



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:51 AM UTC

PDB ID : 7K08 / pdb_00007k08
EMDB ID : EMD-22589
Title : Cryo-EM structure of the nonameric EscV cytosolic domain from the type III secretion system
Authors : Majewski, D.D.; Lyons, B.J.E.; Atkinson, C.E.; Strynadka, N.C.J.
Deposited on : 2020-09-03
Resolution : 4.70 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:

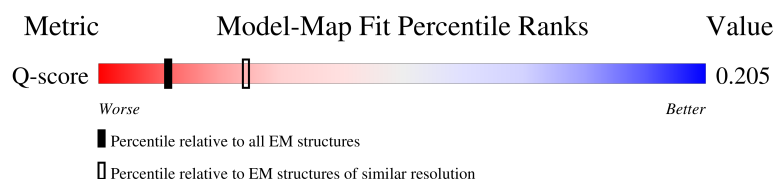
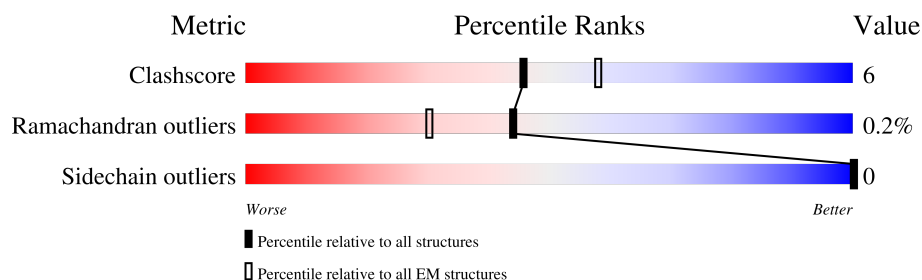
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.70 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	1989 (4.20 - 5.20)

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	A	342	
1	B	342	
1	C	342	
1	D	342	

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Mol	Chain	Length	Quality of chain
1	E	342	27% 70% 21% 6%
1	F	342	27% 70% 22% 5%
1	G	342	27% 69% 23% 6%
1	H	342	29% 70% 22% 6%
1	I	342	27% 70% 22% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 48735 atoms, of which 24606 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 Translocator EscV.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	B	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	C	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	D	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	E	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	F	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	G	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	H	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		
1	I	332	Total	C	H	N	O	S	0	0
			5415	1714	2734	448	512	7		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	expression tag	UNP B7UMA7
A	335	SER	-	expression tag	UNP B7UMA7
A	336	HIS	-	expression tag	UNP B7UMA7
A	337	MET	-	expression tag	UNP B7UMA7
B	334	GLY	-	expression tag	UNP B7UMA7
B	335	SER	-	expression tag	UNP B7UMA7
B	336	HIS	-	expression tag	UNP B7UMA7
B	337	MET	-	expression tag	UNP B7UMA7
C	334	GLY	-	expression tag	UNP B7UMA7
C	335	SER	-	expression tag	UNP B7UMA7
C	336	HIS	-	expression tag	UNP B7UMA7
C	337	MET	-	expression tag	UNP B7UMA7

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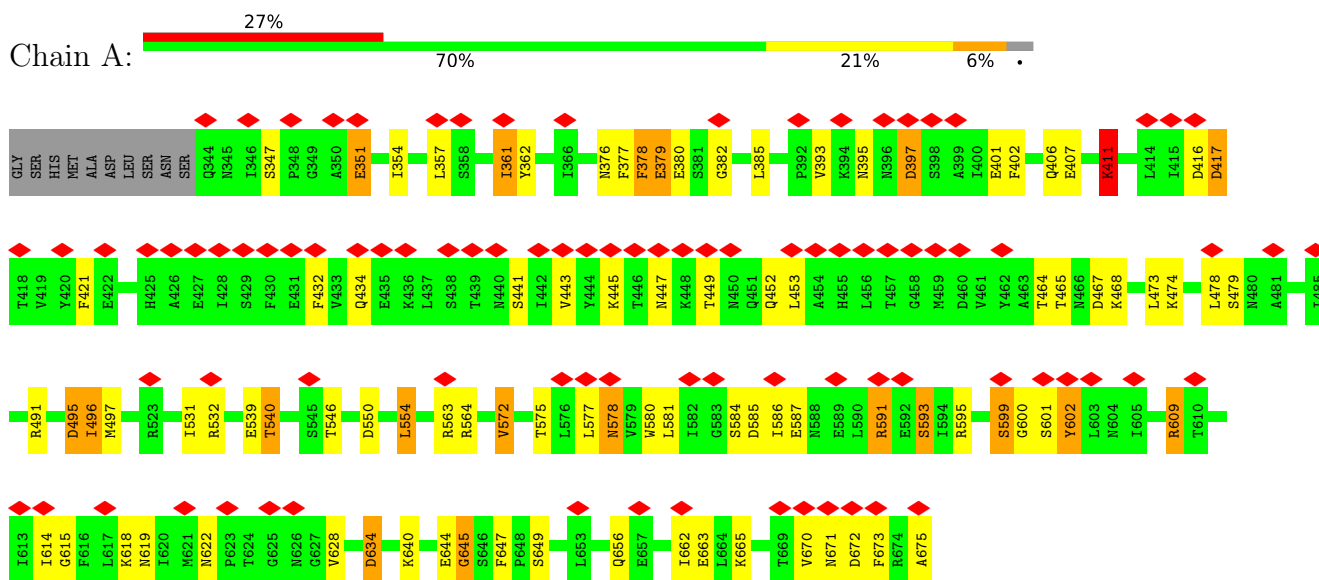
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Chain	Residue	Modelled	Actual	Comment	Reference
D	334	GLY	-	expression tag	UNP B7UMA7
D	335	SER	-	expression tag	UNP B7UMA7
D	336	HIS	-	expression tag	UNP B7UMA7
D	337	MET	-	expression tag	UNP B7UMA7
E	334	GLY	-	expression tag	UNP B7UMA7
E	335	SER	-	expression tag	UNP B7UMA7
E	336	HIS	-	expression tag	UNP B7UMA7
E	337	MET	-	expression tag	UNP B7UMA7
F	334	GLY	-	expression tag	UNP B7UMA7
F	335	SER	-	expression tag	UNP B7UMA7
F	336	HIS	-	expression tag	UNP B7UMA7
F	337	MET	-	expression tag	UNP B7UMA7
G	334	GLY	-	expression tag	UNP B7UMA7
G	335	SER	-	expression tag	UNP B7UMA7
G	336	HIS	-	expression tag	UNP B7UMA7
G	337	MET	-	expression tag	UNP B7UMA7
H	334	GLY	-	expression tag	UNP B7UMA7
H	335	SER	-	expression tag	UNP B7UMA7
H	336	HIS	-	expression tag	UNP B7UMA7
H	337	MET	-	expression tag	UNP B7UMA7
I	334	GLY	-	expression tag	UNP B7UMA7
I	335	SER	-	expression tag	UNP B7UMA7
I	336	HIS	-	expression tag	UNP B7UMA7
I	337	MET	-	expression tag	UNP B7UMA7

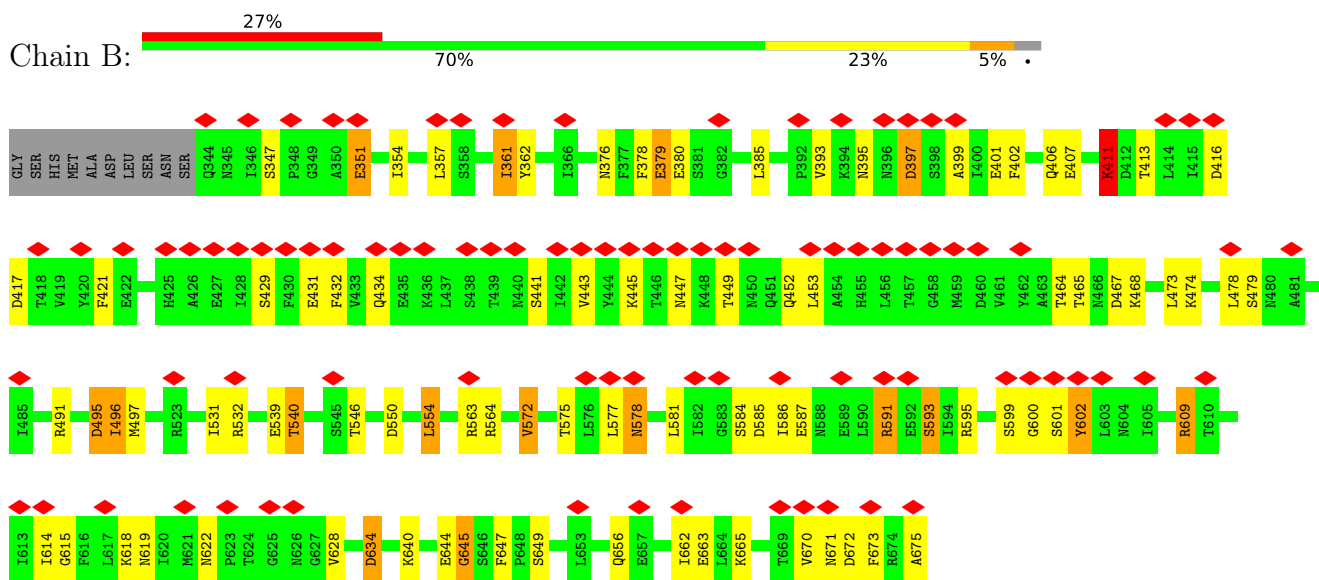
3 Residue-property plots

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: Translocator EscV

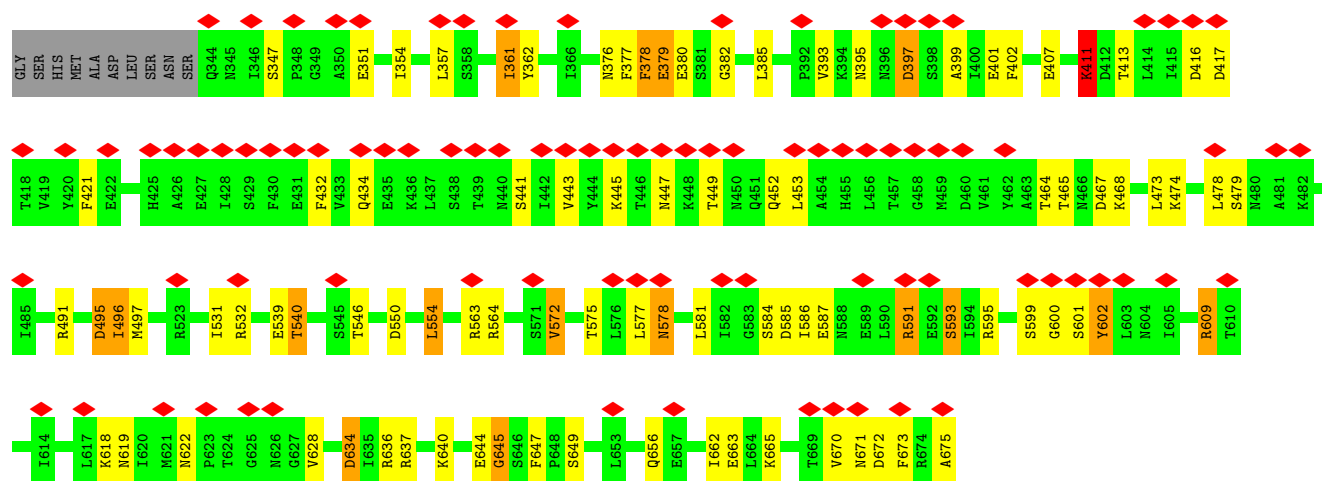


• Molecule 1: Translocator EscV



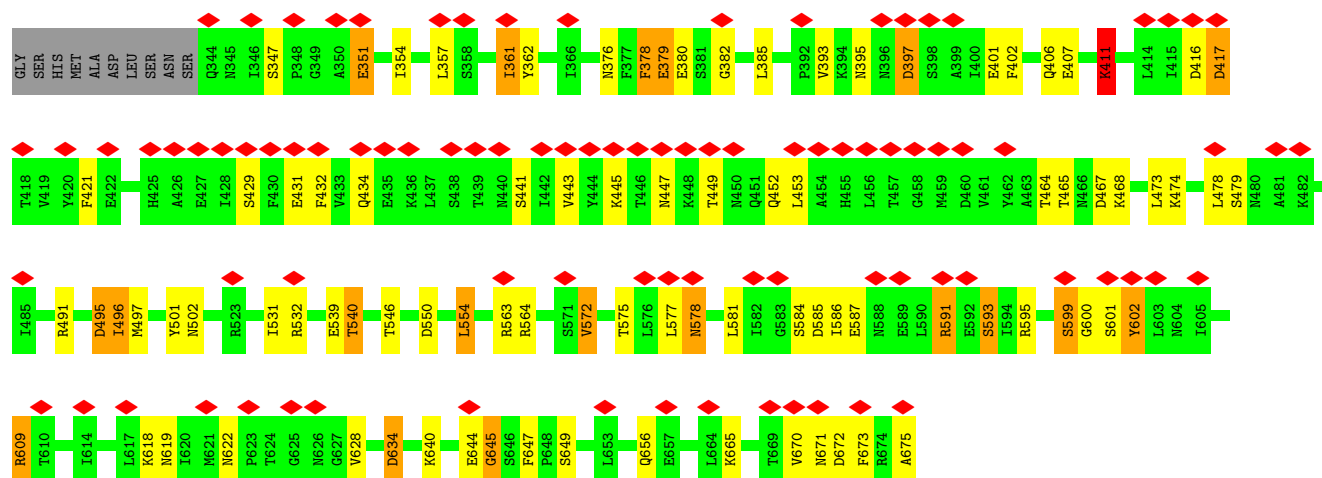
• Molecule 1: Translocator EscV

Chain C: 



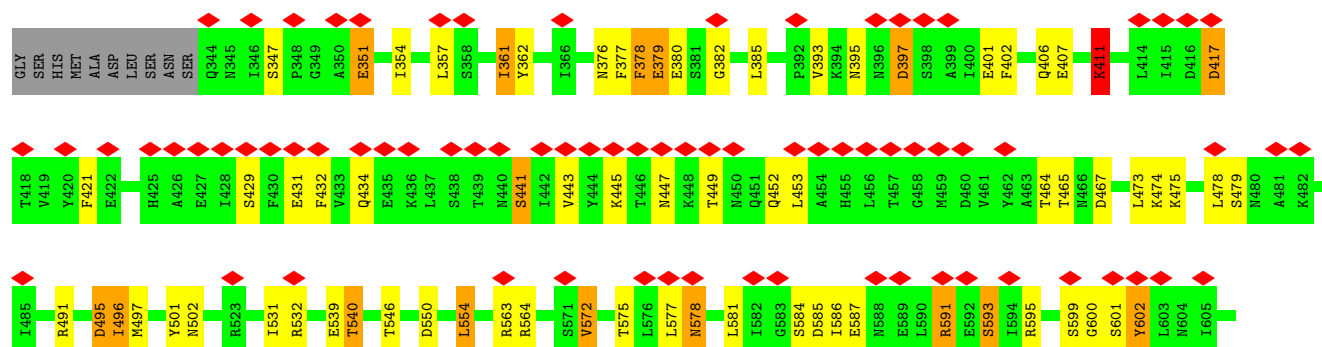
• Molecule 1: Translocator EscV

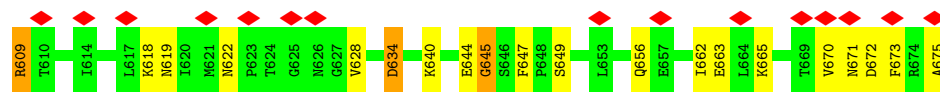
Chain D: 



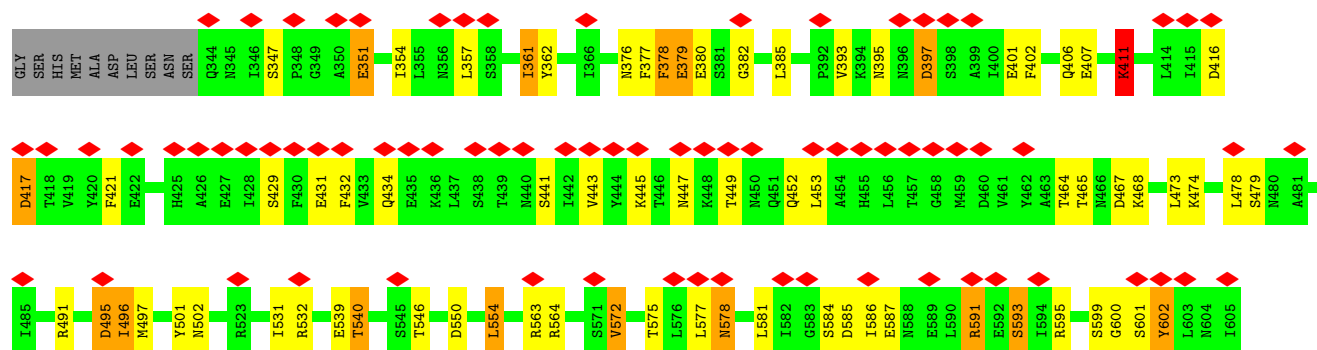
• Molecule 1: Translocator EscV

Chain E: 

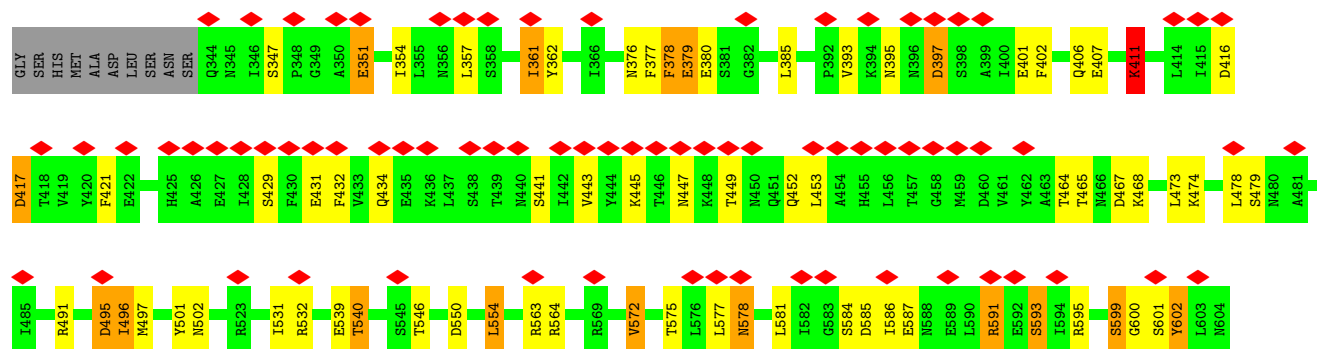




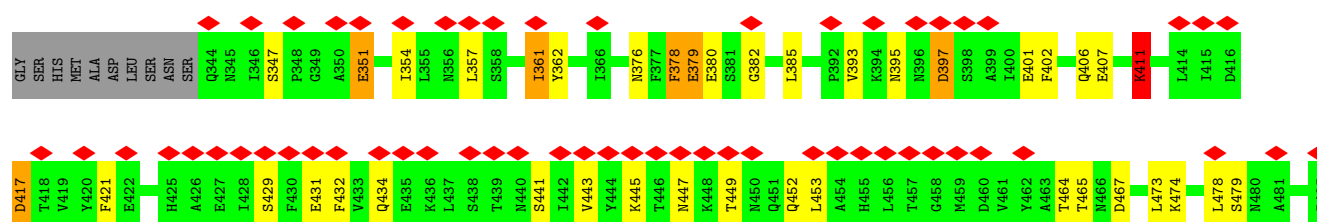
• Molecule 1: Translocator EscV

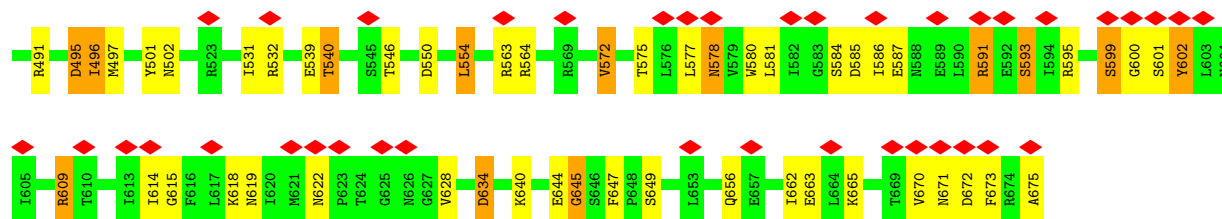


• Molecule 1: Translocator EscV

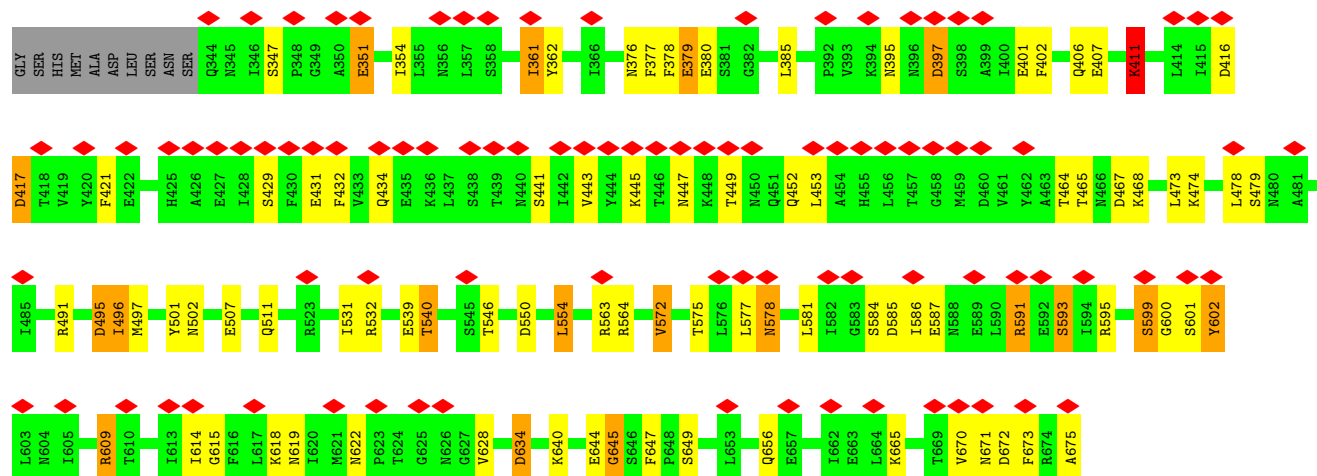


• Molecule 1: Translocator EscV





• Molecule 1: Translocator EscV



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C9	Depositor
Number of particles used	83566	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.017	Depositor
Map size ($\text{\AA}$)	272.64, 272.64, 272.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85200006, 0.85200006, 0.85200006	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	A	1.37	2/2724 (0.1%)	1.70	65/3685 (1.8%)
1	B	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
1	C	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
1	D	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
1	E	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
1	F	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
1	G	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
1	H	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
1	I	1.37	2/2724 (0.1%)	1.70	66/3685 (1.8%)
All	All	1.37	18/24516 (0.1%)	1.70	593/33165 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	11
1	C	0	11
1	D	0	11
1	E	0	11
1	F	0	11
1	G	0	11
1	H	0	11
1	I	0	11
All	All	0	99

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	609	ARG	CZ-NH1	-5.38	1.25	1.32
1	I	609	ARG	CZ-NH1	-5.37	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	609	ARG	CZ-NH1	-5.35	1.25	1.32
1	H	609	ARG	CZ-NH1	-5.35	1.25	1.32
1	F	609	ARG	CZ-NH1	-5.35	1.25	1.32
1	E	609	ARG	CZ-NH1	-5.34	1.25	1.32
1	B	609	ARG	CZ-NH1	-5.31	1.25	1.32
1	G	609	ARG	CZ-NH1	-5.31	1.25	1.32
1	A	609	ARG	CZ-NH1	-5.29	1.25	1.32
1	E	609	ARG	CD-NE	5.17	1.53	1.46
1	D	609	ARG	CD-NE	5.16	1.53	1.46
1	I	609	ARG	CD-NE	5.15	1.53	1.46
1	B	609	ARG	CD-NE	5.15	1.53	1.46
1	C	609	ARG	CD-NE	5.13	1.53	1.46
1	G	609	ARG	CD-NE	5.13	1.53	1.46
1	F	609	ARG	CD-NE	5.11	1.53	1.46
1	H	609	ARG	CD-NE	5.10	1.53	1.46
1	A	609	ARG	CD-NE	5.08	1.53	1.46

All (593) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	ARG	CA-C-N	18.30	152.44	122.62
1	B	532	ARG	C-N-CA	18.30	152.44	122.62
1	C	532	ARG	CA-C-N	18.29	152.43	122.62
1	C	532	ARG	C-N-CA	18.29	152.43	122.62
1	G	532	ARG	CA-C-N	18.28	152.41	122.62
1	G	532	ARG	C-N-CA	18.28	152.41	122.62
1	I	532	ARG	CA-C-N	18.28	152.41	122.62
1	I	532	ARG	C-N-CA	18.28	152.41	122.62
1	D	532	ARG	CA-C-N	18.27	152.41	122.62
1	D	532	ARG	C-N-CA	18.27	152.41	122.62
1	H	532	ARG	CA-C-N	18.26	152.39	122.62
1	H	532	ARG	C-N-CA	18.26	152.39	122.62
1	F	532	ARG	CA-C-N	18.26	152.39	122.62
1	F	532	ARG	C-N-CA	18.26	152.39	122.62
1	A	532	ARG	CA-C-N	18.25	152.37	122.62
1	A	532	ARG	C-N-CA	18.25	152.37	122.62
1	E	532	ARG	CA-C-N	18.25	152.37	122.62
1	E	532	ARG	C-N-CA	18.25	152.37	122.62
1	G	645	GLY	O-C-N	-12.15	114.36	123.35
1	F	645	GLY	O-C-N	-12.11	114.39	123.35
1	C	645	GLY	O-C-N	-12.11	114.39	123.35
1	D	645	GLY	O-C-N	-12.07	114.42	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	645	GLY	O-C-N	-12.07	114.42	123.35
1	B	645	GLY	O-C-N	-12.06	114.42	123.35
1	I	645	GLY	O-C-N	-12.05	114.43	123.35
1	H	645	GLY	O-C-N	-12.03	114.45	123.35
1	E	645	GLY	O-C-N	-12.02	114.46	123.35
1	H	645	GLY	CA-C-O	-9.05	113.42	120.76
1	E	645	GLY	CA-C-O	-9.05	113.43	120.76
1	D	645	GLY	CA-C-O	-9.02	113.45	120.76
1	C	645	GLY	CA-C-O	-9.02	113.46	120.76
1	A	645	GLY	CA-C-O	-9.01	113.46	120.76
1	F	645	GLY	CA-C-O	-9.00	113.47	120.76
1	B	645	GLY	CA-C-O	-8.99	113.47	120.76
1	G	645	GLY	CA-C-O	-8.99	113.48	120.76
1	I	645	GLY	CA-C-O	-8.97	113.50	120.76
1	B	495	ASP	N-CA-C	-8.88	102.03	113.12
1	E	495	ASP	N-CA-C	-8.88	102.03	113.12
1	H	495	ASP	N-CA-C	-8.86	102.05	113.12
1	C	495	ASP	N-CA-C	-8.86	102.05	113.12
1	I	495	ASP	N-CA-C	-8.85	102.06	113.12
1	G	495	ASP	N-CA-C	-8.85	102.06	113.12
1	D	495	ASP	N-CA-C	-8.84	102.07	113.12
1	F	495	ASP	N-CA-C	-8.84	102.08	113.12
1	A	495	ASP	N-CA-C	-8.83	102.08	113.12
1	I	351	GLU	CA-C-N	8.54	128.97	120.52
1	I	351	GLU	C-N-CA	8.54	128.97	120.52
1	B	351	GLU	CA-C-N	8.53	128.96	120.52
1	B	351	GLU	C-N-CA	8.53	128.96	120.52
1	E	351	GLU	CA-C-N	8.53	128.96	120.52
1	E	351	GLU	C-N-CA	8.53	128.96	120.52
1	D	351	GLU	CA-C-N	8.51	128.94	120.52
1	D	351	GLU	C-N-CA	8.51	128.94	120.52
1	H	351	GLU	CA-C-N	8.50	128.94	120.52
1	H	351	GLU	C-N-CA	8.50	128.94	120.52
1	A	351	GLU	CA-C-N	8.50	128.94	120.52
1	A	351	GLU	C-N-CA	8.50	128.94	120.52
1	G	351	GLU	CA-C-N	8.48	128.91	120.52
1	G	351	GLU	C-N-CA	8.48	128.91	120.52
1	F	351	GLU	CA-C-N	8.47	128.91	120.52
1	F	351	GLU	C-N-CA	8.47	128.91	120.52
1	C	351	GLU	CA-C-N	8.47	128.90	120.52
1	C	351	GLU	C-N-CA	8.47	128.90	120.52
1	D	378	PHE	CA-CB-CG	-7.64	106.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	PHE	CA-CB-CG	-7.61	106.19	113.80
1	F	378	PHE	CA-CB-CG	-7.61	106.19	113.80
1	A	378	PHE	CA-CB-CG	-7.60	106.20	113.80
1	G	378	PHE	CA-CB-CG	-7.60	106.20	113.80
1	H	378	PHE	CA-CB-CG	-7.60	106.20	113.80
1	I	378	PHE	CA-CB-CG	-7.59	106.21	113.80
1	E	378	PHE	CA-CB-CG	-7.58	106.22	113.80
1	C	378	PHE	CA-CB-CG	-7.56	106.24	113.80
1	D	478	LEU	N-CA-C	-7.54	103.03	112.90
1	H	402	PHE	CA-CB-CG	-7.54	106.27	113.80
1	E	478	LEU	N-CA-C	-7.53	103.03	112.90
1	C	402	PHE	CA-CB-CG	-7.53	106.27	113.80
1	G	402	PHE	CA-CB-CG	-7.53	106.27	113.80
1	A	402	PHE	CA-CB-CG	-7.52	106.28	113.80
1	C	478	LEU	N-CA-C	-7.52	103.05	112.90
1	F	478	LEU	N-CA-C	-7.52	103.05	112.90
1	A	478	LEU	N-CA-C	-7.52	103.05	112.90
1	E	402	PHE	CA-CB-CG	-7.52	106.28	113.80
1	G	478	LEU	N-CA-C	-7.51	103.06	112.90
1	F	402	PHE	CA-CB-CG	-7.51	106.29	113.80
1	I	478	LEU	N-CA-C	-7.50	103.07	112.90
1	B	478	LEU	N-CA-C	-7.50	103.08	112.90
1	H	478	LEU	N-CA-C	-7.50	103.08	112.90
1	I	402	PHE	CA-CB-CG	-7.50	106.30	113.80
1	D	402	PHE	CA-CB-CG	-7.47	106.33	113.80
1	B	402	PHE	CA-CB-CG	-7.46	106.34	113.80
1	B	554	LEU	CA-C-N	-7.35	109.21	121.92
1	B	554	LEU	C-N-CA	-7.35	109.21	121.92
1	F	554	LEU	CA-C-N	-7.34	109.22	121.92
1	F	554	LEU	C-N-CA	-7.34	109.22	121.92
1	C	554	LEU	CA-C-N	-7.33	109.23	121.92
1	C	554	LEU	C-N-CA	-7.33	109.23	121.92
1	H	554	LEU	CA-C-N	-7.33	109.23	121.92
1	H	554	LEU	C-N-CA	-7.33	109.23	121.92
1	D	554	LEU	CA-C-N	-7.33	109.24	121.92
1	D	554	LEU	C-N-CA	-7.33	109.24	121.92
1	E	554	LEU	CA-C-N	-7.32	109.25	121.92
1	E	554	LEU	C-N-CA	-7.32	109.25	121.92
1	A	554	LEU	CA-C-N	-7.32	109.25	121.92
1	A	554	LEU	C-N-CA	-7.32	109.25	121.92
1	G	554	LEU	CA-C-N	-7.32	109.26	121.92
1	G	554	LEU	C-N-CA	-7.32	109.26	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	554	LEU	CA-C-N	-7.31	109.28	121.92
1	I	554	LEU	C-N-CA	-7.31	109.28	121.92
1	I	647	PHE	CA-C-N	7.30	127.46	119.87
1	I	647	PHE	C-N-CA	7.30	127.46	119.87
1	B	647	PHE	CA-C-N	7.29	127.45	119.87
1	B	647	PHE	C-N-CA	7.29	127.45	119.87
1	D	647	PHE	CA-C-N	7.29	127.45	119.87
1	D	647	PHE	C-N-CA	7.29	127.45	119.87
1	G	647	PHE	CA-C-N	7.28	127.44	119.87
1	G	647	PHE	C-N-CA	7.28	127.44	119.87
1	A	647	PHE	CA-C-N	7.27	127.43	119.87
1	A	647	PHE	C-N-CA	7.27	127.43	119.87
1	E	647	PHE	CA-C-N	7.27	127.43	119.87
1	E	647	PHE	C-N-CA	7.27	127.43	119.87
1	C	647	PHE	CA-C-N	7.26	127.42	119.87
1	C	647	PHE	C-N-CA	7.26	127.42	119.87
1	F	647	PHE	CA-C-N	7.24	127.40	119.87
1	F	647	PHE	C-N-CA	7.24	127.40	119.87
1	H	647	PHE	CA-C-N	7.24	127.40	119.87
1	H	647	PHE	C-N-CA	7.24	127.40	119.87
1	I	411	LYS	CA-C-O	-7.17	112.42	120.66
1	B	411	LYS	CA-C-O	-7.14	112.44	120.66
1	G	411	LYS	CA-C-O	-7.14	112.45	120.66
1	C	411	LYS	CA-C-O	-7.14	112.45	120.66
1	D	411	LYS	CA-C-O	-7.13	112.45	120.66
1	A	411	LYS	CA-C-O	-7.12	112.47	120.66
1	E	411	LYS	CA-C-O	-7.11	112.48	120.66
1	F	411	LYS	CA-C-O	-7.11	112.49	120.66
1	H	411	LYS	CA-C-O	-7.09	112.50	120.66
1	F	634	ASP	N-CA-C	-6.81	103.65	112.23
1	I	634	ASP	N-CA-C	-6.80	103.66	112.23
1	H	634	ASP	N-CA-C	-6.80	103.66	112.23
1	B	634	ASP	N-CA-C	-6.78	103.69	112.23
1	D	634	ASP	N-CA-C	-6.78	103.69	112.23
1	C	634	ASP	N-CA-C	-6.77	103.69	112.23
1	G	634	ASP	N-CA-C	-6.77	103.70	112.23
1	E	634	ASP	N-CA-C	-6.76	103.71	112.23
1	A	634	ASP	N-CA-C	-6.75	103.72	112.23
1	G	441	SER	N-CA-C	-6.71	101.04	110.50
1	D	441	SER	N-CA-C	-6.70	101.05	110.50
1	C	441	SER	N-CA-C	-6.70	101.06	110.50
1	E	441	SER	N-CA-C	-6.70	101.06	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	441	SER	N-CA-C	-6.69	101.07	110.50
1	B	441	SER	N-CA-C	-6.66	101.10	110.50
1	F	441	SER	N-CA-C	-6.66	101.10	110.50
1	H	441	SER	N-CA-C	-6.66	101.12	110.50
1	A	441	SER	N-CA-C	-6.65	101.13	110.50
1	F	421	PHE	N-CA-C	6.58	118.45	109.11
1	D	421	PHE	N-CA-C	6.56	118.43	109.11
1	C	421	PHE	N-CA-C	6.55	118.42	109.11
1	B	421	PHE	N-CA-C	6.55	118.41	109.11
1	G	421	PHE	N-CA-C	6.54	118.40	109.11
1	A	421	PHE	N-CA-C	6.53	118.39	109.11
1	E	421	PHE	N-CA-C	6.53	118.38	109.11
1	H	421	PHE	N-CA-C	6.53	118.38	109.11
1	I	421	PHE	N-CA-C	6.51	118.35	109.11
1	H	361	ILE	CA-C-O	-6.46	114.23	120.30
1	B	361	ILE	CA-C-O	-6.40	114.28	120.30
1	F	347	SER	CA-C-N	6.39	126.01	119.56
1	F	347	SER	C-N-CA	6.39	126.01	119.56
1	F	361	ILE	CA-C-O	-6.39	114.29	120.30
1	G	361	ILE	CA-C-O	-6.39	114.30	120.30
1	E	361	ILE	CA-C-O	-6.38	114.30	120.30
1	A	361	ILE	CA-C-O	-6.38	114.31	120.30
1	I	361	ILE	CA-C-O	-6.38	114.31	120.30
1	I	347	SER	CA-C-N	6.37	126.00	119.56
1	I	347	SER	C-N-CA	6.37	126.00	119.56
1	C	361	ILE	CA-C-O	-6.37	114.31	120.30
1	C	347	SER	CA-C-N	6.35	125.98	119.56
1	C	347	SER	C-N-CA	6.35	125.98	119.56
1	G	602	TYR	N-CA-C	-6.35	103.50	111.11
1	G	347	SER	CA-C-N	6.34	125.97	119.56
1	G	347	SER	C-N-CA	6.34	125.97	119.56
1	A	347	SER	CA-C-N	6.34	125.97	119.56
1	A	347	SER	C-N-CA	6.34	125.97	119.56
1	F	602	TYR	N-CA-C	-6.34	103.50	111.11
1	D	361	ILE	CA-C-O	-6.33	114.35	120.30
1	E	347	SER	CA-C-N	6.33	125.96	119.56
1	E	347	SER	C-N-CA	6.33	125.96	119.56
1	I	602	TYR	N-CA-C	-6.33	103.52	111.11
1	B	347	SER	CA-C-N	6.32	125.95	119.56
1	B	347	SER	C-N-CA	6.32	125.95	119.56
1	E	602	TYR	N-CA-C	-6.31	103.54	111.11
1	H	347	SER	CA-C-N	6.30	125.93	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	347	SER	C-N-CA	6.30	125.93	119.56
1	D	602	TYR	N-CA-C	-6.30	103.55	111.11
1	H	602	TYR	N-CA-C	-6.30	103.55	111.11
1	B	602	TYR	N-CA-C	-6.29	103.57	111.11
1	D	347	SER	CA-C-N	6.28	125.90	119.56
1	D	347	SER	C-N-CA	6.28	125.90	119.56
1	D	385	LEU	CA-C-N	6.28	126.24	119.78
1	D	385	LEU	C-N-CA	6.28	126.24	119.78
1	C	602	TYR	N-CA-C	-6.27	103.59	111.11
1	A	602	TYR	N-CA-C	-6.27	103.59	111.11
1	H	417	ASP	N-CA-C	-6.26	104.00	113.89
1	H	385	LEU	CA-C-N	6.26	126.23	119.78
1	H	385	LEU	C-N-CA	6.26	126.23	119.78
1	C	385	LEU	CA-C-N	6.25	126.22	119.78
1	C	385	LEU	C-N-CA	6.25	126.22	119.78
1	F	385	LEU	CA-C-N	6.25	126.22	119.78
1	F	385	LEU	C-N-CA	6.25	126.22	119.78
1	G	417	ASP	N-CA-C	-6.25	104.01	113.89
1	E	385	LEU	CA-C-N	6.25	126.22	119.78
1	E	385	LEU	C-N-CA	6.25	126.22	119.78
1	I	417	ASP	N-CA-C	-6.24	104.03	113.89
1	C	417	ASP	N-CA-C	-6.24	104.03	113.89
1	A	385	LEU	CA-C-N	6.24	126.20	119.78
1	A	385	LEU	C-N-CA	6.24	126.20	119.78
1	E	649	SER	CA-C-N	-6.24	118.10	122.59
1	E	649	SER	C-N-CA	-6.24	118.10	122.59
1	F	417	ASP	N-CA-C	-6.24	104.04	113.89
1	B	417	ASP	N-CA-C	-6.23	104.05	113.89
1	F	649	SER	CA-C-N	-6.22	118.11	122.59
1	F	649	SER	C-N-CA	-6.22	118.11	122.59
1	E	417	ASP	N-CA-C	-6.22	104.06	113.89
1	B	385	LEU	CA-C-N	6.22	126.19	119.78
1	B	385	LEU	C-N-CA	6.22	126.19	119.78
1	I	644	GLU	N-CA-C	-6.21	104.51	111.28
1	A	417	ASP	N-CA-C	-6.21	104.08	113.89
1	D	417	ASP	N-CA-C	-6.21	104.09	113.89
1	I	385	LEU	CA-C-N	6.20	126.17	119.78
1	I	385	LEU	C-N-CA	6.20	126.17	119.78
1	D	554	LEU	CA-C-O	-6.19	111.76	119.38
1	H	554	LEU	CA-C-O	-6.19	111.76	119.38
1	G	554	LEU	CA-C-O	-6.18	111.77	119.38
1	A	649	SER	CA-C-N	-6.18	118.14	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	SER	C-N-CA	-6.18	118.14	122.59
1	D	649	SER	CA-C-N	-6.18	118.14	122.59
1	D	649	SER	C-N-CA	-6.18	118.14	122.59
1	G	385	LEU	CA-C-N	6.18	126.15	119.78
1	G	385	LEU	C-N-CA	6.18	126.15	119.78
1	E	644	GLU	N-CA-C	-6.17	104.55	111.28
1	A	644	GLU	N-CA-C	-6.16	104.56	111.28
1	D	644	GLU	N-CA-C	-6.16	104.56	111.28
1	C	644	GLU	N-CA-C	-6.16	104.57	111.28
1	B	649	SER	CA-C-N	-6.16	118.16	122.59
1	B	649	SER	C-N-CA	-6.16	118.16	122.59
1	I	554	LEU	CA-C-O	-6.16	111.81	119.38
1	I	649	SER	CA-C-N	-6.15	118.16	122.59
1	I	649	SER	C-N-CA	-6.15	118.16	122.59
1	E	554	LEU	CA-C-O	-6.15	111.81	119.38
1	G	644	GLU	N-CA-C	-6.15	104.58	111.28
1	B	554	LEU	CA-C-O	-6.15	111.82	119.38
1	A	554	LEU	CA-C-O	-6.14	111.82	119.38
1	B	644	GLU	N-CA-C	-6.14	104.58	111.28
1	C	554	LEU	CA-C-O	-6.14	111.82	119.38
1	C	649	SER	CA-C-N	-6.14	118.17	122.59
1	C	649	SER	C-N-CA	-6.14	118.17	122.59
1	H	649	SER	CA-C-N	-6.14	118.17	122.59
1	H	649	SER	C-N-CA	-6.14	118.17	122.59
1	F	554	LEU	CA-C-O	-6.13	111.84	119.38
1	G	649	SER	CA-C-N	-6.13	118.18	122.59
1	G	649	SER	C-N-CA	-6.13	118.18	122.59
1	F	644	GLU	N-CA-C	-6.12	104.61	111.28
1	H	644	GLU	N-CA-C	-6.12	104.61	111.28
1	B	453	LEU	N-CA-C	-6.12	103.95	112.45
1	D	453	LEU	N-CA-C	-6.12	103.95	112.45
1	G	379	GLU	CA-C-O	-6.12	114.40	120.82
1	G	453	LEU	N-CA-C	-6.12	103.95	112.45
1	H	673	PHE	CA-CB-CG	6.11	119.91	113.80
1	F	453	LEU	N-CA-C	-6.11	103.97	112.45
1	G	673	PHE	CA-CB-CG	6.11	119.91	113.80
1	I	379	GLU	CA-C-O	-6.11	114.41	120.82
1	C	673	PHE	CA-CB-CG	6.10	119.90	113.80
1	C	453	LEU	N-CA-C	-6.10	103.97	112.45
1	F	379	GLU	CA-C-O	-6.10	114.42	120.82
1	E	593	SER	CA-C-N	-6.09	111.00	121.97
1	E	593	SER	C-N-CA	-6.09	111.00	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	453	LEU	N-CA-C	-6.09	103.98	112.45
1	A	379	GLU	CA-C-O	-6.09	114.42	120.82
1	I	453	LEU	N-CA-C	-6.09	103.98	112.45
1	I	673	PHE	CA-CB-CG	6.09	119.89	113.80
1	D	379	GLU	CA-C-O	-6.09	114.43	120.82
1	D	593	SER	CA-C-N	-6.09	111.01	121.97
1	D	593	SER	C-N-CA	-6.09	111.01	121.97
1	A	453	LEU	N-CA-C	-6.08	103.99	112.45
1	B	379	GLU	CA-C-O	-6.08	114.43	120.82
1	E	453	LEU	N-CA-C	-6.08	103.99	112.45
1	C	593	SER	CA-C-N	-6.08	111.02	121.97
1	C	593	SER	C-N-CA	-6.08	111.02	121.97
1	C	379	GLU	CA-C-O	-6.08	114.43	120.82
1	E	673	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	673	PHE	CA-CB-CG	6.08	119.88	113.80
1	B	673	PHE	CA-CB-CG	6.07	119.87	113.80
1	G	593	SER	CA-C-N	-6.07	111.05	121.97
1	G	593	SER	C-N-CA	-6.07	111.05	121.97
1	H	379	GLU	CA-C-O	-6.07	114.45	120.82
1	E	379	GLU	CA-C-O	-6.07	114.45	120.82
1	B	593	SER	CA-C-N	-6.07	111.05	121.97
1	B	593	SER	C-N-CA	-6.07	111.05	121.97
1	D	673	PHE	CA-CB-CG	6.06	119.86	113.80
1	H	593	SER	CA-C-N	-6.05	111.07	121.97
1	H	593	SER	C-N-CA	-6.05	111.07	121.97
1	F	673	PHE	CA-CB-CG	6.05	119.85	113.80
1	I	593	SER	CA-C-N	-6.05	111.08	121.97
1	I	593	SER	C-N-CA	-6.05	111.08	121.97
1	A	593	SER	CA-C-N	-6.05	111.08	121.97
1	A	593	SER	C-N-CA	-6.05	111.08	121.97
1	F	593	SER	CA-C-N	-6.04	111.10	121.97
1	F	593	SER	C-N-CA	-6.04	111.10	121.97
1	C	618	LYS	N-CA-C	-6.03	104.78	111.71
1	B	618	LYS	N-CA-C	-6.01	104.80	111.71
1	G	618	LYS	N-CA-C	-6.00	104.81	111.71
1	I	618	LYS	N-CA-C	-6.00	104.81	111.71
1	D	618	LYS	N-CA-C	-6.00	104.81	111.71
1	E	618	LYS	N-CA-C	-5.99	104.82	111.71
1	F	618	LYS	N-CA-C	-5.99	104.82	111.71
1	G	622	ASN	CA-C-N	5.99	125.67	119.56
1	G	622	ASN	C-N-CA	5.99	125.67	119.56
1	H	618	LYS	N-CA-C	-5.98	104.83	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	622	ASN	CA-C-N	5.97	125.65	119.56
1	F	622	ASN	C-N-CA	5.97	125.65	119.56
1	I	622	ASN	CA-C-N	5.97	125.65	119.56
1	I	622	ASN	C-N-CA	5.97	125.65	119.56
1	H	539	GLU	CB-CG-CD	5.96	122.73	112.60
1	C	539	GLU	CB-CG-CD	5.95	122.72	112.60
1	A	622	ASN	CA-C-N	5.95	125.63	119.56
1	A	622	ASN	C-N-CA	5.95	125.63	119.56
1	E	622	ASN	CA-C-N	5.95	125.63	119.56
1	E	622	ASN	C-N-CA	5.95	125.63	119.56
1	A	539	GLU	CB-CG-CD	5.95	122.71	112.60
1	A	618	LYS	N-CA-C	-5.94	104.88	111.71
1	B	539	GLU	CB-CG-CD	5.94	122.69	112.60
1	E	539	GLU	CB-CG-CD	5.94	122.69	112.60
1	I	539	GLU	CB-CG-CD	5.94	122.69	112.60
1	D	539	GLU	CB-CG-CD	5.93	122.69	112.60
1	D	622	ASN	CA-C-N	5.93	125.61	119.56
1	D	622	ASN	C-N-CA	5.93	125.61	119.56
1	H	622	ASN	CA-C-N	5.93	125.61	119.56
1	H	622	ASN	C-N-CA	5.93	125.61	119.56
1	F	539	GLU	CB-CG-CD	5.93	122.67	112.60
1	B	622	ASN	CA-C-N	5.92	125.60	119.56
1	B	622	ASN	C-N-CA	5.92	125.60	119.56
1	G	539	GLU	CB-CG-CD	5.91	122.65	112.60
1	C	622	ASN	CA-C-N	5.90	125.58	119.56
1	C	622	ASN	C-N-CA	5.90	125.58	119.56
1	G	595	ARG	N-CA-C	-5.89	101.01	110.14
1	E	595	ARG	N-CA-C	-5.87	101.04	110.14
1	H	347	SER	N-CA-C	5.87	119.83	110.73
1	F	595	ARG	N-CA-C	-5.87	101.05	110.14
1	B	395	ASN	CA-C-N	-5.86	112.39	120.71
1	B	395	ASN	C-N-CA	-5.86	112.39	120.71
1	C	395	ASN	CA-C-N	-5.86	112.39	120.71
1	C	395	ASN	C-N-CA	-5.86	112.39	120.71
1	I	395	ASN	CA-C-N	-5.86	112.39	120.71
1	I	395	ASN	C-N-CA	-5.86	112.39	120.71
1	I	347	SER	N-CA-C	5.86	119.81	110.73
1	D	595	ARG	N-CA-C	-5.85	101.07	110.14
1	A	595	ARG	N-CA-C	-5.85	101.07	110.14
1	G	347	SER	N-CA-C	5.85	119.80	110.73
1	D	347	SER	N-CA-C	5.85	119.80	110.73
1	I	595	ARG	N-CA-C	-5.85	101.07	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	347	SER	N-CA-C	5.85	119.80	110.73
1	G	395	ASN	CA-C-N	-5.85	112.41	120.71
1	G	395	ASN	C-N-CA	-5.85	112.41	120.71
1	H	595	ARG	N-CA-C	-5.85	101.08	110.14
1	A	347	SER	N-CA-C	5.85	119.79	110.73
1	B	595	ARG	N-CA-C	-5.84	101.08	110.14
1	E	395	ASN	CA-C-N	-5.84	112.41	120.71
1	E	395	ASN	C-N-CA	-5.84	112.41	120.71
1	C	595	ARG	N-CA-C	-5.84	101.08	110.14
1	F	347	SER	N-CA-C	5.84	119.78	110.73
1	I	531	ILE	CB-CA-C	-5.84	106.68	113.22
1	A	395	ASN	CA-C-N	-5.84	112.42	120.71
1	A	395	ASN	C-N-CA	-5.84	112.42	120.71
1	C	347	SER	N-CA-C	5.84	119.78	110.73
1	B	347	SER	N-CA-C	5.83	119.77	110.73
1	F	395	ASN	CA-C-N	-5.82	112.45	120.71
1	F	395	ASN	C-N-CA	-5.82	112.45	120.71
1	B	531	ILE	CB-CA-C	-5.82	106.71	113.22
1	D	540	THR	CA-C-O	-5.81	114.72	120.82
1	D	395	ASN	CA-C-N	-5.81	112.46	120.71
1	D	395	ASN	C-N-CA	-5.81	112.46	120.71
1	G	531	ILE	CB-CA-C	-5.80	106.72	113.22
1	H	395	ASN	CA-C-N	-5.80	112.47	120.71
1	H	395	ASN	C-N-CA	-5.80	112.47	120.71
1	H	531	ILE	CB-CA-C	-5.80	106.72	113.22
1	E	531	ILE	CB-CA-C	-5.80	106.72	113.22
1	F	540	THR	CA-C-O	-5.80	114.73	120.82
1	D	531	ILE	CB-CA-C	-5.80	106.73	113.22
1	A	531	ILE	CB-CA-C	-5.79	106.74	113.22
1	B	540	THR	CA-C-O	-5.79	114.74	120.82
1	D	578	ASN	CA-C-N	-5.79	115.64	122.93
1	D	578	ASN	C-N-CA	-5.79	115.64	122.93
1	E	578	ASN	CA-C-N	-5.79	115.64	122.93
1	E	578	ASN	C-N-CA	-5.79	115.64	122.93
1	B	578	ASN	CA-C-N	-5.78	115.64	122.93
1	B	578	ASN	C-N-CA	-5.78	115.64	122.93
1	C	540	THR	CA-C-O	-5.78	114.75	120.82
1	I	540	THR	CA-C-O	-5.78	114.75	120.82
1	A	578	ASN	CA-C-N	-5.78	115.65	122.93
1	A	578	ASN	C-N-CA	-5.78	115.65	122.93
1	C	531	ILE	CB-CA-C	-5.78	106.75	113.22
1	F	531	ILE	CB-CA-C	-5.78	106.75	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	578	ASN	CA-C-N	-5.77	115.66	122.93
1	F	578	ASN	C-N-CA	-5.77	115.66	122.93
1	H	578	ASN	CA-C-N	-5.77	115.66	122.93
1	H	578	ASN	C-N-CA	-5.77	115.66	122.93
1	C	578	ASN	CA-C-N	-5.77	115.67	122.93
1	C	578	ASN	C-N-CA	-5.77	115.67	122.93
1	I	578	ASN	CA-C-N	-5.75	115.68	122.93
1	I	578	ASN	C-N-CA	-5.75	115.68	122.93
1	G	578	ASN	CA-C-N	-5.75	115.68	122.93
1	G	578	ASN	C-N-CA	-5.75	115.68	122.93
1	A	540	THR	CA-C-O	-5.75	114.79	120.82
1	E	540	THR	CA-C-O	-5.74	114.79	120.82
1	C	479	SER	N-CA-C	-5.74	105.03	111.28
1	H	540	THR	CA-C-O	-5.74	114.80	120.82
1	G	479	SER	N-CA-C	-5.74	105.03	111.28
1	G	540	THR	CA-C-O	-5.73	114.80	120.82
1	I	479	SER	N-CA-C	-5.72	105.04	111.28
1	D	479	SER	N-CA-C	-5.72	105.05	111.28
1	F	479	SER	N-CA-C	-5.72	105.05	111.28
1	H	479	SER	N-CA-C	-5.72	105.05	111.28
1	E	479	SER	N-CA-C	-5.69	105.08	111.28
1	B	479	SER	N-CA-C	-5.68	105.08	111.28
1	H	640	LYS	N-CA-C	-5.68	105.09	111.28
1	G	640	LYS	N-CA-C	-5.68	105.09	111.28
1	A	479	SER	N-CA-C	-5.67	105.09	111.28
1	D	640	LYS	N-CA-C	-5.66	105.11	111.28
1	A	640	LYS	N-CA-C	-5.65	105.12	111.28
1	B	640	LYS	N-CA-C	-5.65	105.12	111.28
1	I	640	LYS	N-CA-C	-5.65	105.12	111.28
1	E	640	LYS	N-CA-C	-5.65	105.12	111.28
1	A	593	SER	CA-C-O	-5.64	113.07	119.78
1	C	640	LYS	N-CA-C	-5.62	105.15	111.28
1	G	593	SER	CA-C-O	-5.62	113.09	119.78
1	H	593	SER	CA-C-O	-5.61	113.10	119.78
1	F	640	LYS	N-CA-C	-5.61	105.17	111.28
1	A	496	ILE	N-CA-C	-5.60	102.35	109.58
1	C	593	SER	CA-C-O	-5.60	113.12	119.78
1	C	496	ILE	N-CA-C	-5.59	102.37	109.58
1	F	593	SER	CA-C-O	-5.59	113.13	119.78
1	E	593	SER	CA-C-O	-5.58	113.13	119.78
1	I	443	VAL	N-CA-CB	-5.58	104.63	111.67
1	D	593	SER	CA-C-O	-5.58	113.14	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	443	VAL	N-CA-CB	-5.58	104.64	111.67
1	B	496	ILE	N-CA-C	-5.58	102.39	109.58
1	B	593	SER	CA-C-O	-5.58	113.14	119.78
1	G	496	ILE	N-CA-C	-5.57	102.39	109.58
1	D	496	ILE	N-CA-C	-5.57	102.39	109.58
1	A	443	VAL	N-CA-CB	-5.57	104.65	111.67
1	E	496	ILE	N-CA-C	-5.57	102.40	109.58
1	F	443	VAL	N-CA-CB	-5.57	104.66	111.67
1	H	496	ILE	N-CA-C	-5.57	102.40	109.58
1	I	593	SER	CA-C-O	-5.56	113.16	119.78
1	C	443	VAL	N-CA-CB	-5.56	104.66	111.67
1	G	443	VAL	N-CA-CB	-5.56	104.66	111.67
1	I	496	ILE	N-CA-C	-5.56	102.40	109.58
1	F	496	ILE	N-CA-C	-5.55	102.41	109.58
1	B	443	VAL	N-CA-CB	-5.54	104.69	111.67
1	E	443	VAL	N-CA-CB	-5.54	104.69	111.67
1	D	443	VAL	N-CA-CB	-5.54	104.69	111.67
1	I	577	LEU	N-CA-C	5.48	118.55	109.46
1	B	379	GLU	O-C-N	-5.47	116.43	122.07
1	H	577	LEU	N-CA-C	5.47	118.55	109.46
1	B	577	LEU	N-CA-C	5.47	118.53	109.46
1	D	577	LEU	N-CA-C	5.47	118.53	109.46
1	G	577	LEU	N-CA-C	5.46	118.53	109.46
1	C	577	LEU	N-CA-C	5.46	118.53	109.46
1	F	379	GLU	O-C-N	-5.46	116.45	122.07
1	E	379	GLU	O-C-N	-5.45	116.45	122.07
1	A	577	LEU	N-CA-C	5.45	118.51	109.46
1	F	577	LEU	N-CA-C	5.45	118.51	109.46
1	I	397	ASP	CA-CB-CG	-5.45	107.15	112.60
1	H	397	ASP	CA-CB-CG	-5.44	107.16	112.60
1	E	577	LEU	N-CA-C	5.44	118.49	109.46
1	C	379	GLU	O-C-N	-5.43	116.47	122.07
1	F	397	ASP	CA-CB-CG	-5.43	107.17	112.60
1	C	397	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	397	ASP	CA-CB-CG	-5.43	107.17	112.60
1	G	397	ASP	CA-CB-CG	-5.42	107.17	112.60
1	I	379	GLU	O-C-N	-5.42	116.48	122.07
1	H	379	GLU	O-C-N	-5.42	116.49	122.07
1	G	581	LEU	N-CA-C	5.42	118.07	109.24
1	A	379	GLU	O-C-N	-5.41	116.50	122.07
1	D	379	GLU	O-C-N	-5.41	116.49	122.07
1	C	581	LEU	N-CA-C	5.41	118.06	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	397	ASP	CA-CB-CG	-5.41	107.19	112.60
1	E	397	ASP	CA-CB-CG	-5.41	107.19	112.60
1	B	581	LEU	N-CA-C	5.41	118.05	109.24
1	H	581	LEU	N-CA-C	5.41	118.05	109.24
1	F	581	LEU	N-CA-C	5.40	118.05	109.24
1	D	581	LEU	N-CA-C	5.40	118.04	109.24
1	B	397	ASP	CA-CB-CG	-5.39	107.21	112.60
1	E	581	LEU	N-CA-C	5.39	118.03	109.24
1	I	581	LEU	N-CA-C	5.38	118.02	109.24
1	A	581	LEU	N-CA-C	5.38	118.01	109.24
1	G	379	GLU	O-C-N	-5.38	116.53	122.07
1	B	362	TYR	N-CA-C	5.36	118.08	110.10
1	C	362	TYR	N-CA-C	5.36	118.08	110.10
1	H	362	TYR	N-CA-C	5.35	118.07	110.10
1	A	362	TYR	N-CA-C	5.35	118.07	110.10
1	H	572	VAL	CA-C-O	-5.35	114.48	120.95
1	B	572	VAL	CA-C-O	-5.34	114.49	120.95
1	F	362	TYR	N-CA-C	5.34	118.05	110.10
1	I	362	TYR	N-CA-C	5.33	118.05	110.10
1	A	572	VAL	CA-C-O	-5.33	114.50	120.95
1	G	572	VAL	CA-C-O	-5.33	114.50	120.95
1	E	362	TYR	N-CA-C	5.33	118.04	110.10
1	D	362	TYR	N-CA-C	5.33	118.04	110.10
1	F	572	VAL	CA-C-O	-5.33	114.51	120.95
1	B	546	THR	N-CA-C	-5.32	106.74	113.18
1	C	572	VAL	CA-C-O	-5.32	114.52	120.95
1	I	572	VAL	CA-C-O	-5.31	114.52	120.95
1	D	572	VAL	CA-C-O	-5.31	114.53	120.95
1	E	572	VAL	CA-C-O	-5.30	114.53	120.95
1	G	362	TYR	N-CA-C	5.30	118.00	110.10
1	C	546	THR	N-CA-C	-5.30	106.77	113.18
1	G	546	THR	N-CA-C	-5.29	106.77	113.18
1	H	546	THR	N-CA-C	-5.28	106.79	113.18
1	A	546	THR	N-CA-C	-5.27	106.80	113.18
1	D	546	THR	N-CA-C	-5.27	106.80	113.18
1	E	546	THR	N-CA-C	-5.27	106.81	113.18
1	I	546	THR	N-CA-C	-5.27	106.81	113.18
1	F	546	THR	N-CA-C	-5.26	106.81	113.18
1	I	354	ILE	N-CA-C	5.21	115.62	108.12
1	B	619	ASN	CA-C-N	5.21	127.48	120.50
1	B	619	ASN	C-N-CA	5.21	127.48	120.50
1	H	591	ARG	N-CA-C	-5.20	105.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	619	ASN	CA-C-N	5.19	127.46	120.50
1	D	619	ASN	C-N-CA	5.19	127.46	120.50
1	D	354	ILE	N-CA-C	5.19	115.59	108.12
1	E	354	ILE	N-CA-C	5.19	115.59	108.12
1	H	619	ASN	CA-C-N	5.19	127.45	120.50
1	H	619	ASN	C-N-CA	5.19	127.45	120.50
1	A	619	ASN	CA-C-N	5.18	127.44	120.50
1	A	619	ASN	C-N-CA	5.18	127.44	120.50
1	G	619	ASN	CA-C-N	5.18	127.44	120.50
1	G	619	ASN	C-N-CA	5.18	127.44	120.50
1	B	354	ILE	N-CA-C	5.18	115.58	108.12
1	F	354	ILE	N-CA-C	5.18	115.58	108.12
1	C	354	ILE	N-CA-C	5.17	115.57	108.12
1	E	619	ASN	CA-C-N	5.17	127.43	120.50
1	E	619	ASN	C-N-CA	5.17	127.43	120.50
1	I	619	ASN	CA-C-N	5.17	127.43	120.50
1	I	619	ASN	C-N-CA	5.17	127.43	120.50
1	G	354	ILE	N-CA-C	5.17	115.56	108.12
1	F	619	ASN	CA-C-N	5.16	127.42	120.50
1	F	619	ASN	C-N-CA	5.16	127.42	120.50
1	A	354	ILE	N-CA-C	5.16	115.55	108.12
1	C	619	ASN	CA-C-N	5.16	127.42	120.50
1	C	619	ASN	C-N-CA	5.16	127.42	120.50
1	C	591	ARG	N-CA-C	-5.16	105.74	111.36
1	F	591	ARG	N-CA-C	-5.16	105.74	111.36
1	H	354	ILE	N-CA-C	5.15	115.54	108.12
1	I	591	ARG	N-CA-C	-5.15	105.75	111.36
1	A	591	ARG	N-CA-C	-5.15	105.75	111.36
1	E	591	ARG	N-CA-C	-5.15	105.75	111.36
1	G	591	ARG	N-CA-C	-5.15	105.75	111.36
1	B	591	ARG	N-CA-C	-5.13	105.77	111.36
1	D	591	ARG	N-CA-C	-5.10	105.80	111.36
1	H	467	ASP	CA-CB-CG	5.10	117.70	112.60
1	F	467	ASP	N-CA-C	-5.09	105.82	112.23
1	G	467	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	467	ASP	N-CA-C	-5.07	105.84	112.23
1	F	467	ASP	CA-CB-CG	5.07	117.67	112.60
1	G	445	LYS	CA-C-N	-5.07	114.29	122.81
1	G	445	LYS	C-N-CA	-5.07	114.29	122.81
1	A	445	LYS	CA-C-N	-5.07	114.30	122.81
1	A	445	LYS	C-N-CA	-5.07	114.30	122.81
1	B	467	ASP	CA-CB-CG	5.07	117.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	445	LYS	CA-C-N	-5.07	114.30	122.81
1	E	445	LYS	C-N-CA	-5.07	114.30	122.81
1	F	445	LYS	CA-C-N	-5.07	114.30	122.81
1	F	445	LYS	C-N-CA	-5.07	114.30	122.81
1	H	445	LYS	CA-C-N	-5.07	114.30	122.81
1	H	445	LYS	C-N-CA	-5.07	114.30	122.81
1	B	445	LYS	CA-C-N	-5.06	114.30	122.81
1	B	445	LYS	C-N-CA	-5.06	114.30	122.81
1	D	467	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	467	ASP	N-CA-C	-5.06	105.85	112.23
1	H	467	ASP	N-CA-C	-5.06	105.85	112.23
1	C	445	LYS	CA-C-N	-5.06	114.31	122.81
1	C	445	LYS	C-N-CA	-5.06	114.31	122.81
1	E	467	ASP	N-CA-C	-5.06	105.86	112.23
1	C	467	ASP	N-CA-C	-5.05	105.86	112.23
1	D	445	LYS	CA-C-N	-5.05	114.33	122.81
1	D	445	LYS	C-N-CA	-5.05	114.33	122.81
1	E	467	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	467	ASP	CA-CB-CG	5.05	117.65	112.60
1	I	445	LYS	CA-C-N	-5.04	114.34	122.81
1	I	445	LYS	C-N-CA	-5.04	114.34	122.81
1	I	467	ASP	CA-CB-CG	5.04	117.64	112.60
1	I	467	ASP	N-CA-C	-5.04	105.88	112.23
1	B	467	ASP	N-CA-C	-5.03	105.89	112.23
1	C	467	ASP	CA-CB-CG	5.03	117.62	112.60

There are no chirality outliers.

All (99) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	ILE	Peptide,Mainchain
1	A	379	GLU	Mainchain
1	A	411	LYS	Peptide,Mainchain
1	A	540	THR	Mainchain
1	A	554	LEU	Mainchain
1	A	572	VAL	Mainchain
1	A	593	SER	Mainchain
1	A	645	GLY	Peptide,Mainchain
1	B	361	ILE	Peptide,Mainchain
1	B	379	GLU	Mainchain
1	B	411	LYS	Peptide,Mainchain
1	B	540	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	B	554	LEU	Mainchain
1	B	572	VAL	Mainchain
1	B	593	SER	Mainchain
1	B	645	GLY	Peptide,Mainchain
1	C	361	ILE	Peptide,Mainchain
1	C	379	GLU	Mainchain
1	C	411	LYS	Peptide,Mainchain
1	C	540	THR	Mainchain
1	C	554	LEU	Mainchain
1	C	572	VAL	Mainchain
1	C	593	SER	Mainchain
1	C	645	GLY	Peptide,Mainchain
1	D	361	ILE	Peptide,Mainchain
1	D	379	GLU	Mainchain
1	D	411	LYS	Peptide,Mainchain
1	D	540	THR	Mainchain
1	D	554	LEU	Mainchain
1	D	572	VAL	Mainchain
1	D	593	SER	Mainchain
1	D	645	GLY	Peptide,Mainchain
1	E	361	ILE	Peptide,Mainchain
1	E	379	GLU	Mainchain
1	E	411	LYS	Peptide,Mainchain
1	E	540	THR	Mainchain
1	E	554	LEU	Mainchain
1	E	572	VAL	Mainchain
1	E	593	SER	Mainchain
1	E	645	GLY	Peptide,Mainchain
1	F	361	ILE	Peptide,Mainchain
1	F	379	GLU	Mainchain
1	F	411	LYS	Peptide,Mainchain
1	F	540	THR	Mainchain
1	F	554	LEU	Mainchain
1	F	572	VAL	Mainchain
1	F	593	SER	Mainchain
1	F	645	GLY	Peptide,Mainchain
1	G	361	ILE	Peptide,Mainchain
1	G	379	GLU	Mainchain
1	G	411	LYS	Peptide,Mainchain
1	G	540	THR	Mainchain
1	G	554	LEU	Mainchain
1	G	572	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	G	593	SER	Mainchain
1	G	645	GLY	Peptide,Mainchain
1	H	361	ILE	Peptide,Mainchain
1	H	379	GLU	Mainchain
1	H	411	LYS	Peptide,Mainchain
1	H	540	THR	Mainchain
1	H	554	LEU	Mainchain
1	H	572	VAL	Mainchain
1	H	593	SER	Mainchain
1	H	645	GLY	Peptide,Mainchain
1	I	361	ILE	Peptide,Mainchain
1	I	379	GLU	Mainchain
1	I	411	LYS	Peptide,Mainchain
1	I	540	THR	Mainchain
1	I	554	LEU	Mainchain
1	I	572	VAL	Mainchain
1	I	593	SER	Mainchain
1	I	645	GLY	Peptide,Mainchain

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	A	2681	2734	2732	35	0
1	B	2681	2734	2732	33	0
1	C	2681	2734	2732	33	0
1	D	2681	2734	2732	33	0
1	E	2681	2734	2732	36	0
1	F	2681	2734	2732	35	0
1	G	2681	2734	2732	37	0
1	H	2681	2734	2732	35	0
1	I	2681	2734	2732	34	0
All	All	24129	24606	24588	302	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 6.

All (302) 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:F:575:THR:OG1	1:F:665:LYS:NZ	2.17	0.73
1:D:575:THR:OG1	1:D:665:LYS:NZ	2.18	0.72
1:H:575:THR:OG1	1:H:665:LYS:NZ	2.17	0.71
1:A:575:THR:OG1	1:A:665:LYS:NZ	2.18	0.71
1:C:575:THR:OG1	1:C:665:LYS:NZ	2.18	0.68
1:B:575:THR:OG1	1:B:665:LYS:NZ	2.17	0.68
1:E:575:THR:OG1	1:E:665:LYS:NZ	2.18	0.67
1:I:575:THR:OG1	1:I:665:LYS:NZ	2.18	0.67
1:G:575:THR:OG1	1:G:665:LYS:NZ	2.18	0.66
1:H:599:SER:OG	1:H:600:GLY:N	2.29	0.65
1:G:599:SER:OG	1:G:600:GLY:N	2.29	0.65
1:E:599:SER:OG	1:E:600:GLY:N	2.29	0.65
1:C:599:SER:OG	1:C:600:GLY:N	2.29	0.65
1:I:599:SER:OG	1:I:600:GLY:N	2.29	0.64
1:F:599:SER:OG	1:F:600:GLY:N	2.29	0.63
1:B:599:SER:OG	1:B:600:GLY:N	2.29	0.62
1:E:397:ASP:OD1	1:E:397:ASP:N	2.31	0.62
1:G:397:ASP:OD1	1:G:397:ASP:N	2.31	0.62
1:F:397:ASP:OD1	1:F:397:ASP:N	2.31	0.62
1:D:397:ASP:N	1:D:397:ASP:OD1	2.31	0.62
1:A:599:SER:OG	1:A:600:GLY:N	2.29	0.61
1:D:599:SER:OG	1:D:600:GLY:N	2.29	0.61
1:C:397:ASP:OD1	1:C:397:ASP:N	2.31	0.61
1:H:397:ASP:OD1	1:H:397:ASP:N	2.31	0.61
1:B:397:ASP:N	1:B:397:ASP:OD1	2.31	0.60
1:I:397:ASP:N	1:I:397:ASP:OD1	2.31	0.59
1:A:397:ASP:OD1	1:A:397:ASP:N	2.31	0.58
1:G:376:ASN:O	1:G:380:GLU:N	2.36	0.57
1:F:376:ASN:O	1:F:380:GLU:N	2.36	0.57
1:H:376:ASN:O	1:H:380:GLU:N	2.36	0.57
1:E:376:ASN:O	1:E:380:GLU:N	2.36	0.56
1:I:376:ASN:O	1:I:380:GLU:N	2.36	0.56
1:A:376:ASN:O	1:A:380:GLU:N	2.36	0.55
1:D:376:ASN:O	1:D:380:GLU:N	2.36	0.55
1:B:376:ASN:O	1:B:380:GLU:N	2.36	0.55
1:C:376:ASN:O	1:C:380:GLU:N	2.36	0.55
1:B:634:ASP:OD1	1:B:634:ASP:N	2.40	0.54
1:A:634:ASP:OD1	1:A:634:ASP:N	2.41	0.54
1:C:634:ASP:OD1	1:C:634:ASP:N	2.41	0.54
1:I:601:SER:O	1:I:602:TYR:C	2.53	0.52
1:H:601:SER:O	1:H:602:TYR:C	2.53	0.52
1:G:601:SER:O	1:G:602:TYR:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:634:ASP:OD1	1:I:634:ASP:N	2.41	0.52
1:F:601:SER:O	1:F:602:TYR:C	2.53	0.51
1:E:601:SER:O	1:E:602:TYR:C	2.53	0.51
1:D:464:THR:O	1:D:465:THR:C	2.54	0.51
1:C:464:THR:O	1:C:465:THR:C	2.54	0.51
1:D:634:ASP:OD1	1:D:634:ASP:N	2.40	0.51
1:E:464:THR:O	1:E:465:THR:C	2.54	0.51
1:B:464:THR:O	1:B:465:THR:C	2.54	0.51
1:A:464:THR:O	1:A:465:THR:C	2.54	0.50
1:C:601:SER:O	1:C:602:TYR:C	2.53	0.50
1:D:601:SER:O	1:D:602:TYR:C	2.53	0.50
1:I:464:THR:O	1:I:465:THR:C	2.54	0.50
1:F:464:THR:O	1:F:465:THR:C	2.54	0.50
1:G:586:ILE:O	1:G:587:GLU:C	2.54	0.50
1:G:464:THR:O	1:G:465:THR:C	2.54	0.50
1:G:634:ASP:OD1	1:G:634:ASP:N	2.40	0.50
1:H:464:THR:O	1:H:465:THR:C	2.54	0.50
1:A:586:ILE:O	1:A:587:GLU:C	2.54	0.50
1:D:584:SER:O	1:D:585:ASP:C	2.55	0.50
1:B:601:SER:O	1:B:602:TYR:C	2.53	0.49
1:I:584:SER:O	1:I:585:ASP:C	2.55	0.49
1:A:601:SER:O	1:A:602:TYR:C	2.53	0.49
1:B:584:SER:O	1:B:585:ASP:C	2.55	0.49
1:D:586:ILE:O	1:D:587:GLU:C	2.54	0.49
1:C:586:ILE:O	1:C:587:GLU:C	2.54	0.49
1:F:584:SER:O	1:F:585:ASP:C	2.55	0.49
1:E:586:ILE:O	1:E:587:GLU:C	2.54	0.49
1:I:416:ASP:OD1	1:I:468:LYS:NZ	2.44	0.49
1:H:586:ILE:O	1:H:587:GLU:C	2.54	0.48
1:I:401:GLU:OE1	1:I:411:LYS:NZ	2.46	0.48
1:H:550:ASP:C	1:H:550:ASP:OD1	2.56	0.48
1:G:584:SER:O	1:G:585:ASP:C	2.55	0.48
1:B:586:ILE:O	1:B:587:GLU:C	2.54	0.48
1:F:586:ILE:O	1:F:587:GLU:C	2.54	0.48
1:G:401:GLU:OE1	1:G:411:LYS:NZ	2.46	0.48
1:G:407:GLU:OE1	1:H:564:ARG:NH1	2.47	0.48
1:B:401:GLU:OE1	1:B:411:LYS:NZ	2.47	0.48
1:C:584:SER:O	1:C:585:ASP:C	2.55	0.48
1:A:401:GLU:OE1	1:A:411:LYS:NZ	2.47	0.48
1:A:591:ARG:NH1	1:A:634:ASP:OD1	2.47	0.48
1:B:407:GLU:OE1	1:C:564:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:GLU:OE1	1:F:564:ARG:NH1	2.47	0.48
1:A:407:GLU:OE1	1:B:564:ARG:NH1	2.47	0.47
1:C:591:ARG:NH1	1:C:634:ASP:OD1	2.47	0.47
1:D:401:GLU:OE1	1:D:411:LYS:NZ	2.47	0.47
1:D:407:GLU:OE1	1:E:564:ARG:NH1	2.47	0.47
1:H:401:GLU:OE1	1:H:411:LYS:NZ	2.47	0.47
1:B:432:PHE:O	1:B:434:GLN:NE2	2.47	0.47
1:D:432:PHE:O	1:D:434:GLN:NE2	2.47	0.47
1:H:407:GLU:OE1	1:I:564:ARG:NH1	2.47	0.47
1:A:564:ARG:NH1	1:I:407:GLU:OE1	2.47	0.47
1:B:550:ASP:OD1	1:B:550:ASP:C	2.56	0.47
1:C:407:GLU:OE1	1:D:564:ARG:NH1	2.47	0.47
1:E:584:SER:O	1:E:585:ASP:C	2.55	0.47
1:G:550:ASP:OD1	1:G:550:ASP:C	2.56	0.47
1:G:591:ARG:NH1	1:G:634:ASP:OD1	2.47	0.47
1:H:432:PHE:O	1:H:434:GLN:NE2	2.47	0.47
1:F:591:ARG:NH1	1:F:634:ASP:OD1	2.47	0.47
1:I:432:PHE:O	1:I:434:GLN:NE2	2.47	0.47
1:A:432:PHE:O	1:A:434:GLN:NE2	2.47	0.47
1:A:584:SER:O	1:A:585:ASP:C	2.55	0.47
1:C:432:PHE:O	1:C:434:GLN:NE2	2.47	0.47
1:E:401:GLU:OE1	1:E:411:LYS:NZ	2.46	0.47
1:H:591:ARG:NH1	1:H:634:ASP:OD1	2.47	0.47
1:G:432:PHE:O	1:G:434:GLN:NE2	2.47	0.47
1:I:591:ARG:NH1	1:I:634:ASP:OD1	2.47	0.47
1:A:416:ASP:OD1	1:A:468:LYS:NZ	2.44	0.47
1:F:407:GLU:OE1	1:G:564:ARG:NH1	2.47	0.47
1:E:432:PHE:O	1:E:434:GLN:NE2	2.47	0.47
1:F:432:PHE:O	1:F:434:GLN:NE2	2.47	0.47
1:B:591:ARG:NH1	1:B:634:ASP:OD1	2.47	0.47
1:E:634:ASP:OD1	1:E:634:ASP:N	2.40	0.47
1:F:550:ASP:C	1:F:550:ASP:OD1	2.56	0.47
1:H:584:SER:O	1:H:585:ASP:C	2.55	0.47
1:C:550:ASP:OD1	1:C:550:ASP:C	2.56	0.46
1:D:591:ARG:NH1	1:D:634:ASP:OD1	2.47	0.46
1:E:591:ARG:NH1	1:E:634:ASP:OD1	2.47	0.46
1:H:634:ASP:OD1	1:H:634:ASP:N	2.41	0.46
1:G:563:ARG:NH2	1:G:656:GLN:O	2.49	0.46
1:E:550:ASP:OD1	1:E:550:ASP:C	2.56	0.46
1:H:473:LEU:O	1:H:474:LYS:C	2.56	0.46
1:H:563:ARG:NH2	1:H:656:GLN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:ASP:C	1:D:550:ASP:OD1	2.56	0.46
1:F:563:ARG:NH2	1:F:656:GLN:O	2.49	0.46
1:G:473:LEU:O	1:G:474:LYS:C	2.56	0.46
1:I:586:ILE:O	1:I:587:GLU:C	2.54	0.46
1:E:496:ILE:O	1:E:497:MET:HB2	2.16	0.46
1:I:563:ARG:NH2	1:I:656:GLN:O	2.49	0.46
1:D:496:ILE:O	1:D:497:MET:HB2	2.16	0.46
1:A:496:ILE:O	1:A:497:MET:HB2	2.16	0.45
1:B:496:ILE:O	1:B:497:MET:HB2	2.16	0.45
1:F:401:GLU:OE1	1:F:411:LYS:NZ	2.47	0.45
1:E:563:ARG:NH2	1:E:656:GLN:O	2.49	0.45
1:C:401:GLU:OE1	1:C:411:LYS:NZ	2.47	0.45
1:H:496:ILE:O	1:H:497:MET:HB2	2.16	0.45
1:A:563:ARG:NH2	1:A:656:GLN:O	2.49	0.45
1:C:496:ILE:O	1:C:497:MET:HB2	2.16	0.45
1:B:563:ARG:NH2	1:B:656:GLN:O	2.49	0.45
1:I:473:LEU:O	1:I:474:LYS:C	2.56	0.45
1:D:563:ARG:NH2	1:D:656:GLN:O	2.49	0.45
1:C:473:LEU:O	1:C:474:LYS:C	2.56	0.45
1:A:550:ASP:C	1:A:550:ASP:OD1	2.56	0.45
1:B:473:LEU:O	1:B:474:LYS:C	2.56	0.45
1:F:473:LEU:O	1:F:474:LYS:C	2.56	0.45
1:F:496:ILE:O	1:F:497:MET:HB2	2.16	0.45
1:C:563:ARG:NH2	1:C:656:GLN:O	2.49	0.45
1:G:496:ILE:O	1:G:497:MET:HB2	2.16	0.45
1:H:670:VAL:HG22	1:H:672:ASP:H	1.82	0.45
1:A:452:GLN:CD	1:A:452:GLN:H	2.26	0.44
1:D:670:VAL:HG22	1:D:672:ASP:H	1.82	0.44
1:I:496:ILE:O	1:I:497:MET:HB2	2.16	0.44
1:G:670:VAL:HG22	1:G:672:ASP:H	1.82	0.44
1:F:447:ASN:ND2	1:F:449:THR:OG1	2.51	0.44
1:D:473:LEU:O	1:D:474:LYS:C	2.56	0.44
1:G:417:ASP:OD1	1:G:417:ASP:N	2.47	0.44
1:G:452:GLN:H	1:G:452:GLN:CD	2.26	0.44
1:B:447:ASN:ND2	1:B:449:THR:OG1	2.51	0.44
1:C:447:ASN:ND2	1:C:449:THR:OG1	2.51	0.44
1:G:447:ASN:ND2	1:G:449:THR:OG1	2.51	0.44
1:G:585:ASP:O	1:G:609:ARG:NH2	2.51	0.44
1:H:452:GLN:H	1:H:452:GLN:CD	2.26	0.44
1:A:473:LEU:O	1:A:474:LYS:C	2.56	0.44
1:E:473:LEU:O	1:E:474:LYS:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:452:GLN:H	1:I:452:GLN:CD	2.26	0.44
1:B:585:ASP:O	1:B:609:ARG:NH2	2.51	0.44
1:F:417:ASP:OD1	1:F:417:ASP:N	2.47	0.44
1:B:452:GLN:H	1:B:452:GLN:CD	2.25	0.43
1:C:452:GLN:CD	1:C:452:GLN:H	2.26	0.43
1:D:452:GLN:H	1:D:452:GLN:CD	2.26	0.43
1:E:441:SER:OG	1:E:475:LYS:O	2.33	0.43
1:H:585:ASP:O	1:H:609:ARG:NH2	2.51	0.43
1:A:670:VAL:HG22	1:A:672:ASP:H	1.82	0.43
1:C:585:ASP:O	1:C:609:ARG:NH2	2.51	0.43
1:E:670:VAL:HG22	1:E:672:ASP:H	1.82	0.43
1:F:585:ASP:O	1:F:609:ARG:NH2	2.51	0.43
1:A:447:ASN:ND2	1:A:449:THR:OG1	2.51	0.43
1:A:585:ASP:O	1:A:609:ARG:NH2	2.51	0.43
1:C:670:VAL:HG22	1:C:672:ASP:H	1.82	0.43
1:G:609:ARG:NH1	1:G:675:ALA:OXT	2.52	0.43
1:G:671:ASN:OD1	1:G:671:ASN:N	2.51	0.43
1:I:670:VAL:HG22	1:I:672:ASP:H	1.82	0.43
1:A:609:ARG:NH1	1:A:675:ALA:OXT	2.52	0.43
1:D:416:ASP:OD1	1:D:468:LYS:NZ	2.44	0.43
1:D:447:ASN:ND2	1:D:449:THR:OG1	2.51	0.43
1:F:670:VAL:HG22	1:F:672:ASP:H	1.83	0.43
1:H:609:ARG:NH1	1:H:675:ALA:OXT	2.52	0.43
1:E:447:ASN:ND2	1:E:449:THR:OG1	2.51	0.43
1:H:417:ASP:OD1	1:H:417:ASP:N	2.47	0.43
1:I:609:ARG:NH1	1:I:675:ALA:OXT	2.52	0.43
1:B:670:VAL:HG22	1:B:672:ASP:H	1.82	0.43
1:A:671:ASN:OD1	1:A:671:ASN:N	2.51	0.43
1:H:671:ASN:OD1	1:H:671:ASN:N	2.51	0.43
1:I:585:ASP:O	1:I:609:ARG:NH2	2.51	0.43
1:B:609:ARG:NH1	1:B:675:ALA:OXT	2.52	0.43
1:E:609:ARG:NH1	1:E:675:ALA:OXT	2.52	0.43
1:F:452:GLN:H	1:F:452:GLN:CD	2.26	0.43
1:F:609:ARG:NH1	1:F:675:ALA:OXT	2.52	0.43
1:I:447:ASN:ND2	1:I:449:THR:OG1	2.51	0.43
1:C:671:ASN:OD1	1:C:671:ASN:N	2.51	0.43
1:F:671:ASN:OD1	1:F:671:ASN:N	2.51	0.43
1:H:662:ILE:O	1:H:663:GLU:C	2.62	0.43
1:B:416:ASP:OD1	1:B:468:LYS:NZ	2.44	0.43
1:D:609:ARG:NH1	1:D:675:ALA:OXT	2.52	0.43
1:H:447:ASN:ND2	1:H:449:THR:OG1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ASN:OD1	1:B:671:ASN:N	2.51	0.42
1:E:452:GLN:H	1:E:452:GLN:CD	2.26	0.42
1:E:417:ASP:OD1	1:E:417:ASP:N	2.47	0.42
1:E:671:ASN:OD1	1:E:671:ASN:N	2.51	0.42
1:I:671:ASN:OD1	1:I:671:ASN:N	2.51	0.42
1:E:585:ASP:O	1:E:609:ARG:NH2	2.51	0.42
1:F:416:ASP:OD1	1:F:468:LYS:NZ	2.44	0.42
1:B:491:ARG:NH1	1:B:495:ASP:OD1	2.53	0.42
1:A:491:ARG:NH1	1:A:495:ASP:OD1	2.53	0.42
1:G:357:LEU:O	1:G:393:VAL:N	2.53	0.42
1:C:609:ARG:NH1	1:C:675:ALA:OXT	2.52	0.42
1:F:634:ASP:OD1	1:F:634:ASP:N	2.41	0.42
1:H:491:ARG:NH1	1:H:495:ASP:OD1	2.53	0.42
1:C:491:ARG:NH1	1:C:495:ASP:OD1	2.53	0.42
1:D:671:ASN:OD1	1:D:671:ASN:N	2.51	0.42
1:E:357:LEU:O	1:E:393:VAL:N	2.53	0.42
1:E:491:ARG:NH1	1:E:495:ASP:OD1	2.53	0.42
1:F:491:ARG:NH1	1:F:495:ASP:OD1	2.53	0.42
1:H:357:LEU:O	1:H:393:VAL:N	2.53	0.42
1:A:662:ILE:O	1:A:663:GLU:C	2.62	0.42
1:I:417:ASP:OD1	1:I:417:ASP:N	2.47	0.42
1:I:550:ASP:OD1	1:I:550:ASP:C	2.56	0.42
1:C:416:ASP:OD1	1:C:468:LYS:NZ	2.44	0.41
1:E:377:PHE:O	1:E:378:PHE:C	2.63	0.41
1:C:662:ILE:O	1:C:663:GLU:C	2.62	0.41
1:G:501:TYR:HB2	1:G:502:ASN:HA	2.03	0.41
1:A:578:ASN:O	1:A:628:VAL:N	2.53	0.41
1:C:357:LEU:O	1:C:393:VAL:N	2.53	0.41
1:D:491:ARG:NH1	1:D:495:ASP:OD1	2.53	0.41
1:E:662:ILE:O	1:E:663:GLU:C	2.62	0.41
1:G:662:ILE:O	1:G:663:GLU:C	2.62	0.41
1:D:429:SER:HB3	1:D:431:GLU:OE1	2.20	0.41
1:E:351:GLU:OE1	1:E:406:GLN:HG2	2.21	0.41
1:I:614:ILE:O	1:I:615:GLY:C	2.63	0.41
1:H:351:GLU:OE1	1:H:406:GLN:HG2	2.21	0.41
1:A:357:LEU:O	1:A:393:VAL:N	2.53	0.41
1:B:578:ASN:O	1:B:628:VAL:N	2.53	0.41
1:F:377:PHE:O	1:F:378:PHE:C	2.63	0.41
1:H:614:ILE:O	1:H:615:GLY:C	2.63	0.41
1:I:351:GLU:OE1	1:I:406:GLN:HG2	2.21	0.41
1:I:376:ASN:O	1:I:377:PHE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:O	1:B:393:VAL:N	2.53	0.41
1:C:376:ASN:O	1:C:377:PHE:C	2.63	0.41
1:E:501:TYR:HB2	1:E:502:ASN:HA	2.03	0.41
1:F:357:LEU:O	1:F:393:VAL:N	2.53	0.41
1:G:376:ASN:O	1:G:377:PHE:C	2.63	0.41
1:A:614:ILE:O	1:A:615:GLY:C	2.63	0.41
1:D:351:GLU:OE1	1:D:406:GLN:HG2	2.21	0.41
1:D:417:ASP:OD1	1:D:417:ASP:N	2.47	0.41
1:D:501:TYR:HB2	1:D:502:ASN:HA	2.02	0.41
1:D:578:ASN:O	1:D:628:VAL:N	2.53	0.41
1:F:578:ASN:O	1:F:628:VAL:N	2.53	0.41
1:G:351:GLU:OE1	1:G:406:GLN:HG2	2.21	0.41
1:D:357:LEU:O	1:D:393:VAL:N	2.53	0.41
1:D:585:ASP:O	1:D:609:ARG:NH2	2.51	0.41
1:E:376:ASN:O	1:E:377:PHE:C	2.63	0.41
1:G:429:SER:HB3	1:G:431:GLU:OE1	2.21	0.41
1:G:491:ARG:NH1	1:G:495:ASP:OD1	2.53	0.41
1:G:636:ARG:O	1:G:637:ARG:C	2.64	0.41
1:H:429:SER:HB3	1:H:431:GLU:OE1	2.20	0.41
1:H:501:TYR:HB2	1:H:502:ASN:HA	2.02	0.41
1:I:429:SER:HB3	1:I:431:GLU:OE1	2.21	0.41
1:I:491:ARG:NH1	1:I:495:ASP:OD1	2.53	0.41
1:I:578:ASN:O	1:I:628:VAL:N	2.53	0.41
1:A:351:GLU:OE1	1:A:406:GLN:HG2	2.21	0.41
1:A:378:PHE:O	1:A:382:GLY:HA2	2.21	0.41
1:B:429:SER:HB3	1:B:431:GLU:OE1	2.20	0.41
1:E:578:ASN:O	1:E:628:VAL:N	2.53	0.41
1:F:429:SER:HB3	1:F:431:GLU:OE1	2.21	0.41
1:G:377:PHE:O	1:G:378:PHE:C	2.63	0.40
1:H:378:PHE:O	1:H:382:GLY:HA2	2.22	0.40
1:A:417:ASP:OD1	1:A:417:ASP:N	2.47	0.40
1:C:578:ASN:O	1:C:628:VAL:N	2.53	0.40
1:F:351:GLU:OE1	1:F:406:GLN:HG2	2.21	0.40
1:F:501:TYR:HB2	1:F:502:ASN:HA	2.03	0.40
1:G:416:ASP:OD1	1:G:468:LYS:NZ	2.44	0.40
1:G:578:ASN:O	1:G:628:VAL:N	2.53	0.40
1:G:614:ILE:O	1:G:615:GLY:C	2.63	0.40
1:A:377:PHE:O	1:A:378:PHE:C	2.63	0.40
1:C:378:PHE:O	1:C:382:GLY:HA2	2.21	0.40
1:F:378:PHE:O	1:F:382:GLY:HA2	2.21	0.40
1:H:578:ASN:O	1:H:628:VAL:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:501:TYR:HB2	1:I:502:ASN:HA	2.03	0.40
1:A:580:TRP:CD1	1:A:580:TRP:N	2.90	0.40
1:B:351:GLU:OE1	1:B:406:GLN:HG2	2.21	0.40
1:B:399:ALA:HA	1:B:413:THR:HA	2.04	0.40
1:C:399:ALA:HA	1:C:413:THR:HA	2.04	0.40
1:D:378:PHE:O	1:D:382:GLY:HA2	2.22	0.40
1:E:378:PHE:O	1:E:382:GLY:HA2	2.22	0.40
1:E:429:SER:HB3	1:E:431:GLU:OE1	2.20	0.40
1:F:636:ARG:O	1:F:637:ARG:C	2.64	0.40
1:H:580:TRP:CD1	1:H:580:TRP:N	2.90	0.40
1:B:614:ILE:O	1:B:615:GLY:C	2.63	0.40
1:B:662:ILE:O	1:B:663:GLU:C	2.62	0.40
1:C:636:ARG:O	1:C:637:ARG:C	2.64	0.40
1:I:507:GLU:O	1:I:511:GLN:N	2.55	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	A	330/342 (96%)	313 (95%)	16 (5%)	1 (0%)	36	72
1	B	330/342 (96%)	313 (95%)	17 (5%)	0	100	100
1	C	330/342 (96%)	313 (95%)	17 (5%)	0	100	100
1	D	330/342 (96%)	313 (95%)	16 (5%)	1 (0%)	36	72
1	E	330/342 (96%)	313 (95%)	17 (5%)	0	100	100
1	F	330/342 (96%)	313 (95%)	17 (5%)	0	100	100
1	G	330/342 (96%)	313 (95%)	16 (5%)	1 (0%)	36	72
1	H	330/342 (96%)	313 (95%)	16 (5%)	1 (0%)	36	72
1	I	330/342 (96%)	313 (95%)	16 (5%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2970/3078 (96%)	2817 (95%)	148 (5%)	5 (0%)	44	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	599	SER
1	D	599	SER
1	G	599	SER
1	H	599	SER
1	I	599	SER

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	A	13/314 (4%)	13 (100%)	0	100	100
1	B	195/314 (62%)	195 (100%)	0	100	100
1	E	1/314 (0%)	1 (100%)	0	100	100
1	F	306/314 (98%)	306 (100%)	0	100	100
1	G	260/314 (83%)	260 (100%)	0	100	100
1	H	306/314 (98%)	306 (100%)	0	100	100
1	I	306/314 (98%)	306 (100%)	0	100	100
All	All	1387/2198 (63%)	1387 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	661	ASN
1	B	360	ASN
1	B	528	ASN
1	F	356	ASN

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Mol	Chain	Res	Type
1	F	360	ASN
1	F	391	ASN
1	F	528	ASN
1	F	661	ASN
1	G	356	ASN
1	G	360	ASN
1	G	391	ASN
1	G	528	ASN
1	G	661	ASN
1	H	356	ASN
1	H	360	ASN
1	H	391	ASN
1	H	528	ASN
1	H	661	ASN
1	I	356	ASN
1	I	360	ASN
1	I	391	ASN
1	I	528	ASN
1	I	661	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

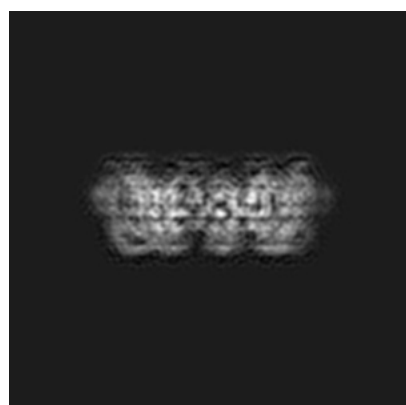
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22589. These allow visual inspection of the internal detail of the map and identification of artifacts.

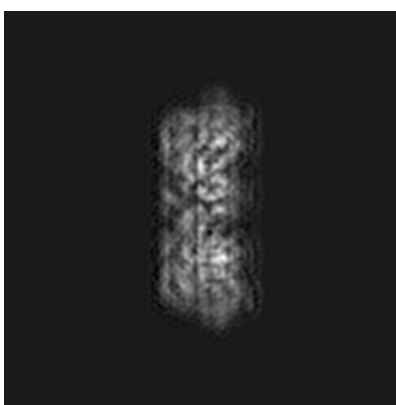
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

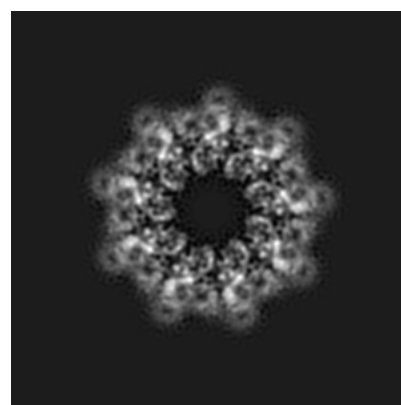
6.1.1 Primary map



X



Y

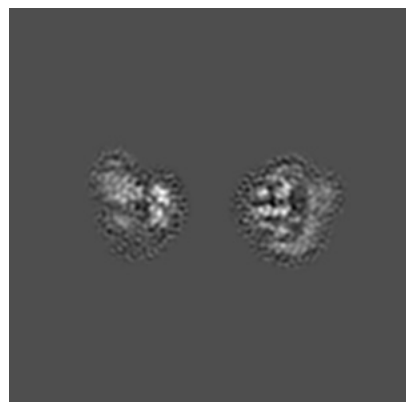


Z

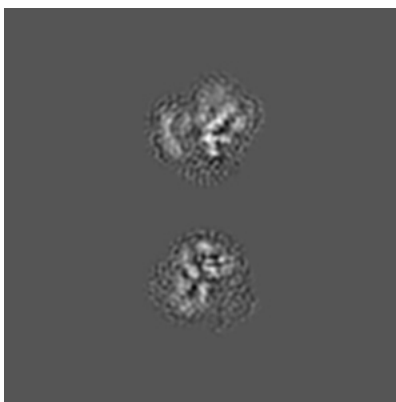
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

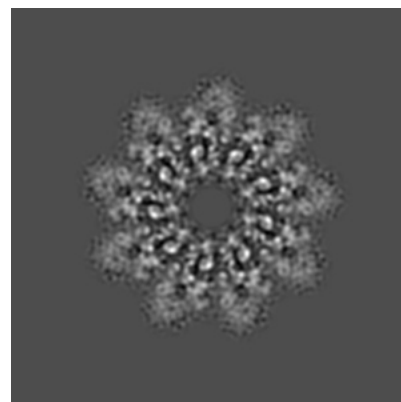
6.2.1 Primary map



X Index: 160



Y Index: 160

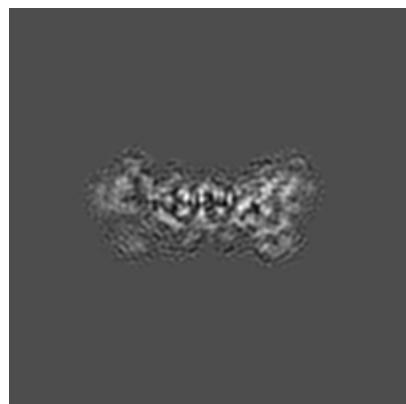


Z Index: 160

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

6.3 Largest variance slices [i](#)

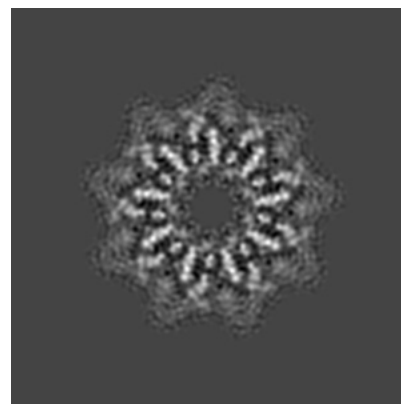
6.3.1 Primary map



X Index: 121



Y Index: 203

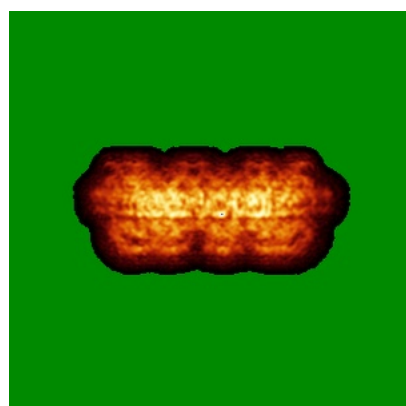


Z Index: 157

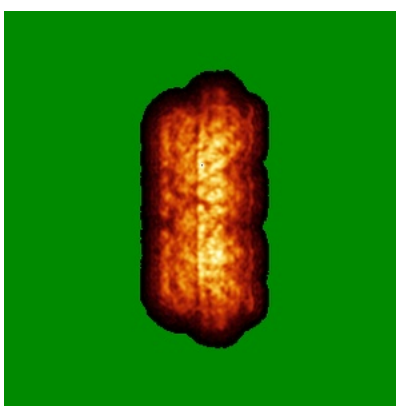
The images above show the largest variance slices of the map in three orthogonal directions.

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

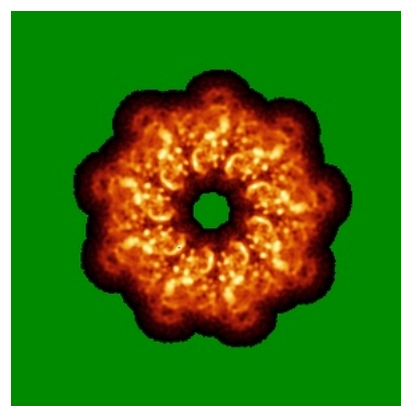
6.4.1 Primary map



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

This section was not generated.

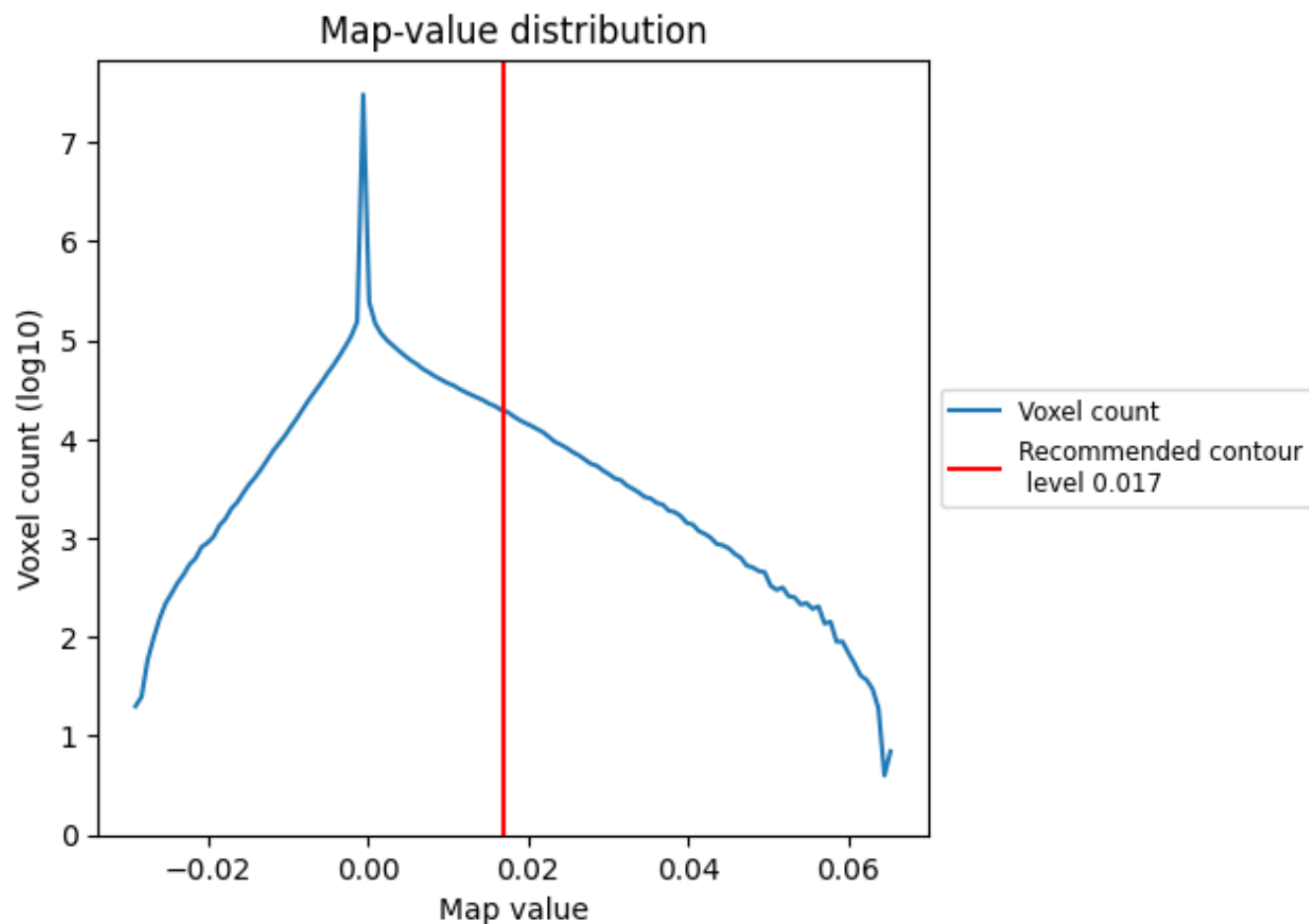
6.6 Mask visualisation

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

7 Map analysis [i](#)

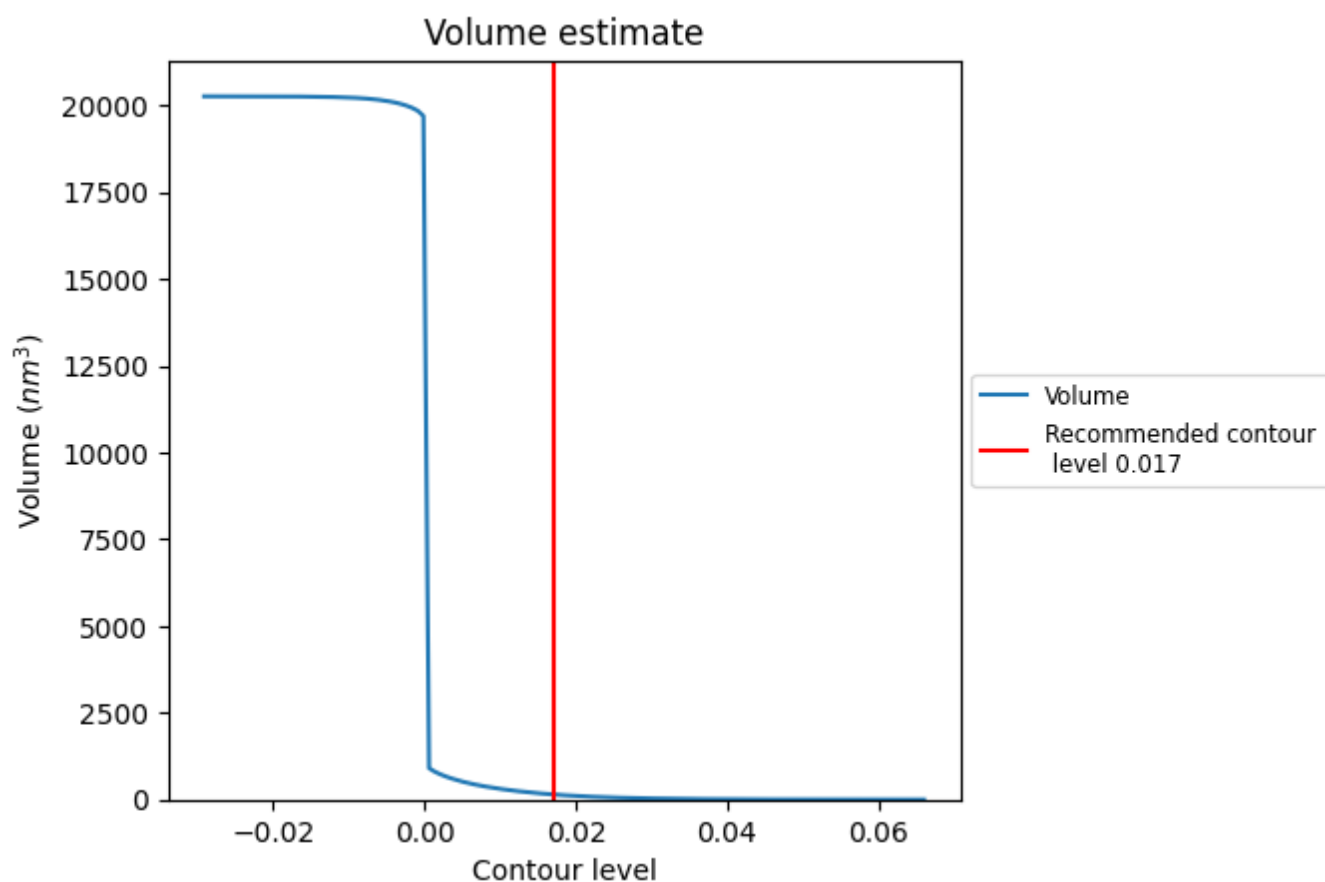
This section contains the results of statistical analysis of the map.

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.

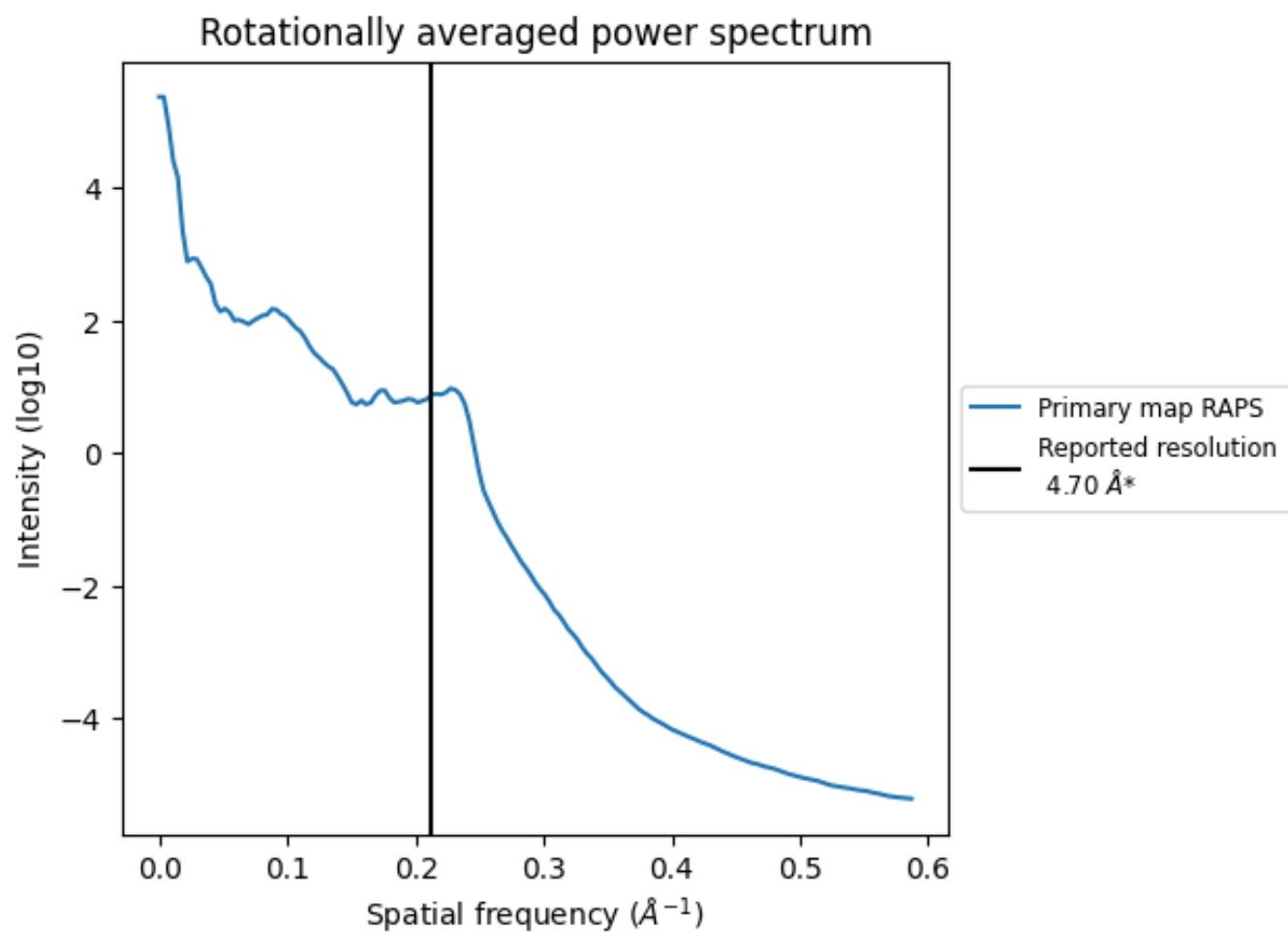
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 ⓘ

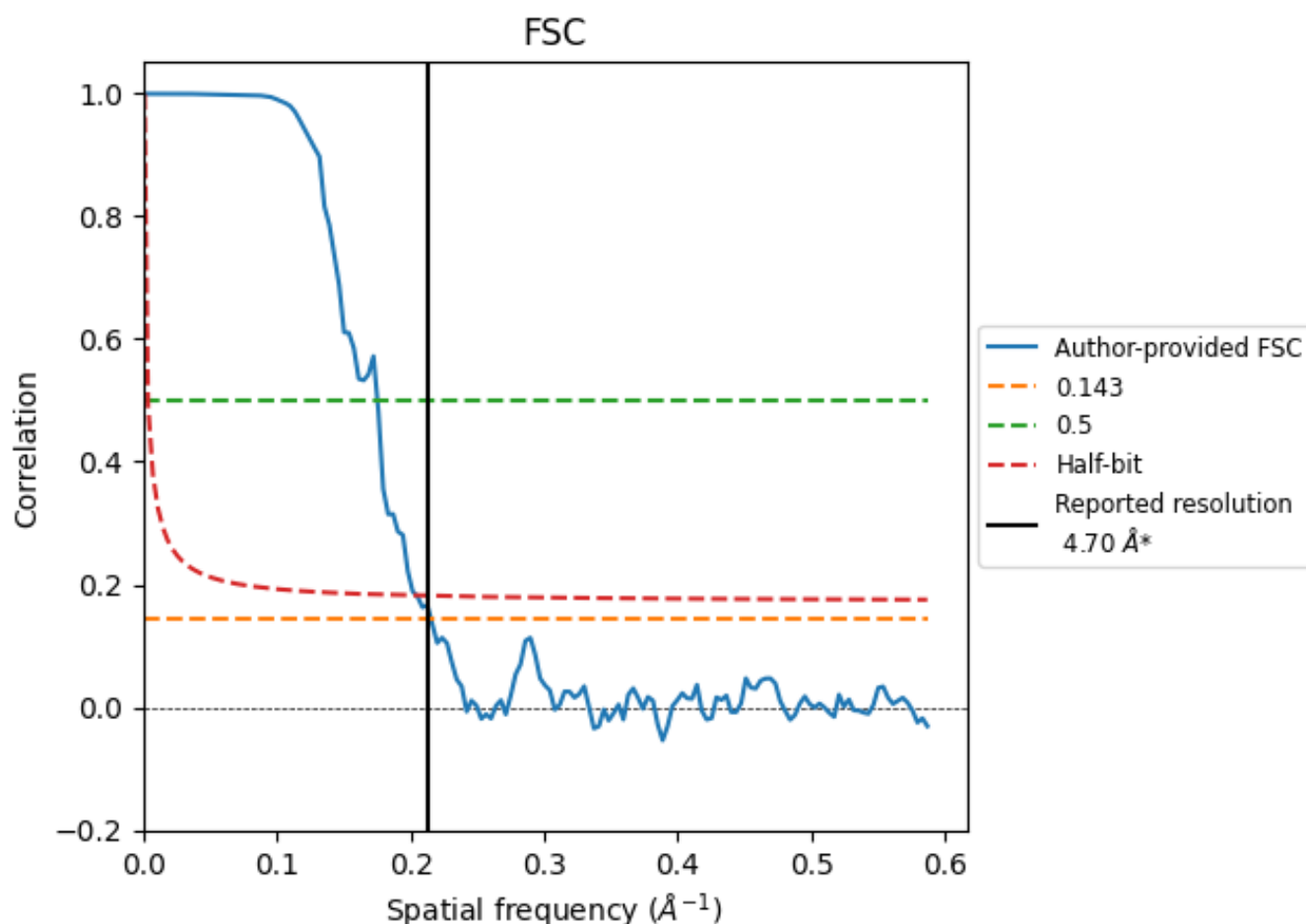


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.64	5.70	4.89
Unmasked-calculated*	-	-	-

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

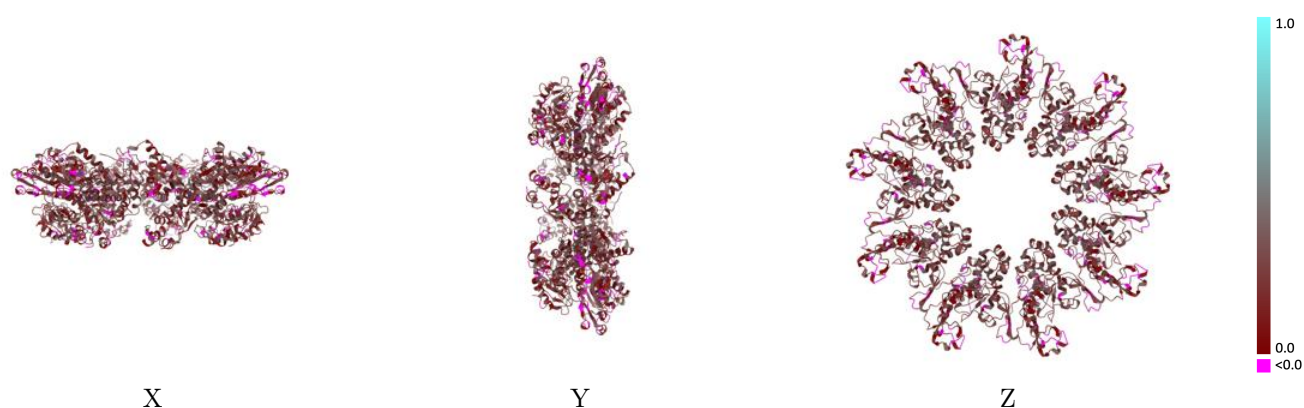
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-22589 and PDB model 7K08. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

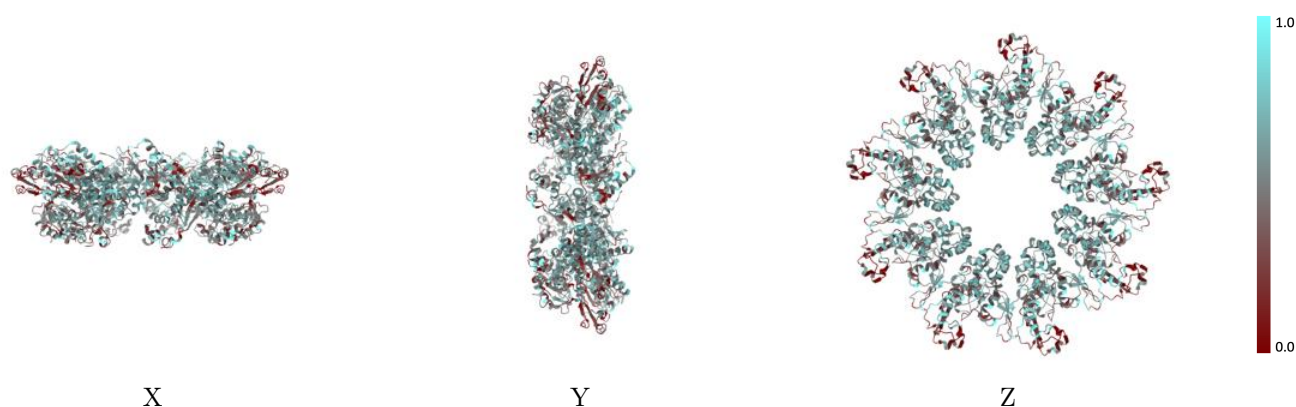
This section was not generated.

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



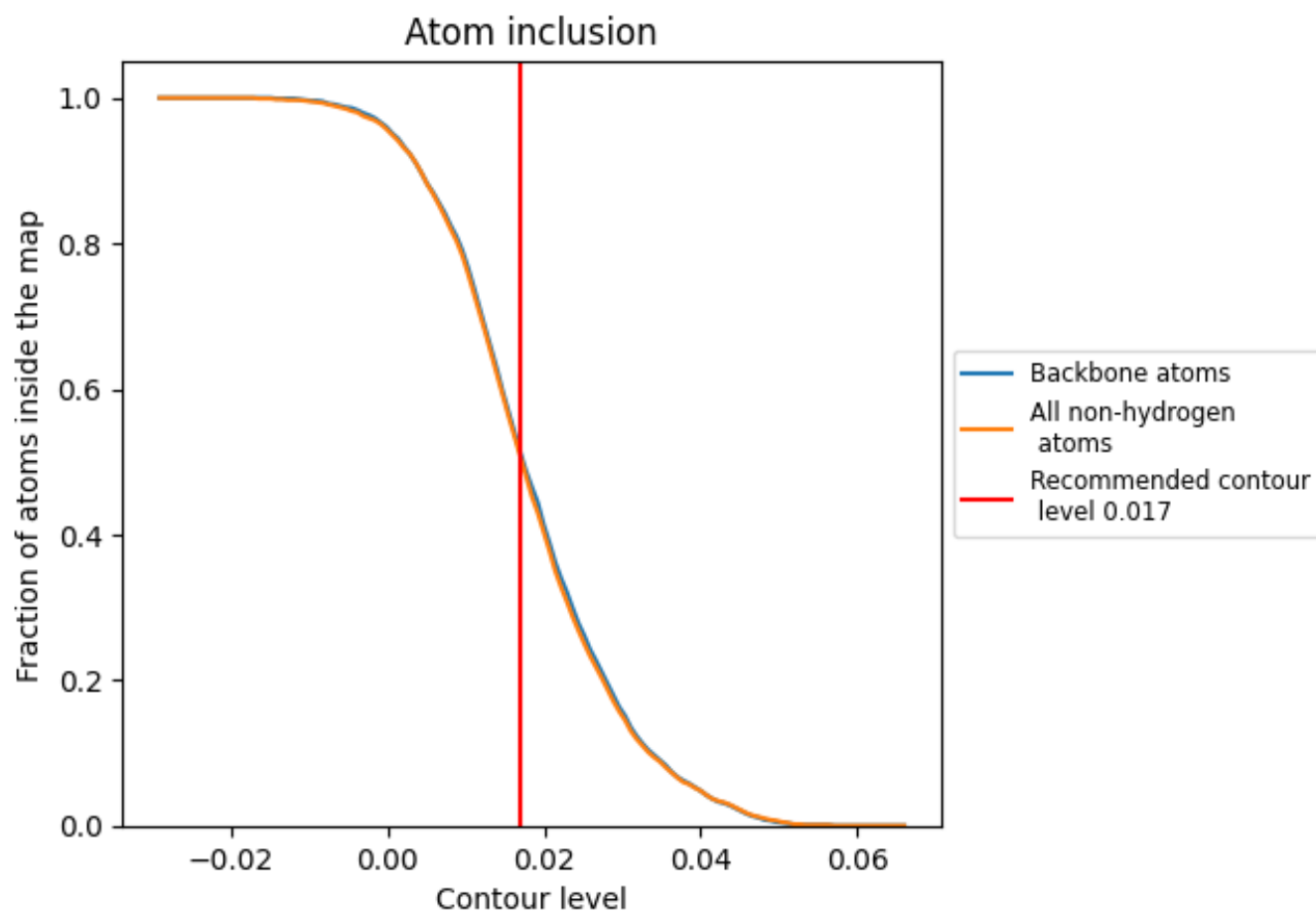
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 51% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5070	0.2050
A	0.5190	0.2060
B	0.5190	0.2040
C	0.5190	0.2050
D	0.5210	0.2050
E	0.5210	0.2050
F	0.5180	0.2050
G	0.5160	0.2050
H	0.5180	0.2060
I	0.5180	0.2050

1.0

0.0

<0.0