



## Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 02:21 am GMT

PDB ID : 5UP4  
EMDB ID : EMD-8582  
Title : Structure of the HIV-1 Capsid Protein and spacer peptide 1 by Cryo-EM  
Authors : Perilla, J.R.; Schirra, R.; Zhang, P.; Schulten, K.  
Deposited on : 2017-02-01  
Resolution : 9.00 Å(reported)  
Based on initial models : 2KOD, 3J34

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:

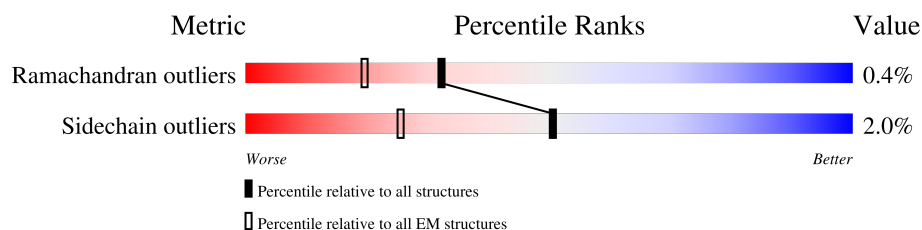
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 9.00 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	221	<div> <div>41%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	C	221	<div> <div>38%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	D	221	<div> <div>44%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	E	221	<div> <div>37%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	F	221	<div> <div>39%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	G	221	<div> <div>31%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	H	221	<div> <div>39%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	I	221	<div> <div>41%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	J	221	<div> <div>42%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	221	<div> <div>40%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	L	221	<div> <div>37%</div> <div>85%</div> <div>15%</div> <div>.</div> </div>
1	M	221	<div> <div>32%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	N	221	<div> <div>31%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	O	221	<div> <div>35%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	P	221	<div> <div>33%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	Q	221	<div> <div>29%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>
1	R	221	<div> <div>31%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	S	221	<div> <div>25%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31068 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 HIV-1 Capsid Protein and spacer peptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	K	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	L	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	M	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	N	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	O	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	P	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	Q	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	R	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	S	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	C	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	D	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	E	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	F	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	G	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	H	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	I	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		

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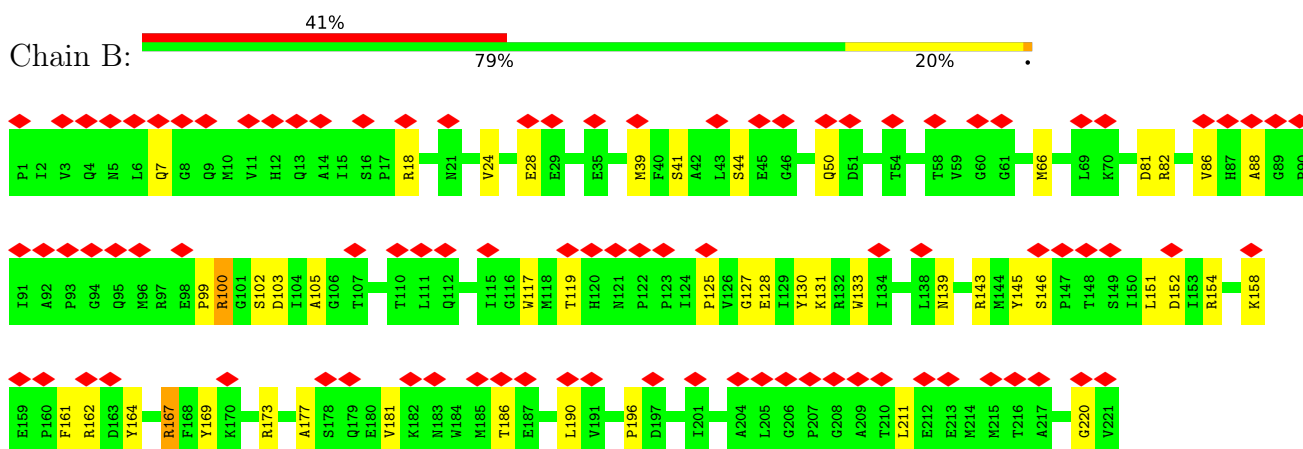
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		

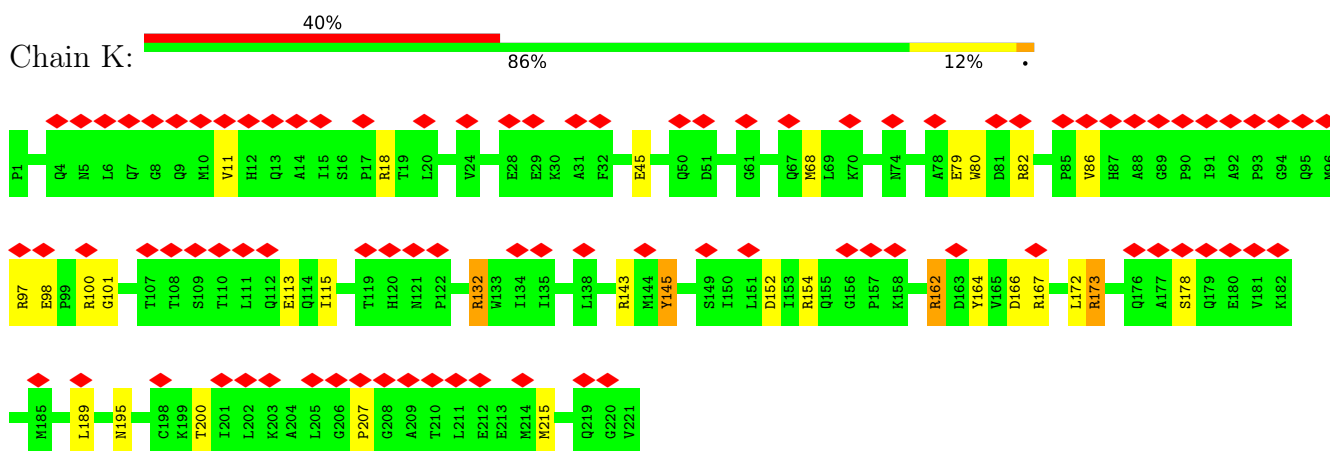
### 3 Residue-property plots

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.

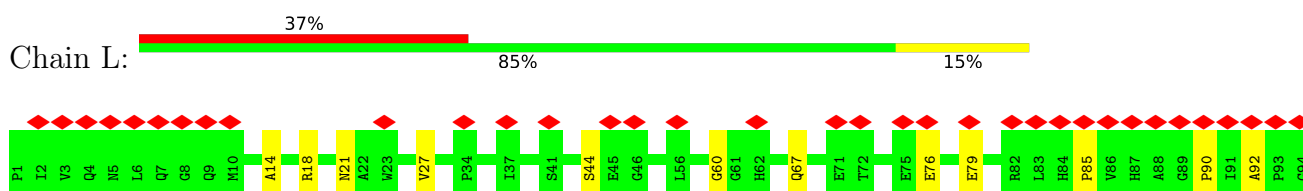
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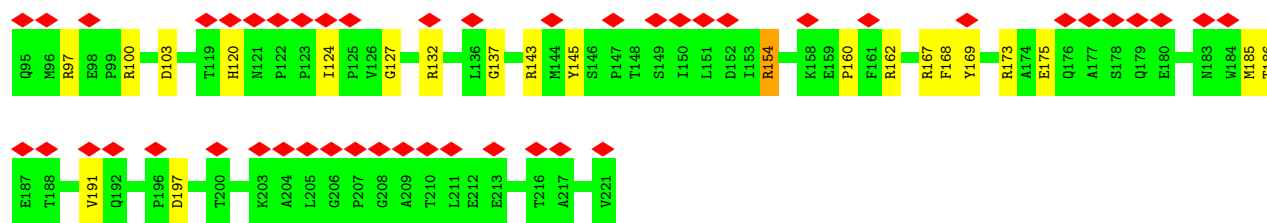


- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

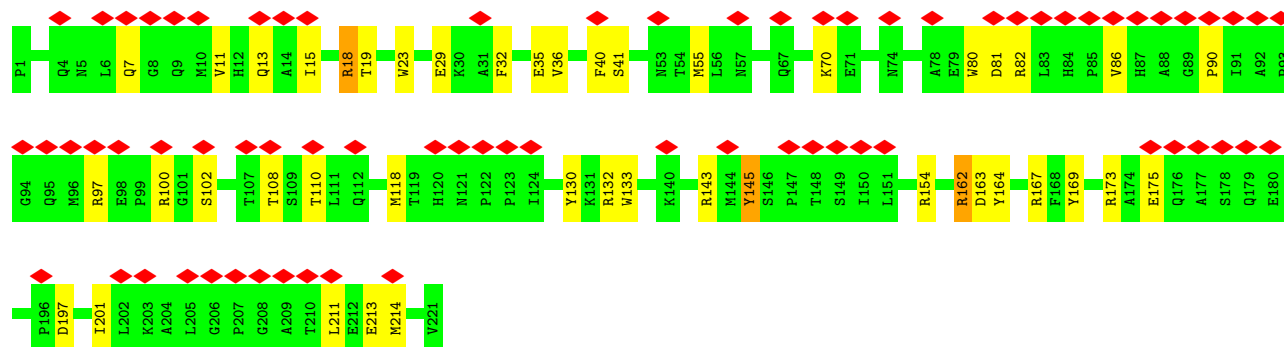
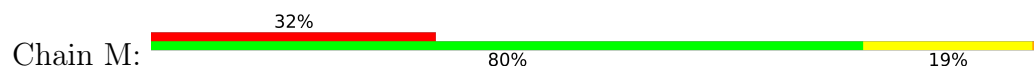


- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

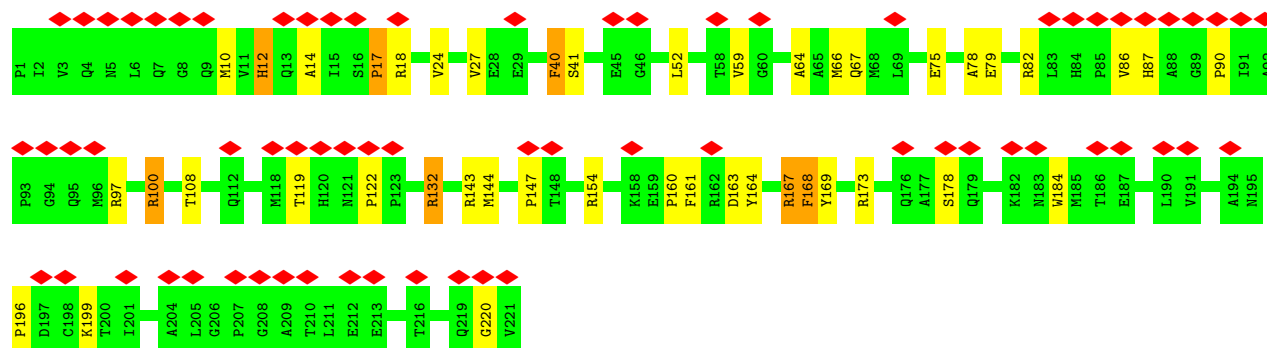
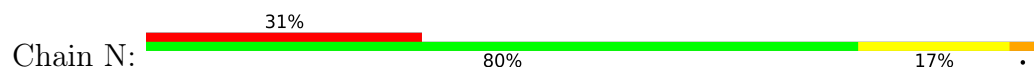




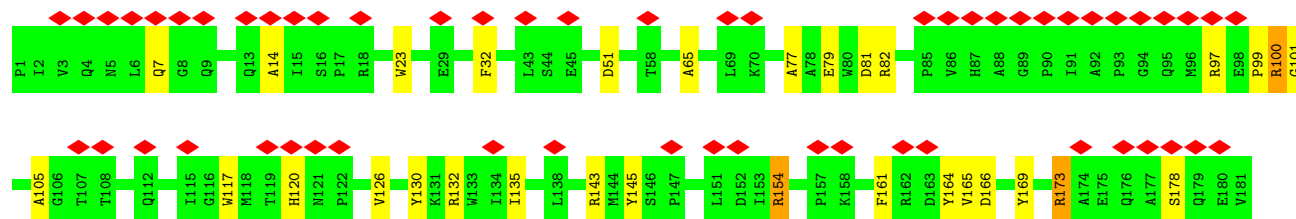
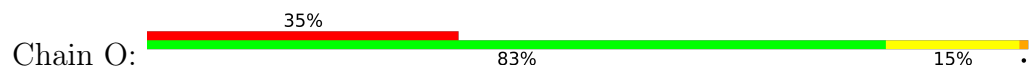
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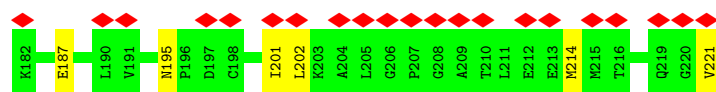


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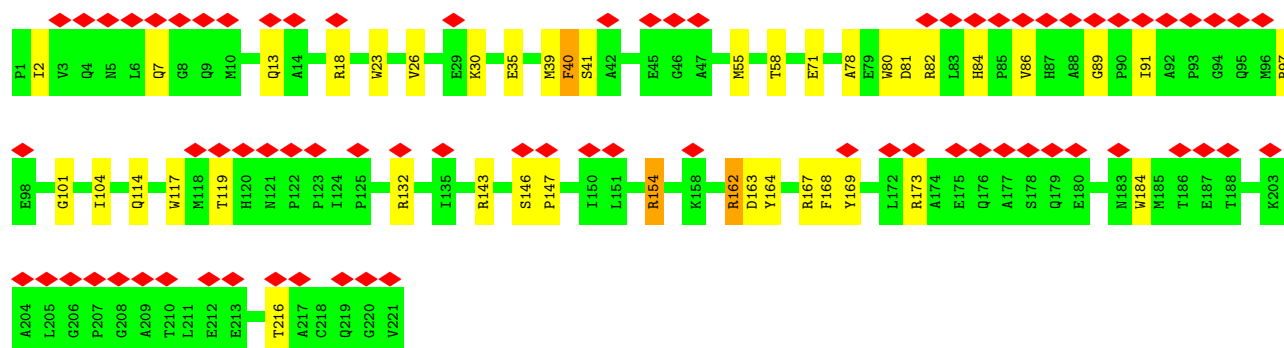
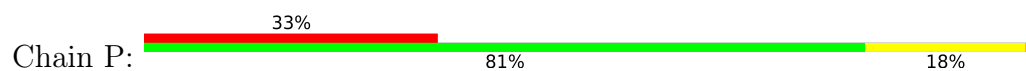


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

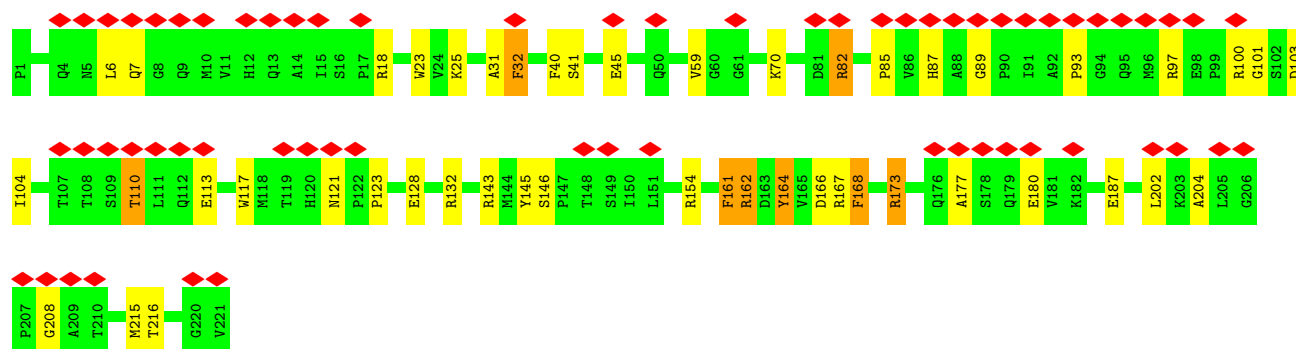
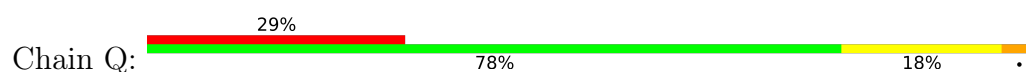




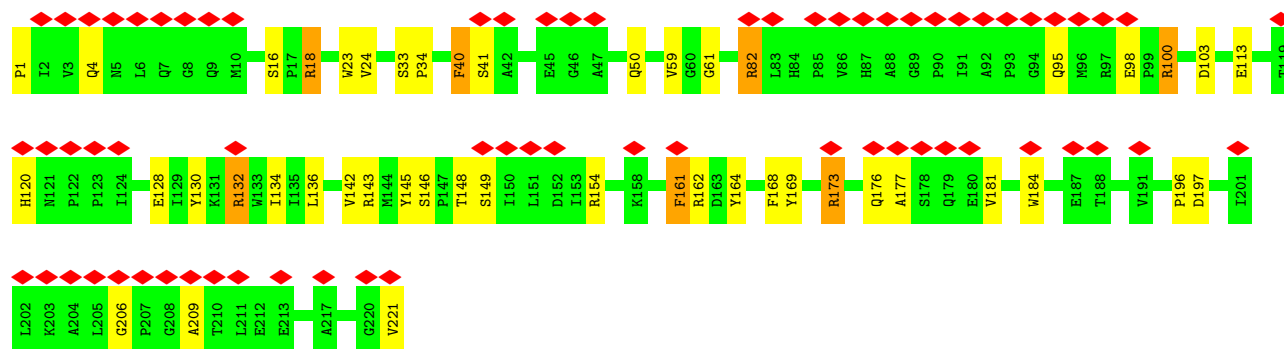
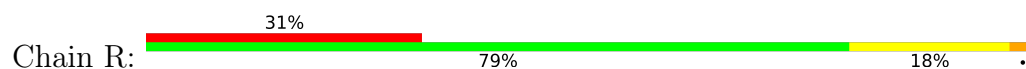
- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



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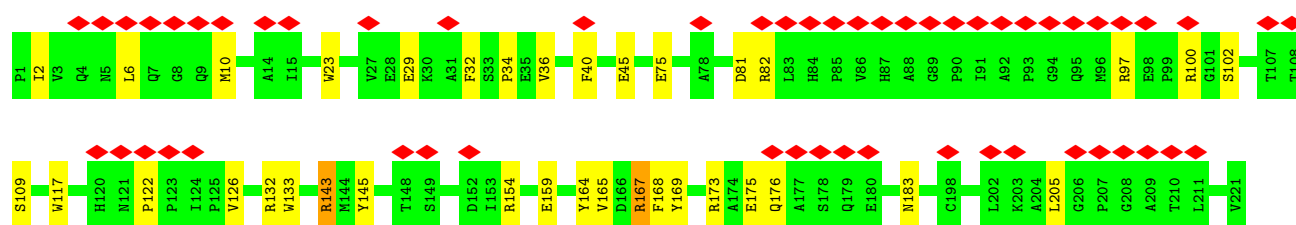
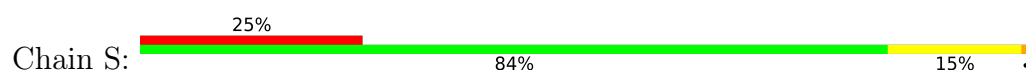


- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

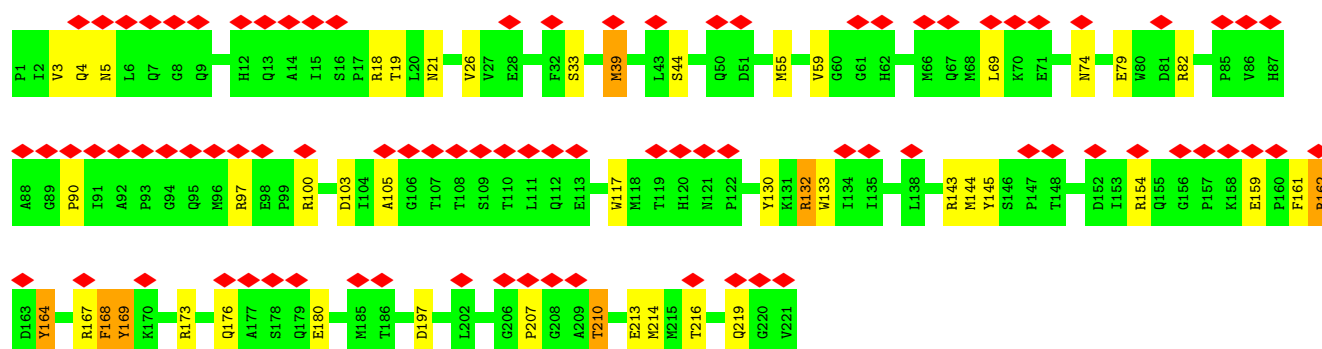
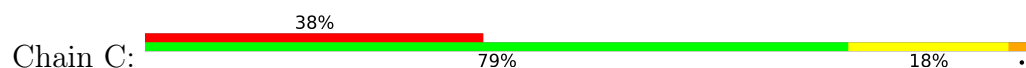


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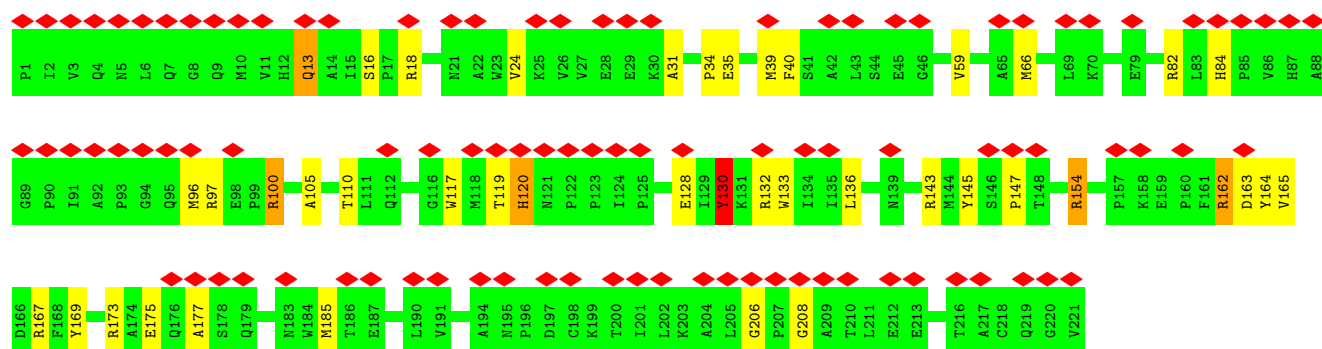
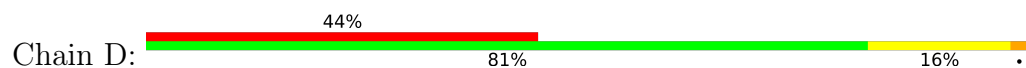




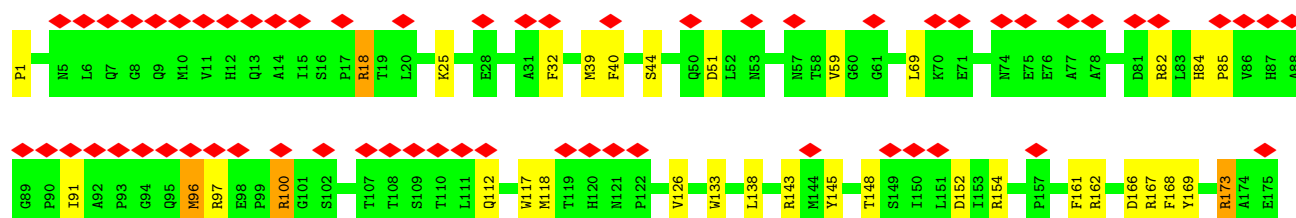
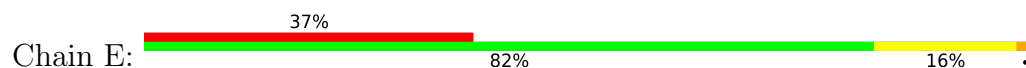
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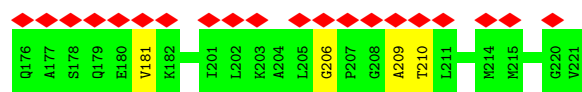


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

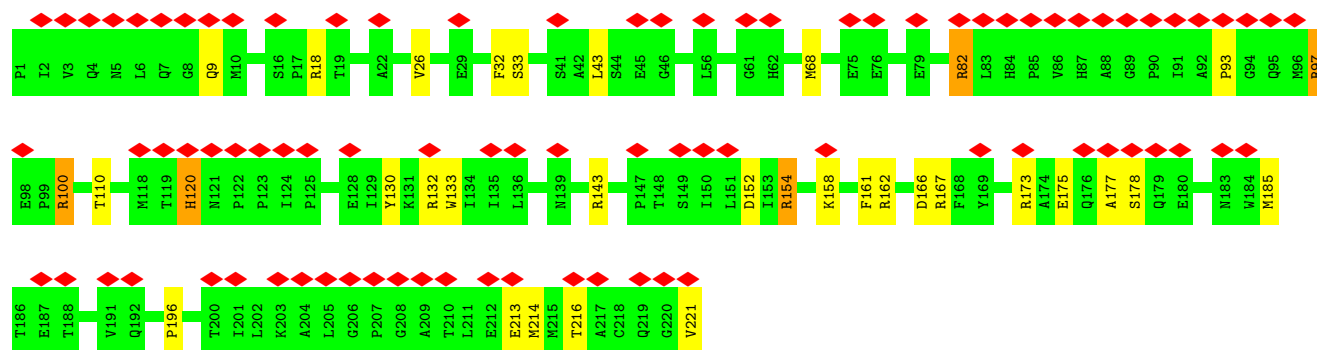
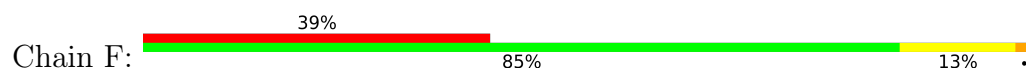


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

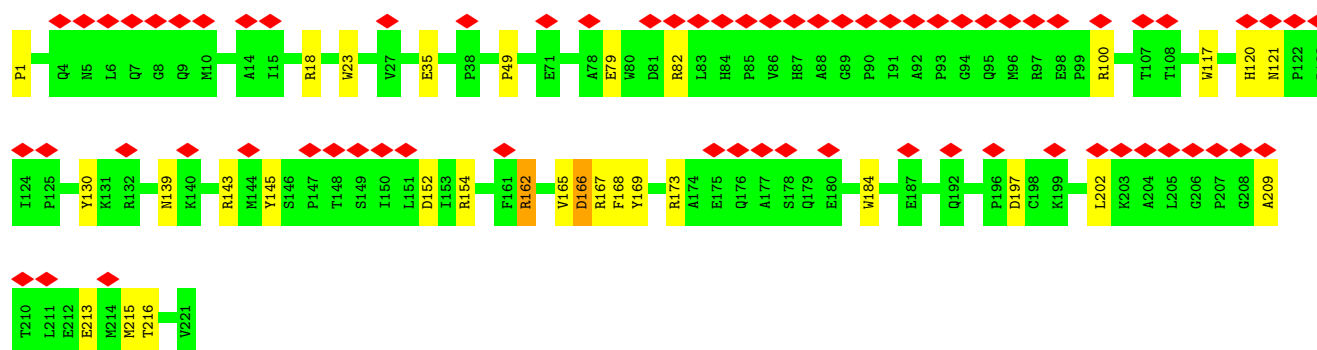
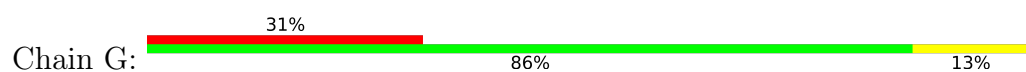




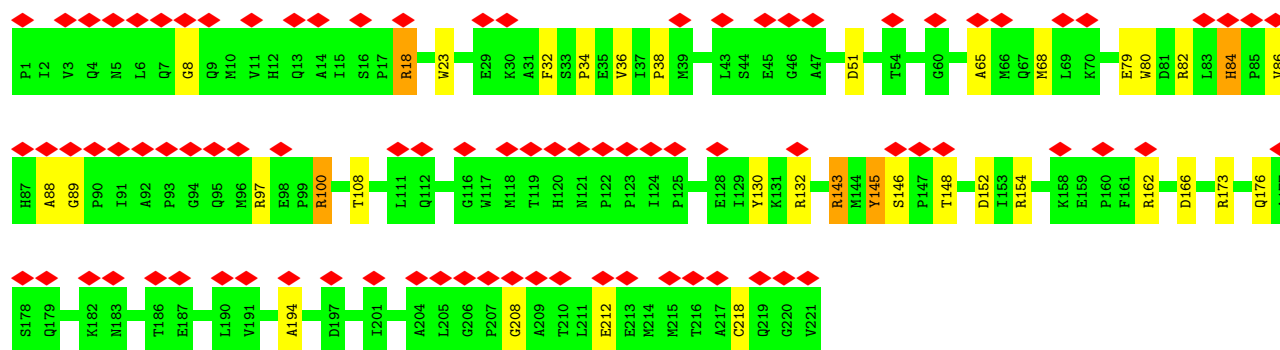
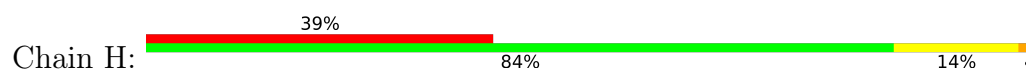
- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



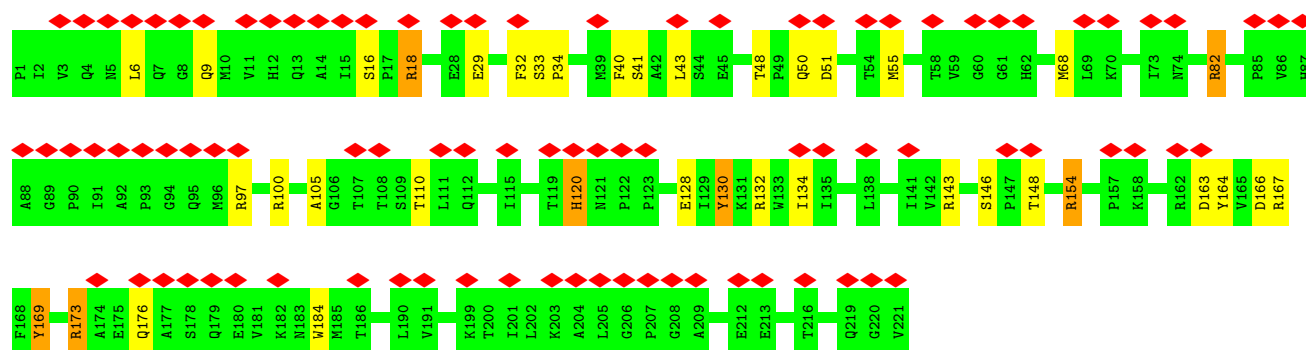
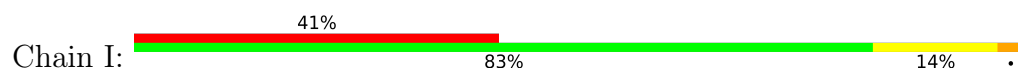
- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



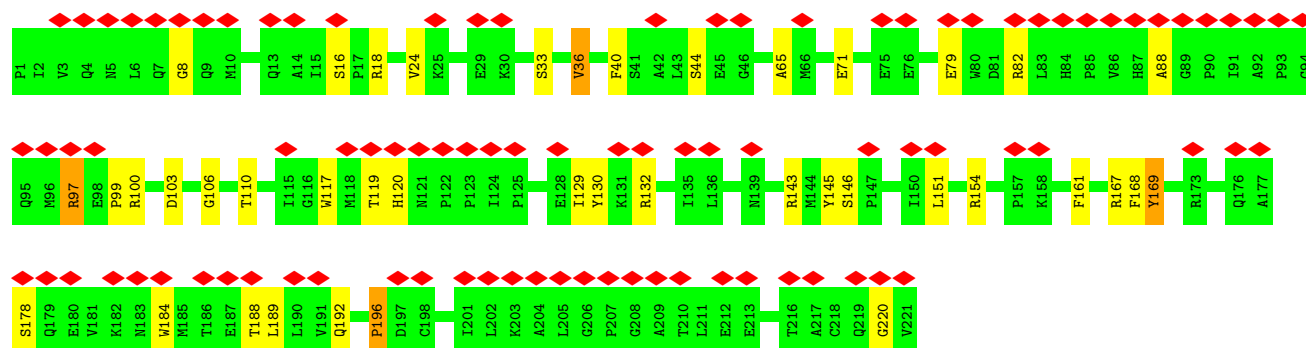
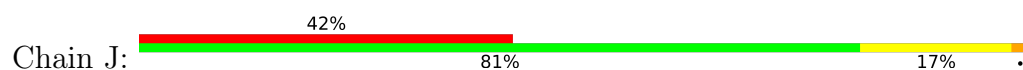
- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=128.88°, rise=13.46 Å, axial sym=C1	Depositor
Number of segments used	14000	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 ( $e^-/\text{\AA}^2$ )	23	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	545.60004, 545.60004, 545.60004	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	B	1.65	9/1765 (0.5%)	1.98	42/2398 (1.8%)
1	C	1.64	11/1765 (0.6%)	1.93	39/2398 (1.6%)
1	D	1.60	9/1765 (0.5%)	2.03	43/2398 (1.8%)
1	E	1.63	7/1765 (0.4%)	2.00	39/2398 (1.6%)
1	F	1.58	5/1765 (0.3%)	1.91	35/2398 (1.5%)
1	G	1.64	7/1765 (0.4%)	1.91	40/2398 (1.7%)
1	H	1.65	8/1765 (0.5%)	1.90	31/2398 (1.3%)
1	I	1.63	9/1765 (0.5%)	2.15	38/2398 (1.6%)
1	J	1.66	16/1765 (0.9%)	1.95	34/2398 (1.4%)
1	K	1.65	9/1765 (0.5%)	1.99	30/2398 (1.3%)
1	L	1.67	10/1765 (0.6%)	1.90	29/2398 (1.2%)
1	M	1.63	13/1765 (0.7%)	1.88	38/2398 (1.6%)
1	N	1.62	10/1765 (0.6%)	1.93	45/2398 (1.9%)
1	O	1.61	6/1765 (0.3%)	1.97	42/2398 (1.8%)
1	P	1.63	11/1765 (0.6%)	1.96	37/2398 (1.5%)
1	Q	1.60	14/1765 (0.8%)	2.04	37/2398 (1.5%)
1	R	1.67	15/1765 (0.8%)	1.89	32/2398 (1.3%)
1	S	1.64	13/1765 (0.7%)	2.04	37/2398 (1.5%)
All	All	1.63	182/31770 (0.6%)	1.97	668/43164 (1.5%)

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	B	0	3
1	C	0	7
1	D	0	7
1	E	0	5
1	F	0	5
1	H	0	7
1	I	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	K	0	6
1	L	0	1
1	M	0	6
1	N	0	6
1	O	0	5
1	P	0	3
1	Q	0	8
1	R	0	6
1	S	0	3
All	All	0	87

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	38	PRO	N-CD	-8.91	1.35	1.47
1	E	44	SER	CA-CB	8.81	1.66	1.52
1	H	8	GLY	CA-C	8.51	1.65	1.51
1	N	17	PRO	N-CD	-8.20	1.36	1.47
1	M	102	SER	CA-CB	8.07	1.65	1.52
1	H	23	TRP	CD2-CE2	7.99	1.50	1.41
1	O	178	SER	CA-CB	7.96	1.64	1.52
1	K	178	SER	CA-CB	7.78	1.64	1.52
1	L	127	GLY	CA-C	-7.72	1.39	1.51
1	G	168	PHE	CB-CG	7.68	1.64	1.51
1	P	23	TRP	NE1-CE2	-7.67	1.27	1.37
1	S	34	PRO	N-CD	-7.56	1.37	1.47
1	B	127	GLY	N-CA	7.33	1.57	1.46
1	S	109	SER	CA-CB	7.22	1.63	1.52
1	L	44	SER	CA-CB	7.21	1.63	1.52
1	I	16	SER	CA-CB	7.20	1.63	1.52
1	J	196	PRO	CA-C	-7.16	1.38	1.52
1	L	175	GLU	CD-OE1	7.09	1.33	1.25
1	J	8	GLY	CA-C	-6.97	1.40	1.51
1	M	169	TYR	CG-CD1	6.95	1.48	1.39
1	J	129	ILE	CA-CB	-6.87	1.39	1.54
1	C	161	PHE	CG-CD1	6.85	1.49	1.38
1	H	145	TYR	CB-CG	6.81	1.61	1.51
1	R	41	SER	CB-OG	6.81	1.51	1.42
1	J	106	GLY	CA-C	-6.79	1.41	1.51
1	L	85	PRO	N-CD	-6.61	1.38	1.47
1	B	28	GLU	CD-OE2	-6.59	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	178	SER	CA-CB	6.58	1.62	1.52
1	C	213	GLU	CG-CD	6.55	1.61	1.51
1	I	134	ILE	C-O	6.49	1.35	1.23
1	P	146	SER	CB-OG	6.47	1.50	1.42
1	L	145	TYR	CG-CD1	6.46	1.47	1.39
1	S	45	GLU	CG-CD	-6.43	1.42	1.51
1	R	146	SER	CA-CB	6.43	1.62	1.52
1	F	178	SER	CB-OG	6.42	1.50	1.42
1	E	1	PRO	N-CA	6.41	1.58	1.47
1	Q	45	GLU	C-N	6.38	1.44	1.33
1	I	34	PRO	N-CD	6.34	1.56	1.47
1	C	180	GLU	CG-CD	-6.32	1.42	1.51
1	M	175	GLU	CD-OE1	6.28	1.32	1.25
1	L	90	PRO	N-CD	6.26	1.56	1.47
1	O	130	TYR	CG-CD1	6.25	1.47	1.39
1	R	206	GLY	CA-C	-6.21	1.42	1.51
1	G	145	TYR	CE2-CZ	6.19	1.46	1.38
1	D	16	SER	CB-OG	6.18	1.50	1.42
1	O	101	GLY	CA-C	-6.17	1.42	1.51
1	Q	208	GLY	N-CA	6.14	1.55	1.46
1	P	80	TRP	CD2-CE2	6.09	1.48	1.41
1	J	146	SER	CA-CB	-6.04	1.43	1.52
1	Q	113	GLU	CD-OE2	6.04	1.32	1.25
1	P	132	ARG	CD-NE	6.00	1.56	1.46
1	D	165	VAL	CB-CG2	6.00	1.65	1.52
1	M	41	SER	CB-OG	6.00	1.50	1.42
1	R	120	HIS	CG-CD2	6.00	1.46	1.35
1	S	169	TYR	CG-CD1	6.00	1.47	1.39
1	I	120	HIS	CA-CB	6.00	1.67	1.53
1	P	184	TRP	NE1-CE2	-5.97	1.29	1.37
1	B	169	TYR	CE1-CZ	5.97	1.46	1.38
1	R	154	ARG	CA-CB	5.96	1.67	1.53
1	B	41	SER	CB-OG	5.94	1.50	1.42
1	K	79	GLU	CD-OE2	-5.93	1.19	1.25
1	G	169	TYR	CB-CG	5.92	1.60	1.51
1	H	89	GLY	C-N	5.92	1.45	1.34
1	L	60	GLY	CA-C	-5.90	1.42	1.51
1	J	40	PHE	CG-CD2	5.90	1.47	1.38
1	Q	117	TRP	CD2-CE3	-5.89	1.31	1.40
1	C	97	ARG	CZ-NH1	-5.87	1.25	1.33
1	O	164	TYR	CG-CD1	5.86	1.46	1.39
1	I	29	GLU	CA-CB	5.83	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	TYR	CE2-CZ	5.83	1.46	1.38
1	G	35	GLU	CB-CG	5.83	1.63	1.52
1	N	160	PRO	CA-C	-5.82	1.41	1.52
1	J	117	TRP	CD2-CE2	5.76	1.48	1.41
1	F	9	GLN	CG-CD	5.76	1.64	1.51
1	Q	32	PHE	CB-CG	-5.72	1.41	1.51
1	F	158	LYS	N-CA	-5.70	1.34	1.46
1	R	61	GLY	N-CA	5.70	1.54	1.46
1	Q	145	TYR	CG-CD2	5.67	1.46	1.39
1	R	128	GLU	CD-OE2	5.66	1.31	1.25
1	B	128	GLU	CD-OE2	5.66	1.31	1.25
1	S	122	PRO	CA-CB	5.66	1.64	1.53
1	M	213	GLU	CG-CD	-5.66	1.43	1.51
1	R	136	LEU	C-N	5.64	1.43	1.33
1	H	130	TYR	CG-CD1	5.59	1.46	1.39
1	I	43	LEU	CA-CB	5.58	1.66	1.53
1	O	169	TYR	CB-CG	5.57	1.60	1.51
1	Q	82	ARG	CB-CG	5.57	1.67	1.52
1	P	114	GLN	CG-CD	5.55	1.63	1.51
1	G	130	TYR	CE2-CZ	-5.54	1.31	1.38
1	M	163	ASP	CA-CB	5.53	1.66	1.53
1	N	18	ARG	CZ-NH1	5.52	1.40	1.33
1	S	143	ARG	CZ-NH2	-5.52	1.25	1.33
1	D	128	GLU	CD-OE2	-5.50	1.19	1.25
1	M	110	THR	CA-CB	5.49	1.67	1.53
1	J	16	SER	CA-CB	5.47	1.61	1.52
1	J	220	GLY	N-CA	5.47	1.54	1.46
1	D	34	PRO	N-CD	-5.47	1.40	1.47
1	N	164	TYR	CB-CG	-5.46	1.43	1.51
1	P	89	GLY	CA-C	-5.45	1.43	1.51
1	Q	128	GLU	CB-CG	5.45	1.62	1.52
1	D	206	GLY	N-CA	-5.44	1.37	1.46
1	E	145	TYR	CG-CD2	5.43	1.46	1.39
1	F	33	SER	CA-CB	5.42	1.61	1.52
1	Q	187	GLU	CG-CD	-5.41	1.43	1.51
1	S	6	LEU	CA-CB	5.41	1.66	1.53
1	K	101	GLY	CA-C	-5.40	1.43	1.51
1	C	145	TYR	CB-CG	-5.40	1.43	1.51
1	E	100	ARG	C-N	5.39	1.42	1.33
1	R	161	PHE	CG-CD1	5.38	1.46	1.38
1	K	115	ILE	CA-CB	-5.37	1.42	1.54
1	N	161	PHE	CG-CD1	5.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	145	TYR	CG-CD2	5.37	1.46	1.39
1	Q	123	PRO	N-CA	-5.36	1.38	1.47
1	S	117	TRP	CG-CD2	-5.36	1.34	1.43
1	M	145	TYR	CZ-OH	5.36	1.47	1.37
1	O	117	TRP	NE1-CE2	5.36	1.44	1.37
1	D	117	TRP	CZ2-CH2	5.34	1.47	1.37
1	Q	89	GLY	N-CA	5.34	1.54	1.46
1	L	137	GLY	N-CA	5.33	1.54	1.46
1	N	75	GLU	CD-OE1	5.33	1.31	1.25
1	N	199	LYS	CA-CB	5.33	1.65	1.53
1	J	154	ARG	CZ-NH2	-5.33	1.26	1.33
1	S	117	TRP	CG-CD1	5.29	1.44	1.36
1	R	154	ARG	CD-NE	5.29	1.55	1.46
1	R	113	GLU	CG-CD	-5.29	1.44	1.51
1	F	93	PRO	N-CD	-5.28	1.40	1.47
1	C	33	SER	CB-OG	5.26	1.49	1.42
1	D	24	VAL	CB-CG2	5.26	1.63	1.52
1	D	35	GLU	CB-CG	5.26	1.62	1.52
1	E	206	GLY	CA-C	5.26	1.60	1.51
1	J	145	TYR	CG-CD2	5.26	1.46	1.39
1	S	40	PHE	CA-CB	5.25	1.65	1.53
1	L	160	PRO	N-CD	-5.25	1.40	1.47
1	I	130	TYR	CG-CD2	5.25	1.46	1.39
1	D	164	TYR	CG-CD2	5.25	1.46	1.39
1	J	71	GLU	CD-OE2	5.24	1.31	1.25
1	E	133	TRP	NE1-CE2	5.24	1.44	1.37
1	J	44	SER	N-CA	5.23	1.56	1.46
1	S	82	ARG	CZ-NH1	-5.21	1.26	1.33
1	P	143	ARG	NE-CZ	5.21	1.39	1.33
1	P	35	GLU	CB-CG	5.20	1.62	1.52
1	M	145	TYR	CE1-CZ	5.20	1.45	1.38
1	C	44	SER	CA-CB	5.19	1.60	1.52
1	R	33	SER	CA-CB	5.18	1.60	1.52
1	M	164	TYR	CA-CB	5.18	1.65	1.53
1	C	117	TRP	CE2-CZ2	-5.18	1.30	1.39
1	G	1	PRO	N-CD	5.18	1.55	1.47
1	H	86	VAL	CB-CG2	5.18	1.63	1.52
1	B	99	PRO	N-CD	5.18	1.55	1.47
1	I	33	SER	CA-CB	5.18	1.60	1.52
1	K	113	GLU	CG-CD	5.17	1.59	1.51
1	J	36	VAL	CB-CG2	5.16	1.63	1.52
1	B	133	TRP	CG-CD2	5.15	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	102	SER	CB-OG	5.15	1.49	1.42
1	N	67	GLN	CA-CB	5.14	1.65	1.53
1	I	146	SER	CA-CB	5.14	1.60	1.52
1	B	146	SER	CB-OG	5.13	1.49	1.42
1	S	75	GLU	CB-CG	5.13	1.61	1.52
1	Q	101	GLY	CA-C	-5.12	1.43	1.51
1	H	208	GLY	CA-C	-5.12	1.43	1.51
1	N	12	HIS	CB-CG	5.11	1.59	1.50
1	J	33	SER	CA-CB	5.11	1.60	1.52
1	R	221	VAL	C-OXT	5.10	1.33	1.23
1	N	161	PHE	CG-CD2	5.10	1.46	1.38
1	K	98	GLU	CG-CD	-5.10	1.44	1.51
1	K	207	PRO	N-CA	5.09	1.55	1.47
1	G	184	TRP	CG-CD1	5.08	1.43	1.36
1	P	117	TRP	CG-CD2	-5.08	1.35	1.43
1	Q	93	PRO	C-N	5.07	1.42	1.33
1	L	79	GLU	CB-CG	5.07	1.61	1.52
1	Q	23	TRP	CZ2-CH2	5.05	1.47	1.37
1	M	35	GLU	CD-OE1	5.04	1.31	1.25
1	M	130	TYR	CE1-CZ	5.04	1.45	1.38
1	C	168	PHE	CG-CD1	5.04	1.46	1.38
1	K	145	TYR	CZ-OH	5.04	1.46	1.37
1	C	105	ALA	CA-CB	5.04	1.63	1.52
1	C	162	ARG	CD-NE	5.03	1.54	1.46
1	E	97	ARG	CZ-NH2	-5.03	1.26	1.33
1	R	16	SER	C-N	5.02	1.43	1.34
1	P	30	LYS	CB-CG	5.01	1.66	1.52
1	S	36	VAL	CB-CG2	5.00	1.63	1.52
1	K	45	GLU	CA-CB	5.00	1.65	1.53

All (668) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	97	ARG	NE-CZ-NH2	-24.06	108.27	120.30
1	D	162	ARG	NE-CZ-NH1	23.43	132.01	120.30
1	O	82	ARG	NE-CZ-NH2	-23.09	108.75	120.30
1	D	143	ARG	NE-CZ-NH1	22.89	131.75	120.30
1	B	173	ARG	NE-CZ-NH1	22.83	131.71	120.30
1	E	82	ARG	NE-CZ-NH1	22.10	131.35	120.30
1	L	173	ARG	NE-CZ-NH1	22.02	131.31	120.30
1	Q	154	ARG	NE-CZ-NH1	21.38	130.99	120.30
1	I	97	ARG	NE-CZ-NH1	21.37	130.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	173	ARG	NE-CZ-NH2	-21.02	109.79	120.30
1	S	167	ARG	NE-CZ-NH1	20.77	130.68	120.30
1	L	132	ARG	NE-CZ-NH1	20.50	130.55	120.30
1	I	167	ARG	NE-CZ-NH1	19.41	130.01	120.30
1	S	167	ARG	NE-CZ-NH2	-19.37	110.61	120.30
1	E	167	ARG	NE-CZ-NH1	19.20	129.90	120.30
1	S	100	ARG	NE-CZ-NH1	19.02	129.81	120.30
1	I	100	ARG	NE-CZ-NH1	18.90	129.75	120.30
1	I	82	ARG	NE-CZ-NH1	18.89	129.75	120.30
1	D	167	ARG	NE-CZ-NH1	18.81	129.70	120.30
1	Q	162	ARG	NE-CZ-NH1	18.57	129.59	120.30
1	D	162	ARG	NE-CZ-NH2	-18.35	111.12	120.30
1	Q	162	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	P	82	ARG	NE-CZ-NH1	18.24	129.42	120.30
1	I	173	ARG	NE-CZ-NH1	17.72	129.16	120.30
1	S	100	ARG	NE-CZ-NH2	-17.66	111.47	120.30
1	K	173	ARG	NE-CZ-NH2	-16.89	111.86	120.30
1	H	173	ARG	NE-CZ-NH1	16.70	128.65	120.30
1	F	132	ARG	NE-CZ-NH2	-16.70	111.95	120.30
1	B	173	ARG	NE-CZ-NH2	-16.51	112.05	120.30
1	C	173	ARG	NE-CZ-NH1	16.42	128.51	120.30
1	J	132	ARG	NE-CZ-NH1	16.19	128.39	120.30
1	J	100	ARG	NE-CZ-NH1	16.13	128.37	120.30
1	P	18	ARG	NE-CZ-NH1	16.00	128.30	120.30
1	H	97	ARG	NE-CZ-NH2	-15.63	112.49	120.30
1	K	100	ARG	NE-CZ-NH1	15.47	128.03	120.30
1	G	173	ARG	NE-CZ-NH2	-15.23	112.68	120.30
1	G	82	ARG	NE-CZ-NH1	15.17	127.89	120.30
1	K	82	ARG	NE-CZ-NH1	15.15	127.87	120.30
1	I	18	ARG	NE-CZ-NH1	15.13	127.86	120.30
1	I	82	ARG	NE-CZ-NH2	-14.99	112.80	120.30
1	I	100	ARG	NE-CZ-NH2	-14.72	112.94	120.30
1	N	97	ARG	NE-CZ-NH1	14.57	127.58	120.30
1	C	100	ARG	NE-CZ-NH1	14.23	127.42	120.30
1	K	132	ARG	NE-CZ-NH2	-14.15	113.23	120.30
1	P	169	TYR	CB-CG-CD1	-14.04	112.58	121.00
1	L	173	ARG	NE-CZ-NH2	-14.03	113.29	120.30
1	N	173	ARG	NE-CZ-NH1	13.75	127.17	120.30
1	E	143	ARG	NE-CZ-NH1	13.49	127.04	120.30
1	K	132	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	I	32	PHE	CB-CG-CD2	13.37	130.16	120.80
1	I	18	ARG	NE-CZ-NH2	-13.18	113.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	18	ARG	NE-CZ-NH1	13.17	126.88	120.30
1	C	132	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	O	173	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	O	51	ASP	CB-CG-OD1	12.56	129.60	118.30
1	S	81	ASP	CB-CG-OD1	-12.52	107.03	118.30
1	K	173	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	J	145	TYR	CB-CG-CD2	12.41	128.44	121.00
1	E	18	ARG	NE-CZ-NH2	-12.33	114.13	120.30
1	B	82	ARG	NE-CZ-NH1	12.27	126.43	120.30
1	P	132	ARG	NE-CZ-NH1	12.23	126.41	120.30
1	L	132	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	N	168	PHE	CB-CG-CD1	12.15	129.30	120.80
1	S	132	ARG	NE-CZ-NH2	-12.15	114.23	120.30
1	C	154	ARG	NE-CZ-NH1	12.13	126.36	120.30
1	M	82	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	J	100	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	R	130	TYR	CB-CG-CD2	-12.05	113.77	121.00
1	Q	173	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	H	173	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	D	167	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	E	145	TYR	CB-CG-CD2	-11.94	113.84	121.00
1	J	145	TYR	CB-CG-CD1	-11.92	113.85	121.00
1	B	162	ARG	NE-CZ-NH1	11.89	126.25	120.30
1	F	82	ARG	NE-CZ-NH2	11.80	126.20	120.30
1	E	82	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	M	167	ARG	NE-CZ-NH2	-11.49	114.55	120.30
1	I	154	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	F	97	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	R	162	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	Q	40	PHE	CB-CG-CD1	-11.21	112.95	120.80
1	G	173	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	F	167	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	F	167	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	B	167	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	D	97	ARG	NE-CZ-NH1	11.05	125.82	120.30
1	R	130	TYR	CB-CG-CD1	11.04	127.62	121.00
1	O	82	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	O	154	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	F	154	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	E	100	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	F	100	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	E	168	PHE	CB-CG-CD1	10.75	128.32	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	P	168	PHE	CB-CG-CD2	10.71	128.30	120.80
1	J	82	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	B	100	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	E	167	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	R	173	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	L	97	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	I	164	TYR	CB-CG-CD1	10.46	127.27	121.00
1	S	173	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	P	82	ARG	NH1-CZ-NH2	-10.43	107.93	119.40
1	N	168	PHE	CB-CG-CD2	-10.40	113.52	120.80
1	O	161	PHE	CB-CG-CD2	10.31	128.02	120.80
1	D	173	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	N	82	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	Q	18	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	J	169	TYR	CB-CG-CD2	-10.19	114.89	121.00
1	D	154	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	F	97	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	Q	100	ARG	NE-CZ-NH2	-10.05	115.28	120.30
1	F	130	TYR	CB-CG-CD1	10.04	127.03	121.00
1	L	100	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	D	143	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	L	167	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	J	97	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	S	81	ASP	CB-CG-OD2	9.91	127.22	118.30
1	Q	82	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	G	100	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	P	162	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	O	173	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	B	152	ASP	CB-CG-OD1	9.79	127.11	118.30
1	O	161	PHE	CB-CG-CD1	-9.78	113.95	120.80
1	N	173	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	S	97	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	G	82	ARG	NH1-CZ-NH2	-9.71	108.72	119.40
1	R	100	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	I	32	PHE	CB-CG-CD1	-9.66	114.04	120.80
1	F	82	ARG	NH1-CZ-NH2	-9.60	108.85	119.40
1	R	197	ASP	CB-CG-OD1	9.56	126.91	118.30
1	H	18	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	G	100	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	H	97	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	Q	173	ARG	NE-CZ-NH1	9.44	125.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	161	PHE	CB-CG-CD2	9.43	127.40	120.80
1	P	169	TYR	CG-CD1-CE1	-9.41	113.77	121.30
1	B	82	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	I	40	PHE	CB-CG-CD2	-9.25	114.33	120.80
1	F	132	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	K	167	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	N	143	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	C	18	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	Q	100	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	R	40	PHE	CB-CG-CD1	9.08	127.15	120.80
1	F	18	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	R	120	HIS	CA-CB-CG	9.05	128.99	113.60
1	B	145	TYR	CB-CG-CD1	9.04	126.42	121.00
1	E	154	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	O	100	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	H	82	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	K	215	MET	CG-SD-CE	-8.96	85.86	100.20
1	I	167	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	M	143	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	D	173	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	G	152	ASP	CB-CG-OD1	8.85	126.26	118.30
1	G	169	TYR	CB-CG-CD1	-8.78	115.73	121.00
1	M	164	TYR	CB-CG-CD1	-8.76	115.75	121.00
1	Q	164	TYR	CB-CG-CD1	8.67	126.20	121.00
1	R	168	PHE	CB-CG-CD1	-8.64	114.75	120.80
1	P	168	PHE	CB-CG-CD1	-8.61	114.77	120.80
1	J	97	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	M	18	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	S	154	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	B	154	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	D	18	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	R	161	PHE	CB-CG-CD2	-8.45	114.89	120.80
1	F	152	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	162	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	O	132	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	B	18	ARG	NE-CZ-NH2	8.33	124.46	120.30
1	B	100	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	H	162	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	Q	164	TYR	CB-CG-CD2	-8.29	116.03	121.00
1	Q	154	ARG	NH1-CZ-NH2	-8.27	110.30	119.40
1	F	82	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	C	162	ARG	NE-CZ-NH1	8.25	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	169	TYR	CB-CG-CD1	8.21	125.92	121.00
1	J	184	TRP	CB-CG-CD1	-8.17	116.38	127.00
1	M	40	PHE	CB-CG-CD1	-8.15	115.09	120.80
1	M	80	TRP	CB-CG-CD2	-8.13	116.03	126.60
1	C	161	PHE	CB-CG-CD2	-8.12	115.11	120.80
1	Q	168	PHE	CB-CG-CD1	8.11	126.47	120.80
1	H	51	ASP	CB-CG-OD1	8.09	125.58	118.30
1	S	168	PHE	CB-CG-CD2	8.07	126.45	120.80
1	D	132	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	E	152	ASP	CB-CG-OD2	7.98	125.48	118.30
1	G	145	TYR	CB-CG-CD1	7.98	125.79	121.00
1	I	68	MET	CG-SD-CE	-7.95	87.49	100.20
1	O	145	TYR	CB-CG-CD2	-7.91	116.25	121.00
1	N	161	PHE	CB-CG-CD2	7.88	126.31	120.80
1	O	132	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	M	40	PHE	CB-CG-CD2	7.81	126.27	120.80
1	M	82	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	E	168	PHE	CB-CG-CD2	-7.78	115.35	120.80
1	G	165	VAL	CG1-CB-CG2	-7.75	98.50	110.90
1	N	167	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	G	167	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	K	143	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	F	110	THR	CA-CB-CG2	-7.62	101.73	112.40
1	O	130	TYR	CB-CG-CD2	7.58	125.55	121.00
1	S	154	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	F	133	TRP	CB-CG-CD2	-7.57	116.77	126.60
1	Q	110	THR	CA-CB-OG1	7.56	124.88	109.00
1	M	80	TRP	CB-CG-CD1	7.56	136.83	127.00
1	O	100	ARG	NH1-CZ-NH2	-7.56	111.09	119.40
1	N	132	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	D	164	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	E	39	MET	CG-SD-CE	-7.54	88.14	100.20
1	I	166	ASP	CB-CG-OD2	7.53	125.08	118.30
1	B	145	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	G	167	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	Q	145	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	K	152	ASP	CB-CG-OD1	7.46	125.01	118.30
1	C	197	ASP	CB-CG-OD1	-7.46	111.59	118.30
1	F	120	HIS	CA-CB-CG	7.46	126.28	113.60
1	R	132	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	E	162	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	Q	215	MET	CG-SD-CE	-7.38	88.39	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	168	PHE	CB-CG-CD1	-7.38	115.63	120.80
1	P	97	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	66	MET	CG-SD-CE	-7.35	88.43	100.20
1	G	215	MET	CG-SD-CE	-7.32	88.48	100.20
1	D	82	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	R	103	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	F	162	ARG	CG-CD-NE	-7.27	96.54	111.80
1	K	100	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	E	32	PHE	N-CA-CB	7.18	123.52	110.60
1	N	66	MET	CG-SD-CE	-7.17	88.73	100.20
1	E	209	ALA	CB-CA-C	7.13	120.79	110.10
1	H	65	ALA	N-CA-CB	-7.12	100.13	110.10
1	K	68	MET	CA-CB-CG	7.09	125.36	113.30
1	C	59	VAL	CA-CB-CG2	-7.09	100.27	110.90
1	D	100	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	K	166	ASP	CB-CG-OD2	7.07	124.66	118.30
1	S	23	TRP	CB-CG-CD1	-7.07	117.81	127.00
1	J	132	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	P	163	ASP	CB-CG-OD1	7.06	124.65	118.30
1	F	130	TYR	CB-CG-CD2	-7.05	116.77	121.00
1	H	100	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	Q	97	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	J	168	PHE	CB-CG-CD2	7.02	125.71	120.80
1	H	68	MET	CG-SD-CE	-7.01	88.98	100.20
1	R	162	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	K	162	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	M	143	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	H	130	TYR	CB-CG-CD2	6.96	125.17	121.00
1	M	197	ASP	CB-CG-OD1	6.91	124.51	118.30
1	C	132	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	L	103	ASP	O-C-N	-6.89	111.68	122.70
1	N	100	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	P	81	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	E	51	ASP	CB-CG-OD1	6.84	124.45	118.30
1	S	132	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	F	133	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	M	201	ILE	CA-CB-CG1	6.79	123.91	111.00
1	L	185	MET	CG-SD-CE	-6.77	89.37	100.20
1	F	18	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	I	132	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	N	52	LEU	CB-CG-CD1	6.75	122.47	111.00
1	P	167	ARG	NE-CZ-NH2	-6.74	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	40	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	D	143	ARG	NH1-CZ-NH2	-6.69	112.04	119.40
1	J	130	TYR	CB-CG-CD1	6.69	125.01	121.00
1	S	117	TRP	CH2-CZ2-CE2	-6.68	110.72	117.40
1	O	166	ASP	CB-CG-OD1	6.67	124.30	118.30
1	N	100	ARG	NH1-CZ-NH2	-6.66	112.07	119.40
1	N	143	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	E	126	VAL	CA-CB-CG1	-6.65	100.93	110.90
1	H	79	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	R	23	TRP	O-C-N	-6.64	112.07	122.70
1	M	164	TYR	CB-CG-CD2	6.60	124.96	121.00
1	D	164	TYR	CB-CG-CD2	6.59	124.95	121.00
1	E	181	VAL	CA-CB-CG2	-6.57	101.05	110.90
1	P	167	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	G	154	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	L	191	VAL	CG1-CB-CG2	-6.54	100.43	110.90
1	K	18	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	J	8	GLY	O-C-N	-6.53	112.25	122.70
1	D	143	ARG	CD-NE-CZ	6.52	132.72	123.60
1	K	162	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	Q	166	ASP	CB-CG-OD1	6.51	124.16	118.30
1	N	87	HIS	N-CA-CB	6.50	122.30	110.60
1	E	100	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	P	55	MET	CG-SD-CE	6.49	110.58	100.20
1	L	168	PHE	CB-CG-CD2	6.49	125.34	120.80
1	C	216	THR	CA-CB-CG2	-6.47	103.34	112.40
1	C	26	VAL	CA-CB-CG2	-6.47	101.20	110.90
1	E	91	ILE	N-CA-C	-6.47	93.54	111.00
1	G	130	TYR	CG-CD1-CE1	-6.47	116.13	121.30
1	I	169	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	N	18	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	P	7	GLN	N-CA-C	6.43	128.36	111.00
1	D	185	MET	CG-SD-CE	-6.42	89.92	100.20
1	B	103	ASP	CB-CG-OD1	6.40	124.06	118.30
1	O	201	ILE	O-C-N	-6.40	112.45	122.70
1	J	119	THR	CA-CB-CG2	-6.39	103.45	112.40
1	M	110	THR	CA-CB-CG2	-6.39	103.46	112.40
1	O	117	TRP	CD1-CG-CD2	6.38	111.40	106.30
1	D	169	TYR	CZ-CE2-CD2	-6.38	114.06	119.80
1	Q	145	TYR	CB-CG-CD1	6.38	124.83	121.00
1	Q	167	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	G	130	TYR	CD1-CE1-CZ	6.37	125.54	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	194	ALA	N-CA-CB	6.37	119.02	110.10
1	K	86	VAL	CG1-CB-CG2	-6.36	100.73	110.90
1	N	169	TYR	CD1-CE1-CZ	6.36	125.52	119.80
1	L	103	ASP	CB-CG-OD1	6.36	124.02	118.30
1	M	154	ARG	O-C-N	-6.35	112.54	122.70
1	C	173	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	G	143	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	S	133	TRP	CE3-CZ3-CH2	-6.34	114.22	121.20
1	I	105	ALA	N-CA-CB	-6.33	101.24	110.10
1	O	195	ASN	CA-CB-CG	6.32	127.31	113.40
1	J	18	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	66	MET	CG-SD-CE	-6.32	90.09	100.20
1	L	168	PHE	CB-CG-CD1	-6.32	116.38	120.80
1	M	23	TRP	CH2-CZ2-CE2	6.31	123.71	117.40
1	O	145	TYR	CB-CG-CD1	6.31	124.78	121.00
1	P	154	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	I	173	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
1	B	117	TRP	CD1-CG-CD2	6.29	111.33	106.30
1	I	51	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	S	145	TYR	CG-CD2-CE2	-6.27	116.29	121.30
1	L	132	ARG	CD-NE-CZ	6.26	132.37	123.60
1	O	202	LEU	CB-CG-CD2	6.26	121.65	111.00
1	J	189	LEU	CB-CG-CD2	6.26	121.64	111.00
1	R	169	TYR	CB-CG-CD1	6.26	124.75	121.00
1	H	18	ARG	CD-NE-CZ	6.26	132.36	123.60
1	P	173	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	L	169	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	H	36	VAL	CA-CB-CG2	-6.25	101.53	110.90
1	F	100	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	E	161	PHE	CB-CG-CD1	-6.18	116.47	120.80
1	G	145	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	Q	202	LEU	CB-CG-CD1	6.17	121.49	111.00
1	N	122	PRO	N-CA-CB	6.17	110.70	103.30
1	J	40	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	P	18	ARG	NH1-CZ-NH2	-6.15	112.63	119.40
1	I	132	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	K	82	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
1	F	185	MET	CG-SD-CE	-6.14	90.37	100.20
1	Q	104	ILE	O-C-N	-6.13	112.88	122.70
1	J	130	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	B	119	THR	CA-CB-CG2	-6.13	103.82	112.40
1	J	65	ALA	N-CA-CB	-6.13	101.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	143	ARG	NH1-CZ-NH2	-6.13	112.66	119.40
1	H	143	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	K	18	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	M	154	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	O	214	MET	CG-SD-CE	-6.11	90.43	100.20
1	D	117	TRP	CG-CD2-CE3	-6.10	128.41	133.90
1	B	39	MET	CG-SD-CE	-6.09	90.46	100.20
1	R	143	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	L	14	ALA	N-CA-CB	6.07	118.60	110.10
1	N	14	ALA	O-C-N	-6.07	112.99	122.70
1	G	139	ASN	CB-CG-ND2	6.07	131.26	116.70
1	I	132	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	M	162	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	J	161	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	M	55	MET	CG-SD-CE	-6.05	90.52	100.20
1	N	108	THR	CA-CB-CG2	-6.05	103.93	112.40
1	O	154	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	M	81	ASP	CB-CG-OD1	6.04	123.73	118.30
1	R	149	SER	N-CA-CB	-6.03	101.45	110.50
1	O	130	TYR	CG-CD2-CE2	6.02	126.12	121.30
1	B	44	SER	N-CA-CB	6.02	119.53	110.50
1	S	82	ARG	CD-NE-CZ	6.02	132.03	123.60
1	L	154	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	Q	59	VAL	O-C-N	-6.02	112.97	123.20
1	C	161	PHE	CB-CG-CD1	6.02	125.01	120.80
1	F	152	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	S	117	TRP	CE2-CD2-CG	6.00	112.10	107.30
1	S	175	GLU	OE1-CD-OE2	-5.99	116.12	123.30
1	H	32	PHE	CB-CG-CD2	-5.99	116.61	120.80
1	O	105	ALA	N-CA-CB	5.96	118.44	110.10
1	B	88	ALA	C-N-CA	5.94	134.78	122.30
1	D	163	ASP	CB-CG-OD2	5.94	123.64	118.30
1	M	167	ARG	CD-NE-CZ	5.94	131.91	123.60
1	E	18	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	P	80	TRP	CB-CG-CD1	5.92	134.70	127.00
1	K	166	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	D	105	ALA	CB-CA-C	5.91	118.97	110.10
1	C	167	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	C	5	ASN	O-C-N	-5.89	113.27	122.70
1	K	97	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	M	86	VAL	CB-CA-C	5.89	122.59	111.40
1	O	100	ARG	NE-CZ-NH2	5.89	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	209	ALA	CB-CA-C	-5.89	101.27	110.10
1	O	65	ALA	N-CA-CB	-5.88	101.86	110.10
1	D	169	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	K	97	ARG	CD-NE-CZ	5.87	131.82	123.60
1	F	32	PHE	CB-CG-CD1	5.87	124.91	120.80
1	I	110	THR	N-CA-CB	5.86	121.43	110.30
1	N	178	SER	O-C-N	-5.86	113.33	122.70
1	B	133	TRP	CD2-CE2-CZ2	-5.85	115.28	122.30
1	N	154	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	M	132	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	I	154	ARG	NH1-CZ-NH2	-5.84	112.97	119.40
1	L	76	GLU	O-C-N	-5.84	113.36	122.70
1	J	132	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	G	23	TRP	CB-CG-CD1	-5.83	119.43	127.00
1	B	161	PHE	CB-CG-CD2	-5.82	116.72	120.80
1	I	6	LEU	CB-CG-CD2	5.82	120.89	111.00
1	G	117	TRP	CD2-CE3-CZ3	-5.81	111.25	118.80
1	E	96	MET	CG-SD-CE	-5.80	90.91	100.20
1	H	36	VAL	CA-CB-CG1	5.80	119.61	110.90
1	Q	41	SER	N-CA-CB	5.80	119.20	110.50
1	F	143	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	Q	85	PRO	N-CA-CB	5.80	110.26	103.30
1	B	181	VAL	CG1-CB-CG2	-5.79	101.63	110.90
1	P	114	GLN	CG-CD-OE1	-5.79	110.01	121.60
1	P	132	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	C	164	TYR	CB-CG-CD1	5.79	124.48	121.00
1	I	51	ASP	CB-CG-OD1	5.79	123.51	118.30
1	J	184	TRP	CB-CG-CD2	5.79	134.12	126.60
1	B	86	VAL	CA-CB-CG1	5.78	119.56	110.90
1	M	133	TRP	CG-CD1-NE1	-5.78	104.33	110.10
1	E	210	THR	CA-CB-CG2	-5.78	104.31	112.40
1	M	173	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	O	32	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	P	119	THR	CA-CB-CG2	-5.76	104.33	112.40
1	O	97	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	B	105	ALA	N-CA-CB	-5.75	102.04	110.10
1	E	145	TYR	CB-CG-CD1	5.75	124.45	121.00
1	E	97	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	G	202	LEU	CB-CG-CD1	-5.75	101.23	111.00
1	I	167	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
1	H	148	THR	N-CA-CB	5.74	121.21	110.30
1	C	167	ARG	CG-CD-NE	-5.74	99.74	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	THR	CA-CB-CG2	-5.74	104.37	112.40
1	J	188	THR	O-C-N	-5.73	113.53	122.70
1	D	105	ALA	N-CA-CB	-5.73	102.08	110.10
1	O	77	ALA	N-CA-CB	-5.72	102.10	110.10
1	E	18	ARG	CD-NE-CZ	5.71	131.60	123.60
1	L	143	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	69	LEU	CB-CG-CD1	5.71	120.70	111.00
1	L	27	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	R	134	ILE	CA-CB-CG1	-5.70	100.17	111.00
1	Q	25	LYS	N-CA-CB	-5.70	100.35	110.60
1	C	210	THR	CA-CB-OG1	5.70	120.96	109.00
1	P	26	VAL	CA-CB-CG2	-5.69	102.37	110.90
1	R	40	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	S	143	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	N	59	VAL	CA-CB-CG1	-5.67	102.40	110.90
1	F	175	GLU	N-CA-CB	5.67	120.80	110.60
1	M	81	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	S	165	VAL	CA-CB-CG1	5.66	119.39	110.90
1	E	173	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	P	40	PHE	CB-CG-CD2	5.66	124.76	120.80
1	B	143	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	D	130	TYR	CB-CG-CD1	5.65	124.39	121.00
1	P	164	TYR	CB-CG-CD1	5.64	124.39	121.00
1	J	167	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	S	2	ILE	O-C-N	-5.63	113.70	122.70
1	H	23	TRP	CB-CG-CD1	-5.62	119.70	127.00
1	C	214	MET	CG-SD-CE	-5.61	91.22	100.20
1	J	24	VAL	CA-CB-CG2	-5.61	102.48	110.90
1	N	86	VAL	CA-CB-CG2	5.61	119.31	110.90
1	N	78	ALA	CB-CA-C	5.60	118.50	110.10
1	E	25	LYS	O-C-N	-5.60	113.75	122.70
1	R	98	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	R	24	VAL	CA-CB-CG1	-5.58	102.53	110.90
1	C	133	TRP	CH2-CZ2-CE2	5.58	122.98	117.40
1	J	169	TYR	CZ-CE2-CD2	-5.57	114.79	119.80
1	N	10	MET	CA-CB-CG	5.57	122.77	113.30
1	P	2	ILE	O-C-N	-5.56	113.80	122.70
1	K	97	ARG	CG-CD-NE	-5.56	100.12	111.80
1	F	161	PHE	CB-CG-CD1	-5.56	116.91	120.80
1	G	23	TRP	CD1-CG-CD2	5.56	110.75	106.30
1	M	97	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	G	162	ARG	CD-NE-CZ	5.55	131.37	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	81	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	N	24	VAL	CA-CB-CG2	-5.54	102.58	110.90
1	R	177	ALA	O-C-N	-5.54	113.83	122.70
1	L	162	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	168	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	C	39	MET	CG-SD-CE	-5.54	91.34	100.20
1	G	167	ARG	CG-CD-NE	-5.54	100.17	111.80
1	K	11	VAL	CA-CB-CG2	-5.53	102.60	110.90
1	I	184	TRP	CZ3-CH2-CZ2	-5.53	114.96	121.60
1	M	29	GLU	O-C-N	-5.53	113.85	122.70
1	J	143	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	M	133	TRP	CD1-CG-CD2	5.53	110.72	106.30
1	O	214	MET	CA-CB-CG	5.52	122.69	113.30
1	C	103	ASP	CB-CG-OD1	5.52	123.27	118.30
1	P	169	TYR	CD1-CG-CD2	5.52	123.97	117.90
1	B	164	TYR	CB-CG-CD1	5.52	124.31	121.00
1	R	181	VAL	CA-CB-CG1	5.52	119.17	110.90
1	O	99	PRO	O-C-N	-5.51	113.88	122.70
1	G	23	TRP	CB-CA-C	5.51	121.42	110.40
1	D	208	GLY	O-C-N	-5.51	113.89	122.70
1	P	162	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	G	154	ARG	CD-NE-CZ	5.50	131.30	123.60
1	G	117	TRP	CE2-CD2-CE3	5.50	125.30	118.70
1	P	78	ALA	CB-CA-C	5.50	118.35	110.10
1	G	130	TYR	O-C-N	-5.50	113.90	122.70
1	S	205	LEU	CB-CA-C	-5.49	99.77	110.20
1	C	169	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	C	219	GLN	N-CA-CB	5.48	120.46	110.60
1	N	132	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	O	221	VAL	CA-CB-CG1	5.47	119.10	110.90
1	Q	103	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	C	19	THR	OG1-CB-CG2	-5.46	97.44	110.00
1	N	144	MET	CA-CB-CG	5.46	122.59	113.30
1	J	192	GLN	CA-CB-CG	5.46	125.41	113.40
1	E	59	VAL	CG1-CB-CG2	-5.46	102.17	110.90
1	R	142	VAL	CA-CB-CG1	5.45	119.07	110.90
1	G	166	ASP	CB-CG-OD2	5.45	123.20	118.30
1	O	23	TRP	CE2-CD2-CG	-5.44	102.94	107.30
1	F	214	MET	CG-SD-CE	-5.44	91.50	100.20
1	D	175	GLU	N-CA-CB	5.43	120.38	110.60
1	D	120	HIS	O-C-N	-5.43	114.02	122.70
1	N	27	VAL	CG1-CB-CG2	-5.43	102.22	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	29	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	G	162	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	R	184	TRP	CZ3-CH2-CZ2	-5.41	115.10	121.60
1	F	154	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	O	82	ARG	NH1-CZ-NH2	5.41	125.35	119.40
1	J	151	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	L	18	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	P	154	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	117	TRP	O-C-N	-5.38	114.09	122.70
1	N	163	ASP	CB-CG-OD2	5.38	123.14	118.30
1	H	108	THR	CA-CB-CG2	5.37	119.92	112.40
1	B	130	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	D	120	HIS	CA-CB-CG	5.36	122.72	113.60
1	K	143	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	N	163	ASP	O-C-N	-5.36	114.13	122.70
1	G	213	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	J	169	TYR	CG-CD1-CE1	-5.36	117.01	121.30
1	E	118	MET	CG-SD-CE	-5.35	91.63	100.20
1	N	17	PRO	N-CD-CG	5.35	111.23	103.20
1	I	166	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	E	40	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	M	108	THR	CA-CB-CG2	-5.34	104.92	112.40
1	I	48	THR	CA-CB-CG2	-5.34	104.92	112.40
1	G	121	ASN	CB-CA-C	5.34	121.09	110.40
1	H	166	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	P	104	ILE	O-C-N	-5.34	114.16	122.70
1	E	138	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	C	133	TRP	CG-CD2-CE3	-5.33	129.10	133.90
1	D	39	MET	CA-CB-CG	5.33	122.37	113.30
1	C	74	ASN	CB-CG-OD1	5.33	132.26	121.60
1	E	69	LEU	O-C-N	-5.33	114.18	122.70
1	G	130	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	P	58	THR	O-C-N	-5.33	114.18	122.70
1	N	168	PHE	CG-CD1-CE1	5.32	126.65	120.80
1	Q	204	ALA	N-CA-CB	-5.31	102.66	110.10
1	G	18	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	Q	146	SER	CB-CA-C	-5.31	100.01	110.10
1	C	161	PHE	CD1-CE1-CZ	5.31	126.47	120.10
1	F	26	VAL	CA-CB-CG1	-5.30	102.95	110.90
1	B	181	VAL	CA-CB-CG1	5.30	118.84	110.90
1	S	164	TYR	CG-CD1-CE1	-5.30	117.06	121.30
1	D	119	THR	CA-CB-OG1	5.29	120.11	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	100	ARG	NH1-CZ-NH2	-5.29	113.59	119.40
1	G	162	ARG	CA-CB-CG	5.28	125.02	113.40
1	I	55	MET	CG-SD-CE	-5.28	91.75	100.20
1	B	151	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	O	165	VAL	CA-CB-CG1	5.28	118.82	110.90
1	J	103	ASP	CB-CG-OD1	5.27	123.05	118.30
1	D	31	ALA	CB-CA-C	5.27	118.01	110.10
1	N	87	HIS	O-C-N	-5.27	114.27	122.70
1	N	220	GLY	N-CA-C	5.27	126.28	113.10
1	S	164	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	C	3	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	H	18	ARG	NH1-CZ-NH2	-5.27	113.61	119.40
1	S	169	TYR	CB-CG-CD2	5.27	124.16	121.00
1	N	184	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	B	211	LEU	CB-CG-CD2	5.26	119.94	111.00
1	C	145	TYR	CG-CD1-CE1	5.26	125.51	121.30
1	P	39	MET	CG-SD-CE	-5.25	91.80	100.20
1	S	183	ASN	CB-CA-C	-5.25	99.90	110.40
1	C	167	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	C	55	MET	O-C-N	-5.25	114.31	122.70
1	C	144	MET	N-CA-CB	-5.24	101.17	110.60
1	N	40	PHE	CG-CD2-CE2	-5.24	115.04	120.80
1	H	152	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	88	ALA	O-C-N	-5.23	114.31	123.20
1	L	197	ASP	CB-CG-OD2	5.23	123.00	118.30
1	S	82	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	J	99	PRO	N-CD-CG	5.23	111.04	103.20
1	F	213	GLU	CG-CD-OE1	-5.22	107.85	118.30
1	B	220	GLY	CA-C-O	-5.22	111.21	120.60
1	Q	161	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	B	81	ASP	CB-CG-OD1	5.21	122.99	118.30
1	O	14	ALA	O-C-N	-5.21	114.37	122.70
1	Q	31	ALA	N-CA-CB	-5.21	102.81	110.10
1	D	119	THR	CA-CB-CG2	-5.19	105.13	112.40
1	I	9	GLN	CB-CG-CD	5.19	125.10	111.60
1	H	162	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	S	126	VAL	CA-CB-CG1	-5.19	103.12	110.90
1	R	59	VAL	CA-CB-CG2	5.18	118.67	110.90
1	R	18	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	I	184	TRP	CH2-CZ2-CE2	5.18	122.58	117.40
1	L	92	ALA	N-CA-CB	5.18	117.35	110.10
1	F	68	MET	CB-CA-C	5.17	120.75	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	SER	O-C-N	-5.17	114.43	122.70
1	M	169	TYR	CB-CG-CD2	5.17	124.10	121.00
1	N	119	THR	CA-CB-CG2	-5.17	105.17	112.40
1	H	80	TRP	CE3-CZ3-CH2	-5.17	115.52	121.20
1	O	51	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	H	88	ALA	CB-CA-C	5.16	117.84	110.10
1	G	216	THR	N-CA-CB	5.16	120.10	110.30
1	M	36	VAL	CA-CB-CG1	5.16	118.64	110.90
1	R	4	GLN	C-N-CA	5.15	134.57	121.70
1	K	189	LEU	CB-CA-C	-5.15	100.42	110.20
1	S	159	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	P	71	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	D	133	TRP	CB-CG-CD1	5.14	133.69	127.00
1	O	126	VAL	CA-CB-CG1	-5.14	103.19	110.90
1	H	212	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	S	169	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	139	ASN	CB-CA-C	5.14	120.67	110.40
1	H	146	SER	CB-CA-C	-5.13	100.34	110.10
1	C	197	ASP	CB-CG-OD2	5.13	122.91	118.30
1	K	80	TRP	CA-C-O	5.12	130.86	120.10
1	P	80	TRP	CB-CG-CD2	-5.12	119.94	126.60
1	Q	143	ARG	CA-C-O	5.12	130.85	120.10
1	O	135	ILE	CA-CB-CG2	5.12	121.13	110.90
1	F	143	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	158	LYS	CB-CA-C	-5.12	100.17	110.40
1	D	59	VAL	CA-CB-CG2	-5.11	103.23	110.90
1	D	133	TRP	CB-CG-CD2	-5.11	119.96	126.60
1	D	136	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	I	163	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	190	LEU	N-CA-CB	-5.10	100.20	110.40
1	Q	6	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	K	195	ASN	CB-CA-C	5.10	120.59	110.40
1	O	79	GLU	OE1-CD-OE2	-5.10	117.19	123.30
1	E	112	GLN	O-C-N	-5.09	114.55	122.70
1	M	7	GLN	N-CA-CB	5.09	119.77	110.60
1	N	86	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	M	118	MET	CG-SD-CE	5.09	108.34	100.20
1	M	163	ASP	CA-CB-CG	-5.09	102.21	113.40
1	S	23	TRP	CB-CG-CD2	5.09	133.21	126.60
1	C	159	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	M	19	THR	N-CA-CB	5.08	119.95	110.30
1	B	131	LYS	O-C-N	-5.08	114.57	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	132	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	N	14	ALA	CB-CA-C	5.07	117.70	110.10
1	G	197	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	E	148	THR	CA-CB-CG2	-5.06	105.31	112.40
1	Q	168	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	B	24	VAL	CA-CB-CG1	5.05	118.48	110.90
1	N	100	ARG	O-C-N	-5.05	114.61	123.20
1	S	102	SER	O-C-N	-5.05	114.61	122.70
1	M	214	MET	CA-CB-CG	5.05	121.89	113.30
1	O	130	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	L	79	GLU	CG-CD-OE1	5.05	128.40	118.30
1	G	79	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	R	209	ALA	CB-CA-C	-5.04	102.53	110.10
1	D	13	GLN	CG-CD-OE1	-5.04	111.51	121.60
1	B	161	PHE	CB-CG-CD1	5.04	124.33	120.80
1	K	200	THR	CA-CB-CG2	-5.04	105.35	112.40
1	D	96	MET	N-CA-CB	5.04	119.66	110.60
1	L	186	THR	OG1-CB-CG2	-5.03	98.43	110.00
1	F	43	LEU	O-C-N	-5.03	114.66	122.70
1	L	124	ILE	N-CA-C	-5.02	97.44	111.00
1	I	176	GLN	CG-CD-OE1	-5.02	111.55	121.60
1	P	101	GLY	O-C-N	5.02	130.73	122.70
1	R	82	ARG	CD-NE-CZ	5.02	130.62	123.60
1	H	84	HIS	CA-CB-CG	-5.01	105.08	113.60
1	Q	180	GLU	OE1-CD-OE2	-5.01	117.29	123.30
1	N	79	GLU	OE1-CD-OE2	-5.00	117.29	123.30
1	R	154	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	S	10	MET	CG-SD-CE	-5.00	92.19	100.20
1	N	64	ALA	N-CA-CB	5.00	117.10	110.10

There are no chirality outliers.

All (87) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	186	THR	Mainchain
1	C	130	TYR	Sidechain
1	C	132	ARG	Sidechain
1	C	162	ARG	Sidechain
1	C	164	TYR	Sidechain
1	C	168	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	C	169	TYR	Sidechain
1	C	82	ARG	Sidechain
1	D	100	ARG	Sidechain
1	D	120	HIS	Sidechain
1	D	130	TYR	Sidechain
1	D	145	TYR	Sidechain
1	D	154	ARG	Sidechain
1	D	162	ARG	Sidechain
1	D	84	HIS	Sidechain
1	E	100	ARG	Sidechain
1	E	169	TYR	Sidechain
1	E	173	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	84	HIS	Sidechain
1	F	100	ARG	Sidechain
1	F	154	ARG	Sidechain
1	F	173	ARG	Sidechain
1	F	82	ARG	Sidechain
1	F	97	ARG	Sidechain
1	H	100	ARG	Sidechain
1	H	132	ARG	Sidechain
1	H	143	ARG	Sidechain
1	H	145	TYR	Sidechain
1	H	154	ARG	Sidechain
1	H	18	ARG	Sidechain
1	H	84	HIS	Sidechain
1	I	130	TYR	Sidechain
1	I	143	ARG	Sidechain
1	I	154	ARG	Sidechain
1	I	169	TYR	Sidechain
1	I	173	ARG	Sidechain
1	I	41	SER	Mainchain
1	I	82	ARG	Sidechain
1	J	169	TYR	Sidechain
1	J	97	ARG	Sidechain
1	K	132	ARG	Sidechain
1	K	145	TYR	Sidechain
1	K	154	ARG	Sidechain
1	K	162	ARG	Sidechain
1	K	164	TYR	Sidechain
1	K	173	ARG	Sidechain
1	L	154	ARG	Sidechain

*Continued on next page...*

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Mol	Chain	Res	Type	Group
1	M	100	ARG	Sidechain
1	M	145	TYR	Sidechain
1	M	162	ARG	Sidechain
1	M	18	ARG	Sidechain
1	M	211	LEU	Mainchain
1	M	32	PHE	Sidechain
1	N	100	ARG	Sidechain
1	N	12	HIS	Sidechain
1	N	132	ARG	Sidechain
1	N	167	ARG	Sidechain
1	N	168	PHE	Sidechain
1	N	40	PHE	Sidechain
1	O	100	ARG	Sidechain
1	O	120	HIS	Sidechain
1	O	143	ARG	Sidechain
1	O	154	ARG	Sidechain
1	O	173	ARG	Sidechain
1	P	154	ARG	Sidechain
1	P	162	ARG	Sidechain
1	P	40	PHE	Sidechain
1	Q	161	PHE	Sidechain
1	Q	162	ARG	Sidechain
1	Q	164	TYR	Sidechain
1	Q	168	PHE	Sidechain
1	Q	173	ARG	Sidechain
1	Q	32	PHE	Sidechain
1	Q	82	ARG	Sidechain
1	Q	87	HIS	Sidechain
1	R	100	ARG	Sidechain
1	R	132	ARG	Sidechain
1	R	161	PHE	Sidechain
1	R	173	ARG	Sidechain
1	R	40	PHE	Sidechain
1	R	82	ARG	Sidechain
1	S	143	ARG	Sidechain
1	S	167	ARG	Sidechain
1	S	32	PHE	Sidechain

## 5.2 Too-close contacts

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1726	0	1725	0	0
1	C	1726	0	1725	0	0
1	D	1726	0	1725	0	0
1	E	1726	0	1725	0	0
1	F	1726	0	1725	0	0
1	G	1726	0	1725	0	0
1	H	1726	0	1725	0	0
1	I	1726	0	1725	0	0
1	J	1726	0	1725	0	0
1	K	1726	0	1725	0	0
1	L	1726	0	1725	0	0
1	M	1726	0	1725	0	0
1	N	1726	0	1725	0	0
1	O	1726	0	1725	0	0
1	P	1726	0	1725	0	0
1	Q	1726	0	1725	0	0
1	R	1726	0	1725	0	0
1	S	1726	0	1725	0	0
All	All	31068	0	31050	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	B	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	14 52
1	C	219/221 (99%)	207 (94%)	11 (5%)	1 (0%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	219/221 (99%)	213 (97%)	4 (2%)	2 (1%)	14	52
1	E	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
1	F	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	14	52
1	G	219/221 (99%)	209 (95%)	9 (4%)	1 (0%)	25	64
1	H	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	I	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	J	219/221 (99%)	210 (96%)	8 (4%)	1 (0%)	25	64
1	K	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	L	219/221 (99%)	210 (96%)	8 (4%)	1 (0%)	25	64
1	M	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	14	52
1	N	219/221 (99%)	207 (94%)	11 (5%)	1 (0%)	25	64
1	O	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	P	219/221 (99%)	206 (94%)	11 (5%)	2 (1%)	14	52
1	Q	219/221 (99%)	210 (96%)	8 (4%)	1 (0%)	25	64
1	R	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	S	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
All	All	3942/3978 (99%)	3783 (96%)	143 (4%)	16 (0%)	32	68

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	147	PRO
1	D	177	ALA
1	F	177	ALA
1	G	120	HIS
1	B	177	ALA
1	L	120	HIS
1	Q	177	ALA
1	J	88	ALA
1	F	120	HIS
1	M	15	ILE
1	M	90	PRO
1	C	207	PRO
1	B	125	PRO
1	P	91	ILE
1	D	147	PRO

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Mol	Chain	Res	Type
1	P	147	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	B	188/188 (100%)	185 (98%)	3 (2%)	58	73
1	C	188/188 (100%)	181 (96%)	7 (4%)	29	49
1	D	188/188 (100%)	186 (99%)	2 (1%)	70	80
1	E	188/188 (100%)	185 (98%)	3 (2%)	58	73
1	F	188/188 (100%)	184 (98%)	4 (2%)	48	66
1	G	188/188 (100%)	185 (98%)	3 (2%)	58	73
1	H	188/188 (100%)	185 (98%)	3 (2%)	58	73
1	I	188/188 (100%)	183 (97%)	5 (3%)	40	58
1	J	188/188 (100%)	183 (97%)	5 (3%)	40	58
1	K	188/188 (100%)	187 (100%)	1 (0%)	86	89
1	L	188/188 (100%)	186 (99%)	2 (1%)	70	80
1	M	188/188 (100%)	185 (98%)	3 (2%)	58	73
1	N	188/188 (100%)	184 (98%)	4 (2%)	48	66
1	O	188/188 (100%)	186 (99%)	2 (1%)	70	80
1	P	188/188 (100%)	183 (97%)	5 (3%)	40	58
1	Q	188/188 (100%)	183 (97%)	5 (3%)	40	58
1	R	188/188 (100%)	179 (95%)	9 (5%)	21	43
1	S	188/188 (100%)	187 (100%)	1 (0%)	86	89
All	All	3384/3384 (100%)	3317 (98%)	67 (2%)	50	68

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	GLN

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Mol	Chain	Res	Type
1	B	50	GLN
1	B	196	PRO
1	K	172	LEU
1	L	21	ASN
1	L	67	GLN
1	M	11	VAL
1	M	13	GLN
1	M	70	LYS
1	N	17	PRO
1	N	41	SER
1	N	90	PRO
1	N	196	PRO
1	O	7	GLN
1	O	187	GLU
1	P	13	GLN
1	P	41	SER
1	P	84	HIS
1	P	86	VAL
1	P	216	THR
1	Q	7	GLN
1	Q	70	LYS
1	Q	110	THR
1	Q	121	ASN
1	Q	216	THR
1	R	1	PRO
1	R	18	ARG
1	R	34	PRO
1	R	50	GLN
1	R	95	GLN
1	R	148	THR
1	R	164	TYR
1	R	176	GLN
1	R	196	PRO
1	S	176	GLN
1	C	4	GLN
1	C	21	ASN
1	C	39	MET
1	C	79	GLU
1	C	90	PRO
1	C	176	GLN
1	C	210	THR
1	D	13	GLN

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Mol	Chain	Res	Type
1	D	130	TYR
1	E	85	PRO
1	E	96	MET
1	E	166	ASP
1	F	166	ASP
1	F	196	PRO
1	F	216	THR
1	F	221	VAL
1	G	49	PRO
1	G	162	ARG
1	G	166	ASP
1	H	34	PRO
1	H	176	GLN
1	H	218	CYS
1	I	18	ARG
1	I	50	GLN
1	I	120	HIS
1	I	128	GLU
1	I	148	THR
1	J	36	VAL
1	J	79	GLU
1	J	110	THR
1	J	120	HIS
1	J	196	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

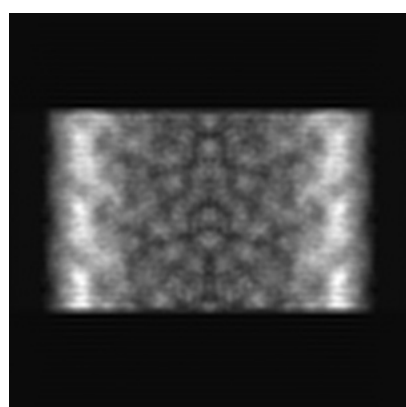
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8582. These allow visual inspection of the internal detail of the map and identification of artifacts.

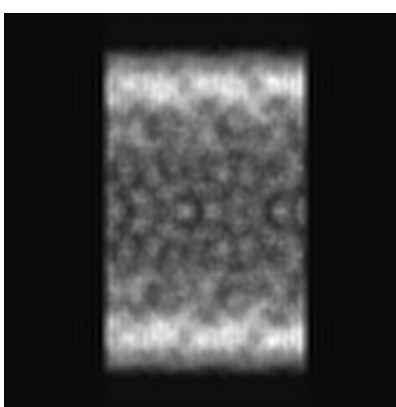
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

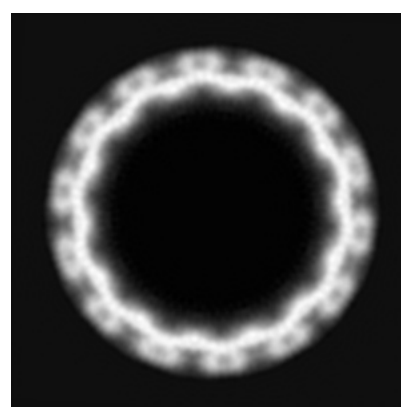
#### 6.1.1 Primary map



X



Y

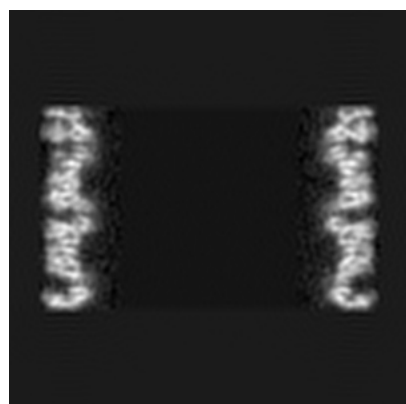


Z

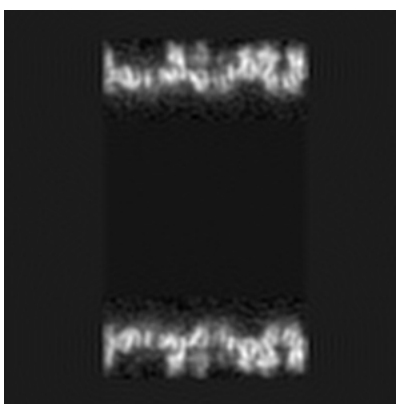
The images above show the map projected in three orthogonal directions.

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

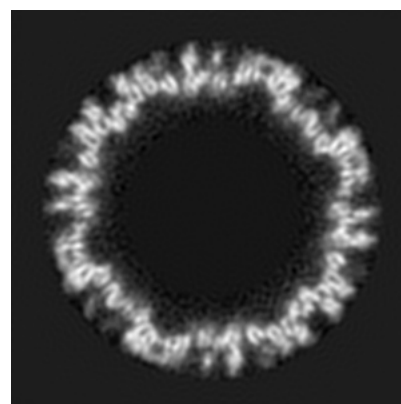
#### 6.2.1 Primary map



X Index: 248



Y Index: 248

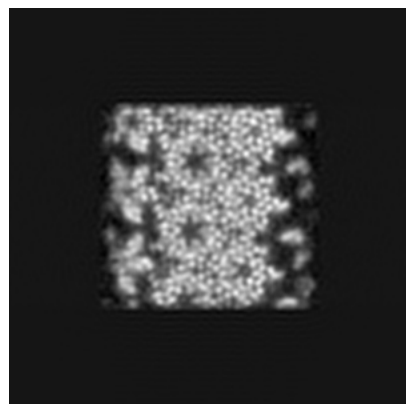


Z Index: 248

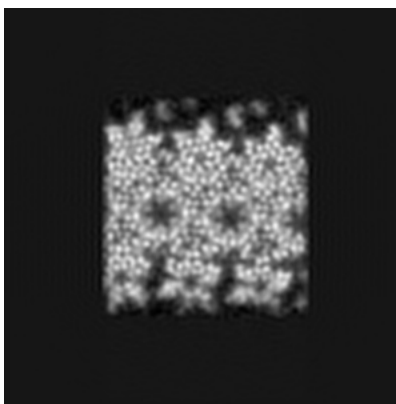
The images above show central slices of the map in three orthogonal directions.

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

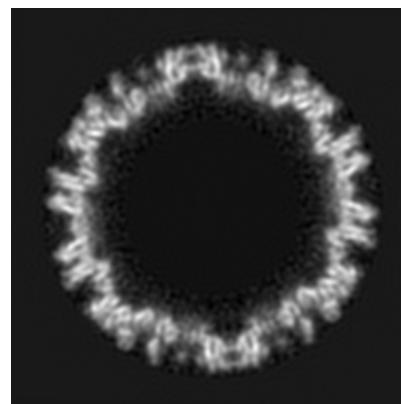
### 6.3.1 Primary map



X Index: 411



Y Index: 409

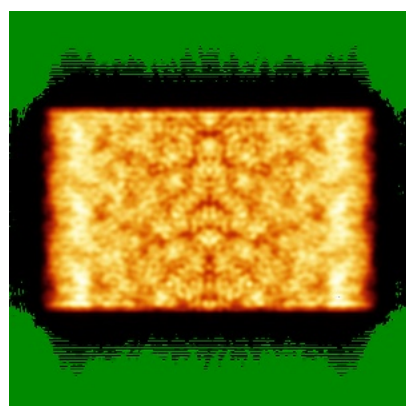


Z Index: 366

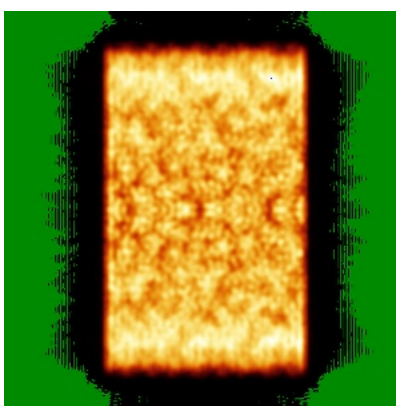
The images above show the largest variance slices of the map in three orthogonal directions.

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

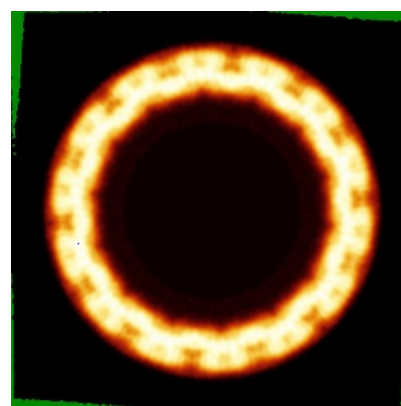
### 6.4.1 Primary map



X



Y

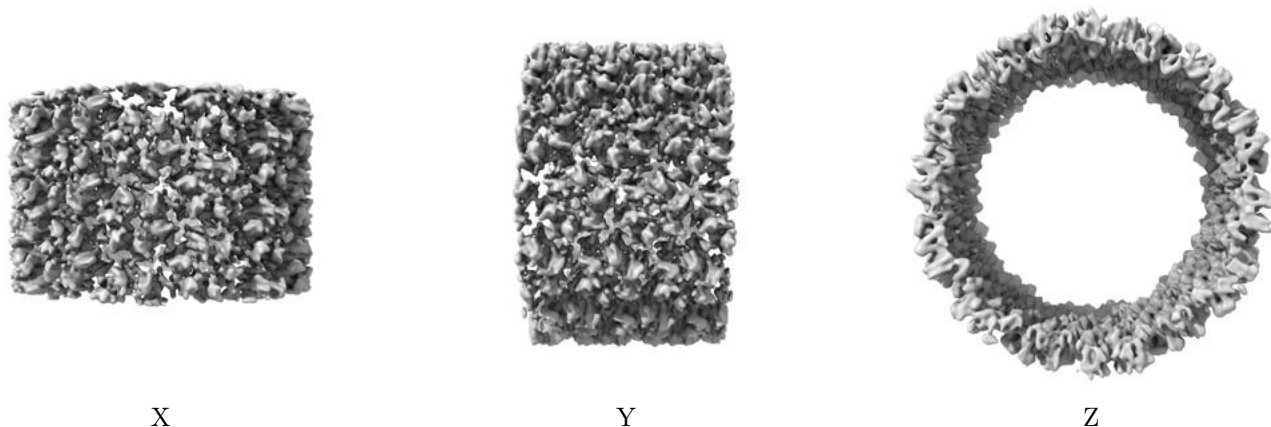


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

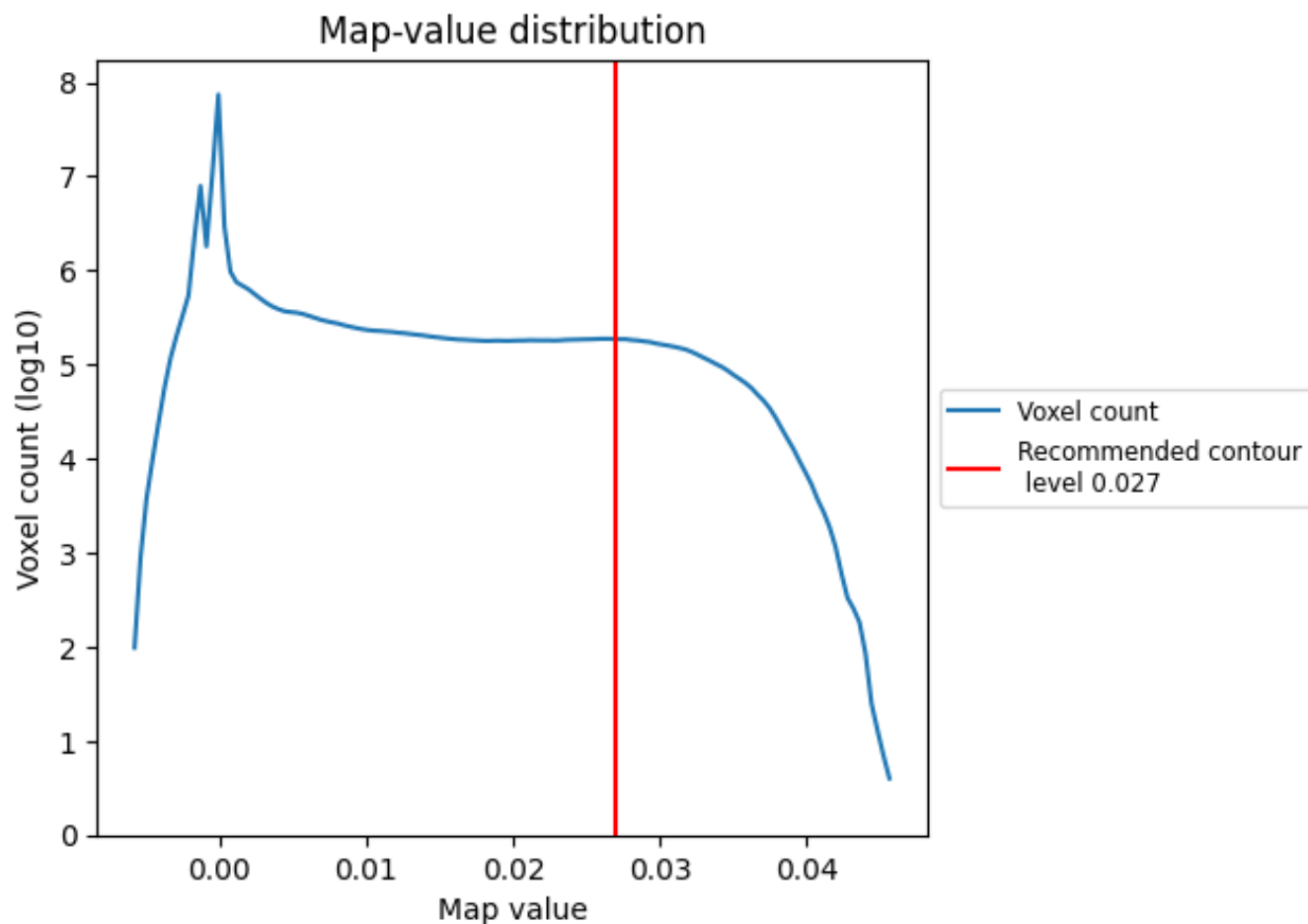
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

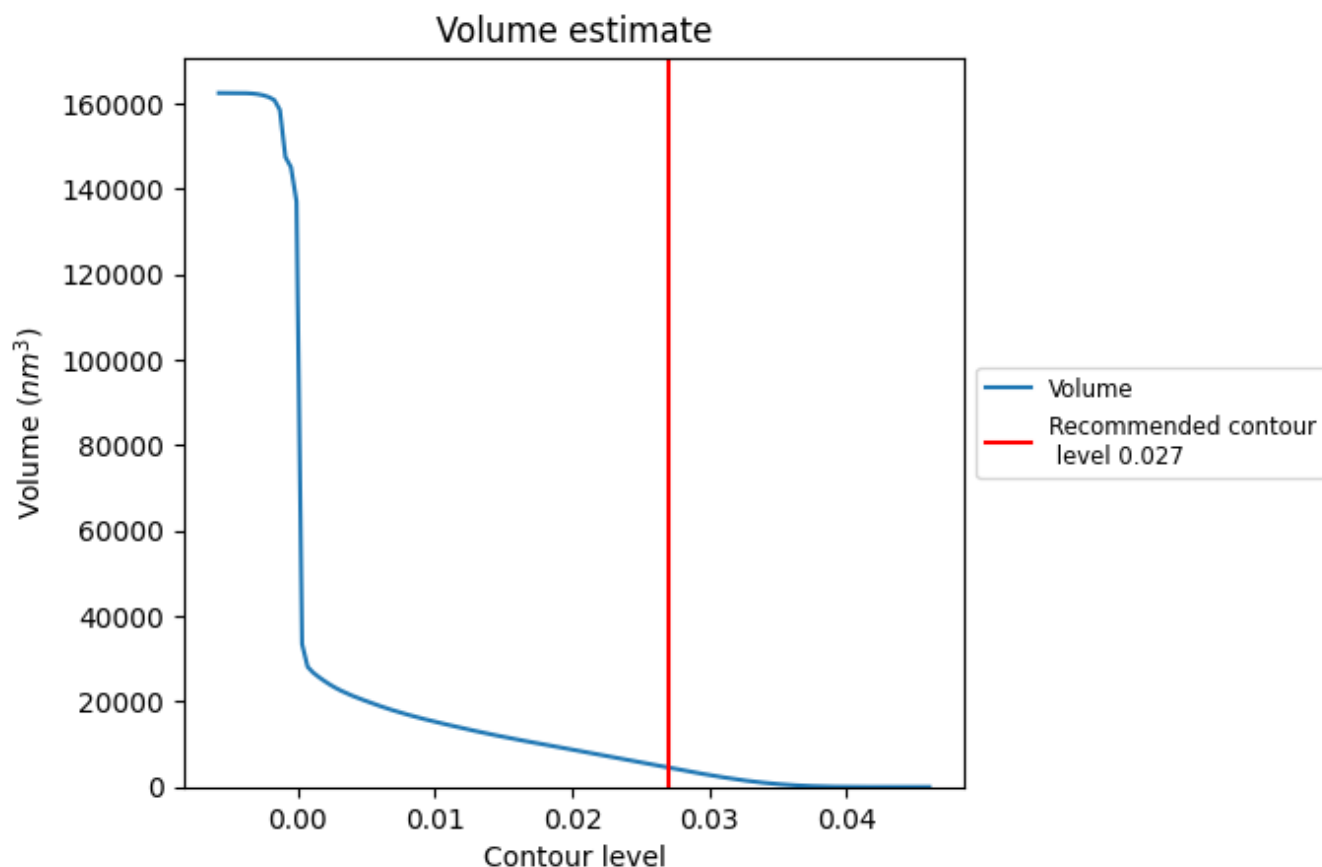
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

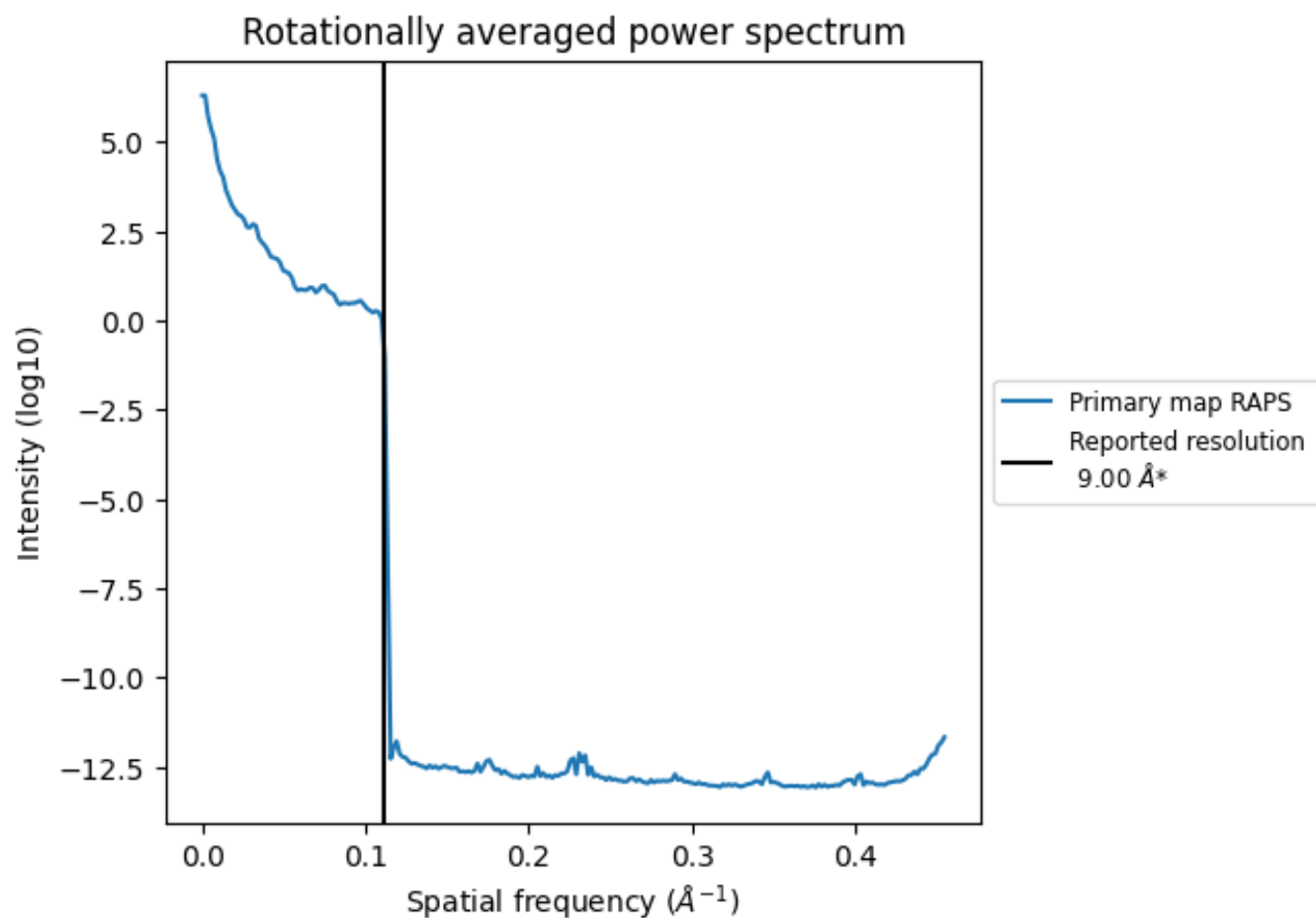
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4556 nm<sup>3</sup>; this corresponds to an approximate mass of 4116 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 ⓘ



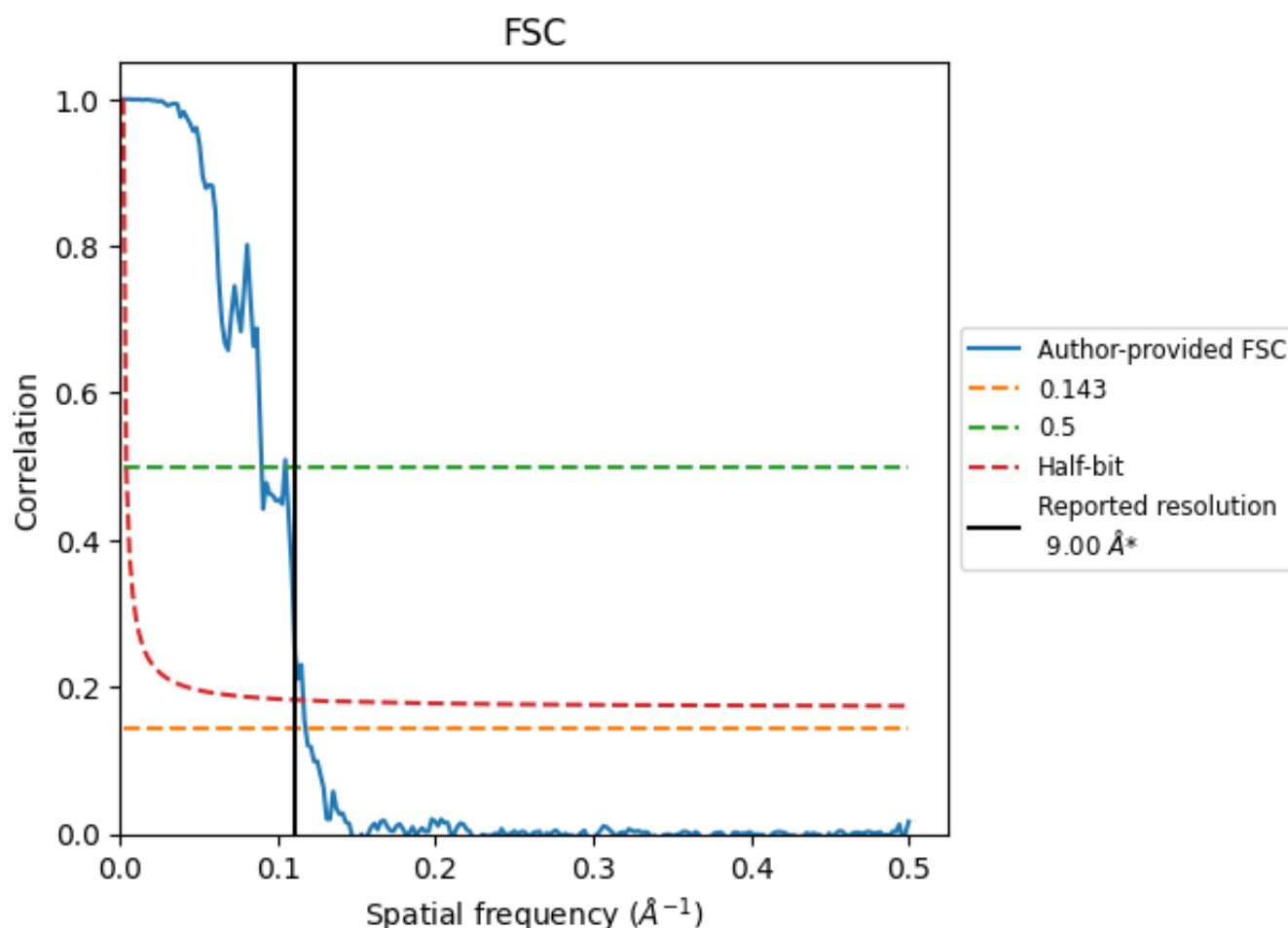
\*Reported resolution corresponds to spatial frequency of 0.111 Å<sup>-1</sup>



## 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 0.111 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

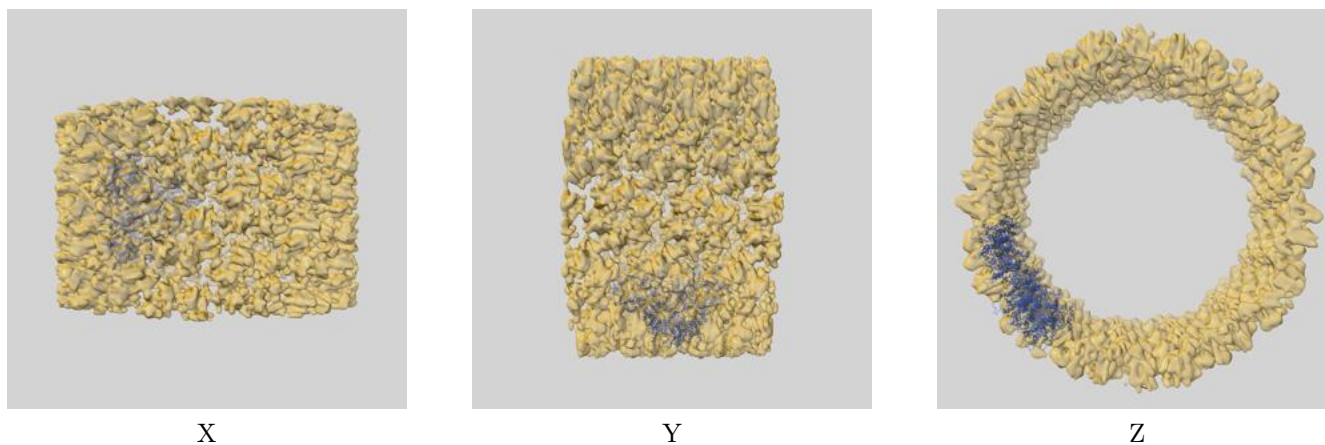
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	8.50	11.14	8.61
Unmasked-calculated*	-	-	-

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

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

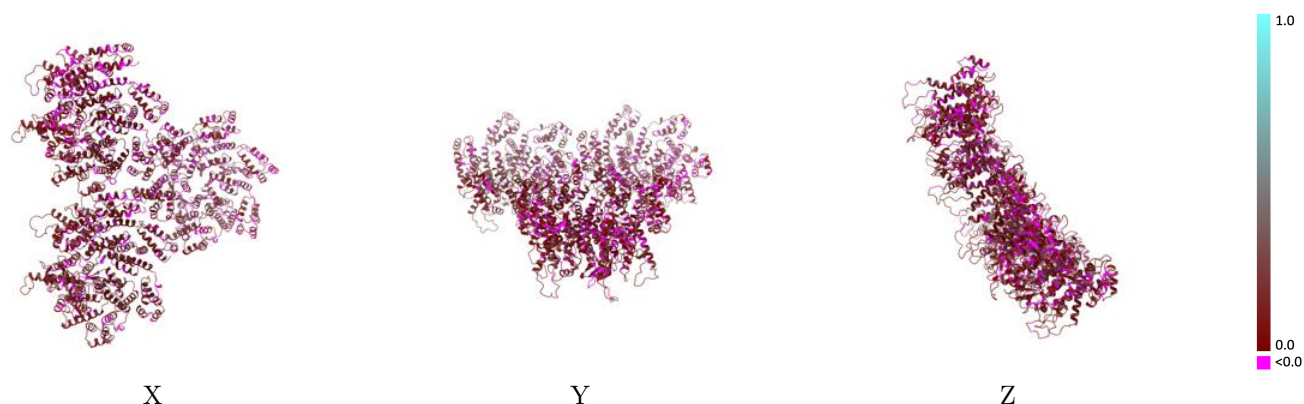
This section contains information regarding the fit between EMDB map EMD-8582 and PDB model 5UP4. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



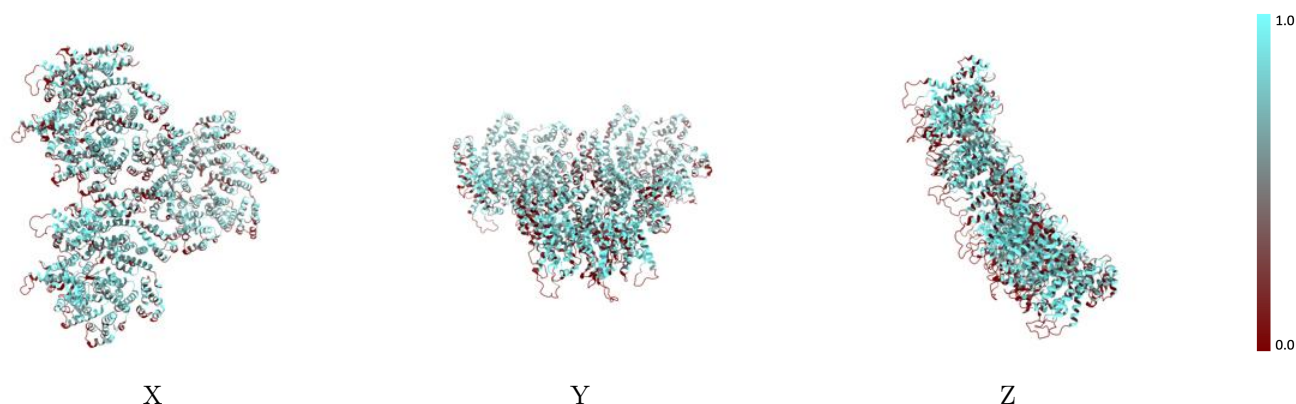
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



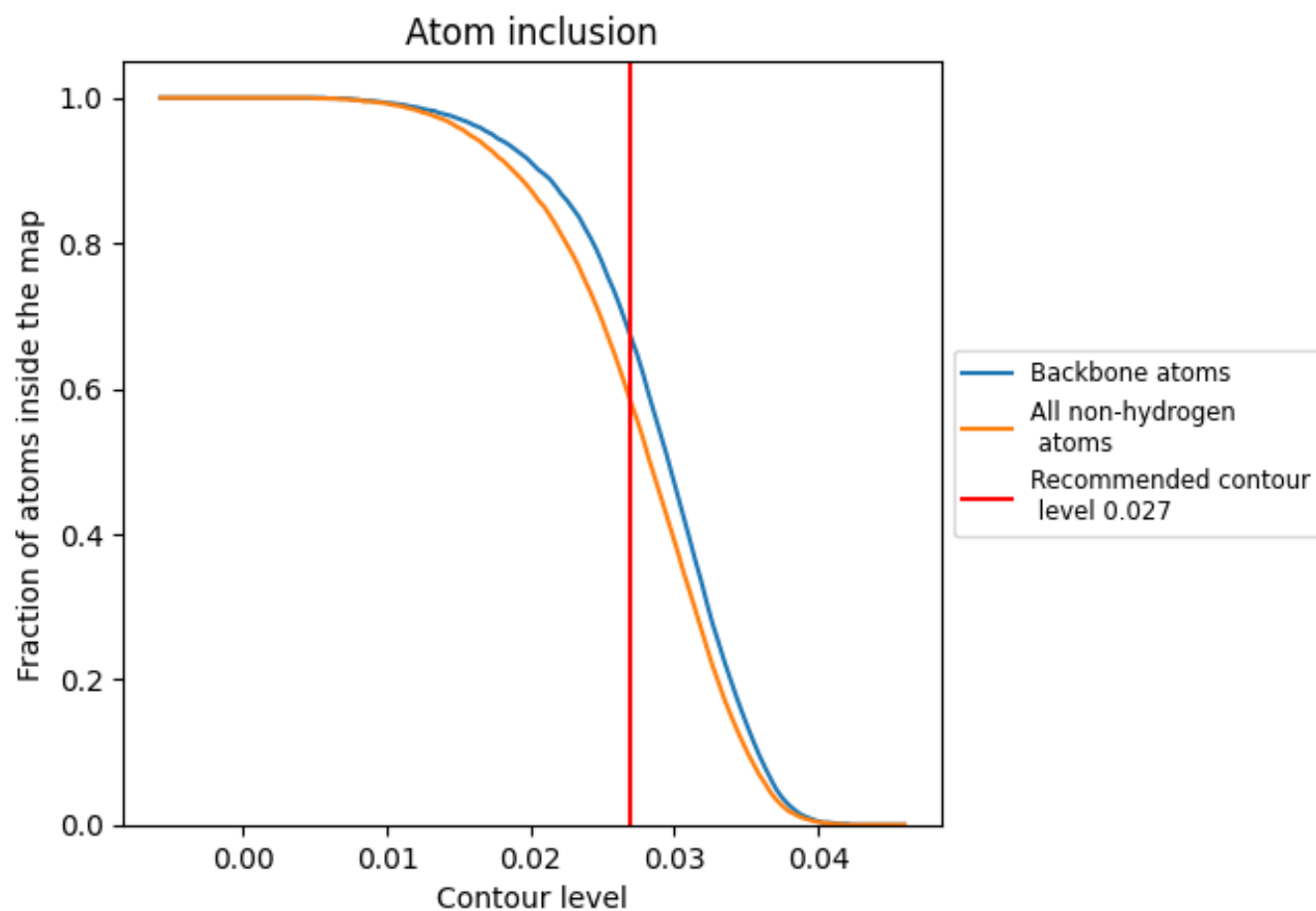
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 58% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5800	 0.0970
B	 0.5590	 0.0680
C	 0.5660	 0.0830
D	 0.5330	 0.0740
E	 0.5750	 0.0990
F	 0.5470	 0.0940
G	 0.6090	 0.1090
H	 0.5640	 0.0630
I	 0.5480	 0.0780
J	 0.5350	 0.0920
K	 0.5650	 0.0860
L	 0.5560	 0.1010
M	 0.6120	 0.1080
N	 0.6220	 0.1090
O	 0.5850	 0.0940
P	 0.5940	 0.1090
Q	 0.6120	 0.1230
R	 0.6020	 0.1260
S	 0.6540	 0.1340

