



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 03:34 pm GMT

PDB ID : 7AOY  
EMDB ID : EMD-11847  
Title : Helical arrangement of Bunyamwera virus nucleocapsid protein within a native ribonucleoprotein  
Authors : Hopkins, F.R.; Fontana, J.; Barr, J.N.  
Deposited on : 2020-10-15  
Resolution : 13.00 Å(reported)  
Based on initial model : 3ZLA

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

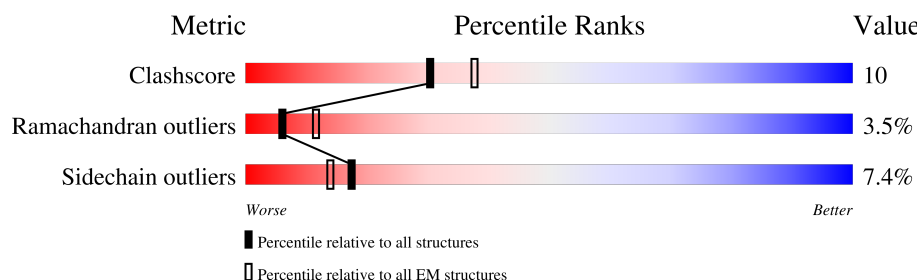
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	233	
1	B	233	
1	C	233	
1	D	233	
1	E	233	
1	F	233	
1	G	233	
1	H	233	

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Mol	Chain	Length	Quality of chain
1	I	233	<div><div></div><div>6%</div><div>61%</div><div>28%</div><div>8%</div><div>••</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16587 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.

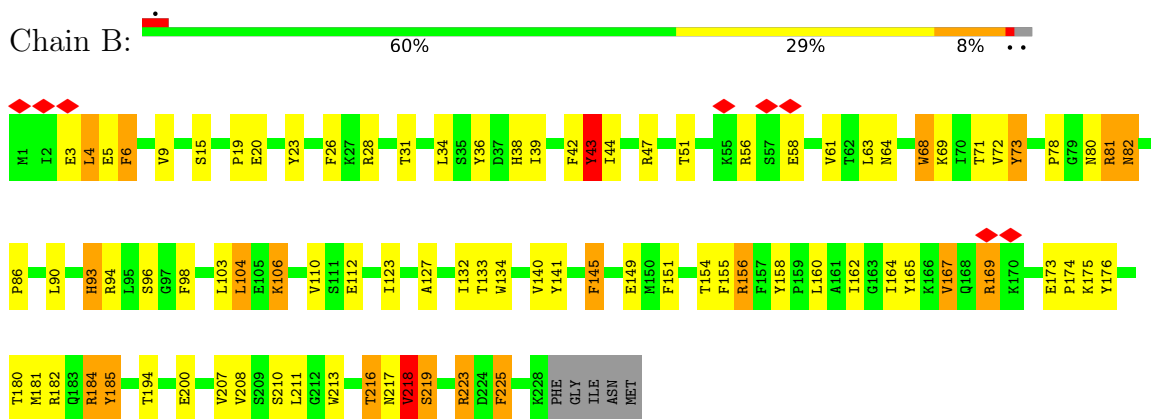
- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	A	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	C	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	D	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	E	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	F	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	G	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	H	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	I	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		

### 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.

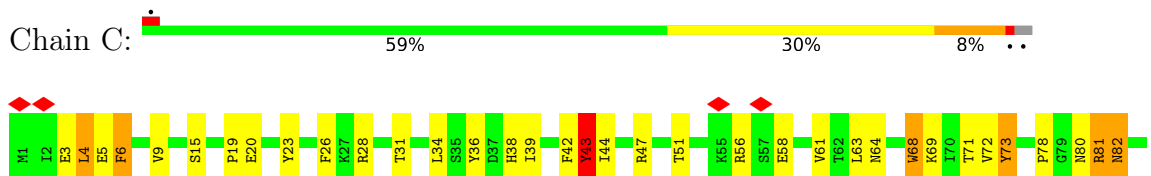
#### • Molecule 1: Nucleoprotein

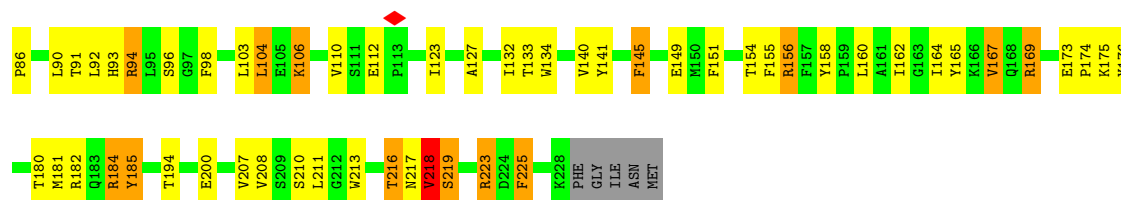


#### • Molecule 1: Nucleoprotein

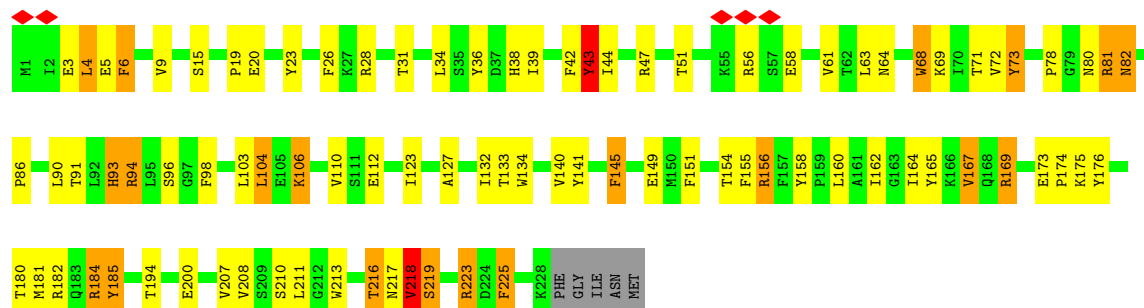


#### • Molecule 1: Nucleoprotein

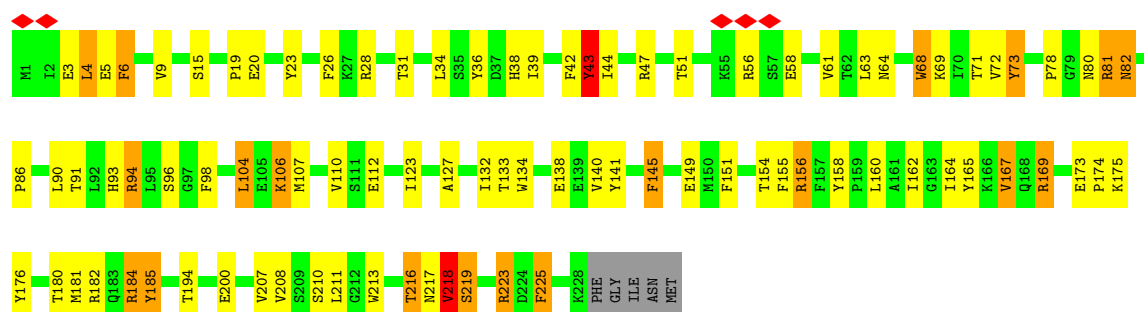




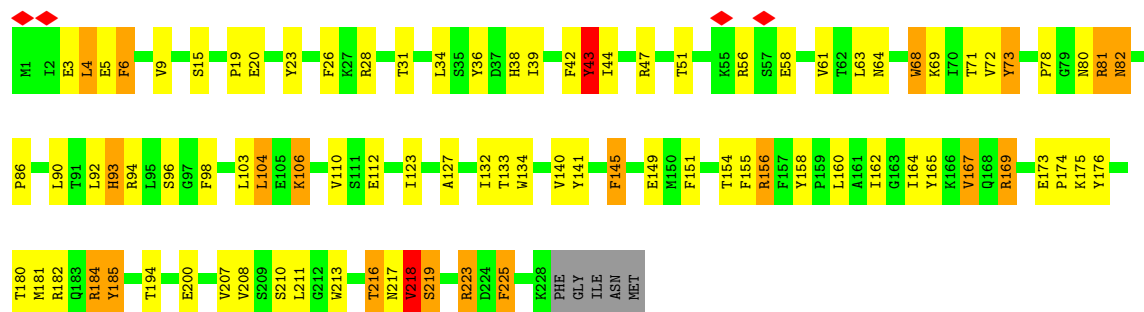
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

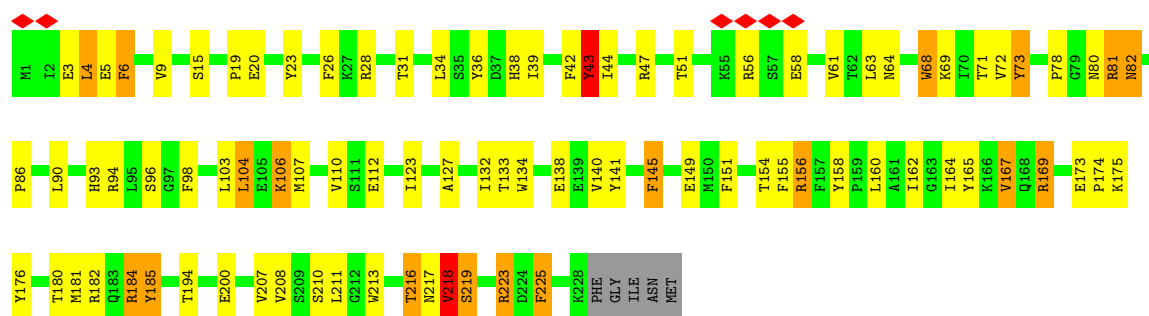


• Molecule 1: Nucleoprotein



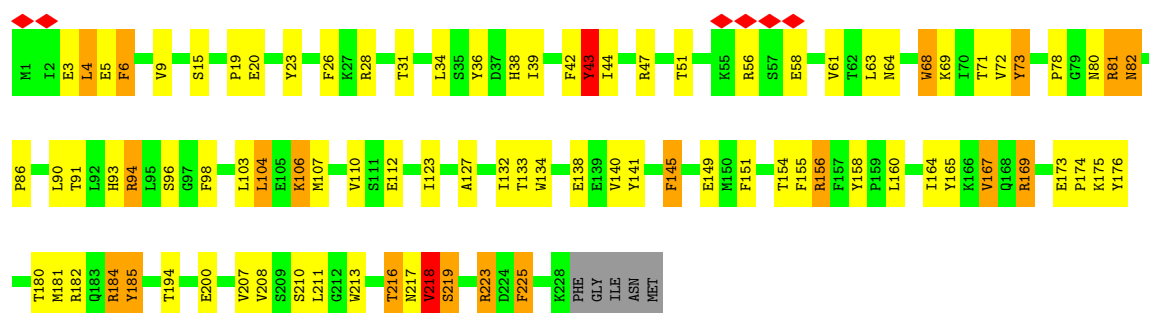
• Molecule 1: Nucleoprotein

Chain G:  59% 30% 8% ..



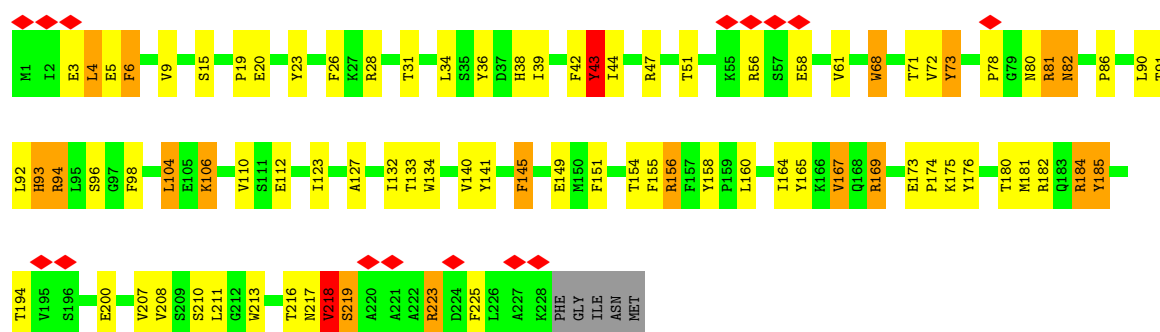
• Molecule 1: Nucleoprotein

Chain H:  59% 30% 8% ..



• Molecule 1: Nucleoprotein

Chain I:  61% 28% 8% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5077	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 ( $e^-/\text{\AA}^2$ )	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.28, 4.28, 4.28	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	1.74	17/1887 (0.9%)	1.96	53/2551 (2.1%)
1	B	1.74	17/1887 (0.9%)	1.96	53/2551 (2.1%)
1	C	1.74	17/1887 (0.9%)	1.96	52/2551 (2.0%)
1	D	1.74	17/1887 (0.9%)	1.96	53/2551 (2.1%)
1	E	1.74	17/1887 (0.9%)	1.96	53/2551 (2.1%)
1	F	1.74	17/1887 (0.9%)	1.96	53/2551 (2.1%)
1	G	1.74	17/1887 (0.9%)	1.96	52/2551 (2.0%)
1	H	1.74	17/1887 (0.9%)	1.96	53/2551 (2.1%)
1	I	1.74	17/1887 (0.9%)	1.96	54/2551 (2.1%)
All	All	1.74	153/16983 (0.9%)	1.96	476/22959 (2.1%)

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	7
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	7
1	F	0	7
1	G	0	7
1	H	0	7
1	I	0	7
All	All	0	63

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	156	ARG	CZ-NH1	7.35	1.42	1.33
1	B	156	ARG	CZ-NH1	7.30	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	ARG	CZ-NH1	7.30	1.42	1.33
1	F	156	ARG	CZ-NH1	7.30	1.42	1.33
1	H	156	ARG	CZ-NH1	7.29	1.42	1.33
1	D	156	ARG	CZ-NH1	7.27	1.42	1.33
1	C	156	ARG	CZ-NH1	7.27	1.42	1.33
1	E	156	ARG	CZ-NH1	7.26	1.42	1.33
1	I	156	ARG	CZ-NH1	7.24	1.42	1.33
1	E	169	ARG	CZ-NH1	6.50	1.41	1.33
1	C	169	ARG	CZ-NH1	6.49	1.41	1.33
1	D	169	ARG	CZ-NH1	6.49	1.41	1.33
1	G	169	ARG	CZ-NH1	6.49	1.41	1.33
1	B	169	ARG	CZ-NH1	6.49	1.41	1.33
1	F	169	ARG	CZ-NH1	6.49	1.41	1.33
1	I	169	ARG	CZ-NH1	6.49	1.41	1.33
1	H	169	ARG	CZ-NH1	6.49	1.41	1.33
1	A	169	ARG	CZ-NH1	6.48	1.41	1.33
1	A	165	TYR	CB-CG	6.39	1.61	1.51
1	F	165	TYR	CB-CG	6.37	1.61	1.51
1	G	165	TYR	CB-CG	6.36	1.61	1.51
1	D	165	TYR	CB-CG	6.35	1.61	1.51
1	E	165	TYR	CB-CG	6.35	1.61	1.51
1	B	165	TYR	CB-CG	6.35	1.61	1.51
1	H	165	TYR	CB-CG	6.35	1.61	1.51
1	C	165	TYR	CB-CG	6.33	1.61	1.51
1	I	165	TYR	CB-CG	6.33	1.61	1.51
1	C	20	GLU	CB-CG	5.98	1.63	1.52
1	F	20	GLU	CB-CG	5.97	1.63	1.52
1	H	20	GLU	CB-CG	5.97	1.63	1.52
1	D	20	GLU	CB-CG	5.96	1.63	1.52
1	B	20	GLU	CB-CG	5.96	1.63	1.52
1	E	20	GLU	CB-CG	5.95	1.63	1.52
1	I	20	GLU	CB-CG	5.95	1.63	1.52
1	H	223	ARG	CZ-NH2	5.94	1.40	1.33
1	A	20	GLU	CB-CG	5.94	1.63	1.52
1	G	20	GLU	CB-CG	5.94	1.63	1.52
1	C	223	ARG	CZ-NH2	5.91	1.40	1.33
1	A	223	ARG	CZ-NH2	5.90	1.40	1.33
1	F	223	ARG	CZ-NH2	5.89	1.40	1.33
1	E	223	ARG	CZ-NH2	5.89	1.40	1.33
1	B	223	ARG	CZ-NH2	5.88	1.40	1.33
1	D	223	ARG	CZ-NH2	5.87	1.40	1.33
1	I	223	ARG	CZ-NH2	5.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	223	ARG	CZ-NH2	5.84	1.40	1.33
1	D	173	GLU	CG-CD	5.83	1.60	1.51
1	G	173	GLU	CG-CD	5.81	1.60	1.51
1	B	173	GLU	CG-CD	5.80	1.60	1.51
1	E	173	GLU	CG-CD	5.80	1.60	1.51
1	H	173	GLU	CG-CD	5.80	1.60	1.51
1	F	173	GLU	CG-CD	5.79	1.60	1.51
1	C	173	GLU	CG-CD	5.79	1.60	1.51
1	I	173	GLU	CG-CD	5.79	1.60	1.51
1	A	173	GLU	CG-CD	5.78	1.60	1.51
1	F	15	SER	CA-CB	5.73	1.61	1.52
1	G	15	SER	CA-CB	5.73	1.61	1.52
1	H	15	SER	CA-CB	5.72	1.61	1.52
1	D	15	SER	CA-CB	5.72	1.61	1.52
1	E	15	SER	CA-CB	5.72	1.61	1.52
1	A	15	SER	CA-CB	5.71	1.61	1.52
1	B	15	SER	CA-CB	5.71	1.61	1.52
1	I	15	SER	CA-CB	5.69	1.61	1.52
1	C	15	SER	CA-CB	5.69	1.61	1.52
1	G	182	ARG	CZ-NH2	5.68	1.40	1.33
1	H	182	ARG	CZ-NH2	5.67	1.40	1.33
1	I	182	ARG	CZ-NH2	5.67	1.40	1.33
1	E	182	ARG	CZ-NH2	5.67	1.40	1.33
1	A	217	ASN	CA-CB	5.66	1.67	1.53
1	H	184	ARG	CZ-NH1	5.65	1.40	1.33
1	A	182	ARG	CZ-NH2	5.65	1.40	1.33
1	B	182	ARG	CZ-NH2	5.64	1.40	1.33
1	D	217	ASN	CA-CB	5.64	1.67	1.53
1	G	217	ASN	CA-CB	5.64	1.67	1.53
1	F	217	ASN	CA-CB	5.64	1.67	1.53
1	B	217	ASN	CA-CB	5.64	1.67	1.53
1	I	217	ASN	CA-CB	5.63	1.67	1.53
1	C	217	ASN	CA-CB	5.63	1.67	1.53
1	F	182	ARG	CZ-NH2	5.63	1.40	1.33
1	C	36	TYR	CZ-OH	5.63	1.47	1.37
1	D	182	ARG	CZ-NH2	5.63	1.40	1.33
1	E	217	ASN	CA-CB	5.62	1.67	1.53
1	B	184	ARG	CZ-NH1	5.62	1.40	1.33
1	A	184	ARG	CZ-NH1	5.62	1.40	1.33
1	G	36	TYR	CZ-OH	5.62	1.47	1.37
1	H	217	ASN	CA-CB	5.62	1.67	1.53
1	C	182	ARG	CZ-NH2	5.62	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	184	ARG	CZ-NH1	5.62	1.40	1.33
1	F	36	TYR	CZ-OH	5.62	1.47	1.37
1	I	36	TYR	CZ-OH	5.62	1.47	1.37
1	I	184	ARG	CZ-NH1	5.61	1.40	1.33
1	B	36	TYR	CZ-OH	5.60	1.47	1.37
1	D	184	ARG	CZ-NH1	5.60	1.40	1.33
1	F	184	ARG	CZ-NH1	5.60	1.40	1.33
1	D	26	PHE	CG-CD1	5.60	1.47	1.38
1	I	26	PHE	CG-CD1	5.60	1.47	1.38
1	A	36	TYR	CZ-OH	5.59	1.47	1.37
1	G	184	ARG	CZ-NH1	5.59	1.40	1.33
1	H	36	TYR	CZ-OH	5.59	1.47	1.37
1	C	184	ARG	CZ-NH1	5.58	1.40	1.33
1	G	26	PHE	CG-CD1	5.58	1.47	1.38
1	E	26	PHE	CG-CD1	5.58	1.47	1.38
1	B	26	PHE	CG-CD1	5.56	1.47	1.38
1	D	36	TYR	CZ-OH	5.56	1.47	1.37
1	E	36	TYR	CZ-OH	5.56	1.47	1.37
1	H	26	PHE	CG-CD1	5.55	1.47	1.38
1	C	26	PHE	CG-CD1	5.54	1.47	1.38
1	A	26	PHE	CG-CD1	5.54	1.47	1.38
1	F	26	PHE	CG-CD1	5.53	1.47	1.38
1	I	165	TYR	CE2-CZ	5.40	1.45	1.38
1	E	165	TYR	CE2-CZ	5.39	1.45	1.38
1	A	165	TYR	CE2-CZ	5.38	1.45	1.38
1	C	165	TYR	CE2-CZ	5.38	1.45	1.38
1	B	165	TYR	CE2-CZ	5.36	1.45	1.38
1	G	80	ASN	CA-CB	5.36	1.67	1.53
1	G	165	TYR	CE2-CZ	5.35	1.45	1.38
1	H	165	TYR	CE2-CZ	5.35	1.45	1.38
1	F	80	ASN	CA-CB	5.34	1.67	1.53
1	C	80	ASN	CA-CB	5.34	1.67	1.53
1	I	80	ASN	CA-CB	5.34	1.67	1.53
1	B	80	ASN	CA-CB	5.34	1.67	1.53
1	E	80	ASN	CA-CB	5.34	1.67	1.53
1	A	80	ASN	CA-CB	5.33	1.67	1.53
1	F	165	TYR	CE2-CZ	5.33	1.45	1.38
1	D	80	ASN	CA-CB	5.33	1.67	1.53
1	D	165	TYR	CE2-CZ	5.33	1.45	1.38
1	H	80	ASN	CA-CB	5.31	1.67	1.53
1	D	200	GLU	CB-CG	5.23	1.62	1.52
1	A	200	GLU	CB-CG	5.22	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	200	GLU	CB-CG	5.21	1.62	1.52
1	H	200	GLU	CB-CG	5.20	1.62	1.52
1	C	200	GLU	CB-CG	5.20	1.62	1.52
1	I	200	GLU	CB-CG	5.20	1.62	1.52
1	E	200	GLU	CB-CG	5.20	1.62	1.52
1	F	112	GLU	CD-OE1	5.20	1.31	1.25
1	B	200	GLU	CB-CG	5.19	1.62	1.52
1	E	112	GLU	CD-OE1	5.18	1.31	1.25
1	C	112	GLU	CD-OE1	5.18	1.31	1.25
1	G	200	GLU	CB-CG	5.17	1.61	1.52
1	B	112	GLU	CD-OE1	5.14	1.31	1.25
1	D	112	GLU	CD-OE1	5.13	1.31	1.25
1	A	112	GLU	CD-OE1	5.12	1.31	1.25
1	I	112	GLU	CD-OE1	5.12	1.31	1.25
1	H	112	GLU	CD-OE1	5.12	1.31	1.25
1	G	112	GLU	CD-OE1	5.12	1.31	1.25
1	D	96	SER	CA-CB	5.05	1.60	1.52
1	C	96	SER	CA-CB	5.05	1.60	1.52
1	A	96	SER	CA-CB	5.04	1.60	1.52
1	B	96	SER	CA-CB	5.03	1.60	1.52
1	H	96	SER	CA-CB	5.02	1.60	1.52
1	F	96	SER	CA-CB	5.02	1.60	1.52
1	E	96	SER	CA-CB	5.01	1.60	1.52
1	I	96	SER	CA-CB	5.01	1.60	1.52
1	G	96	SER	CA-CB	5.01	1.60	1.52

All (476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	184	ARG	NE-CZ-NH2	12.71	126.65	120.30
1	A	184	ARG	NE-CZ-NH2	12.66	126.63	120.30
1	E	184	ARG	NE-CZ-NH2	12.65	126.63	120.30
1	C	184	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	B	184	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	H	184	ARG	NE-CZ-NH2	12.62	126.61	120.30
1	I	184	ARG	NE-CZ-NH2	12.62	126.61	120.30
1	D	184	ARG	NE-CZ-NH2	12.61	126.61	120.30
1	G	184	ARG	NE-CZ-NH2	12.56	126.58	120.30
1	H	223	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	F	223	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	A	223	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	D	223	ARG	NE-CZ-NH1	11.90	126.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	ARG	NE-CZ-NH1	11.89	126.24	120.30
1	B	223	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	E	223	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	I	223	ARG	NE-CZ-NH1	11.87	126.24	120.30
1	G	223	ARG	NE-CZ-NH1	11.85	126.22	120.30
1	G	47	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	D	47	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	H	47	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	F	47	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	47	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	I	47	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	B	47	ARG	NE-CZ-NH2	-10.33	115.14	120.30
1	C	47	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	E	47	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	28	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	G	28	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	F	28	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	H	28	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	I	28	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	28	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	C	28	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	D	28	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	E	28	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	I	182	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	G	182	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	H	182	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	E	182	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	182	ARG	NE-CZ-NH2	-9.63	115.49	120.30
1	B	182	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	D	182	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	C	182	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	F	182	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	I	182	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	A	182	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	G	182	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	H	182	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	B	182	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	E	182	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	F	182	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	C	182	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	D	182	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	C	165	TYR	CB-CG-CD2	-8.61	115.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	165	TYR	CB-CG-CD2	-8.60	115.84	121.00
1	I	165	TYR	CB-CG-CD2	-8.59	115.84	121.00
1	B	165	TYR	CB-CG-CD2	-8.57	115.86	121.00
1	D	165	TYR	CB-CG-CD2	-8.57	115.86	121.00
1	E	165	TYR	CB-CG-CD2	-8.56	115.87	121.00
1	G	4	LEU	CB-CG-CD2	8.55	125.54	111.00
1	C	4	LEU	CB-CG-CD2	8.55	125.53	111.00
1	H	4	LEU	CB-CG-CD2	8.55	125.53	111.00
1	A	4	LEU	CB-CG-CD2	8.55	125.53	111.00
1	D	4	LEU	CB-CG-CD2	8.54	125.53	111.00
1	B	4	LEU	CB-CG-CD2	8.54	125.52	111.00
1	I	4	LEU	CB-CG-CD2	8.54	125.52	111.00
1	H	165	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	G	165	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	E	4	LEU	CB-CG-CD2	8.52	125.49	111.00
1	F	4	LEU	CB-CG-CD2	8.52	125.49	111.00
1	A	165	TYR	CB-CG-CD2	-8.51	115.89	121.00
1	H	81	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	E	81	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	F	81	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	C	81	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	I	81	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	D	81	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	81	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	F	42	PHE	CB-CG-CD1	8.41	126.69	120.80
1	E	42	PHE	CB-CG-CD1	8.41	126.69	120.80
1	G	81	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	81	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	42	PHE	CB-CG-CD1	8.36	126.65	120.80
1	B	42	PHE	CB-CG-CD1	8.35	126.64	120.80
1	I	42	PHE	CB-CG-CD1	8.34	126.64	120.80
1	D	42	PHE	CB-CG-CD1	8.33	126.63	120.80
1	G	42	PHE	CB-CG-CD1	8.32	126.62	120.80
1	A	42	PHE	CB-CG-CD1	8.31	126.62	120.80
1	H	42	PHE	CB-CG-CD1	8.30	126.61	120.80
1	C	145	PHE	CB-CG-CD1	-8.30	114.99	120.80
1	G	145	PHE	CB-CG-CD1	-8.26	115.02	120.80
1	F	145	PHE	CB-CG-CD1	-8.25	115.02	120.80
1	H	145	PHE	CB-CG-CD1	-8.25	115.03	120.80
1	I	145	PHE	CB-CG-CD1	-8.24	115.03	120.80
1	A	145	PHE	CB-CG-CD1	-8.24	115.03	120.80
1	D	145	PHE	CB-CG-CD1	-8.24	115.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	PHE	CB-CG-CD1	-8.23	115.04	120.80
1	E	145	PHE	CB-CG-CD1	-8.22	115.04	120.80
1	A	73	TYR	CB-CG-CD1	7.52	125.51	121.00
1	I	73	TYR	CB-CG-CD1	7.52	125.51	121.00
1	E	73	TYR	CB-CG-CD1	7.50	125.50	121.00
1	H	73	TYR	CB-CG-CD1	7.49	125.49	121.00
1	B	73	TYR	CB-CG-CD1	7.48	125.49	121.00
1	F	184	ARG	NH1-CZ-NH2	-7.46	111.19	119.40
1	E	184	ARG	NH1-CZ-NH2	-7.46	111.20	119.40
1	C	184	ARG	NH1-CZ-NH2	-7.45	111.20	119.40
1	A	184	ARG	NH1-CZ-NH2	-7.45	111.21	119.40
1	G	73	TYR	CB-CG-CD1	7.45	125.47	121.00
1	B	184	ARG	NH1-CZ-NH2	-7.44	111.21	119.40
1	D	184	ARG	NH1-CZ-NH2	-7.44	111.21	119.40
1	H	184	ARG	NH1-CZ-NH2	-7.44	111.22	119.40
1	I	184	ARG	NH1-CZ-NH2	-7.44	111.22	119.40
1	C	73	TYR	CB-CG-CD1	7.43	125.46	121.00
1	F	73	TYR	CB-CG-CD1	7.43	125.46	121.00
1	D	73	TYR	CB-CG-CD1	7.42	125.45	121.00
1	G	184	ARG	NH1-CZ-NH2	-7.42	111.23	119.40
1	G	42	PHE	CB-CG-CD2	-7.41	115.61	120.80
1	A	42	PHE	CB-CG-CD2	-7.41	115.61	120.80
1	E	42	PHE	CB-CG-CD2	-7.41	115.62	120.80
1	D	42	PHE	CB-CG-CD2	-7.40	115.62	120.80
1	I	42	PHE	CB-CG-CD2	-7.40	115.62	120.80
1	B	42	PHE	CB-CG-CD2	-7.39	115.62	120.80
1	F	42	PHE	CB-CG-CD2	-7.39	115.63	120.80
1	C	42	PHE	CB-CG-CD2	-7.39	115.63	120.80
1	H	158	TYR	CB-CG-CD2	7.38	125.43	121.00
1	H	42	PHE	CB-CG-CD2	-7.38	115.63	120.80
1	I	158	TYR	CB-CG-CD2	7.36	125.42	121.00
1	A	158	TYR	CB-CG-CD2	7.36	125.42	121.00
1	E	158	TYR	CB-CG-CD2	7.36	125.41	121.00
1	F	158	TYR	CB-CG-CD2	7.35	125.41	121.00
1	G	56	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	158	TYR	CB-CG-CD2	7.33	125.40	121.00
1	C	56	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	C	158	TYR	CB-CG-CD2	7.33	125.39	121.00
1	D	158	TYR	CB-CG-CD2	7.33	125.39	121.00
1	G	158	TYR	CB-CG-CD2	7.30	125.38	121.00
1	E	56	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	56	ARG	NE-CZ-NH2	-7.29	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	D	56	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	H	56	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	F	56	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	I	56	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	G	155	PHE	CB-CG-CD2	-6.88	115.98	120.80
1	C	155	PHE	CB-CG-CD2	-6.85	116.01	120.80
1	H	155	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	I	155	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	D	155	PHE	CB-CG-CD2	-6.82	116.02	120.80
1	B	155	PHE	CB-CG-CD2	-6.82	116.02	120.80
1	E	155	PHE	CB-CG-CD2	-6.82	116.03	120.80
1	A	155	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	F	155	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	D	185	TYR	CG-CD1-CE1	-6.64	115.99	121.30
1	F	6	PHE	CB-CG-CD2	-6.63	116.16	120.80
1	C	6	PHE	CB-CG-CD2	-6.63	116.16	120.80
1	I	6	PHE	CB-CG-CD2	-6.63	116.16	120.80
1	E	185	TYR	CG-CD1-CE1	-6.62	116.00	121.30
1	F	71	THR	CA-CB-CG2	6.61	121.65	112.40
1	B	185	TYR	CG-CD1-CE1	-6.61	116.02	121.30
1	G	71	THR	CA-CB-CG2	6.61	121.65	112.40
1	I	71	THR	CA-CB-CG2	6.61	121.65	112.40
1	A	185	TYR	CG-CD1-CE1	-6.60	116.02	121.30
1	B	71	THR	CA-CB-CG2	6.60	121.64	112.40
1	E	71	THR	CA-CB-CG2	6.60	121.64	112.40
1	E	6	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	A	6	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	D	71	THR	CA-CB-CG2	6.59	121.63	112.40
1	H	6	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	H	71	THR	CA-CB-CG2	6.59	121.62	112.40
1	H	185	TYR	CG-CD1-CE1	-6.59	116.03	121.30
1	A	71	THR	CA-CB-CG2	6.59	121.62	112.40
1	C	185	TYR	CG-CD1-CE1	-6.59	116.03	121.30
1	G	6	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	G	185	TYR	CG-CD1-CE1	-6.59	116.03	121.30
1	C	71	THR	CA-CB-CG2	6.59	121.62	112.40
1	B	6	PHE	CB-CG-CD2	-6.58	116.19	120.80
1	I	185	TYR	CG-CD1-CE1	-6.58	116.03	121.30
1	F	185	TYR	CG-CD1-CE1	-6.58	116.04	121.30
1	D	6	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	A	219	SER	N-CA-CB	6.47	120.20	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	219	SER	N-CA-CB	6.43	120.15	110.50
1	B	219	SER	N-CA-CB	6.43	120.14	110.50
1	C	219	SER	N-CA-CB	6.42	120.14	110.50
1	G	219	SER	N-CA-CB	6.42	120.14	110.50
1	I	219	SER	N-CA-CB	6.42	120.12	110.50
1	E	219	SER	N-CA-CB	6.41	120.12	110.50
1	F	219	SER	N-CA-CB	6.41	120.11	110.50
1	D	219	SER	N-CA-CB	6.41	120.11	110.50
1	D	43	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	F	145	PHE	CB-CG-CD2	6.15	125.11	120.80
1	G	145	PHE	CB-CG-CD2	6.15	125.10	120.80
1	G	43	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	C	145	PHE	CB-CG-CD2	6.14	125.10	120.80
1	C	43	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	F	43	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	B	43	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	E	43	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	61	VAL	CA-CB-CG2	-6.12	101.72	110.90
1	H	61	VAL	CA-CB-CG2	-6.12	101.72	110.90
1	I	61	VAL	CA-CB-CG2	-6.12	101.72	110.90
1	G	61	VAL	CA-CB-CG2	-6.12	101.73	110.90
1	B	61	VAL	CA-CB-CG2	-6.11	101.73	110.90
1	C	61	VAL	CA-CB-CG2	-6.11	101.73	110.90
1	B	145	PHE	CB-CG-CD2	6.11	125.08	120.80
1	F	61	VAL	CA-CB-CG2	-6.11	101.74	110.90
1	A	43	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	D	61	VAL	CA-CB-CG2	-6.11	101.74	110.90
1	E	61	VAL	CA-CB-CG2	-6.11	101.74	110.90
1	H	43	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	A	145	PHE	CB-CG-CD2	6.10	125.07	120.80
1	D	145	PHE	CB-CG-CD2	6.10	125.07	120.80
1	I	43	TYR	CB-CG-CD2	-6.09	117.34	121.00
1	A	68	TRP	CB-CG-CD2	-6.08	118.69	126.60
1	E	145	PHE	CB-CG-CD2	6.07	125.05	120.80
1	H	145	PHE	CB-CG-CD2	6.07	125.05	120.80
1	I	145	PHE	CB-CG-CD2	6.06	125.05	120.80
1	E	68	TRP	CB-CG-CD2	-6.06	118.72	126.60
1	B	68	TRP	CB-CG-CD2	-6.05	118.73	126.60
1	F	68	TRP	CB-CG-CD2	-6.04	118.74	126.60
1	C	68	TRP	CB-CG-CD2	-6.04	118.75	126.60
1	G	68	TRP	CB-CG-CD2	-6.04	118.75	126.60
1	G	127	ALA	CB-CA-C	-6.04	101.05	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	68	TRP	CB-CG-CD2	-6.03	118.76	126.60
1	D	68	TRP	CB-CG-CD2	-6.02	118.78	126.60
1	H	68	TRP	CB-CG-CD2	-6.02	118.78	126.60
1	D	127	ALA	CB-CA-C	-6.01	101.09	110.10
1	C	127	ALA	CB-CA-C	-6.00	101.10	110.10
1	E	127	ALA	CB-CA-C	-6.00	101.10	110.10
1	F	127	ALA	CB-CA-C	-6.00	101.10	110.10
1	G	73	TYR	N-CA-CB	6.00	121.40	110.60
1	B	127	ALA	CB-CA-C	-6.00	101.11	110.10
1	A	127	ALA	CB-CA-C	-5.99	101.11	110.10
1	H	127	ALA	CB-CA-C	-5.99	101.12	110.10
1	I	127	ALA	CB-CA-C	-5.99	101.12	110.10
1	B	73	TYR	N-CA-CB	5.98	121.36	110.60
1	F	73	TYR	N-CA-CB	5.97	121.35	110.60
1	E	73	TYR	N-CA-CB	5.97	121.35	110.60
1	H	73	TYR	N-CA-CB	5.96	121.34	110.60
1	C	73	TYR	N-CA-CB	5.96	121.33	110.60
1	I	73	TYR	N-CA-CB	5.96	121.33	110.60
1	D	73	TYR	N-CA-CB	5.96	121.33	110.60
1	E	185	TYR	CD1-CE1-CZ	5.96	125.17	119.80
1	A	73	TYR	N-CA-CB	5.95	121.30	110.60
1	B	185	TYR	CD1-CE1-CZ	5.94	125.14	119.80
1	H	185	TYR	CD1-CE1-CZ	5.93	125.13	119.80
1	A	185	TYR	CD1-CE1-CZ	5.92	125.13	119.80
1	C	185	TYR	CD1-CE1-CZ	5.92	125.12	119.80
1	G	185	TYR	CD1-CE1-CZ	5.92	125.12	119.80
1	I	185	TYR	CD1-CE1-CZ	5.91	125.12	119.80
1	D	185	TYR	CD1-CE1-CZ	5.91	125.11	119.80
1	F	185	TYR	CD1-CE1-CZ	5.91	125.12	119.80
1	G	167	VAL	CA-CB-CG2	5.88	119.72	110.90
1	H	167	VAL	CA-CB-CG2	5.88	119.72	110.90
1	B	167	VAL	CA-CB-CG2	5.87	119.71	110.90
1	E	167	VAL	CA-CB-CG2	5.87	119.71	110.90
1	F	167	VAL	CA-CB-CG2	5.87	119.71	110.90
1	C	167	VAL	CA-CB-CG2	5.87	119.70	110.90
1	A	167	VAL	CA-CB-CG2	5.87	119.70	110.90
1	D	167	VAL	CA-CB-CG2	5.87	119.70	110.90
1	I	167	VAL	CA-CB-CG2	5.87	119.70	110.90
1	G	156	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	F	156	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	156	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	156	ARG	NE-CZ-NH2	5.79	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	156	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	C	156	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	D	156	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	H	104	LEU	CB-CG-CD1	5.73	120.75	111.00
1	D	210	SER	C-N-CA	5.73	136.03	121.70
1	C	104	LEU	CB-CG-CD1	5.73	120.74	111.00
1	F	223	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	H	156	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	I	210	SER	C-N-CA	5.73	136.02	121.70
1	A	104	LEU	CB-CG-CD1	5.72	120.73	111.00
1	G	176	TYR	CG-CD2-CE2	-5.72	116.72	121.30
1	G	104	LEU	CB-CG-CD1	5.72	120.72	111.00
1	H	210	SER	C-N-CA	5.72	136.00	121.70
1	B	210	SER	C-N-CA	5.72	135.99	121.70
1	E	210	SER	C-N-CA	5.72	135.99	121.70
1	B	104	LEU	CB-CG-CD1	5.71	120.71	111.00
1	F	210	SER	C-N-CA	5.71	135.98	121.70
1	A	223	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	210	SER	C-N-CA	5.71	135.97	121.70
1	C	210	SER	C-N-CA	5.70	135.96	121.70
1	F	104	LEU	CB-CG-CD1	5.70	120.69	111.00
1	I	104	LEU	CB-CG-CD1	5.70	120.69	111.00
1	D	104	LEU	CB-CG-CD1	5.70	120.69	111.00
1	D	223	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	176	TYR	CG-CD2-CE2	-5.70	116.74	121.30
1	G	210	SER	C-N-CA	5.69	135.94	121.70
1	B	176	TYR	CG-CD2-CE2	-5.69	116.75	121.30
1	E	104	LEU	CB-CG-CD1	5.69	120.68	111.00
1	I	176	TYR	CG-CD2-CE2	-5.69	116.75	121.30
1	C	223	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	F	176	TYR	CG-CD2-CE2	-5.67	116.76	121.30
1	G	223	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	H	176	TYR	CG-CD2-CE2	-5.67	116.76	121.30
1	I	156	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	C	176	TYR	CG-CD2-CE2	-5.66	116.77	121.30
1	D	176	TYR	CG-CD2-CE2	-5.66	116.77	121.30
1	E	223	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	I	72	VAL	CA-CB-CG1	5.66	119.39	110.90
1	H	223	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	43	TYR	CB-CG-CD1	5.66	124.39	121.00
1	D	72	VAL	CA-CB-CG1	5.66	119.38	110.90
1	E	72	VAL	CA-CB-CG1	5.66	119.38	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	TYR	CG-CD2-CE2	-5.65	116.78	121.30
1	B	72	VAL	CA-CB-CG1	5.65	119.38	110.90
1	B	223	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	F	72	VAL	CA-CB-CG1	5.65	119.38	110.90
1	A	72	VAL	CA-CB-CG1	5.65	119.37	110.90
1	H	98	PHE	N-CA-CB	5.65	120.76	110.60
1	I	98	PHE	N-CA-CB	5.64	120.76	110.60
1	A	43	TYR	CB-CG-CD1	5.64	124.39	121.00
1	C	72	VAL	CA-CB-CG1	5.64	119.36	110.90
1	D	98	PHE	N-CA-CB	5.64	120.75	110.60
1	H	72	VAL	CA-CB-CG1	5.64	119.36	110.90
1	C	98	PHE	N-CA-CB	5.64	120.75	110.60
1	G	98	PHE	N-CA-CB	5.64	120.75	110.60
1	I	223	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	I	43	TYR	CB-CG-CD1	5.64	124.38	121.00
1	B	98	PHE	N-CA-CB	5.64	120.74	110.60
1	F	98	PHE	N-CA-CB	5.64	120.74	110.60
1	G	72	VAL	CA-CB-CG1	5.64	119.36	110.90
1	A	98	PHE	N-CA-CB	5.63	120.74	110.60
1	E	98	PHE	N-CA-CB	5.63	120.74	110.60
1	G	43	TYR	CB-CG-CD1	5.63	124.38	121.00
1	D	43	TYR	CB-CG-CD1	5.62	124.38	121.00
1	D	218	VAL	C-N-CA	5.62	135.76	121.70
1	E	43	TYR	CB-CG-CD1	5.62	124.38	121.00
1	F	43	TYR	CB-CG-CD1	5.62	124.37	121.00
1	B	43	TYR	CB-CG-CD1	5.62	124.37	121.00
1	E	218	VAL	C-N-CA	5.62	135.74	121.70
1	H	218	VAL	C-N-CA	5.61	135.72	121.70
1	F	218	VAL	C-N-CA	5.61	135.72	121.70
1	I	218	VAL	C-N-CA	5.61	135.72	121.70
1	B	218	VAL	C-N-CA	5.61	135.72	121.70
1	C	218	VAL	C-N-CA	5.61	135.72	121.70
1	G	218	VAL	C-N-CA	5.60	135.71	121.70
1	A	218	VAL	C-N-CA	5.60	135.69	121.70
1	H	43	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	207	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	C	207	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	H	207	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	F	207	VAL	CG1-CB-CG2	-5.54	102.04	110.90
1	G	207	VAL	CG1-CB-CG2	-5.54	102.04	110.90
1	E	207	VAL	CG1-CB-CG2	-5.54	102.04	110.90
1	D	207	VAL	CG1-CB-CG2	-5.53	102.05	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	VAL	CG1-CB-CG2	-5.53	102.05	110.90
1	I	207	VAL	CG1-CB-CG2	-5.52	102.06	110.90
1	G	155	PHE	CD1-CG-CD2	5.51	125.47	118.30
1	H	155	PHE	CD1-CG-CD2	5.50	125.46	118.30
1	D	155	PHE	CD1-CG-CD2	5.50	125.45	118.30
1	C	155	PHE	CD1-CG-CD2	5.50	125.45	118.30
1	E	155	PHE	CD1-CG-CD2	5.49	125.44	118.30
1	B	155	PHE	CD1-CG-CD2	5.49	125.44	118.30
1	I	155	PHE	CD1-CG-CD2	5.49	125.43	118.30
1	A	155	PHE	CD1-CG-CD2	5.47	125.41	118.30
1	F	155	PHE	CD1-CG-CD2	5.46	125.40	118.30
1	C	82	ASN	N-CA-CB	5.46	120.43	110.60
1	G	82	ASN	N-CA-CB	5.45	120.40	110.60
1	B	82	ASN	N-CA-CB	5.45	120.40	110.60
1	H	82	ASN	N-CA-CB	5.45	120.40	110.60
1	I	82	ASN	N-CA-CB	5.44	120.39	110.60
1	A	82	ASN	N-CA-CB	5.44	120.39	110.60
1	D	82	ASN	N-CA-CB	5.43	120.38	110.60
1	F	82	ASN	N-CA-CB	5.43	120.38	110.60
1	E	82	ASN	N-CA-CB	5.42	120.36	110.60
1	E	225	PHE	CB-CG-CD1	5.42	124.59	120.80
1	E	43	TYR	CG-CD2-CE2	5.41	125.62	121.30
1	H	43	TYR	CG-CD2-CE2	5.40	125.62	121.30
1	I	43	TYR	CG-CD2-CE2	5.40	125.62	121.30
1	D	225	PHE	CB-CG-CD1	5.39	124.57	120.80
1	H	225	PHE	CB-CG-CD1	5.38	124.57	120.80
1	A	43	TYR	CG-CD2-CE2	5.38	125.60	121.30
1	B	43	TYR	CG-CD2-CE2	5.37	125.60	121.30
1	F	43	TYR	CG-CD2-CE2	5.37	125.60	121.30
1	G	43	TYR	CG-CD2-CE2	5.37	125.60	121.30
1	C	23	TYR	CZ-CE2-CD2	5.37	124.63	119.80
1	B	225	PHE	CB-CG-CD1	5.37	124.56	120.80
1	F	23	TYR	CZ-CE2-CD2	5.37	124.63	119.80
1	D	43	TYR	CG-CD2-CE2	5.36	125.59	121.30
1	G	225	PHE	CB-CG-CD1	5.36	124.55	120.80
1	A	225	PHE	CB-CG-CD1	5.35	124.55	120.80
1	I	225	PHE	CB-CG-CD1	5.35	124.55	120.80
1	C	225	PHE	CB-CG-CD1	5.35	124.54	120.80
1	E	23	TYR	CZ-CE2-CD2	5.35	124.61	119.80
1	F	43	TYR	O-C-N	5.34	131.25	122.70
1	C	43	TYR	CG-CD2-CE2	5.34	125.57	121.30
1	D	23	TYR	CZ-CE2-CD2	5.34	124.61	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	TYR	CZ-CE2-CD2	5.34	124.60	119.80
1	I	23	TYR	CZ-CE2-CD2	5.34	124.60	119.80
1	F	225	PHE	CB-CG-CD1	5.33	124.53	120.80
1	I	43	TYR	O-C-N	5.32	131.21	122.70
1	B	43	TYR	O-C-N	5.32	131.21	122.70
1	G	43	TYR	O-C-N	5.32	131.21	122.70
1	G	23	TYR	CZ-CE2-CD2	5.31	124.58	119.80
1	H	23	TYR	CZ-CE2-CD2	5.31	124.58	119.80
1	A	23	TYR	CZ-CE2-CD2	5.30	124.57	119.80
1	D	43	TYR	O-C-N	5.30	131.18	122.70
1	A	43	TYR	O-C-N	5.30	131.17	122.70
1	C	43	TYR	O-C-N	5.29	131.17	122.70
1	E	43	TYR	O-C-N	5.29	131.17	122.70
1	H	43	TYR	O-C-N	5.27	131.13	122.70
1	A	98	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	C	98	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	E	210	SER	N-CA-CB	5.26	118.39	110.50
1	H	210	SER	N-CA-CB	5.26	118.39	110.50
1	I	73	TYR	CD1-CG-CD2	-5.25	112.12	117.90
1	A	210	SER	N-CA-CB	5.25	118.38	110.50
1	F	98	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	B	210	SER	N-CA-CB	5.25	118.37	110.50
1	H	73	TYR	CD1-CG-CD2	-5.24	112.13	117.90
1	F	207	VAL	CA-CB-CG1	5.24	118.76	110.90
1	C	207	VAL	CA-CB-CG1	5.24	118.75	110.90
1	D	210	SER	N-CA-CB	5.24	118.36	110.50
1	B	73	TYR	CD1-CG-CD2	-5.24	112.14	117.90
1	E	207	VAL	CA-CB-CG1	5.23	118.75	110.90
1	G	210	SER	N-CA-CB	5.23	118.35	110.50
1	E	73	TYR	CD1-CG-CD2	-5.23	112.15	117.90
1	B	98	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	A	73	TYR	CD1-CG-CD2	-5.23	112.15	117.90
1	C	210	SER	N-CA-CB	5.23	118.34	110.50
1	G	207	VAL	CA-CB-CG1	5.23	118.74	110.90
1	F	210	SER	N-CA-CB	5.22	118.34	110.50
1	D	73	TYR	CD1-CG-CD2	-5.22	112.16	117.90
1	B	207	VAL	CA-CB-CG1	5.22	118.73	110.90
1	H	207	VAL	CA-CB-CG1	5.22	118.73	110.90
1	A	207	VAL	CA-CB-CG1	5.22	118.72	110.90
1	I	207	VAL	CA-CB-CG1	5.21	118.72	110.90
1	I	210	SER	N-CA-CB	5.21	118.32	110.50
1	F	73	TYR	CD1-CG-CD2	-5.21	112.17	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	H	98	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	I	98	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	G	73	TYR	CD1-CG-CD2	-5.20	112.18	117.90
1	D	207	VAL	CA-CB-CG1	5.20	118.69	110.90
1	E	98	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	C	73	TYR	CD1-CG-CD2	-5.18	112.20	117.90
1	D	98	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	D	58	GLU	N-CA-CB	5.18	119.92	110.60
1	G	58	GLU	N-CA-CB	5.17	119.91	110.60
1	C	58	GLU	N-CA-CB	5.17	119.90	110.60
1	H	58	GLU	N-CA-CB	5.17	119.90	110.60
1	F	58	GLU	N-CA-CB	5.17	119.90	110.60
1	A	58	GLU	N-CA-CB	5.16	119.89	110.60
1	E	58	GLU	N-CA-CB	5.16	119.89	110.60
1	B	58	GLU	N-CA-CB	5.16	119.88	110.60
1	G	98	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	D	169	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	I	58	GLU	N-CA-CB	5.15	119.88	110.60
1	G	169	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	F	90	LEU	CB-CG-CD1	5.13	119.72	111.00
1	B	169	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	H	169	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	F	169	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	I	169	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	90	LEU	CB-CG-CD1	5.12	119.71	111.00
1	D	90	LEU	CB-CG-CD1	5.12	119.70	111.00
1	E	90	LEU	CB-CG-CD1	5.12	119.71	111.00
1	B	90	LEU	CB-CG-CD1	5.12	119.70	111.00
1	I	90	LEU	CB-CG-CD1	5.12	119.70	111.00
1	C	90	LEU	CB-CG-CD1	5.11	119.69	111.00
1	C	169	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	G	90	LEU	CB-CG-CD1	5.11	119.69	111.00
1	H	90	LEU	CB-CG-CD1	5.11	119.69	111.00
1	A	169	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	H	158	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	I	93	HIS	CA-CB-CG	5.03	122.15	113.60
1	F	93	HIS	CA-CB-CG	5.02	122.13	113.60
1	A	158	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	D	93	HIS	CA-CB-CG	5.01	122.12	113.60
1	I	158	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	B	93	HIS	CA-CB-CG	5.01	122.11	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	158	TYR	CB-CG-CD1	-5.00	118.00	121.00

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	169	ARG	Sidechain
1	A	184	ARG	Sidechain
1	A	185	TYR	Sidechain
1	A	43	TYR	Sidechain
1	A	73	TYR	Sidechain
1	A	94	ARG	Sidechain
1	B	141	TYR	Sidechain
1	B	169	ARG	Sidechain
1	B	184	ARG	Sidechain
1	B	185	TYR	Sidechain
1	B	43	TYR	Sidechain
1	B	73	TYR	Sidechain
1	B	94	ARG	Sidechain
1	C	141	TYR	Sidechain
1	C	169	ARG	Sidechain
1	C	184	ARG	Sidechain
1	C	185	TYR	Sidechain
1	C	43	TYR	Sidechain
1	C	73	TYR	Sidechain
1	C	94	ARG	Sidechain
1	D	141	TYR	Sidechain
1	D	169	ARG	Sidechain
1	D	184	ARG	Sidechain
1	D	185	TYR	Sidechain
1	D	43	TYR	Sidechain
1	D	73	TYR	Sidechain
1	D	94	ARG	Sidechain
1	E	141	TYR	Sidechain
1	E	169	ARG	Sidechain
1	E	184	ARG	Sidechain
1	E	185	TYR	Sidechain
1	E	43	TYR	Sidechain
1	E	73	TYR	Sidechain
1	E	94	ARG	Sidechain
1	F	141	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	F	169	ARG	Sidechain
1	F	184	ARG	Sidechain
1	F	185	TYR	Sidechain
1	F	43	TYR	Sidechain
1	F	73	TYR	Sidechain
1	F	94	ARG	Sidechain
1	G	141	TYR	Sidechain
1	G	169	ARG	Sidechain
1	G	184	ARG	Sidechain
1	G	185	TYR	Sidechain
1	G	43	TYR	Sidechain
1	G	73	TYR	Sidechain
1	G	94	ARG	Sidechain
1	H	141	TYR	Sidechain
1	H	169	ARG	Sidechain
1	H	184	ARG	Sidechain
1	H	185	TYR	Sidechain
1	H	43	TYR	Sidechain
1	H	73	TYR	Sidechain
1	H	94	ARG	Sidechain
1	I	141	TYR	Sidechain
1	I	169	ARG	Sidechain
1	I	184	ARG	Sidechain
1	I	185	TYR	Sidechain
1	I	43	TYR	Sidechain
1	I	73	TYR	Sidechain
1	I	94	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1843	0	1863	40	0
1	B	1843	0	1863	63	0
1	C	1843	0	1863	65	0
1	D	1843	0	1863	63	0
1	E	1843	0	1863	63	0
1	F	1843	0	1863	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1843	0	1863	64	0
1	H	1843	0	1863	64	0
1	I	1843	0	1863	39	0
All	All	16587	0	16767	331	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 10.

All (331) 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:225:PHE:HD2	1:D:181:MET:HE3	1.28	0.97
1:C:225:PHE:CD2	1:D:181:MET:HE3	2.04	0.92
1:G:225:PHE:HD2	1:H:181:MET:HE3	1.36	0.90
1:D:225:PHE:HD2	1:E:181:MET:HE3	1.36	0.90
1:B:225:PHE:CD2	1:C:181:MET:SD	2.65	0.90
1:H:225:PHE:CD2	1:I:181:MET:SD	2.65	0.90
1:E:225:PHE:CD2	1:F:181:MET:SD	2.65	0.90
1:D:225:PHE:CD2	1:E:181:MET:SD	2.65	0.90
1:F:225:PHE:CD2	1:G:181:MET:SD	2.65	0.90
1:G:225:PHE:CD2	1:H:181:MET:SD	2.65	0.90
1:B:181:MET:SD	1:A:225:PHE:CD2	2.65	0.89
1:C:225:PHE:CD2	1:D:181:MET:SD	2.65	0.89
1:B:181:MET:CE	1:A:225:PHE:CD2	2.57	0.88
1:H:225:PHE:CD2	1:I:181:MET:CE	2.57	0.88
1:B:225:PHE:CD2	1:C:181:MET:CE	2.57	0.88
1:D:225:PHE:CD2	1:E:181:MET:CE	2.57	0.88
1:F:225:PHE:CD2	1:G:181:MET:CE	2.56	0.88
1:C:225:PHE:CD2	1:D:181:MET:CE	2.57	0.87
1:E:225:PHE:CD2	1:F:181:MET:CE	2.56	0.87
1:B:225:PHE:HD2	1:C:181:MET:HE3	1.36	0.87
1:G:225:PHE:CD2	1:H:181:MET:CE	2.56	0.86
1:H:225:PHE:HD2	1:I:181:MET:HE3	1.37	0.86
1:E:225:PHE:HD2	1:F:181:MET:HE3	1.42	0.85
1:E:225:PHE:HD2	1:F:181:MET:CE	1.92	0.82
1:F:225:PHE:HD2	1:G:181:MET:CE	1.92	0.82
1:B:181:MET:CE	1:A:225:PHE:HD2	1.92	0.81
1:B:225:PHE:HD2	1:C:181:MET:CE	1.92	0.81
1:H:225:PHE:HD2	1:I:181:MET:CE	1.92	0.81
1:G:225:PHE:HD2	1:H:181:MET:CE	1.92	0.80
1:B:225:PHE:CD2	1:C:181:MET:HE3	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:HD2	1:D:181:MET:CE	1.92	0.79
1:G:225:PHE:CD2	1:H:181:MET:HE3	2.16	0.78
1:B:181:MET:HE1	1:A:225:PHE:CE2	2.18	0.78
1:D:225:PHE:CD2	1:E:181:MET:HE3	2.16	0.77
1:B:160:LEU:HD21	1:A:225:PHE:CZ	2.20	0.77
1:F:225:PHE:CZ	1:G:160:LEU:HD21	2.20	0.77
1:H:225:PHE:CD2	1:I:181:MET:HE3	2.18	0.77
1:C:225:PHE:CZ	1:D:160:LEU:HD21	2.20	0.77
1:D:225:PHE:HD2	1:E:181:MET:CE	1.92	0.77
1:G:225:PHE:CZ	1:H:160:LEU:HD21	2.20	0.77
1:H:225:PHE:CZ	1:I:160:LEU:HD21	2.20	0.77
1:D:225:PHE:CZ	1:E:160:LEU:HD21	2.20	0.77
1:E:225:PHE:CZ	1:F:160:LEU:HD21	2.20	0.76
1:G:225:PHE:CE2	1:H:181:MET:SD	2.79	0.76
1:H:225:PHE:CE2	1:I:181:MET:SD	2.79	0.76
1:B:225:PHE:CZ	1:C:160:LEU:HD21	2.20	0.76
1:B:181:MET:SD	1:A:225:PHE:CE2	2.79	0.76
1:C:225:PHE:CE2	1:D:181:MET:SD	2.79	0.76
1:D:225:PHE:CE2	1:E:181:MET:SD	2.79	0.75
1:B:225:PHE:CE2	1:C:181:MET:SD	2.79	0.75
1:E:225:PHE:CE2	1:F:181:MET:SD	2.79	0.74
1:F:225:PHE:CE2	1:G:181:MET:SD	2.79	0.74
1:F:225:PHE:CE2	1:G:181:MET:HE1	2.23	0.73
1:F:225:PHE:HD2	1:G:181:MET:HE3	1.52	0.72
1:E:225:PHE:CD2	1:F:181:MET:HE3	2.24	0.71
1:B:216:THR:HG21	1:C:175:LYS:HG3	1.73	0.70
1:F:216:THR:HG21	1:G:175:LYS:HG3	1.73	0.70
1:E:216:THR:HG21	1:F:175:LYS:HG3	1.73	0.70
1:B:175:LYS:HG3	1:A:216:THR:HG21	1.73	0.70
1:C:225:PHE:CE2	1:D:181:MET:CE	2.75	0.70
1:H:216:THR:HG21	1:I:175:LYS:HG3	1.73	0.70
1:B:225:PHE:CE2	1:C:181:MET:CE	2.75	0.69
1:C:216:THR:HG21	1:D:175:LYS:HG3	1.73	0.69
1:D:225:PHE:CE2	1:E:181:MET:CE	2.75	0.69
1:B:181:MET:CE	1:A:225:PHE:CE2	2.75	0.69
1:G:216:THR:HG21	1:H:175:LYS:HG3	1.73	0.69
1:G:225:PHE:CE2	1:H:181:MET:CE	2.75	0.69
1:D:216:THR:HG21	1:E:175:LYS:HG3	1.73	0.69
1:E:225:PHE:CE2	1:F:181:MET:CE	2.75	0.69
1:F:225:PHE:CE2	1:G:181:MET:CE	2.75	0.69
1:H:225:PHE:CE2	1:I:181:MET:CE	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:MET:HE3	1:A:225:PHE:HD2	1.59	0.67
1:D:140:VAL:HG13	1:D:208:VAL:HG12	1.77	0.67
1:H:140:VAL:HG13	1:H:208:VAL:HG12	1.77	0.67
1:G:140:VAL:HG13	1:G:208:VAL:HG12	1.77	0.66
1:C:140:VAL:HG13	1:C:208:VAL:HG12	1.77	0.66
1:E:140:VAL:HG13	1:E:208:VAL:HG12	1.77	0.66
1:F:225:PHE:HE2	1:G:181:MET:HE1	1.60	0.66
1:A:140:VAL:HG13	1:A:208:VAL:HG12	1.77	0.66
1:I:140:VAL:HG13	1:I:208:VAL:HG12	1.77	0.66
1:B:140:VAL:HG13	1:B:208:VAL:HG12	1.77	0.66
1:B:181:MET:HE1	1:A:225:PHE:HE2	1.58	0.65
1:F:140:VAL:HG13	1:F:208:VAL:HG12	1.77	0.65
1:H:106:LYS:O	1:H:110:VAL:HG22	1.98	0.65
1:B:216:THR:CG2	1:C:175:LYS:HG3	2.27	0.64
1:A:106:LYS:O	1:A:110:VAL:HG22	1.97	0.64
1:D:216:THR:CG2	1:E:175:LYS:HG3	2.27	0.64
1:B:175:LYS:HG3	1:A:216:THR:CG2	2.27	0.64
1:E:225:PHE:CE2	1:F:181:MET:HE1	2.32	0.64
1:C:106:LYS:O	1:C:110:VAL:HG22	1.97	0.64
1:G:216:THR:CG2	1:H:175:LYS:HG3	2.27	0.64
1:H:216:THR:CG2	1:I:175:LYS:HG3	2.27	0.64
1:E:106:LYS:O	1:E:110:VAL:HG22	1.97	0.64
1:E:216:THR:CG2	1:F:175:LYS:HG3	2.27	0.64
1:F:216:THR:CG2	1:G:175:LYS:HG3	2.27	0.64
1:B:175:LYS:HD2	1:A:216:THR:CG2	2.28	0.64
1:I:106:LYS:O	1:I:110:VAL:HG22	1.97	0.64
1:G:106:LYS:O	1:G:110:VAL:HG22	1.98	0.64
1:G:216:THR:CG2	1:H:175:LYS:HD2	2.28	0.64
1:E:216:THR:CG2	1:F:175:LYS:HD2	2.28	0.63
1:F:216:THR:CG2	1:G:175:LYS:HD2	2.28	0.63
1:D:106:LYS:O	1:D:110:VAL:HG22	1.97	0.63
1:B:106:LYS:O	1:B:110:VAL:HG22	1.97	0.63
1:C:216:THR:CG2	1:D:175:LYS:HD2	2.28	0.63
1:B:216:THR:CG2	1:C:175:LYS:HD2	2.28	0.63
1:F:106:LYS:O	1:F:110:VAL:HG22	1.97	0.63
1:C:216:THR:CG2	1:D:175:LYS:HG3	2.27	0.63
1:H:216:THR:CG2	1:I:175:LYS:HD2	2.28	0.63
1:D:216:THR:CG2	1:E:175:LYS:HD2	2.28	0.63
1:E:225:PHE:HE2	1:F:181:MET:HE1	1.65	0.60
1:I:133:THR:HG22	1:I:134:TRP:H	1.68	0.59
1:B:133:THR:HG22	1:B:134:TRP:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:THR:HG22	1:C:134:TRP:H	1.68	0.58
1:F:133:THR:HG22	1:F:134:TRP:H	1.68	0.58
1:H:225:PHE:CE2	1:I:181:MET:HE1	2.38	0.58
1:H:133:THR:HG22	1:H:134:TRP:H	1.68	0.58
1:E:133:THR:HG22	1:E:134:TRP:H	1.68	0.58
1:G:133:THR:HG22	1:G:134:TRP:H	1.68	0.57
1:D:133:THR:HG22	1:D:134:TRP:H	1.68	0.57
1:A:133:THR:HG22	1:A:134:TRP:H	1.68	0.56
1:D:216:THR:CG2	1:E:175:LYS:CG	2.84	0.56
1:B:225:PHE:CE2	1:C:160:LEU:HD21	2.41	0.56
1:B:225:PHE:CE2	1:C:181:MET:HE1	2.41	0.56
1:F:225:PHE:CE2	1:G:160:LEU:HD21	2.41	0.56
1:H:225:PHE:CE2	1:I:160:LEU:HD21	2.41	0.56
1:G:216:THR:CG2	1:H:175:LYS:CG	2.84	0.55
1:B:216:THR:CG2	1:C:175:LYS:CG	2.84	0.55
1:C:216:THR:CG2	1:D:175:LYS:CG	2.84	0.55
1:E:216:THR:CG2	1:F:175:LYS:CG	2.84	0.55
1:H:216:THR:CG2	1:I:175:LYS:CG	2.84	0.55
1:E:225:PHE:CE2	1:F:160:LEU:HD21	2.41	0.55
1:B:175:LYS:CG	1:A:216:THR:CG2	2.84	0.55
1:F:216:THR:CG2	1:G:175:LYS:CG	2.84	0.55
1:D:225:PHE:CE2	1:E:160:LEU:HD21	2.41	0.55
1:H:225:PHE:HE2	1:I:181:MET:HE1	1.70	0.55
1:G:225:PHE:CE2	1:H:160:LEU:HD21	2.41	0.55
1:D:225:PHE:HE2	1:E:181:MET:HE1	1.71	0.55
1:G:225:PHE:HE2	1:H:181:MET:HE1	1.71	0.54
1:B:160:LEU:HD21	1:A:225:PHE:CE2	2.41	0.54
1:C:225:PHE:CE2	1:D:160:LEU:HD21	2.41	0.54
1:G:225:PHE:CE2	1:H:181:MET:HE1	2.41	0.54
1:B:225:PHE:HE2	1:C:181:MET:HE1	1.71	0.53
1:D:225:PHE:CE2	1:E:181:MET:HE1	2.41	0.53
1:G:216:THR:HG23	1:H:175:LYS:HD2	1.90	0.53
1:B:175:LYS:HD2	1:A:216:THR:HG23	1.90	0.53
1:C:216:THR:HG23	1:D:175:LYS:HD2	1.90	0.52
1:D:216:THR:HG23	1:E:175:LYS:HD2	1.90	0.52
1:H:216:THR:HG23	1:I:175:LYS:HD2	1.90	0.52
1:B:216:THR:HG23	1:C:175:LYS:HD2	1.90	0.52
1:F:216:THR:HG23	1:G:175:LYS:HD2	1.90	0.52
1:E:216:THR:HG23	1:F:175:LYS:HD2	1.90	0.52
1:F:44:ILE:HG21	1:G:9:VAL:HG13	1.92	0.52
1:B:9:VAL:HG13	1:A:44:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:HG21	1:C:9:VAL:HG13	1.92	0.51
1:D:44:ILE:HG21	1:E:9:VAL:HG13	1.92	0.51
1:C:44:ILE:HG21	1:D:9:VAL:HG13	1.92	0.51
1:G:44:ILE:HG21	1:H:9:VAL:HG13	1.92	0.51
1:B:225:PHE:HD2	1:C:181:MET:SD	2.29	0.51
1:E:44:ILE:HG21	1:F:9:VAL:HG13	1.92	0.50
1:H:44:ILE:HG21	1:I:9:VAL:HG13	1.92	0.50
1:A:43:TYR:CG	1:A:145:PHE:CZ	3.01	0.48
1:D:43:TYR:CG	1:D:145:PHE:CZ	3.01	0.48
1:H:43:TYR:CG	1:H:145:PHE:CZ	3.01	0.48
1:E:43:TYR:CG	1:E:145:PHE:CZ	3.01	0.48
1:E:63:LEU:HD22	1:F:6:PHE:CE2	2.49	0.48
1:F:43:TYR:CG	1:F:145:PHE:CZ	3.01	0.48
1:G:43:TYR:CG	1:G:145:PHE:CZ	3.01	0.48
1:B:63:LEU:HD22	1:C:6:PHE:CE2	2.49	0.48
1:C:43:TYR:CG	1:C:145:PHE:CZ	3.01	0.48
1:B:223:ARG:HE	1:B:223:ARG:HA	1.79	0.48
1:H:223:ARG:HE	1:H:223:ARG:HA	1.79	0.48
1:I:43:TYR:CG	1:I:145:PHE:CZ	3.01	0.48
1:A:223:ARG:HE	1:A:223:ARG:HA	1.79	0.48
1:C:63:LEU:HD22	1:D:6:PHE:CE2	2.49	0.48
1:D:223:ARG:HE	1:D:223:ARG:HA	1.79	0.48
1:E:223:ARG:HE	1:E:223:ARG:HA	1.79	0.48
1:H:63:LEU:HD22	1:I:6:PHE:CE2	2.49	0.48
1:B:43:TYR:CG	1:B:145:PHE:CZ	3.01	0.48
1:G:223:ARG:HE	1:G:223:ARG:HA	1.79	0.48
1:B:6:PHE:CE2	1:A:63:LEU:HD22	2.49	0.47
1:G:63:LEU:HD22	1:H:6:PHE:CE2	2.49	0.47
1:C:223:ARG:HE	1:C:223:ARG:HA	1.79	0.47
1:D:63:LEU:HD22	1:E:6:PHE:CE2	2.49	0.47
1:F:63:LEU:HD22	1:G:6:PHE:CE2	2.49	0.47
1:F:223:ARG:HE	1:F:223:ARG:HA	1.79	0.47
1:I:223:ARG:HE	1:I:223:ARG:HA	1.79	0.47
1:F:225:PHE:CD2	1:G:181:MET:HE3	2.36	0.47
1:C:223:ARG:HA	1:C:223:ARG:NE	2.31	0.46
1:F:223:ARG:HA	1:F:223:ARG:NE	2.31	0.46
1:I:223:ARG:HA	1:I:223:ARG:NE	2.31	0.46
1:B:223:ARG:HA	1:B:223:ARG:NE	2.31	0.46
1:G:223:ARG:HA	1:G:223:ARG:NE	2.31	0.46
1:E:216:THR:HG22	1:F:175:LYS:HD2	1.98	0.46
1:E:223:ARG:HA	1:E:223:ARG:NE	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:HD2	1:A:216:THR:HG22	1.98	0.45
1:F:225:PHE:HD2	1:G:181:MET:SD	2.29	0.45
1:D:223:ARG:HA	1:D:223:ARG:NE	2.31	0.45
1:G:69:LYS:HE2	1:H:3:GLU:OE1	2.17	0.45
1:H:216:THR:HG22	1:I:175:LYS:HD2	1.98	0.45
1:D:69:LYS:HE2	1:E:3:GLU:OE1	2.17	0.45
1:C:69:LYS:HE2	1:D:3:GLU:OE1	2.17	0.45
1:C:216:THR:CG2	1:D:175:LYS:CD	2.95	0.45
1:B:225:PHE:HE2	1:C:160:LEU:HD11	1.82	0.45
1:F:225:PHE:HE2	1:G:160:LEU:HD11	1.82	0.45
1:H:223:ARG:HA	1:H:223:ARG:NE	2.31	0.45
1:A:223:ARG:HA	1:A:223:ARG:NE	2.31	0.45
1:D:216:THR:CG2	1:E:175:LYS:CD	2.95	0.45
1:G:216:THR:CG2	1:H:175:LYS:CD	2.95	0.45
1:B:3:GLU:OE1	1:A:69:LYS:HE2	2.17	0.45
1:C:225:PHE:HE2	1:D:160:LEU:HD11	1.82	0.45
1:G:216:THR:HG22	1:H:175:LYS:HD2	1.98	0.45
1:H:69:LYS:HE2	1:I:3:GLU:OE1	2.17	0.45
1:D:225:PHE:HE2	1:E:160:LEU:HD11	1.82	0.45
1:F:69:LYS:HE2	1:G:3:GLU:OE1	2.17	0.45
1:F:216:THR:HG22	1:G:175:LYS:HD2	1.98	0.45
1:G:225:PHE:HE2	1:H:160:LEU:HD11	1.82	0.45
1:I:38:HIS:CD2	1:I:68:TRP:HB2	2.52	0.44
1:B:160:LEU:HD11	1:A:225:PHE:HE2	1.82	0.44
1:E:225:PHE:HE2	1:F:160:LEU:HD11	1.82	0.44
1:B:38:HIS:CD2	1:B:68:TRP:HB2	2.52	0.44
1:D:216:THR:HG22	1:E:175:LYS:HD2	1.98	0.44
1:F:216:THR:CG2	1:G:175:LYS:CD	2.95	0.44
1:B:216:THR:HG22	1:C:175:LYS:HD2	1.98	0.44
1:A:38:HIS:CD2	1:A:68:TRP:HB2	2.52	0.44
1:G:38:HIS:CD2	1:G:68:TRP:HB2	2.52	0.44
1:H:225:PHE:HE2	1:I:160:LEU:HD11	1.82	0.44
1:B:69:LYS:HE2	1:C:3:GLU:OE1	2.17	0.44
1:C:216:THR:HG22	1:D:175:LYS:HD2	1.98	0.44
1:B:44:ILE:HG21	1:C:9:VAL:CG1	2.48	0.44
1:E:31:THR:HA	1:E:34:LEU:HB3	1.99	0.44
1:E:38:HIS:CD2	1:E:68:TRP:HB2	2.52	0.44
1:E:69:LYS:HE2	1:F:3:GLU:OE1	2.17	0.44
1:D:38:HIS:CD2	1:D:68:TRP:HB2	2.52	0.44
1:C:31:THR:HA	1:C:34:LEU:HB3	1.99	0.44
1:C:164:ILE:HA	1:C:167:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ILE:HG21	1:E:9:VAL:CG1	2.48	0.44
1:E:216:THR:CG2	1:F:175:LYS:CD	2.95	0.44
1:F:38:HIS:CD2	1:F:68:TRP:HB2	2.52	0.44
1:G:164:ILE:HA	1:G:167:VAL:HG22	2.00	0.44
1:H:38:HIS:CD2	1:H:68:TRP:HB2	2.52	0.44
1:C:38:HIS:CD2	1:C:68:TRP:HB2	2.52	0.43
1:F:31:THR:HA	1:F:34:LEU:HB3	1.99	0.43
1:H:31:THR:HA	1:H:34:LEU:HB3	1.99	0.43
1:I:31:THR:HA	1:I:34:LEU:HB3	1.99	0.43
1:B:44:ILE:HD11	1:B:123:ILE:HB	2.00	0.43
1:D:31:THR:HA	1:D:34:LEU:HB3	1.99	0.43
1:G:31:THR:HA	1:G:34:LEU:HB3	1.99	0.43
1:B:181:MET:HE1	1:A:225:PHE:CD2	2.39	0.43
1:B:216:THR:CG2	1:C:175:LYS:CD	2.95	0.43
1:E:44:ILE:HG21	1:F:9:VAL:CG1	2.48	0.43
1:F:44:ILE:HG21	1:G:9:VAL:CG1	2.48	0.43
1:F:44:ILE:HD11	1:F:123:ILE:HB	2.00	0.43
1:H:216:THR:CG2	1:I:175:LYS:CD	2.95	0.43
1:I:164:ILE:HA	1:I:167:VAL:HG22	2.00	0.43
1:B:164:ILE:HA	1:B:167:VAL:HG22	2.00	0.43
1:C:44:ILE:HD11	1:C:123:ILE:HB	2.01	0.43
1:C:225:PHE:HE2	1:D:181:MET:HE1	1.84	0.43
1:G:44:ILE:HG21	1:H:9:VAL:CG1	2.48	0.43
1:H:164:ILE:HA	1:H:167:VAL:HG22	2.00	0.43
1:B:31:THR:HA	1:B:34:LEU:HB3	1.99	0.43
1:G:107:MET:HE2	1:G:138:GLU:HB3	2.01	0.43
1:I:44:ILE:HD11	1:I:123:ILE:HB	2.01	0.43
1:A:164:ILE:HA	1:A:167:VAL:HG22	2.00	0.43
1:G:44:ILE:HD11	1:G:123:ILE:HB	2.00	0.43
1:A:31:THR:HA	1:A:34:LEU:HB3	1.99	0.43
1:A:107:MET:HE2	1:A:138:GLU:HB3	2.01	0.43
1:D:164:ILE:HA	1:D:167:VAL:HG22	2.00	0.43
1:E:44:ILE:HD11	1:E:123:ILE:HB	2.01	0.43
1:F:164:ILE:HA	1:F:167:VAL:HG22	2.00	0.43
1:B:9:VAL:CG1	1:A:44:ILE:HG21	2.48	0.43
1:B:175:LYS:CD	1:A:216:THR:CG2	2.95	0.43
1:E:64:ASN:HB3	1:F:5:GLU:HA	2.01	0.43
1:H:44:ILE:HG21	1:I:9:VAL:CG1	2.48	0.43
1:C:44:ILE:HG21	1:D:9:VAL:CG1	2.48	0.42
1:A:39:ILE:HG22	1:A:43:TYR:CE2	2.55	0.42
1:D:44:ILE:HD11	1:D:123:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:ILE:HG22	1:H:43:TYR:CE2	2.55	0.42
1:D:39:ILE:HG22	1:D:43:TYR:CE2	2.55	0.42
1:E:39:ILE:HG22	1:E:43:TYR:CE2	2.55	0.42
1:H:44:ILE:HD11	1:H:123:ILE:HB	2.00	0.42
1:I:39:ILE:HG22	1:I:43:TYR:CE2	2.55	0.42
1:A:44:ILE:HD11	1:A:123:ILE:HB	2.00	0.42
1:E:133:THR:HB	1:E:213:TRP:CD1	2.55	0.42
1:D:133:THR:HB	1:D:213:TRP:CD1	2.55	0.42
1:B:5:GLU:HA	1:A:64:ASN:HB3	2.01	0.42
1:C:133:THR:HB	1:C:213:TRP:CD1	2.55	0.42
1:G:133:THR:HB	1:G:213:TRP:CD1	2.55	0.42
1:I:133:THR:HB	1:I:213:TRP:CD1	2.55	0.42
1:B:133:THR:HB	1:B:213:TRP:CD1	2.55	0.42
1:F:39:ILE:HG22	1:F:43:TYR:CE2	2.55	0.42
1:G:64:ASN:HB3	1:H:5:GLU:HA	2.01	0.42
1:C:39:ILE:HG22	1:C:43:TYR:CE2	2.55	0.42
1:C:64:ASN:HB3	1:D:5:GLU:HA	2.01	0.42
1:B:39:ILE:HG22	1:B:43:TYR:CE2	2.55	0.42
1:E:164:ILE:HA	1:E:167:VAL:HG22	2.00	0.42
1:H:133:THR:HB	1:H:213:TRP:CD1	2.55	0.42
1:A:133:THR:HB	1:A:213:TRP:CD1	2.55	0.41
1:C:225:PHE:HD2	1:D:181:MET:SD	2.29	0.41
1:G:39:ILE:HG22	1:G:43:TYR:CE2	2.55	0.41
1:I:160:LEU:HD13	1:I:180:THR:HG21	2.02	0.41
1:C:160:LEU:HD13	1:C:180:THR:HG21	2.02	0.41
1:F:133:THR:HB	1:F:213:TRP:CD1	2.55	0.41
1:F:160:LEU:HD13	1:F:180:THR:HG21	2.02	0.41
1:G:160:LEU:HD13	1:G:180:THR:HG21	2.02	0.41
1:B:64:ASN:HB3	1:C:5:GLU:HA	2.01	0.41
1:A:160:LEU:HD13	1:A:180:THR:HG21	2.02	0.41
1:B:160:LEU:HD13	1:B:180:THR:HG21	2.02	0.41
1:F:64:ASN:HB3	1:G:5:GLU:HA	2.01	0.41
1:D:64:ASN:HB3	1:E:5:GLU:HA	2.01	0.41
1:H:160:LEU:HD13	1:H:180:THR:HG21	2.02	0.41
1:D:160:LEU:HD13	1:D:180:THR:HG21	2.02	0.41
1:E:160:LEU:HD13	1:E:180:THR:HG21	2.02	0.41
1:H:64:ASN:HB3	1:I:5:GLU:HA	2.01	0.41
1:H:107:MET:HE2	1:H:138:GLU:HB3	2.03	0.41
1:B:39:ILE:HG21	1:B:103:LEU:HD11	2.03	0.41
1:C:39:ILE:HG21	1:C:103:LEU:HD11	2.03	0.41
1:E:107:MET:HE2	1:E:138:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:THR:H	1:H:94:ARG:HB2	1.86	0.41
1:H:39:ILE:HG21	1:H:103:LEU:HD11	2.03	0.41
1:D:91:THR:H	1:D:94:ARG:HB2	1.86	0.40
1:I:92:LEU:C	1:I:92:LEU:HD13	2.42	0.40
1:A:91:THR:H	1:A:94:ARG:HB2	1.87	0.40
1:C:92:LEU:HD13	1:C:92:LEU:C	2.42	0.40
1:E:91:THR:H	1:E:94:ARG:HB2	1.86	0.40
1:G:39:ILE:HG21	1:G:103:LEU:HD11	2.03	0.40
1:A:92:LEU:C	1:A:92:LEU:HD13	2.42	0.40
1:F:39:ILE:HG21	1:F:103:LEU:HD11	2.03	0.40
1:D:39:ILE:HG21	1:D:103:LEU:HD11	2.03	0.40
1:F:92:LEU:HD13	1:F:92:LEU:C	2.42	0.40
1:C:91:THR:H	1:C:94:ARG:HB2	1.87	0.40
1:I:91:THR:H	1:I:94:ARG:HB2	1.86	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	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	B	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	C	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	D	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	E	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	F	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	G	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	H	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25
1	I	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2034/2097 (97%)	1854 (91%)	108 (5%)	72 (4%)	6	25

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	B	211	LEU
1	B	218	VAL
1	B	219	SER
1	A	82	ASN
1	A	211	LEU
1	A	218	VAL
1	A	219	SER
1	C	82	ASN
1	C	211	LEU
1	C	218	VAL
1	C	219	SER
1	D	82	ASN
1	D	211	LEU
1	D	218	VAL
1	D	219	SER
1	E	82	ASN
1	E	211	LEU
1	E	218	VAL
1	E	219	SER
1	F	82	ASN
1	F	211	LEU
1	F	218	VAL
1	F	219	SER
1	G	82	ASN
1	G	211	LEU
1	G	218	VAL
1	G	219	SER
1	H	82	ASN
1	H	211	LEU
1	H	218	VAL
1	H	219	SER
1	I	82	ASN
1	I	211	LEU
1	I	218	VAL
1	I	219	SER
1	B	132	ILE

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Mol	Chain	Res	Type
1	B	156	ARG
1	A	132	ILE
1	A	156	ARG
1	C	132	ILE
1	C	156	ARG
1	D	132	ILE
1	D	156	ARG
1	E	132	ILE
1	E	156	ARG
1	F	132	ILE
1	F	156	ARG
1	G	132	ILE
1	G	156	ARG
1	H	132	ILE
1	H	156	ARG
1	I	132	ILE
1	I	156	ARG
1	B	86	PRO
1	A	86	PRO
1	C	86	PRO
1	D	86	PRO
1	E	86	PRO
1	F	86	PRO
1	G	86	PRO
1	H	86	PRO
1	I	86	PRO
1	B	19	PRO
1	A	19	PRO
1	C	19	PRO
1	D	19	PRO
1	E	19	PRO
1	F	19	PRO
1	G	19	PRO
1	H	19	PRO
1	I	19	PRO

### 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	199/203 (98%)	184 (92%)	15 (8%)	13	38
1	B	199/203 (98%)	184 (92%)	15 (8%)	13	38
1	C	199/203 (98%)	184 (92%)	15 (8%)	13	38
1	D	199/203 (98%)	184 (92%)	15 (8%)	13	38
1	E	199/203 (98%)	184 (92%)	15 (8%)	13	38
1	F	199/203 (98%)	184 (92%)	15 (8%)	13	38
1	G	199/203 (98%)	184 (92%)	15 (8%)	13	38
1	H	199/203 (98%)	185 (93%)	14 (7%)	15	40
1	I	199/203 (98%)	185 (93%)	14 (7%)	15	40
All	All	1791/1827 (98%)	1658 (93%)	133 (7%)	17	38

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	LEU
1	B	51	THR
1	B	78	PRO
1	B	81	ARG
1	B	93	HIS
1	B	104	LEU
1	B	106	LYS
1	B	149	GLU
1	B	151	PHE
1	B	154	THR
1	B	162	ILE
1	B	174	PRO
1	B	194	THR
1	B	216	THR
1	B	218	VAL
1	A	4	LEU
1	A	51	THR
1	A	78	PRO
1	A	81	ARG
1	A	93	HIS
1	A	104	LEU
1	A	106	LYS
1	A	149	GLU
1	A	151	PHE

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Mol	Chain	Res	Type
1	A	154	THR
1	A	162	ILE
1	A	174	PRO
1	A	194	THR
1	A	216	THR
1	A	218	VAL
1	C	4	LEU
1	C	51	THR
1	C	78	PRO
1	C	81	ARG
1	C	93	HIS
1	C	104	LEU
1	C	106	LYS
1	C	149	GLU
1	C	151	PHE
1	C	154	THR
1	C	162	ILE
1	C	174	PRO
1	C	194	THR
1	C	216	THR
1	C	218	VAL
1	D	4	LEU
1	D	51	THR
1	D	78	PRO
1	D	81	ARG
1	D	93	HIS
1	D	104	LEU
1	D	106	LYS
1	D	149	GLU
1	D	151	PHE
1	D	154	THR
1	D	162	ILE
1	D	174	PRO
1	D	194	THR
1	D	216	THR
1	D	218	VAL
1	E	4	LEU
1	E	51	THR
1	E	78	PRO
1	E	81	ARG
1	E	93	HIS
1	E	104	LEU

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Mol	Chain	Res	Type
1	E	106	LYS
1	E	149	GLU
1	E	151	PHE
1	E	154	THR
1	E	162	ILE
1	E	174	PRO
1	E	194	THR
1	E	216	THR
1	E	218	VAL
1	F	4	LEU
1	F	51	THR
1	F	78	PRO
1	F	81	ARG
1	F	93	HIS
1	F	104	LEU
1	F	106	LYS
1	F	149	GLU
1	F	151	PHE
1	F	154	THR
1	F	162	ILE
1	F	174	PRO
1	F	194	THR
1	F	216	THR
1	F	218	VAL
1	G	4	LEU
1	G	51	THR
1	G	78	PRO
1	G	81	ARG
1	G	93	HIS
1	G	104	LEU
1	G	106	LYS
1	G	149	GLU
1	G	151	PHE
1	G	154	THR
1	G	162	ILE
1	G	174	PRO
1	G	194	THR
1	G	216	THR
1	G	218	VAL
1	H	4	LEU
1	H	51	THR
1	H	78	PRO

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Mol	Chain	Res	Type
1	H	81	ARG
1	H	93	HIS
1	H	104	LEU
1	H	106	LYS
1	H	149	GLU
1	H	151	PHE
1	H	154	THR
1	H	174	PRO
1	H	194	THR
1	H	216	THR
1	H	218	VAL
1	I	4	LEU
1	I	51	THR
1	I	78	PRO
1	I	81	ARG
1	I	93	HIS
1	I	104	LEU
1	I	106	LYS
1	I	149	GLU
1	I	151	PHE
1	I	154	THR
1	I	174	PRO
1	I	194	THR
1	I	216	THR
1	I	218	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	HIS
1	B	130	ASN
1	A	38	HIS
1	A	130	ASN
1	C	38	HIS
1	C	130	ASN
1	D	38	HIS
1	D	130	ASN
1	E	38	HIS
1	E	130	ASN
1	F	38	HIS
1	F	130	ASN
1	G	38	HIS

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Mol	Chain	Res	Type
1	G	130	ASN
1	H	38	HIS
1	H	130	ASN
1	I	38	HIS
1	I	130	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

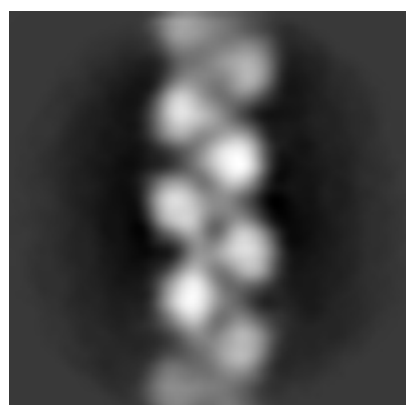
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11847. These allow visual inspection of the internal detail of the map and identification of artifacts.

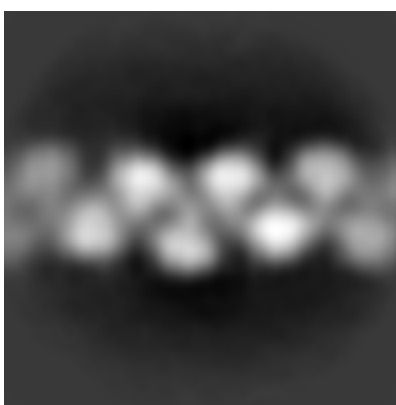
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

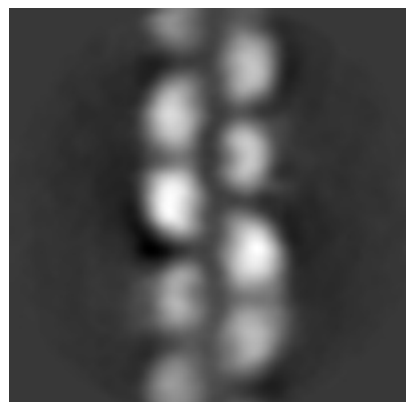


Z

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

### 6.2 Central slices [i](#)

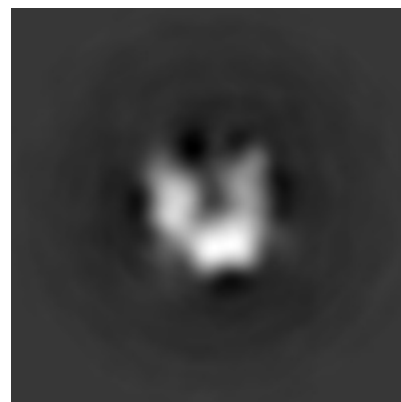
#### 6.2.1 Primary map



X Index: 32



Y Index: 32

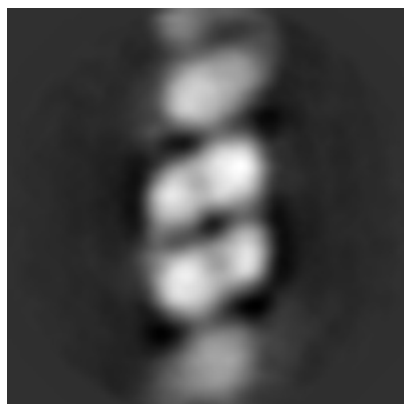


Z Index: 32

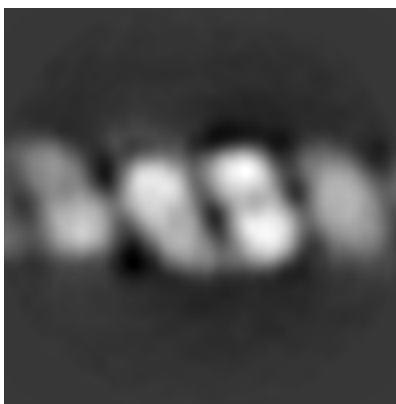
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

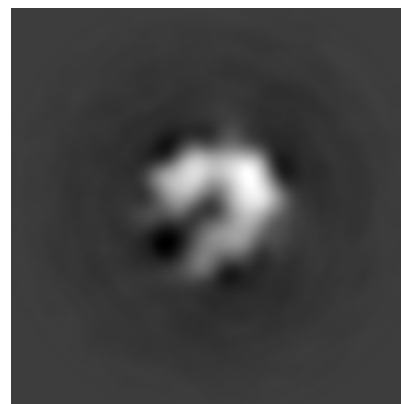
### 6.3.1 Primary map



X Index: 37



Y Index: 37



Z Index: 38

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

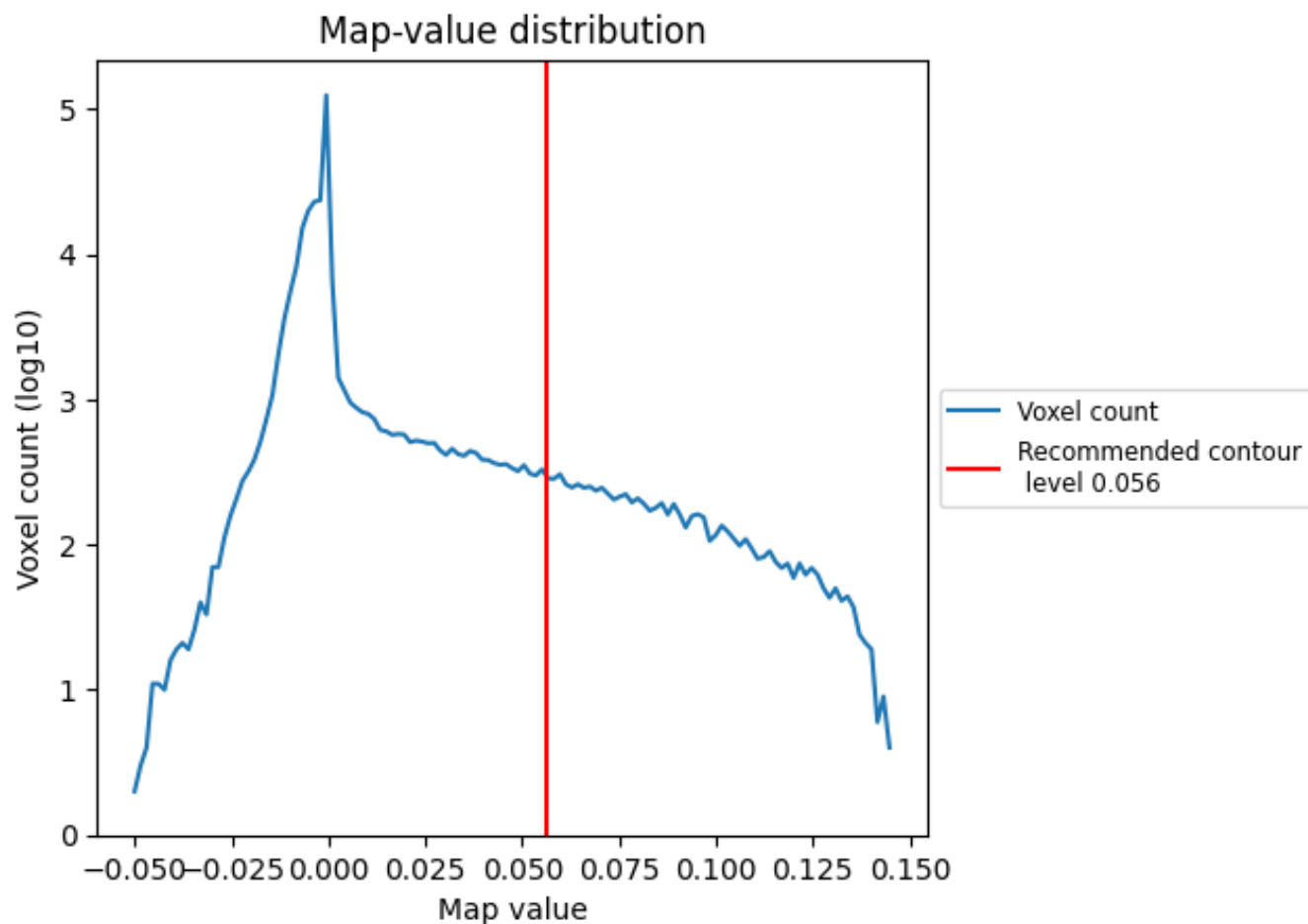
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

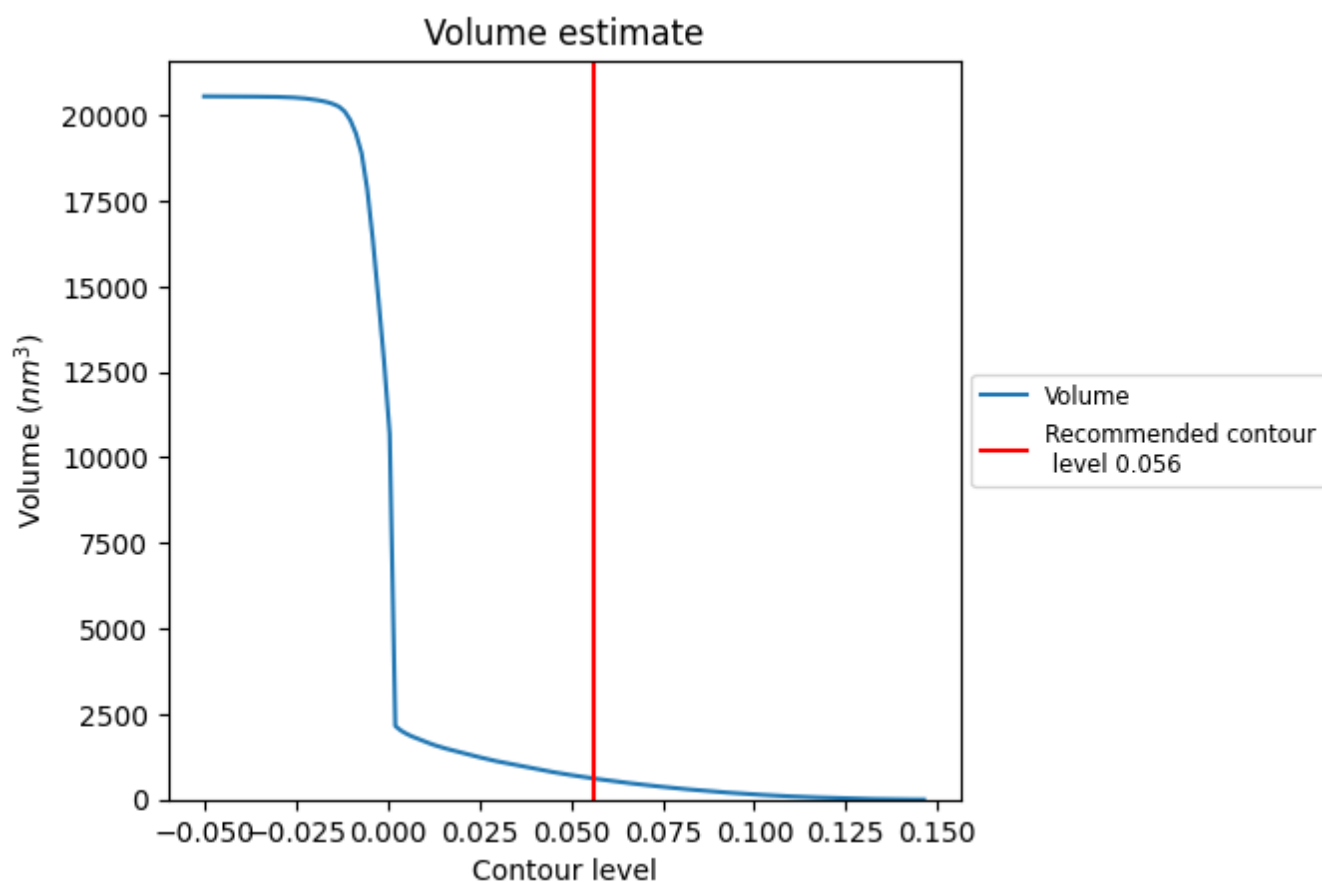
This section contains the results of statistical analysis of the map.

### 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.

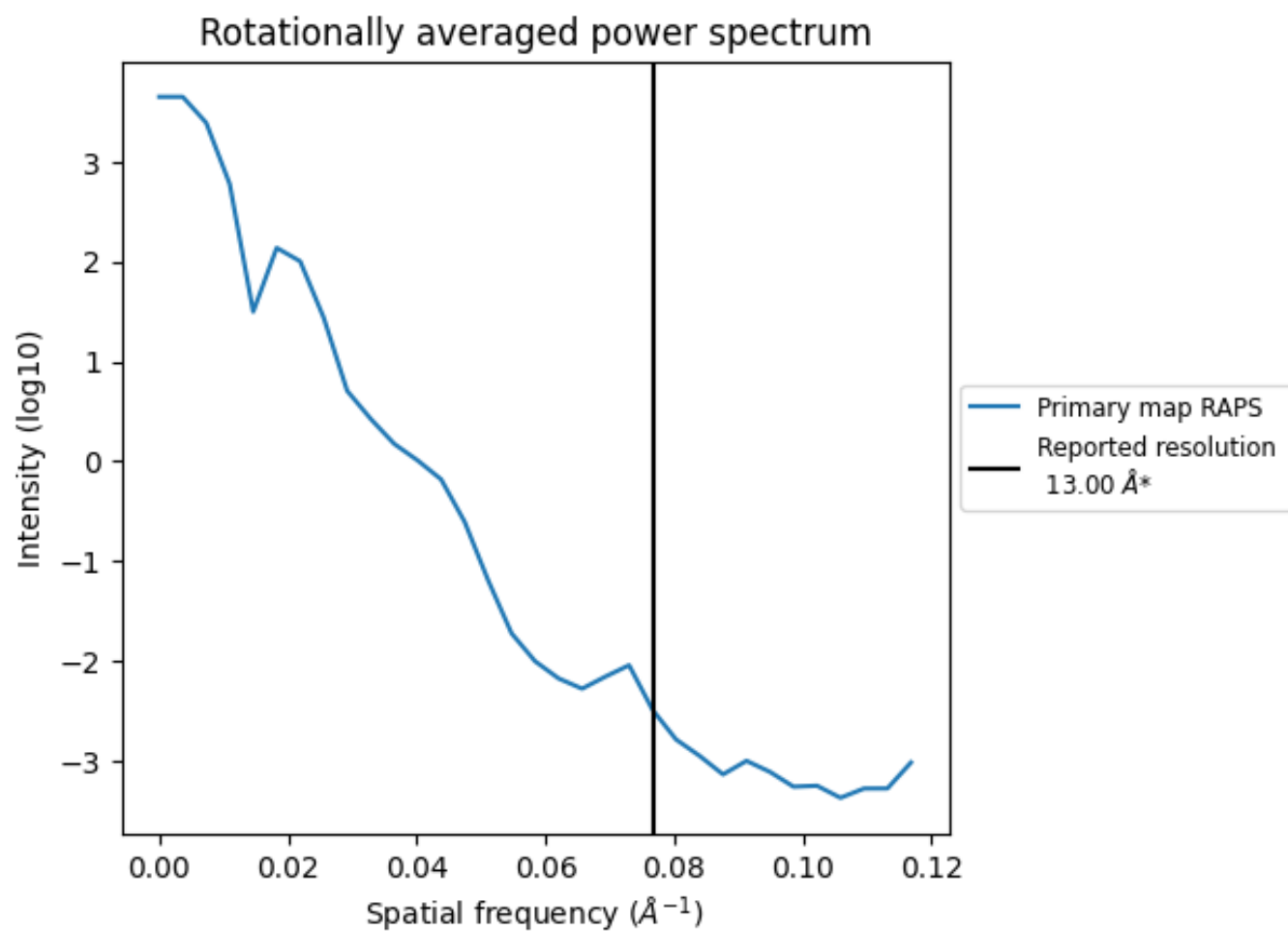
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm<sup>3</sup>; this corresponds to an approximate mass of 561 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 ⓘ



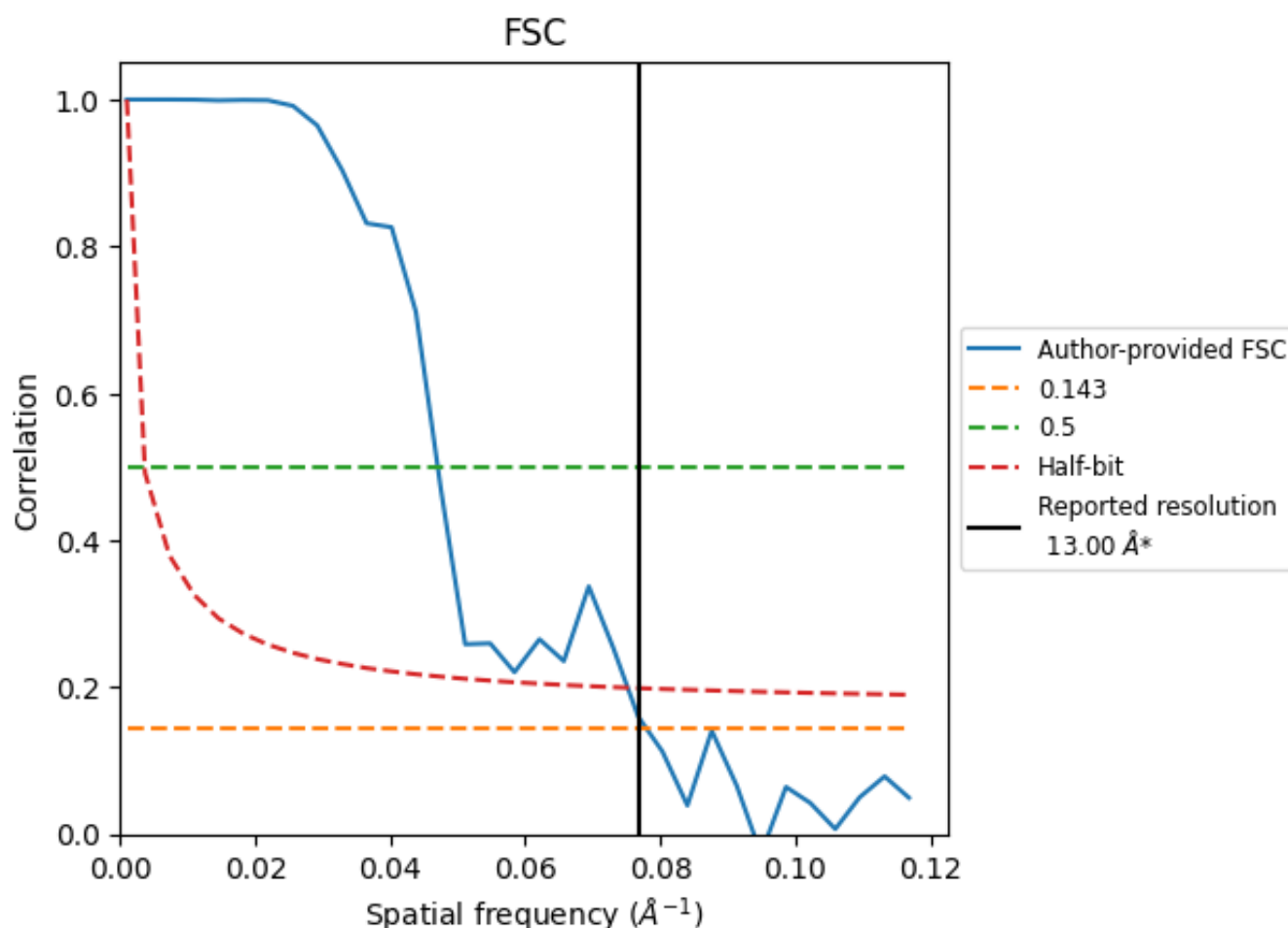
\*Reported resolution corresponds to spatial frequency of 0.077 Å<sup>-1</sup>



## 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 0.077  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

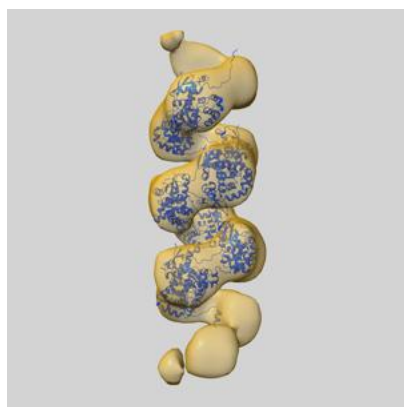
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	13.00	-	-
Author-provided FSC curve	12.84	21.28	13.32
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11847 and PDB model 7AOY. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

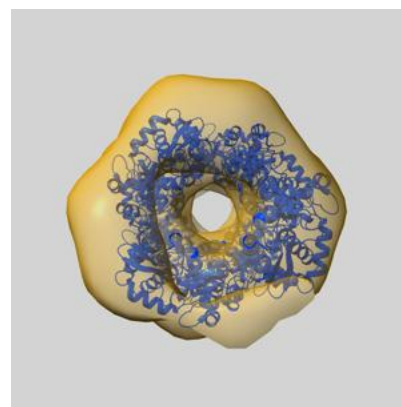
### 9.1 Map-model overlay [i](#)



X



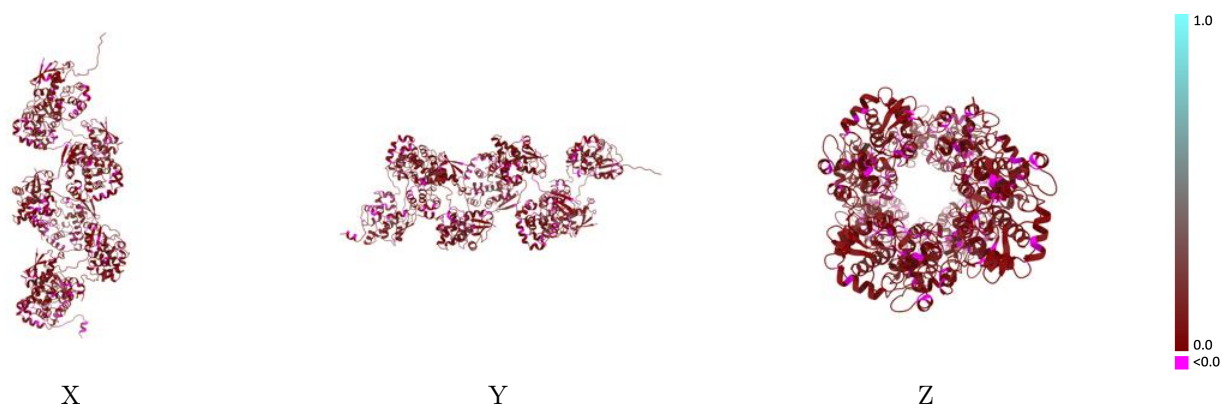
Y



Z

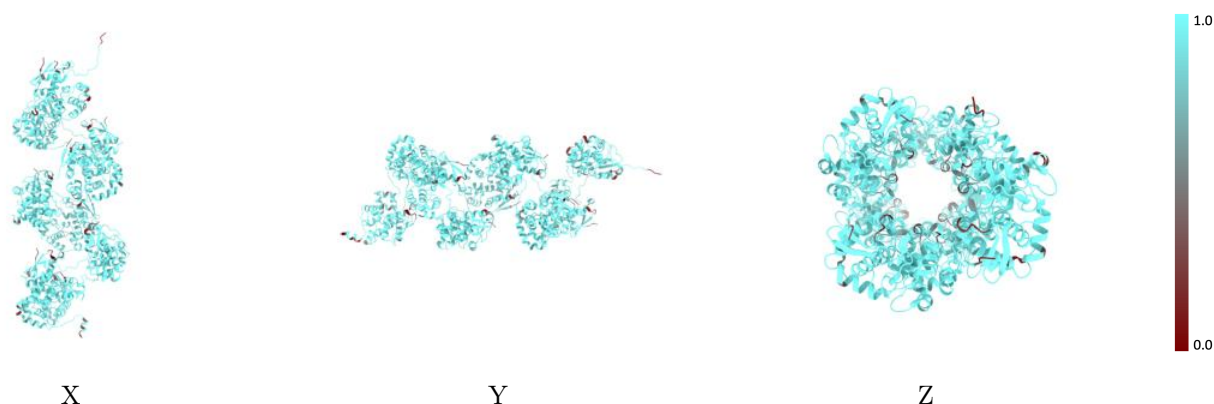
The images above show the 3D surface view of the map at the recommended contour level 0.056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



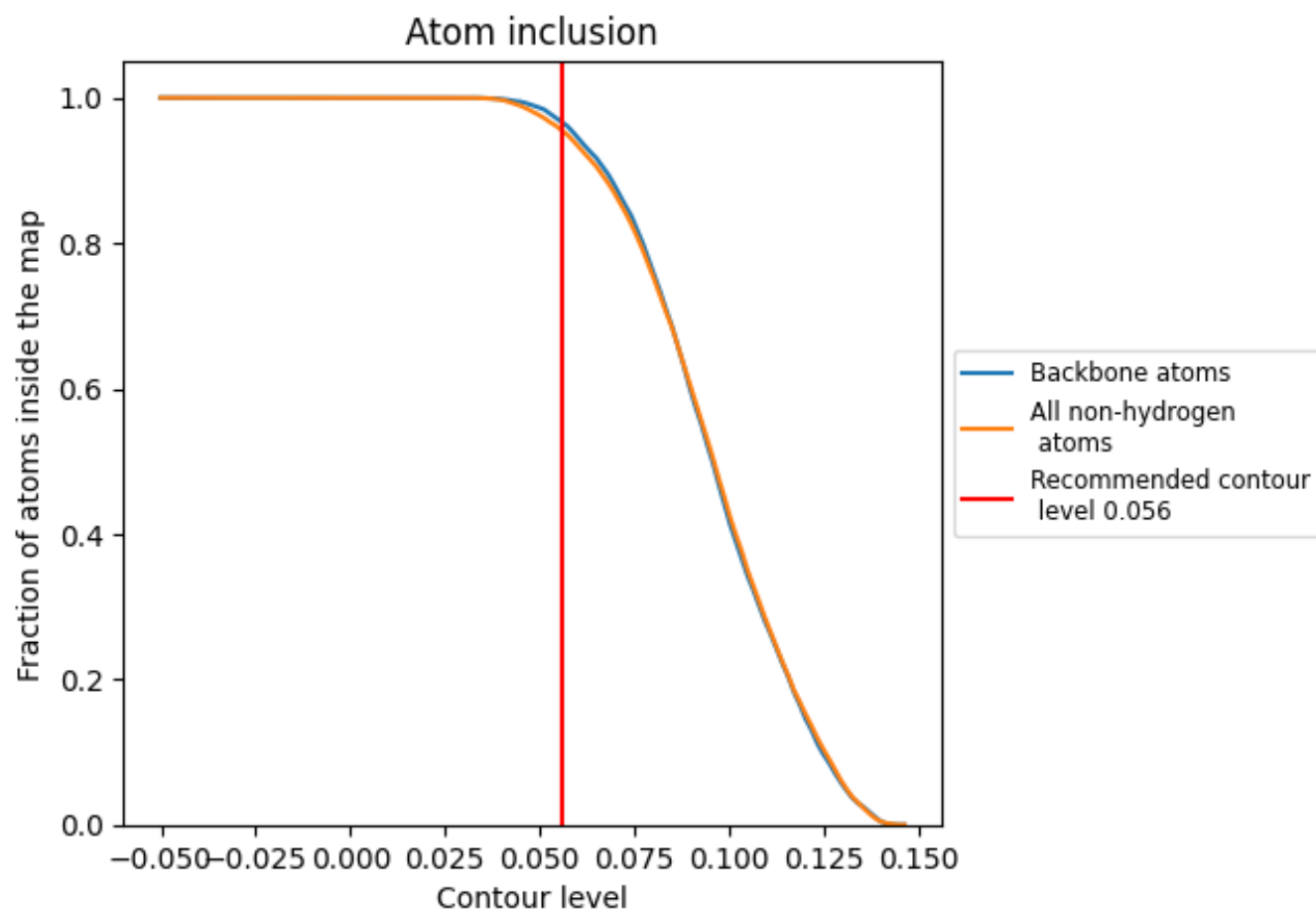
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.056).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9545</div>	<div><div></div>0.0720</div>
A	<div><div></div>0.9241</div>	<div><div></div>0.0730</div>
B	<div><div></div>0.9490</div>	<div><div></div>0.0760</div>
C	<div><div></div>0.9634</div>	<div><div></div>0.0720</div>
D	<div><div></div>0.9640</div>	<div><div></div>0.0710</div>
E	<div><div></div>0.9701</div>	<div><div></div>0.0720</div>
F	<div><div></div>0.9712</div>	<div><div></div>0.0710</div>
G	<div><div></div>0.9667</div>	<div><div></div>0.0720</div>
H	<div><div></div>0.9540</div>	<div><div></div>0.0740</div>
I	<div><div></div>0.9279</div>	<div><div></div>0.0710</div>

1.0

0.0

<0.0