1f:7:LYS:HD2	2.18	0.44
3:1c:117:ASP:O	3:1d:7:LYS:HD2	2.18	0.44
4:2D:156:ASP:OD1	4:2D:156:ASP:N	2.47	0.44
2:1C:92:GLU:O	4:2C:154:LYS:CE	2.66	0.44
3:1c:124:GLU:CB	3:1d:7:LYS:HE2	2.47	0.43
4:2A:191:ASP:OD1	4:2A:191:ASP:N	2.48	0.43
4:2C:14:ILE:O	4:2D:686:SER:CB	2.66	0.43
4:2D:14:ILE:O	4:2E:686:SER:CB	2.66	0.43
3:1d:81:ASN:HB3	3:1e:49:MET:HE3	2.00	0.43
4:2F:191:ASP:OD1	4:2F:191:ASP:N	2.48	0.43
4:2A:406:THR:CG2	4:2B:554:THR:HG23	2.09	0.43
1:0B:26:GLU:OE2	1:0B:48:LYS:NZ	2.52	0.43
1:0E:142:GLU:OE2	3:1c:8:PHE:CE2	2.71	0.43
2:1C:202:ASN:OD1	2:1C:202:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:14:ILE:O	4:2F:686:SER:CB	2.67	0.43
2:1B:222:ASN:CG	2:1B:227:PHE:CE2	2.94	0.43
3:1a:49:MET:HE3	3:1f:81:ASN:HB3	2.01	0.43
4:2A:169:LEU:HA	4:2A:170:PRO:HD3	1.94	0.43
3:2a:109:TRP:HA	3:2a:110:PRO:HD3	1.64	0.43
1:0A:26:GLU:OE2	1:0A:48:LYS:NZ	2.52	0.43
2:1D:92:GLU:O	4:2D:154:LYS:CE	2.67	0.43
3:1d:124:GLU:CB	3:1e:7:LYS:HE2	2.47	0.43
3:1e:124:GLU:CB	3:1f:7:LYS:HE2	2.47	0.43
1:0C:26:GLU:OE2	1:0C:48:LYS:NZ	2.52	0.43
4:2D:191:ASP:OD1	4:2D:191:ASP:N	2.48	0.43
2:1F:92:GLU:O	4:2F:154:LYS:CE	2.66	0.43
3:2c:109:TRP:HA	3:2c:110:PRO:HD3	1.63	0.43
3:1d:119:LYS:O	3:1e:8:PHE:HA	2.19	0.43
4:2A:420:ASN:O	4:2A:421:PHE:C	2.57	0.43
1:0F:26:GLU:OE2	1:0F:48:LYS:NZ	2.52	0.42
3:1a:12:VAL:HG22	3:1a:90:ILE:HG12	2.01	0.42
3:1b:12:VAL:HG22	3:1b:90:ILE:HG12	2.01	0.42
3:1c:12:VAL:HG22	3:1c:90:ILE:HG12	2.01	0.42
4:2A:404:ALA:HB1	4:2A:411:GLU:HB2	2.01	0.42
1:0E:26:GLU:OE2	1:0E:48:LYS:NZ	2.52	0.42
3:1f:12:VAL:HG22	3:1f:90:ILE:HG12	2.01	0.42
4:2B:404:ALA:HB1	4:2B:411:GLU:HB2	2.01	0.42
4:2F:404:ALA:HB1	4:2F:411:GLU:HB2	2.01	0.42
1:0E:66:PRO:HG3	3:1b:19:ILE:HD11	2.01	0.42
3:1a:119:LYS:O	3:1b:8:PHE:HA	2.19	0.42
4:2A:581:ASP:OD1	4:2A:581:ASP:C	2.62	0.42
4:2C:420:ASN:O	4:2C:421:PHE:C	2.57	0.42
4:2D:45:ASP:OD1	4:2D:45:ASP:N	2.49	0.42
1:0D:26:GLU:OE2	1:0D:48:LYS:NZ	2.51	0.42
3:1d:12:VAL:HG22	3:1d:90:ILE:HG12	2.01	0.42
3:1e:12:VAL:HG22	3:1e:90:ILE:HG12	2.01	0.42
4:2C:404:ALA:HB1	4:2C:411:GLU:HB2	2.01	0.42
4:2D:404:ALA:HB1	4:2D:411:GLU:HB2	2.01	0.42
4:2E:156:ASP:OD1	4:2E:156:ASP:N	2.47	0.42
4:2E:404:ALA:HB1	4:2E:411:GLU:HB2	2.01	0.42
3:1a:7:LYS:HE2	3:1f:124:GLU:CB	2.49	0.42
1:0D:118:THR:H	1:0D:121:ASN:HB2	1.85	0.42
2:1C:165:LEU:CD2	2:1C:170:LEU:HD12	2.50	0.42
2:1E:165:LEU:CD2	2:1E:170:LEU:HD12	2.50	0.42
4:2B:581:ASP:OD1	4:2B:581:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2C:366:ILE:O	4:2C:367:LYS:C	2.63	0.42
4:2D:366:ILE:O	4:2D:367:LYS:C	2.63	0.42
2:1F:222:ASN:HB3	2:1F:227:PHE:CE2	2.55	0.42
2:1D:222:ASN:HB3	2:1D:227:PHE:CE2	2.55	0.41
3:1a:117:ASP:O	3:1b:7:LYS:HD2	2.20	0.41
3:1b:119:LYS:O	3:1c:8:PHE:HA	2.20	0.41
1:0A:66:PRO:HG3	3:1f:19:ILE:HD11	2.01	0.41
2:1A:222:ASN:HB3	2:1A:227:PHE:CE2	2.55	0.41
2:1B:145:ASN:OD1	2:1B:145:ASN:N	2.51	0.41
2:1B:165:LEU:CD2	2:1B:170:LEU:HD12	2.50	0.41
2:1C:222:ASN:HB3	2:1C:227:PHE:CE2	2.55	0.41
4:2B:366:ILE:O	4:2B:367:LYS:C	2.62	0.41
1:0C:66:PRO:HG3	3:1d:19:ILE:HD11	2.01	0.41
1:0E:118:THR:H	1:0E:121:ASN:HB2	1.85	0.41
2:1B:92:GLU:O	4:2B:154:LYS:CE	2.68	0.41
4:2F:581:ASP:OD1	4:2F:581:ASP:C	2.62	0.41
3:2d:109:TRP:HA	3:2d:110:PRO:HD3	1.64	0.41
1:0B:66:PRO:HG3	3:1e:19:ILE:HD11	2.01	0.41
4:2F:214:ILE:HB	4:2F:215:PRO:HD3	2.03	0.41
2:1B:222:ASN:HB3	2:1B:227:PHE:CE2	2.55	0.41
2:1E:202:ASN:OD1	2:1E:202:ASN:N	2.50	0.41
4:2A:366:ILE:O	4:2A:367:LYS:C	2.62	0.41
4:2D:214:ILE:HB	4:2D:215:PRO:HD3	2.03	0.41
4:2E:214:ILE:HB	4:2E:215:PRO:HD3	2.03	0.41
4:2F:366:ILE:O	4:2F:367:LYS:C	2.63	0.41
2:1A:92:GLU:O	4:2A:154:LYS:CE	2.68	0.41
2:1D:165:LEU:CD2	2:1D:170:LEU:HD12	2.50	0.41
2:1E:92:GLU:O	4:2E:154:LYS:CE	2.68	0.41
4:2A:14:ILE:O	4:2B:686:SER:CB	2.68	0.41
3:1e:119:LYS:O	3:1f:8:PHE:HA	2.21	0.41
4:2C:214:ILE:HB	4:2C:215:PRO:HD3	2.03	0.41
1:0A:118:THR:H	1:0A:121:ASN:HB2	1.85	0.41
2:1B:222:ASN:HD22	2:1B:227:PHE:HE2	1.20	0.41
2:1C:170:LEU:HD11	2:1C:179:ILE:HD11	2.03	0.41
2:1D:170:LEU:HD11	2:1D:179:ILE:HD11	2.03	0.41
2:1E:222:ASN:HB3	2:1E:227:PHE:CE2	2.55	0.41
4:2A:214:ILE:HB	4:2A:215:PRO:HD3	2.03	0.41
3:2b:111:LEU:CD2	3:2c:33:ILE:CG1	2.99	0.41
1:0F:128:LEU:HD23	1:0F:128:LEU:HA	1.95	0.41
4:2E:366:ILE:O	4:2E:367:LYS:C	2.63	0.41
4:2B:214:ILE:HB	4:2B:215:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:169:LEU:HA	4:2E:170:PRO:HD3	1.94	0.40
1:0F:118:THR:H	1:0F:121:ASN:HB2	1.85	0.40
2:1D:107:ASP:OD1	2:1D:107:ASP:C	2.64	0.40
2:1F:165:LEU:CD2	2:1F:170:LEU:HD12	2.50	0.40
4:2C:581:ASP:OD1	4:2C:581:ASP:C	2.62	0.40
1:0D:66:PRO:HG3	3:1c:19:ILE:HD11	2.02	0.40
2:1E:170:LEU:HD11	2:1E:179:ILE:HD11	2.03	0.40
2:1B:107:ASP:C	2:1B:107:ASP:OD1	2.64	0.40
4:2F:45:ASP:OD1	4:2F:45:ASP:N	2.49	0.40
1:0C:118:THR:H	1:0C:121:ASN:HB2	1.85	0.40
3:1e:81:ASN:HB3	3:1f:49:MET:HE3	2.00	0.40
4:2B:14:ILE:O	4:2C:686:SER:CB	2.68	0.40
4:2F:169:LEU:HA	4:2F:170:PRO:HD3	1.94	0.40
3:2a:33:ILE:HD11	3:2f:111:LEU:CD1	2.51	0.40
3:2a:33:ILE:CG1	3:2f:111:LEU:CD2	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0A	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0B	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0C	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0D	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0E	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0F	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
2	1A	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1B	282/284 (99%)	279 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1C	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1D	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1E	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1F	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
3	1a	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1b	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1c	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1d	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1e	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1f	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	2a	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2b	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2c	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2d	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2e	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2f	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
4	2A	651/692 (94%)	638 (98%)	13 (2%)	0	100	100
4	2B	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
4	2C	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
4	2D	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
4	2E	651/692 (94%)	638 (98%)	13 (2%)	0	100	100
4	2F	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
All	All	8436/8742 (96%)	8264 (98%)	172 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0A	186/186 (100%)	185 (100%)	1 (0%)	81	92
1	0B	186/186 (100%)	185 (100%)	1 (0%)	81	92
1	0C	186/186 (100%)	185 (100%)	1 (0%)	81	92
1	0D	186/186 (100%)	185 (100%)	1 (0%)	81	92
1	0E	186/186 (100%)	185 (100%)	1 (0%)	81	92
1	0F	186/186 (100%)	185 (100%)	1 (0%)	81	92
2	1A	264/264 (100%)	264 (100%)	0	100	100
2	1B	264/264 (100%)	264 (100%)	0	100	100
2	1C	264/264 (100%)	264 (100%)	0	100	100
2	1D	264/264 (100%)	264 (100%)	0	100	100
2	1E	264/264 (100%)	264 (100%)	0	100	100
2	1F	264/264 (100%)	264 (100%)	0	100	100
3	1a	127/128 (99%)	127 (100%)	0	100	100
3	1b	127/128 (99%)	127 (100%)	0	100	100
3	1c	127/128 (99%)	127 (100%)	0	100	100
3	1d	127/128 (99%)	127 (100%)	0	100	100
3	1e	127/128 (99%)	127 (100%)	0	100	100
3	1f	127/128 (99%)	127 (100%)	0	100	100
3	2a	127/128 (99%)	127 (100%)	0	100	100
3	2b	127/128 (99%)	127 (100%)	0	100	100
3	2c	127/128 (99%)	127 (100%)	0	100	100
3	2d	127/128 (99%)	127 (100%)	0	100	100
3	2e	127/128 (99%)	127 (100%)	0	100	100
3	2f	127/128 (99%)	127 (100%)	0	100	100
4	2A	547/593 (92%)	547 (100%)	0	100	100
4	2B	547/593 (92%)	547 (100%)	0	100	100
4	2C	547/593 (92%)	547 (100%)	0	100	100
4	2D	547/593 (92%)	547 (100%)	0	100	100
4	2E	547/593 (92%)	547 (100%)	0	100	100
4	2F	547/593 (92%)	547 (100%)	0	100	100
All	All	7506/7794 (96%)	7500 (100%)	6 (0%)	87	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0A	82	LEU
1	0B	82	LEU
1	0C	82	LEU
1	0D	82	LEU
1	0E	82	LEU
1	0F	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	0A	15	GLN
1	0A	68	ASN
1	0A	189	ASN
1	0B	15	GLN
1	0B	68	ASN
1	0B	189	ASN
1	0C	15	GLN
1	0C	68	ASN
1	0C	189	ASN
1	0D	15	GLN
1	0D	68	ASN
1	0D	189	ASN
1	0E	15	GLN
1	0E	68	ASN
1	0E	189	ASN
1	0F	15	GLN
1	0F	68	ASN
1	0F	189	ASN
2	1A	169	HIS
2	1A	181	GLN
2	1A	206	HIS
2	1B	169	HIS
2	1B	181	GLN
2	1C	169	HIS
2	1C	181	GLN
2	1D	169	HIS
2	1D	181	GLN
2	1D	206	HIS
2	1E	169	HIS
2	1E	181	GLN
2	1E	206	HIS
2	1F	169	HIS
2	1F	181	GLN

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Mol	Chain	Res	Type
2	1F	206	HIS
3	1a	81	ASN
3	1a	123	ASN
3	1b	81	ASN
3	1b	123	ASN
3	1c	81	ASN
3	1c	123	ASN
3	1d	81	ASN
3	1d	123	ASN
3	1e	81	ASN
3	1e	123	ASN
3	1f	81	ASN
3	1f	123	ASN
4	2A	36	GLN
4	2A	219	ASN
4	2A	245	GLN
4	2A	552	HIS
4	2B	36	GLN
4	2B	219	ASN
4	2B	245	GLN
4	2B	420	ASN
4	2B	552	HIS
4	2C	36	GLN
4	2C	219	ASN
4	2C	245	GLN
4	2C	420	ASN
4	2C	552	HIS
4	2D	36	GLN
4	2D	219	ASN
4	2D	245	GLN
4	2D	420	ASN
4	2D	552	HIS
4	2E	36	GLN
4	2E	219	ASN
4	2E	245	GLN
4	2E	552	HIS
4	2F	36	GLN
4	2F	219	ASN
4	2F	245	GLN
4	2F	552	HIS
3	2b	53	GLN
3	2c	53	GLN

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Mol	Chain	Res	Type
3	2d	53	GLN
3	2e	9	HIS
3	2e	53	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	0A	1
1	0B	1
1	0C	1
1	0D	1
1	0E	1
1	0F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	0A	82:LEU	C	83:ASN	N	1.17
1	0B	82:LEU	C	83:ASN	N	1.17
1	0C	82:LEU	C	83:ASN	N	1.17
1	0D	82:LEU	C	83:ASN	N	1.17
1	0E	82:LEU	C	83:ASN	N	1.17
1	0F	82:LEU	C	83:ASN	N	1.17

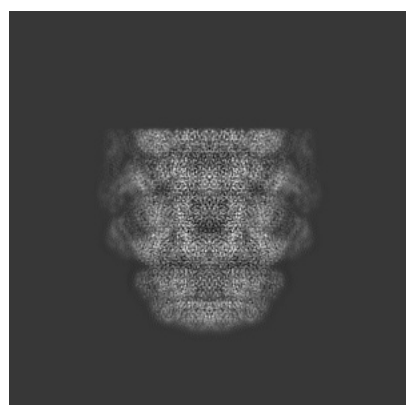
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11734. These allow visual inspection of the internal detail of the map and identification of artifacts.

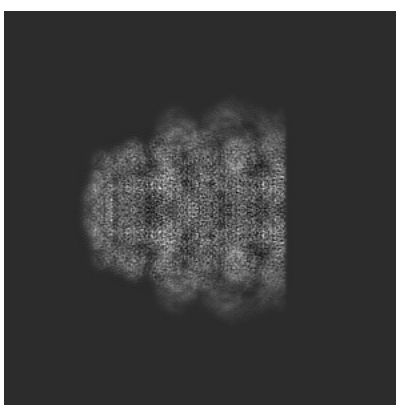
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

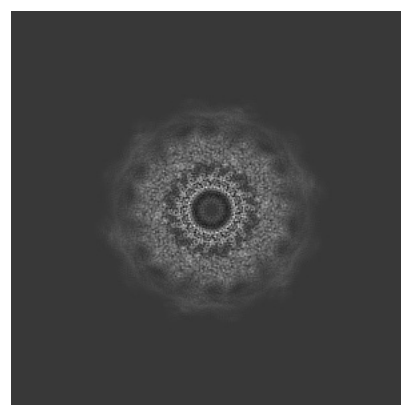
6.1.1 Primary map



X



Y



Z

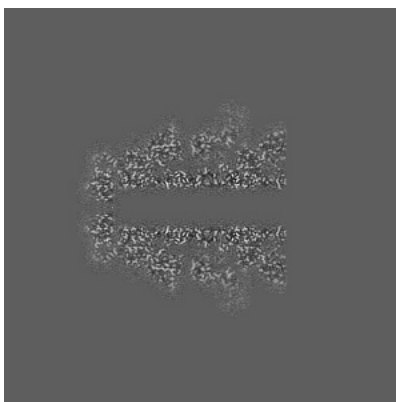
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

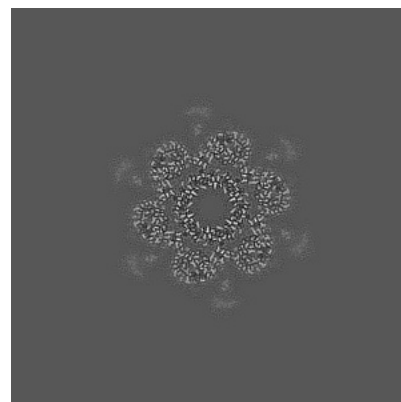
6.2.1 Primary map



X Index: 200



Y Index: 200

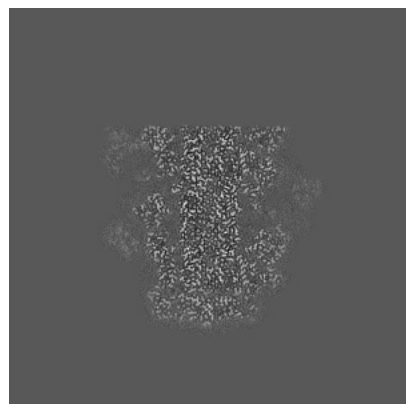


Z Index: 200

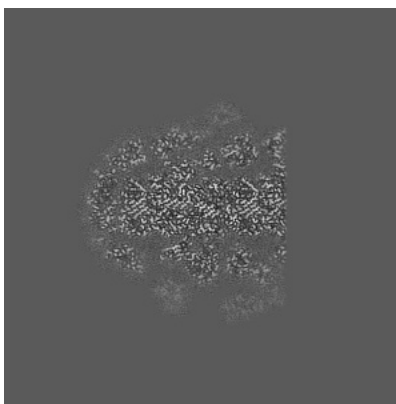
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

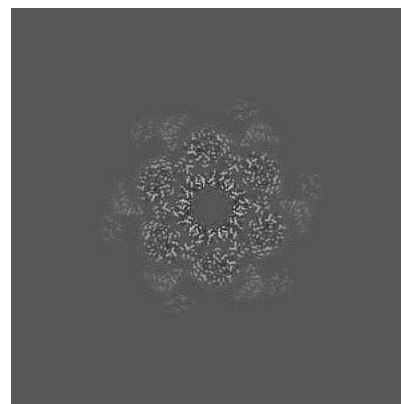
6.3.1 Primary map



X Index: 179



Y Index: 177

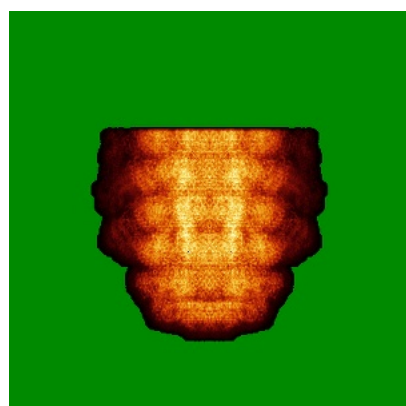


Z Index: 234

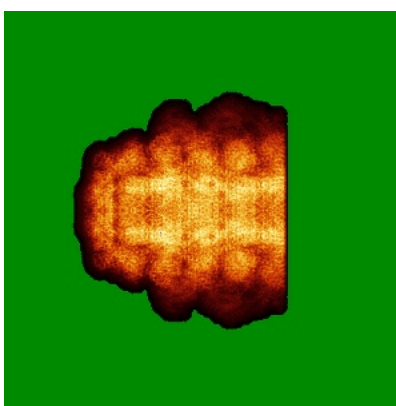
The images above show the largest variance slices of the map in three orthogonal directions.

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

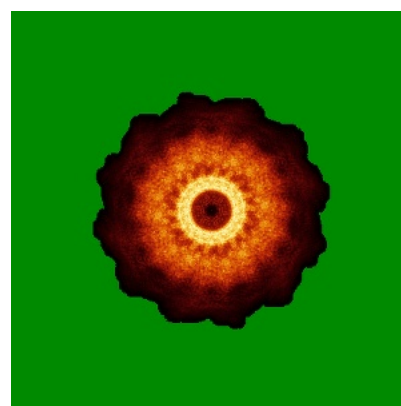
6.4.1 Primary map



X



Y

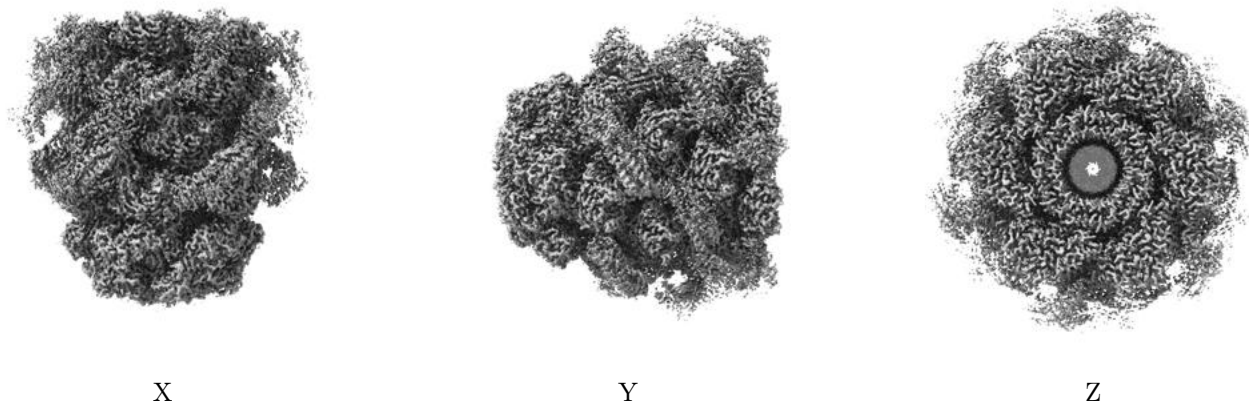


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

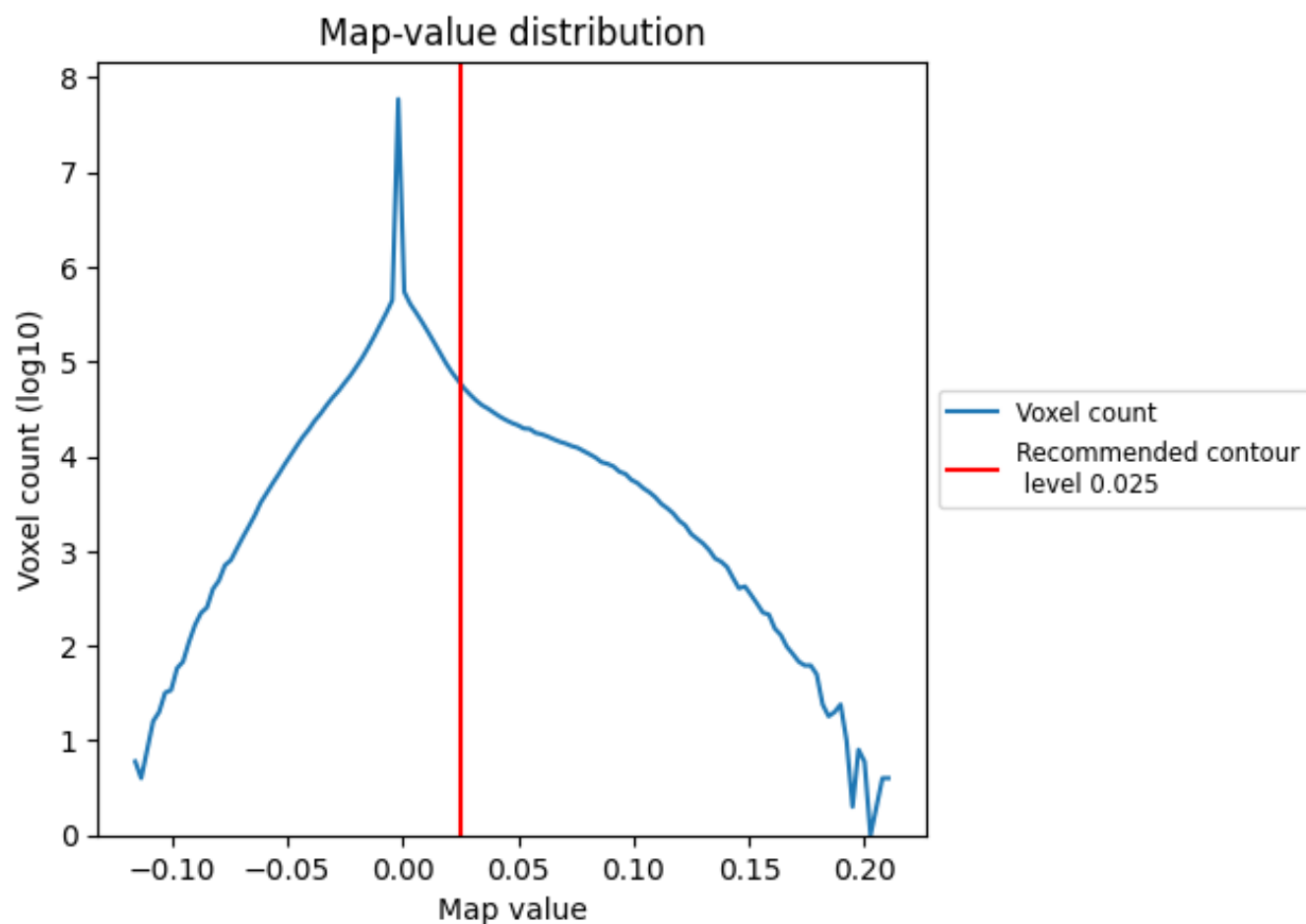
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

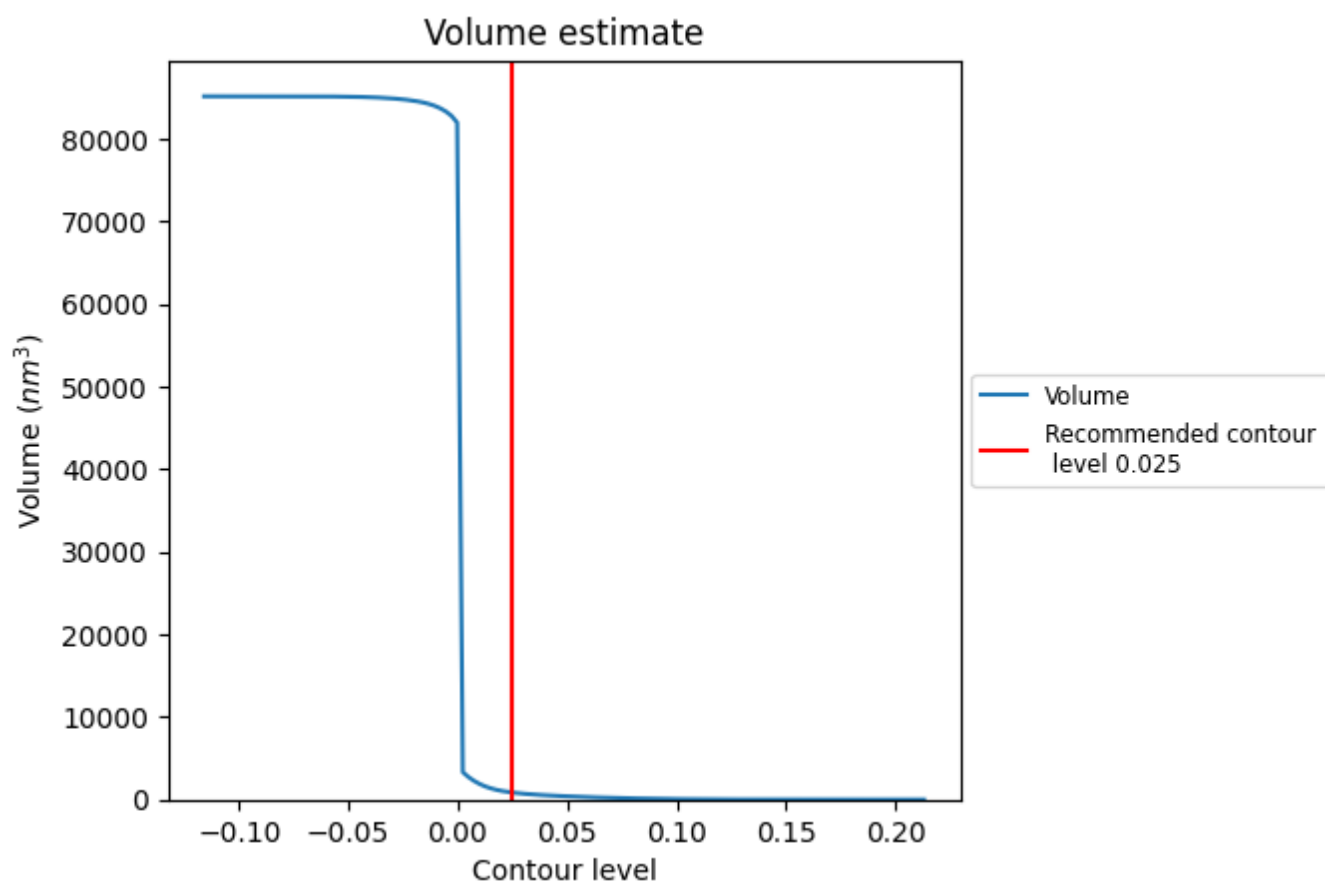
This section contains the results of statistical analysis of the map.

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.

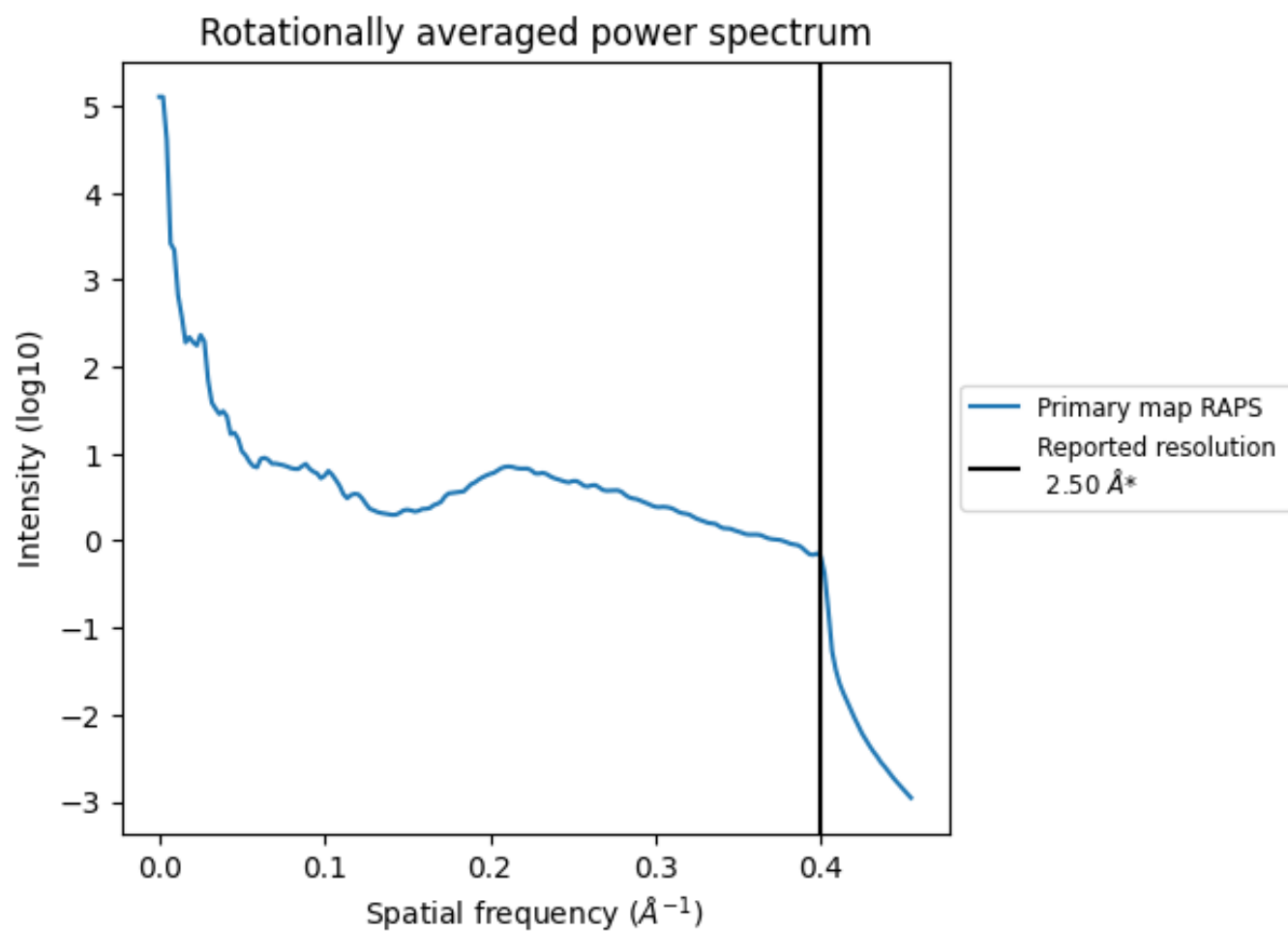
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 851 nm³; this corresponds to an approximate mass of 769 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

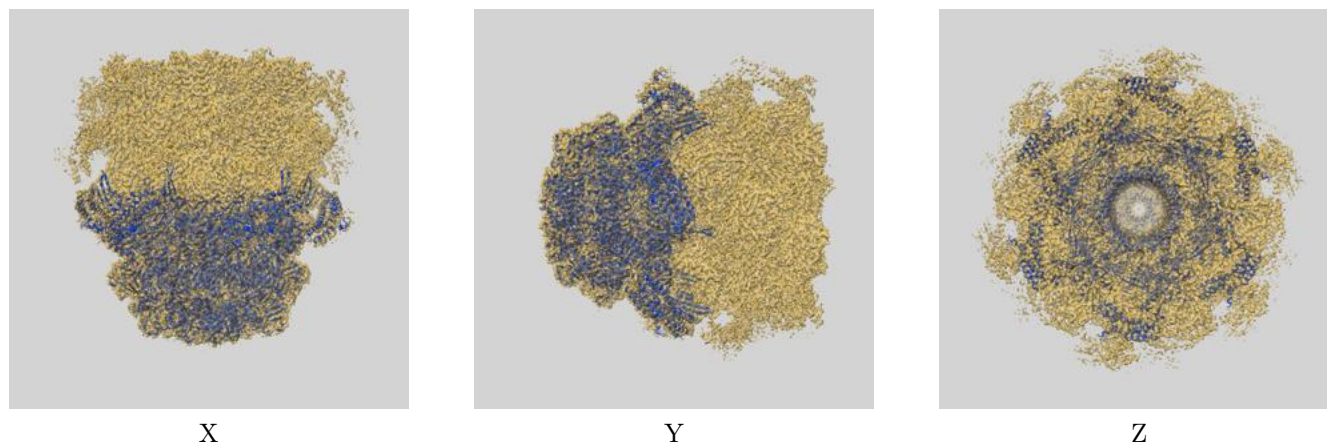
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

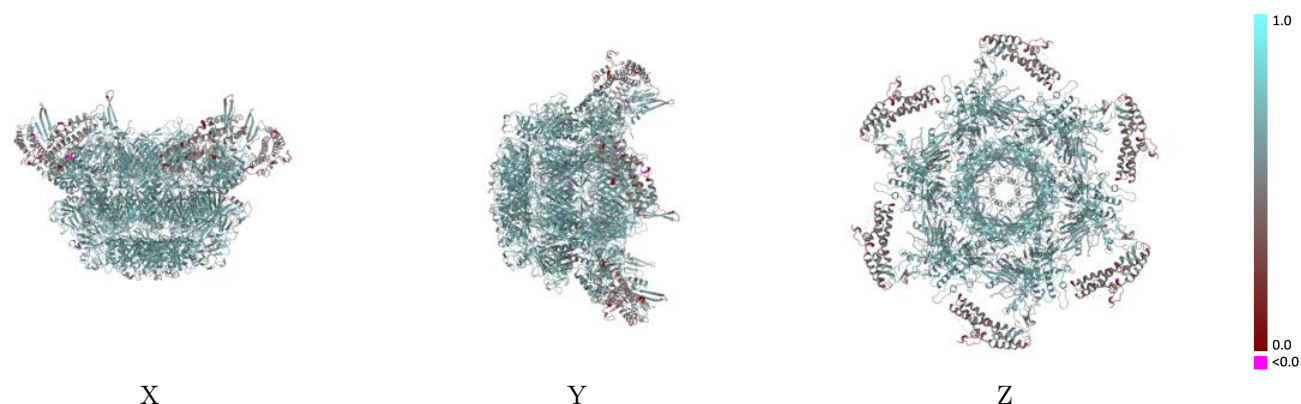
This section contains information regarding the fit between EMDB map EMD-11734 and PDB model 7ADZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



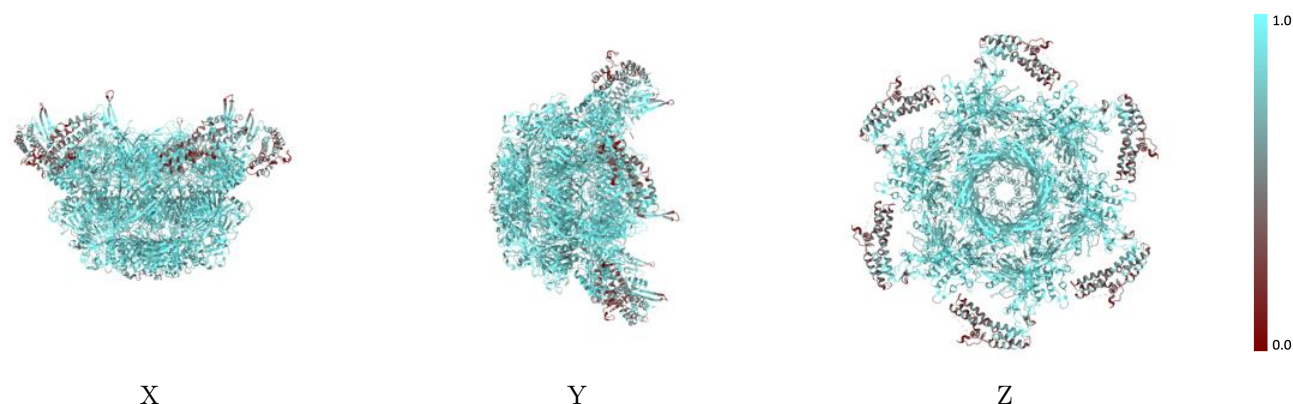
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



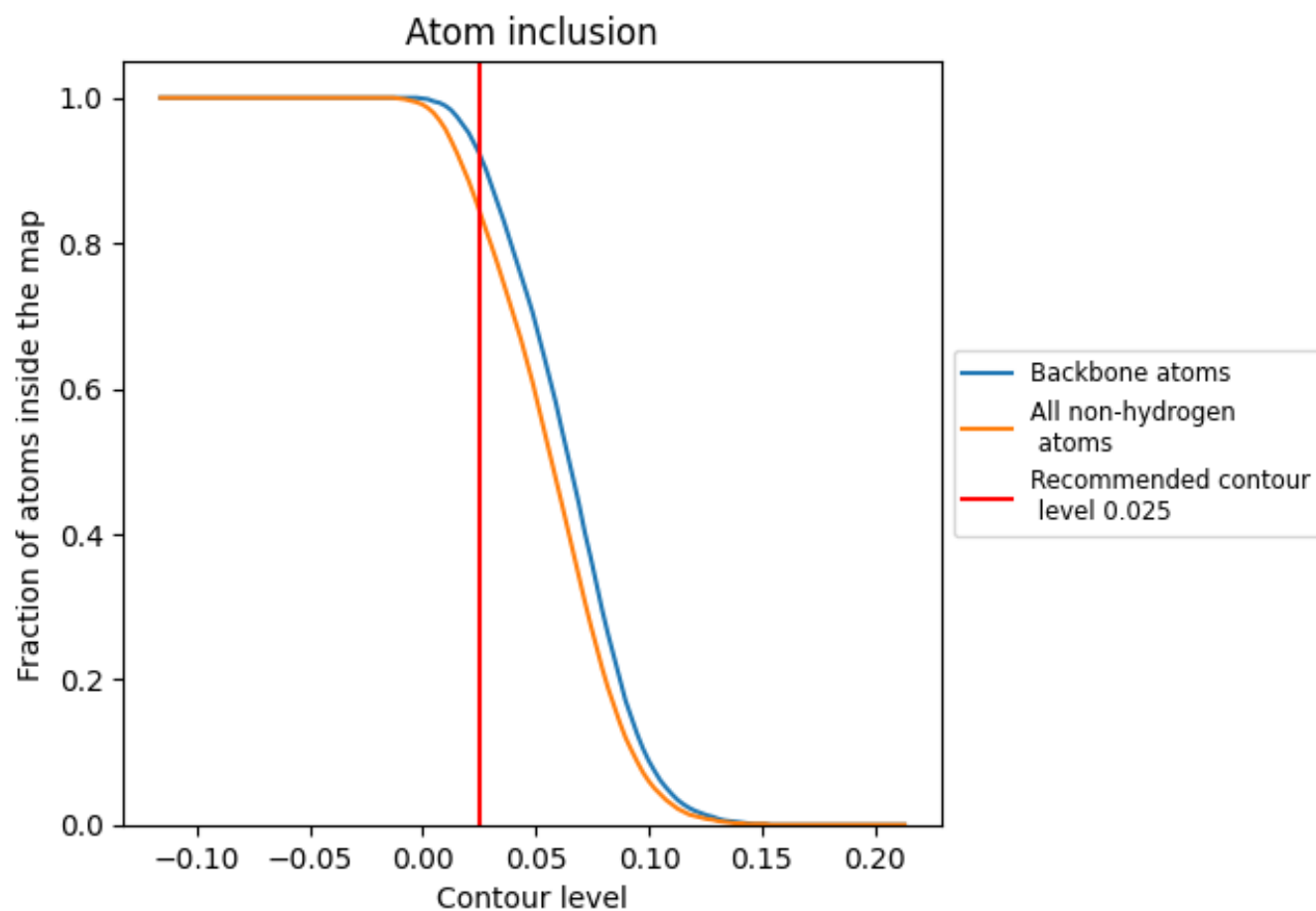
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.6110
0A	 0.9080	 0.6570
0B	 0.9060	 0.6540
0C	 0.9080	 0.6530
0D	 0.9080	 0.6580
0E	 0.9070	 0.6530
0F	 0.9080	 0.6520
1A	 0.8620	 0.6070
1B	 0.8720	 0.6080
1C	 0.8670	 0.6090
1D	 0.8640	 0.6070
1E	 0.8730	 0.6070
1F	 0.8670	 0.6080
1a	 0.9360	 0.6880
1b	 0.9340	 0.6820
1c	 0.9330	 0.6830
1d	 0.9370	 0.6890
1e	 0.9340	 0.6830
1f	 0.9330	 0.6840
2A	 0.7730	 0.5710
2B	 0.7730	 0.5710
2C	 0.7790	 0.5690
2D	 0.7740	 0.5710
2E	 0.7750	 0.5700
2F	 0.7770	 0.5690
2a	 0.9350	 0.6660
2b	 0.9350	 0.6630
2c	 0.9370	 0.6650
2d	 0.9330	 0.6660
2e	 0.9360	 0.6640
2f	 0.9380	 0.6660

