



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 07:11 am GMT

PDB ID : 6HE5  
EMDB ID : EMD-0210  
Title : 20S core particle of PAN-proteasomes  
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.  
Deposited on : 2018-08-20  
Resolution : 4.12 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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) : 2.31.2

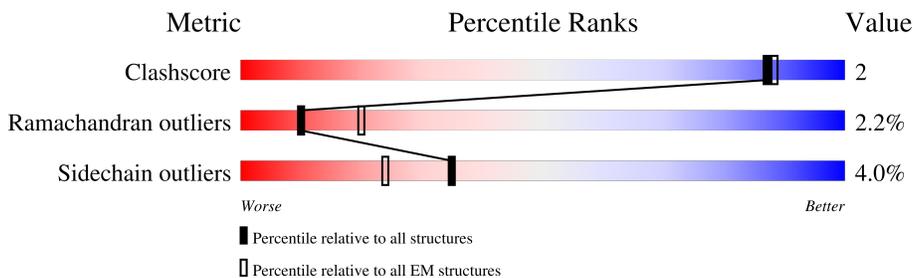
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.12 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	247	
1	B	247	
1	C	247	
1	D	247	
1	E	247	
1	F	247	
1	G	247	
2	1	210	

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Mol	Chain	Length	Quality of chain
2	2	210	<p>57% 70% 21% 5%</p>
2	3	210	<p>56% 71% 20% 5%</p>
2	4	210	<p>57% 71% 21% 5%</p>
2	5	210	<p>58% 69% 22% 5%</p>
2	6	210	<p>56% 65% 25% 5%</p>
2	7	210	<p>60% 69% 22% 5%</p>
3	H	401	<p>98%</p>
3	I	401	<p>98%</p>
3	J	401	<p>98%</p>
3	K	401	<p>98%</p>
3	L	401	<p>98%</p>
3	M	401	<p>98%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24633 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	242	1907	1211	321	368	7	0	0
1	B	242	1907	1211	321	368	7	0	0
1	C	242	1907	1211	321	368	7	0	0
1	D	242	1907	1211	321	368	7	0	0
1	E	242	1907	1211	321	368	7	0	0
1	F	242	1907	1211	321	368	7	0	0
1	G	242	1907	1211	321	368	7	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O29760
A	1	GLY	-	expression tag	UNP O29760
B	0	MET	-	initiating methionine	UNP O29760
B	1	GLY	-	expression tag	UNP O29760
C	0	MET	-	initiating methionine	UNP O29760
C	1	GLY	-	expression tag	UNP O29760
D	0	MET	-	initiating methionine	UNP O29760
D	1	GLY	-	expression tag	UNP O29760
E	0	MET	-	initiating methionine	UNP O29760
E	1	GLY	-	expression tag	UNP O29760
F	0	MET	-	initiating methionine	UNP O29760
F	1	GLY	-	expression tag	UNP O29760
G	0	MET	-	initiating methionine	UNP O29760
G	1	GLY	-	expression tag	UNP O29760

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	202	1552	982	260	304	6	0	0
2	2	202	1552	982	260	304	6	0	0
2	3	202	1552	982	260	304	6	0	0
2	4	202	1552	982	260	304	6	0	0
2	5	202	1552	982	260	304	6	0	0
2	6	202	1552	982	260	304	6	0	0
2	7	202	1552	982	260	304	6	0	0

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	10	MET	-	initiating methionine	UNP Q9P996
1	214	HIS	-	expression tag	UNP Q9P996
1	215	HIS	-	expression tag	UNP Q9P996
1	216	HIS	-	expression tag	UNP Q9P996
1	217	HIS	-	expression tag	UNP Q9P996
1	218	HIS	-	expression tag	UNP Q9P996
1	219	HIS	-	expression tag	UNP Q9P996
2	10	MET	-	initiating methionine	UNP Q9P996
2	214	HIS	-	expression tag	UNP Q9P996
2	215	HIS	-	expression tag	UNP Q9P996
2	216	HIS	-	expression tag	UNP Q9P996
2	217	HIS	-	expression tag	UNP Q9P996
2	218	HIS	-	expression tag	UNP Q9P996
2	219	HIS	-	expression tag	UNP Q9P996
3	10	MET	-	initiating methionine	UNP Q9P996
3	214	HIS	-	expression tag	UNP Q9P996
3	215	HIS	-	expression tag	UNP Q9P996
3	216	HIS	-	expression tag	UNP Q9P996
3	217	HIS	-	expression tag	UNP Q9P996
3	218	HIS	-	expression tag	UNP Q9P996
3	219	HIS	-	expression tag	UNP Q9P996
4	10	MET	-	initiating methionine	UNP Q9P996
4	214	HIS	-	expression tag	UNP Q9P996
4	215	HIS	-	expression tag	UNP Q9P996
4	216	HIS	-	expression tag	UNP Q9P996
4	217	HIS	-	expression tag	UNP Q9P996

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Chain	Residue	Modelled	Actual	Comment	Reference
4	218	HIS	-	expression tag	UNP Q9P996
4	219	HIS	-	expression tag	UNP Q9P996
5	10	MET	-	initiating methionine	UNP Q9P996
5	214	HIS	-	expression tag	UNP Q9P996
5	215	HIS	-	expression tag	UNP Q9P996
5	216	HIS	-	expression tag	UNP Q9P996
5	217	HIS	-	expression tag	UNP Q9P996
5	218	HIS	-	expression tag	UNP Q9P996
5	219	HIS	-	expression tag	UNP Q9P996
6	10	MET	-	initiating methionine	UNP Q9P996
6	214	HIS	-	expression tag	UNP Q9P996
6	215	HIS	-	expression tag	UNP Q9P996
6	216	HIS	-	expression tag	UNP Q9P996
6	217	HIS	-	expression tag	UNP Q9P996
6	218	HIS	-	expression tag	UNP Q9P996
6	219	HIS	-	expression tag	UNP Q9P996
7	10	MET	-	initiating methionine	UNP Q9P996
7	214	HIS	-	expression tag	UNP Q9P996
7	215	HIS	-	expression tag	UNP Q9P996
7	216	HIS	-	expression tag	UNP Q9P996
7	217	HIS	-	expression tag	UNP Q9P996
7	218	HIS	-	expression tag	UNP Q9P996
7	219	HIS	-	expression tag	UNP Q9P996

- Molecule 3 is a protein called Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	I	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	K	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	L	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	M	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	J	9	Total	C	N	O	S	0	0
			70	47	10	12	1		

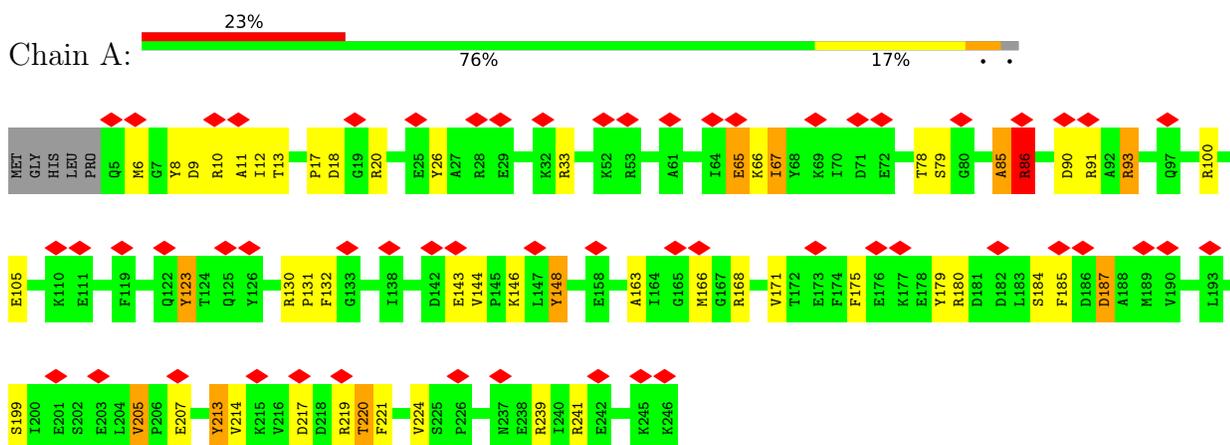
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLY	-	expression tag	UNP O28303
H	-1	HIS	-	expression tag	UNP O28303
H	0	MET	-	expression tag	UNP O28303
H	1	GLY	-	expression tag	UNP O28303
I	-2	GLY	-	expression tag	UNP O28303
I	-1	HIS	-	expression tag	UNP O28303
I	0	MET	-	expression tag	UNP O28303
I	1	GLY	-	expression tag	UNP O28303
K	-2	GLY	-	expression tag	UNP O28303
K	-1	HIS	-	expression tag	UNP O28303
K	0	MET	-	expression tag	UNP O28303
K	1	GLY	-	expression tag	UNP O28303
L	-2	GLY	-	expression tag	UNP O28303
L	-1	HIS	-	expression tag	UNP O28303
L	0	MET	-	expression tag	UNP O28303
L	1	GLY	-	expression tag	UNP O28303
M	-2	GLY	-	expression tag	UNP O28303
M	-1	HIS	-	expression tag	UNP O28303
M	0	MET	-	expression tag	UNP O28303
M	1	GLY	-	expression tag	UNP O28303
J	-2	GLY	-	expression tag	UNP O28303
J	-1	HIS	-	expression tag	UNP O28303
J	0	MET	-	expression tag	UNP O28303
J	1	GLY	-	expression tag	UNP O28303

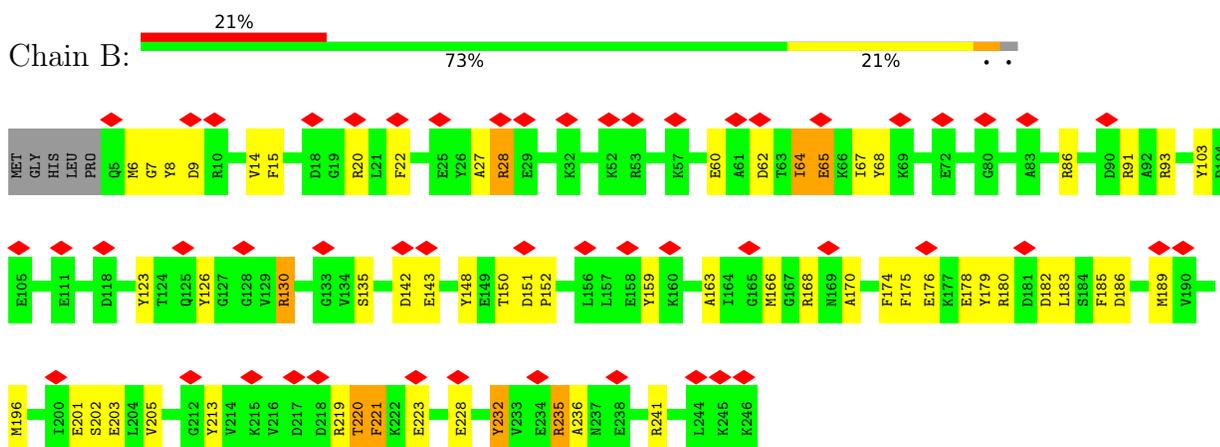
### 3 Residue-property plots

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.

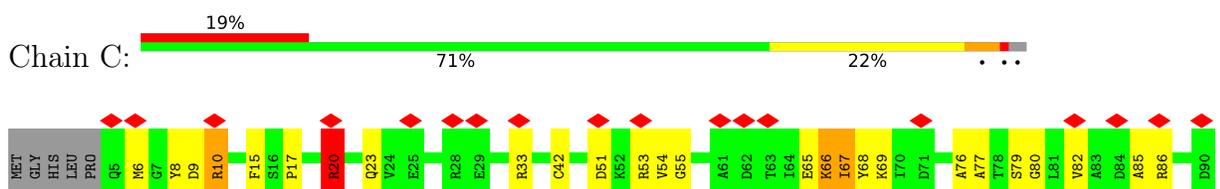
- Molecule 1: Proteasome subunit alpha

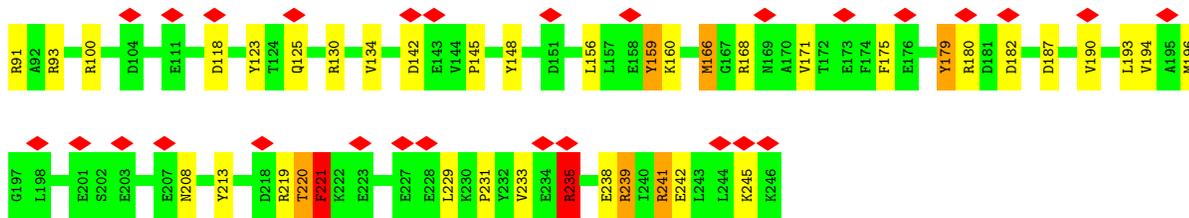


- Molecule 1: Proteasome subunit alpha

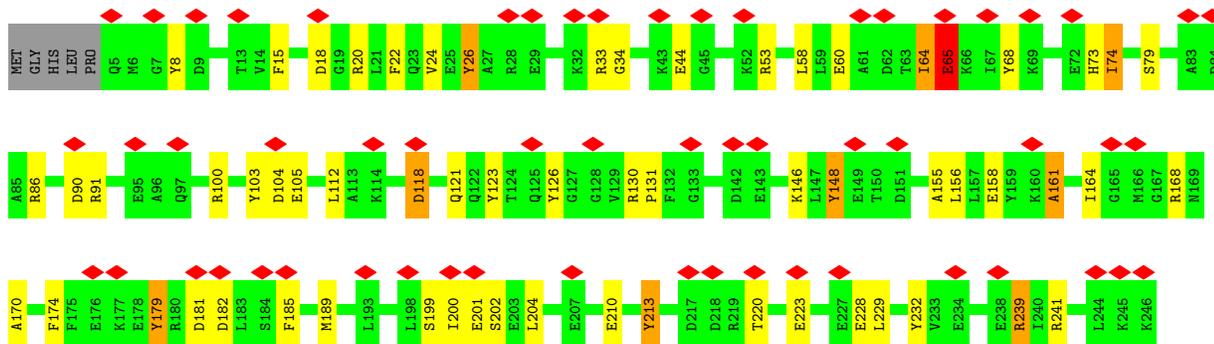


- Molecule 1: Proteasome subunit alpha

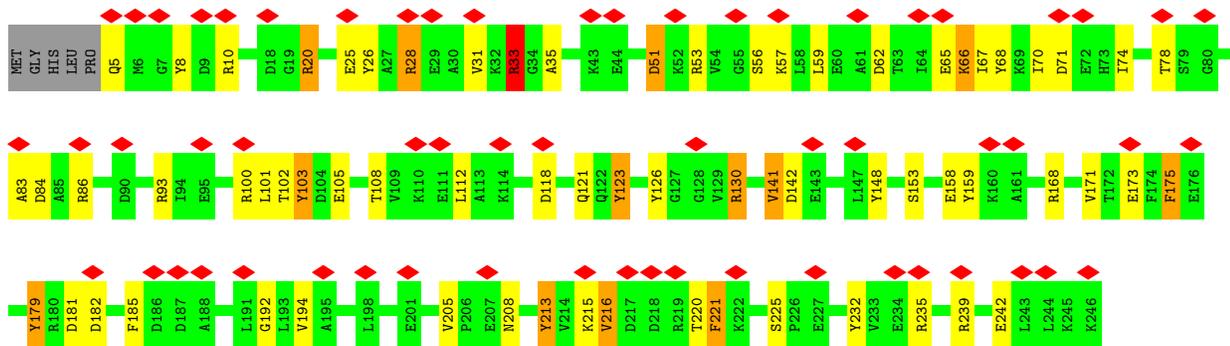




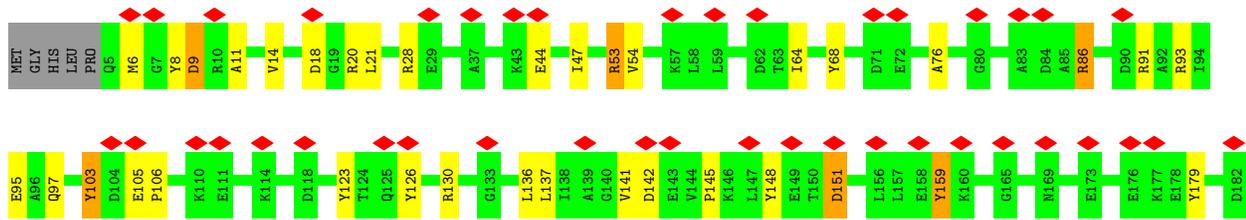
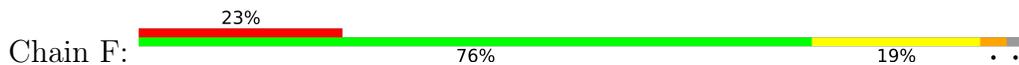
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

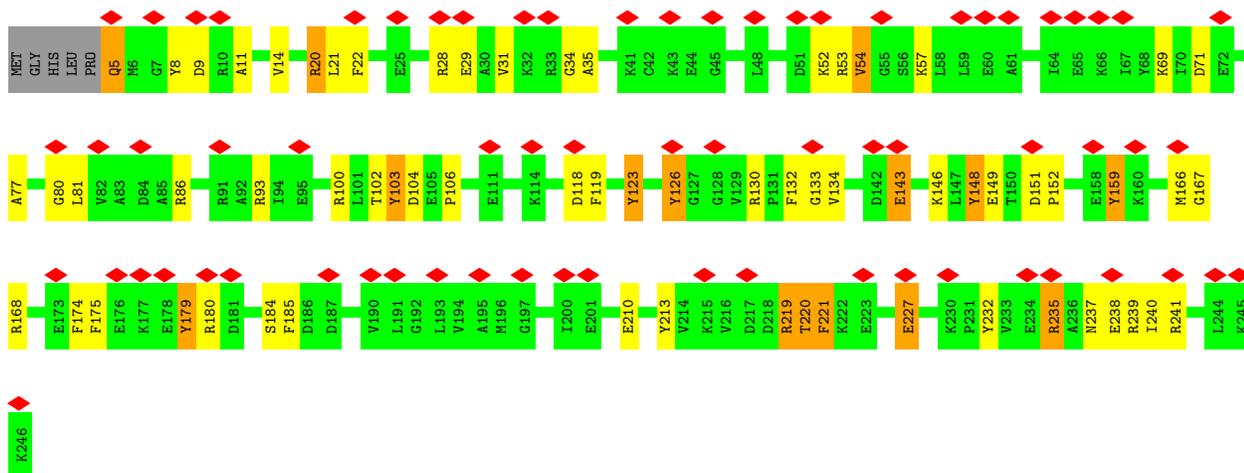


• Molecule 1: Proteasome subunit alpha





• Molecule 1: Proteasome subunit alpha

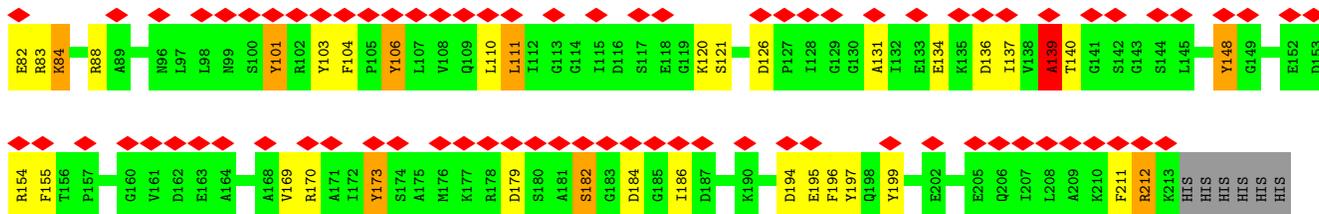


• Molecule 2: Proteasome subunit beta

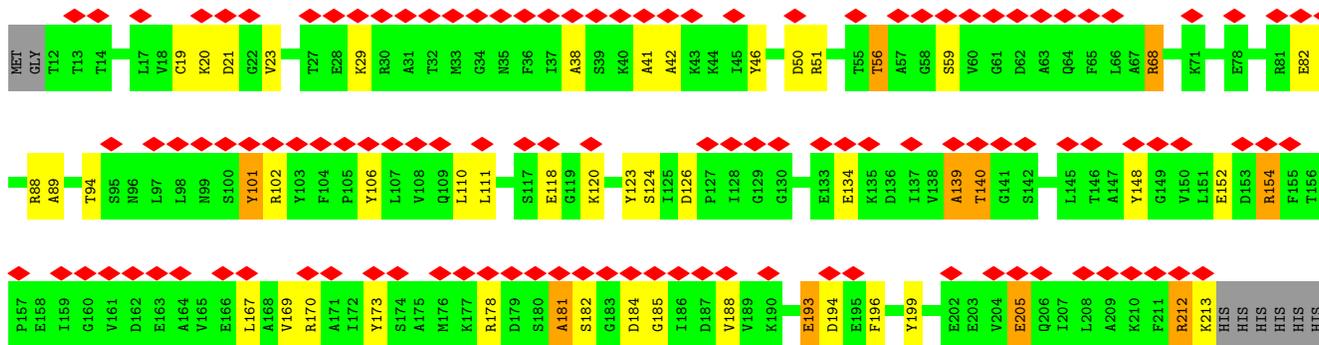


• Molecule 2: Proteasome subunit beta

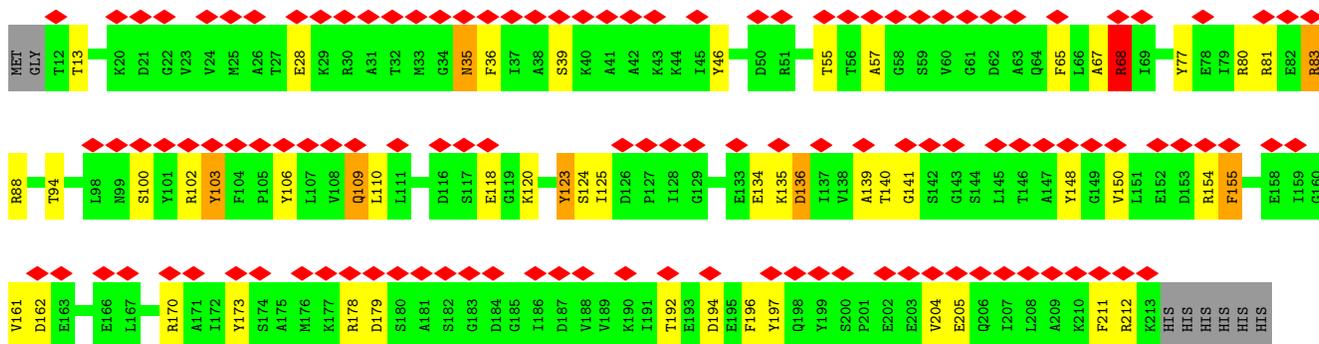




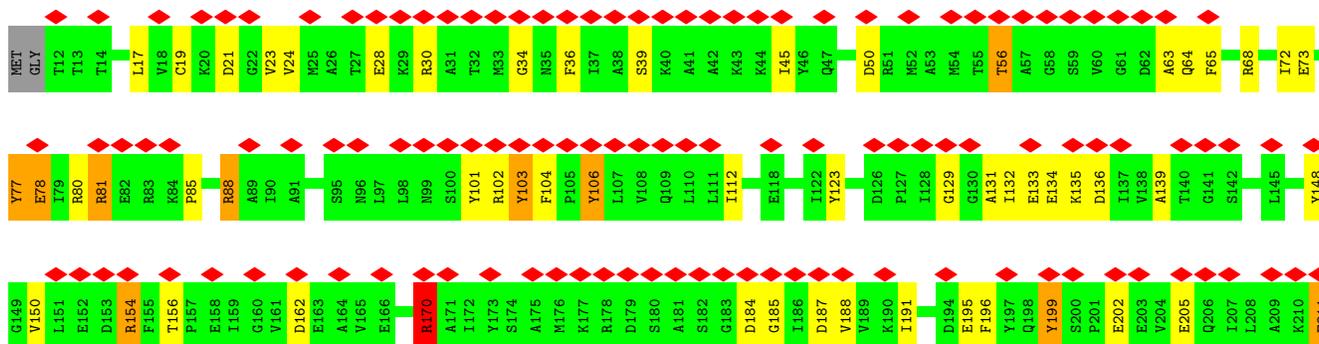
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182989	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0372	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	1.71	21/1934 (1.1%)	1.81	33/2605 (1.3%)
1	B	1.71	21/1934 (1.1%)	1.91	43/2605 (1.7%)
1	C	1.68	13/1934 (0.7%)	1.90	40/2605 (1.5%)
1	D	1.67	15/1934 (0.8%)	1.90	44/2605 (1.7%)
1	E	1.80	24/1934 (1.2%)	1.98	50/2605 (1.9%)
1	F	1.64	14/1934 (0.7%)	1.97	47/2605 (1.8%)
1	G	1.70	20/1934 (1.0%)	1.90	47/2605 (1.8%)
2	1	1.72	10/1572 (0.6%)	2.00	53/2121 (2.5%)
2	2	1.72	16/1572 (1.0%)	2.15	48/2121 (2.3%)
2	3	1.72	10/1572 (0.6%)	2.01	49/2121 (2.3%)
2	4	1.75	12/1572 (0.8%)	2.03	46/2121 (2.2%)
2	5	3.37	23/1572 (1.5%)	2.29	54/2121 (2.5%)
2	6	1.68	14/1572 (0.9%)	2.06	52/2121 (2.5%)
2	7	1.76	12/1572 (0.8%)	2.02	52/2121 (2.5%)
3	H	1.75	1/71 (1.4%)	2.00	2/92 (2.2%)
3	I	1.38	0/71	1.78	1/92 (1.1%)
3	J	1.58	1/71 (1.4%)	1.76	0/92
3	K	1.21	0/71	2.04	2/92 (2.2%)
3	L	1.64	0/71	2.11	2/92 (2.2%)
3	M	1.61	0/71	1.64	0/92
All	All	1.86	227/24968 (0.9%)	1.99	665/33634 (2.0%)

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	8
1	B	0	7
1	C	0	13
1	D	0	6
1	E	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	8
1	G	0	10
2	1	0	4
2	2	0	8
2	3	0	4
2	4	0	6
2	5	0	8
2	6	0	9
2	7	0	7
3	H	0	1
3	I	0	2
3	J	0	1
3	L	0	1
All	All	0	114

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	170	ARG	CZ-NH1	63.12	2.15	1.33
2	5	211	PHE	CG-CD2	48.04	2.10	1.38
2	5	211	PHE	CG-CD1	43.89	2.04	1.38
2	5	211	PHE	CE2-CZ	34.72	2.03	1.37
2	5	211	PHE	CE1-CZ	34.51	2.02	1.37
2	5	211	PHE	CD2-CE2	34.37	2.08	1.39
2	5	211	PHE	CD1-CE1	32.65	2.04	1.39
1	E	5	GLN	N-CA	-22.93	1.00	1.46
1	E	66	LYS	C-N	16.25	1.71	1.34
2	7	212	ARG	NE-CZ	9.61	1.45	1.33
1	G	148	TYR	CE1-CZ	9.55	1.50	1.38
1	A	179	TYR	CB-CG	-8.66	1.38	1.51
1	C	179	TYR	CG-CD1	8.61	1.50	1.39
1	B	241	ARG	CZ-NH1	7.87	1.43	1.33
2	2	73	GLU	CD-OE2	7.87	1.34	1.25
2	6	212	ARG	CZ-NH1	7.76	1.43	1.33
2	3	173	TYR	CE2-CZ	7.60	1.48	1.38
1	G	180	ARG	NE-CZ	7.52	1.42	1.33
1	D	68	TYR	CG-CD1	7.50	1.49	1.39
1	D	8	TYR	CE2-CZ	7.28	1.48	1.38
1	B	219	ARG	NE-CZ	7.26	1.42	1.33
1	G	219	ARG	CD-NE	7.21	1.58	1.46
1	A	168	ARG	CZ-NH2	7.13	1.42	1.33
2	5	80	ARG	CZ-NH1	7.13	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	170	ARG	CZ-NH1	7.12	1.42	1.33
2	3	106	TYR	CG-CD1	7.09	1.48	1.39
1	G	239	ARG	NE-CZ	7.04	1.42	1.33
1	B	235	ARG	CZ-NH1	7.03	1.42	1.33
2	2	81	ARG	CZ-NH1	6.97	1.42	1.33
2	6	106	TYR	CE1-CZ	6.93	1.47	1.38
1	A	148	TYR	CZ-OH	6.91	1.49	1.37
1	A	105	GLU	CD-OE2	6.88	1.33	1.25
2	7	106	TYR	CG-CD2	6.84	1.48	1.39
2	4	118	GLU	CG-CD	6.79	1.62	1.51
2	7	211	PHE	CG-CD1	6.78	1.49	1.38
2	2	106	TYR	CE1-CZ	6.78	1.47	1.38
2	5	101	TYR	CE1-CZ	6.59	1.47	1.38
2	4	197	TYR	CD1-CE1	6.52	1.49	1.39
1	D	241	ARG	CD-NE	6.50	1.57	1.46
1	F	91	ARG	CZ-NH2	6.50	1.41	1.33
2	5	212	ARG	NE-CZ	6.48	1.41	1.33
2	3	59	SER	CA-CB	6.46	1.62	1.52
2	7	77	TYR	CZ-OH	6.45	1.48	1.37
2	2	30	ARG	CZ-NH1	6.43	1.41	1.33
2	7	102	ARG	CZ-NH2	6.42	1.41	1.33
2	4	77	TYR	CE1-CZ	6.41	1.46	1.38
1	E	86	ARG	NE-CZ	6.41	1.41	1.33
1	C	179	TYR	CE2-CZ	6.38	1.46	1.38
2	7	205	GLU	CG-CD	6.32	1.61	1.51
2	5	81	ARG	NE-CZ	6.28	1.41	1.33
1	E	105	GLU	CG-CD	6.27	1.61	1.51
1	A	180	ARG	CD-NE	6.23	1.57	1.46
1	D	232	TYR	CG-CD2	6.22	1.47	1.39
1	G	126	TYR	CE2-CZ	6.19	1.46	1.38
2	2	170	ARG	NE-CZ	6.19	1.41	1.33
1	F	68	TYR	CG-CD1	6.16	1.47	1.39
1	E	10	ARG	CD-NE	6.14	1.56	1.46
1	G	53	ARG	NE-CZ	6.12	1.41	1.33
2	3	152	GLU	CG-CD	6.08	1.61	1.51
2	2	212	ARG	CZ-NH2	6.05	1.41	1.33
2	1	178	ARG	CZ-NH1	6.05	1.41	1.33
1	F	86	ARG	NE-CZ	6.04	1.41	1.33
2	5	134	GLU	CD-OE1	6.04	1.32	1.25
2	4	88	ARG	NE-CZ	6.02	1.40	1.33
1	E	192	GLY	CA-C	-5.99	1.42	1.51
2	4	124	SER	CA-CB	5.99	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	123	TYR	CE2-CZ	5.97	1.46	1.38
1	G	210	GLU	CD-OE2	5.97	1.32	1.25
1	A	241	ARG	CZ-NH1	5.96	1.40	1.33
1	E	53	ARG	CD-NE	5.94	1.56	1.46
2	5	184	ASP	CB-CG	5.94	1.64	1.51
1	B	148	TYR	CB-CG	5.93	1.60	1.51
1	A	219	ARG	CZ-NH1	5.92	1.40	1.33
1	F	241	ARG	CZ-NH1	5.91	1.40	1.33
2	1	36	PHE	CG-CD1	5.90	1.47	1.38
2	5	34	GLY	N-CA	-5.88	1.37	1.46
1	D	223	GLU	CG-CD	5.88	1.60	1.51
1	C	33	ARG	CZ-NH2	5.87	1.40	1.33
2	6	121	SER	CA-CB	5.87	1.61	1.52
2	5	103	TYR	CE1-CZ	5.87	1.46	1.38
2	2	173	TYR	CE2-CZ	5.87	1.46	1.38
2	6	104	PHE	CG-CD1	5.80	1.47	1.38
1	B	148	TYR	CE1-CZ	5.79	1.46	1.38
1	B	180	ARG	CZ-NH2	5.77	1.40	1.33
1	E	148	TYR	CG-CD1	5.76	1.46	1.39
1	E	153	SER	CA-CB	5.76	1.61	1.52
1	F	93	ARG	NE-CZ	5.75	1.40	1.33
1	G	86	ARG	CZ-NH1	5.73	1.40	1.33
2	6	178	ARG	CD-NE	5.72	1.56	1.46
2	4	148	TYR	CD1-CE1	5.71	1.48	1.39
1	B	135	SER	CA-CB	5.71	1.61	1.52
1	E	130	ARG	NE-CZ	5.70	1.40	1.33
2	6	113	GLY	CA-C	-5.70	1.42	1.51
2	4	100	SER	CA-CB	5.69	1.61	1.52
2	1	197	TYR	CE1-CZ	5.67	1.46	1.38
2	3	205	GLU	CB-CG	5.67	1.62	1.52
1	B	213	TYR	CB-CG	5.67	1.60	1.51
1	E	235	ARG	CZ-NH2	5.64	1.40	1.33
2	1	211	PHE	CG-CD1	5.64	1.47	1.38
1	A	10	ARG	NE-CZ	5.63	1.40	1.33
1	E	148	TYR	CZ-OH	5.63	1.47	1.37
2	6	67	ALA	CA-C	-5.62	1.38	1.52
1	B	228	GLU	CD-OE1	-5.60	1.19	1.25
2	5	73	GLU	CD-OE1	5.60	1.31	1.25
1	F	20	ARG	NE-CZ	5.60	1.40	1.33
1	C	86	ARG	CZ-NH1	5.60	1.40	1.33
1	A	33	ARG	CZ-NH1	5.59	1.40	1.33
1	G	103	TYR	CG-CD2	5.59	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	80	ARG	CZ-NH1	5.58	1.40	1.33
1	F	221	PHE	CA-CB	5.57	1.66	1.53
2	5	68	ARG	CZ-NH1	5.57	1.40	1.33
2	5	123	TYR	CZ-OH	5.56	1.47	1.37
2	5	88	ARG	CD-NE	5.54	1.55	1.46
1	E	100	ARG	NE-CZ	5.54	1.40	1.33
1	B	228	GLU	CD-OE2	5.54	1.31	1.25
1	A	86	ARG	CZ-NH2	5.54	1.40	1.33
1	E	242	GLU	CG-CD	5.51	1.60	1.51
1	C	123	TYR	CG-CD2	5.50	1.46	1.39
1	D	60	GLU	CB-CG	5.50	1.62	1.52
1	B	8	TYR	CE2-CZ	5.48	1.45	1.38
2	2	121	SER	CA-CB	5.48	1.61	1.52
1	E	123	TYR	CG-CD1	5.48	1.46	1.39
1	E	232	TYR	CE2-CZ	5.47	1.45	1.38
1	F	219	ARG	CZ-NH1	5.47	1.40	1.33
1	G	20	ARG	CZ-NH2	5.47	1.40	1.33
1	G	185	PHE	CB-CG	-5.46	1.42	1.51
1	B	175	PHE	CB-CG	5.46	1.60	1.51
2	3	184	ASP	C-N	5.46	1.42	1.33
1	A	199	SER	CA-CB	5.44	1.61	1.52
1	A	100	ARG	NE-CZ	5.43	1.40	1.33
1	C	23	GLN	N-CA	-5.43	1.35	1.46
1	G	179	TYR	CE1-CZ	5.40	1.45	1.38
1	D	20	ARG	CZ-NH2	5.40	1.40	1.33
1	A	91	ARG	CZ-NH2	5.40	1.40	1.33
1	A	146	LYS	N-CA	-5.39	1.35	1.46
1	E	173	GLU	CG-CD	-5.39	1.43	1.51
1	F	225	SER	CA-CB	5.39	1.61	1.52
1	G	241	ARG	NE-CZ	5.39	1.40	1.33
1	A	18	ASP	CB-CG	5.39	1.63	1.51
1	C	10	ARG	CZ-NH1	5.39	1.40	1.33
1	E	232	TYR	CG-CD1	5.38	1.46	1.39
1	E	93	ARG	CD-NE	5.38	1.55	1.46
2	6	148	TYR	CG-CD1	5.38	1.46	1.39
1	C	10	ARG	CD-NE	5.38	1.55	1.46
1	C	8	TYR	CE2-CZ	5.37	1.45	1.38
1	G	167	GLY	CA-C	-5.36	1.43	1.51
1	D	100	ARG	CZ-NH2	5.36	1.40	1.33
2	6	211	PHE	CG-CD2	5.35	1.46	1.38
2	2	30	ARG	CD-NE	5.34	1.55	1.46
2	2	101	TYR	CE2-CZ	5.33	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	51	ARG	CD-NE	5.32	1.55	1.46
1	B	148	TYR	CG-CD1	5.32	1.46	1.39
2	3	118	GLU	C-N	5.32	1.42	1.33
1	E	225	SER	CA-CB	5.31	1.60	1.52
1	G	53	ARG	CZ-NH2	5.30	1.40	1.33
1	F	239	ARG	CZ-NH2	5.29	1.40	1.33
2	3	193	GLU	CB-CG	5.29	1.62	1.52
1	B	202	SER	CA-CB	5.29	1.60	1.52
1	E	65	GLU	C-N	5.28	1.46	1.34
2	6	80	ARG	CD-NE	5.28	1.55	1.46
1	G	168	ARG	CZ-NH2	5.28	1.40	1.33
2	6	134	GLU	CD-OE1	5.28	1.31	1.25
2	2	88	ARG	NE-CZ	5.27	1.40	1.33
2	2	82	GLU	CG-CD	5.26	1.59	1.51
2	2	173	TYR	CG-CD1	5.26	1.46	1.39
2	1	212	ARG	NE-CZ	5.25	1.39	1.33
1	C	77	ALA	CA-CB	5.25	1.63	1.52
1	C	100	ARG	NE-CZ	5.25	1.39	1.33
2	3	82	GLU	CG-CD	5.25	1.59	1.51
2	7	178	ARG	NE-CZ	5.25	1.39	1.33
1	E	185	PHE	CG-CD2	5.24	1.46	1.38
1	B	235	ARG	CZ-NH2	5.23	1.39	1.33
1	B	123	TYR	CG-CD1	5.22	1.46	1.39
2	2	84	LYS	CA-CB	5.22	1.65	1.53
2	1	24	VAL	CA-CB	-5.21	1.43	1.54
1	D	228	GLU	CG-CD	5.21	1.59	1.51
2	7	154	ARG	CD-NE	5.21	1.55	1.46
1	G	148	TYR	CB-CG	-5.21	1.43	1.51
1	A	239	ARG	CZ-NH1	5.20	1.39	1.33
2	2	65	PHE	CE1-CZ	5.20	1.47	1.37
3	H	393	LYS	C-N	5.19	1.42	1.33
1	E	93	ARG	CZ-NH2	5.19	1.39	1.33
1	D	158	GLU	CD-OE1	5.19	1.31	1.25
1	F	235	ARG	NE-CZ	5.19	1.39	1.33
1	D	210	GLU	CG-CD	5.18	1.59	1.51
2	4	141	GLY	CA-C	-5.17	1.43	1.51
1	C	130	ARG	NE-CZ	5.17	1.39	1.33
2	5	103	TYR	CZ-OH	5.16	1.46	1.37
2	5	135	LYS	CA-CB	5.16	1.65	1.53
2	5	154	ARG	CZ-NH2	5.16	1.39	1.33
1	F	86	ARG	CZ-NH2	5.15	1.39	1.33
2	4	170	ARG	CZ-NH2	5.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	392	LEU	N-CA	-5.15	1.36	1.46
1	F	53	ARG	CD-NE	5.14	1.55	1.46
1	B	8	TYR	CB-CG	-5.14	1.44	1.51
1	B	15	PHE	CG-CD2	5.14	1.46	1.38
2	6	87	VAL	CB-CG2	5.14	1.63	1.52
1	A	93	ARG	CZ-NH2	5.12	1.39	1.33
2	7	13	THR	CA-C	-5.12	1.39	1.52
2	1	173	TYR	CZ-OH	5.11	1.46	1.37
2	1	148	TYR	CG-CD2	5.11	1.45	1.39
2	4	83	ARG	CZ-NH2	5.10	1.39	1.33
1	B	20	ARG	CD-NE	5.09	1.55	1.46
2	5	28	GLU	CG-CD	5.09	1.59	1.51
1	A	148	TYR	CE2-CZ	5.07	1.45	1.38
1	G	54	VAL	CB-CG2	5.07	1.63	1.52
1	D	130	ARG	CZ-NH2	5.07	1.39	1.33
1	A	20	ARG	CZ-NH2	5.07	1.39	1.33
2	3	89	ALA	CA-C	-5.05	1.39	1.52
2	6	102	ARG	NE-CZ	5.04	1.39	1.33
1	C	168	ARG	NE-CZ	5.04	1.39	1.33
2	4	135	LYS	CA-C	-5.03	1.39	1.52
2	1	30	ARG	CZ-NH1	5.03	1.39	1.33
1	D	44	GLU	N-CA	-5.03	1.36	1.46
1	B	176	GLU	CD-OE1	5.03	1.31	1.25
1	G	53	ARG	CD-NE	5.03	1.54	1.46
1	A	224	VAL	CB-CG1	5.02	1.63	1.52
1	D	131	PRO	N-CA	-5.02	1.38	1.47
2	6	68	ARG	CZ-NH1	5.02	1.39	1.33
1	F	53	ARG	CZ-NH1	5.02	1.39	1.33
2	2	104	PHE	CG-CD1	5.01	1.46	1.38
1	A	184	SER	CA-CB	5.01	1.60	1.52
1	G	227	GLU	CG-CD	5.01	1.59	1.51
2	7	28	GLU	N-CA	-5.01	1.36	1.46
1	E	10	ARG	CZ-NH2	5.01	1.39	1.33
1	B	60	GLU	CD-OE2	5.00	1.31	1.25
2	7	28	GLU	CG-CD	5.00	1.59	1.51

All (665) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	170	ARG	NE-CZ-NH2	-37.83	101.39	120.30
2	5	170	ARG	NE-CZ-NH1	20.34	130.47	120.30
2	2	212	ARG	NE-CZ-NH1	19.40	130.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	ARG	NE-CZ-NH2	-18.12	111.24	120.30
1	D	86	ARG	NE-CZ-NH1	16.07	128.34	120.30
2	3	178	ARG	NE-CZ-NH1	15.92	128.26	120.30
2	2	101	TYR	CB-CG-CD2	-15.54	111.68	121.00
2	5	106	TYR	CB-CG-CD2	15.48	130.29	121.00
1	E	8	TYR	CB-CG-CD1	-14.82	112.11	121.00
2	5	106	TYR	CB-CG-CD1	-14.79	112.12	121.00
2	2	101	TYR	CB-CG-CD1	14.67	129.80	121.00
1	E	130	ARG	NE-CZ-NH2	-14.61	113.00	120.30
2	3	178	ARG	NE-CZ-NH2	-13.79	113.41	120.30
2	4	106	TYR	CB-CG-CD1	13.47	129.08	121.00
1	D	213	TYR	CB-CG-CD1	13.18	128.91	121.00
1	F	126	TYR	CB-CG-CD1	13.05	128.83	121.00
1	F	159	TYR	CB-CG-CD2	-12.76	113.34	121.00
1	B	235	ARG	NE-CZ-NH2	12.74	126.67	120.30
2	2	30	ARG	NE-CZ-NH2	12.66	126.63	120.30
2	5	77	TYR	CB-CG-CD1	-12.54	113.48	121.00
2	6	199	TYR	CB-CG-CD1	12.50	128.50	121.00
2	5	212	ARG	NE-CZ-NH2	-12.38	114.11	120.30
2	2	51	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	B	20	ARG	NE-CZ-NH1	12.16	126.38	120.30
2	6	51	ARG	NE-CZ-NH1	-11.86	114.37	120.30
2	2	83	ARG	NE-CZ-NH2	11.85	126.22	120.30
2	6	199	TYR	CB-CG-CD2	-11.79	113.93	121.00
1	F	130	ARG	NE-CZ-NH1	11.70	126.15	120.30
2	7	211	PHE	CB-CG-CD2	11.67	128.97	120.80
2	4	83	ARG	NE-CZ-NH1	-11.61	114.49	120.30
1	C	219	ARG	NE-CZ-NH2	-11.60	114.50	120.30
2	2	148	TYR	CB-CG-CD1	-11.57	114.06	121.00
1	F	20	ARG	NE-CZ-NH2	11.51	126.06	120.30
2	2	106	TYR	CB-CG-CD1	-11.27	114.24	121.00
2	2	154	ARG	NE-CZ-NH1	-11.05	114.78	120.30
1	F	239	ARG	NE-CZ-NH1	11.02	125.81	120.30
2	2	46	TYR	CB-CG-CD2	-11.00	114.40	121.00
1	F	221	PHE	CB-CG-CD2	-10.98	113.11	120.80
1	G	53	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	F	148	TYR	CB-CG-CD2	-10.79	114.53	121.00
2	4	106	TYR	CB-CG-CD2	-10.77	114.54	121.00
1	C	180	ARG	NE-CZ-NH2	10.77	125.68	120.30
1	E	65	GLU	O-C-N	-10.76	105.49	122.70
2	4	102	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	C	241	ARG	NE-CZ-NH2	10.58	125.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	ARG	NE-CZ-NH2	10.43	125.52	120.30
2	2	68	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	F	159	TYR	CB-CG-CD1	10.40	127.24	121.00
2	3	46	TYR	CB-CG-CD1	-10.40	114.76	121.00
1	A	86	ARG	NE-CZ-NH1	10.39	125.50	120.30
2	6	102	ARG	NE-CZ-NH2	10.32	125.46	120.30
2	1	46	TYR	CB-CG-CD1	10.30	127.18	121.00
2	6	83	ARG	NE-CZ-NH1	-10.29	115.15	120.30
1	E	123	TYR	CB-CG-CD2	-10.29	114.83	121.00
2	5	81	ARG	NE-CZ-NH2	10.29	125.44	120.30
2	7	83	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	A	168	ARG	NE-CZ-NH2	-10.24	115.18	120.30
2	4	154	ARG	NE-CZ-NH1	-10.22	115.19	120.30
2	6	88	ARG	NE-CZ-NH2	10.19	125.39	120.30
1	D	179	TYR	CB-CG-CD2	10.10	127.06	121.00
2	1	102	ARG	NE-CZ-NH2	10.10	125.35	120.30
2	1	46	TYR	CB-CG-CD2	-10.09	114.95	121.00
1	D	103	TYR	CB-CG-CD2	-10.09	114.95	121.00
1	E	86	ARG	NE-CZ-NH1	-10.08	115.26	120.30
2	3	51	ARG	NE-CZ-NH2	10.07	125.33	120.30
1	F	148	TYR	CB-CG-CD1	9.98	126.99	121.00
1	D	185	PHE	CB-CG-CD1	9.98	127.78	120.80
1	C	123	TYR	CB-CG-CD2	-9.96	115.02	121.00
2	4	197	TYR	CB-CG-CD2	-9.92	115.05	121.00
1	B	232	TYR	CB-CG-CD1	-9.85	115.09	121.00
1	B	241	ARG	NE-CZ-NH2	9.85	125.22	120.30
2	5	123	TYR	CB-CG-CD1	-9.78	115.13	121.00
1	B	174	PHE	CB-CG-CD2	-9.71	114.01	120.80
1	C	10	ARG	NE-CZ-NH2	-9.70	115.45	120.30
2	4	173	TYR	CB-CG-CD2	9.68	126.81	121.00
2	7	102	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	E	68	TYR	CB-CG-CD2	-9.63	115.22	121.00
2	5	199	TYR	CB-CG-CD2	-9.47	115.32	121.00
1	G	100	ARG	NE-CZ-NH1	-9.46	115.57	120.30
1	A	26	TYR	CG-CD1-CE1	-9.45	113.74	121.30
2	3	123	TYR	CB-CG-CD2	-9.37	115.38	121.00
1	A	10	ARG	NE-CZ-NH2	9.37	124.98	120.30
2	5	77	TYR	CB-CG-CD2	9.35	126.61	121.00
1	F	179	TYR	CB-CG-CD2	-9.31	115.41	121.00
2	2	81	ARG	NE-CZ-NH1	9.26	124.93	120.30
2	2	103	TYR	CB-CG-CD1	-9.23	115.46	121.00
2	6	178	ARG	NE-CZ-NH2	-9.22	115.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	213	TYR	CB-CG-CD1	9.20	126.52	121.00
2	2	148	TYR	CB-CG-CD2	9.18	126.51	121.00
2	6	81	ARG	NE-CZ-NH2	-9.16	115.72	120.30
2	6	155	PHE	CB-CG-CD1	-9.15	114.39	120.80
1	D	185	PHE	CB-CG-CD2	-9.15	114.39	120.80
1	B	68	TYR	CB-CG-CD2	9.13	126.48	121.00
1	F	86	ARG	NE-CZ-NH2	-9.13	115.73	120.30
2	4	103	TYR	CB-CG-CD2	-9.08	115.55	121.00
1	B	174	PHE	CB-CG-CD1	9.04	127.13	120.80
2	1	211	PHE	CB-CG-CD1	-9.02	114.49	120.80
1	G	53	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	26	TYR	CB-CG-CD1	-8.98	115.61	121.00
1	E	126	TYR	CB-CG-CD2	-8.92	115.65	121.00
1	G	175	PHE	CB-CG-CD2	-8.91	114.56	120.80
2	1	148	TYR	CB-CG-CD1	-8.89	115.67	121.00
2	1	170	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	G	235	ARG	NE-CZ-NH1	-8.88	115.86	120.30
2	2	88	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	A	241	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	C	123	TYR	CB-CG-CD1	8.87	126.32	121.00
1	B	123	TYR	CB-CG-CD2	-8.84	115.70	121.00
2	4	77	TYR	CZ-CE2-CD2	8.79	127.71	119.80
1	D	202	SER	N-CA-CB	8.76	123.64	110.50
2	7	211	PHE	CB-CG-CD1	-8.73	114.69	120.80
1	F	235	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	D	182	ASP	CB-CG-OD1	8.72	126.15	118.30
1	B	123	TYR	CB-CG-CD1	8.62	126.17	121.00
2	5	65	PHE	CB-CG-CD2	8.61	126.82	120.80
1	E	158	GLU	OE1-CD-OE2	8.58	133.59	123.30
1	B	185	PHE	CB-CG-CD1	8.57	126.80	120.80
1	E	126	TYR	CB-CG-CD1	8.54	126.12	121.00
2	3	106	TYR	CB-CG-CD2	-8.52	115.89	121.00
2	1	154	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	F	130	ARG	NE-CZ-NH2	-8.51	116.05	120.30
2	2	30	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	D	33	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	E	26	TYR	CB-CG-CD2	8.45	126.07	121.00
1	D	91	ARG	NE-CZ-NH2	-8.45	116.08	120.30
2	2	81	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	E	148	TYR	CB-CG-CD2	8.31	125.98	121.00
2	1	136	ASP	CB-CG-OD2	-8.31	110.82	118.30
2	3	102	ARG	NE-CZ-NH2	-8.29	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	100	ARG	NE-CZ-NH2	8.28	124.44	120.30
2	6	54	MET	CG-SD-CE	-8.26	86.98	100.20
2	6	68	ARG	NE-CZ-NH2	-8.24	116.18	120.30
2	7	81	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	E	66	LYS	O-C-N	8.24	135.88	122.70
1	E	123	TYR	CB-CG-CD1	8.23	125.94	121.00
2	3	101	TYR	CB-CG-CD1	-8.23	116.06	121.00
1	G	22	PHE	CB-CG-CD2	-8.22	115.04	120.80
1	D	126	TYR	CB-CG-CD2	8.22	125.93	121.00
1	C	15	PHE	CB-CG-CD2	-8.19	115.06	120.80
2	6	81	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	65	GLU	N-CA-CB	8.13	125.24	110.60
1	F	123	TYR	CB-CG-CD2	-8.11	116.13	121.00
1	G	130	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	B	219	ARG	NE-CZ-NH2	8.03	124.32	120.30
2	2	111	LEU	CB-CG-CD1	8.03	124.66	111.00
2	5	154	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	E	65	GLU	C-N-CA	8.01	141.72	121.70
2	6	51	ARG	NE-CZ-NH2	8.01	124.30	120.30
2	5	30	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	D	181	ASP	CB-CG-OD2	-7.95	111.14	118.30
2	5	170	ARG	NH1-CZ-NH2	7.94	128.13	119.40
1	G	179	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	F	221	PHE	CB-CG-CD1	7.91	126.33	120.80
2	3	154	ARG	NE-CZ-NH2	7.90	124.25	120.30
2	4	173	TYR	CB-CG-CD1	-7.89	116.27	121.00
1	E	175	PHE	CB-CG-CD1	7.87	126.31	120.80
2	3	123	TYR	CB-CG-CD1	7.86	125.72	121.00
2	7	103	TYR	CB-CG-CD2	7.83	125.70	121.00
1	D	24	VAL	CA-CB-CG2	-7.80	99.20	110.90
1	C	235	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	C	219	ARG	NE-CZ-NH1	7.69	124.15	120.30
2	7	39	SER	N-CA-CB	7.69	122.03	110.50
1	G	168	ARG	NE-CZ-NH2	-7.69	116.46	120.30
2	1	197	TYR	CB-CG-CD2	7.68	125.61	121.00
1	G	104	ASP	N-CA-CB	7.64	124.36	110.60
2	1	104	PHE	CB-CG-CD1	-7.63	115.46	120.80
2	7	68	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	5	196	PHE	CB-CG-CD1	-7.57	115.50	120.80
2	2	88	ARG	NE-CZ-NH2	7.57	124.08	120.30
2	7	197	TYR	CB-CG-CD2	7.56	125.53	121.00
2	1	211	PHE	CB-CG-CD2	7.54	126.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	52	MET	CG-SD-CE	-7.50	88.20	100.20
2	7	179	ASP	CB-CG-OD2	-7.50	111.55	118.30
2	3	169	VAL	CA-CB-CG2	-7.48	99.69	110.90
1	F	20	ARG	NE-CZ-NH1	-7.47	116.57	120.30
2	2	106	TYR	CB-CG-CD2	7.47	125.48	121.00
2	7	24	VAL	CA-CB-CG2	-7.47	99.70	110.90
1	C	159	TYR	CB-CG-CD2	-7.44	116.54	121.00
2	4	162	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	90	ASP	CB-CG-OD1	-7.39	111.65	118.30
2	6	148	TYR	CG-CD1-CE1	-7.39	115.39	121.30
2	4	196	PHE	N-CA-CB	7.38	123.89	110.60
2	6	101	TYR	CG-CD1-CE1	-7.34	115.42	121.30
2	7	27	THR	CA-CB-CG2	-7.33	102.14	112.40
1	B	219	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	B	185	PHE	CB-CG-CD2	-7.32	115.68	120.80
2	6	104	PHE	CB-CG-CD1	7.32	125.92	120.80
2	6	173	TYR	CB-CG-CD1	-7.24	116.66	121.00
1	B	91	ARG	NE-CZ-NH1	-7.23	116.68	120.30
2	1	82	GLU	N-CA-CB	7.22	123.61	110.60
2	2	77	TYR	CG-CD1-CE1	-7.22	115.52	121.30
1	E	65	GLU	CA-C-N	7.21	133.07	117.20
2	5	123	TYR	CG-CD2-CE2	-7.19	115.55	121.30
2	7	88	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	C	79	SER	N-CA-CB	7.17	121.25	110.50
1	E	93	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	148	TYR	CB-CG-CD2	-7.15	116.71	121.00
2	3	106	TYR	CG-CD1-CE1	-7.15	115.58	121.30
2	6	65	PHE	CB-CG-CD2	-7.12	115.82	120.80
2	5	68	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	2	212	ARG	NH1-CZ-NH2	-7.08	111.61	119.40
2	1	170	ARG	NH1-CZ-NH2	-7.07	111.62	119.40
2	4	65	PHE	CB-CG-CD1	-7.07	115.85	120.80
1	E	185	PHE	CB-CG-CD2	-7.06	115.86	120.80
2	6	173	TYR	CB-CG-CD2	7.06	125.24	121.00
2	1	139	ALA	N-CA-CB	7.06	119.98	110.10
2	3	46	TYR	CG-CD1-CE1	-7.05	115.66	121.30
2	5	24	VAL	CA-CB-CG2	-7.04	100.35	110.90
1	E	108	THR	CA-CB-CG2	-7.03	102.55	112.40
2	7	178	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	B	68	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	B	27	ALA	N-CA-CB	7.02	119.92	110.10
1	F	91	ARG	NE-CZ-NH2	-7.01	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	PHE	CB-CG-CD1	7.00	125.70	120.80
2	2	103	TYR	CD1-CE1-CZ	-7.00	113.50	119.80
2	6	140	THR	N-CA-CB	6.97	123.55	110.30
1	A	224	VAL	CG1-CB-CG2	-6.97	99.74	110.90
2	4	77	TYR	CB-CG-CD2	-6.96	116.83	121.00
2	3	42	ALA	N-CA-CB	6.95	119.82	110.10
1	G	86	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	B	20	ARG	NH1-CZ-NH2	-6.92	111.78	119.40
2	1	102	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	E	66	LYS	CA-C-N	-6.91	101.99	117.20
2	3	199	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	F	11	ALA	N-CA-CB	6.85	119.69	110.10
1	B	103	TYR	CB-CG-CD2	-6.85	116.89	121.00
2	2	139	ALA	N-CA-CB	6.85	119.69	110.10
1	B	91	ARG	NE-CZ-NH2	6.84	123.72	120.30
2	5	199	TYR	CG-CD1-CE1	-6.82	115.85	121.30
2	3	154	ARG	NE-CZ-NH1	-6.81	116.90	120.30
1	F	137	LEU	N-CA-C	-6.80	92.64	111.00
1	C	220	THR	CA-CB-CG2	-6.79	102.89	112.40
2	1	106	TYR	CB-CG-CD2	6.79	125.07	121.00
1	G	118	ASP	CB-CG-OD1	6.77	124.40	118.30
2	4	212	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	D	64	ILE	C-N-CA	6.77	138.62	121.70
1	E	31	VAL	CA-CB-CG2	-6.75	100.78	110.90
1	E	118	ASP	CB-CG-OD1	-6.75	112.23	118.30
2	7	162	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	G	213	TYR	CG-CD2-CE2	-6.73	115.92	121.30
1	C	175	PHE	CB-CG-CD2	-6.72	116.09	120.80
2	1	154	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	2	51	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	5	101	TYR	CG-CD1-CE1	-6.70	115.94	121.30
2	6	123	TYR	CB-CG-CD1	6.69	125.02	121.00
1	B	203	GLU	N-CA-CB	6.69	122.64	110.60
2	5	162	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	F	76	ALA	CB-CA-C	-6.66	100.11	110.10
1	A	166	MET	CG-SD-CE	6.66	110.85	100.20
1	E	28	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	G	219	ARG	N-CA-CB	6.65	122.58	110.60
2	1	71	LYS	O-C-N	-6.65	112.06	122.70
2	3	173	TYR	CB-CG-CD1	-6.65	117.01	121.00
2	4	102	ARG	NH1-CZ-NH2	-6.63	112.10	119.40
2	6	136	ASP	CB-CG-OD1	6.63	124.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	104	PHE	CB-CG-CD1	-6.63	116.16	120.80
2	5	195	GLU	O-C-N	6.62	133.29	122.70
2	5	65	PHE	CB-CG-CD1	-6.62	116.17	120.80
2	1	67	ALA	N-CA-CB	6.61	119.35	110.10
2	7	13	THR	N-CA-CB	6.60	122.84	110.30
1	F	93	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	G	11	ALA	N-CA-CB	6.59	119.32	110.10
2	7	77	TYR	O-C-N	-6.57	112.19	122.70
1	C	118	ASP	CB-CG-OD1	6.57	124.21	118.30
2	4	155	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	D	179	TYR	CB-CG-CD1	-6.56	117.06	121.00
2	7	173	TYR	CB-CG-CD1	6.54	124.92	121.00
2	4	77	TYR	CG-CD2-CE2	-6.54	116.07	121.30
2	4	179	ASP	CB-CG-OD2	6.54	124.18	118.30
2	2	65	PHE	CB-CG-CD1	-6.53	116.23	120.80
1	C	68	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	D	168	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	F	54	VAL	CA-CB-CG1	-6.51	101.13	110.90
1	F	95	GLU	N-CA-CB	6.51	122.32	110.60
2	3	196	PHE	CB-CG-CD2	-6.50	116.25	120.80
2	2	199	TYR	CB-CG-CD2	-6.50	117.10	121.00
2	5	187	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	239	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	D	161	ALA	CB-CA-C	-6.48	100.38	110.10
1	E	8	TYR	CB-CG-CD2	6.48	124.89	121.00
1	E	213	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	G	20	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	7	93	LEU	CB-CG-CD1	6.46	121.99	111.00
2	4	67	ALA	N-CA-CB	6.46	119.15	110.10
1	A	26	TYR	CB-CG-CD2	6.45	124.87	121.00
2	7	197	TYR	CB-CG-CD1	-6.45	117.13	121.00
2	6	46	TYR	CB-CG-CD1	-6.45	117.13	121.00
2	5	30	ARG	NE-CZ-NH1	-6.44	117.08	120.30
2	3	83	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	7	123	TYR	CG-CD1-CE1	-6.42	116.17	121.30
1	E	93	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	2	182	SER	N-CA-CB	6.40	120.10	110.50
1	C	51	ASP	CB-CG-OD2	6.39	124.06	118.30
2	4	194	ASP	CB-CG-OD2	-6.39	112.54	118.30
1	B	189	MET	CG-SD-CE	-6.39	89.98	100.20
2	5	77	TYR	CG-CD2-CE2	-6.38	116.19	121.30
2	1	77	TYR	CB-CG-CD1	-6.38	117.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	123	TYR	CG-CD2-CE2	-6.38	116.20	121.30
1	C	239	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	8	TYR	CB-CG-CD1	6.37	124.82	121.00
2	1	197	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	D	161	ALA	N-CA-CB	6.30	118.92	110.10
1	D	103	TYR	CD1-CG-CD2	6.30	124.83	117.90
1	F	6	MET	CG-SD-CE	-6.30	90.12	100.20
2	6	39	SER	N-CA-CB	6.30	119.95	110.50
2	5	212	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	182	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	68	TYR	CB-CG-CD2	6.29	124.77	121.00
1	F	68	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	E	62	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	1	170	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	62	ASP	CB-CG-OD2	-6.26	112.67	118.30
2	4	81	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	F	44	GLU	CB-CA-C	-6.25	97.90	110.40
1	D	126	TYR	N-CA-CB	6.25	121.85	110.60
1	F	151	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	G	241	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	26	TYR	CB-CG-CD2	6.24	124.75	121.00
2	1	155	PHE	CB-CG-CD1	-6.24	116.44	120.80
2	4	109	GLN	N-CA-CB	6.23	121.82	110.60
2	1	65	PHE	CB-CG-CD1	-6.23	116.44	120.80
2	3	212	ARG	CG-CD-NE	-6.23	98.72	111.80
1	E	103	TYR	CB-CG-CD1	6.21	124.73	121.00
2	3	20	LYS	N-CA-CB	-6.21	99.42	110.60
2	4	161	VAL	CA-CB-CG1	-6.21	101.58	110.90
2	3	120	LYS	N-CA-CB	6.20	121.76	110.60
2	2	199	TYR	CD1-CE1-CZ	-6.19	114.23	119.80
2	4	154	ARG	NE-CZ-NH2	6.18	123.39	120.30
2	6	102	ARG	NH1-CZ-NH2	-6.18	112.61	119.40
1	B	65	GLU	N-CA-CB	6.17	121.71	110.60
1	C	76	ALA	N-CA-CB	6.17	118.74	110.10
2	7	68	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	3	56	THR	CA-CB-CG2	-6.16	103.77	112.40
2	1	173	TYR	CB-CG-CD1	6.16	124.69	121.00
2	4	46	TYR	CB-CG-CD1	-6.16	117.31	121.00
2	6	211	PHE	CB-CG-CD1	-6.13	116.51	120.80
2	5	23	VAL	CA-CB-CG1	6.12	120.09	110.90
1	A	185	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	A	213	TYR	CB-CG-CD1	-6.12	117.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	23	VAL	CA-CB-CG2	-6.12	101.73	110.90
2	2	21	ASP	CB-CG-OD1	-6.11	112.80	118.30
2	1	178	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	E	179	TYR	CB-CG-CD2	-6.10	117.34	121.00
2	1	136	ASP	CB-CG-OD1	6.10	123.79	118.30
1	C	20	ARG	N-CA-CB	6.09	121.57	110.60
1	D	53	ARG	N-CA-C	-6.09	94.56	111.00
2	4	68	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	G	235	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	7	123	TYR	CB-CG-CD1	-6.08	117.35	121.00
2	1	101	TYR	CZ-CE2-CD2	-6.05	114.35	119.80
3	K	397	PHE	N-CA-CB	6.04	121.48	110.60
2	7	164	ALA	CB-CA-C	-6.04	101.04	110.10
2	2	184	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	232	TYR	CB-CG-CD2	6.03	124.62	121.00
1	E	130	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	7	191	ILE	N-CA-C	-6.02	94.75	111.00
1	E	216	VAL	CA-CB-CG2	-6.01	101.89	110.90
1	G	168	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	F	68	TYR	CB-CG-CD1	6.00	124.60	121.00
2	1	132	ILE	CA-CB-CG2	-6.00	98.90	110.90
2	3	46	TYR	CB-CA-C	-5.99	98.42	110.40
2	3	193	GLU	N-CA-CB	5.99	121.38	110.60
2	6	86	THR	CA-CB-OG1	5.98	121.57	109.00
1	G	20	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	7	134	GLU	N-CA-CB	5.98	121.37	110.60
2	6	28	GLU	OE1-CD-OE2	5.98	130.48	123.30
2	3	124	SER	N-CA-C	-5.97	94.87	111.00
2	5	80	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	G	9	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	G	77	ALA	N-CA-CB	5.96	118.45	110.10
1	C	171	VAL	CA-CB-CG2	-5.96	101.96	110.90
1	G	106	PRO	N-CA-CB	5.96	110.45	103.30
3	L	390	PRO	N-CA-CB	5.96	110.45	103.30
1	G	238	GLU	OE1-CD-OE2	5.96	130.45	123.30
1	E	66	LYS	C-N-CA	-5.95	106.82	121.70
1	E	20	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	2	78	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	E	8	TYR	CG-CD1-CE1	-5.95	116.54	121.30
2	3	140	THR	N-CA-CB	5.95	121.60	110.30
1	G	93	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	1	196	PHE	CB-CG-CD1	5.93	124.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	TYR	CG-CD2-CE2	-5.93	116.56	121.30
2	1	173	TYR	CA-CB-CG	5.92	124.65	113.40
2	7	41	ALA	CB-CA-C	-5.91	101.24	110.10
2	1	81	ARG	NE-CZ-NH2	-5.91	117.35	120.30
3	I	397	PHE	CB-CG-CD2	5.91	124.93	120.80
1	B	67	ILE	N-CA-C	-5.90	95.06	111.00
2	6	80	ARG	NE-CZ-NH1	-5.90	117.35	120.30
2	3	50	ASP	CB-CG-OD2	5.90	123.61	118.30
2	5	23	VAL	CA-CB-CG2	-5.89	102.06	110.90
1	E	235	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	C	166	MET	CG-SD-CE	-5.88	90.79	100.20
2	4	178	ARG	NE-CZ-NH1	-5.88	117.36	120.30
2	5	148	TYR	CB-CG-CD1	5.87	124.52	121.00
2	6	77	TYR	CB-CG-CD1	5.87	124.52	121.00
1	A	11	ALA	N-CA-CB	5.87	118.31	110.10
1	B	170	ALA	CB-CA-C	-5.87	101.30	110.10
1	B	186	ASP	CB-CG-OD1	-5.87	113.02	118.30
2	7	195	GLU	N-CA-CB	5.86	121.15	110.60
1	G	22	PHE	CB-CG-CD1	5.85	124.89	120.80
2	6	88	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	F	28	ARG	NE-CZ-NH2	5.85	123.22	120.30
2	2	36	PHE	CB-CG-CD1	-5.84	116.71	120.80
2	7	65	PHE	CB-CG-CD1	-5.84	116.71	120.80
2	2	50	ASP	CB-CG-OD1	-5.83	113.05	118.30
2	2	55	THR	CA-CB-CG2	-5.83	104.24	112.40
1	G	148	TYR	CB-CA-C	-5.82	98.75	110.40
1	C	33	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	G	119	PHE	CB-CG-CD1	-5.82	116.73	120.80
2	5	150	VAL	CA-CB-CG2	-5.81	102.18	110.90
2	6	197	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	G	14	VAL	C-N-CA	5.80	136.20	121.70
2	4	35	ASN	N-CA-CB	5.80	121.04	110.60
1	F	136	LEU	CB-CA-C	-5.79	99.19	110.20
2	1	43	LYS	N-CA-CB	5.79	121.02	110.60
2	6	183	GLY	N-CA-C	-5.79	98.63	113.10
1	E	101	LEU	CB-CG-CD1	5.79	120.84	111.00
2	4	123	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	G	133	GLY	N-CA-C	-5.79	98.64	113.10
2	7	123	TYR	CD1-CE1-CZ	5.78	125.00	119.80
1	F	123	TYR	CG-CD2-CE2	-5.77	116.68	121.30
2	1	63	ALA	N-CA-CB	5.77	118.18	110.10
1	E	25	GLU	OE1-CD-OE2	-5.77	116.38	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	211	PHE	CB-CG-CD1	5.77	124.84	120.80
1	E	182	ASP	CB-CG-OD2	5.76	123.49	118.30
2	5	102	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	C	142	ASP	CB-CG-OD2	5.76	123.48	118.30
2	6	195	GLU	N-CA-CB	5.76	120.97	110.60
2	2	53	ALA	N-CA-CB	5.75	118.15	110.10
2	3	194	ASP	CB-CG-OD1	5.75	123.47	118.30
2	7	194	ASP	CB-CA-C	-5.75	98.91	110.40
1	B	183	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	G	52	LYS	CA-CB-CG	5.74	126.03	113.40
1	G	166	MET	CG-SD-CE	5.74	109.38	100.20
2	2	196	PHE	N-CA-C	-5.72	95.57	111.00
1	C	54	VAL	CB-CA-C	5.71	122.24	111.40
2	3	88	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	A	20	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	90	ASP	CB-CG-OD1	5.70	123.43	118.30
2	4	179	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	6	162	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	D	22	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	4	57	ALA	N-CA-CB	5.66	118.03	110.10
1	G	28	ARG	NE-CZ-NH2	5.66	123.13	120.30
2	1	212	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	118	ASP	N-CA-CB	5.66	120.78	110.60
2	7	134	GLU	CG-CD-OE1	-5.66	106.99	118.30
1	D	104	ASP	CA-C-N	-5.65	104.76	117.20
2	7	62	ASP	CB-CG-OD1	5.65	123.39	118.30
2	4	80	ARG	N-CA-CB	5.65	120.77	110.60
2	3	68	ARG	N-CA-CB	5.64	120.76	110.60
2	5	101	TYR	CD1-CE1-CZ	5.64	124.88	119.80
1	D	182	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	F	220	THR	CA-CB-CG2	-5.63	104.51	112.40
2	6	179	ASP	CA-CB-CG	-5.63	101.01	113.40
1	B	235	ARG	NE-CZ-NH1	-5.63	117.49	120.30
2	1	123	TYR	CZ-CE2-CD2	5.62	124.86	119.80
2	1	197	TYR	CG-CD1-CE1	5.62	125.79	121.30
2	5	72	ILE	CA-CB-CG2	5.62	122.13	110.90
2	2	40	LYS	N-CA-C	-5.60	95.87	111.00
2	6	80	ARG	NE-CZ-NH2	5.59	123.10	120.30
2	6	53	ALA	CB-CA-C	-5.58	101.72	110.10
2	5	50	ASP	CB-CG-OD1	5.58	123.32	118.30
2	4	162	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	196	MET	CG-SD-CE	-5.58	91.28	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	181	ALA	N-CA-CB	5.58	117.91	110.10
2	7	212	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	7	148	TYR	CG-CD2-CE2	-5.57	116.84	121.30
1	A	67	ILE	N-CA-C	-5.57	95.97	111.00
2	1	106	TYR	N-CA-C	-5.57	95.97	111.00
1	D	239	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	2	134	GLU	N-CA-CB	5.56	120.61	110.60
1	B	223	GLU	OE1-CD-OE2	5.56	129.97	123.30
2	3	29	LYS	CB-CA-C	-5.55	99.29	110.40
1	C	6	MET	CG-SD-CE	5.55	109.07	100.20
2	1	39	SER	N-CA-CB	5.54	118.82	110.50
1	C	145	PRO	N-CA-CB	5.54	109.95	103.30
1	B	150	THR	N-CA-C	-5.53	96.06	111.00
1	F	103	TYR	CD1-CE1-CZ	5.53	124.78	119.80
2	6	197	TYR	CB-CG-CD2	5.53	124.32	121.00
2	4	13	THR	O-C-N	-5.53	113.85	122.70
1	G	221	PHE	CG-CD1-CE1	-5.52	114.72	120.80
1	F	196	MET	CG-SD-CE	-5.52	91.36	100.20
2	5	36	PHE	N-CA-CB	5.52	120.54	110.60
2	6	42	ALA	N-CA-CB	5.51	117.81	110.10
1	B	159	TYR	CB-CG-CD2	5.50	124.30	121.00
1	B	201	GLU	CB-CG-CD	-5.50	99.35	114.20
2	1	80	ARG	CG-CD-NE	-5.50	100.26	111.80
1	E	141	VAL	O-C-N	-5.49	113.91	122.70
2	6	101	TYR	CD1-CE1-CZ	5.49	124.74	119.80
1	A	146	LYS	N-CA-CB	5.49	120.48	110.60
1	F	219	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	1	116	ASP	CB-CA-C	5.48	121.36	110.40
2	2	139	ALA	N-CA-C	-5.47	96.22	111.00
1	D	170	ALA	CB-CA-C	-5.47	101.89	110.10
1	D	58	LEU	CB-CG-CD2	5.47	120.30	111.00
2	6	139	ALA	N-CA-C	-5.46	96.26	111.00
1	G	149	GLU	N-CA-C	-5.45	96.29	111.00
1	A	26	TYR	CD1-CE1-CZ	5.45	124.70	119.80
2	2	211	PHE	CB-CG-CD2	5.44	124.61	120.80
2	7	178	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	G	174	PHE	CB-CG-CD1	-5.44	116.99	120.80
2	6	55	THR	CA-CB-CG2	-5.44	104.79	112.40
2	7	134	GLU	OE1-CD-OE2	5.44	129.82	123.30
1	F	185	PHE	CB-CG-CD1	-5.43	117.00	120.80
2	4	36	PHE	CB-CG-CD2	-5.43	117.00	120.80
2	6	15	VAL	CA-CB-CG2	5.43	119.04	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	18	VAL	CA-CB-CG1	5.42	119.04	110.90
1	A	214	VAL	CA-CB-CG1	-5.42	102.77	110.90
2	4	196	PHE	N-CA-C	-5.42	96.37	111.00
2	4	103	TYR	CG-CD2-CE2	-5.42	116.97	121.30
2	5	56	THR	CA-CB-CG2	-5.41	104.82	112.40
2	5	148	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	F	126	TYR	CD1-CG-CD2	-5.41	111.95	117.90
2	1	30	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	E	235	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	F	235	ARG	CD-NE-CZ	-5.41	116.03	123.60
2	1	95	SER	CB-CA-C	-5.40	99.84	110.10
1	G	123	TYR	CG-CD1-CE1	5.40	125.62	121.30
2	3	21	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	6	139	ALA	CB-CA-C	-5.40	102.01	110.10
1	F	214	VAL	CA-CB-CG1	-5.39	102.81	110.90
2	7	103	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	A	93	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	D	148	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	B	142	ASP	CB-CG-OD1	-5.39	113.45	118.30
2	3	83	ARG	CD-NE-CZ	-5.39	116.06	123.60
1	G	29	GLU	CA-CB-CG	-5.38	101.55	113.40
2	1	181	ALA	O-C-N	5.37	131.30	122.70
1	G	232	TYR	CB-CG-CD1	5.37	124.22	121.00
3	K	391	ASP	CB-CG-OD1	-5.37	113.47	118.30
2	4	103	TYR	CD1-CG-CD2	5.37	123.80	117.90
2	7	161	VAL	CA-CB-CG1	-5.37	102.85	110.90
1	C	53	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	C	20	ARG	N-CA-C	-5.36	96.52	111.00
1	F	145	PRO	N-CA-CB	5.36	109.73	103.30
1	F	224	VAL	CA-CB-CG1	5.36	118.93	110.90
2	2	155	PHE	CB-CG-CD1	-5.35	117.06	120.80
2	7	81	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
1	C	241	ARG	NH1-CZ-NH2	-5.34	113.52	119.40
1	G	8	TYR	CB-CG-CD2	5.34	124.21	121.00
1	D	146	LYS	CB-CA-C	-5.34	99.72	110.40
2	6	123	TYR	CB-CA-C	-5.33	99.74	110.40
2	5	80	ARG	NE-CZ-NH1	-5.33	117.64	120.30
2	7	199	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	4	150	VAL	CA-CB-CG2	5.32	118.88	110.90
1	A	85	ALA	N-CA-CB	5.32	117.54	110.10
1	E	181	ASP	CB-CG-OD1	-5.32	113.52	118.30
2	5	103	TYR	CD1-CE1-CZ	-5.32	115.01	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	MET	CG-SD-CE	-5.32	91.69	100.20
2	5	78	GLU	CG-CD-OE1	5.32	128.93	118.30
1	F	91	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	2	49	ALA	N-CA-CB	5.31	117.53	110.10
2	3	139	ALA	N-CA-CB	5.31	117.53	110.10
2	3	139	ALA	N-CA-C	-5.30	96.68	111.00
2	3	111	LEU	CB-CA-C	-5.30	100.14	110.20
2	5	188	VAL	C-N-CA	5.29	134.94	121.70
2	6	45	ILE	N-CA-C	-5.29	96.71	111.00
1	B	28	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	4	211	PHE	CB-CG-CD2	5.28	124.50	120.80
2	7	211	PHE	CD1-CE1-CZ	5.28	126.44	120.10
2	5	112	ILE	N-CA-C	-5.27	96.77	111.00
1	E	26	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	F	218	ASP	CB-CG-OD1	5.26	123.04	118.30
1	F	212	GLY	N-CA-C	-5.25	99.99	113.10
1	G	146	LYS	N-CA-C	-5.25	96.84	111.00
2	1	30	ARG	CD-NE-CZ	5.24	130.94	123.60
2	7	83	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	3	185	GLY	N-CA-C	-5.23	100.02	113.10
1	A	213	TYR	CB-CG-CD2	5.23	124.14	121.00
1	C	242	GLU	CB-CA-C	5.23	120.86	110.40
1	B	93	ARG	CB-CA-C	-5.22	99.95	110.40
1	C	160	LYS	CB-CA-C	-5.22	99.95	110.40
1	A	20	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	G	130	ARG	CD-NE-CZ	-5.21	116.30	123.60
2	5	196	PHE	CB-CG-CD2	5.21	124.45	120.80
2	7	136	ASP	O-C-N	5.21	131.03	122.70
2	7	138	VAL	CA-CB-CG2	-5.20	103.09	110.90
1	B	182	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	187	ASP	N-CA-CB	5.20	119.95	110.60
1	E	28	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	132	PHE	CB-CG-CD1	5.19	124.44	120.80
1	E	213	TYR	CA-CB-CG	5.19	123.27	113.40
2	5	21	ASP	CB-CG-OD2	5.19	122.97	118.30
2	2	173	TYR	CG-CD1-CE1	5.19	125.45	121.30
2	7	170	ARG	C-N-CA	5.19	134.67	121.70
2	7	179	ASP	N-CA-CB	5.19	119.94	110.60
2	3	170	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	3	38	ALA	O-C-N	-5.18	114.41	122.70
2	7	30	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	213	TYR	CD1-CG-CD2	-5.18	112.21	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	B	126	TYR	CG-CD2-CE2	-5.17	117.16	121.30
1	C	85	ALA	N-CA-CB	5.17	117.34	110.10
2	5	211	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	C	82	VAL	CA-CB-CG2	-5.16	103.16	110.90
2	1	148	TYR	CG-CD1-CE1	-5.16	117.17	121.30
3	H	396	MET	N-CA-CB	5.16	119.89	110.60
1	B	126	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	A	205	VAL	CA-CB-CG2	-5.15	103.17	110.90
1	C	166	MET	CA-CB-CG	5.15	122.06	113.30
1	G	219	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	9	ASP	N-CA-CB	5.14	119.86	110.60
1	E	171	VAL	CB-CA-C	5.14	121.17	111.40
3	H	397	PHE	CB-CG-CD1	-5.14	117.20	120.80
2	7	178	ARG	N-CA-CB	5.13	119.84	110.60
1	C	221	PHE	N-CA-CB	5.13	119.83	110.60
1	D	74	ILE	N-CA-CB	5.13	122.60	110.80
2	1	173	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	2	195	GLU	N-CA-CB	5.13	119.83	110.60
1	F	9	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	185	PHE	CB-CG-CD1	-5.12	117.22	120.80
2	3	139	ALA	C-N-CA	5.11	134.49	121.70
1	A	67	ILE	N-CA-CB	5.11	122.56	110.80
1	C	231	PRO	N-CA-CB	5.11	109.42	103.30
1	A	79	SER	N-CA-CB	5.10	118.14	110.50
2	4	211	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
1	D	199	SER	CB-CA-C	-5.09	100.44	110.10
2	5	81	ARG	NE-CZ-NH1	-5.09	117.76	120.30
2	5	129	GLY	C-N-CA	5.08	132.97	122.30
1	G	28	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	175	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	D	33	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	D	213	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	4	39	SER	N-CA-C	-5.08	97.29	111.00
2	5	77	TYR	CZ-CE2-CD2	5.07	124.36	119.80
2	6	80	ARG	O-C-N	-5.07	114.58	122.70
2	2	136	ASP	CB-CG-OD2	-5.07	113.74	118.30
2	1	116	ASP	CB-CG-OD2	-5.07	113.74	118.30
2	3	46	TYR	CB-CG-CD2	5.07	124.04	121.00
2	4	80	ARG	O-C-N	-5.07	114.60	122.70
2	2	126	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	221	PHE	CB-CG-CD1	-5.06	117.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	TYR	CB-CG-CD1	-5.06	117.97	121.00
2	3	134	GLU	CG-CD-OE2	-5.06	108.18	118.30
2	2	194	ASP	CB-CG-OD2	-5.06	113.75	118.30
2	3	188	VAL	CA-CB-CG2	5.06	118.49	110.90
2	3	212	ARG	CD-NE-CZ	5.06	130.68	123.60
2	7	108	VAL	CA-CB-CG1	5.05	118.48	110.90
2	3	94	THR	CA-CB-CG2	-5.05	105.33	112.40
1	G	159	TYR	CB-CG-CD2	-5.05	117.97	121.00
2	6	62	ASP	CB-CG-OD2	5.04	122.84	118.30
2	5	39	SER	N-CA-CB	5.04	118.06	110.50
2	1	41	ALA	CB-CA-C	5.03	117.64	110.10
1	D	15	PHE	CB-CG-CD1	-5.03	117.28	120.80
2	1	156	THR	N-CA-CB	5.03	119.85	110.30
1	D	18	ASP	CB-CG-OD1	-5.03	113.78	118.30
2	3	126	ASP	CB-CG-OD1	-5.03	113.78	118.30
2	1	197	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
3	L	397	PHE	CB-CG-CD1	-5.02	117.28	120.80
2	5	156	THR	N-CA-CB	5.02	119.84	110.30
2	6	52	MET	CA-CB-CG	5.02	121.84	113.30
2	6	133	GLU	CA-CB-CG	5.02	124.44	113.40
2	4	55	THR	N-CA-CB	5.02	119.83	110.30
1	F	44	GLU	N-CA-CB	5.01	119.62	110.60
2	4	204	VAL	CG1-CB-CG2	-5.01	102.88	110.90
2	6	135	LYS	N-CA-CB	5.01	119.62	110.60
1	A	123	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	220	THR	CA-CB-CG2	-5.01	105.39	112.40
1	D	201	GLU	N-CA-CB	5.01	119.61	110.60
1	F	137	LEU	CB-CG-CD2	5.01	119.51	111.00
1	E	84	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	G	69	LYS	N-CA-CB	5.00	119.61	110.60
2	7	196	PHE	N-CA-C	-5.00	97.49	111.00
1	B	236	ALA	N-CA-CB	5.00	117.10	110.10

There are no chirality outliers.

All (114) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	199	TYR	Sidechain
2	1	211	PHE	Sidechain
2	1	77	TYR	Sidechain
2	1	80	ARG	Sidechain
2	2	101	TYR	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	2	139	ALA	Peptide,Mainchain
2	2	148	TYR	Sidechain
2	2	173	TYR	Sidechain
2	2	197	TYR	Sidechain
2	2	77	TYR	Sidechain
2	2	81	ARG	Sidechain
2	3	101	TYR	Sidechain
2	3	148	TYR	Sidechain
2	3	212	ARG	Sidechain
2	3	68	ARG	Sidechain
2	4	103	TYR	Sidechain
2	4	123	TYR	Sidechain
2	4	139	ALA	Peptide
2	4	155	PHE	Sidechain
2	4	68	ARG	Sidechain
2	4	83	ARG	Sidechain
2	5	106	TYR	Sidechain
2	5	132	ILE	Peptide
2	5	139	ALA	Mainchain
2	5	154	ARG	Sidechain
2	5	170	ARG	Sidechain
2	5	199	TYR	Sidechain
2	5	81	ARG	Sidechain
2	5	88	ARG	Sidechain
2	6	101	TYR	Sidechain
2	6	103	TYR	Sidechain
2	6	139	ALA	Peptide
2	6	148	TYR	Sidechain
2	6	173	TYR	Sidechain
2	6	36	PHE	Sidechain
2	6	46	TYR	Sidechain
2	6	77	TYR	Sidechain
2	6	88	ARG	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	199	TYR	Sidechain
2	7	51	ARG	Sidechain
2	7	77	TYR	Sidechain
2	7	83	ARG	Sidechain
2	7	88	ARG	Sidechain
1	A	123	TYR	Sidechain
1	A	148	TYR	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	A	213	TYR	Sidechain
1	A	220	THR	Peptide
1	A	221	PHE	Sidechain
1	A	65	GLU	Peptide
1	A	86	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	14	VAL	Peptide
1	B	179	TYR	Sidechain
1	B	22	PHE	Sidechain
1	B	220	THR	Peptide
1	B	232	TYR	Sidechain
1	B	235	ARG	Sidechain
1	B	86	ARG	Sidechain
1	C	10	ARG	Sidechain
1	C	148	TYR	Sidechain
1	C	159	TYR	Sidechain
1	C	179	TYR	Sidechain
1	C	20	ARG	Sidechain
1	C	213	TYR	Sidechain
1	C	220	THR	Peptide
1	C	221	PHE	Sidechain
1	C	235	ARG	Sidechain
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	C	91	ARG	Sidechain
1	C	93	ARG	Sidechain
1	D	105	GLU	Peptide
1	D	174	PHE	Sidechain
1	D	179	TYR	Sidechain
1	D	213	TYR	Sidechain
1	D	220	THR	Peptide
1	D	239	ARG	Sidechain
1	E	103	TYR	Sidechain
1	E	123	TYR	Sidechain
1	E	159	TYR	Sidechain
1	E	168	ARG	Sidechain
1	E	175	PHE	Sidechain
1	E	179	TYR	Sidechain
1	E	20	ARG	Sidechain
1	E	215	LYS	Peptide
1	E	220	THR	Peptide
1	E	221	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	E	28	ARG	Sidechain
1	F	103	TYR	Sidechain
1	F	14	VAL	Peptide
1	F	159	TYR	Sidechain
1	F	213	TYR	Sidechain
1	F	220	THR	Peptide
1	F	53	ARG	Sidechain
1	F	8	TYR	Sidechain
1	F	86	ARG	Sidechain
1	G	123	TYR	Sidechain
1	G	126	TYR	Sidechain
1	G	148	TYR	Sidechain
1	G	159	TYR	Sidechain
1	G	179	TYR	Sidechain
1	G	220	THR	Peptide
1	G	235	ARG	Sidechain
1	G	34	GLY	Peptide
1	G	35	ALA	Peptide
1	G	5	GLN	Peptide
3	H	394	GLY	Peptide
3	I	394	GLY	Peptide
3	I	397	PHE	Sidechain
3	J	397	PHE	Sidechain
3	L	394	GLY	Peptide

## 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	1907	0	1941	6	0
1	B	1907	0	1941	4	0
1	C	1907	0	1941	9	0
1	D	1907	0	1941	6	0
1	E	1907	0	1940	18	0
1	F	1907	0	1941	2	0
1	G	1907	0	1941	7	0
2	1	1552	0	1580	6	0
2	2	1552	0	1580	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	1552	0	1580	2	0
2	4	1552	0	1580	3	0
2	5	1552	0	1580	27	0
2	6	1552	0	1580	7	0
2	7	1552	0	1580	9	0
3	H	70	0	74	1	0
3	I	70	0	74	0	0
3	J	70	0	74	0	0
3	K	70	0	74	1	0
3	L	70	0	74	1	0
3	M	70	0	74	0	0
All	All	24633	0	25090	101	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 2.

All (101) 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)
2:5:211:PHE:CE1	2:5:211:PHE:CZ	2.02	1.46
2:5:211:PHE:CZ	2:5:211:PHE:CE2	2.03	1.46
2:5:211:PHE:CG	2:5:211:PHE:CD1	2.04	1.45
1:E:66:LYS:C	1:E:67:ILE:N	1.71	1.44
2:5:211:PHE:CE1	2:5:211:PHE:CD1	2.04	1.43
2:5:211:PHE:CE2	2:5:211:PHE:CD2	2.08	1.41
2:5:211:PHE:CG	2:5:211:PHE:CD2	2.10	1.37
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.34	1.11
2:5:170:ARG:CZ	2:5:170:ARG:NH1	2.15	1.10
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.36	1.08
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.37	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CD1	2.24	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.24	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.25	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CE2	2.24	1.04
2:5:170:ARG:NH1	2:5:211:PHE:CD2	2.25	1.04
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.42	1.03
2:5:170:ARG:NH1	2:5:211:PHE:CZ	2.25	1.03
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.42	1.03
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.47	0.98
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.43	0.86
2:5:170:ARG:NH2	2:5:211:PHE:CG	2.46	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:ALA:HB3	1:E:66:LYS:NZ	1.93	0.83
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.52	0.78
1:E:35:ALA:HB3	1:E:66:LYS:HZ2	1.48	0.78
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.51	0.77
1:E:66:LYS:C	1:E:67:ILE:CA	2.53	0.76
1:E:66:LYS:CA	1:E:67:ILE:N	2.49	0.75
2:7:64:GLN:HE22	2:7:68:ARG:HE	1.39	0.71
1:A:163:ALA:HB2	1:A:171:VAL:HG11	1.78	0.65
1:A:13:THR:HA	1:B:130:ARG:HB3	1.83	0.60
2:1:154:ARG:HH12	2:1:166:GLU:HG2	1.71	0.56
1:G:237:ASN:HA	1:G:240:ILE:HD12	1.91	0.53
2:7:54:MET:HE2	2:7:112:ILE:HD11	1.91	0.53
1:A:65:GLU:H	1:A:66:LYS:HA	1.74	0.52
1:C:80:GLY:HA3	1:C:134:VAL:HG12	1.90	0.52
2:1:68:ARG:HH22	2:2:131:ALA:H	1.54	0.52
1:D:79:SER:HB3	1:D:164:ILE:HD12	1.92	0.51
1:G:143:GLU:HA	1:G:219:ARG:HH12	1.77	0.49
1:B:28:ARG:HA	1:B:152:PRO:HG2	1.94	0.48
1:C:229:LEU:O	1:C:233:VAL:HG23	2.13	0.48
2:4:94:THR:HG21	2:4:110:LEU:HD22	1.94	0.48
2:5:56:THR:HG21	2:5:63:ALA:HB1	1.94	0.48
2:4:68:ARG:HH22	2:5:131:ALA:HB3	1.78	0.48
1:G:102:THR:HG23	1:G:103:TYR:CD2	2.49	0.48
1:E:35:ALA:HB3	1:E:66:LYS:HZ3	1.78	0.47
2:7:137:ILE:HD11	2:7:155:PHE:CD1	2.48	0.47
1:E:66:LYS:O	1:E:78:THR:HG22	2.14	0.47
2:6:45:ILE:HD12	2:6:189:VAL:HG11	1.97	0.47
1:B:64:ILE:HG21	3:K:398:VAL:HG11	1.97	0.47
2:3:56:THR:HG23	2:3:110:LEU:HD23	1.97	0.47
2:7:20:LYS:HD3	2:7:158:GLU:HA	1.97	0.46
1:E:33:ARG:HB3	3:H:397:PHE:CD2	2.50	0.46
2:5:78:GLU:HB2	2:5:85:PRO:HD3	1.95	0.46
1:G:81:LEU:HD11	3:L:397:PHE:CE2	2.50	0.46
1:A:12:ILE:HD12	1:A:131:PRO:HD3	1.98	0.45
1:C:238:GLU:HA	1:C:241:ARG:HE	1.82	0.45
2:1:137:ILE:HD11	2:1:155:PHE:CD1	2.52	0.45
1:C:190:VAL:O	1:C:194:VAL:HG23	2.16	0.45
1:D:200:ILE:HD11	1:D:204:LEU:HD23	1.98	0.45
2:6:36:PHE:CD1	2:7:140:THR:HA	2.52	0.44
1:D:148:TYR:CD1	1:D:156:LEU:HD11	2.53	0.44
2:2:169:VAL:HA	2:2:186:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:64:GLN:NE2	2:7:68:ARG:HE	2.09	0.44
1:E:35:ALA:CB	1:E:66:LYS:HZ3	2.31	0.44
1:E:66:LYS:N	1:E:67:ILE:N	2.66	0.44
1:A:78:THR:HG21	1:A:85:ALA:CB	2.48	0.44
1:E:194:VAL:HG11	1:E:239:ARG:HG2	2.00	0.43
2:6:86:THR:HG23	2:6:89:ALA:H	1.83	0.43
2:1:165:VAL:O	2:1:169:VAL:HG23	2.18	0.43
1:D:155:ALA:HB2	1:E:83:ALA:HB2	2.01	0.43
1:F:47:ILE:HD13	1:F:189:MET:HA	2.00	0.43
2:7:207:ILE:HG22	2:7:211:PHE:CZ	2.54	0.43
2:4:125:ILE:HD12	2:4:125:ILE:N	2.34	0.43
2:5:64:GLN:HG2	2:6:131:ALA:H	1.84	0.43
2:7:14:THR:HG22	2:7:27:THR:HG22	2.01	0.43
2:7:179:ASP:HB3	2:7:181:ALA:H	1.83	0.42
1:C:193:LEU:HD23	1:C:233:VAL:HA	2.01	0.42
1:G:227:GLU:CD	1:G:227:GLU:H	2.22	0.42
2:1:137:ILE:HD13	2:1:137:ILE:HA	1.92	0.42
1:C:193:LEU:CD2	1:C:233:VAL:HG22	2.50	0.42
1:D:74:ILE:HG21	1:D:112:LEU:HD23	2.02	0.42
1:E:51:ASP:O	1:E:66:LYS:HG3	2.20	0.42
2:6:122:ILE:HG21	2:6:138:VAL:HG11	2.01	0.42
1:E:59:LEU:HD12	1:E:59:LEU:H	1.84	0.42
1:C:190:VAL:HG21	1:C:235:ARG:HH11	1.85	0.42
1:E:74:ILE:HG21	1:E:112:LEU:HD23	2.02	0.42
1:E:141:VAL:HG11	1:E:216:VAL:HG22	2.02	0.42
1:C:193:LEU:HD21	1:C:233:VAL:HG22	2.02	0.41
1:E:205:VAL:HG22	1:E:208:ASN:HD21	1.84	0.41
1:G:31:VAL:HA	1:G:80:GLY:HA2	2.02	0.41
2:6:12:THR:HG21	2:6:58:GLY:H	1.85	0.41
1:G:132:PHE:HB3	1:G:134:VAL:HG12	2.02	0.41
1:E:70:ILE:HG21	1:E:112:LEU:HD21	2.03	0.41
1:C:17:PRO:HA	1:D:26:TYR:CE1	2.56	0.41
1:F:141:VAL:HG11	1:F:216:VAL:HG22	2.02	0.41
2:6:70:ILE:HD11	2:6:94:THR:HA	2.03	0.41
2:1:95:SER:HB3	2:1:130:GLY:H	1.86	0.40
1:A:205:VAL:HG12	1:A:207:GLU:H	1.87	0.40
1:B:163:ALA:HB3	1:B:168:ARG:HA	2.03	0.40
2:3:154:ARG:HD3	2:3:167:LEU:HD13	2.03	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	240/247 (97%)	227 (95%)	10 (4%)	3 (1%)	12	47
1	B	240/247 (97%)	223 (93%)	12 (5%)	5 (2%)	7	38
1	C	240/247 (97%)	222 (92%)	11 (5%)	7 (3%)	4	32
1	D	240/247 (97%)	223 (93%)	13 (5%)	4 (2%)	9	42
1	E	240/247 (97%)	226 (94%)	13 (5%)	1 (0%)	34	71
1	F	240/247 (97%)	224 (93%)	11 (5%)	5 (2%)	7	38
1	G	240/247 (97%)	225 (94%)	9 (4%)	6 (2%)	5	34
2	1	200/210 (95%)	191 (96%)	5 (2%)	4 (2%)	7	39
2	2	200/210 (95%)	182 (91%)	12 (6%)	6 (3%)	4	31
2	3	200/210 (95%)	181 (90%)	14 (7%)	5 (2%)	5	34
2	4	200/210 (95%)	185 (92%)	12 (6%)	3 (2%)	10	45
2	5	200/210 (95%)	185 (92%)	10 (5%)	5 (2%)	5	34
2	6	200/210 (95%)	180 (90%)	14 (7%)	6 (3%)	4	31
2	7	200/210 (95%)	182 (91%)	15 (8%)	3 (2%)	10	45
3	H	7/401 (2%)	4 (57%)	2 (29%)	1 (14%)	0	4
3	I	7/401 (2%)	5 (71%)	1 (14%)	1 (14%)	0	4
3	J	7/401 (2%)	7 (100%)	0	0	100	100
3	K	7/401 (2%)	5 (71%)	1 (14%)	1 (14%)	0	4
3	L	7/401 (2%)	5 (71%)	0	2 (29%)	0	0
3	M	7/401 (2%)	6 (86%)	1 (14%)	0	100	100
All	All	3122/5605 (56%)	2888 (92%)	166 (5%)	68 (2%)	10	37

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	64	ILE
1	C	20	ARG
1	C	67	ILE
1	E	221	PHE
1	F	64	ILE
1	G	20	ARG
2	2	41	ALA
2	2	106	TYR
2	3	139	ALA
2	4	35	ASN
2	4	140	THR
2	6	139	ALA
2	7	39	SER
3	H	395	VAL
1	B	143	GLU
1	C	66	LYS
1	C	221	PHE
1	C	245	LYS
1	D	34	GLY
1	D	65	GLU
1	D	161	ALA
1	F	9	ASP
1	G	221	PHE
2	2	139	ALA
2	2	182	SER
2	2	212	ARG
2	3	41	ALA
2	6	140	THR
2	7	83	ARG
3	K	392	LEU
1	A	9	ASP
1	A	143	GLU
1	B	221	PHE
1	C	9	ASP
1	F	221	PHE
1	G	54	VAL
1	G	184	SER
2	1	136	ASP
2	2	140	THR
2	3	140	THR
2	3	181	ALA
2	5	191	ILE

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Mol	Chain	Res	Type
2	5	212	ARG
2	6	20	LYS
2	6	136	ASP
2	7	133	GLU
3	I	393	LYS
3	L	395	VAL
1	B	65	GLU
1	F	106	PRO
1	G	143	GLU
2	1	183	GLY
2	1	185	GLY
2	5	136	ASP
2	6	41	ALA
2	1	212	ARG
2	3	193	GLU
2	5	133	GLU
2	6	40	LYS
3	L	391	ASP
1	G	71	ASP
2	4	136	ASP
1	D	64	ILE
1	F	105	GLU
2	5	185	GLY
1	C	55	GLY
1	B	7	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	203/207 (98%)	196 (97%)	7 (3%)	37 60
1	B	203/207 (98%)	196 (97%)	7 (3%)	37 60
1	C	203/207 (98%)	194 (96%)	9 (4%)	28 54
1	D	203/207 (98%)	197 (97%)	6 (3%)	41 63
1	E	203/207 (98%)	193 (95%)	10 (5%)	25 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	203/207 (98%)	195 (96%)	8 (4%)	32	57
1	G	203/207 (98%)	197 (97%)	6 (3%)	41	63
2	1	164/171 (96%)	155 (94%)	9 (6%)	21	49
2	2	164/171 (96%)	156 (95%)	8 (5%)	25	52
2	3	164/171 (96%)	160 (98%)	4 (2%)	49	68
2	4	164/171 (96%)	157 (96%)	7 (4%)	29	55
2	5	164/171 (96%)	157 (96%)	7 (4%)	29	55
2	6	164/171 (96%)	156 (95%)	8 (5%)	25	52
2	7	164/171 (96%)	161 (98%)	3 (2%)	59	76
3	H	8/346 (2%)	7 (88%)	1 (12%)	4	22
3	I	8/346 (2%)	8 (100%)	0	100	100
3	J	8/346 (2%)	5 (62%)	3 (38%)	0	0
3	K	8/346 (2%)	7 (88%)	1 (12%)	4	22
3	L	8/346 (2%)	8 (100%)	0	100	100
3	M	8/346 (2%)	7 (88%)	1 (12%)	4	22
All	All	2617/4722 (55%)	2512 (96%)	105 (4%)	35	56

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	17	PRO
1	A	86	ARG
1	A	130	ARG
1	A	144	VAL
1	A	187	ASP
1	A	217	ASP
1	B	6	MET
1	B	130	ARG
1	B	151	ASP
1	B	166	MET
1	B	178	GLU
1	B	205	VAL
1	B	220	THR
1	C	42	CYS
1	C	67	ILE
1	C	69	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	125	GLN
1	C	156	LEU
1	C	166	MET
1	C	187	ASP
1	C	208	ASN
1	C	239	ARG
1	D	65	GLU
1	D	73	HIS
1	D	118	ASP
1	D	121	GLN
1	D	189	MET
1	D	229	LEU
1	E	33	ARG
1	E	51	ASP
1	E	56	SER
1	E	57	LYS
1	E	71	ASP
1	E	102	THR
1	E	121	GLN
1	E	130	ARG
1	E	142	ASP
1	E	213	TYR
1	F	18	ASP
1	F	21	LEU
1	F	97	GLN
1	F	142	ASP
1	F	151	ASP
1	F	208	ASN
1	F	229	LEU
1	F	238	GLU
1	G	5	GLN
1	G	21	LEU
1	G	57	LYS
1	G	151	ASP
1	G	152	PRO
1	G	220	THR
2	1	27	THR
2	1	28	GLU
2	1	45	ILE
2	1	50	ASP
2	1	64	GLN
2	1	107	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	1	120	LYS
2	1	161	VAL
2	1	202	GLU
2	2	44	LYS
2	2	45	ILE
2	2	84	LYS
2	2	110	LEU
2	2	111	LEU
2	2	120	LYS
2	2	137	ILE
2	2	179	ASP
2	3	19	CYS
2	3	182	SER
2	3	205	GLU
2	3	213	LYS
2	4	28	GLU
2	4	109	GLN
2	4	120	LYS
2	4	134	GLU
2	4	136	ASP
2	4	192	THR
2	4	205	GLU
2	5	17	LEU
2	5	19	CYS
2	5	45	ILE
2	5	77	TYR
2	5	103	TYR
2	5	202	GLU
2	5	205	GLU
2	6	17	LEU
2	6	28	GLU
2	6	45	ILE
2	6	95	SER
2	6	136	ASP
2	6	161	VAL
2	6	202	GLU
2	6	205	GLU
2	7	45	ILE
2	7	64	GLN
2	7	170	ARG
3	H	396	MET
3	K	398	VAL

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Mol	Chain	Res	Type
3	M	398	VAL
3	J	395	VAL
3	J	396	MET
3	J	398	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	HIS
1	C	237	ASN
1	D	99	ASN
1	D	121	GLN
1	E	208	ASN
1	F	208	ASN
1	G	97	GLN
1	G	121	GLN
1	G	237	ASN
2	2	35	ASN
2	4	99	ASN
2	5	35	ASN
2	7	64	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	66:LYS	C	67:ILE	N	1.71

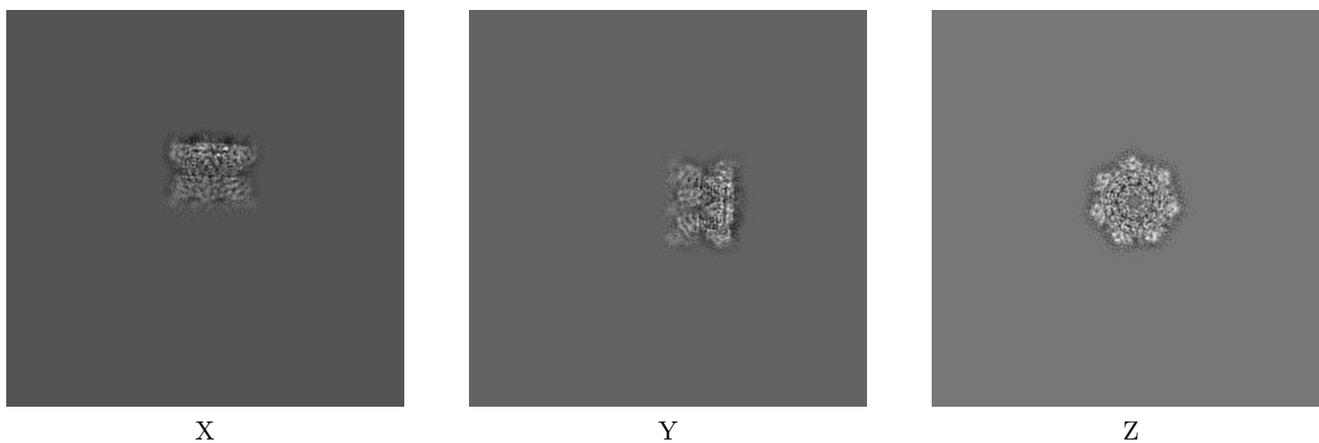
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0210. 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](#)

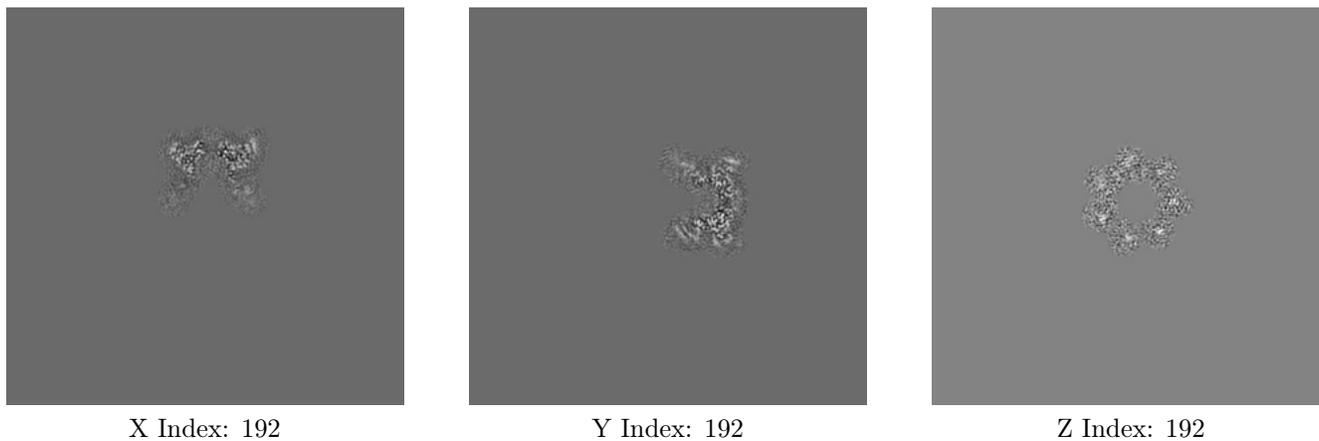
#### 6.1.1 Primary map



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

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

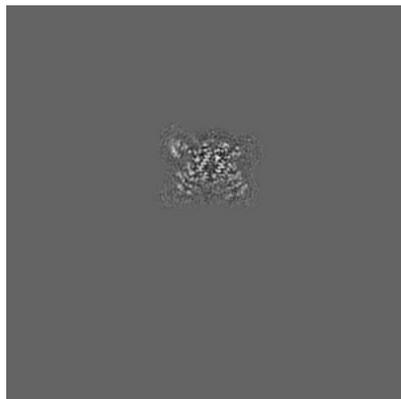
#### 6.2.1 Primary map



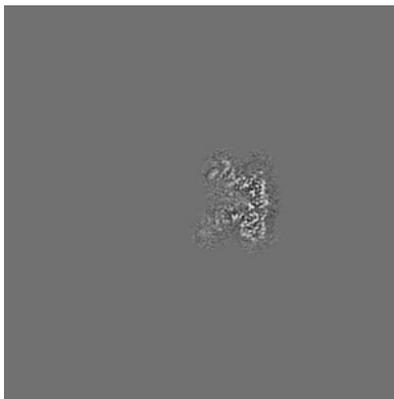
The images above show central slices of the map in three orthogonal directions.

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

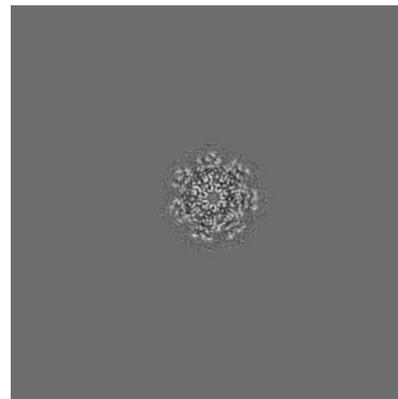
### 6.3.1 Primary map



X Index: 177



Y Index: 212



Z Index: 243

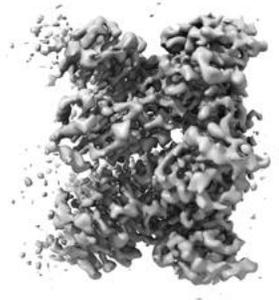
The images above show the largest variance slices of the map in three orthogonal directions.

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

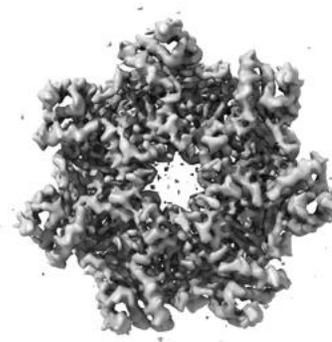
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0372. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

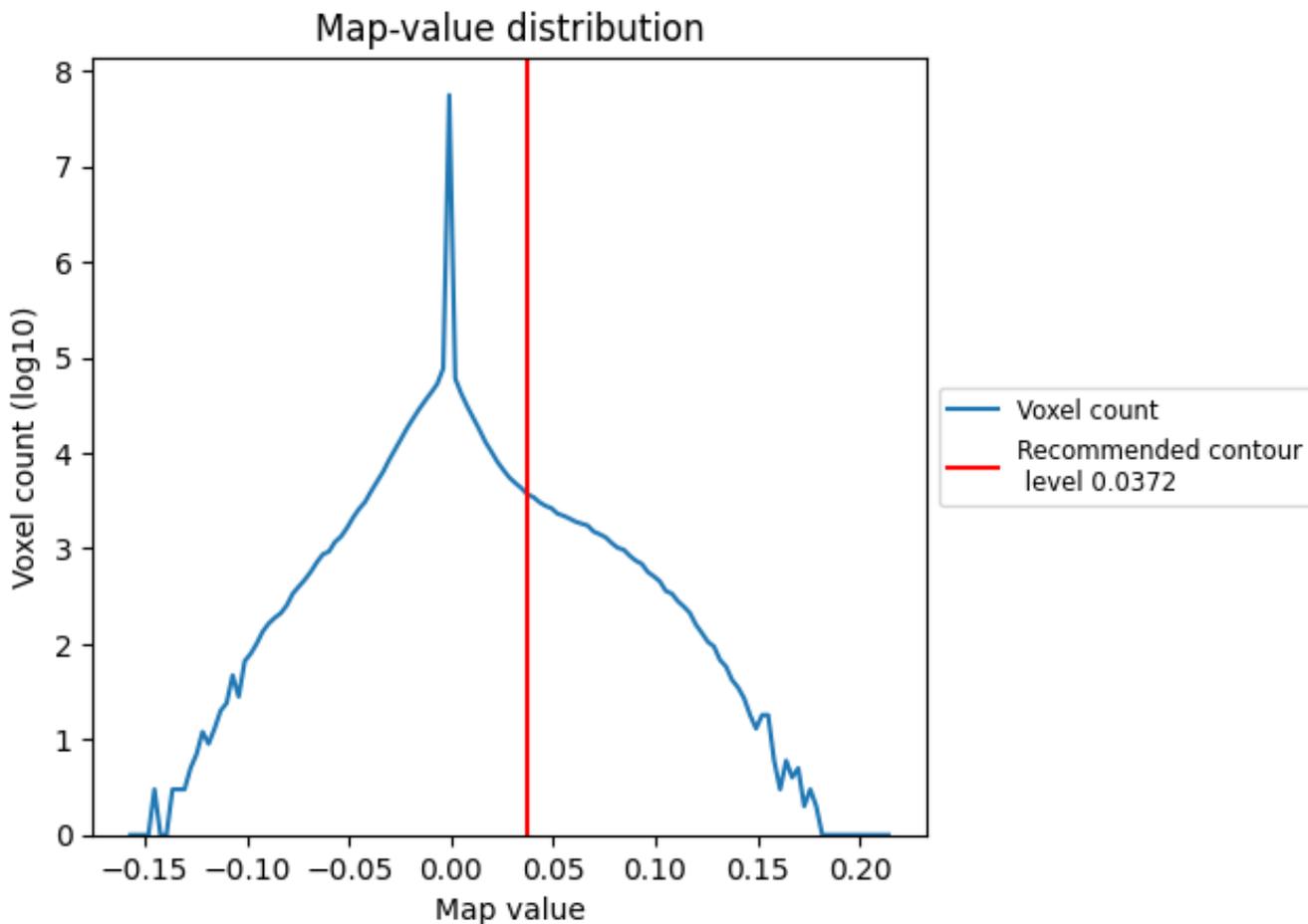
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

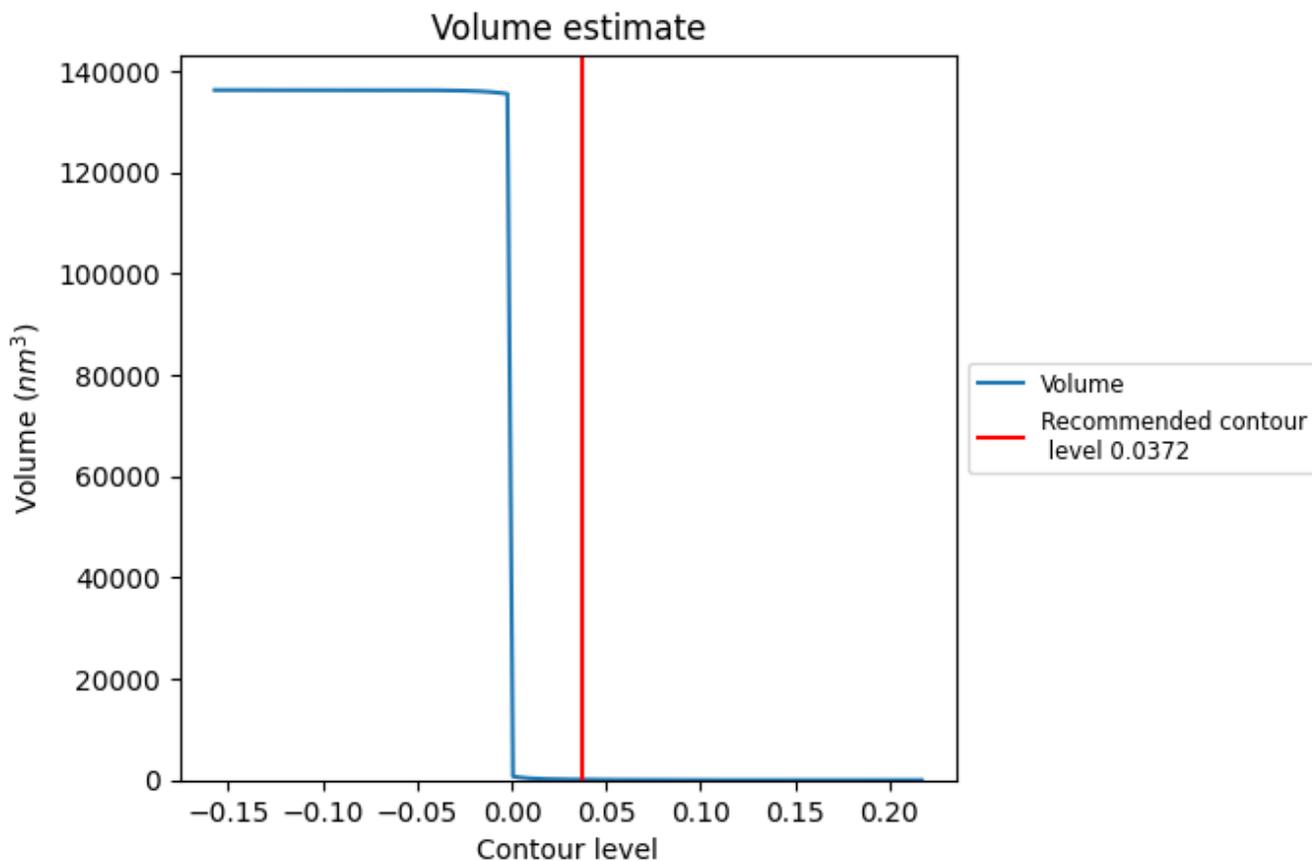
This section contains the results of statistical analysis of the map.

### 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.

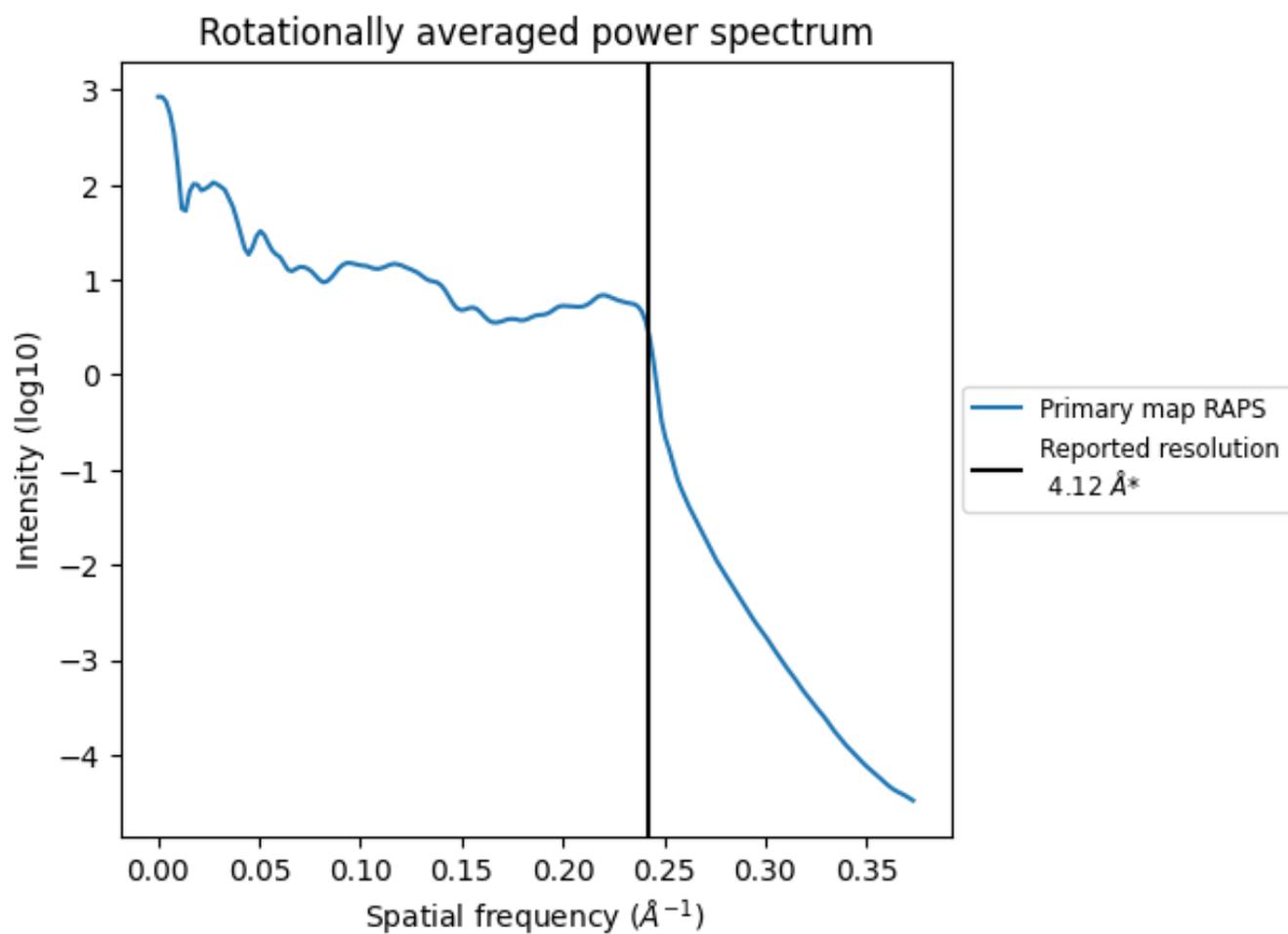
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 99 nm<sup>3</sup>; this corresponds to an approximate mass of 90 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.243 \text{\AA}^{-1}$

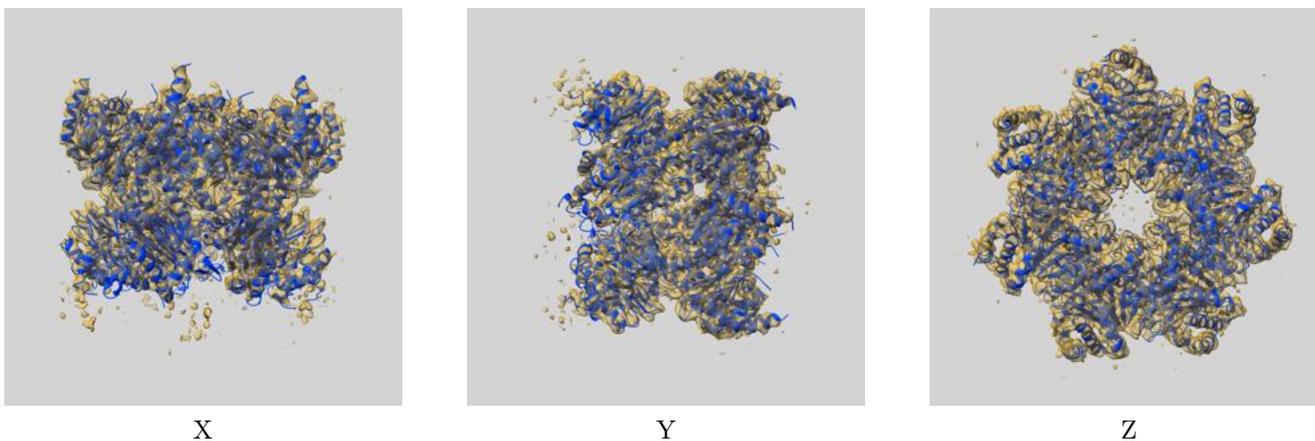
## 8 Fourier-Shell correlation

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

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

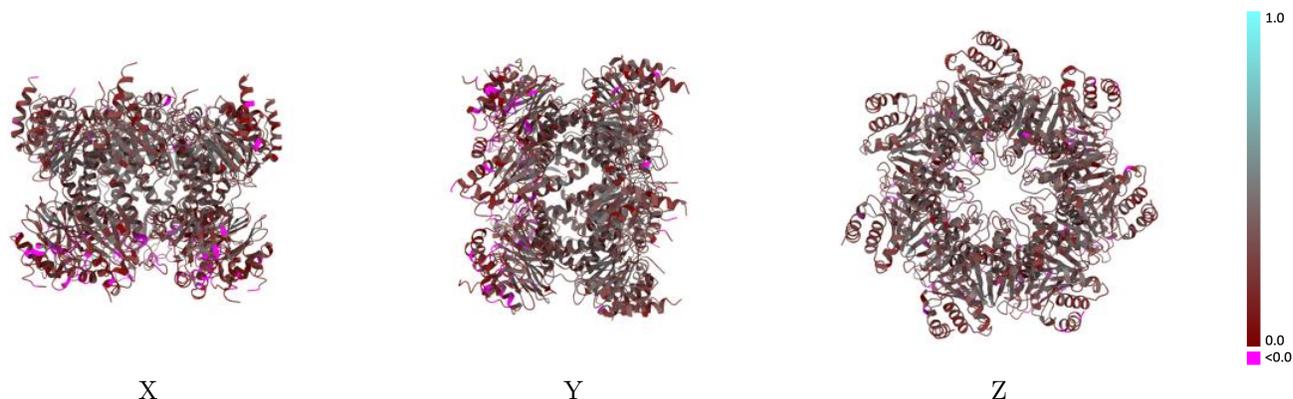
This section contains information regarding the fit between EMDB map EMD-0210 and PDB model 6HE5. Per-residue inclusion information can be found in section 3 on page 8.

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



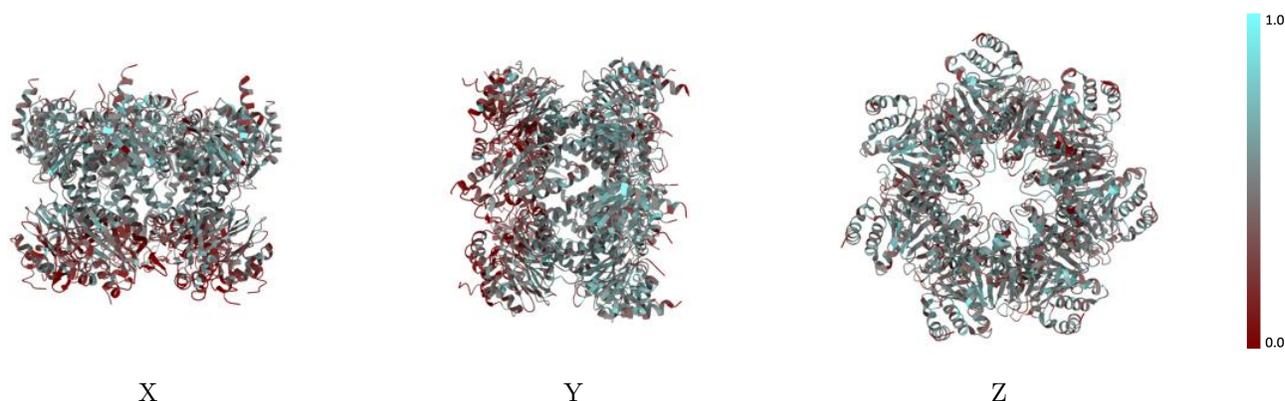
The images above show the 3D surface view of the map at the recommended contour level 0.0372 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



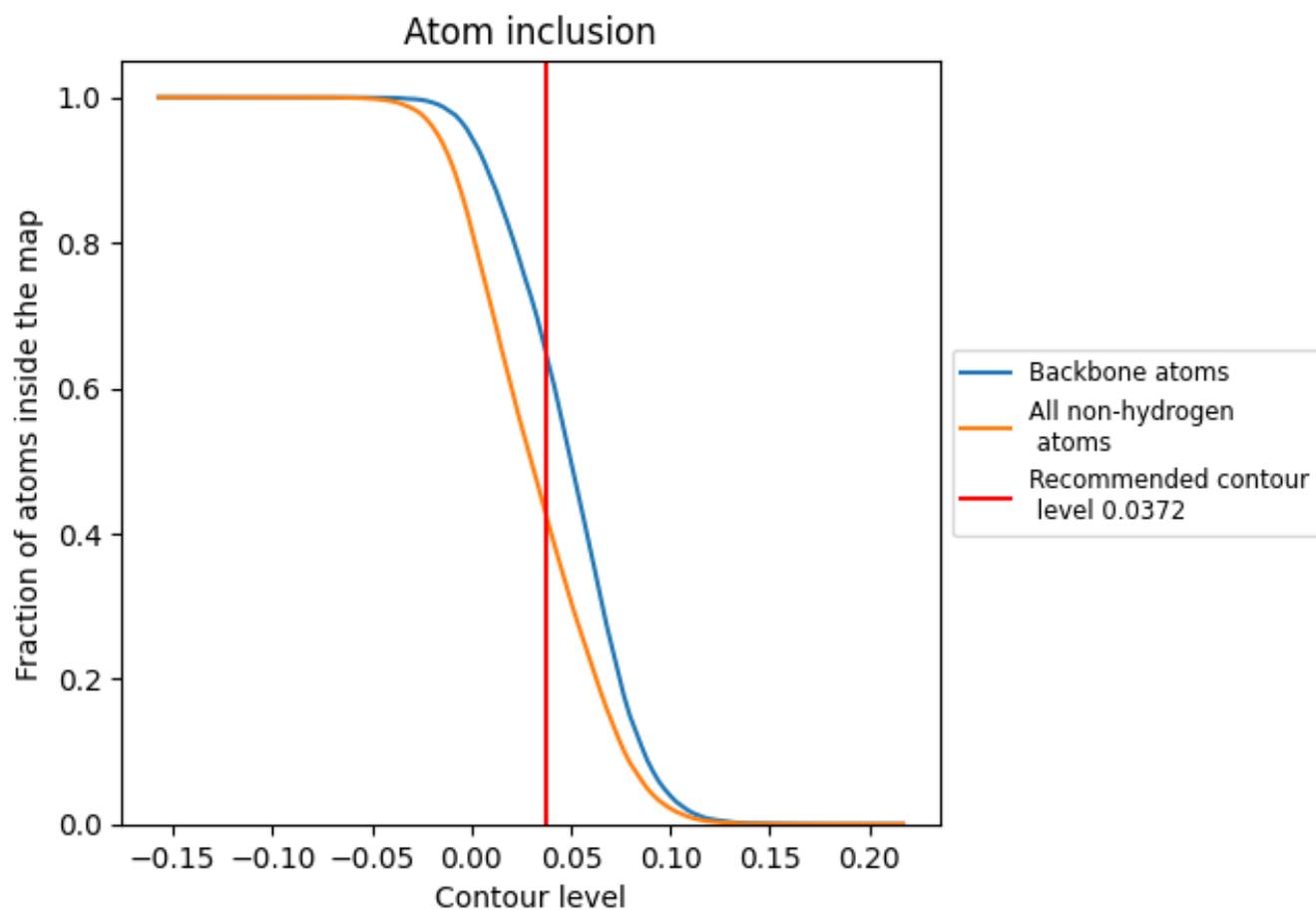
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0372).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 43% 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 (0.0372) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4289	 0.2660
1	 0.3182	 0.2210
2	 0.3366	 0.2170
3	 0.3221	 0.2070
4	 0.3241	 0.2090
5	 0.3215	 0.2000
6	 0.3215	 0.2240
7	 0.3116	 0.2000
A	 0.5204	 0.3060
B	 0.5338	 0.3150
C	 0.5247	 0.3280
D	 0.5284	 0.3110
E	 0.5220	 0.3130
F	 0.5354	 0.3210
G	 0.5016	 0.2970
H	 0.1857	 0.0680
I	 0.2286	 0.2200
J	 0.2143	 0.2510
K	 0.2000	 0.1630
L	 0.0714	 0.1190
M	 0.1857	 0.1990

