Full wwPDB EM Validation Report

Nov 20, 2022 – 07:13 am GMT

PDB ID	:	6HE7
EMDB ID	:	EMD-0211
Title	:	20S proteasome from Archaeoglobus fulgidus
Authors	:	Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on	:	2018-08-20
Resolution	:	3.69 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

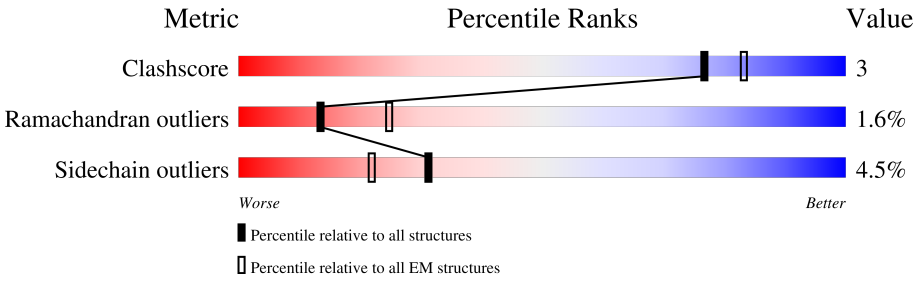
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.69 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	235	23% 69% 27% ·
1	B	235	20% 78% 18% ·
1	C	235	20% 69% 26% ·
1	D	235	24% 69% 26% 5%
1	E	235	23% 67% 29% · ·
1	F	235	23% 74% 20% 6%
1	G	235	20% 68% 26% 6%
2	1	202	50% 68% 28% ·

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Mol	Chain	Length	Quality of chain
2	2	202	51% 71% 24% 5%
2	3	202	48% 68% 28%
2	4	202	50% 69% 25% 6%
2	5	202	51% 71% 23% 5%
2	6	202	53% 67% 29%
2	7	202	50% 68% 28%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23821 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
1	A	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	B	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	C	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	D	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	E	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	F	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	G	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		

- Molecule 2 is a protein called Proteasome subunit beta.

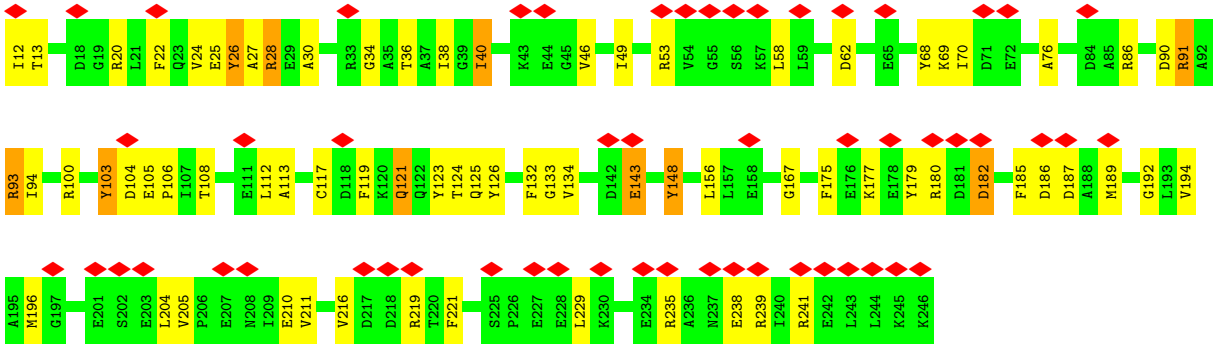
Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	2	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	3	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	4	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	5	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	6	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	7	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		

3 Residue-property plots (i)

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.

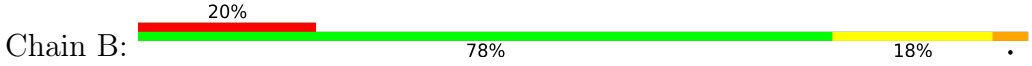
• Molecule 1: Proteasome subunit alpha

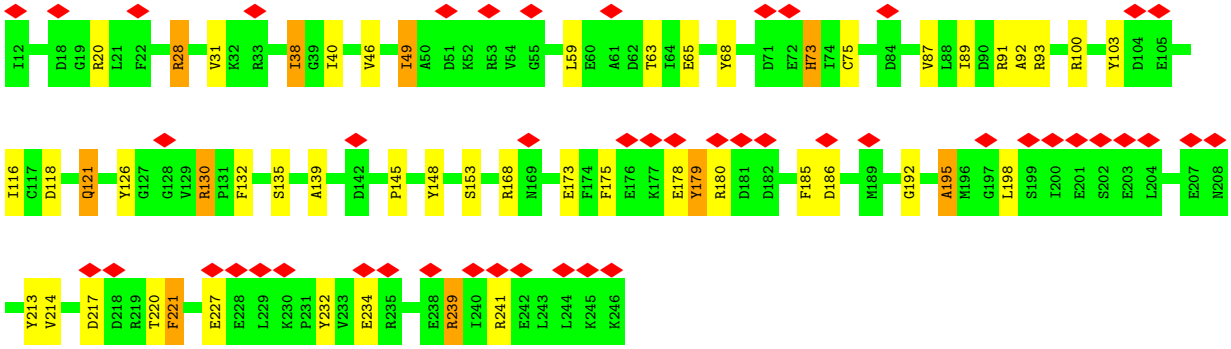
Chain A:



• Molecule 1: Proteasome subunit alpha

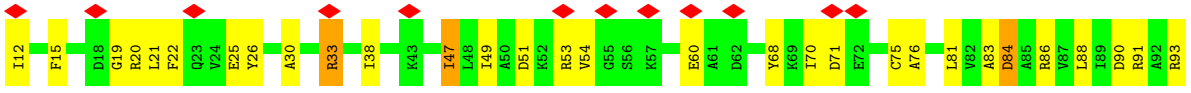
Chain B:

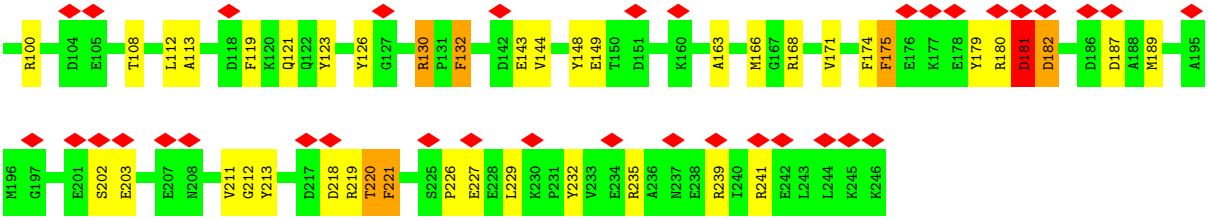




• Molecule 1: Proteasome subunit alpha

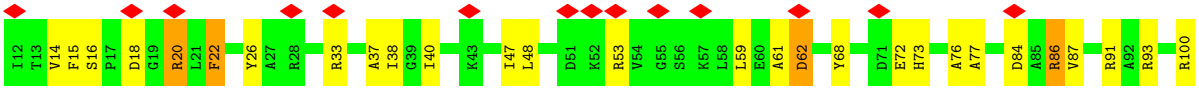
Chain C:

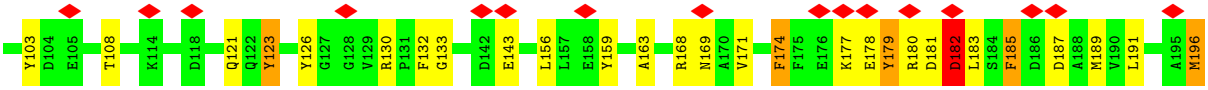


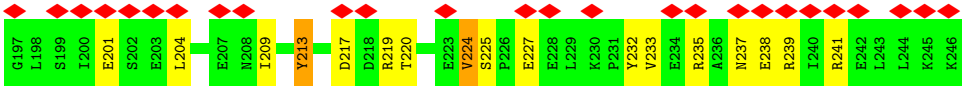


• Molecule 1: Proteasome subunit alpha

Chain D:

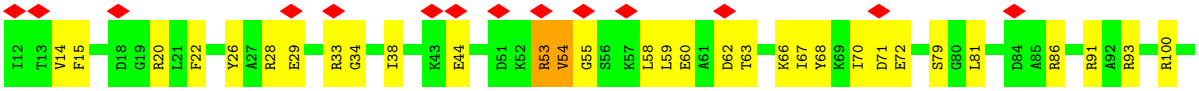


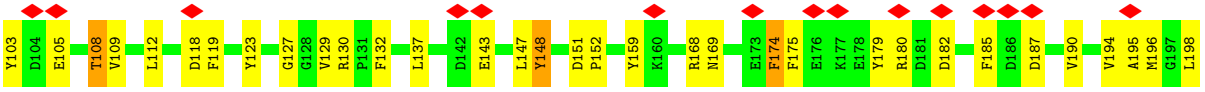


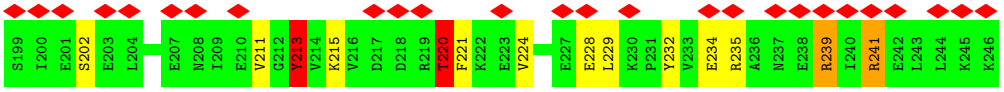


• Molecule 1: Proteasome subunit alpha

Chain E:

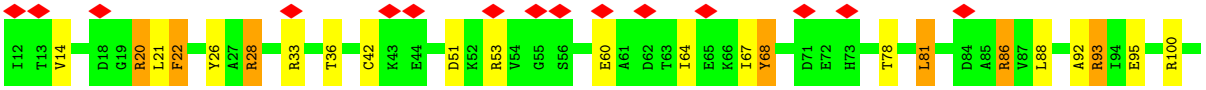


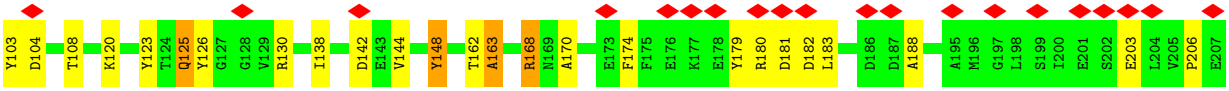


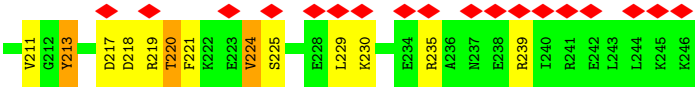


• Molecule 1: Proteasome subunit alpha

Chain F:

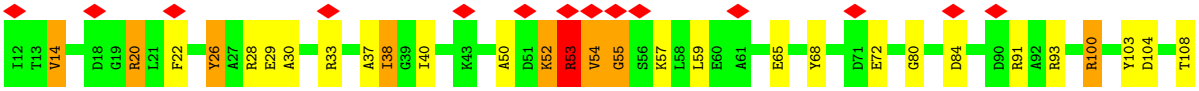


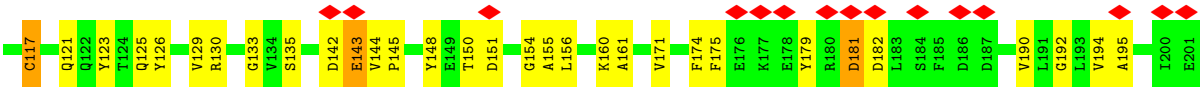




• Molecule 1: Proteasome subunit alpha

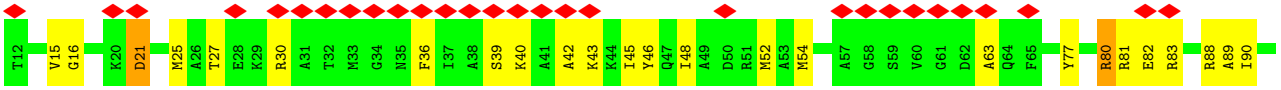
Chain G:

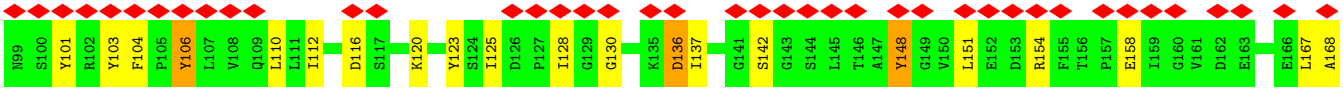


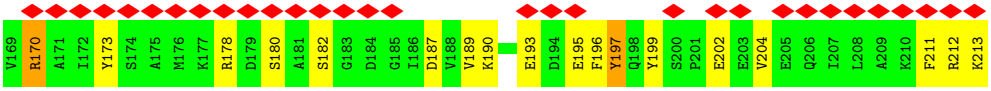


• Molecule 2: Proteasome subunit beta

Chain 1:

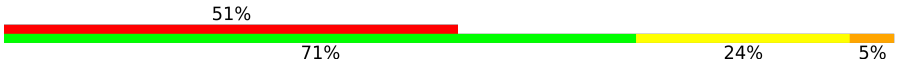


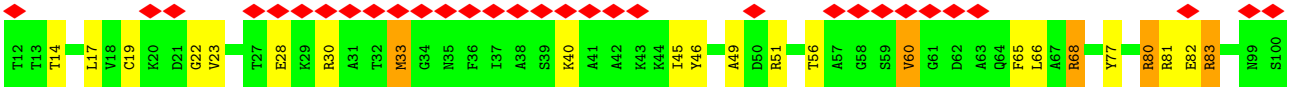


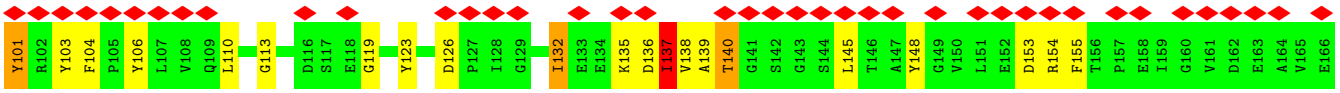


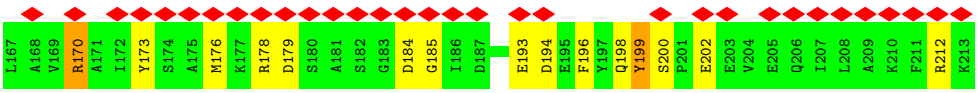
• Molecule 2: Proteasome subunit beta

Chain 2:



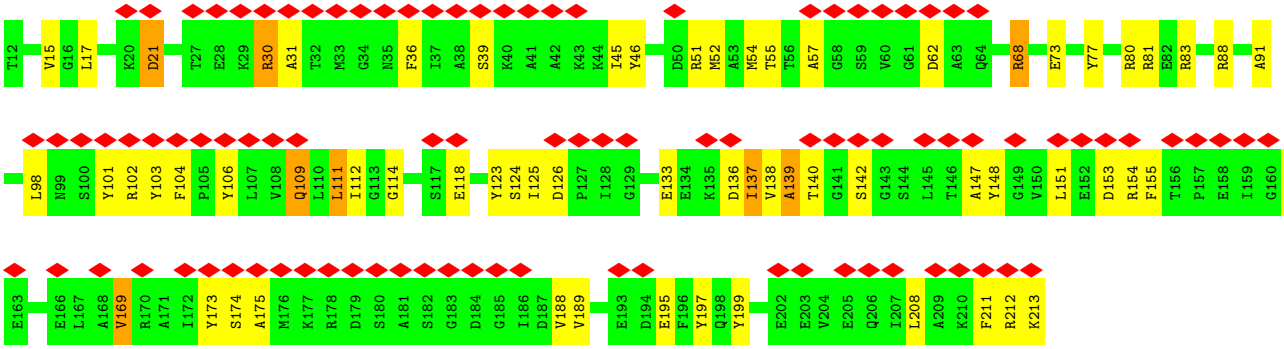






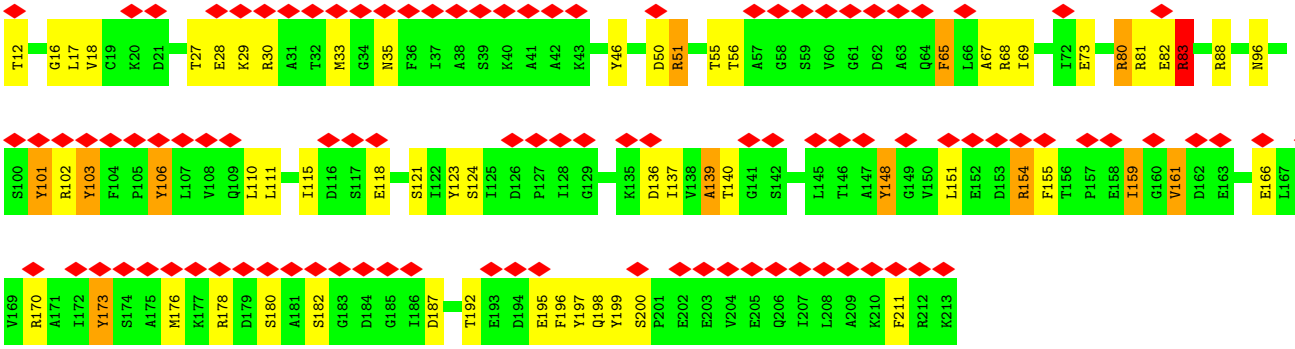
• Molecule 2: Proteasome subunit beta

Chain 3:



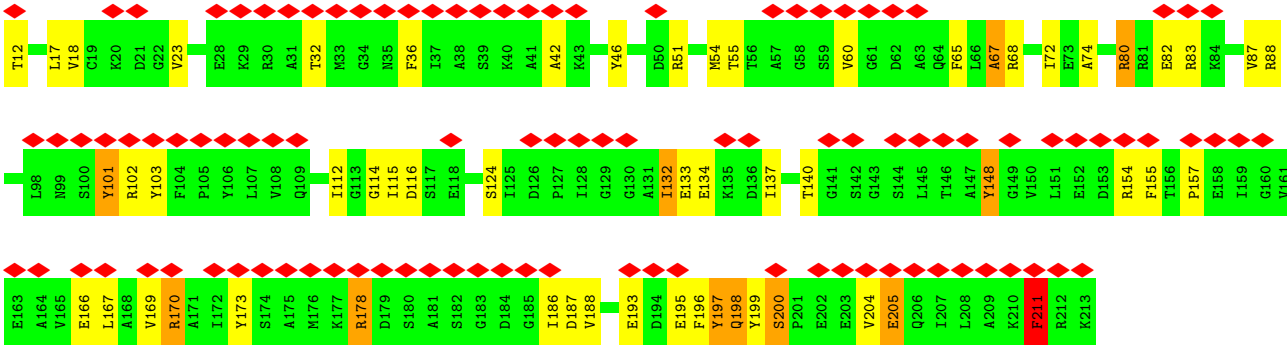
• Molecule 2: Proteasome subunit beta

Chain 4:



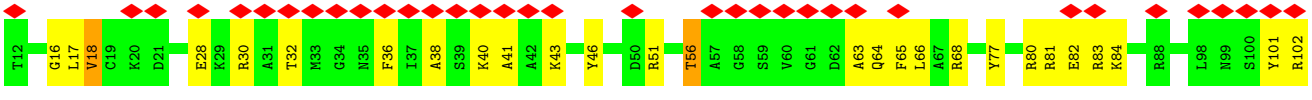
• Molecule 2: Proteasome subunit beta

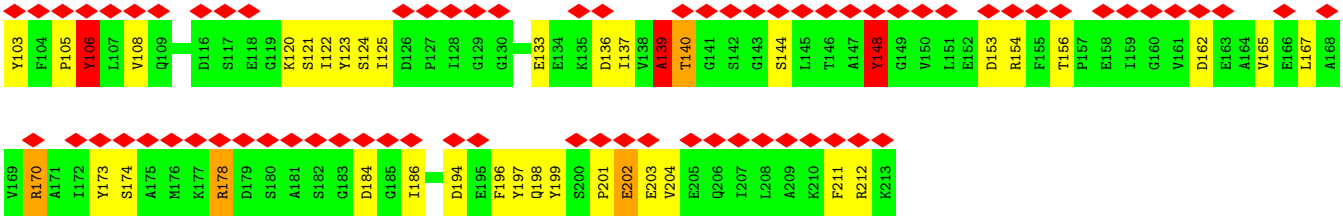
Chain 5:



• Molecule 2: Proteasome subunit beta

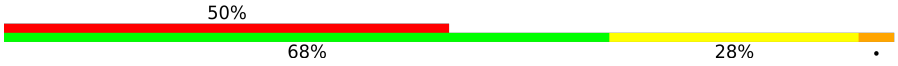
Chain 6:

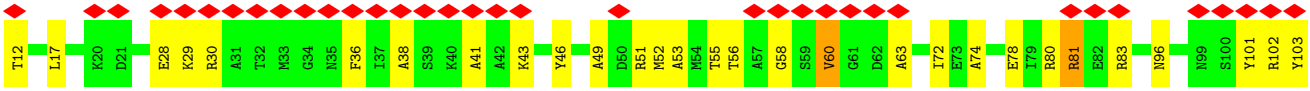


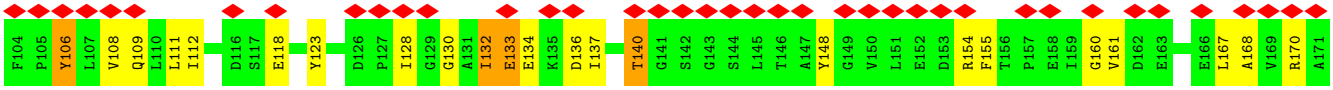


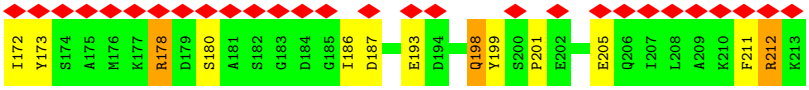
• Molecule 2: Proteasome subunit beta

Chain 7:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	105384	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 ($e^-/Å^2$)	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	0.509	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.08	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	1.72	12/1876 (0.6%)	1.99	46/2528 (1.8%)
1	B	1.69	17/1876 (0.9%)	2.03	37/2528 (1.5%)
1	C	1.73	18/1876 (1.0%)	2.11	52/2528 (2.1%)
1	D	1.74	21/1876 (1.1%)	1.98	50/2528 (2.0%)
1	E	1.75	24/1876 (1.3%)	2.06	49/2528 (1.9%)
1	F	1.71	19/1876 (1.0%)	2.01	51/2528 (2.0%)
1	G	1.75	14/1876 (0.7%)	2.02	58/2528 (2.3%)
2	1	1.80	25/1573 (1.6%)	2.03	41/2121 (1.9%)
2	2	1.79	21/1573 (1.3%)	2.04	54/2121 (2.5%)
2	3	1.84	22/1573 (1.4%)	2.01	49/2121 (2.3%)
2	4	1.81	21/1573 (1.3%)	1.98	45/2121 (2.1%)
2	5	4.08	20/1573 (1.3%)	2.01	41/2121 (1.9%)
2	6	1.81	19/1573 (1.2%)	2.05	44/2121 (2.1%)
2	7	1.69	7/1573 (0.4%)	2.01	38/2121 (1.8%)
All	All	1.99	260/24143 (1.1%)	2.02	655/32543 (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	5
1	C	0	10
1	D	0	10
1	E	0	11
1	F	0	9
1	G	0	12
2	1	0	5
2	2	0	8
2	3	0	4
2	4	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	5	0	10
2	6	0	8
2	7	0	6
All	All	0	115

All (260) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	211	PHE	CG-CD1	105.69	2.97	1.38
2	5	211	PHE	CG-CD2	53.28	2.18	1.38
2	5	211	PHE	CE2-CZ	47.10	2.26	1.37
2	5	211	PHE	CE1-CZ	43.74	2.20	1.37
2	5	211	PHE	CD1-CE1	41.83	2.23	1.39
2	5	211	PHE	CD2-CE2	40.33	2.19	1.39
2	4	103	TYR	CE2-CZ	9.58	1.50	1.38
1	F	179	TYR	CG-CD2	8.66	1.50	1.39
1	E	91	ARG	NE-CZ	8.18	1.43	1.33
2	3	83	ARG	CD-NE	8.10	1.60	1.46
2	6	144	SER	CA-CB	7.93	1.64	1.52
1	B	126	TYR	CZ-OH	7.76	1.51	1.37
2	4	68	ARG	NE-CZ	7.66	1.43	1.33
1	D	123	TYR	CZ-OH	7.66	1.50	1.37
2	6	51	ARG	NE-CZ	7.61	1.43	1.33
2	5	51	ARG	CZ-NH1	7.44	1.42	1.33
1	G	29	GLU	CD-OE1	7.43	1.33	1.25
1	E	44	GLU	C-N	7.42	1.46	1.33
1	E	130	ARG	CZ-NH2	7.34	1.42	1.33
1	B	192	GLY	N-CA	-7.28	1.35	1.46
1	C	202	SER	CB-OG	-7.23	1.32	1.42
1	D	91	ARG	NE-CZ	7.19	1.42	1.33
2	1	212	ARG	NE-CZ	7.18	1.42	1.33
2	1	173	TYR	CG-CD2	7.14	1.48	1.39
2	3	154	ARG	CD-NE	7.09	1.58	1.46
1	E	26	TYR	CE1-CZ	-7.06	1.29	1.38
1	G	133	GLY	CA-C	-7.02	1.40	1.51
2	1	180	SER	CB-OG	7.01	1.51	1.42
1	C	86	ARG	NE-CZ	7.00	1.42	1.33
1	A	119	PHE	N-CA	-6.92	1.32	1.46
1	C	33	ARG	NE-CZ	6.91	1.42	1.33
2	4	101	TYR	CE1-CZ	6.88	1.47	1.38
2	3	197	TYR	CG-CD2	6.83	1.48	1.39
2	3	102	ARG	CZ-NH2	6.83	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	241	ARG	CZ-NH2	6.81	1.41	1.33
2	6	124	SER	CA-CB	6.79	1.63	1.52
1	G	241	ARG	NE-CZ	6.71	1.41	1.33
2	2	22	GLY	N-CA	-6.70	1.35	1.46
2	6	121	SER	CA-CB	6.69	1.62	1.52
1	B	241	ARG	CZ-NH1	6.59	1.41	1.33
2	3	68	ARG	CZ-NH1	6.58	1.41	1.33
2	7	78	GLU	CD-OE2	6.57	1.32	1.25
1	E	33	ARG	CZ-NH2	6.55	1.41	1.33
1	C	227	GLU	CD-OE2	6.54	1.32	1.25
1	D	174	PHE	CB-CG	-6.53	1.40	1.51
2	4	200	SER	CA-CB	6.52	1.62	1.52
1	A	239	ARG	CD-NE	6.50	1.57	1.46
1	A	133	GLY	CA-C	-6.48	1.41	1.51
1	A	91	ARG	NE-CZ	6.47	1.41	1.33
1	D	132	PHE	CG-CD2	6.45	1.48	1.38
2	3	197	TYR	CZ-OH	6.42	1.48	1.37
2	5	82	GLU	CD-OE2	6.39	1.32	1.25
2	4	82	GLU	CG-CD	6.35	1.61	1.51
1	C	174	PHE	CG-CD2	6.35	1.48	1.38
2	2	212	ARG	CZ-NH2	6.34	1.41	1.33
2	3	46	TYR	CE1-CZ	6.34	1.46	1.38
1	E	175	PHE	CG-CD2	6.32	1.48	1.38
2	2	106	TYR	CG-CD2	6.29	1.47	1.39
2	4	159	ILE	C-N	6.29	1.44	1.33
2	4	118	GLU	CD-OE2	6.29	1.32	1.25
1	E	86	ARG	NE-CZ	6.27	1.41	1.33
2	6	40	LYS	CD-CE	6.26	1.67	1.51
2	4	211	PHE	CG-CD1	6.26	1.48	1.38
2	5	65	PHE	CG-CD2	6.25	1.48	1.38
2	1	130	GLY	CA-C	-6.23	1.41	1.51
1	D	201	GLU	CG-CD	6.22	1.61	1.51
1	D	239	ARG	CZ-NH2	6.22	1.41	1.33
1	E	58	LEU	N-CA	-6.22	1.33	1.46
1	F	86	ARG	NE-CZ	6.22	1.41	1.33
2	7	193	GLU	CD-OE2	6.21	1.32	1.25
2	4	124	SER	CA-CB	6.21	1.62	1.52
2	2	200	SER	CA-CB	6.21	1.62	1.52
1	D	72	GLU	CG-CD	6.21	1.61	1.51
2	2	83	ARG	CZ-NH1	6.19	1.41	1.33
2	3	142	SER	CA-CB	6.18	1.62	1.52
1	F	53	ARG	CA-CB	6.17	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	187	ASP	C-N	6.15	1.48	1.34
1	B	28	ARG	CZ-NH2	6.15	1.41	1.33
1	G	239	ARG	CZ-NH1	6.13	1.41	1.33
2	6	202	GLU	CD-OE2	6.10	1.32	1.25
2	2	30	ARG	CZ-NH2	6.09	1.41	1.33
1	G	26	TYR	CG-CD1	6.08	1.47	1.39
2	7	118	GLU	CD-OE1	6.07	1.32	1.25
2	1	83	ARG	NE-CZ	6.06	1.41	1.33
2	3	124	SER	CA-CB	6.05	1.62	1.52
2	1	103	TYR	CG-CD1	6.04	1.47	1.39
2	1	199	TYR	CE2-CZ	6.04	1.46	1.38
2	2	170	ARG	NE-CZ	6.04	1.41	1.33
2	5	114	GLY	CA-C	-6.03	1.42	1.51
2	6	148	TYR	CD2-CE2	6.00	1.48	1.39
2	6	167	LEU	CA-CB	5.98	1.67	1.53
1	B	234	GLU	CD-OE2	-5.97	1.19	1.25
1	C	126	TYR	CE1-CZ	5.96	1.46	1.38
1	E	202	SER	CA-CB	5.95	1.61	1.52
2	3	174	SER	CA-CB	5.95	1.61	1.52
2	6	133	GLU	CD-OE1	5.95	1.32	1.25
1	A	53	ARG	NE-CZ	5.94	1.40	1.33
1	G	91	ARG	CD-NE	5.93	1.56	1.46
2	2	113	GLY	N-CA	-5.92	1.37	1.46
1	F	225	SER	CA-CB	5.90	1.61	1.52
1	A	25	GLU	CD-OE2	5.88	1.32	1.25
2	3	80	ARG	CZ-NH1	5.87	1.40	1.33
1	C	179	TYR	CE2-CZ	5.85	1.46	1.38
1	D	219	ARG	NE-CZ	5.83	1.40	1.33
1	G	53	ARG	CZ-NH2	5.82	1.40	1.33
2	6	106	TYR	CB-CG	5.82	1.60	1.51
2	1	16	GLY	CA-C	-5.81	1.42	1.51
1	D	213	TYR	CZ-OH	5.81	1.47	1.37
1	E	15	PHE	CG-CD1	5.80	1.47	1.38
1	A	239	ARG	NE-CZ	5.80	1.40	1.33
2	3	118	GLU	CB-CG	5.80	1.63	1.52
2	1	158	GLU	CD-OE2	5.79	1.32	1.25
2	4	88	ARG	CD-NE	5.79	1.56	1.46
1	E	168	ARG	NE-CZ	5.78	1.40	1.33
1	D	133	GLY	CA-C	-5.77	1.42	1.51
1	F	104	ASP	CA-CB	5.77	1.66	1.53
2	1	148	TYR	CB-CG	-5.76	1.43	1.51
2	2	80	ARG	NE-CZ	5.76	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	80	ARG	CZ-NH1	5.76	1.40	1.33
2	6	173	TYR	CA-CB	5.76	1.66	1.53
2	4	46	TYR	CZ-OH	5.76	1.47	1.37
1	A	238	GLU	CD-OE1	-5.75	1.19	1.25
1	B	20	ARG	CZ-NH2	5.75	1.40	1.33
1	G	179	TYR	CG-CD1	5.74	1.46	1.39
2	4	148	TYR	CE1-CZ	5.74	1.46	1.38
2	5	103	TYR	CZ-OH	5.72	1.47	1.37
2	1	213	LYS	C-O	5.72	1.34	1.23
2	2	81	ARG	NE-CZ	5.72	1.40	1.33
1	B	20	ARG	NE-CZ	5.71	1.40	1.33
1	D	33	ARG	NE-CZ	5.71	1.40	1.33
2	4	166	GLU	CD-OE2	5.70	1.31	1.25
1	E	152	PRO	N-CD	-5.68	1.39	1.47
1	D	168	ARG	CZ-NH2	5.68	1.40	1.33
2	7	46	TYR	CG-CD1	5.68	1.46	1.39
1	F	179	TYR	CE2-CZ	5.67	1.46	1.38
1	C	100	ARG	NE-CZ	5.67	1.40	1.33
1	E	190	VAL	CB-CG1	5.67	1.64	1.52
1	C	123	TYR	CG-CD1	5.66	1.46	1.39
2	4	73	GLU	CD-OE2	5.65	1.31	1.25
2	1	46	TYR	CG-CD2	5.65	1.46	1.39
1	C	68	TYR	CE2-CZ	5.65	1.45	1.38
1	C	91	ARG	CZ-NH2	5.64	1.40	1.33
1	B	100	ARG	CZ-NH1	5.64	1.40	1.33
2	7	180	SER	CB-OG	5.64	1.49	1.42
1	G	148	TYR	CG-CD1	5.63	1.46	1.39
1	C	212	GLY	CA-C	-5.62	1.42	1.51
1	F	33	ARG	CZ-NH1	5.61	1.40	1.33
2	3	81	ARG	CZ-NH2	5.60	1.40	1.33
1	F	219	ARG	CZ-NH2	5.60	1.40	1.33
2	6	212	ARG	CD-NE	5.59	1.55	1.46
2	5	178	ARG	NE-CZ	5.58	1.40	1.33
1	E	213	TYR	CZ-OH	5.58	1.47	1.37
1	G	91	ARG	CZ-NH2	5.57	1.40	1.33
1	F	93	ARG	NE-CZ	5.55	1.40	1.33
2	4	80	ARG	CD-NE	5.53	1.55	1.46
1	B	130	ARG	NE-CZ	5.53	1.40	1.33
2	5	12	THR	N-CA	5.51	1.57	1.46
1	E	130	ARG	CZ-NH1	5.50	1.40	1.33
1	G	28	ARG	NE-CZ	5.49	1.40	1.33
1	G	192	GLY	CA-C	-5.49	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	114	GLY	CA-C	-5.48	1.43	1.51
1	B	93	ARG	CZ-NH2	5.47	1.40	1.33
1	E	33	ARG	CZ-NH1	5.47	1.40	1.33
2	1	173	TYR	CD2-CE2	5.47	1.47	1.39
1	G	72	GLU	CG-CD	5.47	1.60	1.51
1	E	148	TYR	CG-CD2	5.46	1.46	1.39
2	2	193	GLU	CG-CD	5.46	1.60	1.51
2	1	80	ARG	CD-NE	5.45	1.55	1.46
1	F	20	ARG	CZ-NH2	5.44	1.40	1.33
1	B	232	TYR	CE1-CZ	5.42	1.45	1.38
1	A	180	ARG	CZ-NH2	5.42	1.40	1.33
1	A	24	VAL	CA-CB	-5.39	1.43	1.54
2	1	36	PHE	CG-CD1	5.37	1.46	1.38
2	2	199	TYR	CZ-OH	5.37	1.47	1.37
2	3	36	PHE	CG-CD2	5.36	1.46	1.38
2	6	211	PHE	CG-CD2	5.36	1.46	1.38
2	4	102	ARG	CZ-NH2	5.36	1.40	1.33
1	C	93	ARG	CZ-NH1	5.36	1.40	1.33
2	2	140	THR	C-N	5.36	1.42	1.33
1	E	20	ARG	C-O	5.35	1.33	1.23
1	F	126	TYR	CB-CG	5.34	1.59	1.51
2	5	83	ARG	NE-CZ	5.34	1.40	1.33
1	C	86	ARG	CZ-NH2	5.32	1.40	1.33
2	1	211	PHE	CE2-CZ	5.32	1.47	1.37
1	F	206	PRO	N-CD	5.32	1.55	1.47
2	3	80	ARG	CA-CB	5.31	1.65	1.53
1	C	132	PHE	CE1-CZ	5.31	1.47	1.37
2	5	88	ARG	CD-NE	5.31	1.55	1.46
1	C	25	GLU	CD-OE1	-5.31	1.19	1.25
1	F	168	ARG	CZ-NH2	5.31	1.40	1.33
1	A	210	GLU	CD-OE2	5.30	1.31	1.25
2	5	205	GLU	CD-OE1	5.30	1.31	1.25
1	G	154	GLY	CA-C	-5.29	1.43	1.51
2	6	30	ARG	NE-CZ	5.29	1.40	1.33
1	D	219	ARG	CZ-NH1	5.28	1.40	1.33
2	5	60	VAL	C-N	5.28	1.42	1.33
2	4	211	PHE	CG-CD2	5.27	1.46	1.38
1	B	195	ALA	CA-CB	5.26	1.63	1.52
1	B	103	TYR	CE2-CZ	-5.24	1.31	1.38
2	6	203	GLU	CG-CD	5.24	1.59	1.51
2	1	197	TYR	CG-CD1	5.24	1.46	1.39
2	2	101	TYR	CZ-OH	5.23	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	86	ARG	CZ-NH1	5.23	1.39	1.33
2	6	197	TYR	CE2-CZ	5.23	1.45	1.38
1	E	55	GLY	CA-C	-5.22	1.43	1.51
2	6	106	TYR	CE2-CZ	5.22	1.45	1.38
2	4	96	ASN	CA-CB	5.22	1.66	1.53
2	3	88	ARG	CD-NE	5.21	1.55	1.46
1	F	239	ARG	CZ-NH2	5.21	1.39	1.33
2	5	46	TYR	CE2-CZ	5.21	1.45	1.38
2	3	199	TYR	CG-CD1	5.21	1.46	1.39
2	6	178	ARG	NE-CZ	5.21	1.39	1.33
1	B	65	GLU	CB-CG	5.20	1.62	1.52
2	1	154	ARG	NE-CZ	5.20	1.39	1.33
2	1	199	TYR	CG-CD2	5.20	1.46	1.39
1	D	235	ARG	CD-NE	5.19	1.55	1.46
1	F	42	CYS	CA-CB	5.18	1.65	1.53
2	1	193	GLU	CA-CB	5.18	1.65	1.53
2	4	199	TYR	CG-CD1	5.18	1.45	1.39
1	F	33	ARG	CZ-NH2	5.18	1.39	1.33
2	1	142	SER	CA-CB	5.17	1.60	1.52
2	5	148	TYR	CA-CB	5.17	1.65	1.53
1	F	203	GLU	CD-OE2	5.17	1.31	1.25
1	E	67	ILE	CA-CB	-5.17	1.43	1.54
1	B	173	GLU	CG-CD	5.16	1.59	1.51
2	3	73	GLU	CD-OE1	5.16	1.31	1.25
2	1	88	ARG	NE-CZ	5.15	1.39	1.33
1	D	20	ARG	CD-NE	5.15	1.55	1.46
1	D	191	LEU	C-N	5.15	1.42	1.33
2	1	148	TYR	N-CA	-5.12	1.36	1.46
1	E	234	GLU	CG-CD	5.12	1.59	1.51
2	2	101	TYR	CG-CD1	-5.10	1.32	1.39
1	D	16	SER	CA-CB	5.09	1.60	1.52
2	7	148	TYR	CG-CD2	5.09	1.45	1.39
1	F	239	ARG	NE-CZ	5.08	1.39	1.33
1	C	75	CYS	CB-SG	-5.08	1.73	1.81
2	2	153	ASP	CB-CG	5.06	1.62	1.51
2	1	123	TYR	CB-CG	-5.06	1.44	1.51
1	F	68	TYR	CE2-CZ	5.06	1.45	1.38
2	4	180	SER	CB-OG	5.05	1.48	1.42
1	D	178	GLU	CD-OE2	5.04	1.31	1.25
1	B	227	GLU	CD-OE2	5.03	1.31	1.25
1	C	93	ARG	CZ-NH2	5.03	1.39	1.33
2	3	133	GLU	CA-C	-5.03	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	ARG	NE-CZ	5.03	1.39	1.33
2	1	43	LYS	N-CA	-5.03	1.36	1.46
2	2	19	CYS	CB-SG	5.03	1.90	1.82
2	2	178	ARG	NE-CZ	5.03	1.39	1.33
2	3	173	TYR	CZ-OH	5.03	1.46	1.37
2	3	212	ARG	CZ-NH1	5.02	1.39	1.33
2	4	154	ARG	CG-CD	5.02	1.64	1.51
1	E	234	GLU	N-CA	5.01	1.56	1.46
2	6	56	THR	CB-CG2	5.01	1.68	1.52
1	A	143	GLU	CD-OE2	5.01	1.31	1.25
2	2	202	GLU	CD-OE2	5.01	1.31	1.25
2	2	51	ARG	CD-NE	5.01	1.54	1.46
1	D	93	ARG	NE-CZ	5.00	1.39	1.33
1	B	153	SER	CA-CB	5.00	1.60	1.52
1	E	182	ASP	N-CA	-5.00	1.36	1.46
2	2	68	ARG	CZ-NH1	5.00	1.39	1.33

All (655) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	181	ASP	O-C-N	27.32	166.42	122.70
1	B	180	ARG	NE-CZ-NH2	21.68	131.14	120.30
1	E	180	ARG	NE-CZ-NH2	20.37	130.48	120.30
1	A	123	TYR	CB-CG-CD2	-18.26	110.05	121.00
2	5	211	PHE	CG-CD1-CE1	-18.16	100.83	120.80
2	1	101	TYR	CB-CG-CD1	-17.44	110.53	121.00
1	A	123	TYR	CB-CG-CD1	17.44	131.46	121.00
1	C	181	ASP	CA-C-O	-16.79	84.84	120.10
2	4	178	ARG	NE-CZ-NH1	15.78	128.19	120.30
1	C	181	ASP	CA-C-N	-14.65	84.96	117.20
1	B	179	TYR	CB-CG-CD1	14.45	129.67	121.00
2	1	101	TYR	CB-CG-CD2	14.45	129.67	121.00
2	6	148	TYR	CB-CG-CD1	-14.30	112.42	121.00
1	E	180	ARG	NE-CZ-NH1	-14.27	113.16	120.30
2	6	68	ARG	NE-CZ-NH2	-14.07	113.26	120.30
1	G	20	ARG	NE-CZ-NH2	-13.73	113.43	120.30
1	B	175	PHE	CB-CG-CD1	13.37	130.16	120.80
1	C	20	ARG	NE-CZ-NH2	-13.21	113.69	120.30
2	7	81	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	G	26	TYR	CB-CG-CD1	13.11	128.87	121.00
2	5	46	TYR	CB-CG-CD1	-12.92	113.25	121.00
2	3	80	ARG	NE-CZ-NH1	-12.88	113.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	86	ARG	NE-CZ-NH2	-12.87	113.86	120.30
1	C	182	ASP	N-CA-CB	12.87	133.77	110.60
1	F	28	ARG	NE-CZ-NH1	-12.65	113.98	120.30
2	2	154	ARG	NE-CZ-NH1	-12.57	114.01	120.30
2	6	196	PHE	CB-CG-CD1	12.44	129.51	120.80
1	G	103	TYR	CB-CG-CD2	-12.42	113.55	121.00
1	D	26	TYR	CB-CG-CD2	12.34	128.40	121.00
1	D	179	TYR	CB-CG-CD1	-12.22	113.67	121.00
1	E	26	TYR	CB-CG-CD1	12.14	128.28	121.00
2	3	212	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	B	175	PHE	CB-CG-CD2	-11.97	112.42	120.80
1	A	241	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	E	132	PHE	CB-CG-CD2	-11.96	112.43	120.80
2	6	30	ARG	NE-CZ-NH1	-11.89	114.35	120.30
2	6	77	TYR	CB-CG-CD1	11.65	127.99	121.00
2	4	197	TYR	CB-CG-CD1	-11.41	114.16	121.00
1	B	103	TYR	CB-CG-CD2	11.28	127.77	121.00
1	G	20	ARG	NE-CZ-NH1	11.19	125.90	120.30
1	E	33	ARG	NE-CZ-NH2	-11.19	114.71	120.30
2	4	178	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	G	123	TYR	CB-CG-CD1	11.07	127.64	121.00
2	1	197	TYR	CB-CG-CD1	-11.06	114.36	121.00
1	B	239	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	F	100	ARG	NE-CZ-NH1	10.90	125.75	120.30
2	7	46	TYR	CB-CG-CD2	-10.85	114.49	121.00
2	1	83	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	B	103	TYR	CB-CG-CD1	-10.77	114.53	121.00
1	D	126	TYR	CB-CG-CD1	10.61	127.37	121.00
1	D	91	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	G	174	PHE	CB-CG-CD2	-10.55	113.41	120.80
1	A	179	TYR	CB-CG-CD1	-10.50	114.70	121.00
2	2	103	TYR	CB-CG-CD1	-10.44	114.74	121.00
1	E	132	PHE	CB-CG-CD1	10.42	128.09	120.80
2	3	155	PHE	CB-CG-CD1	-10.39	113.53	120.80
1	A	53	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	B	180	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	F	86	ARG	NE-CZ-NH2	-10.35	115.12	120.30
2	5	197	TYR	CB-CG-CD1	-10.21	114.87	121.00
2	6	199	TYR	CB-CG-CD1	10.18	127.11	121.00
1	E	93	ARG	NE-CZ-NH1	10.10	125.35	120.30
2	6	196	PHE	CB-CG-CD2	-10.10	113.73	120.80
2	5	46	TYR	CB-CG-CD2	10.06	127.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	100	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	G	175	PHE	CB-CG-CD2	-10.03	113.78	120.80
1	F	126	TYR	CB-CG-CD1	-10.02	114.99	121.00
2	3	46	TYR	CB-CG-CD2	-10.00	115.00	121.00
2	4	211	PHE	CB-CG-CD2	9.99	127.79	120.80
2	6	81	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	D	126	TYR	CB-CG-CD2	-9.91	115.06	121.00
2	7	46	TYR	CG-CD1-CE1	-9.84	113.43	121.30
1	E	26	TYR	CB-CG-CD2	-9.83	115.10	121.00
2	1	81	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	C	168	ARG	NE-CZ-NH1	9.76	125.18	120.30
2	6	170	ARG	NE-CZ-NH1	-9.73	115.44	120.30
1	B	168	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	C	175	PHE	CB-CG-CD2	-9.69	114.02	120.80
2	6	102	ARG	NE-CZ-NH2	-9.65	115.47	120.30
2	7	148	TYR	CB-CG-CD2	9.62	126.77	121.00
1	C	187	ASP	CB-CG-OD2	-9.60	109.66	118.30
1	G	100	ARG	NE-CZ-NH2	9.60	125.10	120.30
2	2	212	ARG	NE-CZ-NH2	-9.57	115.51	120.30
2	7	102	ARG	NE-CZ-NH2	9.57	125.08	120.30
1	F	174	PHE	CB-CG-CD1	-9.50	114.15	120.80
2	5	68	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	G	33	ARG	NE-CZ-NH2	-9.49	115.56	120.30
2	6	154	ARG	NE-CZ-NH2	9.46	125.03	120.30
2	2	196	PHE	CB-CG-CD2	9.44	127.41	120.80
2	3	31	ALA	N-CA-CB	9.42	123.28	110.10
1	C	168	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	53	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	C	241	ARG	NE-CZ-NH2	9.31	124.96	120.30
2	7	83	ARG	NE-CZ-NH2	9.29	124.94	120.30
2	7	80	ARG	NE-CZ-NH2	-9.29	115.66	120.30
2	1	80	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	A	186	ASP	CB-CG-OD1	-9.12	110.09	118.30
2	3	199	TYR	CB-CG-CD1	-9.11	115.53	121.00
2	7	51	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	A	100	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	B	132	PHE	CB-CG-CD1	9.02	127.11	120.80
1	D	68	TYR	CB-CG-CD1	-8.96	115.62	121.00
1	E	159	TYR	CB-CG-CD1	8.93	126.36	121.00
2	4	199	TYR	CB-CG-CD2	-8.85	115.69	121.00
1	F	104	ASP	CB-CG-OD2	-8.84	110.34	118.30
2	3	51	ARG	NE-CZ-NH1	-8.83	115.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	77	TYR	CB-CG-CD2	-8.83	115.70	121.00
2	7	101	TYR	CB-CG-CD1	8.79	126.28	121.00
1	C	53	ARG	NE-CZ-NH1	-8.78	115.91	120.30
2	5	199	TYR	CB-CG-CD2	8.73	126.23	121.00
1	F	20	ARG	NE-CZ-NH1	8.72	124.66	120.30
2	2	56	THR	CA-CB-CG2	-8.70	100.22	112.40
1	F	182	ASP	CB-CG-OD1	8.69	126.12	118.30
1	G	26	TYR	CB-CG-CD2	-8.69	115.79	121.00
2	2	103	TYR	CZ-CE2-CD2	-8.67	112.00	119.80
2	2	212	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	F	130	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	C	33	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	G	22	PHE	CB-CG-CD1	-8.61	114.78	120.80
2	3	104	PHE	CB-CG-CD2	-8.56	114.81	120.80
2	1	116	ASP	CB-CG-OD1	-8.53	110.62	118.30
2	5	162	ASP	CB-CG-OD1	-8.52	110.64	118.30
2	1	88	ARG	NE-CZ-NH1	-8.48	116.06	120.30
2	5	103	TYR	CB-CG-CD2	-8.48	115.92	121.00
1	C	239	ARG	NE-CZ-NH2	8.46	124.53	120.30
2	6	199	TYR	CB-CG-CD2	-8.36	115.98	121.00
1	D	232	TYR	CB-CG-CD1	-8.36	115.98	121.00
1	E	86	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	F	68	TYR	CB-CG-CD2	8.35	126.01	121.00
1	G	53	ARG	NE-CZ-NH2	-8.34	116.13	120.30
2	1	30	ARG	NE-CZ-NH2	8.34	124.47	120.30
2	4	187	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	F	182	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	C	26	TYR	CB-CG-CD1	8.29	125.97	121.00
1	C	218	ASP	CB-CG-OD2	8.29	125.76	118.30
1	D	180	ARG	NE-CZ-NH2	8.24	124.42	120.30
2	1	170	ARG	NE-CZ-NH1	-8.21	116.20	120.30
2	4	50	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	C	239	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	G	53	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	D	68	TYR	CB-CG-CD2	8.15	125.89	121.00
2	2	103	TYR	CB-CG-CD2	8.12	125.87	121.00
2	5	68	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	241	ARG	NE-CZ-NH1	-8.06	116.27	120.30
2	1	104	PHE	CG-CD2-CE2	8.05	129.66	120.80
2	3	77	TYR	CB-CG-CD1	-8.05	116.17	121.00
2	4	30	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	A	28	ARG	NE-CZ-NH2	-8.01	116.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	179	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	F	22	PHE	CB-CG-CD1	8.00	126.40	120.80
1	D	100	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	F	179	TYR	CB-CG-CD1	7.94	125.77	121.00
2	7	178	ARG	NE-CZ-NH1	7.93	124.27	120.30
2	2	65	PHE	CB-CG-CD1	-7.93	115.25	120.80
1	D	103	TYR	CZ-CE2-CD2	7.91	126.92	119.80
2	6	153	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	D	179	TYR	CG-CD2-CE2	-7.84	115.03	121.30
1	A	219	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	E	22	PHE	CB-CG-CD1	-7.72	115.39	120.80
1	A	241	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	G	91	ARG	NE-CZ-NH2	-7.71	116.44	120.30
2	4	197	TYR	CB-CG-CD2	7.64	125.58	121.00
1	C	182	ASP	N-CA-C	-7.60	90.48	111.00
1	A	28	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	3	104	PHE	CB-CG-CD1	7.57	126.10	120.80
2	3	173	TYR	CB-CG-CD2	-7.56	116.46	121.00
1	B	139	ALA	N-CA-CB	7.54	120.66	110.10
1	F	180	ARG	NE-CZ-NH1	-7.54	116.53	120.30
2	6	46	TYR	CG-CD1-CE1	-7.54	115.27	121.30
1	C	180	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	20	ARG	NE-CZ-NH1	7.53	124.06	120.30
2	4	173	TYR	CB-CG-CD1	7.53	125.52	121.00
1	B	195	ALA	N-CA-CB	7.48	120.58	110.10
2	2	154	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	91	ARG	NE-CZ-NH1	-7.44	116.58	120.30
2	4	103	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	C	53	ARG	NE-CZ-NH2	7.39	123.99	120.30
2	7	30	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	D	53	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	2	83	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	F	170	ALA	CB-CA-C	-7.36	99.06	110.10
2	7	178	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	185	PHE	CB-CG-CD1	-7.32	115.68	120.80
1	A	148	TYR	CG-CD2-CE2	-7.30	115.46	121.30
1	G	235	ARG	NE-CZ-NH2	7.27	123.94	120.30
2	3	62	ASP	CB-CG-OD2	-7.27	111.75	118.30
2	7	168	ALA	CB-CA-C	-7.27	99.19	110.10
2	1	106	TYR	CB-CG-CD1	-7.21	116.68	121.00
2	3	139	ALA	N-CA-CB	7.20	120.18	110.10
2	6	102	ARG	NE-CZ-NH1	7.20	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	139	ALA	C-N-CA	7.19	139.67	121.70
1	B	221	PHE	CB-CG-CD2	7.18	125.83	120.80
1	G	218	ASP	CB-CG-OD1	-7.17	111.84	118.30
2	2	46	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	F	33	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	1	197	TYR	CB-CG-CD2	7.15	125.29	121.00
2	3	102	ARG	NE-CZ-NH2	-7.15	116.73	120.30
2	6	46	TYR	CB-CG-CD2	-7.14	116.71	121.00
1	A	117	CYS	CA-CB-SG	-7.13	101.16	114.00
1	G	26	TYR	CG-CD2-CE2	7.13	127.01	121.30
2	4	83	ARG	NE-CZ-NH1	7.13	123.87	120.30
2	1	104	PHE	CB-CG-CD1	7.11	125.78	120.80
1	C	90	ASP	CB-CG-OD1	-7.11	111.91	118.30
2	3	139	ALA	C-N-CA	7.10	139.44	121.70
1	F	123	TYR	CB-CG-CD2	7.09	125.25	121.00
1	F	93	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	2	155	PHE	CB-CG-CD2	-7.09	115.84	120.80
1	F	219	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	2	185	GLY	N-CA-C	-7.06	95.45	113.10
2	7	74	ALA	CB-CA-C	-7.06	99.51	110.10
2	7	83	ARG	NE-CZ-NH1	-7.05	116.78	120.30
2	4	56	THR	CA-CB-CG2	-7.04	102.54	112.40
1	E	174	PHE	CB-CG-CD2	7.03	125.72	120.80
1	F	104	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	179	TYR	CB-CG-CD2	-7.00	116.80	121.00
2	1	104	PHE	CZ-CE2-CD2	-7.00	111.70	120.10
2	3	80	ARG	NE-CZ-NH2	6.98	123.79	120.30
2	1	77	TYR	CG-CD2-CE2	-6.97	115.72	121.30
1	E	168	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	2	81	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	26	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	E	53	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	20	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	D	130	ARG	NE-CZ-NH1	6.95	123.77	120.30
2	3	103	TYR	CB-CG-CD1	-6.92	116.85	121.00
2	2	33	MET	CG-SD-CE	-6.91	89.15	100.20
2	5	169	VAL	CG1-CB-CG2	6.87	121.90	110.90
1	B	132	PHE	CB-CG-CD2	-6.87	115.99	120.80
1	C	187	ASP	CB-CG-OD1	6.86	124.47	118.30
2	5	87	VAL	CA-CB-CG1	-6.86	100.62	110.90
2	6	66	LEU	CB-CG-CD1	6.85	122.64	111.00
1	C	76	ALA	N-CA-CB	6.84	119.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	3	140	THR	C-N-CA	6.81	136.61	122.30
2	6	36	PHE	CB-CG-CD1	-6.81	116.03	120.80
2	7	134	GLU	N-CA-CB	6.80	122.84	110.60
1	A	179	TYR	CB-CG-CD2	6.80	125.08	121.00
1	A	26	TYR	CB-CG-CD1	6.79	125.07	121.00
1	G	216	VAL	CA-CB-CG1	6.79	121.08	110.90
1	E	93	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	D	187	ASP	CB-CG-OD2	-6.75	112.22	118.30
2	3	139	ALA	CA-C-N	6.75	132.06	117.20
2	5	187	ASP	CB-CG-OD1	6.75	124.37	118.30
1	F	51	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	A	216	VAL	CA-CB-CG1	6.73	120.99	110.90
1	D	33	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	4	106	TYR	CB-CG-CD2	-6.71	116.98	121.00
1	A	148	TYR	CZ-CE2-CD2	6.68	125.81	119.80
1	E	123	TYR	CG-CD1-CE1	-6.68	115.96	121.30
1	A	125	GLN	N-CA-CB	6.67	122.61	110.60
1	D	14	VAL	CA-CB-CG2	6.67	120.91	110.90
2	2	106	TYR	CG-CD2-CE2	-6.66	115.97	121.30
2	2	173	TYR	CB-CG-CD2	-6.66	117.00	121.00
1	E	232	TYR	CB-CG-CD2	6.65	124.99	121.00
2	3	199	TYR	CA-CB-CG	-6.65	100.76	113.40
2	2	65	PHE	CB-CG-CD2	6.64	125.44	120.80
1	A	108	THR	N-CA-CB	6.62	122.89	110.30
2	5	55	THR	N-CA-CB	6.62	122.88	110.30
1	A	22	PHE	CB-CG-CD1	6.61	125.43	120.80
1	C	51	ASP	CB-CG-OD1	6.60	124.24	118.30
1	G	175	PHE	CB-CG-CD1	6.60	125.42	120.80
2	6	101	TYR	CB-CG-CD2	6.59	124.95	121.00
1	B	239	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	22	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	F	104	ASP	N-CA-CB	6.55	122.39	110.60
1	E	235	ARG	NE-CZ-NH2	6.54	123.57	120.30
2	4	68	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	6	106	TYR	N-CA-C	-6.54	93.36	111.00
1	G	160	LYS	N-CA-CB	6.53	122.35	110.60
2	3	212	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	4	170	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	C	130	ARG	NE-CZ-NH1	6.51	123.55	120.30
2	4	88	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	5	173	TYR	CD1-CE1-CZ	-6.47	113.97	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	F	174	PHE	CB-CG-CD2	6.46	125.33	120.80
1	G	84	ASP	CB-CG-OD1	6.46	124.12	118.30
2	7	36	PHE	CB-CG-CD2	-6.45	116.29	120.80
2	1	89	ALA	CB-CA-C	-6.44	100.43	110.10
2	3	88	ARG	NE-CZ-NH2	6.44	123.52	120.30
2	5	103	TYR	CB-CG-CD1	6.44	124.86	121.00
1	C	148	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	G	232	TYR	CZ-CE2-CD2	6.43	125.59	119.80
2	7	101	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	F	14	VAL	CG1-CB-CG2	-6.43	100.61	110.90
2	1	106	TYR	CB-CG-CD2	6.42	124.85	121.00
2	3	137	ILE	N-CA-CB	-6.41	96.06	110.80
2	5	200	SER	N-CA-CB	6.41	120.11	110.50
2	4	176	MET	CG-SD-CE	-6.40	89.96	100.20
1	D	181	ASP	N-CA-CB	6.38	122.08	110.60
2	1	195	GLU	C-N-CA	6.37	137.63	121.70
2	7	53	ALA	N-CA-CB	6.35	119.00	110.10
1	A	182	ASP	CB-CG-OD2	-6.34	112.59	118.30
2	1	25	MET	CG-SD-CE	-6.33	90.06	100.20
1	A	126	TYR	CB-CG-CD1	6.33	124.80	121.00
1	F	211	VAL	N-CA-C	-6.33	93.92	111.00
2	1	196	PHE	N-CA-C	-6.30	93.99	111.00
1	D	18	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	219	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	G	93	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	D	232	TYR	CG-CD2-CE2	-6.28	116.28	121.30
1	D	91	ARG	NE-CZ-NH1	6.27	123.43	120.30
2	6	18	VAL	CA-CB-CG2	-6.26	101.50	110.90
1	A	187	ASP	N-CA-CB	6.25	121.86	110.60
2	4	103	TYR	CG-CD2-CE2	-6.25	116.30	121.30
1	F	181	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	F	235	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	5	124	SER	N-CA-CB	6.24	119.87	110.50
2	3	211	PHE	CB-CG-CD2	-6.22	116.45	120.80
2	1	54	MET	CG-SD-CE	-6.20	90.27	100.20
2	6	162	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	D	179	TYR	CB-CG-CD2	6.19	124.71	121.00
2	2	123	TYR	CB-CG-CD1	6.18	124.71	121.00
2	2	132	ILE	N-CA-C	-6.18	94.31	111.00
2	4	111	LEU	N-CA-C	-6.18	94.31	111.00
1	C	123	TYR	CB-CG-CD2	6.17	124.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	81	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	186	ASP	CB-CG-OD2	6.16	123.84	118.30
2	2	103	TYR	CG-CD1-CE1	-6.15	116.38	121.30
2	3	62	ASP	CB-CG-OD1	6.15	123.83	118.30
1	D	26	TYR	CB-CG-CD1	-6.15	117.31	121.00
2	7	38	ALA	N-CA-CB	6.14	118.70	110.10
1	E	68	TYR	CB-CG-CD2	-6.14	117.31	121.00
2	2	184	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	5	173	TYR	N-CA-CB	6.14	121.65	110.60
2	2	138	VAL	CG1-CB-CG2	6.13	120.71	110.90
1	A	189	MET	CG-SD-CE	-6.13	90.39	100.20
1	F	67	ILE	N-CA-C	-6.13	94.45	111.00
1	F	36	THR	CA-CB-CG2	-6.12	103.83	112.40
1	D	181	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	126	TYR	CD1-CE1-CZ	6.11	125.30	119.80
2	3	15	VAL	CA-CB-CG1	-6.08	101.78	110.90
1	F	224	VAL	CA-CB-CG2	-6.08	101.79	110.90
1	G	104	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	182	ASP	O-C-N	6.07	132.42	122.70
2	3	36	PHE	CB-CG-CD1	-6.07	116.55	120.80
1	A	46	VAL	CA-CB-CG2	-6.07	101.79	110.90
2	3	111	LEU	N-CA-CB	6.07	122.53	110.40
1	F	26	TYR	CB-CG-CD2	-6.07	117.36	121.00
2	2	101	TYR	CB-CG-CD1	6.06	124.64	121.00
2	6	103	TYR	CB-CG-CD1	-6.06	117.36	121.00
2	1	42	ALA	N-CA-C	-6.05	94.67	111.00
1	F	217	ASP	CB-CG-OD2	6.05	123.74	118.30
2	3	52	MET	N-CA-CB	6.04	121.48	110.60
1	B	89	ILE	N-CA-CB	6.04	124.69	110.80
2	6	173	TYR	O-C-N	6.03	132.35	122.70
1	F	148	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	F	68	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	F	92	ALA	N-CA-CB	6.01	118.52	110.10
1	F	211	VAL	CG1-CB-CG2	6.01	120.52	110.90
2	5	55	THR	CA-CB-CG2	-6.01	103.99	112.40
2	6	108	VAL	CA-CB-CG2	6.01	119.91	110.90
1	G	143	GLU	CB-CA-C	-6.00	98.39	110.40
2	4	65	PHE	CB-CG-CD2	-6.00	116.60	120.80
2	4	198	GLN	N-CA-CB	6.00	121.41	110.60
2	6	197	TYR	CB-CG-CD1	6.00	124.60	121.00
2	3	98	LEU	CB-CG-CD2	6.00	121.20	111.00
1	G	103	TYR	CB-CG-CD1	5.99	124.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	91	ARG	NE-CZ-NH1	5.99	123.29	120.30
2	3	51	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	5	148	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	62	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	19	GLY	O-C-N	-5.96	113.16	122.70
2	2	136	ASP	CB-CG-OD1	5.96	123.67	118.30
2	6	68	ARG	NH1-CZ-NH2	5.95	125.95	119.40
2	7	123	TYR	CG-CD1-CE1	-5.95	116.54	121.30
1	E	187	ASP	CB-CG-OD1	5.94	123.65	118.30
1	E	79	SER	N-CA-CB	5.94	119.40	110.50
2	2	153	ASP	N-CA-CB	5.93	121.28	110.60
1	E	109	VAL	CA-CB-CG1	-5.93	102.00	110.90
2	5	88	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	F	28	ARG	NH1-CZ-NH2	5.90	125.89	119.40
2	2	198	GLN	CA-CB-CG	-5.89	100.45	113.40
1	D	123	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	F	95	GLU	OE1-CD-OE2	-5.88	116.24	123.30
2	4	67	ALA	N-CA-CB	5.88	118.33	110.10
1	G	68	TYR	CB-CG-CD1	5.88	124.53	121.00
2	5	157	PRO	N-CD-CG	5.88	112.01	103.20
1	D	108	THR	CA-CB-CG2	-5.87	104.18	112.40
1	G	55	GLY	CA-C-N	-5.87	104.28	117.20
2	2	153	ASP	CB-CG-OD1	5.87	123.59	118.30
2	3	147	ALA	N-CA-CB	5.87	118.32	110.10
2	1	204	VAL	CA-CB-CG2	-5.86	102.11	110.90
1	C	54	VAL	CA-CB-CG1	-5.86	102.11	110.90
1	F	142	ASP	CB-CG-OD1	5.85	123.57	118.30
1	G	235	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	A	103	TYR	CB-CG-CD1	-5.85	117.49	121.00
2	1	199	TYR	CB-CA-C	-5.84	98.72	110.40
2	7	187	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	A	235	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	C	21	LEU	N-CA-CB	5.83	122.07	110.40
1	B	75	CYS	N-CA-CB	5.83	121.09	110.60
2	5	74	ALA	N-CA-CB	5.83	118.26	110.10
1	D	77	ALA	CB-CA-C	-5.83	101.36	110.10
2	2	106	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	D	189	MET	CG-SD-CE	-5.82	90.88	100.20
2	4	196	PHE	N-CA-C	-5.82	95.28	111.00
1	A	185	PHE	CB-CG-CD2	-5.82	116.73	120.80
2	6	211	PHE	CB-CG-CD2	5.82	124.87	120.80
2	2	198	GLN	CB-CA-C	5.80	122.00	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	110	LEU	CB-CA-C	-5.80	99.18	110.20
2	6	80	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	105	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	G	218	ASP	CB-CG-OD2	5.79	123.51	118.30
2	6	165	VAL	CA-CB-CG2	-5.79	102.22	110.90
1	C	132	PHE	C-N-CA	5.79	134.45	122.30
1	D	174	PHE	CB-CG-CD1	5.78	124.84	120.80
1	G	108	THR	CA-CB-CG2	-5.77	104.33	112.40
1	E	118	ASP	CB-CG-OD1	5.76	123.49	118.30
2	3	175	ALA	N-CA-CB	5.76	118.17	110.10
1	C	182	ASP	CB-CG-OD2	-5.75	113.12	118.30
2	2	145	LEU	CB-CG-CD1	5.75	120.78	111.00
1	B	93	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	213	TYR	CB-CG-CD1	-5.74	117.56	121.00
2	6	194	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	87	VAL	CA-CB-CG1	5.73	119.50	110.90
2	4	27	THR	O-C-N	-5.71	113.56	122.70
2	4	17	LEU	CB-CG-CD2	5.71	120.71	111.00
2	7	55	THR	CA-CB-CG2	-5.71	104.41	112.40
2	2	82	GLU	N-CA-CB	5.70	120.87	110.60
2	4	123	TYR	CD1-CE1-CZ	5.70	124.93	119.80
1	D	62	ASP	N-CA-CB	5.70	120.86	110.60
1	G	161	ALA	N-CA-CB	5.70	118.08	110.10
2	7	106	TYR	N-CA-C	-5.70	95.61	111.00
2	5	197	TYR	N-CA-C	-5.70	95.62	111.00
1	G	55	GLY	O-C-N	5.69	131.80	122.70
2	1	170	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	E	108	THR	CA-CB-CG2	-5.68	104.45	112.40
2	5	211	PHE	CD1-CE1-CZ	5.68	126.92	120.10
2	6	211	PHE	CB-CG-CD1	-5.67	116.83	120.80
2	3	46	TYR	CG-CD1-CE1	5.67	125.83	121.30
2	4	101	TYR	CB-CG-CD1	-5.66	117.60	121.00
2	7	212	ARG	CG-CD-NE	-5.66	99.91	111.80
2	7	170	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	E	147	LEU	CB-CG-CD2	-5.65	101.40	111.00
2	3	57	ALA	N-CA-C	-5.63	95.80	111.00
2	3	101	TYR	CB-CG-CD1	5.63	124.38	121.00
1	C	84	ASP	CB-CG-OD1	5.62	123.36	118.30
2	6	162	ASP	CB-CA-C	-5.62	99.16	110.40
2	1	187	ASP	CB-CG-OD1	5.62	123.35	118.30
1	G	220	THR	N-CA-CB	5.61	120.96	110.30
1	A	205	VAL	N-CA-C	-5.61	95.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	211	PHE	CB-CG-CD1	-5.61	116.87	120.80
1	G	208	ASN	N-CA-CB	5.60	120.69	110.60
1	C	219	ARG	N-CA-CB	5.60	120.67	110.60
1	D	84	ASP	CB-CG-OD1	-5.60	113.26	118.30
2	4	192	THR	CA-CB-CG2	5.60	120.24	112.40
1	F	138	ILE	CA-CB-CG1	5.59	121.63	111.00
2	1	21	ASP	CB-CG-OD1	-5.59	113.26	118.30
2	4	88	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	220	THR	CA-CB-CG2	-5.59	104.58	112.40
2	1	80	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	F	33	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	180	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	D	196	MET	CG-SD-CE	-5.58	91.27	100.20
1	F	126	TYR	N-CA-C	-5.58	95.93	111.00
1	G	80	GLY	CA-C-O	5.58	130.64	120.60
1	E	130	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	123	TYR	CD1-CE1-CZ	5.57	124.82	119.80
1	D	238	GLU	CB-CA-C	-5.56	99.27	110.40
1	G	52	LYS	C-N-CA	5.56	135.60	121.70
2	2	123	TYR	CG-CD1-CE1	-5.56	116.85	121.30
2	3	91	ALA	CB-CA-C	-5.56	101.76	110.10
1	E	239	ARG	CD-NE-CZ	5.55	131.37	123.60
1	B	46	VAL	CB-CA-C	5.55	121.94	111.40
2	5	42	ALA	CB-CA-C	-5.55	101.78	110.10
1	E	29	GLU	O-C-N	-5.54	113.83	122.70
2	1	158	GLU	N-CA-CB	5.54	120.57	110.60
2	5	132	ILE	CG1-CB-CG2	-5.53	99.23	111.40
2	7	108	VAL	CB-CA-C	5.53	121.91	111.40
1	F	230	LYS	CA-C-O	-5.53	108.48	120.10
1	B	135	SER	N-CA-CB	5.53	118.79	110.50
1	E	174	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	F	81	LEU	CB-CG-CD1	5.52	120.38	111.00
1	B	175	PHE	N-CA-CB	-5.51	100.68	110.60
2	7	111	LEU	N-CA-C	-5.51	96.12	111.00
1	A	103	TYR	CB-CG-CD2	5.51	124.30	121.00
2	2	198	GLN	N-CA-C	-5.50	96.14	111.00
2	4	51	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	5	112	ILE	N-CA-C	-5.50	96.14	111.00
2	7	199	TYR	CZ-CE2-CD2	-5.50	114.85	119.80
1	A	93	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	B	221	PHE	CB-CG-CD1	-5.50	116.95	120.80
2	3	46	TYR	CD1-CE1-CZ	-5.50	114.85	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4	199	TYR	CG-CD2-CE2	-5.50	116.90	121.30
1	E	148	TYR	CB-CG-CD2	5.50	124.30	121.00
1	B	145	PRO	N-CA-CB	5.49	109.89	103.30
2	5	134	GLU	N-CA-CB	5.49	120.48	110.60
1	G	228	GLU	OE1-CD-OE2	5.49	129.88	123.30
2	2	170	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	76	ALA	N-CA-CB	5.48	117.78	110.10
1	D	227	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	B	148	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	G	100	ARG	CD-NE-CZ	-5.48	115.92	123.60
2	7	198	GLN	N-CA-C	-5.48	96.22	111.00
2	4	16	GLY	N-CA-C	-5.47	99.42	113.10
2	7	212	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	2	123	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	5	188	VAL	CA-CB-CG2	5.47	119.11	110.90
1	E	71	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	174	PHE	CB-CG-CD2	-5.46	116.98	120.80
2	4	33	MET	C-N-CA	5.46	133.76	122.30
2	2	56	THR	C-N-CA	5.46	135.34	121.70
2	2	45	ILE	N-CA-C	-5.45	96.28	111.00
2	3	30	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	2	137	ILE	CA-CB-CG1	5.44	121.34	111.00
2	3	199	TYR	CG-CD1-CE1	-5.44	116.95	121.30
1	D	76	ALA	N-CA-CB	5.43	117.71	110.10
1	F	213	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	1	25	MET	CA-CB-CG	5.43	122.52	113.30
1	E	28	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	196	MET	CG-SD-CE	-5.42	91.52	100.20
1	G	100	ARG	NH1-CZ-NH2	-5.42	113.43	119.40
2	3	46	TYR	CB-CG-CD1	5.42	124.25	121.00
1	E	119	PHE	CB-CG-CD2	-5.42	117.00	120.80
2	6	16	GLY	N-CA-C	-5.42	99.55	113.10
1	D	103	TYR	CG-CD2-CE2	-5.42	116.97	121.30
2	2	212	ARG	N-CA-CB	5.42	120.35	110.60
2	3	139	ALA	O-C-N	-5.42	114.03	122.70
1	D	59	LEU	CB-CA-C	-5.42	99.91	110.20
2	2	173	TYR	CB-CG-CD1	5.41	124.25	121.00
1	D	219	ARG	N-CA-CB	5.40	120.32	110.60
1	F	22	PHE	CB-CG-CD2	-5.40	117.02	120.80
2	6	77	TYR	CA-CB-CG	5.40	123.66	113.40
2	5	196	PHE	CB-CG-CD2	-5.39	117.02	120.80
1	B	31	VAL	O-C-N	-5.39	114.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	219	ARG	N-CA-CB	5.38	120.29	110.60
1	G	50	ALA	N-CA-CB	5.38	117.63	110.10
2	1	168	ALA	N-CA-CB	5.38	117.63	110.10
2	6	32	THR	CA-CB-CG2	-5.38	104.87	112.40
1	F	60	GLU	CB-CA-C	5.37	121.15	110.40
2	5	80	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	4	106	TYR	N-CA-CB	5.37	120.26	110.60
1	A	62	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	G	93	ARG	CG-CD-NE	-5.36	100.54	111.80
2	2	80	ARG	NE-CZ-NH1	-5.35	117.63	120.30
2	4	55	THR	CA-CB-CG2	-5.34	104.92	112.40
2	6	82	GLU	N-CA-CB	5.34	120.22	110.60
2	2	60	VAL	CB-CA-C	-5.34	101.26	111.40
2	2	23	VAL	CB-CA-C	-5.33	101.26	111.40
2	5	67	ALA	N-CA-CB	5.33	117.56	110.10
1	D	130	ARG	NH1-CZ-NH2	-5.32	113.54	119.40
2	6	139	ALA	CB-CA-C	-5.32	102.12	110.10
2	3	36	PHE	CB-CG-CD2	5.32	124.52	120.80
2	5	198	GLN	N-CA-C	-5.32	96.63	111.00
2	7	160	GLY	O-C-N	-5.32	114.19	122.70
2	2	103	TYR	CG-CD2-CE2	5.31	125.55	121.30
2	5	32	THR	N-CA-C	-5.31	96.66	111.00
2	2	104	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	E	105	GLU	N-CA-C	-5.31	96.67	111.00
2	2	135	LYS	C-N-CA	5.30	134.95	121.70
1	C	181	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	G	217	ASP	CB-CG-OD1	5.30	123.07	118.30
2	7	60	VAL	CA-CB-CG1	5.29	118.84	110.90
1	B	186	ASP	N-CA-CB	5.29	120.12	110.60
1	D	15	PHE	CB-CG-CD2	5.29	124.50	120.80
2	4	197	TYR	CG-CD1-CE1	-5.29	117.07	121.30
2	5	87	VAL	CA-CB-CG2	5.28	118.81	110.90
1	E	228	GLU	N-CA-CB	5.27	120.09	110.60
1	G	213	TYR	CG-CD2-CE2	5.27	125.52	121.30
1	A	100	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	E	60	GLU	OE1-CD-OE2	5.27	129.62	123.30
2	2	126	ASP	CB-CG-OD2	-5.26	113.57	118.30
2	5	101	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	D	159	TYR	CB-CG-CD1	5.25	124.15	121.00
2	2	119	GLY	N-CA-C	-5.25	99.96	113.10
1	D	48	LEU	CB-CA-C	-5.25	100.23	110.20
2	5	88	ARG	NH1-CZ-NH2	-5.24	113.64	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	220	THR	N-CA-C	-5.23	96.87	111.00
2	1	52	MET	CG-SD-CE	-5.21	91.86	100.20
1	A	40	ILE	N-CA-C	-5.21	96.93	111.00
1	B	118	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	106	PRO	N-CD-CG	5.21	111.01	103.20
2	7	112	ILE	N-CA-C	-5.21	96.95	111.00
1	C	149	GLU	N-CA-C	-5.20	96.95	111.00
2	5	88	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	194	VAL	CA-CB-CG2	-5.20	103.10	110.90
1	G	135	SER	N-CA-C	-5.20	96.97	111.00
1	B	46	VAL	O-C-N	5.20	131.01	122.70
1	F	108	THR	CA-CB-CG2	-5.19	105.13	112.40
1	E	118	ASP	N-CA-CB	5.19	119.93	110.60
1	C	113	ALA	CB-CA-C	5.18	117.88	110.10
1	G	181	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	194	VAL	CA-CB-CG1	5.18	118.67	110.90
1	C	68	TYR	CG-CD2-CE2	5.18	125.45	121.30
1	D	241	ARG	CG-CD-NE	-5.18	100.92	111.80
1	G	241	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	E	127	GLY	O-C-N	-5.18	114.39	123.20
2	4	115	ILE	C-N-CA	5.18	134.65	121.70
1	A	69	LYS	CD-CE-NZ	-5.18	99.79	111.70
2	3	199	TYR	CB-CG-CD2	5.18	124.11	121.00
1	C	88	LEU	O-C-N	-5.17	114.43	122.70
2	4	139	ALA	CB-CA-C	-5.17	102.34	110.10
1	F	163	ALA	N-CA-CB	5.17	117.33	110.10
2	1	82	GLU	N-CA-CB	5.17	119.90	110.60
1	G	30	ALA	N-CA-CB	5.16	117.33	110.10
1	E	81	LEU	O-C-N	5.16	130.96	122.70
1	G	135	SER	N-CA-CB	5.15	118.23	110.50
2	2	77	TYR	CB-CG-CD2	-5.15	117.91	121.00
2	3	136	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	D	156	LEU	N-CA-C	-5.15	97.11	111.00
2	2	153	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	7	173	TYR	CZ-CE2-CD2	5.13	124.42	119.80
1	E	68	TYR	CD1-CG-CD2	5.13	123.54	117.90
1	G	123	TYR	CD1-CG-CD2	-5.13	112.26	117.90
1	G	144	VAL	N-CA-C	-5.12	97.16	111.00
2	7	56	THR	CA-CB-CG2	-5.12	105.23	112.40
2	6	139	ALA	N-CA-CB	5.12	117.27	110.10
2	4	67	ALA	CB-CA-C	-5.12	102.42	110.10
1	C	166	MET	N-CA-CB	5.12	119.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	12	ILE	CA-CB-CG2	-5.11	100.68	110.90
1	D	61	ALA	C-N-CA	5.11	134.47	121.70
2	2	49	ALA	N-CA-C	-5.11	97.21	111.00
2	2	155	PHE	CB-CG-CD1	5.11	124.38	120.80
2	4	195	GLU	N-CA-CB	5.11	119.79	110.60
2	7	140	THR	O-C-N	-5.10	114.52	123.20
2	3	21	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	241	ARG	NE-CZ-NH2	5.10	122.85	120.30
2	1	63	ALA	CB-CA-C	-5.09	102.46	110.10
1	C	20	ARG	CG-CD-NE	-5.09	101.11	111.80
2	6	122	ILE	N-CA-CB	5.09	122.51	110.80
2	4	124	SER	N-CA-CB	5.09	118.13	110.50
2	5	18	VAL	CG1-CB-CG2	5.08	119.04	110.90
1	E	220	THR	N-CA-C	-5.08	97.28	111.00
1	A	90	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	204	LEU	CB-CA-C	-5.08	100.55	110.20
2	5	60	VAL	CA-CB-CG1	-5.08	103.28	110.90
1	D	185	PHE	CB-CG-CD1	-5.08	117.25	120.80
2	1	190	LYS	N-CA-C	-5.08	97.29	111.00
1	E	15	PHE	CG-CD2-CE2	5.07	126.38	120.80
1	E	105	GLU	N-CA-CB	5.07	119.72	110.60
1	C	47	ILE	N-CA-CB	5.07	122.46	110.80
2	6	174	SER	N-CA-CB	5.07	118.10	110.50
2	4	103	TYR	CD1-CG-CD2	5.06	123.47	117.90
1	C	219	ARG	CD-NE-CZ	5.06	130.68	123.60
1	G	232	TYR	CG-CD1-CE1	5.06	125.35	121.30
1	G	142	ASP	CB-CG-OD2	5.06	122.85	118.30
2	1	42	ALA	N-CA-CB	5.06	117.18	110.10
2	4	29	LYS	N-CA-CB	5.05	119.70	110.60
1	C	144	VAL	N-CA-C	-5.05	97.36	111.00
2	1	15	VAL	CA-CB-CG1	-5.05	103.32	110.90
2	1	167	LEU	CA-C-O	-5.05	109.49	120.10
1	G	123	TYR	CG-CD2-CE2	5.05	125.34	121.30
2	3	101	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	E	137	LEU	N-CA-CB	5.04	120.48	110.40
2	3	153	ASP	CB-CG-OD1	5.04	122.83	118.30
1	G	117	CYS	CA-CB-SG	-5.03	104.95	114.00
2	1	199	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	3	169	VAL	CG1-CB-CG2	-5.03	102.86	110.90
1	C	30	ALA	N-CA-CB	5.02	117.13	110.10
2	4	161	VAL	CG1-CB-CG2	5.02	118.93	110.90
1	B	40	ILE	N-CA-CB	5.02	122.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	232	TYR	N-CA-CB	5.01	119.62	110.60
1	C	235	ARG	CB-CA-C	-5.01	100.39	110.40
1	A	68	TYR	CB-CG-CD2	5.00	124.00	121.00

There are no chirality outliers.

All (115) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	106	TYR	Sidechain
2	1	148	TYR	Sidechain
2	1	178	ARG	Sidechain
2	1	197	TYR	Sidechain
2	1	80	ARG	Sidechain
2	2	101	TYR	Sidechain
2	2	139	ALA	Mainchain,Peptide
2	2	140	THR	Mainchain
2	2	170	ARG	Sidechain
2	2	199	TYR	Sidechain
2	2	68	ARG	Sidechain
2	2	80	ARG	Sidechain
2	3	123	TYR	Sidechain
2	3	195	GLU	Peptide
2	3	30	ARG	Sidechain
2	3	68	ARG	Sidechain
2	4	101	TYR	Sidechain
2	4	103	TYR	Sidechain
2	4	106	TYR	Sidechain
2	4	139	ALA	Mainchain,Peptide
2	4	140	THR	Mainchain
2	4	173	TYR	Sidechain
2	4	51	ARG	Sidechain
2	4	83	ARG	Sidechain
2	5	101	TYR	Sidechain
2	5	102	ARG	Sidechain
2	5	140	THR	Mainchain
2	5	148	TYR	Sidechain
2	5	170	ARG	Sidechain
2	5	178	ARG	Sidechain
2	5	195	GLU	Peptide
2	5	211	PHE	Sidechain
2	5	36	PHE	Sidechain
2	5	80	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	6	123	TYR	Sidechain
2	6	139	ALA	Peptide
2	6	140	THR	Mainchain
2	6	148	TYR	Sidechain
2	6	170	ARG	Sidechain
2	6	178	ARG	Sidechain
2	6	65	PHE	Sidechain
2	6	83	ARG	Sidechain
2	7	103	TYR	Sidechain
2	7	106	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	140	THR	Mainchain
2	7	212	ARG	Sidechain
2	7	81	ARG	Sidechain
1	A	103	TYR	Sidechain
1	A	148	TYR	Sidechain
1	A	175	PHE	Sidechain
1	A	221	PHE	Sidechain
1	A	26	TYR	Sidechain
1	A	28	ARG	Sidechain
1	A	86	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	179	TYR	Sidechain
1	B	220	THR	Peptide
1	B	239	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	68	TYR	Sidechain
1	C	119	PHE	Sidechain
1	C	130	ARG	Sidechain
1	C	132	PHE	Sidechain
1	C	175	PHE	Sidechain
1	C	181	ASP	Peptide
1	C	213	TYR	Sidechain
1	C	220	THR	Peptide
1	C	221	PHE	Sidechain
1	C	232	TYR	Sidechain
1	C	33	ARG	Sidechain
1	D	123	TYR	Sidechain
1	D	179	TYR	Sidechain
1	D	182	ASP	Peptide
1	D	20	ARG	Sidechain
1	D	22	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	D	220	THR	Mainchain,Peptide
1	D	224	VAL	Peptide
1	D	37	ALA	Peptide
1	D	86	ARG	Sidechain
1	E	103	TYR	Sidechain
1	E	148	TYR	Sidechain
1	E	179	TYR	Sidechain
1	E	185	PHE	Sidechain
1	E	213	TYR	Sidechain
1	E	215	LYS	Mainchain
1	E	220	THR	Peptide
1	E	224	VAL	Peptide
1	E	239	ARG	Sidechain
1	E	241	ARG	Sidechain
1	E	53	ARG	Sidechain
1	F	103	TYR	Sidechain
1	F	148	TYR	Sidechain
1	F	20	ARG	Sidechain
1	F	213	TYR	Sidechain
1	F	220	THR	Peptide
1	F	224	VAL	Mainchain
1	F	28	ARG	Sidechain
1	F	86	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	100	ARG	Sidechain
1	G	126	TYR	Sidechain
1	G	130	ARG	Sidechain
1	G	182	ASP	Peptide
1	G	213	TYR	Sidechain
1	G	220	THR	Peptide
1	G	26	TYR	Sidechain
1	G	37	ALA	Peptide
1	G	52	LYS	Peptide
1	G	53	ARG	Mainchain,Peptide
1	G	54	VAL	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	1850	0	1890	13	0
1	B	1850	0	1890	8	0
1	C	1850	0	1890	9	0
1	D	1850	0	1890	9	0
1	E	1850	0	1890	6	0
1	F	1850	0	1890	4	0
1	G	1850	0	1890	11	0
2	1	1553	0	1579	6	0
2	2	1553	0	1580	7	0
2	3	1553	0	1580	11	0
2	4	1553	0	1580	8	0
2	5	1553	0	1580	47	0
2	6	1553	0	1580	8	0
2	7	1553	0	1580	9	0
All	All	23821	0	24289	144	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 3.

All (144) 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:CD2	2:5:211:PHE:CG	2.18	1.31
2:5:170:ARG:HD3	2:5:211:PHE:CD1	1.66	1.29
2:5:211:PHE:CD2	2:5:211:PHE:CE2	2.19	1.29
2:5:211:PHE:CE1	2:5:211:PHE:CZ	2.20	1.27
2:5:211:PHE:CD1	2:5:211:PHE:CE1	2.22	1.27
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.19	1.24
2:5:211:PHE:CE2	2:5:211:PHE:CZ	2.26	1.22
2:5:170:ARG:NH1	2:5:211:PHE:CD1	2.08	1.21
2:5:170:ARG:HG2	2:5:211:PHE:CE1	1.79	1.18
2:5:170:ARG:CD	2:5:211:PHE:CD1	2.27	1.18
2:5:170:ARG:NE	2:5:211:PHE:CD2	2.16	1.13
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.21	1.08
2:5:170:ARG:NE	2:5:211:PHE:CE2	2.22	1.08
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.22	1.06
2:5:170:ARG:CD	2:5:211:PHE:CG	2.41	1.04
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.42	1.02
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.42	1.02
2:5:170:ARG:NE	2:5:211:PHE:CG	2.30	1.00
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.45	0.98
2:5:170:ARG:HD3	2:5:211:PHE:CG	2.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:170:ARG:CG	2:5:211:PHE:CD1	2.48	0.96
2:5:170:ARG:NH2	2:5:211:PHE:CE2	2.33	0.96
2:5:166:GLU:OE1	2:5:211:PHE:CE1	2.18	0.95
2:1:40:LYS:HE2	2:2:137:ILE:HD11	1.51	0.92
2:5:170:ARG:HG2	2:5:211:PHE:CD1	2.05	0.91
2:5:170:ARG:CG	2:5:211:PHE:CE1	2.53	0.91
2:5:170:ARG:NH2	2:5:211:PHE:CZ	2.38	0.91
2:5:137:ILE:HD11	2:5:155:PHE:CD1	2.06	0.90
2:5:166:GLU:OE1	2:5:211:PHE:HE1	1.54	0.90
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.63	0.80
2:2:137:ILE:HD12	2:2:137:ILE:H	1.46	0.79
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.52	0.76
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.54	0.76
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.69	0.75
2:5:115:ILE:HG21	2:5:193:GLU:HG2	1.70	0.74
1:E:70:ILE:HG21	1:E:112:LEU:HD21	1.73	0.71
1:F:125:GLN:O	1:G:129:VAL:HG23	1.91	0.70
2:1:45:ILE:HD11	2:1:189:VAL:HG22	1.75	0.69
2:5:170:ARG:CD	2:5:211:PHE:CE1	2.83	0.61
1:A:124:THR:HG23	1:B:130:ARG:HH21	1.65	0.61
2:2:17:LEU:HA	2:2:137:ILE:HG22	1.83	0.60
2:5:137:ILE:HD11	2:5:155:PHE:CG	2.37	0.59
1:C:163:ALA:HB2	1:C:171:VAL:HG11	1.84	0.58
2:7:29:LYS:HE3	2:7:201:PRO:HD3	1.85	0.58
1:B:121:GLN:CG	1:C:83:ALA:HB1	2.34	0.58
1:B:38:ILE:HG23	1:B:49:ILE:HG23	1.86	0.57
2:6:43:LYS:HE2	2:6:198:GLN:HE22	1.69	0.57
1:D:163:ALA:HB2	1:D:171:VAL:HG11	1.87	0.56
2:2:137:ILE:HD12	2:2:137:ILE:N	2.18	0.56
2:3:21:ASP:HB2	2:3:161:VAL:HG13	1.89	0.55
1:A:38:ILE:HG23	1:A:49:ILE:HB	1.87	0.55
1:A:70:ILE:HG21	1:A:112:LEU:HD21	1.87	0.54
2:4:65:PHE:CE2	2:4:69:ILE:HD11	2.42	0.54
1:B:121:GLN:HG3	1:C:83:ALA:HB1	1.88	0.54
2:5:115:ILE:HG21	2:5:193:GLU:CG	2.38	0.53
1:C:49:ILE:HG23	1:C:211:VAL:HG22	1.91	0.53
2:5:211:PHE:CG	2:5:211:PHE:CD1	2.97	0.53
2:1:137:ILE:HD12	2:1:151:LEU:HG	1.90	0.52
1:G:171:VAL:HG13	1:G:195:ALA:HB1	1.91	0.52
1:E:211:VAL:HG21	1:E:229:LEU:HD11	1.92	0.52
1:F:88:LEU:HD21	1:F:120:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.77	0.51
2:7:60:VAL:O	2:7:63:ALA:HB3	2.10	0.51
2:1:40:LYS:HE2	2:2:137:ILE:CD1	2.31	0.50
2:4:155:PHE:CE1	2:4:159:ILE:HG21	2.47	0.50
1:C:47:ILE:HD13	1:C:189:MET:HA	1.94	0.50
1:C:108:THR:HG21	2:4:83:ARG:HH22	1.77	0.50
2:5:166:GLU:CD	2:5:211:PHE:CZ	2.85	0.49
2:2:66:LEU:HD23	2:2:110:LEU:HD21	1.95	0.49
2:3:137:ILE:HG23	2:3:151:LEU:HD23	1.94	0.48
2:1:112:ILE:HD12	2:1:125:ILE:HD13	1.95	0.48
1:G:151:ASP:HB2	1:G:155:ALA:HB3	1.96	0.48
2:5:23:VAL:HG23	2:5:115:ILE:HD11	1.96	0.48
2:7:154:ARG:HB2	2:7:167:LEU:HD13	1.96	0.48
2:7:137:ILE:HD11	2:7:155:PHE:CD1	2.49	0.48
1:E:54:VAL:HG23	1:E:59:LEU:HB3	1.96	0.48
1:B:92:ALA:HB2	1:B:116:ILE:HG21	1.96	0.48
1:C:70:ILE:HG21	1:C:112:LEU:HD21	1.94	0.48
1:D:47:ILE:HD11	1:D:185:PHE:CE1	2.49	0.47
2:4:12:THR:N	2:4:182:SER:HG	2.12	0.47
1:D:233:VAL:HG12	1:D:237:ASN:ND2	2.30	0.47
1:A:40:ILE:CD1	1:A:192:GLY:HA3	2.45	0.47
2:5:170:ARG:HA	2:5:211:PHE:CD1	2.49	0.47
1:A:49:ILE:HG12	1:A:211:VAL:HG13	1.96	0.47
2:3:54:MET:HE2	2:3:112:ILE:HD11	1.96	0.47
2:6:186:ILE:HD11	2:6:204:VAL:HG11	1.96	0.47
1:G:190:VAL:O	1:G:194:VAL:HG23	2.15	0.47
2:3:111:LEU:HD13	2:3:138:VAL:HG13	1.97	0.47
1:G:117:CYS:SG	1:G:150:THR:HG23	2.55	0.46
2:7:49:ALA:HB3	2:7:52:MET:SD	2.55	0.46
1:E:174:PHE:CD1	1:E:195:ALA:HB2	2.51	0.46
1:G:204:LEU:H	1:G:237:ASN:HD21	1.63	0.46
2:4:137:ILE:HG23	2:4:151:LEU:HD12	1.98	0.46
1:A:27:ALA:O	1:A:30:ALA:HB3	2.16	0.46
2:4:80:ARG:HD2	2:4:81:ARG:HH12	1.81	0.46
1:A:113:ALA:HB1	1:A:156:LEU:CD1	2.46	0.45
1:C:121:GLN:HE21	1:D:87:VAL:HG21	1.80	0.45
1:D:47:ILE:HD12	1:D:47:ILE:N	2.32	0.45
1:A:132:PHE:HB3	1:A:134:VAL:HG12	1.98	0.45
2:5:186:ILE:HG21	2:5:204:VAL:HG11	1.99	0.45
2:6:64:GLN:HG3	2:7:130:GLY:HA2	1.98	0.45
2:7:172:ILE:HB	2:7:186:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLU:O	1:E:220:THR:HG23	2.16	0.44
1:A:91:ARG:HA	1:A:94:ILE:HD12	1.99	0.44
1:A:113:ALA:HB1	1:A:156:LEU:HD11	1.99	0.43
2:6:125:ILE:HD12	2:6:125:ILE:N	2.33	0.43
1:B:195:ALA:HA	1:B:198:LEU:HD12	1.99	0.43
2:4:18:VAL:HB	2:4:136:ASP:HA	2.00	0.43
1:E:72:GLU:HB2	1:E:100:ARG:HH22	1.82	0.43
1:G:145:PRO:HG3	1:G:216:VAL:HG23	2.00	0.43
2:5:137:ILE:HD11	2:5:155:PHE:CE1	2.52	0.43
2:5:115:ILE:CG2	2:5:193:GLU:HG2	2.42	0.43
2:6:18:VAL:HB	2:6:136:ASP:HA	2.01	0.43
1:D:224:VAL:HG12	1:D:225:SER:H	1.82	0.43
2:3:137:ILE:HG23	2:3:151:LEU:CD2	2.49	0.43
1:A:36:THR:HB	1:A:167:GLY:H	1.84	0.43
1:B:121:GLN:HG2	1:C:83:ALA:HB1	2.00	0.42
1:G:145:PRO:HG3	1:G:216:VAL:CG2	2.49	0.42
2:3:45:ILE:HG12	2:3:55:THR:HG22	2.01	0.42
2:5:132:ILE:HG21	2:5:132:ILE:HD13	1.80	0.42
1:F:163:ALA:HB3	1:F:168:ARG:HA	2.01	0.42
2:7:12:THR:HG21	2:7:58:GLY:H	1.84	0.42
1:D:213:TYR:CE2	1:D:224:VAL:HG22	2.55	0.41
2:3:169:VAL:CG2	2:3:188:VAL:HG21	2.50	0.41
2:4:80:ARG:HD2	2:4:81:ARG:NH1	2.35	0.41
2:6:41:ALA:HB3	2:7:133:GLU:O	2.19	0.41
1:D:204:LEU:HD13	1:D:209:ILE:HD13	2.03	0.41
1:B:73:HIS:O	1:B:214:VAL:HG21	2.19	0.41
2:3:109:GLN:HG2	2:3:126:ASP:HA	2.02	0.41
2:6:84:LYS:HB3	2:6:84:LYS:HE3	1.92	0.41
1:A:12:ILE:HG23	1:G:14:VAL:CG1	2.49	0.41
1:A:121:GLN:O	1:A:124:THR:HG22	2.21	0.41
1:G:121:GLN:HE22	1:G:125:GLN:NE2	2.19	0.41
2:3:169:VAL:HG22	2:3:188:VAL:HG21	2.03	0.41
1:F:183:LEU:HD13	1:F:188:ALA:HA	2.02	0.41
1:G:156:LEU:HD12	1:G:156:LEU:HA	1.94	0.41
2:2:137:ILE:HD13	2:2:148:TYR:CE1	2.56	0.41
2:3:54:MET:CE	2:3:112:ILE:HD11	2.51	0.41
2:3:188:VAL:HG12	2:3:189:VAL:N	2.36	0.41
2:5:154:ARG:HB2	2:5:167:LEU:HD13	2.03	0.41
1:D:40:ILE:HD12	1:D:40:ILE:N	2.36	0.41
2:6:56:THR:HG21	2:6:63:ALA:HB1	2.03	0.40
2:1:48:ILE:HG21	2:1:90:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:54:MET:HE2	2:5:67:ALA:HB2	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	233/235 (99%)	220 (94%)	11 (5%)	2 (1%)	17	54
1	B	233/235 (99%)	219 (94%)	10 (4%)	4 (2%)	9	42
1	C	233/235 (99%)	217 (93%)	12 (5%)	4 (2%)	9	42
1	D	233/235 (99%)	219 (94%)	9 (4%)	5 (2%)	7	38
1	E	233/235 (99%)	212 (91%)	16 (7%)	5 (2%)	7	38
1	F	233/235 (99%)	221 (95%)	9 (4%)	3 (1%)	12	47
1	G	233/235 (99%)	215 (92%)	11 (5%)	7 (3%)	4	32
2	1	200/202 (99%)	186 (93%)	12 (6%)	2 (1%)	15	51
2	2	200/202 (99%)	185 (92%)	13 (6%)	2 (1%)	15	51
2	3	200/202 (99%)	183 (92%)	16 (8%)	1 (0%)	29	66
2	4	200/202 (99%)	188 (94%)	10 (5%)	2 (1%)	15	51
2	5	200/202 (99%)	183 (92%)	15 (8%)	2 (1%)	15	51
2	6	200/202 (99%)	184 (92%)	12 (6%)	4 (2%)	7	39
2	7	200/202 (99%)	183 (92%)	13 (6%)	4 (2%)	7	39
All	All	3031/3059 (99%)	2815 (93%)	169 (6%)	47 (2%)	13	43

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	ILE

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Mol	Chain	Res	Type
1	C	181	ASP
1	D	62	ASP
1	E	221	PHE
1	G	38	ILE
1	G	53	ARG
1	G	54	VAL
2	3	139	ALA
2	6	38	ALA
2	6	106	TYR
2	6	139	ALA
2	6	140	THR
2	7	41	ALA
1	B	73	HIS
1	C	221	PHE
1	D	38	ILE
1	D	183	LEU
1	E	34	GLY
1	F	125	GLN
1	F	221	PHE
1	G	55	GLY
1	G	221	PHE
2	2	83	ARG
1	A	143	GLU
1	B	221	PHE
1	C	143	GLU
2	2	40	LYS
2	4	35	ASN
2	7	133	GLU
2	7	136	ASP
1	B	178	GLU
1	D	73	HIS
1	D	143	GLU
1	E	143	GLU
1	G	143	GLU
2	4	154	ARG
2	5	133	GLU
1	B	38	ILE
1	E	62	ASP
1	F	64	ILE
2	1	21	ASP
2	7	43	LYS
2	1	136	ASP

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Mol	Chain	Res	Type
2	5	200	SER
1	A	34	GLY
1	G	225	SER
1	E	38	ILE

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	198/198 (100%)	190 (96%)	8 (4%)	31	60
1	B	198/198 (100%)	192 (97%)	6 (3%)	41	66
1	C	198/198 (100%)	189 (96%)	9 (4%)	27	57
1	D	198/198 (100%)	191 (96%)	7 (4%)	36	63
1	E	198/198 (100%)	188 (95%)	10 (5%)	24	55
1	F	198/198 (100%)	189 (96%)	9 (4%)	27	57
1	G	198/198 (100%)	190 (96%)	8 (4%)	31	60
2	1	164/164 (100%)	156 (95%)	8 (5%)	25	56
2	2	164/164 (100%)	155 (94%)	9 (6%)	21	53
2	3	164/164 (100%)	156 (95%)	8 (5%)	25	56
2	4	164/164 (100%)	159 (97%)	5 (3%)	41	66
2	5	164/164 (100%)	158 (96%)	6 (4%)	34	61
2	6	164/164 (100%)	153 (93%)	11 (7%)	16	47
2	7	164/164 (100%)	153 (93%)	11 (7%)	16	47
All	All	2534/2534 (100%)	2419 (96%)	115 (4%)	31	57

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	58	LEU
1	A	104	ASP

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Mol	Chain	Res	Type
1	A	121	GLN
1	A	177	LYS
1	A	182	ASP
1	A	196	MET
1	A	229	LEU
1	B	49	ILE
1	B	59	LEU
1	B	63	THR
1	B	121	GLN
1	B	213	TYR
1	B	217	ASP
1	C	22	PHE
1	C	60	GLU
1	C	71	ASP
1	C	81	LEU
1	C	84	ASP
1	C	182	ASP
1	C	203	GLU
1	C	226	PRO
1	C	229	LEU
1	D	121	GLN
1	D	169	ASN
1	D	174	PHE
1	D	177	LYS
1	D	182	ASP
1	D	196	MET
1	D	217	ASP
1	E	14	VAL
1	E	54	VAL
1	E	63	THR
1	E	66	LYS
1	E	108	THR
1	E	129	VAL
1	E	151	ASP
1	E	169	ASN
1	E	198	LEU
1	E	213	TYR
1	F	21	LEU
1	F	22	PHE
1	F	68	TYR
1	F	78	THR
1	F	81	LEU

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Mol	Chain	Res	Type
1	F	144	VAL
1	F	162	THR
1	F	218	ASP
1	F	229	LEU
1	G	14	VAL
1	G	20	ARG
1	G	38	ILE
1	G	40	ILE
1	G	57	LYS
1	G	59	LEU
1	G	65	GLU
1	G	181	ASP
2	1	27	THR
2	1	39	SER
2	1	120	LYS
2	1	128	ILE
2	1	136	ASP
2	1	170	ARG
2	1	182	SER
2	1	202	GLU
2	2	14	THR
2	2	28	GLU
2	2	33	MET
2	2	60	VAL
2	2	132	ILE
2	2	137	ILE
2	2	176	MET
2	2	179	ASP
2	2	194	ASP
2	3	17	LEU
2	3	39	SER
2	3	106	TYR
2	3	109	GLN
2	3	125	ILE
2	3	148	TYR
2	3	208	LEU
2	3	213	LYS
2	4	28	GLU
2	4	110	LEU
2	4	121	SER
2	4	148	TYR
2	4	161	VAL

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Mol	Chain	Res	Type
2	5	17	LEU
2	5	72	ILE
2	5	116	ASP
2	5	197	TYR
2	5	198	GLN
2	5	205	GLU
2	6	17	LEU
2	6	28	GLU
2	6	105	PRO
2	6	106	TYR
2	6	120	LYS
2	6	137	ILE
2	6	148	TYR
2	6	156	THR
2	6	184	ASP
2	6	201	PRO
2	6	202	GLU
2	7	17	LEU
2	7	28	GLU
2	7	72	ILE
2	7	96	ASN
2	7	109	GLN
2	7	128	ILE
2	7	132	ILE
2	7	161	VAL
2	7	178	ARG
2	7	198	GLN
2	7	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	125	GLN
1	A	169	ASN
1	B	121	GLN
1	C	23	GLN
1	C	237	ASN
1	D	169	ASN
1	E	23	GLN
1	E	125	GLN
1	E	237	ASN

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Mol	Chain	Res	Type
1	G	121	GLN
1	G	237	ASN
2	3	64	GLN
2	3	99	ASN
2	6	64	GLN
2	6	96	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

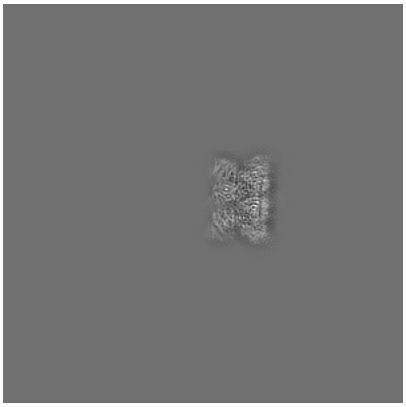
This section contains visualisations of the EMDB entry EMD-0211. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

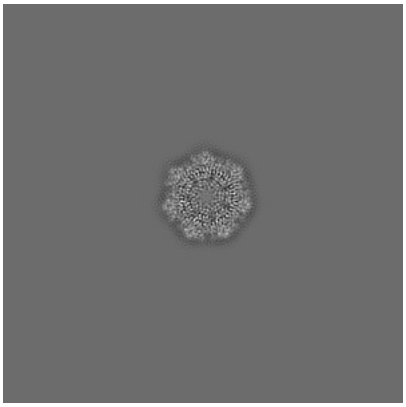
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

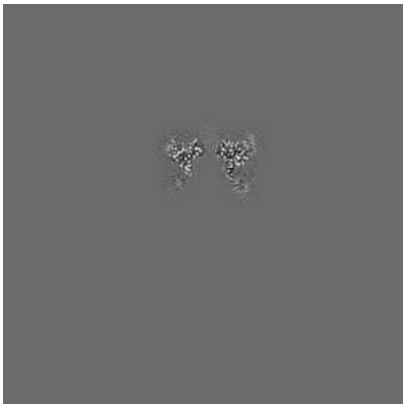


Z

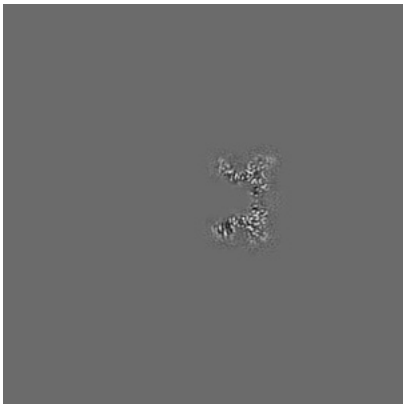
The images above show the map projected in three orthogonal directions.

6.2 Central slices

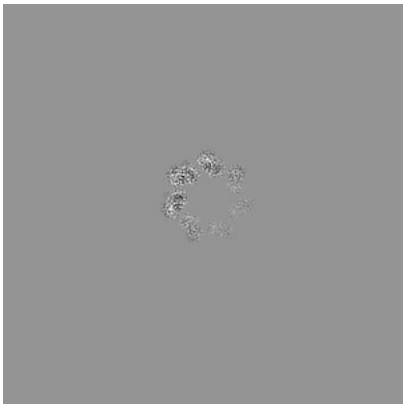
6.2.1 Primary map



X Index: 192



Y Index: 192

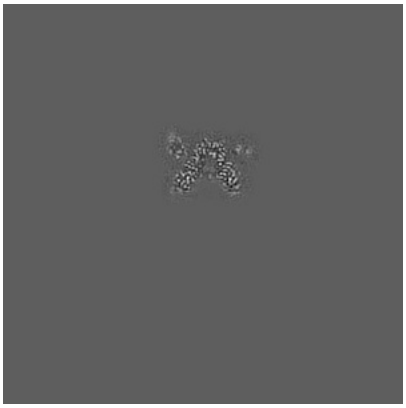


Z Index: 192

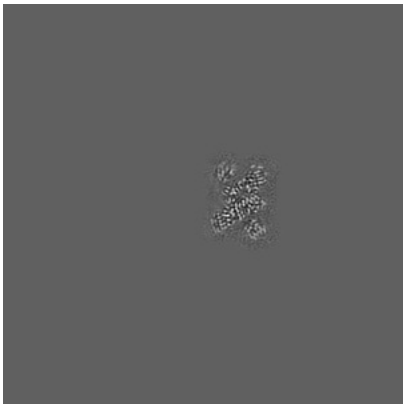
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

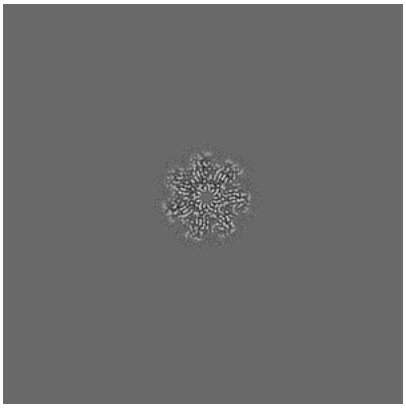
6.3.1 Primary map



X Index: 180



Y Index: 217

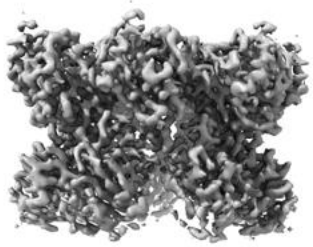


Z Index: 242

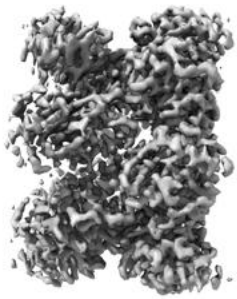
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

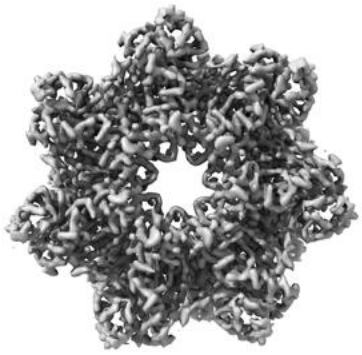
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

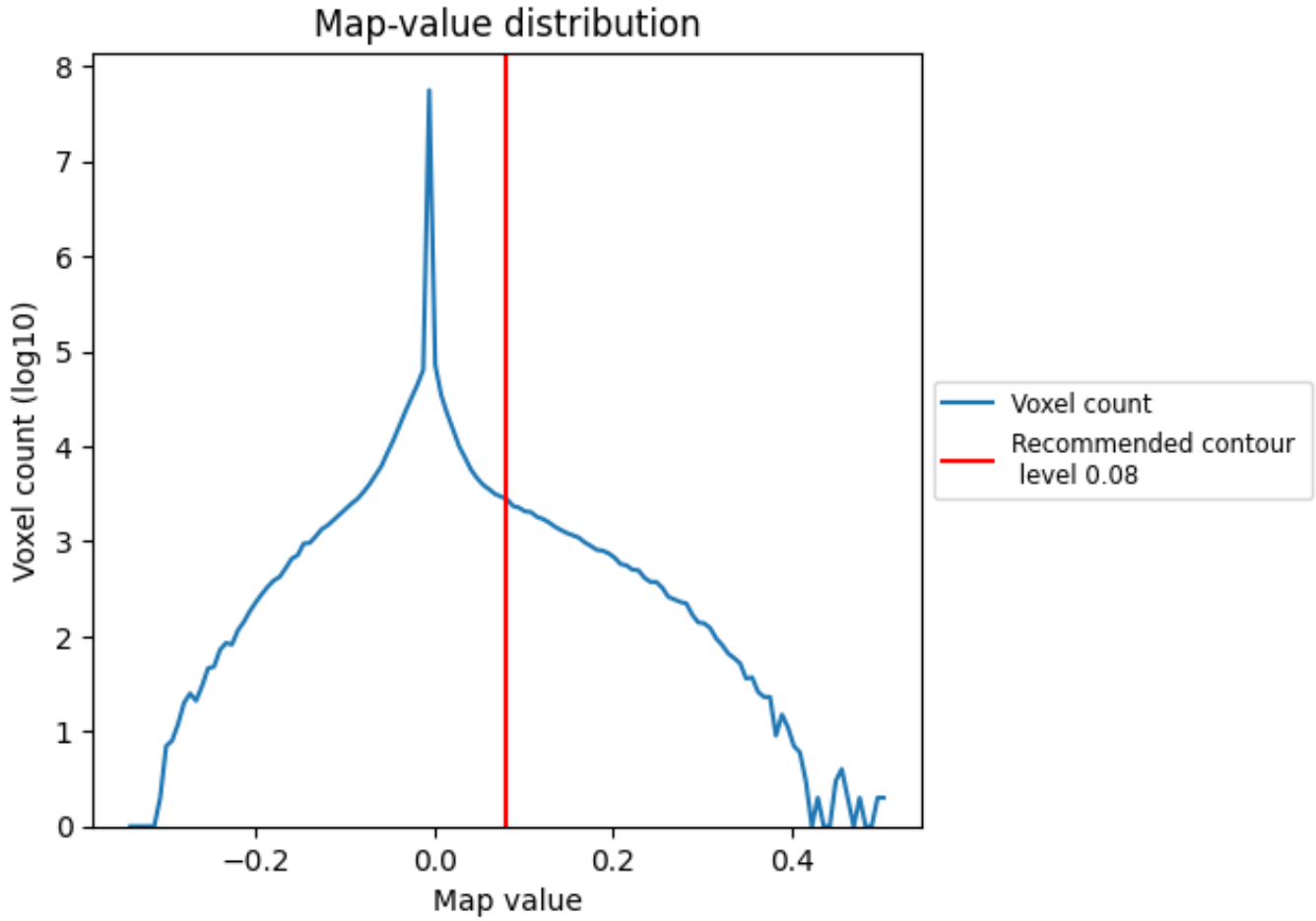
6.5 Mask visualisation (i)

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

7 Map analysis

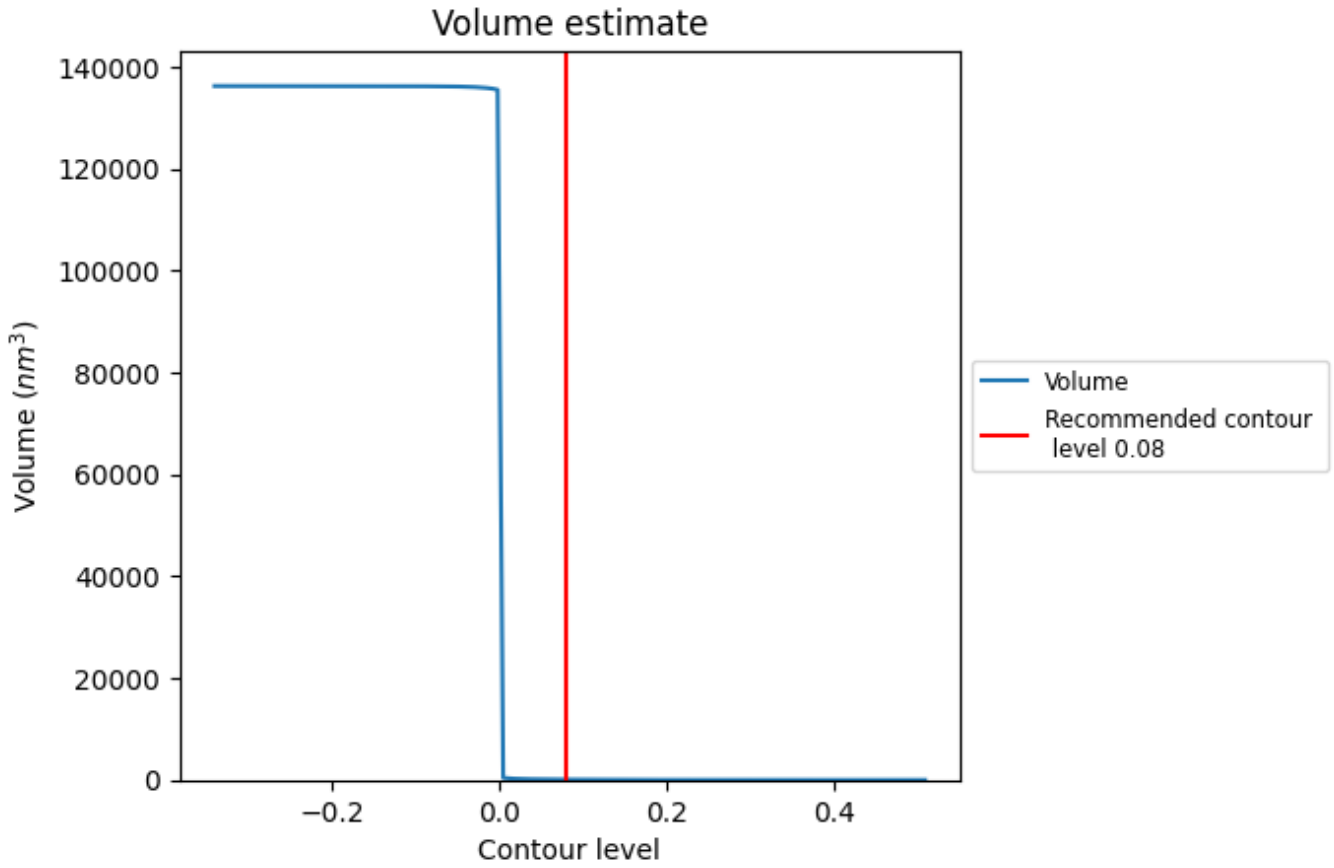
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

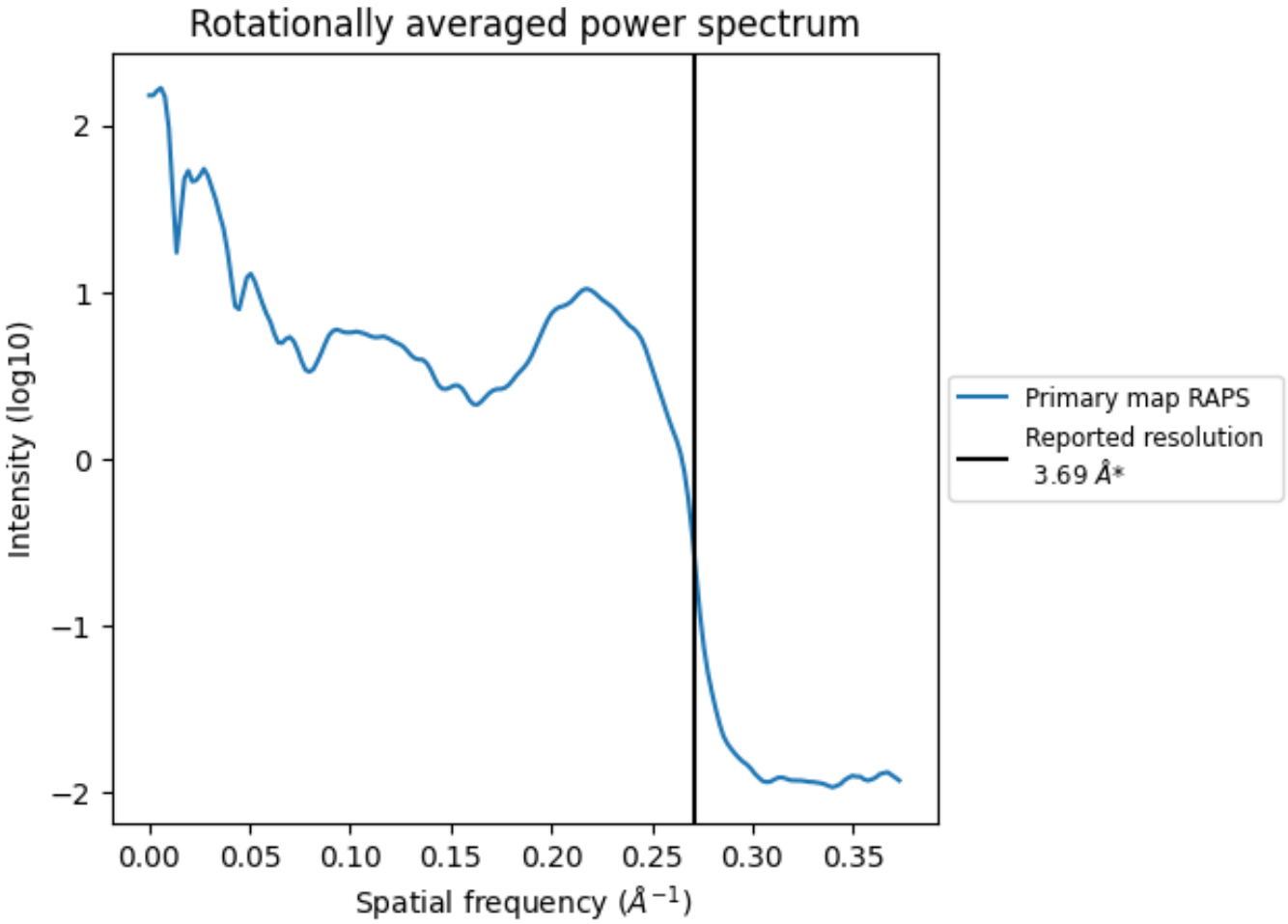
7.2 Volume estimate



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 74 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 0.271 Å^{-1}

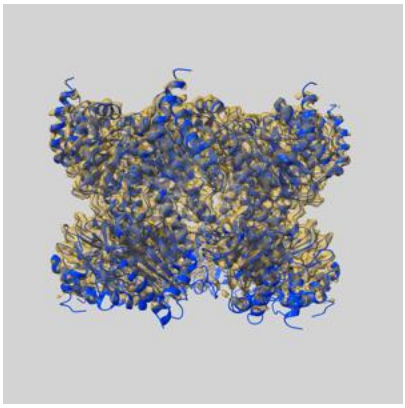
8 Fourier-Shell correlation

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

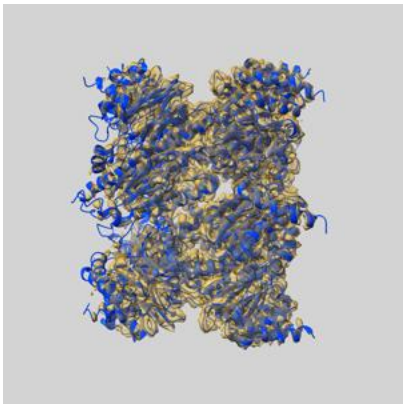
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0211 and PDB model 6HE7. Per-residue inclusion information can be found in section 3 on page 5.

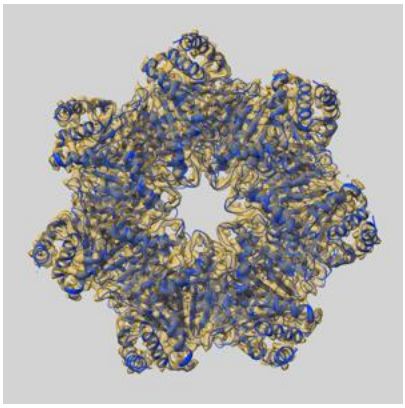
9.1 Map-model overlay



X



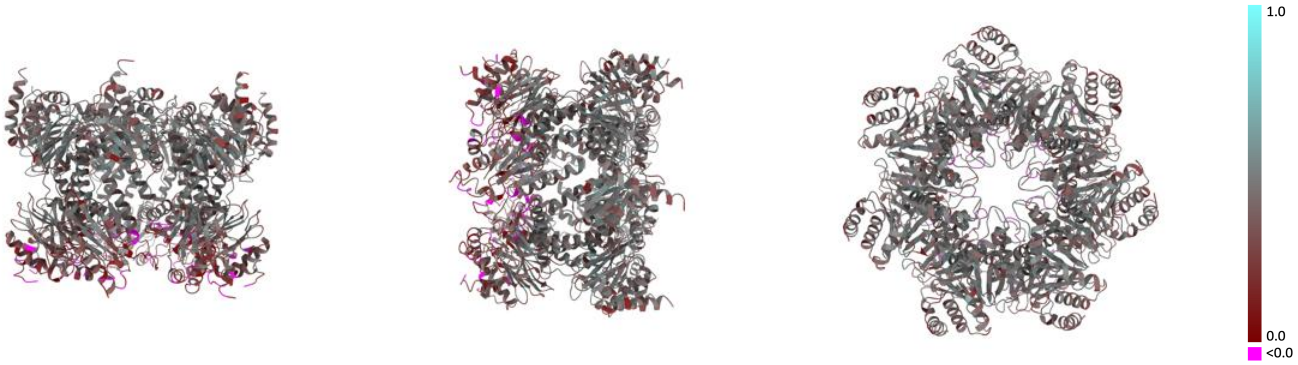
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

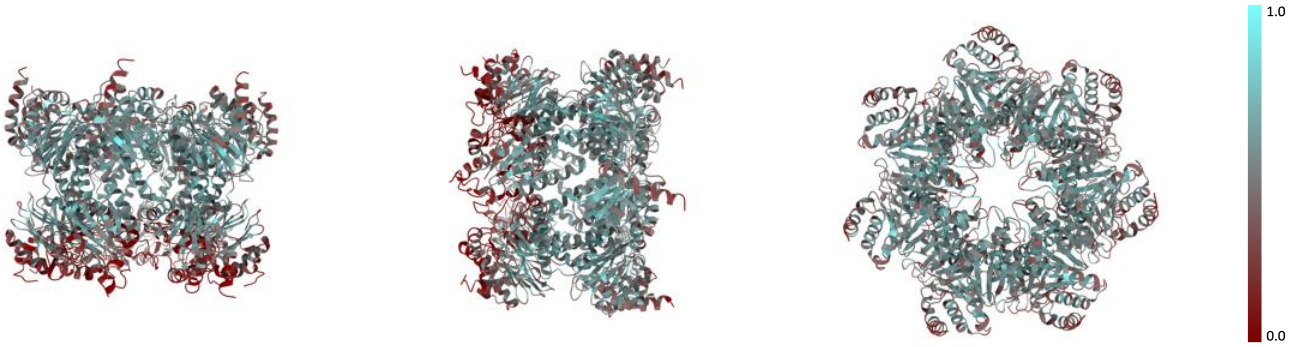
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

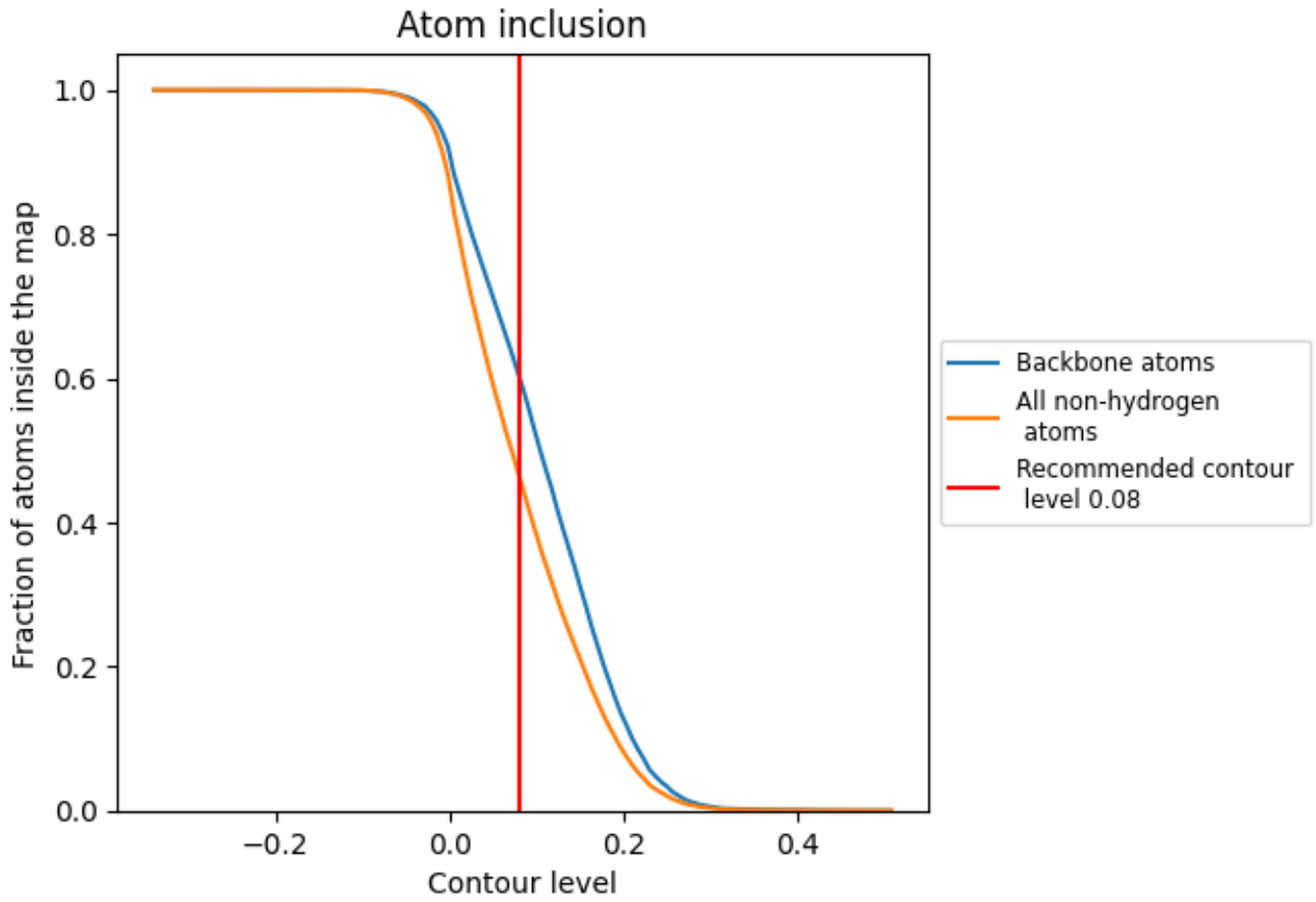
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 47% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4663	0.3830
1	0.3634	0.3250
2	0.3542	0.3070
3	0.3746	0.3410
4	0.3713	0.3320
5	0.3673	0.3160
6	0.3601	0.3270
7	0.3509	0.3140
A	0.5541	0.4330
B	0.5541	0.4340
C	0.5613	0.4340
D	0.5448	0.4350
E	0.5519	0.4380
F	0.5492	0.4250
G	0.5552	0.4350