Preliminary Full wwPDB EM Validation Report ⓘ

Aug 31, 2026 – 01:31 am BST

Deposition ID : D_1292160338

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

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.dev133
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)	:	2.50

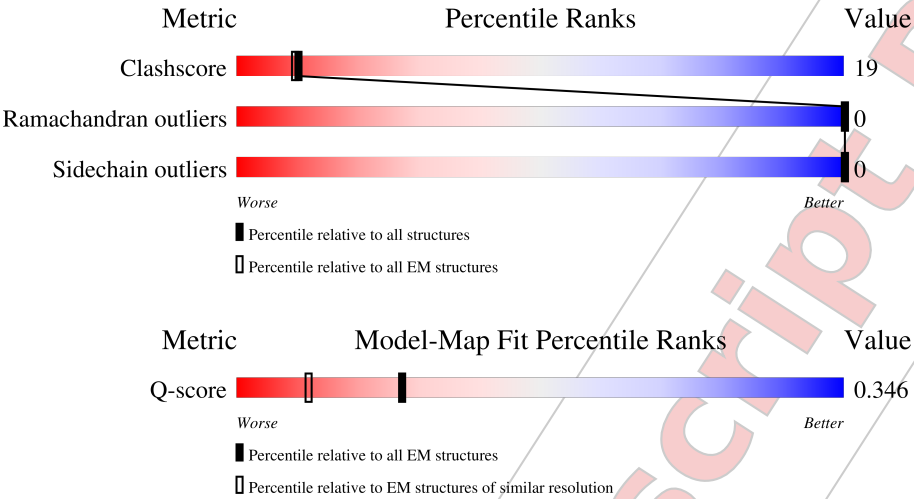
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1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	111	56% 29% 15%
1	B	111	53% 32% 15%
1	C	111	58% 27% 15%
1	D	111	62% 23% 15%
1	E	111	51% 33% 15%

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Mol	Chain	Length	Quality of chain
1	F	111	50% 34% 15%
1	G	111	52% 32% 15%
1	H	111	56% 29% 15%
1	I	111	58% 27% 15%
1	J	111	59% 25% 15%
1	K	111	60% 24% 15%
1	L	111	67% 18% 15%
1	M	111	58% 27% 15%
1	N	111	56% 29% 15%
1	O	111	56% 29% 15%
1	P	111	59% 25% 15%
1	Q	111	58% 27% 15%
1	R	111	59% 25% 15%
1	S	111	67% 18% 15%
1	T	111	59% 25% 15%

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2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15040 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 Serum Amyloid A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	A	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	B	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	C	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	D	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	F	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	G	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	H	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	I	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	J	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	K	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	L	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	M	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	N	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	O	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	P	94	Total 752	C 463	N 143	O 144	S 2	0	0
1	Q	94	Total 752	C 463	N 143	O 144	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	94	Total	C	N	O	S	0	0
			752	463	143	144	2		
1	S	94	Total	C	N	O	S	0	0
			752	463	143	144	2		
1	T	94	Total	C	N	O	S	0	0
			752	463	143	144	2		

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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. 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. 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.

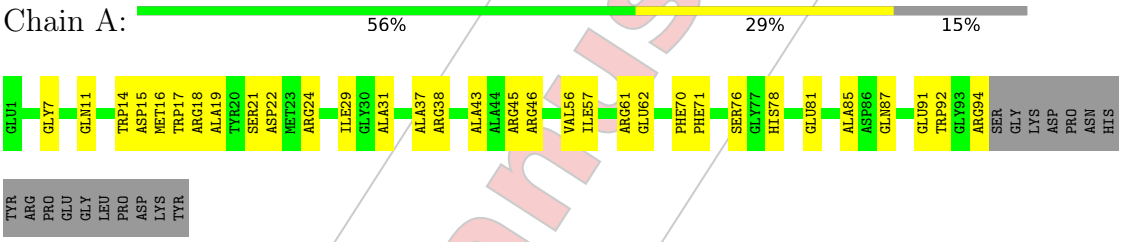
- Molecule 1: Serum Amyloid A

Chain E:



- Molecule 1: Serum Amyloid A

Chain A:



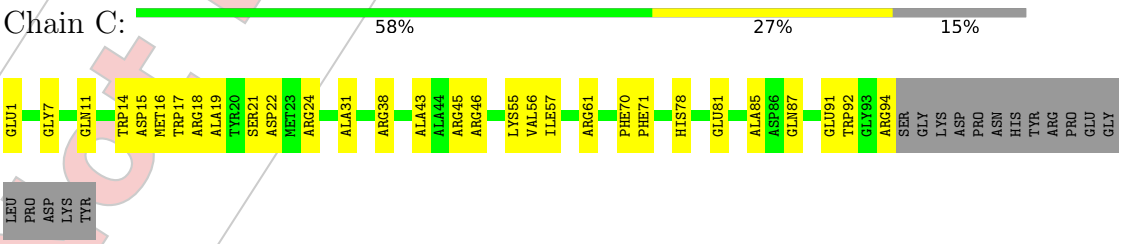
- Molecule 1: Serum Amyloid A

Chain B:



- Molecule 1: Serum Amyloid A

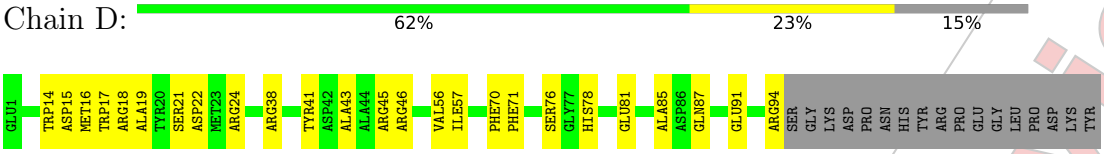
Chain C:



- Molecule 1: Serum Amyloid A

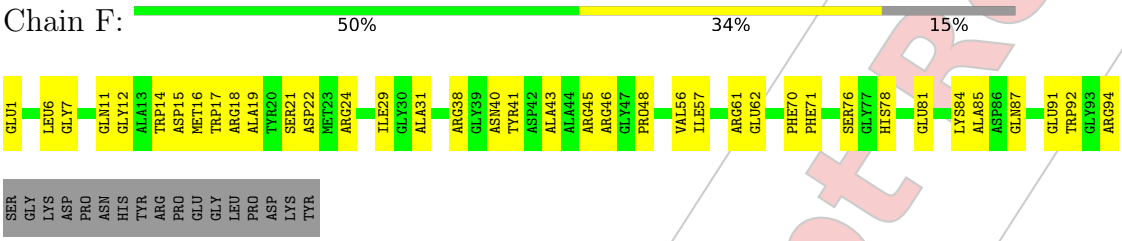
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Chain D:



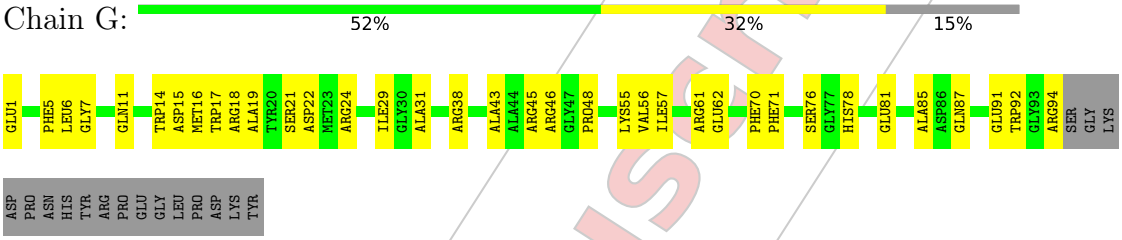
• Molecule 1: Serum Amyloid A

Chain F:



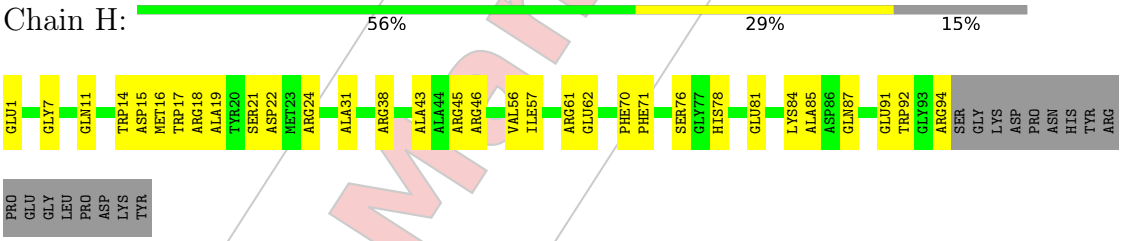
• Molecule 1: Serum Amyloid A

Chain G:



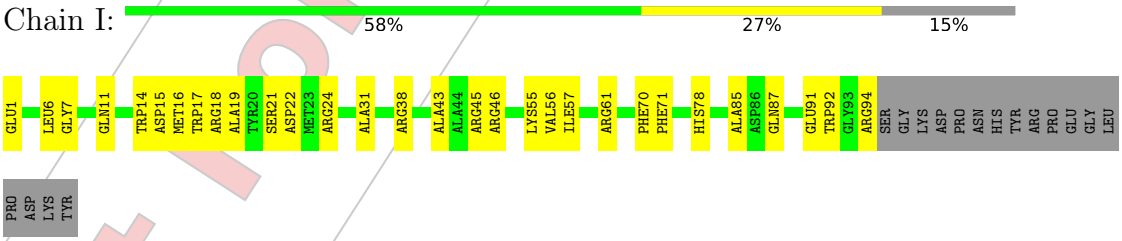
• Molecule 1: Serum Amyloid A

Chain H:



• Molecule 1: Serum Amyloid A

Chain I:



• Molecule 1: Serum Amyloid A

Chain J:



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• Molecule 1: Serum Amyloid A

Chain K:

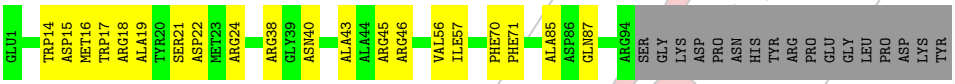




• Molecule 1: Serum Amyloid A

Chain L:

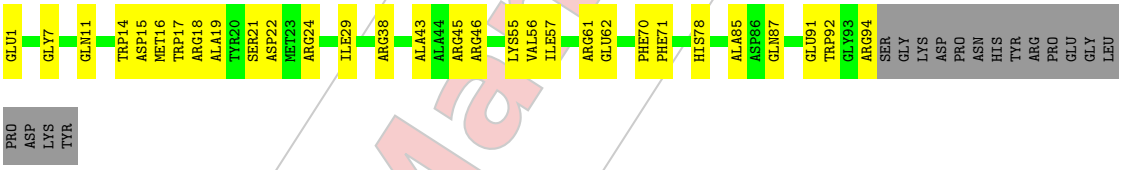




• Molecule 1: Serum Amyloid A

Chain M:

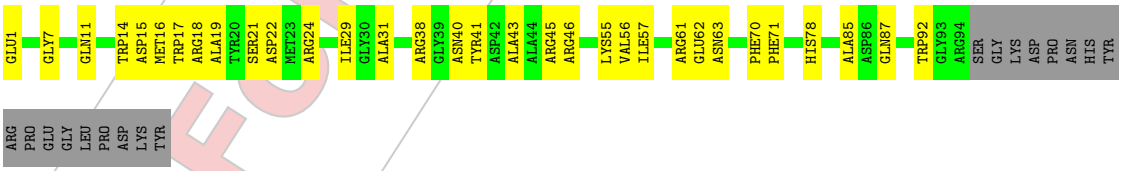




• Molecule 1: Serum Amyloid A

Chain N:





• Molecule 1: Serum Amyloid A

Chain O:





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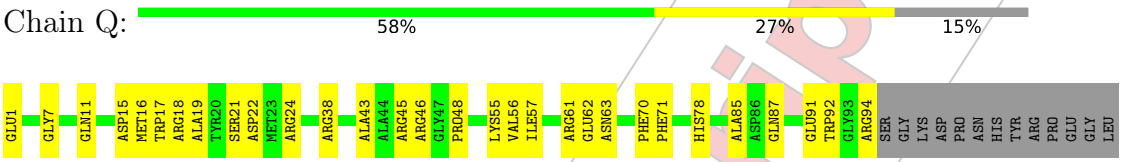
• Molecule 1: Serum Amyloid A

Chain P:



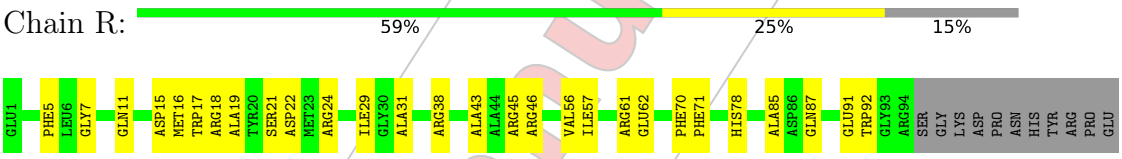
• Molecule 1: Serum Amyloid A

Chain Q:



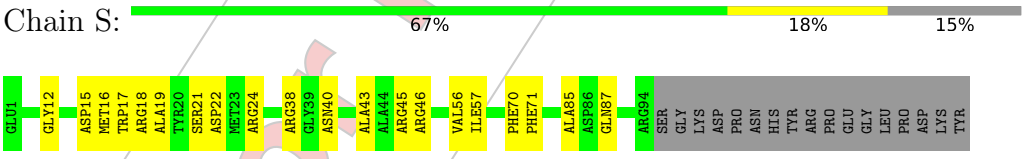
• Molecule 1: Serum Amyloid A

Chain R:



• Molecule 1: Serum Amyloid A

Chain S:



• Molecule 1: Serum Amyloid A

Chain T:



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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	Unknown	
Map size (Å)	469.84, 469.84, 469.84	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1746, 1.1746, 1.1746	Depositor

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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	0.19	0/774	0.45	0/1043
1	B	0.19	0/774	0.45	0/1043
1	C	0.19	0/774	0.45	0/1043
1	D	0.19	0/774	0.45	0/1043
1	E	0.19	0/774	0.45	0/1043
1	F	0.19	0/774	0.45	0/1043
1	G	0.19	0/774	0.45	0/1043
1	H	0.19	0/774	0.45	0/1043
1	I	0.19	0/774	0.45	0/1043
1	J	0.19	0/774	0.45	0/1043
1	K	0.19	0/774	0.45	0/1043
1	L	0.19	0/774	0.45	0/1043
1	M	0.19	0/774	0.45	0/1043
1	N	0.19	0/774	0.45	0/1043
1	O	0.19	0/774	0.45	0/1043
1	P	0.19	0/774	0.45	0/1043
1	Q	0.19	0/774	0.45	0/1043
1	R	0.19	0/774	0.45	0/1043
1	S	0.19	0/774	0.45	0/1043
1	T	0.19	0/774	0.45	0/1043
All	All	0.19	0/15480	0.45	0/20860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

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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	752	0	664	52	0
1	B	752	0	664	58	0
1	C	752	0	664	33	0
1	D	752	0	664	27	0
1	E	752	0	664	64	0
1	F	752	0	664	56	0
1	G	752	0	664	57	0
1	H	752	0	664	49	0
1	I	752	0	664	33	0
1	J	752	0	664	30	0
1	K	752	0	664	34	0
1	L	752	0	664	18	0
1	M	752	0	664	48	0
1	N	752	0	664	43	0
1	O	752	0	664	49	0
1	P	752	0	664	33	0
1	Q	752	0	664	45	0
1	R	752	0	664	36	0
1	S	752	0	664	17	0
1	T	752	0	664	29	0
All	All	15040	0	13280	544	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 19.

All (544) 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:C:56:VAL:HG12	1:C:57:ILE:HG12	1.62	0.81
1:B:56:VAL:HG12	1:B:57:ILE:HG12	1.62	0.81
1:L:56:VAL:HG12	1:L:57:ILE:HG12	1.62	0.81
1:E:56:VAL:HG12	1:E:57:ILE:HG12	1.62	0.81
1:A:56:VAL:HG12	1:A:57:ILE:HG12	1.62	0.81
1:D:56:VAL:HG12	1:D:57:ILE:HG12	1.62	0.81
1:S:56:VAL:HG12	1:S:57:ILE:HG12	1.62	0.81
1:K:56:VAL:HG12	1:K:57:ILE:HG12	1.62	0.80
1:N:56:VAL:HG12	1:N:57:ILE:HG12	1.62	0.80
1:R:56:VAL:HG12	1:R:57:ILE:HG12	1.62	0.80
1:O:56:VAL:HG12	1:O:57:ILE:HG12	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:56:VAL:HG12	1:M:57:ILE:HG12	1.62	0.80
1:Q:56:VAL:HG12	1:Q:57:ILE:HG12	1.62	0.80
1:T:56:VAL:HG12	1:T:57:ILE:HG12	1.62	0.80
1:P:56:VAL:HG12	1:P:57:ILE:HG12	1.62	0.79
1:I:56:VAL:HG12	1:I:57:ILE:HG12	1.62	0.79
1:G:56:VAL:HG12	1:G:57:ILE:HG12	1.62	0.79
1:F:56:VAL:HG12	1:F:57:ILE:HG12	1.62	0.79
1:H:56:VAL:HG12	1:H:57:ILE:HG12	1.62	0.79
1:J:56:VAL:HG12	1:J:57:ILE:HG12	1.62	0.78
1:I:16:MET:HB3	1:I:17:TRP:HE3	1.50	0.76
1:C:16:MET:HB3	1:C:17:TRP:HE3	1.50	0.76
1:F:16:MET:HB3	1:F:17:TRP:HE3	1.50	0.76
1:G:16:MET:HB3	1:G:17:TRP:HE3	1.50	0.76
1:H:16:MET:HB3	1:H:17:TRP:HE3	1.50	0.76
1:J:16:MET:HB3	1:J:17:TRP:HE3	1.50	0.76
1:E:16:MET:HB3	1:E:17:TRP:HE3	1.50	0.76
1:B:16:MET:HB3	1:B:17:TRP:HE3	1.50	0.76
1:A:16:MET:HB3	1:A:17:TRP:HE3	1.50	0.76
1:D:16:MET:HB3	1:D:17:TRP:HE3	1.50	0.76
1:P:16:MET:HB3	1:P:17:TRP:HE3	1.50	0.76
1:L:16:MET:HB3	1:L:17:TRP:HE3	1.50	0.75
1:M:16:MET:HB3	1:M:17:TRP:HE3	1.50	0.75
1:T:16:MET:HB3	1:T:17:TRP:HE3	1.50	0.75
1:K:16:MET:HB3	1:K:17:TRP:HE3	1.50	0.75
1:N:16:MET:HB3	1:N:17:TRP:HE3	1.50	0.75
1:Q:16:MET:HB3	1:Q:17:TRP:HE3	1.50	0.74
1:O:16:MET:HB3	1:O:17:TRP:HE3	1.50	0.74
1:O:24:ARG:HB3	1:R:24:ARG:HH11	1.52	0.74
1:R:16:MET:HB3	1:R:17:TRP:HE3	1.50	0.74
1:S:16:MET:HB3	1:S:17:TRP:HE3	1.50	0.74
1:K:24:ARG:HH11	1:N:24:ARG:HB3	1.54	0.72
1:F:24:ARG:HH11	1:G:24:ARG:HB3	1.56	0.71
1:M:24:ARG:HH11	1:P:24:ARG:HB3	1.57	0.69
1:A:15:ASP:HB2	1:A:38:ARG:HH12	1.57	0.69
1:B:15:ASP:HB2	1:B:38:ARG:HH12	1.57	0.69
1:D:15:ASP:HB2	1:D:38:ARG:HH12	1.58	0.69
1:F:15:ASP:HB2	1:F:38:ARG:HH12	1.57	0.69
1:G:15:ASP:HB2	1:G:38:ARG:HH12	1.58	0.69
1:H:15:ASP:HB2	1:H:38:ARG:HH12	1.58	0.69
1:I:15:ASP:HB2	1:I:38:ARG:HH12	1.58	0.69
1:J:15:ASP:HB2	1:J:38:ARG:HH12	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ASP:HB2	1:E:38:ARG:HH12	1.58	0.69
1:C:15:ASP:HB2	1:C:38:ARG:HH12	1.58	0.69
1:M:15:ASP:HB2	1:M:38:ARG:HH12	1.58	0.69
1:P:15:ASP:HB2	1:P:38:ARG:HH12	1.58	0.69
1:K:15:ASP:HB2	1:K:38:ARG:HH12	1.58	0.68
1:L:15:ASP:HB2	1:L:38:ARG:HH12	1.58	0.68
1:N:15:ASP:HB2	1:N:38:ARG:HH12	1.58	0.68
1:S:15:ASP:HB2	1:S:38:ARG:HH12	1.58	0.68
1:R:15:ASP:HB2	1:R:38:ARG:HH12	1.58	0.68
1:O:15:ASP:HB2	1:O:38:ARG:HH12	1.58	0.68
1:Q:15:ASP:HB2	1:Q:38:ARG:HH12	1.58	0.68
1:R:24:ARG:HB3	1:S:24:ARG:HH11	1.59	0.68
1:T:15:ASP:HB2	1:T:38:ARG:HH12	1.58	0.68
1:B:24:ARG:HH11	1:C:24:ARG:HB3	1.59	0.67
1:A:22:ASP:HA	1:D:22:ASP:O	1.95	0.67
1:H:22:ASP:HA	1:J:22:ASP:O	1.96	0.66
1:E:45:ARG:NH2	1:B:45:ARG:HD2	2.10	0.66
1:E:22:ASP:HA	1:A:22:ASP:O	1.96	0.66
1:E:22:ASP:O	1:B:22:ASP:HA	1.96	0.65
1:O:22:ASP:HA	1:R:22:ASP:O	1.96	0.65
1:G:24:ARG:HH11	1:I:24:ARG:HB3	1.61	0.65
1:E:24:ARG:HB3	1:A:24:ARG:HH11	1.62	0.65
1:Q:45:ARG:CZ	1:T:45:ARG:HD2	2.27	0.65
1:C:16:MET:HB3	1:C:17:TRP:CE3	2.32	0.65
1:O:24:ARG:HH11	1:Q:24:ARG:HB3	1.60	0.64
1:I:16:MET:HB3	1:I:17:TRP:CE3	2.32	0.64
1:S:16:MET:HB3	1:S:17:TRP:CE3	2.32	0.64
1:R:16:MET:HB3	1:R:17:TRP:CE3	2.32	0.64
1:F:22:ASP:HA	1:H:22:ASP:O	1.98	0.64
1:O:16:MET:HB3	1:O:17:TRP:CE3	2.32	0.64
1:L:16:MET:HB3	1:L:17:TRP:CE3	2.32	0.63
1:Q:16:MET:HB3	1:Q:17:TRP:CE3	2.32	0.63
1:K:16:MET:HB3	1:K:17:TRP:CE3	2.32	0.63
1:N:16:MET:HB3	1:N:17:TRP:CE3	2.32	0.63
1:J:16:MET:HB3	1:J:17:TRP:CE3	2.32	0.63
1:M:16:MET:HB3	1:M:17:TRP:CE3	2.32	0.63
1:P:16:MET:HB3	1:P:17:TRP:CE3	2.32	0.63
1:T:16:MET:HB3	1:T:17:TRP:CE3	2.32	0.63
1:F:22:ASP:O	1:G:22:ASP:HA	1.99	0.63
1:H:16:MET:HB3	1:H:17:TRP:CE3	2.32	0.63
1:D:16:MET:HB3	1:D:17:TRP:CE3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:HB3	1:A:17:TRP:CE3	2.32	0.63
1:E:16:MET:HB3	1:E:17:TRP:CE3	2.32	0.63
1:B:16:MET:HB3	1:B:17:TRP:CE3	2.32	0.63
1:F:16:MET:HB3	1:F:17:TRP:CE3	2.32	0.62
1:G:16:MET:HB3	1:G:17:TRP:CE3	2.32	0.62
1:H:24:ARG:HB3	1:J:24:ARG:HH11	1.65	0.62
1:F:45:ARG:CZ	1:G:45:ARG:HD2	2.29	0.62
1:E:45:ARG:CZ	1:B:45:ARG:HD2	2.30	0.62
1:F:45:ARG:NH2	1:G:45:ARG:HD2	2.15	0.60
1:M:45:ARG:HD2	1:N:45:ARG:NH2	2.16	0.60
1:Q:24:ARG:HH11	1:T:24:ARG:HB3	1.66	0.60
1:M:45:ARG:HD2	1:N:45:ARG:CZ	2.31	0.60
1:Q:45:ARG:NH2	1:T:45:ARG:HD2	2.17	0.60
1:M:22:ASP:HA	1:N:22:ASP:O	2.02	0.60
1:H:45:ARG:HD2	1:J:45:ARG:NH2	2.16	0.60
1:M:24:ARG:HB3	1:N:24:ARG:HH11	1.67	0.59
1:A:45:ARG:HD2	1:D:45:ARG:NH2	2.18	0.59
1:F:24:ARG:HB3	1:H:24:ARG:HH11	1.67	0.59
1:G:45:ARG:CZ	1:I:45:ARG:HD2	2.32	0.59
1:B:22:ASP:O	1:C:22:ASP:HA	2.03	0.58
1:K:22:ASP:O	1:N:22:ASP:HA	2.03	0.58
1:B:45:ARG:CZ	1:C:45:ARG:HD2	2.33	0.57
1:E:24:ARG:HH11	1:B:24:ARG:HB3	1.69	0.57
1:M:92:TRP:HA	1:P:92:TRP:O	2.05	0.57
1:R:11:GLN:NE2	1:S:40:ASN:O	2.31	0.57
1:G:45:ARG:NH2	1:I:45:ARG:HD2	2.20	0.56
1:O:22:ASP:O	1:Q:22:ASP:HA	2.04	0.56
1:E:45:ARG:HD2	1:A:45:ARG:NH2	2.21	0.56
1:G:22:ASP:O	1:I:22:ASP:HA	2.06	0.55
1:A:24:ARG:HB3	1:D:24:ARG:HH11	1.70	0.55
1:K:24:ARG:HB3	1:L:24:ARG:HH11	1.70	0.55
1:O:92:TRP:HA	1:Q:92:TRP:O	2.07	0.55
1:E:45:ARG:HD2	1:A:45:ARG:CZ	2.36	0.55
1:K:22:ASP:HA	1:L:22:ASP:O	2.07	0.54
1:O:45:ARG:HD2	1:R:45:ARG:CZ	2.38	0.54
1:F:7:GLY:O	1:G:7:GLY:HA3	2.07	0.54
1:R:22:ASP:HA	1:S:22:ASP:O	2.07	0.54
1:H:45:ARG:HD2	1:J:45:ARG:CZ	2.37	0.54
1:B:45:ARG:NH2	1:C:45:ARG:HD2	2.22	0.54
1:F:45:ARG:HD2	1:H:45:ARG:NH2	2.22	0.54
1:Q:22:ASP:O	1:T:22:ASP:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:45:ARG:O	1:L:45:ARG:HG3	2.08	0.53
1:E:76:SER:HG	1:B:76:SER:HA	1.73	0.53
1:K:45:ARG:O	1:K:45:ARG:HG3	2.09	0.53
1:N:45:ARG:O	1:N:45:ARG:HG3	2.09	0.53
1:D:45:ARG:O	1:D:45:ARG:HG3	2.09	0.53
1:M:45:ARG:HG3	1:M:45:ARG:O	2.09	0.53
1:P:45:ARG:O	1:P:45:ARG:HG3	2.09	0.53
1:E:45:ARG:O	1:E:45:ARG:HG3	2.09	0.53
1:A:45:ARG:HG3	1:A:45:ARG:O	2.09	0.53
1:F:45:ARG:O	1:F:45:ARG:HG3	2.09	0.53
1:H:45:ARG:HG3	1:H:45:ARG:O	2.09	0.53
1:J:45:ARG:O	1:J:45:ARG:HG3	2.09	0.53
1:G:45:ARG:O	1:G:45:ARG:HG3	2.09	0.53
1:B:45:ARG:O	1:B:45:ARG:HG3	2.09	0.53
1:C:45:ARG:HG3	1:C:45:ARG:O	2.09	0.53
1:I:45:ARG:O	1:I:45:ARG:HG3	2.09	0.53
1:M:61:ARG:HH12	1:P:61:ARG:HH21	1.57	0.53
1:B:91:GLU:O	1:C:91:GLU:HA	2.08	0.53
1:S:45:ARG:O	1:S:45:ARG:HG3	2.09	0.52
1:K:45:ARG:HD2	1:L:45:ARG:NH2	2.24	0.52
1:R:45:ARG:HG3	1:R:45:ARG:O	2.09	0.52
1:F:31:ALA:HA	1:G:31:ALA:O	2.10	0.52
1:O:45:ARG:O	1:O:45:ARG:HG3	2.09	0.52
1:K:19:ALA:HB2	1:K:70:PHE:CE2	2.45	0.52
1:L:19:ALA:HB2	1:L:70:PHE:CE2	2.45	0.52
1:Q:45:ARG:O	1:Q:45:ARG:HG3	2.09	0.52
1:N:19:ALA:HB2	1:N:70:PHE:CE2	2.45	0.52
1:P:19:ALA:HB2	1:P:70:PHE:CE2	2.45	0.52
1:A:19:ALA:HB2	1:A:70:PHE:CE2	2.45	0.51
1:D:19:ALA:HB2	1:D:70:PHE:CE2	2.45	0.51
1:M:19:ALA:HB2	1:M:70:PHE:CE2	2.45	0.51
1:O:78:HIS:ND1	1:R:78:HIS:CD2	2.78	0.51
1:E:78:HIS:ND1	1:A:78:HIS:HD2	2.08	0.51
1:B:62:GLU:OE2	1:C:1:GLU:N	2.41	0.51
1:F:45:ARG:HD2	1:H:45:ARG:CZ	2.40	0.51
1:M:91:GLU:O	1:P:91:GLU:HA	2.11	0.51
1:T:45:ARG:HG3	1:T:45:ARG:O	2.09	0.51
1:E:19:ALA:HB2	1:E:70:PHE:CE2	2.46	0.51
1:T:19:ALA:HB2	1:T:70:PHE:CE2	2.45	0.51
1:B:19:ALA:HB2	1:B:70:PHE:CE2	2.45	0.51
1:G:43:ALA:HB1	1:G:46:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:GLU:OE2	1:P:1:GLU:N	2.43	0.51
1:Q:19:ALA:HB2	1:Q:70:PHE:CE2	2.45	0.51
1:E:78:HIS:ND1	1:A:78:HIS:CD2	2.78	0.51
1:C:19:ALA:HB2	1:C:70:PHE:CE2	2.45	0.51
1:F:43:ALA:HB1	1:F:46:ARG:HG3	1.93	0.51
1:H:43:ALA:HB1	1:H:46:ARG:HG3	1.93	0.51
1:I:43:ALA:HB1	1:I:46:ARG:HG3	1.93	0.51
1:J:19:ALA:HB2	1:J:70:PHE:CE2	2.45	0.51
1:J:43:ALA:HB1	1:J:46:ARG:HG3	1.93	0.51
1:E:43:ALA:HB1	1:E:46:ARG:HG3	1.93	0.51
1:B:43:ALA:HB1	1:B:46:ARG:HG3	1.93	0.51
1:D:43:ALA:HB1	1:D:46:ARG:HG3	1.93	0.51
1:O:19:ALA:HB2	1:O:70:PHE:CE2	2.45	0.51
1:A:43:ALA:HB1	1:A:46:ARG:HG3	1.93	0.51
1:C:43:ALA:HB1	1:C:46:ARG:HG3	1.93	0.51
1:H:19:ALA:HB2	1:H:70:PHE:CE2	2.45	0.51
1:E:41:TYR:HB2	1:B:11:GLN:HE21	1.75	0.51
1:F:19:ALA:HB2	1:F:70:PHE:CE2	2.45	0.51
1:G:19:ALA:HB2	1:G:70:PHE:CE2	2.45	0.51
1:O:45:ARG:CZ	1:Q:45:ARG:HD2	2.41	0.51
1:R:19:ALA:HB2	1:R:70:PHE:CE2	2.45	0.51
1:A:45:ARG:HD2	1:D:45:ARG:CZ	2.41	0.50
1:F:78:HIS:ND1	1:H:78:HIS:CD2	2.79	0.50
1:I:19:ALA:HB2	1:I:70:PHE:CE2	2.45	0.50
1:Q:45:ARG:NH1	1:T:45:ARG:HB2	2.27	0.50
1:S:19:ALA:HB2	1:S:70:PHE:CE2	2.45	0.50
1:G:91:GLU:O	1:I:91:GLU:HA	2.11	0.50
1:D:17:TRP:HB3	1:D:70:PHE:CZ	2.47	0.50
1:F:78:HIS:ND1	1:H:78:HIS:HD2	2.10	0.50
1:L:17:TRP:HB3	1:L:70:PHE:CZ	2.47	0.50
1:E:7:GLY:O	1:B:7:GLY:HA3	2.12	0.50
1:E:17:TRP:HB3	1:E:70:PHE:CZ	2.47	0.50
1:A:17:TRP:HB3	1:A:70:PHE:CZ	2.47	0.50
1:B:17:TRP:HB3	1:B:70:PHE:CZ	2.47	0.50
1:K:17:TRP:HB3	1:K:70:PHE:CZ	2.47	0.50
1:K:43:ALA:HB1	1:K:46:ARG:HG3	1.93	0.50
1:L:43:ALA:HB1	1:L:46:ARG:HG3	1.93	0.50
1:N:17:TRP:HB3	1:N:70:PHE:CZ	2.47	0.50
1:Q:17:TRP:HB3	1:Q:70:PHE:CZ	2.47	0.50
1:E:45:ARG:NH1	1:B:45:ARG:HB2	2.27	0.50
1:F:91:GLU:HA	1:H:91:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:43:ALA:HB1	1:N:46:ARG:HG3	1.93	0.50
1:S:43:ALA:HB1	1:S:46:ARG:HG3	1.93	0.50
1:T:17:TRP:HB3	1:T:70:PHE:CZ	2.47	0.50
1:C:17:TRP:HB3	1:C:70:PHE:CZ	2.47	0.50
1:M:17:TRP:HB3	1:M:70:PHE:CZ	2.47	0.50
1:M:43:ALA:HB1	1:M:46:ARG:HG3	1.93	0.50
1:O:17:TRP:HB3	1:O:70:PHE:CZ	2.47	0.50
1:P:43:ALA:HB1	1:P:46:ARG:HG3	1.93	0.50
1:R:17:TRP:HB3	1:R:70:PHE:CZ	2.47	0.50
1:P:17:TRP:HB3	1:P:70:PHE:CZ	2.47	0.50
1:R:43:ALA:HB1	1:R:46:ARG:HG3	1.93	0.50
1:K:92:TRP:HA	1:N:92:TRP:O	2.12	0.50
1:M:45:ARG:CZ	1:P:45:ARG:HD2	2.41	0.50
1:O:43:ALA:HB1	1:O:46:ARG:HG3	1.93	0.50
1:S:17:TRP:HB3	1:S:70:PHE:CZ	2.47	0.50
1:Q:43:ALA:HB1	1:Q:46:ARG:HG3	1.93	0.49
1:E:1:GLU:N	1:A:62:GLU:OE2	2.43	0.49
1:O:45:ARG:HD2	1:R:45:ARG:NH2	2.27	0.49
1:T:43:ALA:HB1	1:T:46:ARG:HG3	1.93	0.49
1:F:17:TRP:HB3	1:F:70:PHE:CZ	2.47	0.49
1:H:17:TRP:HB3	1:H:70:PHE:CZ	2.47	0.49
1:J:17:TRP:HB3	1:J:70:PHE:CZ	2.47	0.49
1:O:78:HIS:ND1	1:R:78:HIS:HD2	2.10	0.49
1:E:91:GLU:HA	1:A:91:GLU:O	2.12	0.49
1:G:17:TRP:HB3	1:G:70:PHE:CZ	2.47	0.49
1:I:17:TRP:HB3	1:I:70:PHE:CZ	2.47	0.49
1:K:45:ARG:CZ	1:N:45:ARG:HD2	2.42	0.49
1:B:78:HIS:HD2	1:C:78:HIS:ND1	2.11	0.49
1:E:40:ASN:O	1:B:11:GLN:NE2	2.42	0.49
1:O:1:GLU:N	1:R:62:GLU:OE2	2.45	0.49
1:A:24:ARG:HA	1:D:24:ARG:O	2.13	0.49
1:F:1:GLU:N	1:H:62:GLU:OE2	2.44	0.49
1:M:87:GLN:CB	1:P:63:ASN:HD21	2.26	0.48
1:F:91:GLU:O	1:G:91:GLU:HA	2.13	0.48
1:K:45:ARG:HD2	1:L:45:ARG:CZ	2.43	0.48
1:B:92:TRP:HA	1:C:92:TRP:O	2.14	0.48
1:M:87:GLN:CG	1:P:63:ASN:HD21	2.26	0.48
1:E:91:GLU:O	1:B:91:GLU:HA	2.14	0.48
1:O:45:ARG:NH2	1:Q:45:ARG:HD2	2.28	0.48
1:M:45:ARG:HB2	1:N:45:ARG:NH1	2.29	0.48
1:O:16:MET:SD	1:R:16:MET:HG3	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ARG:HH12	1:C:61:ARG:HH21	1.61	0.47
1:G:92:TRP:HA	1:I:92:TRP:O	2.14	0.47
1:M:7:GLY:HA3	1:N:7:GLY:O	2.15	0.47
1:B:78:HIS:CD2	1:C:78:HIS:ND1	2.82	0.47
1:M:55:LYS:O	1:P:55:LYS:HA	2.15	0.47
1:E:24:ARG:O	1:B:24:ARG:HA	2.13	0.47
1:O:31:ALA:O	1:R:31:ALA:HA	2.14	0.47
1:F:21:SER:HB2	1:F:71:PHE:CZ	2.50	0.47
1:F:41:TYR:HB2	1:G:11:GLN:HE21	1.79	0.47
1:G:21:SER:HB2	1:G:71:PHE:CZ	2.50	0.47
1:H:21:SER:HB2	1:H:71:PHE:CZ	2.50	0.47
1:H:24:ARG:HA	1:J:24:ARG:O	2.15	0.47
1:I:21:SER:HB2	1:I:71:PHE:CZ	2.50	0.47
1:J:21:SER:HB2	1:J:71:PHE:CZ	2.50	0.47
1:B:16:MET:HG3	1:C:16:MET:SD	2.55	0.47
1:G:7:GLY:O	1:I:7:GLY:HA3	2.14	0.47
1:G:62:GLU:OE2	1:I:1:GLU:N	2.45	0.47
1:M:21:SER:HB2	1:M:71:PHE:CZ	2.50	0.47
1:P:21:SER:HB2	1:P:71:PHE:CZ	2.50	0.47
1:T:21:SER:HB2	1:T:71:PHE:CZ	2.50	0.47
1:N:21:SER:HB2	1:N:71:PHE:CZ	2.50	0.47
1:E:16:MET:SD	1:A:16:MET:HG3	2.55	0.47
1:O:7:GLY:O	1:Q:7:GLY:HA3	2.15	0.47
1:Q:7:GLY:O	1:T:7:GLY:HA3	2.15	0.47
1:Q:21:SER:HB2	1:Q:71:PHE:CZ	2.50	0.47
1:F:40:ASN:O	1:G:11:GLN:NE2	2.38	0.47
1:F:45:ARG:HB2	1:H:45:ARG:NH1	2.29	0.47
1:G:61:ARG:HH12	1:I:61:ARG:HH21	1.63	0.47
1:K:21:SER:HB2	1:K:71:PHE:CZ	2.50	0.47
1:O:21:SER:HB2	1:O:71:PHE:CZ	2.50	0.47
1:R:21:SER:HB2	1:R:71:PHE:CZ	2.50	0.47
1:S:21:SER:HB2	1:S:71:PHE:CZ	2.50	0.47
1:E:45:ARG:HB2	1:A:45:ARG:NH1	2.29	0.46
1:A:45:ARG:HB2	1:D:45:ARG:NH1	2.29	0.46
1:L:21:SER:HB2	1:L:71:PHE:CZ	2.50	0.46
1:M:24:ARG:NH1	1:P:24:ARG:HB3	2.26	0.46
1:O:61:ARG:HH12	1:Q:61:ARG:HH21	1.63	0.46
1:O:29:ILE:HG13	1:R:29:ILE:HD13	1.98	0.46
1:A:76:SER:HA	1:D:76:SER:OG	2.16	0.46
1:B:7:GLY:O	1:C:7:GLY:HA3	2.15	0.46
1:C:21:SER:HB2	1:C:71:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:SER:HB2	1:B:71:PHE:CZ	2.50	0.46
1:F:29:ILE:HD13	1:G:29:ILE:HG13	1.97	0.46
1:K:45:ARG:NH2	1:N:45:ARG:HD2	2.31	0.46
1:O:92:TRP:O	1:R:92:TRP:HA	2.15	0.46
1:E:21:SER:HB2	1:E:71:PHE:CZ	2.50	0.46
1:A:78:HIS:ND1	1:D:78:HIS:CD2	2.84	0.46
1:A:21:SER:HB2	1:A:71:PHE:CZ	2.50	0.46
1:D:21:SER:HB2	1:D:71:PHE:CZ	2.50	0.46
1:F:76:SER:HA	1:H:76:SER:OG	2.16	0.46
1:K:24:ARG:NH1	1:N:24:ARG:HB3	2.28	0.46
1:Q:92:TRP:HA	1:T:92:TRP:O	2.15	0.46
1:F:16:MET:HG3	1:G:16:MET:SD	2.56	0.46
1:E:24:ARG:HA	1:A:24:ARG:O	2.16	0.45
1:B:61:ARG:HH11	1:C:61:ARG:HE	1.62	0.45
1:F:78:HIS:HD2	1:G:78:HIS:ND1	2.14	0.45
1:H:45:ARG:HB2	1:J:45:ARG:NH1	2.31	0.45
1:L:19:ALA:HB2	1:L:70:PHE:CD2	2.51	0.45
1:O:55:LYS:O	1:Q:55:LYS:HA	2.16	0.45
1:E:81:GLU:HA	1:A:81:GLU:O	2.16	0.45
1:H:76:SER:HA	1:J:76:SER:OG	2.16	0.45
1:M:92:TRP:O	1:N:92:TRP:HA	2.16	0.45
1:F:62:GLU:OE2	1:G:1:GLU:N	2.48	0.45
1:H:11:GLN:HE21	1:J:41:TYR:HB2	1.81	0.45
1:J:19:ALA:HB2	1:J:70:PHE:CD2	2.51	0.45
1:K:78:HIS:CD2	1:N:78:HIS:ND1	2.84	0.45
1:P:19:ALA:HB2	1:P:70:PHE:CD2	2.51	0.45
1:H:19:ALA:HB2	1:H:70:PHE:CD2	2.51	0.45
1:K:19:ALA:HB2	1:K:70:PHE:CD2	2.51	0.45
1:M:7:GLY:O	1:P:7:GLY:HA3	2.16	0.45
1:Q:62:GLU:OE2	1:T:1:GLU:N	2.49	0.45
1:A:19:ALA:HB2	1:A:70:PHE:CD2	2.51	0.45
1:K:7:GLY:O	1:N:7:GLY:HA3	2.16	0.45
1:N:19:ALA:HB2	1:N:70:PHE:CD2	2.51	0.45
1:E:19:ALA:HB2	1:E:70:PHE:CD2	2.51	0.45
1:B:19:ALA:HB2	1:B:70:PHE:CD2	2.51	0.45
1:D:19:ALA:HB2	1:D:70:PHE:CD2	2.51	0.45
1:F:19:ALA:HB2	1:F:70:PHE:CD2	2.51	0.45
1:M:19:ALA:HB2	1:M:70:PHE:CD2	2.51	0.45
1:O:24:ARG:HB3	1:R:24:ARG:NH1	2.25	0.45
1:C:19:ALA:HB2	1:C:70:PHE:CD2	2.51	0.45
1:F:24:ARG:HA	1:H:24:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:HIS:CD2	1:G:78:HIS:ND1	2.85	0.45
1:S:19:ALA:HB2	1:S:70:PHE:CD2	2.51	0.45
1:E:76:SER:HA	1:A:76:SER:OG	2.16	0.45
1:B:11:GLN:HB3	1:C:11:GLN:HG3	1.98	0.45
1:F:81:GLU:HA	1:H:81:GLU:O	2.16	0.45
1:G:19:ALA:HB2	1:G:70:PHE:CD2	2.51	0.45
1:O:19:ALA:HB2	1:O:70:PHE:CD2	2.51	0.45
1:R:19:ALA:HB2	1:R:70:PHE:CD2	2.51	0.45
1:Q:19:ALA:HB2	1:Q:70:PHE:CD2	2.51	0.45
1:T:19:ALA:HB2	1:T:70:PHE:CD2	2.51	0.45
1:I:19:ALA:HB2	1:I:70:PHE:CD2	2.51	0.44
1:Q:11:GLN:HB3	1:T:11:GLN:HG3	1.99	0.44
1:F:48:PRO:HD2	1:G:48:PRO:HB3	1.98	0.44
1:K:62:GLU:OE2	1:N:1:GLU:N	2.50	0.44
1:B:24:ARG:NH1	1:C:24:ARG:HB3	2.29	0.44
1:O:7:GLY:HA3	1:R:7:GLY:O	2.17	0.44
1:R:5:PHE:HE2	1:S:12:GLY:H	1.65	0.44
1:G:24:ARG:NH1	1:I:24:ARG:HB3	2.32	0.44
1:M:61:ARG:NH1	1:P:61:ARG:HH21	2.15	0.44
1:O:78:HIS:CD2	1:Q:78:HIS:ND1	2.86	0.44
1:A:11:GLN:HE21	1:D:41:TYR:HB2	1.83	0.44
1:F:61:ARG:HE	1:H:61:ARG:HH11	1.65	0.44
1:K:87:GLN:CG	1:N:63:ASN:HD21	2.31	0.44
1:E:92:TRP:HA	1:B:92:TRP:O	2.17	0.44
1:G:15:ASP:CG	1:G:18:ARG:HD2	2.43	0.44
1:G:16:MET:HG3	1:I:16:MET:SD	2.58	0.44
1:H:15:ASP:CG	1:H:18:ARG:HD2	2.43	0.44
1:J:15:ASP:CG	1:J:18:ARG:HD2	2.43	0.44
1:E:16:MET:HG3	1:B:16:MET:SD	2.58	0.44
1:A:81:GLU:HA	1:D:81:GLU:O	2.18	0.44
1:F:15:ASP:CG	1:F:18:ARG:HD2	2.43	0.44
1:F:76:SER:OG	1:G:76:SER:HA	2.18	0.44
1:H:78:HIS:ND1	1:J:78:HIS:CD2	2.85	0.44
1:H:78:HIS:ND1	1:J:78:HIS:HD2	2.16	0.44
1:G:11:GLN:HB3	1:I:11:GLN:HG3	2.00	0.44
1:I:15:ASP:CG	1:I:18:ARG:HD2	2.43	0.44
1:O:11:GLN:HG3	1:R:11:GLN:HB3	2.00	0.44
1:Q:45:ARG:O	1:T:45:ARG:HA	2.18	0.44
1:Q:48:PRO:HG2	1:T:48:PRO:HB3	2.00	0.44
1:F:61:ARG:HH21	1:H:61:ARG:HH12	1.66	0.43
1:D:15:ASP:CG	1:D:18:ARG:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:NH1	1:C:45:ARG:HB2	2.33	0.43
1:F:6:LEU:HG	1:G:6:LEU:HD22	1.99	0.43
1:F:16:MET:SD	1:H:16:MET:HG3	2.58	0.43
1:G:45:ARG:NH1	1:I:45:ARG:HB2	2.33	0.43
1:O:24:ARG:HA	1:R:24:ARG:O	2.17	0.43
1:O:40:ASN:O	1:Q:11:GLN:NE2	2.44	0.43
1:O:61:ARG:HH21	1:R:61:ARG:HH12	1.65	0.43
1:E:15:ASP:CG	1:E:18:ARG:HD2	2.43	0.43
1:A:15:ASP:CG	1:A:18:ARG:HD2	2.43	0.43
1:K:31:ALA:HA	1:N:31:ALA:O	2.18	0.43
1:E:45:ARG:CZ	1:B:45:ARG:HB2	2.49	0.43
1:F:11:GLN:HB3	1:G:11:GLN:HG3	1.99	0.43
1:O:15:ASP:CG	1:O:18:ARG:HD2	2.43	0.43
1:O:91:GLU:HA	1:R:91:GLU:O	2.19	0.43
1:E:81:GLU:O	1:B:81:GLU:HA	2.19	0.43
1:B:15:ASP:CG	1:B:18:ARG:HD2	2.43	0.43
1:C:15:ASP:CG	1:C:18:ARG:HD2	2.43	0.43
1:M:22:ASP:O	1:P:22:ASP:HA	2.18	0.43
1:M:24:ARG:HA	1:N:24:ARG:O	2.19	0.43
1:Q:15:ASP:CG	1:Q:18:ARG:HD2	2.43	0.43
1:R:15:ASP:CG	1:R:18:ARG:HD2	2.43	0.43
1:S:15:ASP:CG	1:S:18:ARG:HD2	2.43	0.43
1:F:24:ARG:O	1:G:24:ARG:HA	2.18	0.43
1:E:76:SER:OG	1:B:76:SER:HA	2.19	0.43
1:K:61:ARG:HH12	1:N:61:ARG:HH21	1.66	0.43
1:M:78:HIS:HD2	1:P:78:HIS:ND1	2.17	0.43
1:E:78:HIS:CD2	1:B:78:HIS:ND1	2.87	0.43
1:A:78:HIS:ND1	1:D:78:HIS:HD2	2.16	0.43
1:G:61:ARG:HH11	1:I:61:ARG:HE	1.65	0.43
1:H:91:GLU:HA	1:J:91:GLU:O	2.19	0.43
1:L:15:ASP:CG	1:L:18:ARG:HD2	2.43	0.43
1:K:15:ASP:CG	1:K:18:ARG:HD2	2.43	0.43
1:N:15:ASP:CG	1:N:18:ARG:HD2	2.43	0.43
1:Q:61:ARG:HH12	1:T:61:ARG:HH21	1.65	0.43
1:T:15:ASP:CG	1:T:18:ARG:HD2	2.43	0.43
1:E:11:GLN:HG3	1:A:11:GLN:HB3	2.01	0.42
1:F:81:GLU:O	1:G:81:GLU:HA	2.18	0.42
1:F:92:TRP:O	1:H:92:TRP:HA	2.19	0.42
1:K:16:MET:HG3	1:N:16:MET:SD	2.59	0.42
1:M:15:ASP:CG	1:M:18:ARG:HD2	2.43	0.42
1:P:15:ASP:CG	1:P:18:ARG:HD2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ALA:HA	1:C:31:ALA:O	2.18	0.42
1:K:55:LYS:O	1:N:55:LYS:HA	2.19	0.42
1:E:61:ARG:HH21	1:A:61:ARG:HH12	1.67	0.42
1:M:45:ARG:NH2	1:P:45:ARG:HD2	2.34	0.42
1:Q:91:GLU:O	1:T:91:GLU:HA	2.20	0.42
1:G:31:ALA:HA	1:I:31:ALA:O	2.19	0.42
1:O:16:MET:HG3	1:Q:16:MET:SD	2.59	0.42
1:G:78:HIS:HD2	1:I:78:HIS:ND1	2.17	0.42
1:K:11:GLN:NE2	1:L:40:ASN:O	2.43	0.42
1:M:61:ARG:HH11	1:P:61:ARG:HE	1.66	0.42
1:H:7:GLY:HA3	1:J:7:GLY:O	2.20	0.42
1:H:81:GLU:HA	1:J:81:GLU:O	2.19	0.42
1:N:14:TRP:HD1	1:N:16:MET:HG2	1.85	0.42
1:P:14:TRP:HD1	1:P:16:MET:HG2	1.85	0.42
1:F:12:GLY:H	1:G:5:PHE:HE2	1.68	0.42
1:K:14:TRP:HD1	1:K:16:MET:HG2	1.85	0.42
1:M:14:TRP:HD1	1:M:16:MET:HG2	1.85	0.42
1:O:62:GLU:OE2	1:Q:1:GLU:N	2.50	0.42
1:E:61:ARG:HH11	1:B:61:ARG:HE	1.67	0.42
1:L:14:TRP:HD1	1:L:16:MET:HG2	1.85	0.42
1:G:55:LYS:O	1:I:55:LYS:HA	2.20	0.42
1:K:78:HIS:HD2	1:N:78:HIS:ND1	2.18	0.42
1:M:11:GLN:HE21	1:N:41:TYR:HB2	1.84	0.42
1:C:14:TRP:HD1	1:C:16:MET:HG2	1.85	0.42
1:E:29:ILE:HD13	1:B:29:ILE:HG13	2.02	0.41
1:E:61:ARG:HE	1:A:61:ARG:HH11	1.65	0.41
1:A:14:TRP:HD1	1:A:16:MET:HG2	1.85	0.41
1:B:14:TRP:HD1	1:B:16:MET:HG2	1.85	0.41
1:D:14:TRP:HD1	1:D:16:MET:HG2	1.85	0.41
1:G:78:HIS:CD2	1:I:78:HIS:ND1	2.88	0.41
1:E:14:TRP:HD1	1:E:16:MET:HG2	1.85	0.41
1:M:78:HIS:CD2	1:P:78:HIS:ND1	2.88	0.41
1:O:63:ASN:HD21	1:R:87:GLN:CB	2.33	0.41
1:E:24:ARG:HE	1:A:24:ARG:NH1	2.18	0.41
1:B:81:GLU:O	1:C:81:GLU:HA	2.20	0.41
1:Q:16:MET:HG3	1:T:16:MET:SD	2.60	0.41
1:Q:55:LYS:O	1:T:55:LYS:HA	2.20	0.41
1:E:6:LEU:HG	1:B:6:LEU:HD22	2.02	0.41
1:A:91:GLU:HA	1:D:91:GLU:O	2.20	0.41
1:M:11:GLN:NE2	1:N:40:ASN:O	2.46	0.41
1:O:63:ASN:HD21	1:R:87:GLN:CG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:GLN:HB3	1:B:11:GLN:HG3	2.02	0.41
1:E:92:TRP:O	1:A:92:TRP:HA	2.21	0.41
1:H:31:ALA:O	1:J:31:ALA:HA	2.21	0.41
1:M:1:GLU:N	1:N:62:GLU:OE2	2.53	0.41
1:E:70:PHE:HB2	1:A:70:PHE:CD1	2.56	0.41
1:B:85:ALA:HB1	1:B:87:GLN:HE21	1.85	0.41
1:C:85:ALA:HB1	1:C:87:GLN:HE21	1.85	0.41
1:F:61:ARG:HH11	1:G:61:ARG:HE	1.66	0.41
1:H:16:MET:SD	1:J:16:MET:HG3	2.61	0.41
1:M:11:GLN:HG3	1:N:11:GLN:HB3	2.03	0.41
1:M:16:MET:HG3	1:P:16:MET:SD	2.60	0.41
1:O:1:GLU:HG3	1:Q:1:GLU:HA	2.02	0.41
1:E:7:GLY:HA3	1:A:7:GLY:O	2.21	0.41
1:E:85:ALA:HB1	1:E:87:GLN:HE21	1.85	0.41
1:H:1:GLU:N	1:J:62:GLU:OE2	2.52	0.41
1:O:85:ALA:HB1	1:O:87:GLN:HE21	1.85	0.41
1:P:85:ALA:HB1	1:P:87:GLN:HE21	1.85	0.41
1:E:24:ARG:HB3	1:A:24:ARG:NH1	2.33	0.41
1:E:29:ILE:HG13	1:A:29:ILE:HD13	2.02	0.41
1:A:85:ALA:HB1	1:A:87:GLN:HE21	1.85	0.41
1:D:85:ALA:HB1	1:D:87:GLN:HE21	1.85	0.41
1:F:84:LYS:HD2	1:H:84:LYS:HG2	2.03	0.41
1:F:85:ALA:HB1	1:F:87:GLN:HE21	1.85	0.41
1:G:85:ALA:HB1	1:G:87:GLN:HE21	1.85	0.41
1:H:85:ALA:HB1	1:H:87:GLN:HE21	1.85	0.41
1:M:11:GLN:HB3	1:P:11:GLN:HG3	2.02	0.41
1:M:85:ALA:HB1	1:M:87:GLN:HE21	1.85	0.41
1:O:87:GLN:CG	1:Q:63:ASN:HD21	2.34	0.41
1:Q:85:ALA:HB1	1:Q:87:GLN:HE21	1.85	0.41
1:R:45:ARG:HD2	1:S:45:ARG:NH2	2.36	0.41
1:R:85:ALA:HB1	1:R:87:GLN:HE21	1.85	0.41
1:S:85:ALA:HB1	1:S:87:GLN:HE21	1.85	0.41
1:T:85:ALA:HB1	1:T:87:GLN:HE21	1.85	0.41
1:E:61:ARG:NH2	1:A:91:GLU:OE1	2.54	0.41
1:B:55:LYS:O	1:C:55:LYS:HA	2.21	0.41
1:F:45:ARG:NH1	1:G:45:ARG:HB2	2.36	0.41
1:I:85:ALA:HB1	1:I:87:GLN:HE21	1.85	0.41
1:J:85:ALA:HB1	1:J:87:GLN:HE21	1.85	0.41
1:O:61:ARG:O	1:Q:61:ARG:HA	2.21	0.41
1:F:14:TRP:HD1	1:F:16:MET:HG2	1.85	0.40
1:G:14:TRP:HD1	1:G:16:MET:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:TRP:HD1	1:I:16:MET:HG2	1.85	0.40
1:M:16:MET:SD	1:N:16:MET:HG3	2.61	0.40
1:N:85:ALA:HB1	1:N:87:GLN:HE21	1.85	0.40
1:O:91:GLU:O	1:Q:91:GLU:HA	2.21	0.40
1:E:41:TYR:HB2	1:B:11:GLN:NE2	2.37	0.40
1:F:61:ARG:NH2	1:H:91:GLU:OE1	2.53	0.40
1:G:6:LEU:HG	1:I:6:LEU:HD22	2.02	0.40
1:H:14:TRP:HD1	1:H:16:MET:HG2	1.85	0.40
1:H:91:GLU:OE2	1:H:94:ARG:HD2	2.22	0.40
1:K:85:ALA:HB1	1:K:87:GLN:HE21	1.85	0.40
1:E:84:LYS:HG2	1:B:84:LYS:HD2	2.03	0.40
1:E:91:GLU:OE2	1:E:94:ARG:HD2	2.22	0.40
1:B:91:GLU:OE2	1:B:94:ARG:HD2	2.22	0.40
1:C:91:GLU:OE2	1:C:94:ARG:HD2	2.22	0.40
1:F:91:GLU:OE2	1:F:94:ARG:HD2	2.22	0.40
1:G:91:GLU:OE2	1:G:94:ARG:HD2	2.22	0.40
1:I:91:GLU:OE2	1:I:94:ARG:HD2	2.22	0.40
1:J:14:TRP:HD1	1:J:16:MET:HG2	1.85	0.40
1:J:91:GLU:OE2	1:J:94:ARG:HD2	2.22	0.40
1:L:85:ALA:HB1	1:L:87:GLN:HE21	1.85	0.40
1:E:12:GLY:H	1:B:5:PHE:HE2	1.68	0.40
1:E:37:ALA:HA	1:A:37:ALA:O	2.21	0.40
1:A:91:GLU:OE2	1:A:94:ARG:HD2	2.22	0.40
1:D:91:GLU:OE2	1:D:94:ARG:HD2	2.22	0.40
1:Q:91:GLU:OE2	1:Q:94:ARG:HD2	2.22	0.40
1:T:91:GLU:OE2	1:T:94:ARG:HD2	2.22	0.40
1:E:31:ALA:O	1:A:31:ALA:HA	2.21	0.40
1:E:94:ARG:HB2	1:B:94:ARG:HA	2.04	0.40
1:A:16:MET:SD	1:D:16:MET:HG3	2.62	0.40
1:F:15:ASP:OD2	1:F:18:ARG:HD2	2.22	0.40
1:G:15:ASP:OD2	1:G:18:ARG:HD2	2.22	0.40
1:H:15:ASP:OD2	1:H:18:ARG:HD2	2.22	0.40
1:K:15:ASP:OD2	1:K:18:ARG:HD2	2.22	0.40
1:M:15:ASP:OD2	1:M:18:ARG:HD2	2.22	0.40
1:M:29:ILE:HG13	1:N:29:ILE:HD13	2.04	0.40
1:M:91:GLU:OE2	1:M:94:ARG:HD2	2.22	0.40
1:N:15:ASP:OD2	1:N:18:ARG:HD2	2.22	0.40
1:O:61:ARG:NH1	1:Q:61:ARG:HH21	2.20	0.40
1:O:91:GLU:OE2	1:O:94:ARG:HD2	2.22	0.40
1:P:15:ASP:OD2	1:P:18:ARG:HD2	2.22	0.40
1:T:14:TRP:HD1	1:T:16:MET:HG2	1.85	0.40

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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	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	B	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	C	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	D	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	E	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	F	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	G	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	H	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	I	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	J	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	K	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	L	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	M	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	N	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	O	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	P	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	Q	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	R	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	S	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	T	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
All	All	1840/2220 (83%)	1820 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

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5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	67/82 (82%)	67 (100%)	0	100	100
1	B	67/82 (82%)	67 (100%)	0	100	100
1	C	67/82 (82%)	67 (100%)	0	100	100
1	D	67/82 (82%)	67 (100%)	0	100	100
1	E	67/82 (82%)	67 (100%)	0	100	100
1	F	67/82 (82%)	67 (100%)	0	100	100
1	G	67/82 (82%)	67 (100%)	0	100	100
1	H	67/82 (82%)	67 (100%)	0	100	100
1	I	67/82 (82%)	67 (100%)	0	100	100
1	J	67/82 (82%)	67 (100%)	0	100	100
1	K	67/82 (82%)	67 (100%)	0	100	100
1	L	67/82 (82%)	67 (100%)	0	100	100
1	M	67/82 (82%)	67 (100%)	0	100	100
1	N	67/82 (82%)	67 (100%)	0	100	100
1	O	67/82 (82%)	67 (100%)	0	100	100
1	P	67/82 (82%)	67 (100%)	0	100	100
1	Q	67/82 (82%)	67 (100%)	0	100	100
1	R	67/82 (82%)	67 (100%)	0	100	100
1	S	67/82 (82%)	67 (100%)	0	100	100
1	T	67/82 (82%)	67 (100%)	0	100	100
All	All	1340/1640 (82%)	1340 (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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	36	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	A	36	HIS
1	B	36	HIS
1	D	36	HIS
1	D	78	HIS
1	F	36	HIS
1	H	36	HIS
1	J	11	GLN
1	J	36	HIS
1	J	78	HIS
1	K	36	HIS
1	K	78	HIS
1	L	36	HIS
1	L	78	HIS
1	M	90	ASN
1	N	36	HIS
1	N	63	ASN
1	O	36	HIS
1	O	63	ASN
1	P	63	ASN
1	Q	36	HIS
1	Q	63	ASN
1	R	36	HIS
1	R	78	HIS
1	S	36	HIS
1	S	78	HIS
1	T	63	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

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5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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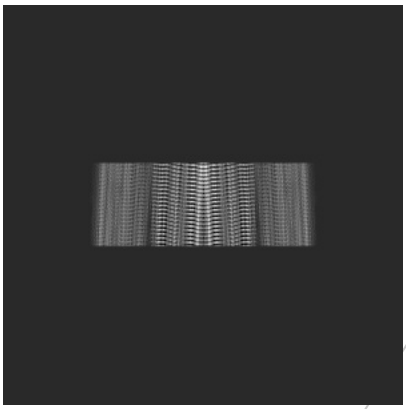
6 Map visualisation

This section contains visualisations of the EMDB entry D_1292160338. These allow visual inspection of the internal detail of the map and identification of artifacts.

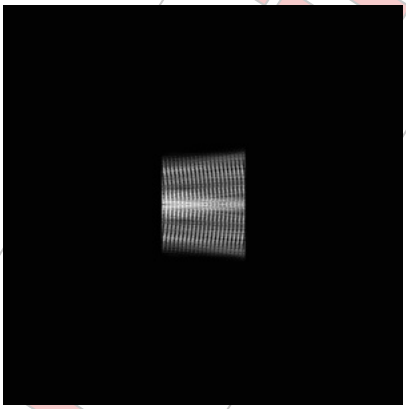
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

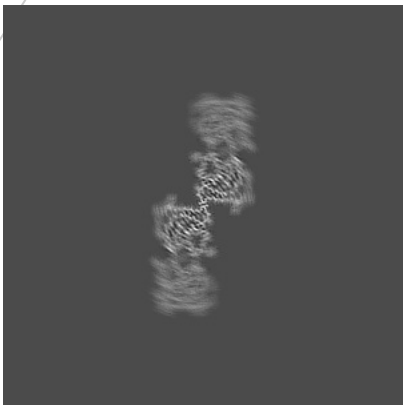
6.1.1 Primary map



X

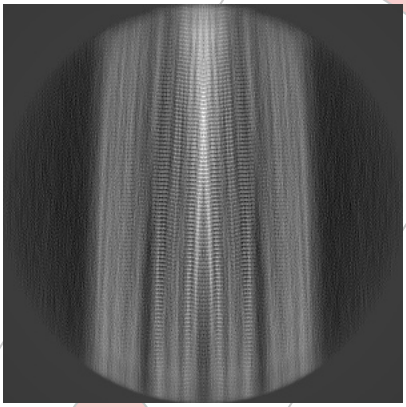


Y

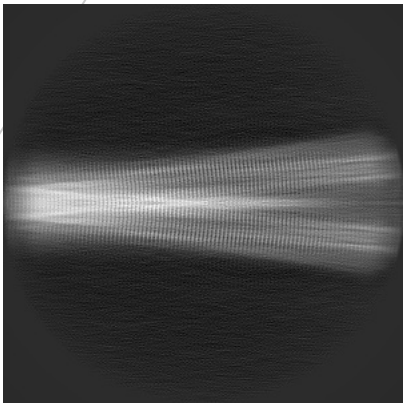


Z

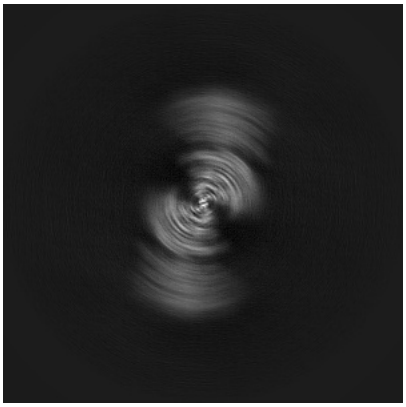
6.1.2 Raw map



X



Y



Z

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

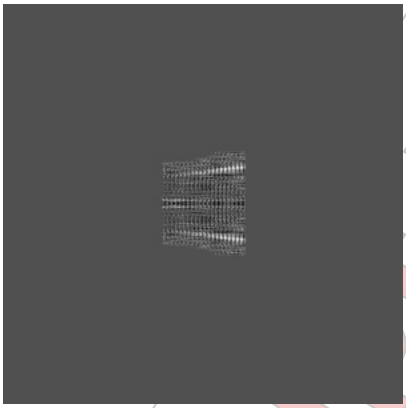
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6.2 Central slices (i)

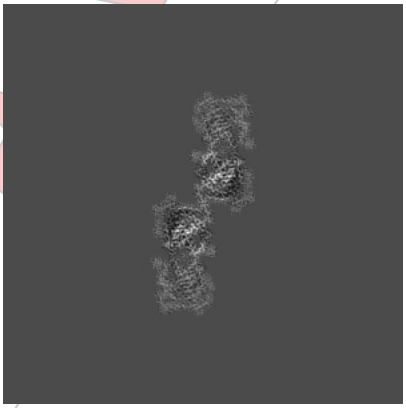
6.2.1 Primary map



X Index: 200

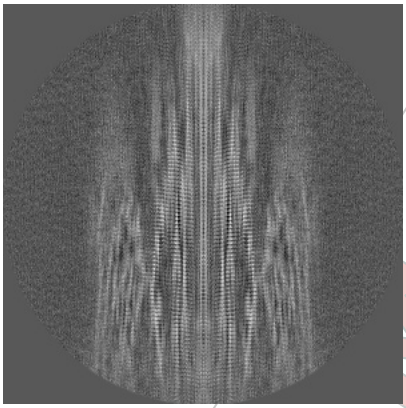


Y Index: 200

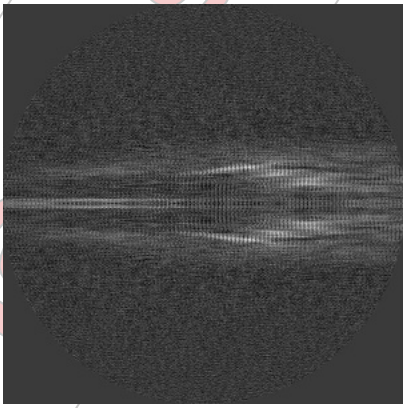


Z Index: 200

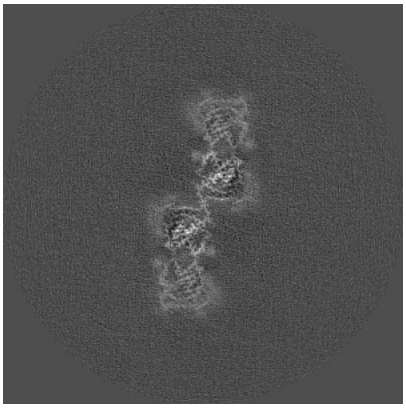
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

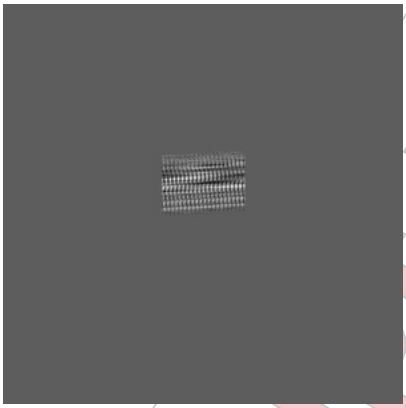
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6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 199

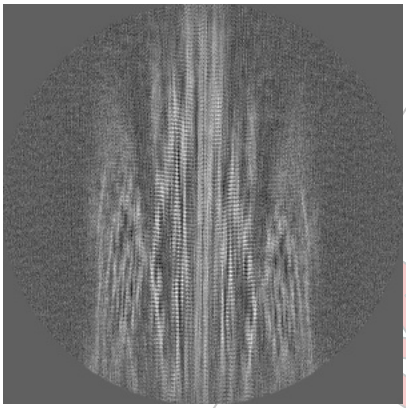


Y Index: 228

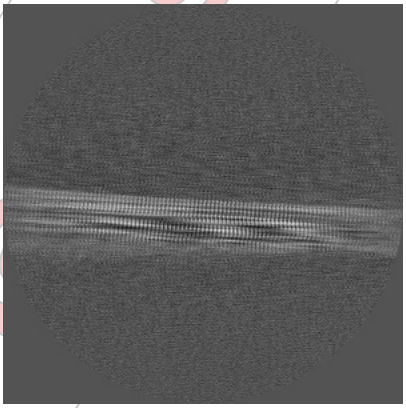


Z Index: 199

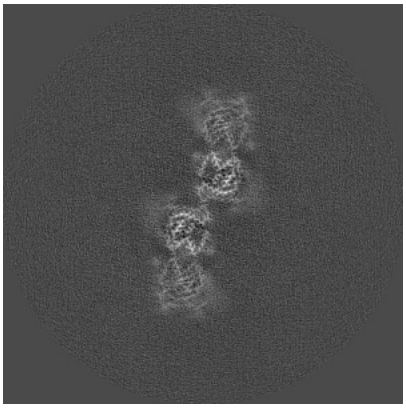
6.3.2 Raw map



X Index: 198



Y Index: 174



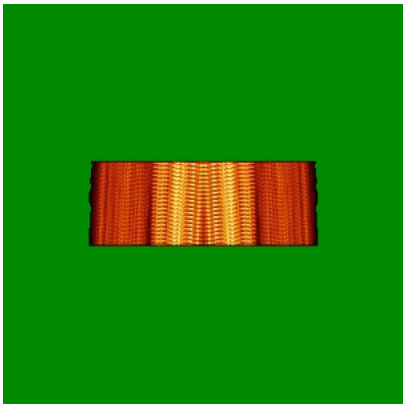
Z Index: 203

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

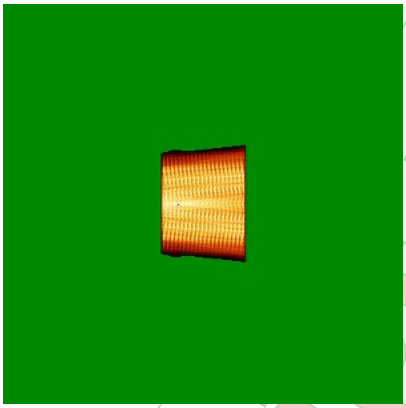
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6.4 Orthogonal standard-deviation projections (False-color)

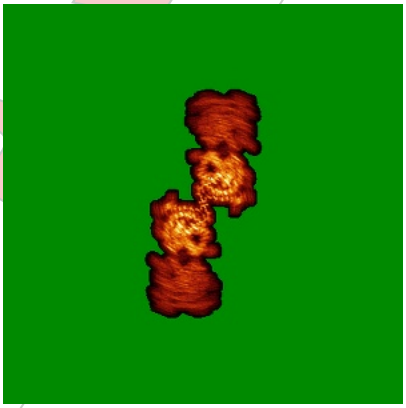
6.4.1 Primary map



X

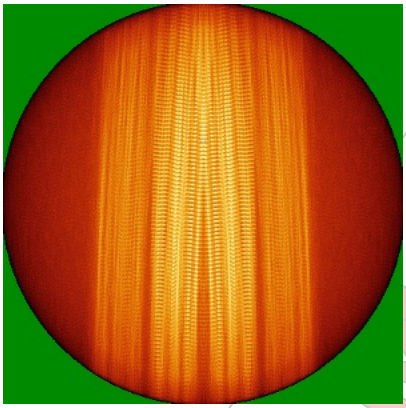


Y

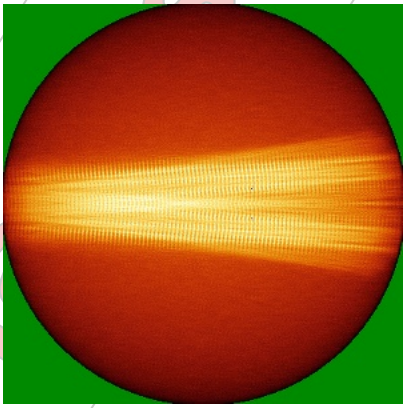


Z

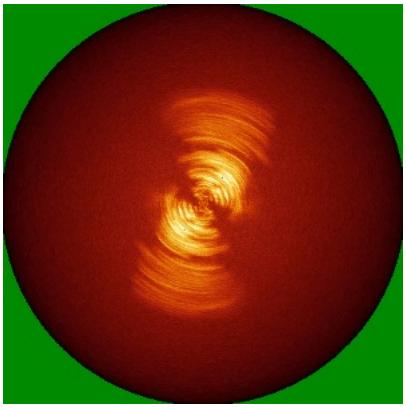
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

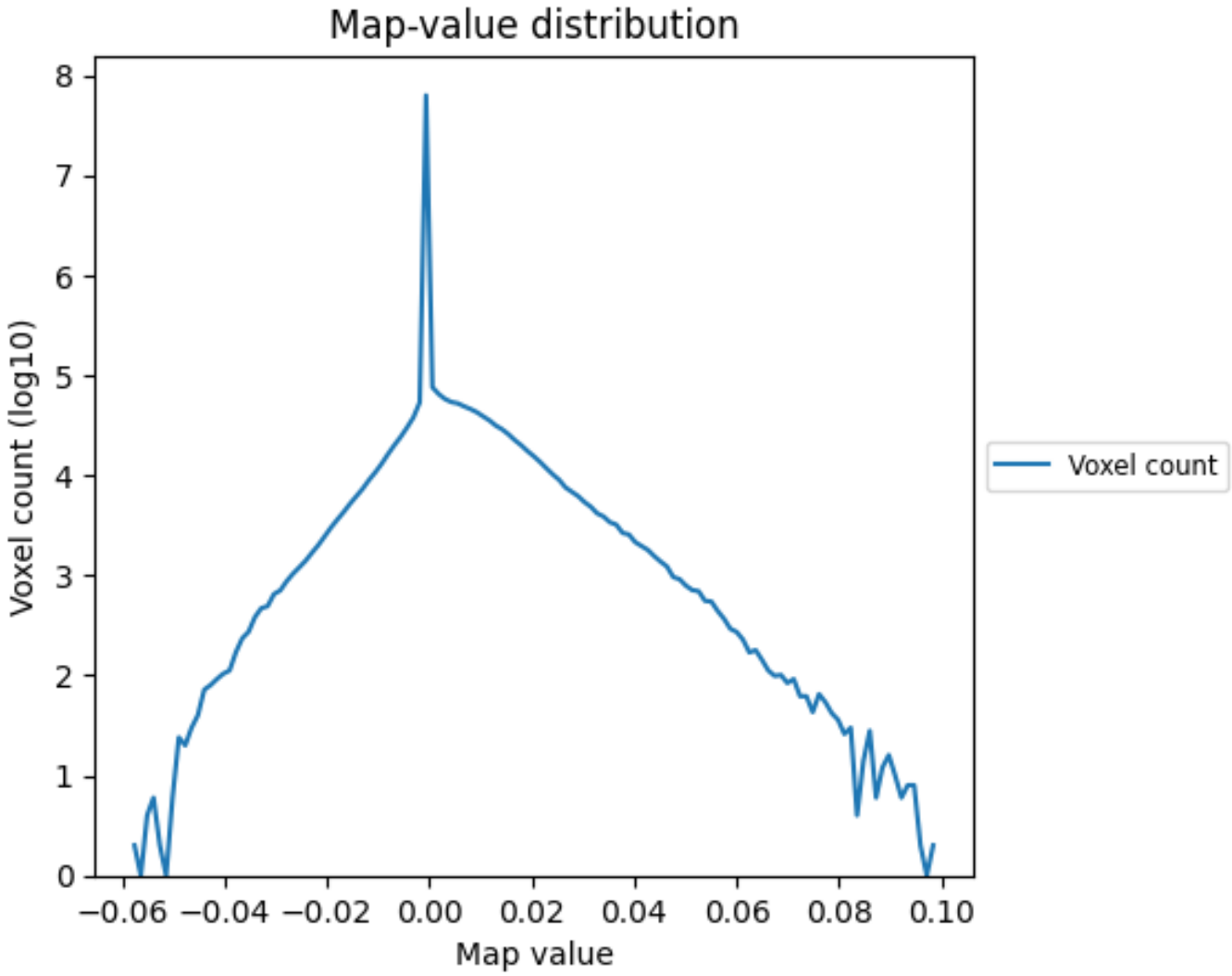
This section was not generated. No masks/segmentation were deposited.

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7 Map analysis

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

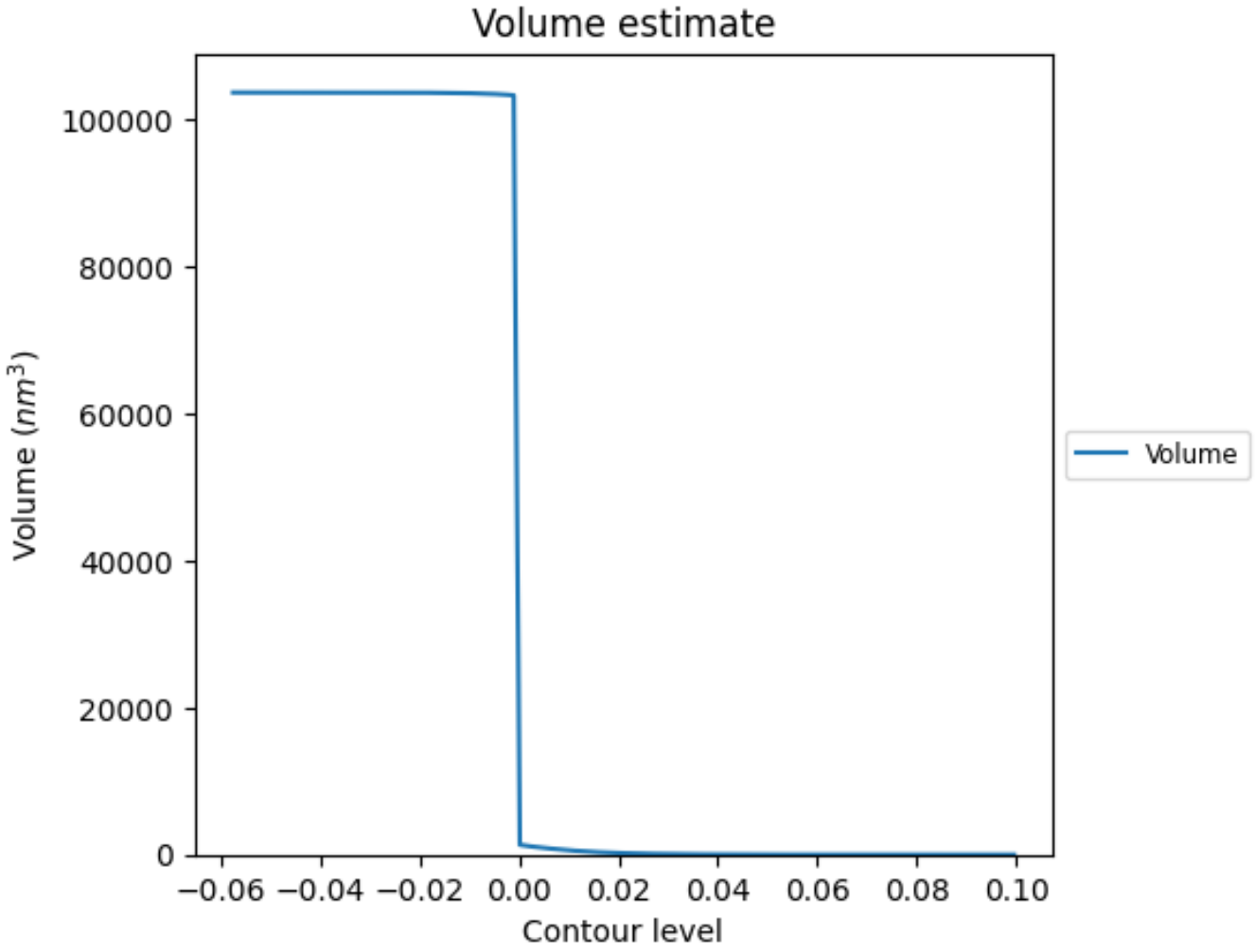
7.1 Map-value distribution



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.

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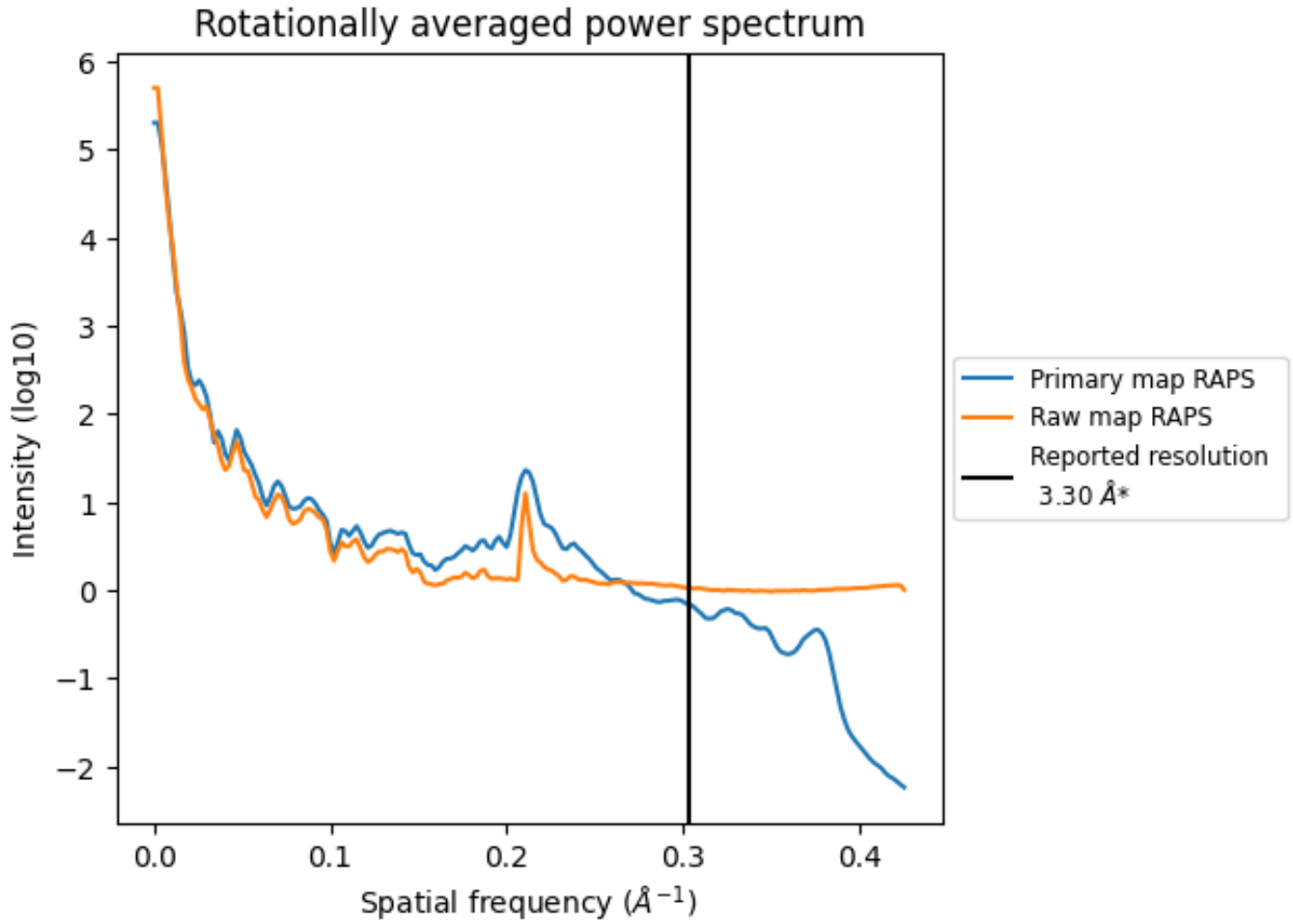
7.2 Volume estimate (i)



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.

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7.3 Rotationally averaged power spectrum (i)



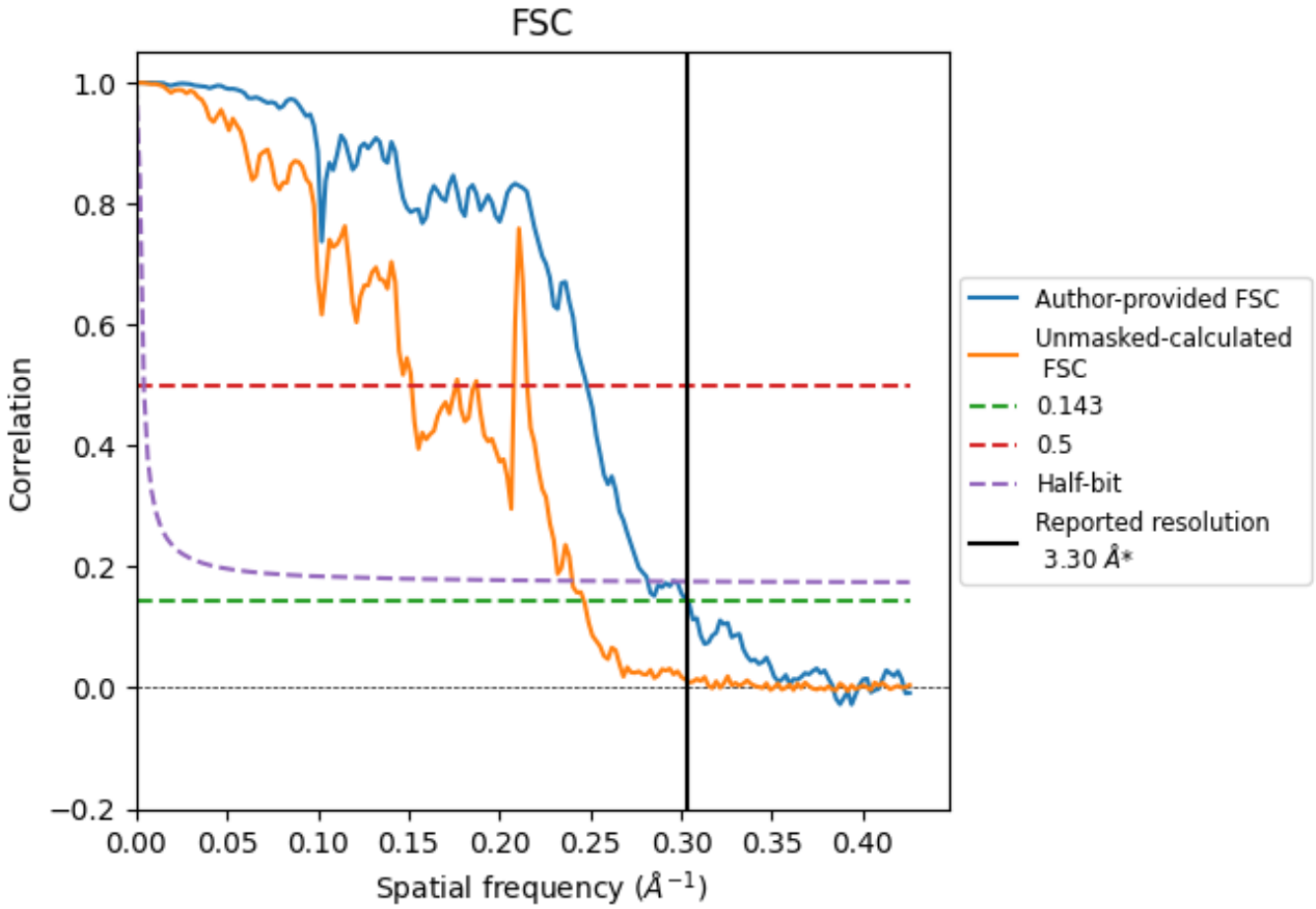
*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.30	4.03	3.55
Unmasked-calculated*	4.06	6.60	4.16

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

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9 Map-model fit

This section was not generated.

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