Full wwPDB EM Validation Report

Feb 12, 2024 – 09:44 AM EST

PDB ID	:	3J1E
EMDB ID	:	EMD-5395
Title	:	Cryo-EM structure of 9-fold symmetric rATcpn-beta in apo state
Authors	:	Zhang, K.; Wang, L.; Liu, Y.X.; Wang, X.; Gao, B.; Hu, Z.J.; Ji, G.; Chan, K.Y.; Schulten, K.; Dong, Z.Y.; Sun, F.
Deposited on	:	2012-02-06
Resolution	:	8.30 Å(reported)
Based on initial model	:	3KO1

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:

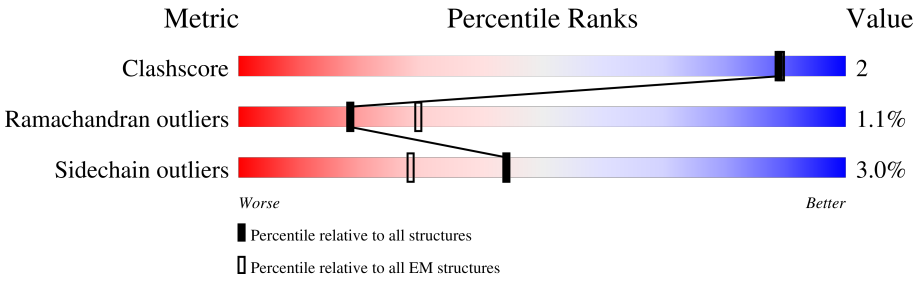
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 8.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	553	12% 70% 18% • 9%
1	B	553	11% 69% 19% • 9%
1	C	553	10% 70% 20% • 9%
1	D	553	11% 69% 19% • 9%
1	E	553	12% 73% 16% • 9%
1	F	553	12% 71% 18% • 9%
1	G	553	11% 71% 17% • 9%
1	H	553	12% 69% 20% • 9%

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Mol	Chain	Length	Quality of chain
1	I	553	11% 74% 15% • 9%
1	K	553	10% 73% 15% • 9%
1	L	553	10% 71% 17% • • 9%
1	M	553	12% 72% 18% • 9%
1	N	553	11% 71% 18% • 9%
1	O	553	11% 72% 17% • 9%
1	P	553	11% 69% 19% • 9%
1	Q	553	11% 72% 17% • 9%
1	R	553	12% 73% 17% • 9%
1	S	553	12% 68% 20% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 69282 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 Chaperonin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	B	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	C	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	D	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	E	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	F	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	G	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	H	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	I	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	K	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	L	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	M	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	N	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	O	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	P	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	Q	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	R	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		

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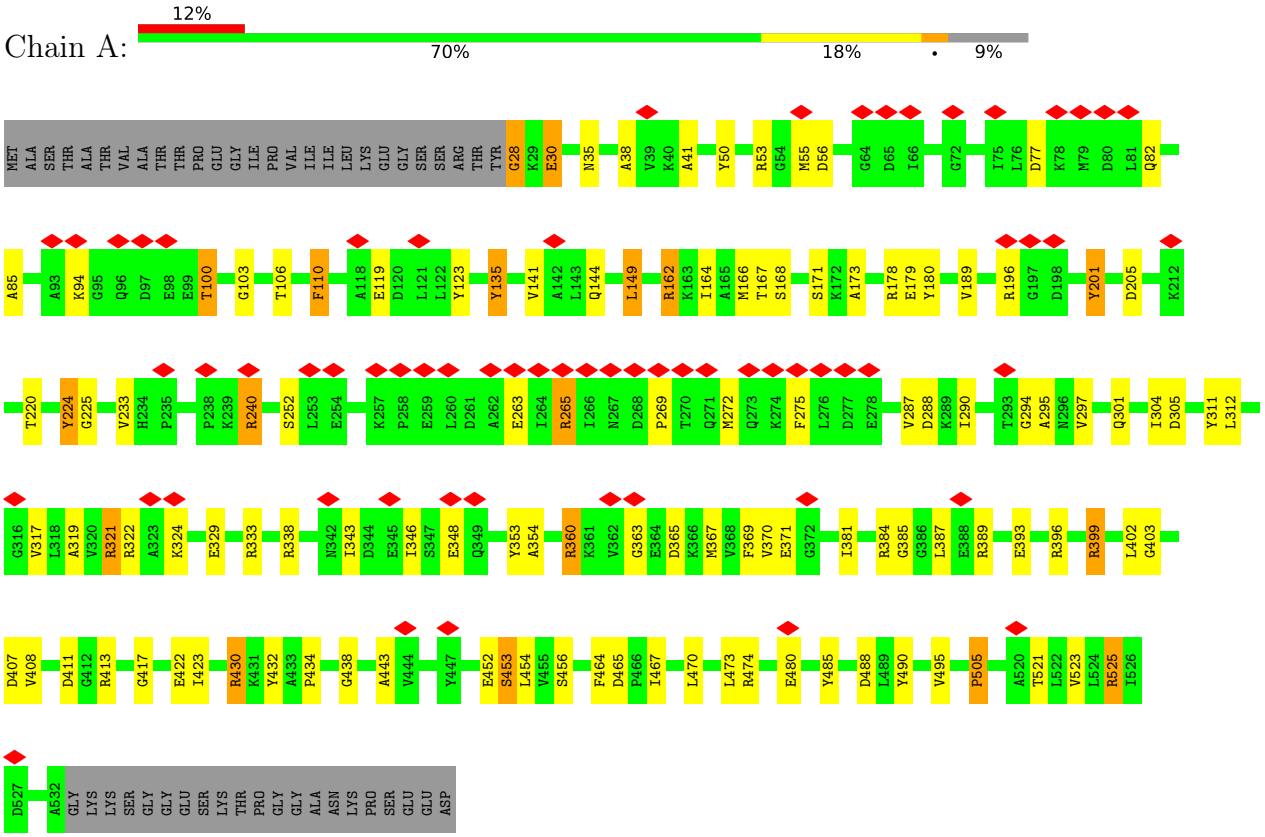
Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		

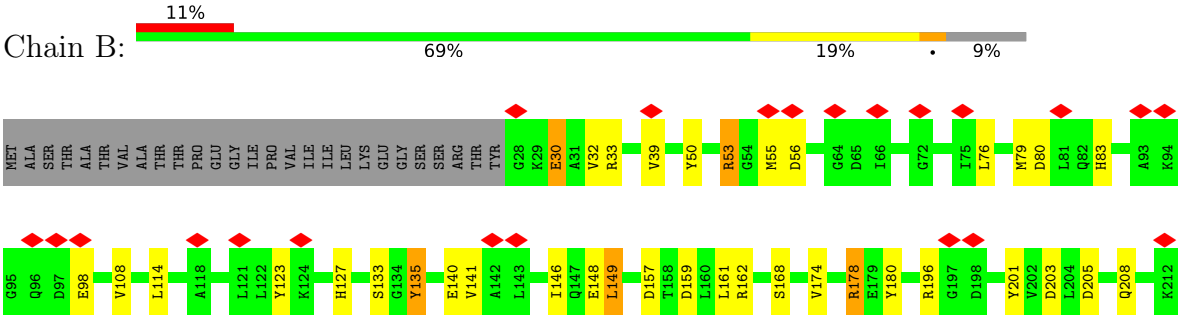
3 Residue-property plots (i)

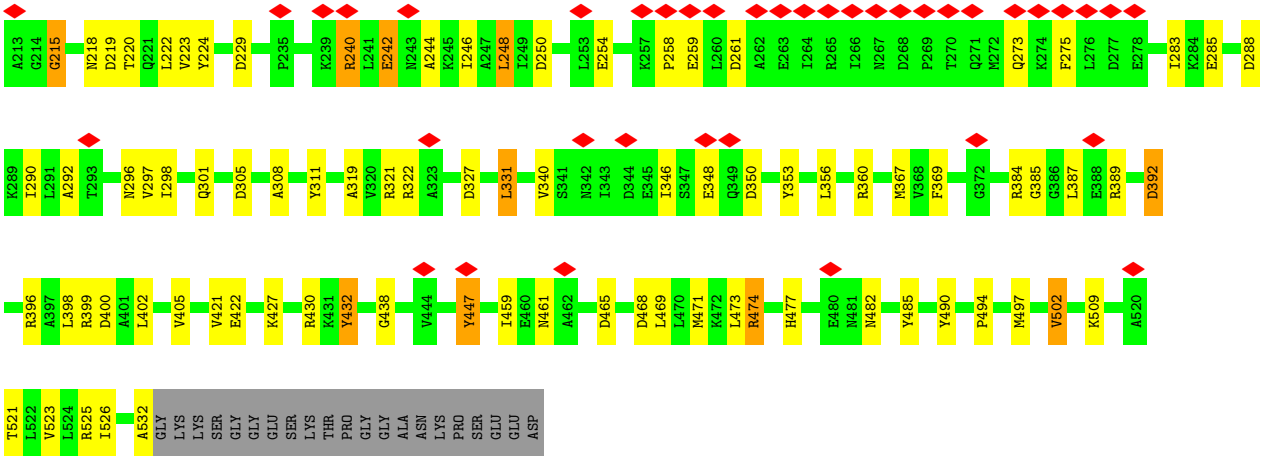
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Chaperonin beta subunit



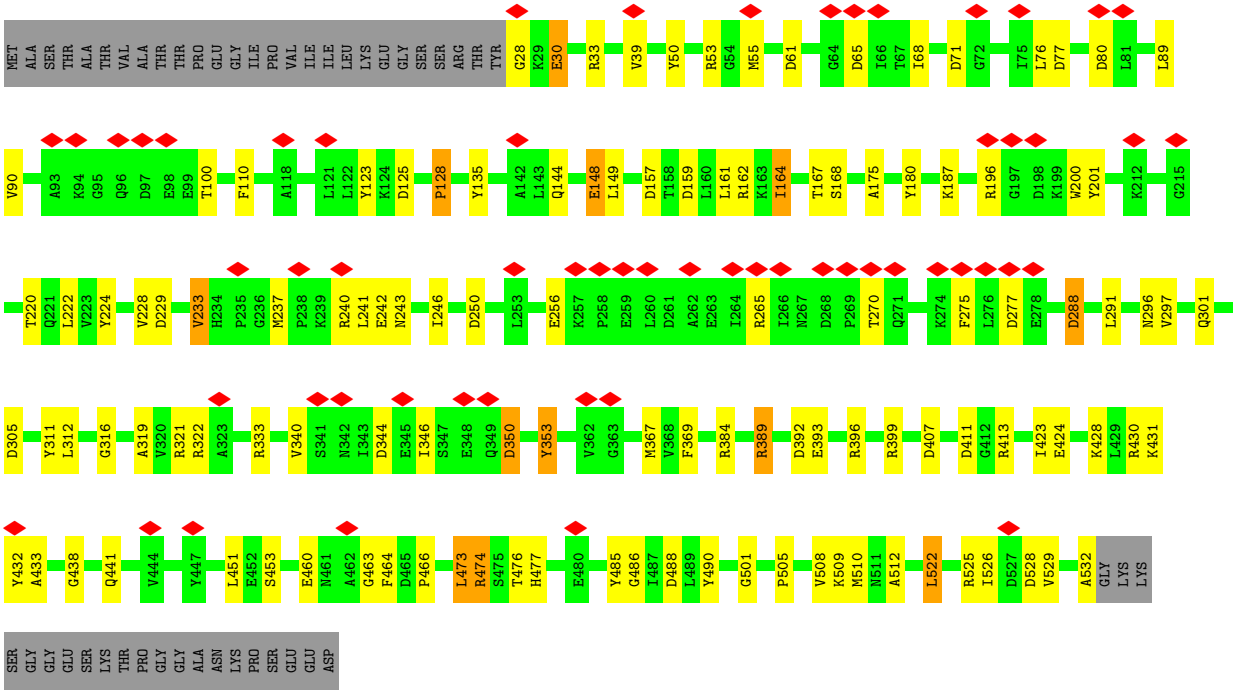
• Molecule 1: Chaperonin beta subunit





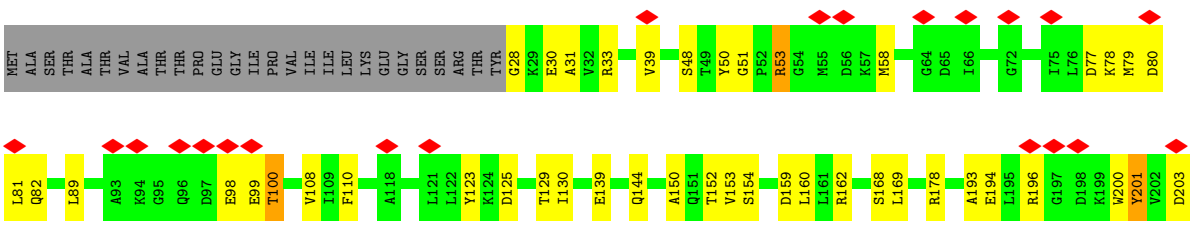
• Molecule 1: Chaperonin beta subunit

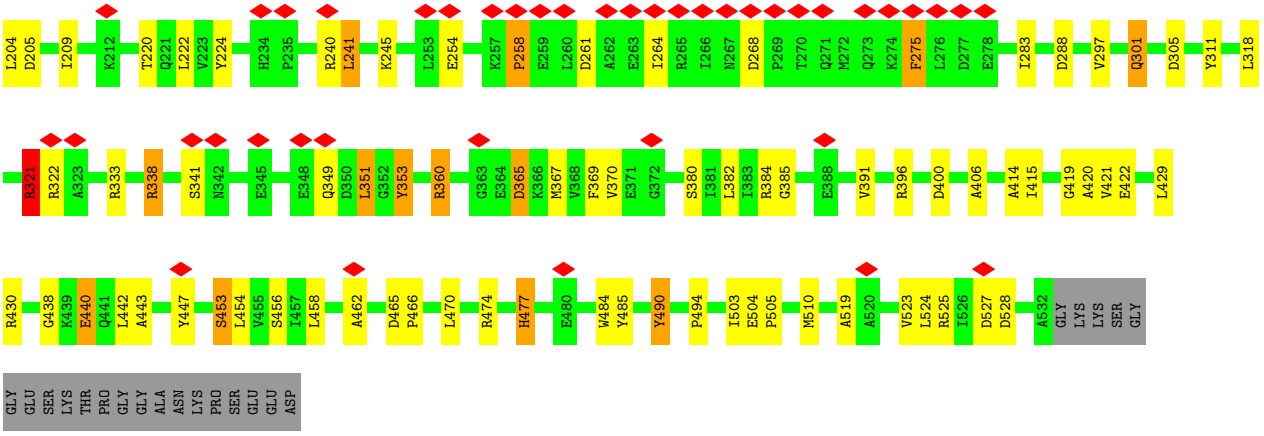
Chain C:



• Molecule 1: Chaperonin beta subunit

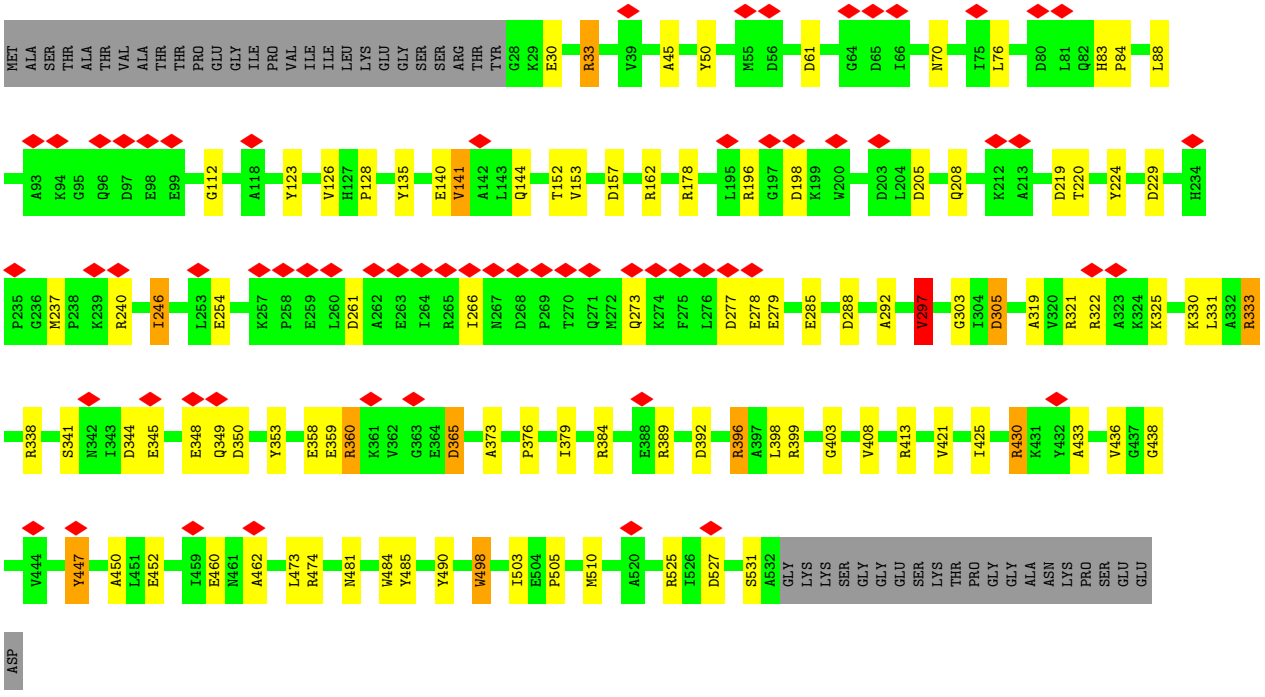
Chain D:





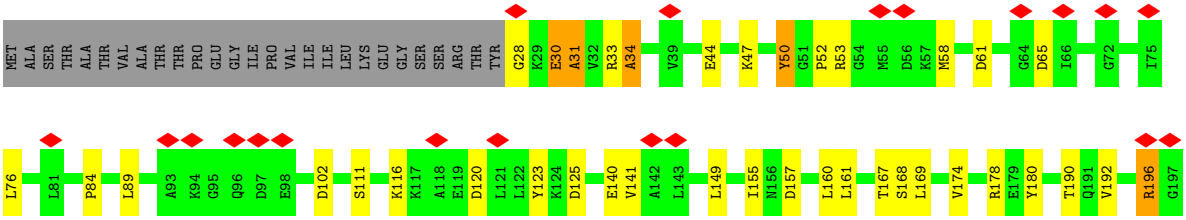
• Molecule 1: Chaperonin beta subunit

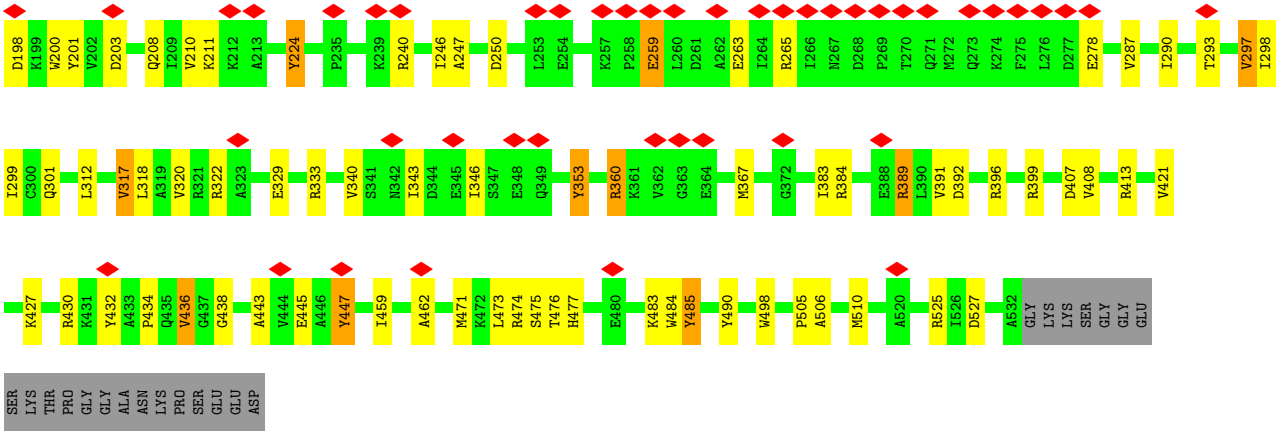
Chain E:



• Molecule 1: Chaperonin beta subunit

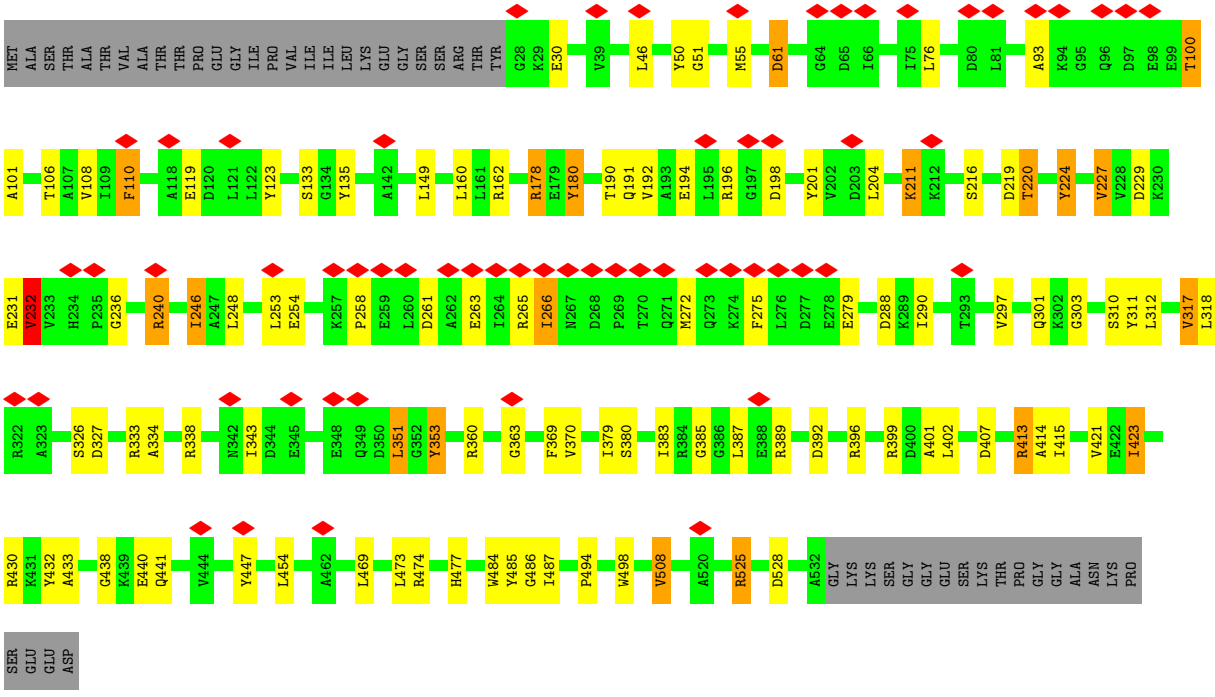
Chain F:





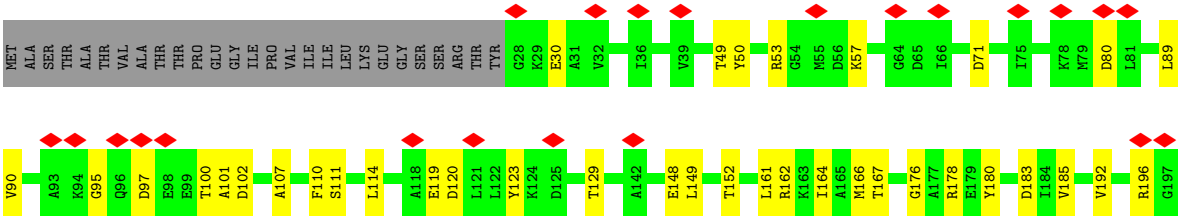
• Molecule 1: Chaperonin beta subunit

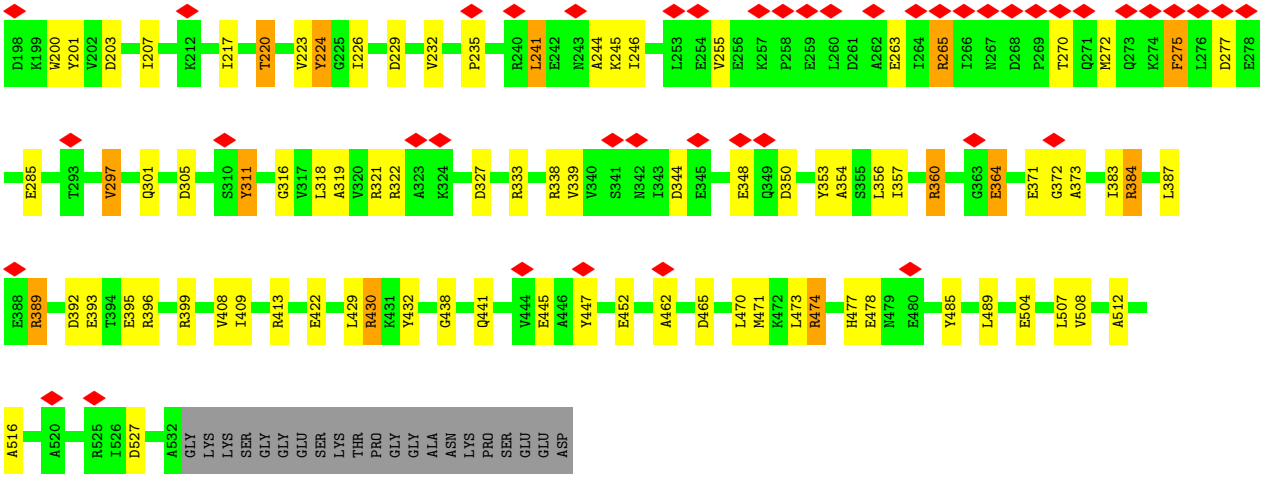
Chain G:



• Molecule 1: Chaperonin beta subunit

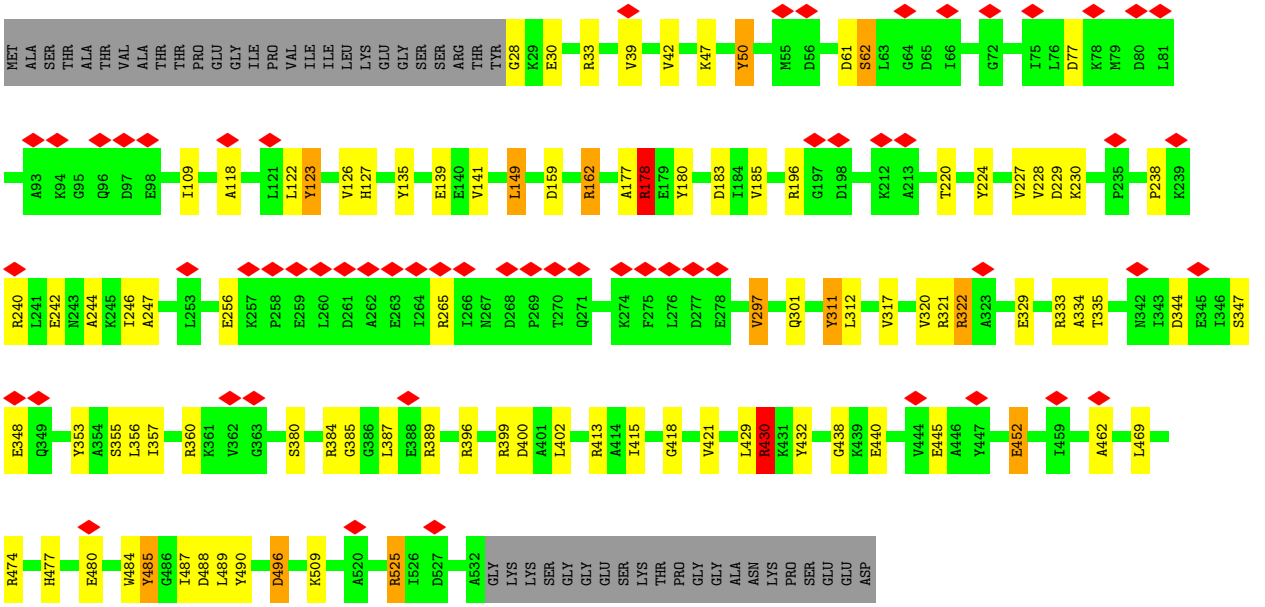
Chain H:





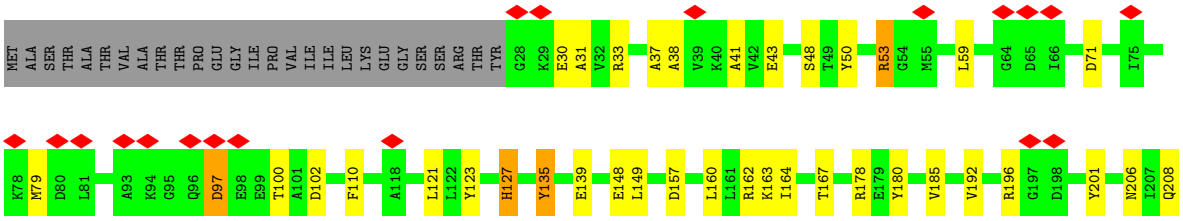
• Molecule 1: Chaperonin beta subunit

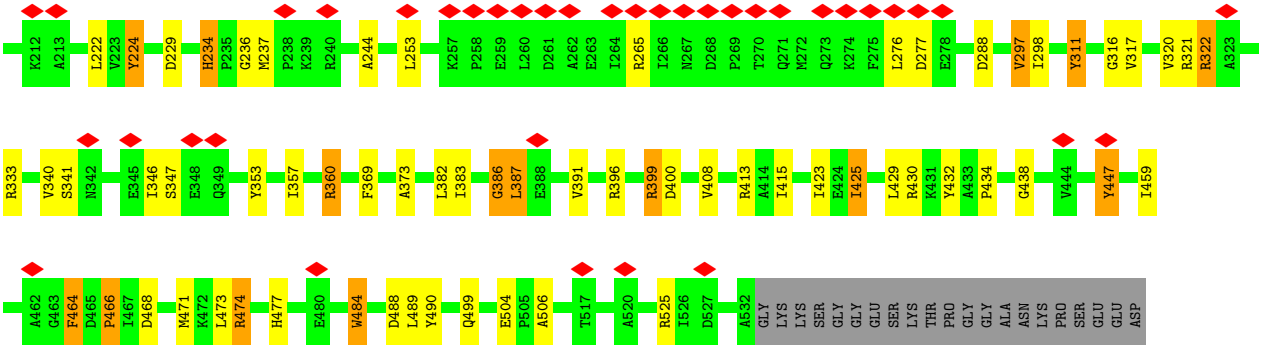
Chain I:



• Molecule 1: Chaperonin beta subunit

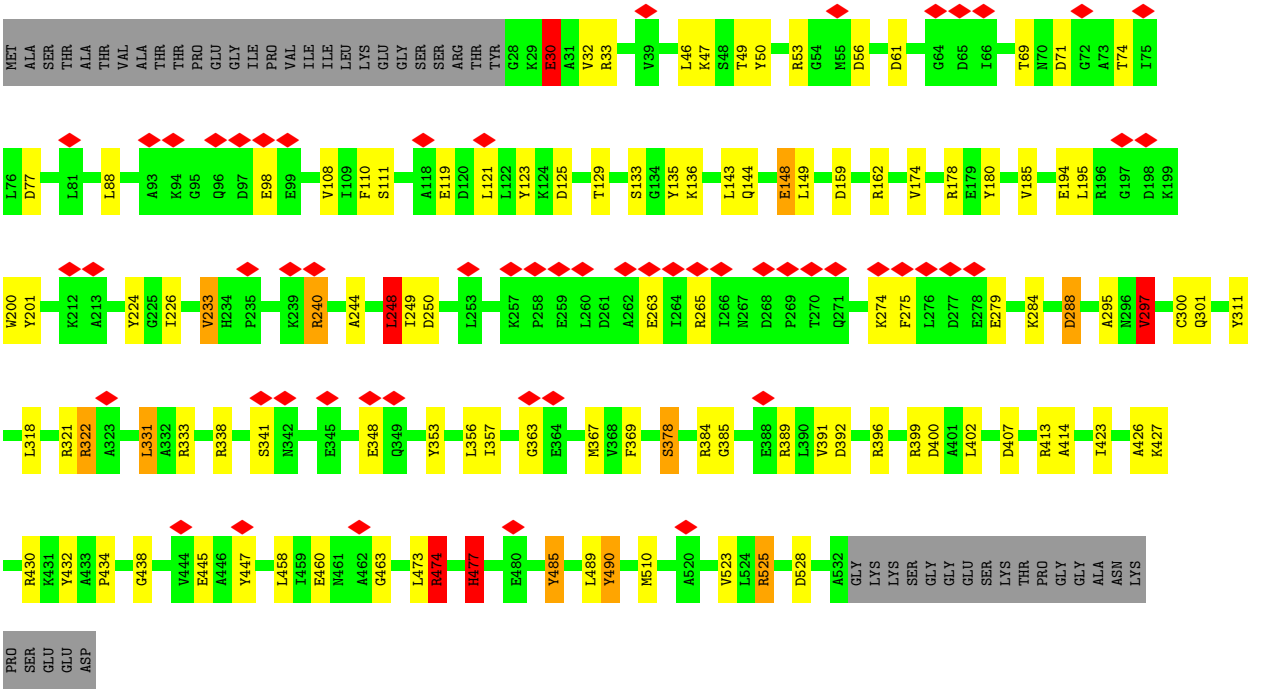
Chain K:





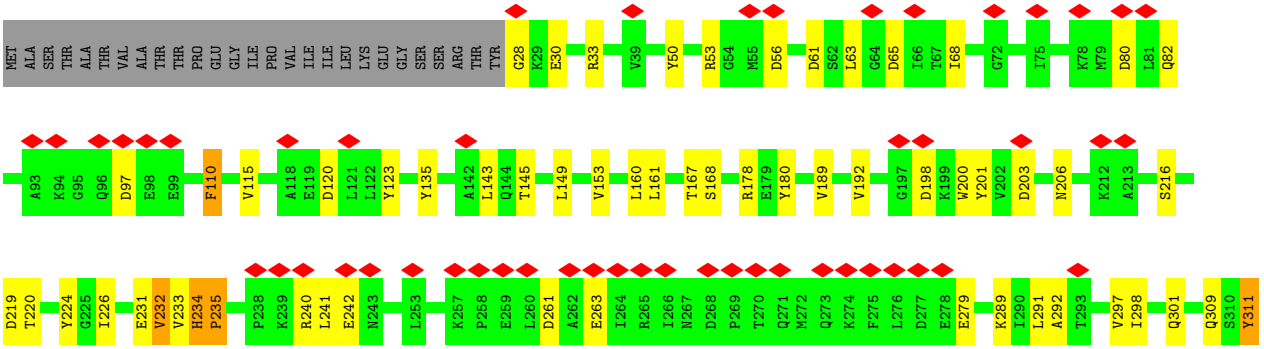
• Molecule 1: Chaperonin beta subunit

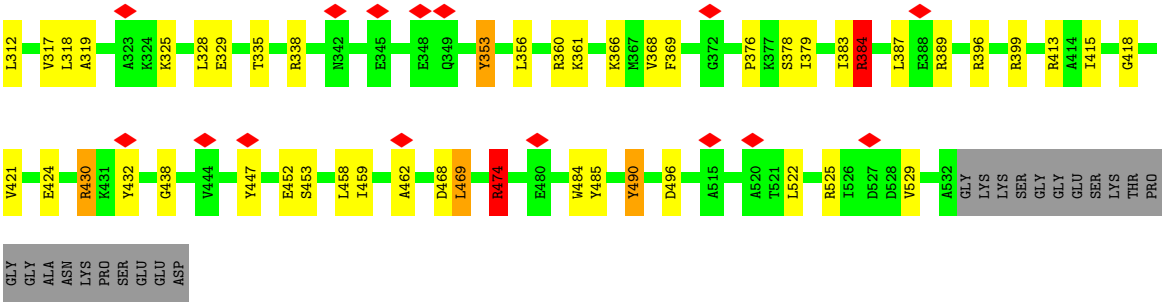
Chain L:



• Molecule 1: Chaperonin beta subunit

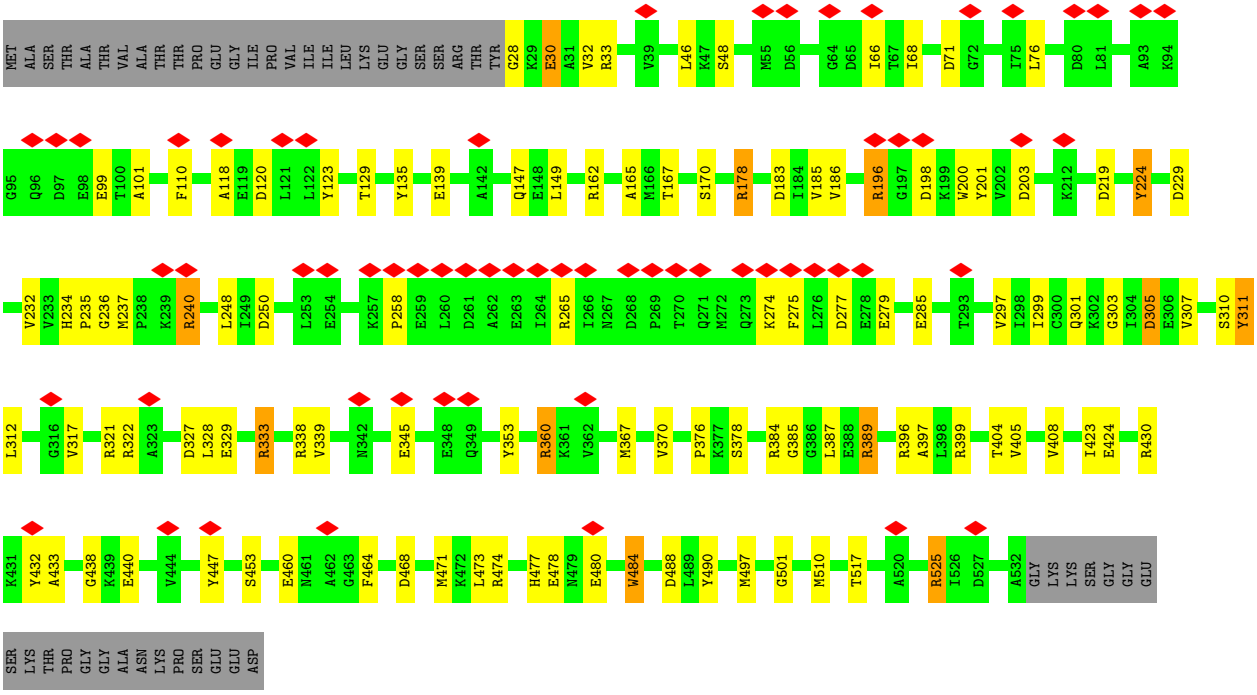
Chain M:





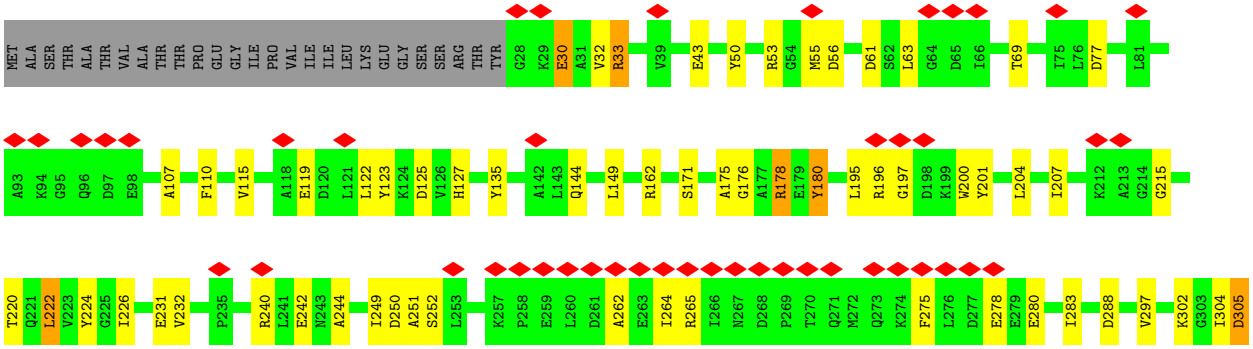
• Molecule 1: Chaperonin beta subunit

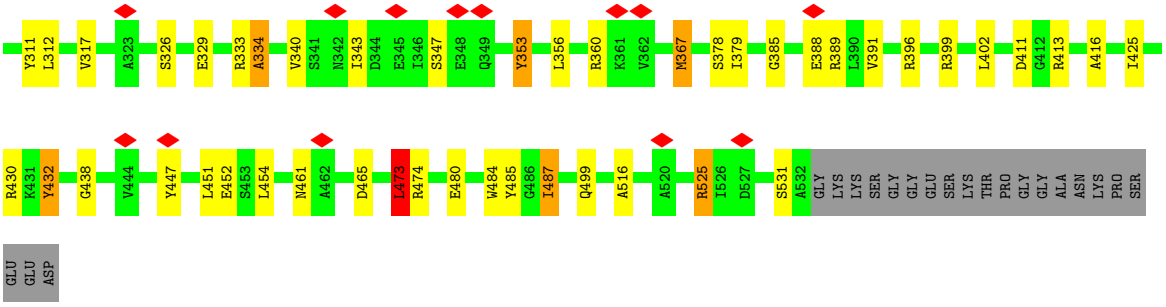
Chain N:



• Molecule 1: Chaperonin beta subunit

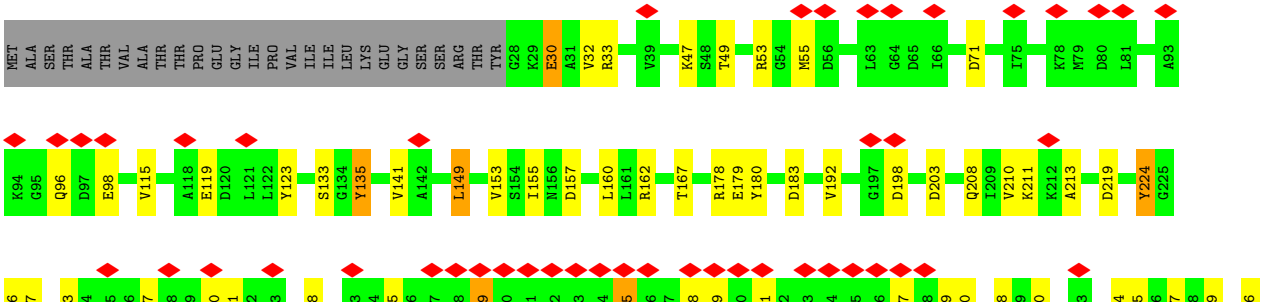
Chain O:





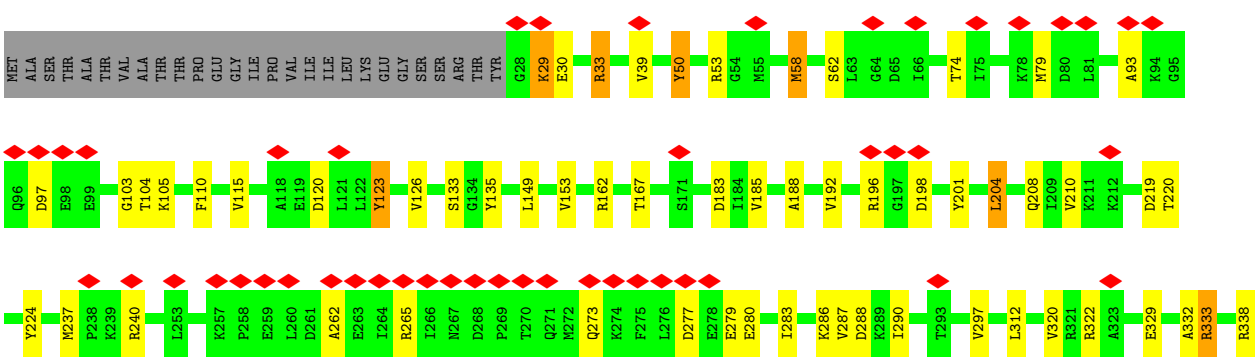
• Molecule 1: Chaperonin beta subunit

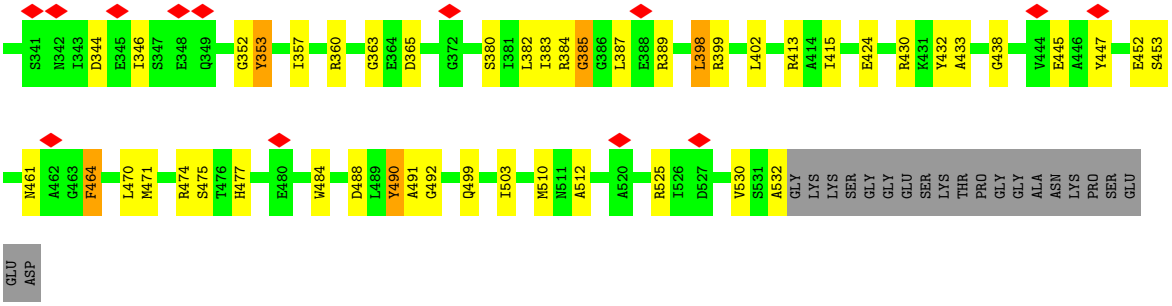
Chain P:



• Molecule 1: Chaperonin beta subunit

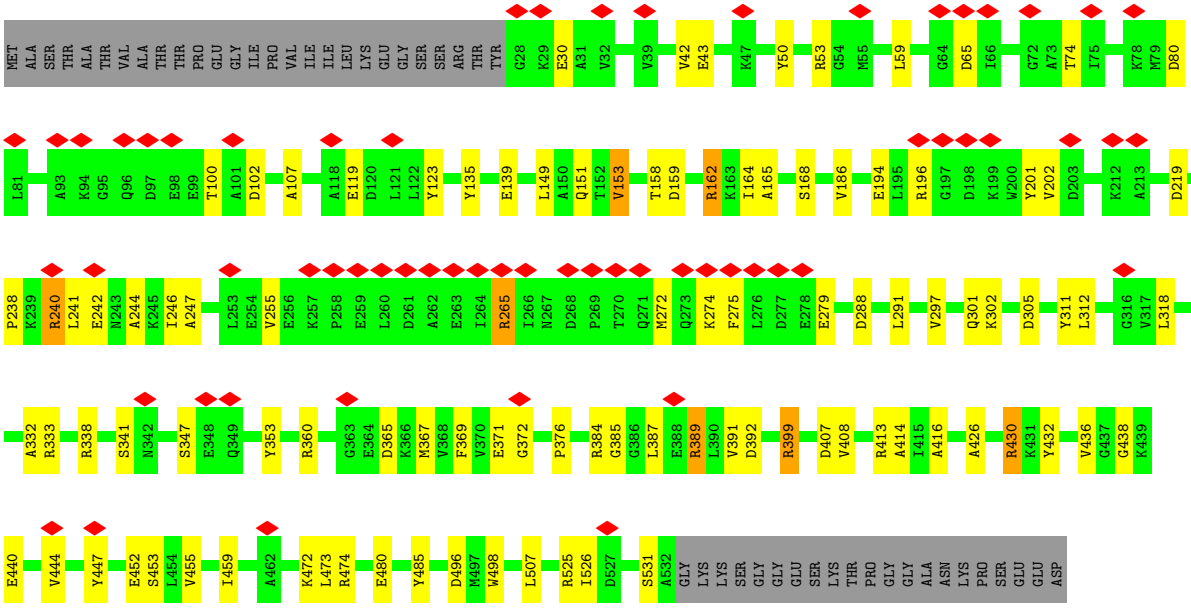
Chain Q:





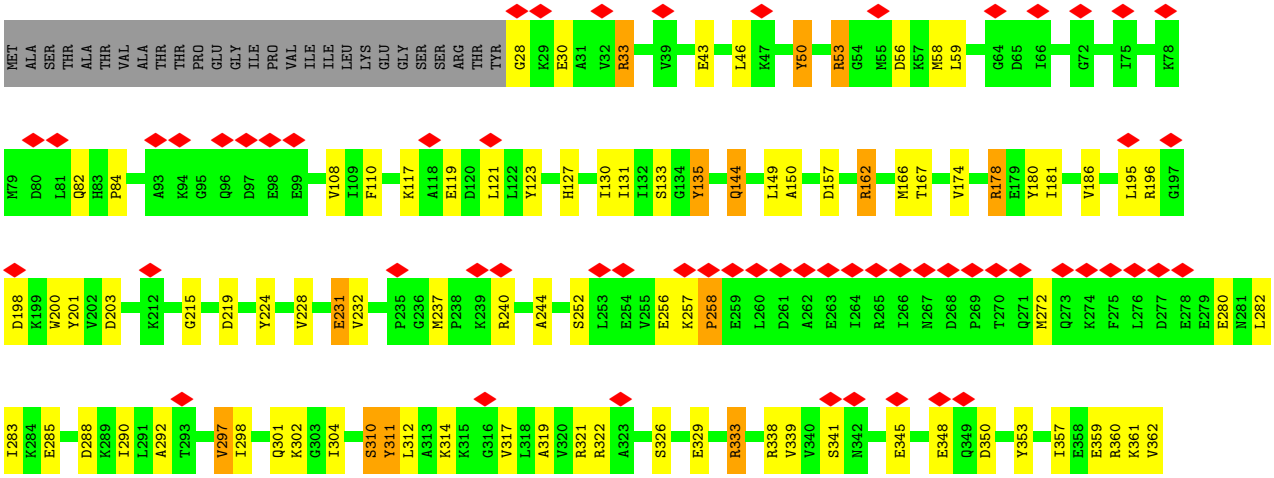
• Molecule 1: Chaperonin beta subunit

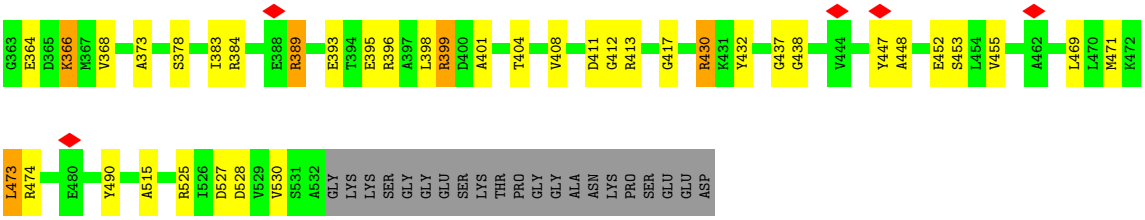
Chain R:



• Molecule 1: Chaperonin beta subunit

Chain S:




G363 E364 D365 K366 M367 V368 A373 S378 I383 R384 E388 R389 E393 T394 E395 R396 A397 L398 R399 D400 A401 T404 V408 D411 G412 R413 G417 R430 K431 Y432 G437 G438 V444 Y447 A448 E452 S453 L454 V455 A462 L469 L470 M471 K472
L473 B474 E480 Y490 A515 R525 I526 D527 D528 V529 V530 S531 A532 GLY LYS LYS SER GLY GLY GLU SER LYS THR PRO GLY GLY ALA ASN LYS PRO SER GLU GLU ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C9	Depositor
Number of particles used	23285	Depositor
Resolution determination method	Not provided	
CTF correction method	The whole micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	96000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	21.001	Depositor
Minimum map value	-12.849	Depositor
Average map value	0.219	Depositor
Map value standard deviation	2.045	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	298.56, 298.56, 298.56	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.8659999, 1.8659999, 1.8659999	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.57	17/3886 (0.4%)	1.94	86/5245 (1.6%)
1	B	1.58	20/3886 (0.5%)	1.92	79/5245 (1.5%)
1	C	1.59	21/3886 (0.5%)	1.95	95/5245 (1.8%)
1	D	1.61	22/3886 (0.6%)	1.97	93/5245 (1.8%)
1	E	1.59	22/3886 (0.6%)	1.94	94/5245 (1.8%)
1	F	1.58	20/3886 (0.5%)	1.92	80/5245 (1.5%)
1	G	1.57	19/3886 (0.5%)	1.90	80/5245 (1.5%)
1	H	1.57	21/3886 (0.5%)	1.93	90/5245 (1.7%)
1	I	1.57	20/3886 (0.5%)	1.95	82/5245 (1.6%)
1	K	1.59	21/3886 (0.5%)	1.93	82/5245 (1.6%)
1	L	1.58	20/3886 (0.5%)	1.93	84/5245 (1.6%)
1	M	1.58	15/3886 (0.4%)	1.90	73/5245 (1.4%)
1	N	1.59	17/3886 (0.4%)	1.99	85/5245 (1.6%)
1	O	1.60	17/3886 (0.4%)	1.93	72/5245 (1.4%)
1	P	1.60	21/3886 (0.5%)	1.91	74/5245 (1.4%)
1	Q	1.60	21/3886 (0.5%)	1.97	71/5245 (1.4%)
1	R	1.57	15/3886 (0.4%)	1.86	76/5245 (1.4%)
1	S	1.59	18/3886 (0.5%)	1.90	88/5245 (1.7%)
All	All	1.58	347/69948 (0.5%)	1.93	1484/94410 (1.6%)

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	11
1	B	0	15
1	C	0	5
1	D	0	11
1	E	0	10
1	F	0	10
1	G	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	8
1	I	0	8
1	K	0	12
1	L	0	8
1	M	0	10
1	N	0	15
1	O	0	7
1	P	0	9
1	Q	0	14
1	R	0	10
1	S	0	11
All	All	0	185

All (347) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	28	GLY	N-CA	8.99	1.59	1.46
1	O	347	SER	CA-CB	8.74	1.66	1.52
1	B	133	SER	CA-CB	8.45	1.65	1.52
1	R	279	GLU	CD-OE2	8.16	1.34	1.25
1	C	28	GLY	N-CA	8.16	1.58	1.46
1	G	413	ARG	CD-NE	8.07	1.60	1.46
1	F	490	TYR	CG-CD2	8.05	1.49	1.39
1	F	168	SER	CA-CB	8.01	1.65	1.52
1	K	48	SER	CA-CB	8.00	1.65	1.52
1	R	372	GLY	CA-C	-7.94	1.39	1.51
1	P	432	TYR	CZ-OH	7.84	1.51	1.37
1	N	353	TYR	CE1-CZ	7.84	1.48	1.38
1	D	28	GLY	N-CA	7.78	1.57	1.46
1	M	28	GLY	N-CA	7.73	1.57	1.46
1	D	154	SER	CA-CB	7.23	1.63	1.52
1	G	133	SER	CA-CB	7.16	1.63	1.52
1	R	447	TYR	CE2-CZ	7.10	1.47	1.38
1	N	311	TYR	CE2-CZ	7.09	1.47	1.38
1	D	453	SER	CA-CB	7.04	1.63	1.52
1	N	170	SER	CA-CB	7.03	1.63	1.52
1	E	338	ARG	CD-NE	6.97	1.58	1.46
1	P	353	TYR	CB-CG	-6.97	1.41	1.51
1	C	490	TYR	CZ-OH	6.87	1.49	1.37
1	C	180	TYR	CE2-CZ	6.80	1.47	1.38
1	R	440	GLU	CD-OE2	6.76	1.33	1.25
1	R	474	ARG	CD-NE	6.73	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	498	TRP	CE3-CZ3	6.72	1.49	1.38
1	S	310	SER	CB-OG	-6.71	1.33	1.42
1	G	240	ARG	CD-NE	6.69	1.57	1.46
1	A	240	ARG	CD-NE	6.67	1.57	1.46
1	P	53	ARG	CD-NE	6.64	1.57	1.46
1	C	196	ARG	CD-NE	6.60	1.57	1.46
1	C	168	SER	CA-CB	6.57	1.62	1.52
1	F	445	GLU	CB-CG	6.57	1.64	1.52
1	R	341	SER	CA-CB	6.56	1.62	1.52
1	O	119	GLU	CB-CG	6.55	1.64	1.52
1	H	285	GLU	CD-OE1	6.55	1.32	1.25
1	Q	389	ARG	CD-NE	6.54	1.57	1.46
1	P	133	SER	CA-CB	6.54	1.62	1.52
1	D	48	SER	CA-CB	6.51	1.62	1.52
1	O	176	GLY	CA-C	-6.51	1.41	1.51
1	R	369	PHE	CG-CD1	6.50	1.48	1.38
1	H	364	GLU	CB-CG	6.49	1.64	1.52
1	H	200	TRP	CZ2-CH2	6.47	1.49	1.37
1	K	386	GLY	CA-C	-6.47	1.41	1.51
1	A	453	SER	CB-OG	6.46	1.50	1.42
1	H	311	TYR	CE2-CZ	6.39	1.46	1.38
1	Q	33	ARG	CD-NE	6.38	1.57	1.46
1	S	329	GLU	CD-OE2	6.38	1.32	1.25
1	E	490	TYR	CE1-CZ	6.37	1.46	1.38
1	D	275	PHE	CE2-CZ	6.35	1.49	1.37
1	K	353	TYR	CE1-CZ	6.33	1.46	1.38
1	F	287	VAL	CB-CG1	6.32	1.66	1.52
1	D	485	TYR	CB-CG	-6.32	1.42	1.51
1	C	180	TYR	CB-CG	-6.30	1.42	1.51
1	M	353	TYR	CE1-CZ	6.30	1.46	1.38
1	E	83	HIS	CB-CG	6.29	1.61	1.50
1	N	345	GLU	CA-CB	6.28	1.67	1.53
1	L	333	ARG	CD-NE	6.25	1.57	1.46
1	K	447	TYR	CZ-OH	6.23	1.48	1.37
1	G	180	TYR	CG-CD2	6.23	1.47	1.39
1	K	148	GLU	CD-OE2	6.23	1.32	1.25
1	B	348	GLU	CD-OE1	6.22	1.32	1.25
1	N	285	GLU	CG-CD	6.20	1.61	1.51
1	A	252	SER	CA-CB	6.20	1.62	1.52
1	E	360	ARG	CD-NE	6.18	1.56	1.46
1	Q	445	GLU	CD-OE2	6.18	1.32	1.25
1	C	486	GLY	CA-C	-6.17	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	401	ALA	CA-CB	6.14	1.65	1.52
1	H	200	TRP	CB-CG	6.14	1.61	1.50
1	N	303	GLY	CA-C	-6.13	1.42	1.51
1	A	403	GLY	CA-C	-6.10	1.42	1.51
1	D	419	GLY	CA-C	6.08	1.61	1.51
1	B	218	ASN	CB-CG	6.07	1.65	1.51
1	F	432	TYR	CE2-CZ	6.06	1.46	1.38
1	N	432	TYR	CG-CD2	6.06	1.47	1.39
1	O	252	SER	CB-OG	6.06	1.50	1.42
1	I	329	GLU	CD-OE1	6.06	1.32	1.25
1	S	133	SER	CA-CB	6.06	1.62	1.52
1	F	475	SER	CB-OG	6.05	1.50	1.42
1	E	531	SER	CB-OG	6.04	1.50	1.42
1	E	254	GLU	CD-OE1	6.04	1.32	1.25
1	O	178	ARG	CD-NE	6.04	1.56	1.46
1	N	135	TYR	CZ-OH	6.04	1.48	1.37
1	R	384	ARG	CD-NE	6.04	1.56	1.46
1	B	369	PHE	CG-CD2	6.03	1.47	1.38
1	A	28	GLY	N-CA	6.03	1.55	1.46
1	S	258	PRO	N-CA	-6.03	1.37	1.47
1	A	168	SER	CA-CB	6.02	1.61	1.52
1	F	28	GLY	N-CA	6.02	1.55	1.46
1	P	388	GLU	CB-CG	6.01	1.63	1.52
1	Q	433	ALA	C-N	-6.01	1.22	1.34
1	L	430	ARG	CD-NE	6.01	1.56	1.46
1	G	353	TYR	CG-CD2	6.01	1.47	1.39
1	C	187	LYS	CA-CB	6.00	1.67	1.53
1	G	216	SER	CB-OG	6.00	1.50	1.42
1	F	201	TYR	CG-CD2	5.99	1.47	1.39
1	I	242	GLU	CG-CD	5.99	1.60	1.51
1	F	224	TYR	CD2-CE2	5.98	1.48	1.39
1	G	119	GLU	CB-CG	5.95	1.63	1.52
1	D	200	TRP	CE3-CZ3	5.93	1.48	1.38
1	H	176	GLY	N-CA	-5.92	1.37	1.46
1	M	279	GLU	CG-CD	5.92	1.60	1.51
1	H	119	GLU	CG-CD	5.92	1.60	1.51
1	Q	363	GLY	N-CA	-5.92	1.37	1.46
1	C	200	TRP	CE3-CZ3	5.92	1.48	1.38
1	N	378	SER	CB-OG	5.91	1.50	1.42
1	B	322	ARG	CD-NE	5.91	1.56	1.46
1	C	243	ASN	CA-CB	5.91	1.68	1.53
1	H	447	TYR	CD1-CE1	5.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	224	TYR	CG-CD2	5.89	1.46	1.39
1	C	466	PRO	N-CD	-5.89	1.39	1.47
1	I	256	GLU	CD-OE1	5.87	1.32	1.25
1	D	474	ARG	CZ-NH1	5.86	1.40	1.33
1	P	265	ARG	CD-NE	5.85	1.56	1.46
1	H	445	GLU	CG-CD	5.84	1.60	1.51
1	G	253	LEU	N-CA	-5.84	1.34	1.46
1	O	402	LEU	CA-C	-5.84	1.37	1.52
1	I	311	TYR	CG-CD2	5.84	1.46	1.39
1	I	347	SER	CA-CB	5.82	1.61	1.52
1	K	33	ARG	NE-CZ	5.82	1.40	1.33
1	B	174	VAL	CB-CG2	5.81	1.65	1.52
1	L	427	LYS	CA-CB	5.81	1.66	1.53
1	L	148	GLU	CD-OE1	5.80	1.32	1.25
1	N	501	GLY	CA-C	-5.80	1.42	1.51
1	P	119	GLU	CG-CD	5.80	1.60	1.51
1	F	140	GLU	CB-CG	5.78	1.63	1.52
1	A	399	ARG	CD-NE	5.78	1.56	1.46
1	F	259	GLU	CG-CD	5.77	1.60	1.51
1	M	338	ARG	CD-NE	5.76	1.56	1.46
1	B	180	TYR	CE1-CZ	5.76	1.46	1.38
1	I	348	GLU	CD-OE1	5.74	1.31	1.25
1	M	168	SER	CA-CB	5.74	1.61	1.52
1	I	452	GLU	CD-OE1	5.72	1.31	1.25
1	B	254	GLU	CB-CG	5.72	1.63	1.52
1	E	140	GLU	CB-CG	5.72	1.63	1.52
1	L	119	GLU	CD-OE1	5.72	1.31	1.25
1	E	460	GLU	CD-OE1	5.71	1.31	1.25
1	A	311	TYR	CE1-CZ	5.71	1.46	1.38
1	R	194	GLU	CD-OE1	5.71	1.31	1.25
1	K	432	TYR	CB-CG	-5.71	1.43	1.51
1	I	445	GLU	CG-CD	5.71	1.60	1.51
1	C	316	GLY	CA-C	5.70	1.60	1.51
1	P	316	GLY	CA-C	-5.70	1.42	1.51
1	M	123	TYR	CE1-CZ	5.70	1.46	1.38
1	M	453	SER	N-CA	5.70	1.57	1.46
1	I	28	GLY	N-CA	5.69	1.54	1.46
1	M	216	SER	CB-OG	5.69	1.49	1.42
1	P	460	GLU	CG-CD	5.69	1.60	1.51
1	N	235	PRO	N-CA	-5.68	1.37	1.47
1	B	485	TYR	CB-CG	-5.68	1.43	1.51
1	Q	103	GLY	N-CA	5.67	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	280	GLU	CD-OE2	5.67	1.31	1.25
1	H	285	GLU	CG-CD	-5.66	1.43	1.51
1	H	371	GLU	CB-CG	5.66	1.62	1.52
1	K	347	SER	CB-OG	-5.65	1.34	1.42
1	L	240	ARG	CA-CB	5.63	1.66	1.53
1	G	50	TYR	CE1-CZ	5.63	1.45	1.38
1	C	322	ARG	CD-NE	5.63	1.56	1.46
1	I	440	GLU	CD-OE2	5.63	1.31	1.25
1	P	464	PHE	CG-CD2	5.62	1.47	1.38
1	L	445	GLU	CD-OE1	5.61	1.31	1.25
1	K	447	TYR	CE2-CZ	5.61	1.45	1.38
1	Q	279	GLU	CG-CD	5.61	1.60	1.51
1	D	321	ARG	CD-NE	5.59	1.55	1.46
1	Q	413	ARG	CD-NE	5.59	1.55	1.46
1	O	531	SER	CA-CB	5.59	1.61	1.52
1	M	180	TYR	CB-CG	5.59	1.60	1.51
1	R	371	GLU	CD-OE1	-5.59	1.19	1.25
1	C	353	TYR	CE1-CZ	-5.58	1.31	1.38
1	C	53	ARG	CD-NE	5.57	1.55	1.46
1	H	201	TYR	CZ-OH	5.57	1.47	1.37
1	E	436	VAL	CA-CB	-5.56	1.43	1.54
1	O	201	TYR	CG-CD2	5.54	1.46	1.39
1	D	318	LEU	CA-CB	5.54	1.66	1.53
1	P	371	GLU	CD-OE1	5.53	1.31	1.25
1	E	490	TYR	CE2-CZ	5.52	1.45	1.38
1	G	326	SER	CA-CB	5.52	1.61	1.52
1	S	417	GLY	N-CA	5.52	1.54	1.46
1	L	378	SER	CA-CB	5.52	1.61	1.52
1	G	51	GLY	CA-C	-5.51	1.43	1.51
1	A	50	TYR	CA-CB	5.50	1.66	1.53
1	I	353	TYR	CE2-CZ	5.50	1.45	1.38
1	K	178	ARG	CD-NE	5.50	1.55	1.46
1	Q	385	GLY	C-N	5.49	1.43	1.33
1	A	396	ARG	CD-NE	5.49	1.55	1.46
1	A	294	GLY	CA-C	-5.49	1.43	1.51
1	B	389	ARG	NE-CZ	5.49	1.40	1.33
1	E	345	GLU	CD-OE2	5.49	1.31	1.25
1	D	224	TYR	CD2-CE2	5.47	1.47	1.39
1	M	242	GLU	CD-OE2	5.47	1.31	1.25
1	F	200	TRP	NE1-CE2	-5.47	1.30	1.37
1	F	263	GLU	CD-OE2	-5.47	1.19	1.25
1	H	201	TYR	CD1-CE1	5.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	148	GLU	CB-CG	5.45	1.62	1.52
1	M	418	GLY	CA-C	5.45	1.60	1.51
1	H	235	PRO	N-CD	5.44	1.55	1.47
1	E	384	ARG	CD-NE	5.44	1.55	1.46
1	Q	402	LEU	CA-CB	5.44	1.66	1.53
1	C	128	PRO	CA-CB	-5.44	1.42	1.53
1	K	316	GLY	N-CA	-5.44	1.37	1.46
1	C	529	VAL	CB-CG1	5.43	1.64	1.52
1	I	360	ARG	CD-NE	5.43	1.55	1.46
1	E	376	PRO	CA-C	-5.43	1.42	1.52
1	B	494	PRO	N-CD	-5.42	1.40	1.47
1	H	110	PHE	CE1-CZ	5.42	1.47	1.37
1	I	380	SER	CA-CB	5.42	1.61	1.52
1	B	461	ASN	CB-CG	5.42	1.63	1.51
1	P	208	GLN	CA-CB	5.42	1.65	1.53
1	Q	380	SER	CB-OG	-5.42	1.35	1.42
1	H	178	ARG	N-CA	-5.41	1.35	1.46
1	I	62	SER	CA-CB	5.41	1.61	1.52
1	O	127	HIS	CB-CG	5.41	1.59	1.50
1	I	353	TYR	CE1-CZ	5.41	1.45	1.38
1	Q	133	SER	CA-CB	5.40	1.61	1.52
1	B	30	GLU	CG-CD	5.40	1.60	1.51
1	R	347	SER	CB-OG	5.39	1.49	1.42
1	S	280	GLU	C-N	5.38	1.46	1.34
1	P	33	ARG	CG-CD	5.38	1.65	1.51
1	F	192	VAL	CB-CG1	5.38	1.64	1.52
1	C	488	ASP	CA-CB	5.37	1.65	1.53
1	Q	475	SER	CB-OG	5.37	1.49	1.42
1	A	464	PHE	CB-CG	-5.37	1.42	1.51
1	I	135	TYR	CA-CB	5.36	1.65	1.53
1	P	353	TYR	CZ-OH	5.35	1.47	1.37
1	E	292	ALA	CA-CB	5.35	1.63	1.52
1	P	135	TYR	CG-CD2	5.34	1.46	1.39
1	S	412	GLY	CA-C	-5.33	1.43	1.51
1	D	490	TYR	CD2-CE2	5.33	1.47	1.39
1	E	452	GLU	CB-CG	5.33	1.62	1.52
1	A	179	GLU	CG-CD	5.32	1.59	1.51
1	G	263	GLU	CD-OE2	5.31	1.31	1.25
1	F	52	PRO	N-CD	5.31	1.55	1.47
1	E	349	GLN	CG-CD	5.31	1.63	1.51
1	K	396	ARG	CD-NE	5.30	1.55	1.46
1	H	504	GLU	CD-OE1	5.30	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	480	GLU	CB-CG	5.30	1.62	1.52
1	D	98	GLU	CG-CD	5.30	1.59	1.51
1	E	359	GLU	CD-OE1	5.30	1.31	1.25
1	L	353	TYR	CZ-OH	5.29	1.46	1.37
1	F	471	MET	CA-CB	5.28	1.65	1.53
1	D	440	GLU	CB-CG	5.27	1.62	1.52
1	Q	461	ASN	CA-CB	5.27	1.66	1.53
1	A	467	ILE	CA-CB	-5.27	1.42	1.54
1	H	447	TYR	CZ-OH	5.27	1.46	1.37
1	G	441	GLN	CG-CD	5.26	1.63	1.51
1	S	341	SER	CA-CB	5.26	1.60	1.52
1	O	171	SER	CA-CB	5.25	1.60	1.52
1	Q	453	SER	CA-CB	5.25	1.60	1.52
1	I	430	ARG	CD-NE	5.25	1.55	1.46
1	Q	492	GLY	N-CA	5.25	1.53	1.46
1	A	432	TYR	CG-CD2	5.25	1.46	1.39
1	R	123	TYR	CE1-CZ	5.25	1.45	1.38
1	L	284	LYS	C-N	5.25	1.46	1.34
1	M	235	PRO	N-CD	-5.24	1.40	1.47
1	L	348	GLU	CB-CG	5.24	1.62	1.52
1	B	180	TYR	CZ-OH	5.24	1.46	1.37
1	S	326	SER	CA-CB	5.23	1.60	1.52
1	D	168	SER	CA-CB	-5.23	1.45	1.52
1	D	527	ASP	CB-CG	-5.23	1.40	1.51
1	G	258	PRO	N-CD	-5.23	1.40	1.47
1	S	437	GLY	C-N	5.23	1.42	1.33
1	S	364	GLU	CG-CD	5.23	1.59	1.51
1	S	119	GLU	CB-CG	5.23	1.62	1.52
1	D	194	GLU	CD-OE1	5.22	1.31	1.25
1	M	53	ARG	CD-NE	5.22	1.55	1.46
1	P	179	GLU	CB-CG	5.22	1.62	1.52
1	O	388	GLU	CB-CG	5.22	1.62	1.52
1	G	525	ARG	CZ-NH1	-5.21	1.26	1.33
1	S	144	GLN	CA-CB	5.21	1.65	1.53
1	P	135	TYR	CE1-CZ	5.21	1.45	1.38
1	K	396	ARG	CZ-NH1	5.20	1.39	1.33
1	M	200	TRP	NE1-CE2	5.20	1.44	1.37
1	A	201	TYR	CE1-CZ	5.20	1.45	1.38
1	B	208	GLN	N-CA	-5.20	1.35	1.46
1	K	50	TYR	CB-CG	-5.20	1.43	1.51
1	K	504	GLU	CB-CG	5.20	1.62	1.52
1	S	180	TYR	CE2-CZ	5.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	ALA	CA-CB	5.19	1.63	1.52
1	O	278	GLU	CD-OE1	5.18	1.31	1.25
1	F	30	GLU	CB-CG	5.16	1.61	1.52
1	B	201	TYR	CB-CG	5.16	1.59	1.51
1	I	311	TYR	CZ-OH	5.16	1.46	1.37
1	Q	105	LYS	CA-CB	5.16	1.65	1.53
1	E	112	GLY	CA-C	5.16	1.60	1.51
1	F	278	GLU	CD-OE2	5.16	1.31	1.25
1	M	413	ARG	CZ-NH1	5.16	1.39	1.33
1	C	311	TYR	CG-CD2	5.15	1.45	1.39
1	S	348	GLU	C-N	5.15	1.45	1.34
1	L	460	GLU	CG-CD	-5.14	1.44	1.51
1	H	316	GLY	N-CA	-5.14	1.38	1.46
1	O	115	VAL	CB-CG2	5.14	1.63	1.52
1	B	140	GLU	CD-OE1	5.13	1.31	1.25
1	N	433	ALA	C-N	5.13	1.44	1.34
1	C	180	TYR	CZ-OH	5.13	1.46	1.37
1	H	393	GLU	CB-CG	5.13	1.61	1.52
1	D	224	TYR	CB-CG	-5.12	1.44	1.51
1	E	303	GLY	CA-C	-5.12	1.43	1.51
1	R	447	TYR	CG-CD1	5.12	1.45	1.39
1	K	466	PRO	N-CD	5.12	1.55	1.47
1	P	518	GLU	CD-OE2	-5.12	1.20	1.25
1	L	363	GLY	CA-C	-5.12	1.43	1.51
1	I	418	GLY	CA-C	-5.11	1.43	1.51
1	B	168	SER	CA-CB	5.11	1.60	1.52
1	G	204	LEU	N-CA	-5.11	1.36	1.46
1	N	432	TYR	CE2-CZ	5.11	1.45	1.38
1	O	197	GLY	CA-C	5.09	1.59	1.51
1	I	50	TYR	CD2-CE2	5.09	1.47	1.39
1	S	231	GLU	CB-CG	5.09	1.61	1.52
1	N	198	ASP	CB-CG	-5.08	1.41	1.51
1	Q	62	SER	CA-CB	5.08	1.60	1.52
1	L	200	TRP	CZ2-CH2	5.08	1.47	1.37
1	L	279	GLU	CB-CG	5.08	1.61	1.52
1	D	201	TYR	CG-CD2	5.08	1.45	1.39
1	B	98	GLU	CB-CG	5.08	1.61	1.52
1	F	485	TYR	CE2-CZ	5.07	1.45	1.38
1	L	434	PRO	CA-C	-5.07	1.42	1.52
1	L	32	VAL	CA-CB	-5.07	1.44	1.54
1	Q	464	PHE	CG-CD1	5.07	1.46	1.38
1	K	37	ALA	CA-CB	5.07	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	50	TYR	CG-CD2	5.07	1.45	1.39
1	E	330	LYS	N-CA	5.07	1.56	1.46
1	H	452	GLU	CD-OE2	5.07	1.31	1.25
1	F	498	TRP	CG-CD2	5.07	1.52	1.43
1	G	110	PHE	CA-CB	5.07	1.65	1.53
1	Q	490	TYR	CZ-OH	5.06	1.46	1.37
1	R	302	LYS	C-N	5.06	1.42	1.33
1	C	123	TYR	CB-CG	-5.06	1.44	1.51
1	K	163	LYS	CA-CB	5.06	1.65	1.53
1	L	338	ARG	CA-CB	5.06	1.65	1.53
1	N	484	TRP	NE1-CE2	5.05	1.44	1.37
1	K	333	ARG	CD-NE	5.05	1.55	1.46
1	P	424	GLU	CB-CG	5.05	1.61	1.52
1	D	123	TYR	CB-CG	-5.04	1.44	1.51
1	O	215	GLY	CA-C	-5.04	1.43	1.51
1	R	531	SER	CB-OG	5.04	1.48	1.42
1	O	333	ARG	CD-NE	5.04	1.55	1.46
1	D	353	TYR	CZ-OH	5.03	1.46	1.37
1	G	321	ARG	CD-NE	5.03	1.54	1.46
1	G	224	TYR	CB-CG	-5.02	1.44	1.51
1	L	194	GLU	CB-CG	5.01	1.61	1.52
1	N	28	GLY	N-CA	5.01	1.53	1.46
1	P	224	TYR	CB-CG	-5.01	1.44	1.51
1	P	280	GLU	CD-OE1	5.00	1.31	1.25
1	A	263	GLU	CB-CG	5.00	1.61	1.52
1	K	297	VAL	CB-CG1	5.00	1.63	1.52
1	O	123	TYR	CE1-CZ	5.00	1.45	1.38

All (1484) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	265	ARG	NE-CZ-NH2	21.33	130.97	120.30
1	E	474	ARG	NE-CZ-NH2	18.96	129.78	120.30
1	Q	413	ARG	NE-CZ-NH1	-18.84	110.88	120.30
1	C	413	ARG	NE-CZ-NH1	-18.20	111.20	120.30
1	D	53	ARG	NE-CZ-NH1	17.94	129.27	120.30
1	M	201	TYR	CB-CG-CD1	-17.71	110.38	121.00
1	I	178	ARG	NE-CZ-NH2	17.67	129.13	120.30
1	C	413	ARG	NE-CZ-NH2	17.06	128.83	120.30
1	E	384	ARG	NE-CZ-NH1	16.98	128.79	120.30
1	O	162	ARG	NE-CZ-NH2	-16.42	112.09	120.30
1	Q	240	ARG	NE-CZ-NH2	-16.00	112.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	178	ARG	NE-CZ-NH2	15.77	128.18	120.30
1	D	525	ARG	NE-CZ-NH1	15.65	128.13	120.30
1	L	135	TYR	CB-CG-CD1	-15.27	111.84	121.00
1	I	240	ARG	NE-CZ-NH1	15.17	127.89	120.30
1	I	399	ARG	NE-CZ-NH2	15.16	127.88	120.30
1	P	338	ARG	NE-CZ-NH2	-14.94	112.83	120.30
1	B	33	ARG	NE-CZ-NH1	14.70	127.65	120.30
1	P	240	ARG	NE-CZ-NH1	14.55	127.58	120.30
1	O	53	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	N	432	TYR	CB-CG-CD2	-14.41	112.36	121.00
1	L	338	ARG	NE-CZ-NH2	-14.39	113.10	120.30
1	N	178	ARG	NE-CZ-NH2	14.38	127.49	120.30
1	D	196	ARG	NE-CZ-NH1	-14.38	113.11	120.30
1	P	384	ARG	NE-CZ-NH2	-14.36	113.12	120.30
1	F	389	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	B	430	ARG	NE-CZ-NH1	14.28	127.44	120.30
1	O	360	ARG	NE-CZ-NH1	-14.28	113.16	120.30
1	C	33	ARG	NE-CZ-NH2	-14.21	113.19	120.30
1	A	338	ARG	NE-CZ-NH2	-14.18	113.21	120.30
1	A	135	TYR	CB-CG-CD2	14.14	129.48	121.00
1	N	265	ARG	NE-CZ-NH1	-14.12	113.24	120.30
1	G	135	TYR	CB-CG-CD2	14.03	129.42	121.00
1	I	430	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	R	413	ARG	NE-CZ-NH2	14.00	127.30	120.30
1	Q	110	PHE	CB-CG-CD2	13.89	130.53	120.80
1	L	240	ARG	NE-CZ-NH2	-13.85	113.37	120.30
1	B	180	TYR	CB-CG-CD1	-13.71	112.77	121.00
1	P	321	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	E	196	ARG	NE-CZ-NH2	13.55	127.08	120.30
1	G	180	TYR	CB-CG-CD2	-13.56	112.87	121.00
1	K	399	ARG	NE-CZ-NH2	13.55	127.08	120.30
1	C	135	TYR	CB-CG-CD1	-13.43	112.94	121.00
1	I	474	ARG	NE-CZ-NH2	13.34	126.97	120.30
1	B	384	ARG	NE-CZ-NH1	13.27	126.93	120.30
1	N	311	TYR	CB-CG-CD1	13.26	128.96	121.00
1	S	360	ARG	NE-CZ-NH2	13.19	126.90	120.30
1	G	178	ARG	NE-CZ-NH2	13.19	126.89	120.30
1	N	389	ARG	NE-CZ-NH1	13.11	126.85	120.30
1	B	322	ARG	NE-CZ-NH2	-13.07	113.76	120.30
1	M	178	ARG	NE-CZ-NH2	13.07	126.84	120.30
1	S	240	ARG	NE-CZ-NH1	13.02	126.81	120.30
1	N	311	TYR	CB-CG-CD2	-13.01	113.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	360	ARG	NE-CZ-NH1	-13.01	113.80	120.30
1	P	333	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	G	265	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	D	196	ARG	NE-CZ-NH2	12.88	126.74	120.30
1	Q	240	ARG	NE-CZ-NH1	12.85	126.73	120.30
1	G	275	PHE	CB-CG-CD2	12.77	129.74	120.80
1	B	33	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	F	474	ARG	NE-CZ-NH1	-12.76	113.92	120.30
1	G	432	TYR	CB-CG-CD1	12.71	128.62	121.00
1	A	135	TYR	CB-CG-CD1	-12.68	113.39	121.00
1	K	322	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	R	321	ARG	NE-CZ-NH2	-12.63	113.98	120.30
1	D	321	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	H	53	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	D	396	ARG	NE-CZ-NH2	-12.53	114.03	120.30
1	B	396	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	K	413	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	R	399	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	R	162	ARG	NE-CZ-NH2	-12.47	114.06	120.30
1	H	53	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	I	384	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	M	360	ARG	NE-CZ-NH1	-12.37	114.11	120.30
1	P	338	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	Q	360	ARG	NE-CZ-NH1	-12.30	114.15	120.30
1	P	384	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	L	135	TYR	CB-CG-CD2	12.25	128.35	121.00
1	R	321	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	K	162	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	L	338	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	K	360	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	B	135	TYR	CB-CG-CD1	-12.13	113.72	121.00
1	S	338	ARG	NE-CZ-NH1	12.07	126.33	120.30
1	M	490	TYR	CB-CG-CD2	-12.06	113.77	121.00
1	I	396	ARG	NE-CZ-NH1	12.02	126.31	120.30
1	O	399	ARG	NE-CZ-NH2	12.02	126.31	120.30
1	M	525	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	K	265	ARG	NE-CZ-NH2	11.93	126.26	120.30
1	F	196	ARG	NE-CZ-NH2	11.89	126.25	120.30
1	Q	201	TYR	CB-CG-CD2	-11.86	113.89	121.00
1	B	240	ARG	NE-CZ-NH2	-11.85	114.37	120.30
1	C	50	TYR	CB-CG-CD2	-11.85	113.89	121.00
1	I	224	TYR	CB-CG-CD1	-11.84	113.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	350	ASP	CB-CG-OD2	11.82	128.94	118.30
1	L	162	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	K	396	ARG	NE-CZ-NH1	11.75	126.18	120.30
1	N	360	ARG	NE-CZ-NH2	11.75	126.17	120.30
1	M	50	TYR	CB-CG-CD2	-11.68	113.99	121.00
1	O	525	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	O	180	TYR	CB-CG-CD2	-11.63	114.02	121.00
1	B	396	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	B	240	ARG	NE-CZ-NH1	11.55	126.07	120.30
1	F	474	ARG	NE-CZ-NH2	11.53	126.06	120.30
1	H	120	ASP	CB-CG-OD2	-11.49	107.96	118.30
1	L	33	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	A	474	ARG	NE-CZ-NH1	-11.46	114.57	120.30
1	F	333	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	H	322	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	K	399	ARG	NE-CZ-NH1	-11.43	114.59	120.30
1	Q	33	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	D	275	PHE	CB-CG-CD1	11.24	128.67	120.80
1	E	322	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	H	311	TYR	CB-CG-CD2	-11.15	114.31	121.00
1	O	53	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	Q	110	PHE	CB-CG-CD1	-11.14	113.00	120.80
1	O	196	ARG	NE-CZ-NH2	11.13	125.87	120.30
1	M	396	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	I	360	ARG	NE-CZ-NH1	-11.02	114.79	120.30
1	D	275	PHE	CB-CG-CD2	-10.94	113.14	120.80
1	I	311	TYR	CB-CG-CD2	-10.91	114.45	121.00
1	R	240	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	D	205	ASP	CB-CG-OD2	10.90	128.11	118.30
1	E	321	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	K	400	ASP	CB-CG-OD1	-10.86	108.52	118.30
1	E	384	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	A	162	ARG	NE-CZ-NH2	10.75	125.67	120.30
1	P	333	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	N	432	TYR	CB-CG-CD1	10.70	127.42	121.00
1	O	178	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	S	178	ARG	NE-CZ-NH2	10.64	125.62	120.30
1	A	360	ARG	NE-CZ-NH1	-10.63	114.98	120.30
1	B	305	ASP	CB-CG-OD1	10.63	127.86	118.30
1	D	201	TYR	CB-CG-CD2	10.62	127.37	121.00
1	A	413	ARG	NE-CZ-NH2	10.62	125.61	120.30
1	A	322	ARG	NE-CZ-NH2	-10.57	115.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	396	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	G	224	TYR	CB-CG-CD1	-10.51	114.70	121.00
1	O	353	TYR	CB-CG-CD2	10.50	127.30	121.00
1	Q	344	ASP	CB-CG-OD1	10.50	127.75	118.30
1	M	413	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	Q	196	ARG	NE-CZ-NH2	10.47	125.53	120.30
1	N	135	TYR	CB-CG-CD2	10.45	127.27	121.00
1	N	196	ARG	NE-CZ-NH1	-10.41	115.09	120.30
1	O	196	ARG	NE-CZ-NH1	-10.41	115.09	120.30
1	H	396	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	L	399	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	B	201	TYR	CB-CG-CD2	-10.32	114.81	121.00
1	G	275	PHE	CB-CG-CD1	-10.32	113.58	120.80
1	R	275	PHE	CB-CG-CD2	-10.31	113.58	120.80
1	E	219	ASP	CB-CG-OD2	10.29	127.56	118.30
1	O	125	ASP	CB-CG-OD2	10.28	127.55	118.30
1	C	135	TYR	CB-CG-CD2	10.27	127.16	121.00
1	E	360	ARG	NE-CZ-NH1	-10.23	115.19	120.30
1	F	178	ARG	NE-CZ-NH2	10.22	125.41	120.30
1	Q	344	ASP	CB-CG-OD2	-10.19	109.13	118.30
1	K	311	TYR	CB-CG-CD2	10.18	127.11	121.00
1	D	178	ARG	NE-CZ-NH2	10.13	125.37	120.30
1	N	162	ARG	NE-CZ-NH2	-10.13	115.24	120.30
1	A	413	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	A	338	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	F	53	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	D	353	TYR	CB-CG-CD1	-10.06	114.96	121.00
1	F	447	TYR	CB-CG-CD2	-10.06	114.96	121.00
1	K	474	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	M	65	ASP	CB-CG-OD1	10.02	127.32	118.30
1	P	430	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	S	123	TYR	CB-CG-CD1	-9.95	115.03	121.00
1	L	224	TYR	CB-CG-CD2	-9.86	115.09	121.00
1	O	413	ARG	NE-CZ-NH1	-9.85	115.37	120.30
1	C	224	TYR	CB-CG-CD1	-9.85	115.09	121.00
1	K	178	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	S	178	ARG	NE-CZ-NH1	-9.81	115.40	120.30
1	G	162	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	C	384	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	N	322	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	R	196	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	B	322	ARG	NE-CZ-NH1	9.76	125.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	430	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	L	384	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	H	183	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	C	53	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	N	353	TYR	CB-CG-CD2	-9.68	115.19	121.00
1	A	322	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	S	353	TYR	CB-CG-CD2	-9.64	115.22	121.00
1	A	474	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	D	201	TYR	CB-CG-CD1	-9.62	115.23	121.00
1	I	178	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	L	162	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	F	396	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	D	53	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	P	389	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	G	447	TYR	CB-CG-CD2	-9.49	115.31	121.00
1	F	240	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	490	TYR	CB-CG-CD2	-9.45	115.33	121.00
1	M	432	TYR	CG-CD2-CE2	-9.44	113.75	121.30
1	A	240	ARG	NE-CZ-NH2	9.41	125.00	120.30
1	H	485	TYR	CB-CG-CD1	9.39	126.64	121.00
1	G	360	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	R	53	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	F	201	TYR	CB-CG-CD2	9.32	126.59	121.00
1	I	474	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	Q	338	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	201	TYR	CG-CD1-CE1	-9.29	113.86	121.30
1	H	71	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	S	399	ARG	NE-CZ-NH1	-9.26	115.67	120.30
1	L	224	TYR	CG-CD2-CE2	-9.26	113.89	121.30
1	C	196	ARG	NE-CZ-NH2	9.25	124.92	120.30
1	D	447	TYR	CB-CG-CD1	9.25	126.55	121.00
1	I	196	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	S	490	TYR	CB-CG-CD2	-9.22	115.47	121.00
1	K	321	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	D	178	ARG	NE-CZ-NH1	-9.20	115.70	120.30
1	L	240	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	N	430	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	F	360	ARG	NE-CZ-NH1	-9.14	115.73	120.30
1	M	240	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	F	360	ARG	NE-CZ-NH2	9.11	124.85	120.30
1	Q	224	TYR	CB-CG-CD2	9.09	126.46	121.00
1	P	288	ASP	CB-CG-OD1	9.08	126.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	373	ALA	N-CA-CB	-9.08	97.39	110.10
1	Q	79	MET	CG-SD-CE	-9.07	85.69	100.20
1	F	203	ASP	CB-CG-OD2	9.05	126.45	118.30
1	C	369	PHE	CB-CG-CD2	9.00	127.10	120.80
1	H	432	TYR	CB-CG-CD1	-9.00	115.60	121.00
1	I	123	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	R	196	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	I	50	TYR	CB-CG-CD1	-8.95	115.63	121.00
1	D	305	ASP	CB-CG-OD2	-8.94	110.25	118.30
1	M	110	PHE	CB-CG-CD1	-8.93	114.55	120.80
1	S	360	ARG	NE-CZ-NH1	-8.93	115.83	120.30
1	D	33	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	L	430	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	B	180	TYR	CB-CG-CD2	8.91	126.35	121.00
1	N	497	MET	CG-SD-CE	-8.89	85.97	100.20
1	N	488	ASP	CB-CG-OD2	8.87	126.29	118.30
1	Q	490	TYR	CB-CG-CD1	-8.87	115.68	121.00
1	N	277	ASP	CB-CG-OD1	8.86	126.27	118.30
1	F	525	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	201	TYR	CB-CG-CD1	-8.81	115.71	121.00
1	K	102	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	Q	322	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	C	321	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	H	183	ASP	CB-CG-OD1	8.74	126.16	118.30
1	R	219	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	L	311	TYR	CG-CD2-CE2	-8.71	114.33	121.30
1	E	447	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	L	485	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	D	447	TYR	CB-CG-CD2	-8.64	115.82	121.00
1	I	396	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	P	430	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	F	180	TYR	CB-CG-CD2	-8.62	115.83	121.00
1	G	399	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	A	178	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	H	430	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	E	353	TYR	CB-CG-CD1	8.59	126.15	121.00
1	I	265	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	M	384	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	E	338	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	C	396	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	I	496	ASP	CB-CG-OD2	8.56	126.00	118.30
1	M	201	TYR	CB-CG-CD2	8.55	126.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	474	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	O	180	TYR	CG-CD1-CE1	-8.51	114.50	121.30
1	F	485	TYR	CG-CD2-CE2	8.50	128.10	121.30
1	D	333	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	K	135	TYR	CB-CG-CD1	-8.48	115.91	121.00
1	E	178	ARG	NE-CZ-NH2	8.47	124.54	120.30
1	O	465	ASP	CB-CG-OD1	8.47	125.92	118.30
1	L	178	ARG	NE-CZ-NH1	-8.47	116.07	120.30
1	G	327	ASP	CB-CG-OD1	8.45	125.90	118.30
1	R	219	ASP	CB-CG-OD1	8.45	125.90	118.30
1	E	413	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	I	50	TYR	CG-CD2-CE2	-8.44	114.55	121.30
1	K	400	ASP	CB-CG-OD2	8.43	125.89	118.30
1	K	320	VAL	CA-CB-CG1	8.42	123.53	110.90
1	L	413	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	K	180	TYR	CB-CG-CD2	8.41	126.04	121.00
1	L	430	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	O	389	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	I	322	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	F	490	TYR	CB-CG-CD2	-8.36	115.99	121.00
1	H	485	TYR	CB-CG-CD2	-8.33	116.00	121.00
1	C	474	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	I	228	VAL	CA-CB-CG2	-8.32	98.42	110.90
1	O	288	ASP	CB-CG-OD2	8.32	125.79	118.30
1	K	53	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	I	488	ASP	CB-CG-OD2	-8.29	110.83	118.30
1	E	277	ASP	CB-CG-OD2	8.29	125.76	118.30
1	P	322	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	B	275	PHE	CB-CG-CD1	-8.28	115.01	120.80
1	D	360	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	A	525	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	H	353	TYR	CB-CG-CD2	-8.24	116.05	121.00
1	K	464	PHE	CB-CG-CD2	-8.24	115.03	120.80
1	B	201	TYR	CD1-CE1-CZ	-8.24	112.39	119.80
1	F	178	ARG	NE-CZ-NH1	-8.23	116.18	120.30
1	R	407	ASP	CB-CG-OD1	8.23	125.70	118.30
1	Q	353	TYR	CB-CG-CD1	-8.22	116.07	121.00
1	A	490	TYR	CB-CG-CD1	-8.21	116.07	121.00
1	E	61	ASP	CB-CG-OD1	8.21	125.69	118.30
1	P	490	TYR	CB-CG-CD2	8.21	125.92	121.00
1	A	224	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	C	201	TYR	CB-CG-CD1	8.19	125.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	237	MET	CG-SD-CE	-8.18	87.11	100.20
1	P	490	TYR	CB-CG-CD1	-8.18	116.09	121.00
1	S	53	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	Q	365	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	G	413	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	S	50	TYR	CG-CD1-CE1	-8.15	114.78	121.30
1	N	360	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	A	110	PHE	CB-CG-CD2	8.13	126.49	120.80
1	O	33	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	D	220	THR	CA-CB-CG2	-8.13	101.02	112.40
1	O	311	TYR	CB-CG-CD2	-8.13	116.12	121.00
1	I	162	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	P	307	VAL	CG1-CB-CG2	-8.11	97.92	110.90
1	A	205	ASP	CB-CG-OD2	8.11	125.60	118.30
1	D	338	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	M	219	ASP	CB-CG-OD1	-8.10	111.01	118.30
1	S	162	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	E	485	TYR	CB-CG-CD2	-8.09	116.14	121.00
1	B	311	TYR	CB-CG-CD1	8.09	125.85	121.00
1	L	400	ASP	CB-CG-OD2	8.08	125.57	118.30
1	K	237	MET	CG-SD-CE	-8.08	87.27	100.20
1	S	201	TYR	CB-CG-CD2	-8.07	116.16	121.00
1	C	224	TYR	CB-CG-CD2	8.07	125.84	121.00
1	F	50	TYR	CB-CG-CD1	-8.06	116.16	121.00
1	K	157	ASP	CB-CG-OD2	8.05	125.55	118.30
1	C	157	ASP	CB-CG-OD2	8.04	125.53	118.30
1	H	327	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	B	135	TYR	CG-CD2-CE2	-8.03	114.88	121.30
1	G	413	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	F	50	TYR	CG-CD2-CE2	-8.01	114.89	121.30
1	C	157	ASP	CB-CG-OD1	-8.01	111.09	118.30
1	A	384	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	F	407	ASP	CB-CG-OD2	7.99	125.49	118.30
1	O	353	TYR	CB-CG-CD1	-7.98	116.21	121.00
1	H	97	ASP	CB-CG-OD1	7.98	125.48	118.30
1	O	110	PHE	CB-CG-CD2	7.98	126.39	120.80
1	G	229	ASP	CB-CG-OD1	7.98	125.48	118.30
1	S	162	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	Q	338	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	L	396	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	H	201	TYR	CB-CG-CD2	-7.94	116.24	121.00
1	H	275	PHE	CB-CG-CD1	7.94	126.36	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	224	TYR	CB-CG-CD1	-7.91	116.25	121.00
1	A	123	TYR	CG-CD2-CE2	-7.90	114.98	121.30
1	Q	322	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	O	43	GLU	OE1-CD-OE2	-7.85	113.88	123.30
1	A	196	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	F	525	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	F	353	TYR	CB-CG-CD2	7.84	125.70	121.00
1	K	229	ASP	CB-CG-OD2	7.84	125.36	118.30
1	K	201	TYR	CB-CG-CD1	-7.83	116.30	121.00
1	A	321	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	S	135	TYR	CB-CG-CD2	7.82	125.69	121.00
1	F	490	TYR	CB-CG-CD1	7.81	125.69	121.00
1	G	123	TYR	CB-CG-CD1	-7.81	116.31	121.00
1	P	413	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	A	189	VAL	CG1-CB-CG2	-7.78	98.45	110.90
1	E	135	TYR	CB-CG-CD1	-7.78	116.33	121.00
1	Q	58	MET	CG-SD-CE	-7.78	87.75	100.20
1	Q	360	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	I	196	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	L	396	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C	240	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	L	432	TYR	CB-CG-CD1	7.72	125.64	121.00
1	O	432	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	O	360	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	M	328	LEU	CB-CG-CD2	7.71	124.10	111.00
1	E	490	TYR	CB-CG-CD2	-7.69	116.39	121.00
1	R	413	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	R	525	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	O	50	TYR	CD1-CE1-CZ	-7.68	112.89	119.80
1	C	322	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	N	229	ASP	CB-CG-OD1	7.65	125.18	118.30
1	G	407	ASP	CB-CG-OD1	7.63	125.17	118.30
1	E	344	ASP	CB-CG-OD1	-7.63	111.44	118.30
1	K	525	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	K	373	ALA	N-CA-CB	7.62	120.76	110.10
1	D	80	ASP	CB-CG-OD2	7.61	125.15	118.30
1	K	31	ALA	N-CA-CB	-7.60	99.45	110.10
1	D	77	ASP	CB-CG-OD2	7.60	125.14	118.30
1	Q	201	TYR	CG-CD2-CE2	-7.59	115.23	121.30
1	G	485	TYR	CB-CG-CD1	7.58	125.55	121.00
1	O	55	MET	CG-SD-CE	-7.58	88.07	100.20
1	G	265	ARG	NE-CZ-NH2	7.58	124.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	178	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	N	322	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	I	224	TYR	CB-CG-CD2	7.54	125.53	121.00
1	N	203	ASP	CB-CG-OD1	7.54	125.09	118.30
1	F	389	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	Q	424	GLU	OE1-CD-OE2	-7.53	114.27	123.30
1	P	525	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	162	ARG	O-C-N	-7.52	110.67	122.70
1	S	123	TYR	CB-CG-CD2	7.52	125.51	121.00
1	C	525	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	Q	384	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	B	465	ASP	CB-CG-OD1	7.50	125.05	118.30
1	H	196	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	R	311	TYR	CB-CG-CD1	-7.48	116.51	121.00
1	M	120	ASP	CB-CG-OD2	7.48	125.03	118.30
1	M	485	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	N	333	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	M	161	LEU	CB-CG-CD2	7.47	123.69	111.00
1	E	490	TYR	CB-CG-CD1	7.44	125.47	121.00
1	N	183	ASP	CB-CG-OD1	7.42	124.98	118.30
1	B	275	PHE	CB-CG-CD2	7.42	126.00	120.80
1	D	39	VAL	CA-CB-CG1	7.41	122.01	110.90
1	R	274	LYS	O-C-N	-7.40	110.85	122.70
1	M	110	PHE	CB-CG-CD2	7.38	125.97	120.80
1	Q	219	ASP	CB-CG-OD1	7.38	124.94	118.30
1	Q	224	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	N	478	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	A	224	TYR	CB-CG-CD1	7.35	125.41	121.00
1	N	399	ARG	NE-CZ-NH1	-7.35	116.63	120.30
1	G	180	TYR	CG-CD1-CE1	-7.34	115.42	121.30
1	I	126	VAL	CG1-CB-CG2	-7.34	99.15	110.90
1	N	464	PHE	CB-CG-CD2	-7.33	115.67	120.80
1	S	321	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	O	135	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	K	369	PHE	CB-CG-CD1	7.31	125.92	120.80
1	I	265	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	S	240	ARG	CD-NE-CZ	7.29	133.81	123.60
1	M	198	ASP	CB-CG-OD1	7.29	124.86	118.30
1	N	275	PHE	CB-CG-CD2	7.29	125.90	120.80
1	L	311	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	A	287	VAL	CA-CB-CG2	7.25	121.78	110.90
1	D	474	ARG	NE-CZ-NH2	7.24	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	D	169	LEU	O-C-N	-7.23	111.13	122.70
1	D	380	SER	N-CA-CB	7.23	121.35	110.50
1	A	333	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	L	288	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	I	322	ARG	NH1-CZ-NH2	-7.22	111.46	119.40
1	H	110	PHE	CB-CG-CD1	-7.20	115.76	120.80
1	A	288	ASP	CB-CG-OD2	7.20	124.78	118.30
1	D	240	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	F	53	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	53	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	85	ALA	N-CA-CB	7.16	120.13	110.10
1	D	525	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	Q	120	ASP	CB-CG-OD2	7.15	124.74	118.30
1	S	348	GLU	OE1-CD-OE2	-7.15	114.72	123.30
1	C	430	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	333	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	M	369	PHE	CB-CG-CD1	-7.13	115.81	120.80
1	E	196	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	A	53	ARG	NE-CZ-NH2	7.11	123.86	120.30
1	O	56	ASP	CB-CG-OD1	7.11	124.70	118.30
1	M	432	TYR	CZ-CE2-CD2	7.11	126.20	119.80
1	C	53	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	C	430	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	S	166	MET	CG-SD-CE	-7.11	88.83	100.20
1	N	471	MET	CG-SD-CE	-7.10	88.83	100.20
1	N	237	MET	CG-SD-CE	-7.10	88.84	100.20
1	P	277	ASP	O-C-N	-7.10	111.34	122.70
1	C	432	TYR	CB-CG-CD1	-7.10	116.74	121.00
1	F	141	VAL	CA-CB-CG2	-7.09	100.26	110.90
1	R	240	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	Q	389	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	D	510	MET	CA-CB-CG	7.09	125.35	113.30
1	Q	430	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	R	53	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	432	TYR	CG-CD1-CE1	-7.07	115.64	121.30
1	Q	452	GLU	OE1-CD-OE2	-7.07	114.81	123.30
1	N	339	VAL	CA-CB-CG2	7.06	121.49	110.90
1	I	509	LYS	O-C-N	-7.06	111.41	122.70
1	E	399	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	B	244	ALA	N-CA-CB	-7.03	100.26	110.10
1	S	186	VAL	CA-CB-CG2	-7.03	100.36	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	399	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	L	447	TYR	CZ-CE2-CD2	-7.02	113.48	119.80
1	A	240	ARG	NH1-CZ-NH2	-7.02	111.68	119.40
1	H	196	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	K	123	TYR	CG-CD2-CE2	-7.01	115.69	121.30
1	C	485	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	B	384	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	S	157	ASP	CB-CG-OD2	7.00	124.60	118.30
1	G	219	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	I	183	ASP	CB-CG-OD1	7.00	124.60	118.30
1	Q	532	ALA	CB-CA-C	-7.00	99.60	110.10
1	D	153	VAL	CA-CB-CG2	-6.98	100.42	110.90
1	A	265	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	H	465	ASP	CB-CG-OD1	6.98	124.58	118.30
1	O	391	VAL	CG1-CB-CG2	-6.98	99.74	110.90
1	F	329	GLU	OE1-CD-OE2	-6.97	114.93	123.30
1	L	490	TYR	CB-CG-CD1	6.97	125.19	121.00
1	C	396	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	I	490	TYR	CG-CD2-CE2	-6.97	115.73	121.30
1	Q	123	TYR	CB-CG-CD1	6.96	125.18	121.00
1	L	275	PHE	CB-CG-CD2	6.96	125.67	120.80
1	D	50	TYR	CB-CG-CD1	-6.96	116.83	121.00
1	P	396	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	H	203	ASP	CB-CG-OD1	6.94	124.55	118.30
1	N	178	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	P	360	ARG	CD-NE-CZ	6.94	133.32	123.60
1	S	196	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	K	277	ASP	CB-CG-OD2	6.94	124.55	118.30
1	H	80	ASP	CB-CG-OD1	-6.94	112.06	118.30
1	L	318	LEU	CB-CG-CD2	6.93	122.79	111.00
1	R	272	MET	CG-SD-CE	-6.93	89.11	100.20
1	C	159	ASP	CB-CG-OD1	6.93	124.53	118.30
1	H	373	ALA	CB-CA-C	6.92	120.49	110.10
1	K	490	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	L	201	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	L	53	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	K	484	TRP	CB-CG-CD2	6.90	135.57	126.60
1	H	399	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	S	430	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	288	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	L	233	VAL	CA-CB-CG1	6.88	121.22	110.90
1	Q	399	ARG	CD-NE-CZ	6.88	133.23	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	31	ALA	CB-CA-C	-6.88	99.79	110.10
1	D	485	TYR	CB-CG-CD2	-6.88	116.88	121.00
1	G	135	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	K	387	LEU	CB-CG-CD1	-6.87	99.32	111.00
1	L	111	SER	N-CA-CB	6.86	120.80	110.50
1	L	50	TYR	CG-CD2-CE2	-6.86	115.81	121.30
1	B	421	VAL	CA-CB-CG2	-6.85	100.62	110.90
1	G	392	ASP	CB-CG-OD2	6.85	124.47	118.30
1	N	405	VAL	CA-CB-CG1	6.85	121.17	110.90
1	E	33	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	F	34	ALA	N-CA-CB	-6.84	100.53	110.10
1	K	490	TYR	CB-CG-CD1	6.83	125.10	121.00
1	Q	365	ASP	CB-CG-OD1	6.83	124.44	118.30
1	B	327	ASP	CB-CG-OD2	6.82	124.44	118.30
1	O	123	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	P	380	SER	N-CA-CB	6.82	120.72	110.50
1	S	196	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	L	133	SER	N-CA-CB	-6.79	100.31	110.50
1	S	525	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	265	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	I	335	THR	CA-CB-CG2	-6.76	102.94	112.40
1	Q	97	ASP	CB-CG-OD1	6.76	124.38	118.30
1	E	485	TYR	CB-CG-CD1	6.75	125.05	121.00
1	O	123	TYR	CZ-CE2-CD2	-6.75	113.73	119.80
1	S	333	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	I	301	GLN	C-N-CA	6.75	138.57	121.70
1	K	311	TYR	CB-CG-CD1	-6.75	116.95	121.00
1	P	71	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	I	220	THR	CA-CB-CG2	-6.70	103.02	112.40
1	C	344	ASP	CB-CG-OD2	6.70	124.33	118.30
1	G	261	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	B	525	ARG	O-C-N	-6.67	112.02	122.70
1	K	110	PHE	CB-CG-CD1	-6.67	116.13	120.80
1	R	444	VAL	CG1-CB-CG2	-6.66	100.24	110.90
1	K	43	GLU	OE1-CD-OE2	-6.65	115.31	123.30
1	D	384	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	430	ARG	NH1-CZ-NH2	-6.64	112.09	119.40
1	E	527	ASP	CB-CG-OD1	6.64	124.27	118.30
1	G	380	SER	CB-CA-C	-6.63	97.50	110.10
1	K	391	VAL	CA-CB-CG1	6.62	120.82	110.90
1	Q	499	GLN	CG-CD-OE1	6.61	134.82	121.60
1	O	311	TYR	CB-CG-CD1	6.61	124.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	69	THR	O-C-N	-6.60	112.14	122.70
1	G	123	TYR	CB-CG-CD2	6.60	124.96	121.00
1	P	432	TYR	CG-CD2-CE2	-6.60	116.02	121.30
1	E	484	TRP	CB-CG-CD2	6.60	135.18	126.60
1	I	320	VAL	CA-CB-CG1	6.60	120.80	110.90
1	S	515	ALA	N-CA-CB	-6.59	100.87	110.10
1	N	353	TYR	CG-CD2-CE2	-6.58	116.03	121.30
1	A	123	TYR	CZ-CE2-CD2	6.58	125.72	119.80
1	H	322	ARG	NH1-CZ-NH2	-6.58	112.17	119.40
1	N	183	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	E	474	ARG	NH1-CZ-NH2	-6.56	112.19	119.40
1	R	474	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	B	350	ASP	CB-CG-OD2	6.55	124.19	118.30
1	H	224	TYR	CG-CD1-CE1	-6.55	116.06	121.30
1	P	180	TYR	CG-CD2-CE2	-6.55	116.06	121.30
1	S	198	ASP	CB-CG-OD2	6.55	124.19	118.30
1	C	485	TYR	CB-CG-CD1	6.55	124.93	121.00
1	I	229	ASP	CB-CG-OD1	6.54	124.19	118.30
1	S	322	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	Q	288	ASP	CB-CG-OD2	6.54	124.19	118.30
1	S	322	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	N	339	VAL	CG1-CB-CG2	-6.53	100.45	110.90
1	E	229	ASP	N-CA-CB	-6.53	98.85	110.60
1	H	166	MET	CG-SD-CE	-6.53	89.76	100.20
1	I	380	SER	O-C-N	-6.53	112.26	122.70
1	D	50	TYR	CB-CG-CD2	6.52	124.91	121.00
1	I	61	ASP	CB-CG-OD2	6.51	124.16	118.30
1	M	474	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	P	183	ASP	CB-CG-OD1	6.50	124.15	118.30
1	G	360	ARG	N-CA-CB	6.50	122.29	110.60
1	F	203	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	D	369	PHE	CB-CG-CD2	-6.49	116.25	120.80
1	H	275	PHE	CG-CD2-CE2	6.49	127.94	120.80
1	A	180	TYR	CG-CD1-CE1	-6.49	116.11	121.30
1	K	160	LEU	CB-CG-CD1	6.49	122.03	111.00
1	D	367	MET	CG-SD-CE	-6.48	89.83	100.20
1	A	490	TYR	CD1-CG-CD2	6.48	125.03	117.90
1	R	123	TYR	CD1-CE1-CZ	-6.48	113.97	119.80
1	P	434	PRO	N-CD-CG	6.47	112.91	103.20
1	N	200	TRP	CA-CB-CG	6.47	125.99	113.70
1	O	61	ASP	CB-CG-OD1	6.47	124.12	118.30
1	F	161	LEU	CB-CG-CD2	6.47	122.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	321	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	E	198	ASP	CB-CG-OD2	6.46	124.12	118.30
1	S	180	TYR	CB-CG-CD2	6.46	124.88	121.00
1	P	96	GLN	O-C-N	-6.46	112.36	122.70
1	D	209	ILE	O-C-N	-6.45	112.38	122.70
1	P	344	ASP	O-C-N	-6.44	112.40	122.70
1	M	203	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	B	141	VAL	CG1-CB-CG2	-6.43	100.60	110.90
1	A	360	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	L	61	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	M	458	LEU	CB-CG-CD1	6.43	121.93	111.00
1	N	468	ASP	CB-CG-OD1	6.43	124.09	118.30
1	K	162	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	L	69	THR	CA-CB-OG1	6.42	122.48	109.00
1	N	484	TRP	CA-CB-CG	6.42	125.90	113.70
1	M	468	ASP	CB-CG-OD1	6.42	124.08	118.30
1	O	454	LEU	CB-CG-CD2	-6.41	100.10	111.00
1	L	474	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	L	77	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	L	288	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	159	ASP	CB-CG-OD1	6.39	124.06	118.30
1	F	58	MET	CG-SD-CE	6.39	110.43	100.20
1	N	279	GLU	O-C-N	-6.39	112.47	122.70
1	C	532	ALA	N-CA-CB	-6.39	101.16	110.10
1	S	240	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	H	389	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	F	50	TYR	CB-CG-CD2	6.38	124.83	121.00
1	B	229	ASP	CB-CG-OD2	6.38	124.04	118.30
1	R	322	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	S	33	ARG	NE-CZ-NH2	6.37	123.49	120.30
1	C	411	ASP	CB-CG-OD2	6.37	124.03	118.30
1	D	283	ILE	CA-CB-CG1	6.37	123.10	111.00
1	G	484	TRP	CB-CG-CD1	-6.37	118.72	127.00
1	C	233	VAL	CA-CB-CG1	6.36	120.44	110.90
1	O	334	ALA	N-CA-CB	6.36	119.01	110.10
1	F	391	VAL	CA-CB-CG1	6.36	120.44	110.90
1	P	203	ASP	CB-CG-OD1	6.34	124.01	118.30
1	D	338	ARG	NH1-CZ-NH2	-6.34	112.43	119.40
1	B	400	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	H	474	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	F	392	ASP	CB-CG-OD1	6.33	124.00	118.30
1	N	250	ASP	CB-CG-OD2	-6.33	112.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	485	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	A	407	ASP	CB-CG-OD2	6.32	123.99	118.30
1	K	396	ARG	NH1-CZ-NH2	-6.32	112.45	119.40
1	C	71	ASP	C-N-CA	6.31	135.54	122.30
1	N	510	MET	CA-CB-CG	-6.31	102.58	113.30
1	E	348	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	A	480	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	G	288	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	261	ASP	CB-CG-OD1	6.30	123.97	118.30
1	F	421	VAL	CG1-CB-CG2	-6.30	100.83	110.90
1	S	447	TYR	CZ-CE2-CD2	-6.30	114.13	119.80
1	K	157	ASP	CB-CG-OD1	-6.29	112.63	118.30
1	C	180	TYR	CZ-CE2-CD2	-6.29	114.14	119.80
1	S	333	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	G	333	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	H	270	THR	O-C-N	-6.29	112.64	122.70
1	S	393	GLU	OE1-CD-OE2	-6.29	115.76	123.30
1	B	402	LEU	N-CA-CB	6.28	122.96	110.40
1	G	219	ASP	CB-CG-OD2	6.28	123.95	118.30
1	R	123	TYR	CG-CD2-CE2	-6.28	116.28	121.30
1	E	350	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	417	GLY	O-C-N	-6.27	112.54	123.20
1	C	33	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	N	384	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	D	523	VAL	CA-CB-CG2	-6.27	101.50	110.90
1	G	402	LEU	CB-CG-CD2	6.26	121.65	111.00
1	G	508	VAL	CA-CB-CG2	-6.26	101.52	110.90
1	K	382	LEU	CB-CG-CD2	-6.25	100.37	111.00
1	N	307	VAL	CG1-CB-CG2	-6.25	100.89	110.90
1	C	237	MET	CG-SD-CE	-6.25	90.20	100.20
1	L	528	ASP	CB-CG-OD1	6.24	123.92	118.30
1	R	265	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	D	268	ASP	CB-CG-OD1	6.24	123.91	118.30
1	K	489	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	R	159	ASP	CB-CG-OD2	6.23	123.90	118.30
1	R	360	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	D	125	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	348	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	K	288	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	N	118	ALA	CB-CA-C	-6.21	100.78	110.10
1	C	180	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	F	208	GLN	CA-CB-CG	6.21	127.06	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	152	THR	N-CA-CB	6.21	122.09	110.30
1	H	180	TYR	CB-CG-CD2	6.19	124.72	121.00
1	D	264	ILE	CA-CB-CG1	6.19	122.76	111.00
1	Q	104	THR	CA-CB-CG2	-6.19	103.73	112.40
1	Q	352	GLY	CA-C-O	6.19	131.74	120.60
1	F	61	ASP	CB-CG-OD1	6.19	123.87	118.30
1	L	407	ASP	CB-CG-OD2	6.18	123.86	118.30
1	D	400	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	I	139	GLU	OE1-CD-OE2	-6.18	115.89	123.30
1	L	477	HIS	CA-CB-CG	6.18	124.10	113.60
1	I	353	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	I	141	VAL	CG1-CB-CG2	-6.17	101.03	110.90
1	R	389	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	L	33	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	E	399	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	B	178	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	D	224	TYR	CG-CD2-CE2	-6.16	116.37	121.30
1	G	266	ILE	CG1-CB-CG2	-6.16	97.86	111.40
1	I	334	ALA	O-C-N	-6.15	112.86	122.70
1	K	276	LEU	CB-CG-CD2	6.15	121.45	111.00
1	M	61	ASP	CB-CG-OD1	6.15	123.83	118.30
1	R	50	TYR	CG-CD2-CE2	-6.15	116.38	121.30
1	B	384	ARG	N-CA-C	-6.15	94.41	111.00
1	M	413	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
1	Q	413	ARG	NH1-CZ-NH2	6.14	126.16	119.40
1	Q	389	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
1	P	491	ALA	N-CA-CB	-6.14	101.51	110.10
1	I	149	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	O	135	TYR	CG-CD1-CE1	-6.12	116.40	121.30
1	M	80	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	P	210	VAL	CG1-CB-CG2	-6.12	101.10	110.90
1	K	178	ARG	NH1-CZ-NH2	-6.12	112.67	119.40
1	C	77	ASP	CB-CG-OD1	6.12	123.80	118.30
1	S	56	ASP	CB-CG-OD1	6.11	123.80	118.30
1	H	185	VAL	CA-CB-CG2	-6.11	101.73	110.90
1	I	118	ALA	CB-CA-C	-6.11	100.94	110.10
1	K	471	MET	CG-SD-CE	-6.11	90.43	100.20
1	C	110	PHE	CB-CG-CD1	-6.11	116.53	120.80
1	A	171	SER	O-C-N	-6.10	112.94	122.70
1	D	123	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	N	460	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	A	324	LYS	O-C-N	-6.09	112.95	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	178	ARG	CG-CD-NE	-6.09	99.01	111.80
1	F	490	TYR	CG-CD2-CE2	-6.09	116.43	121.30
1	A	56	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	M	33	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	P	155	ILE	O-C-N	-6.08	112.98	122.70
1	K	415	ILE	O-C-N	-6.07	112.98	122.70
1	N	424	GLU	O-C-N	-6.07	112.98	122.70
1	C	65	ASP	CB-CG-OD1	-6.07	112.83	118.30
1	R	165	ALA	N-CA-CB	6.07	118.60	110.10
1	M	201	TYR	CG-CD1-CE1	-6.07	116.45	121.30
1	F	485	TYR	CB-CG-CD1	6.06	124.64	121.00
1	Q	93	ALA	N-CA-CB	-6.05	101.63	110.10
1	B	162	ARG	CD-NE-CZ	6.05	132.07	123.60
1	S	384	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
1	O	262	ALA	N-CA-CB	6.05	118.56	110.10
1	A	55	MET	CG-SD-CE	-6.04	90.53	100.20
1	A	485	TYR	CB-CG-CD2	6.04	124.62	121.00
1	A	488	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	B	482	ASN	N-CA-CB	6.04	121.47	110.60
1	G	311	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	S	473	LEU	CB-CG-CD2	6.04	121.27	111.00
1	M	424	GLU	O-C-N	-6.04	113.04	122.70
1	H	353	TYR	CG-CD1-CE1	-6.03	116.48	121.30
1	E	126	VAL	CG1-CB-CG2	-6.03	101.25	110.90
1	I	413	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	P	32	VAL	CG1-CB-CG2	-6.02	101.26	110.90
1	N	423	ILE	O-C-N	-6.02	113.07	122.70
1	S	368	VAL	CG1-CB-CG2	-6.01	101.28	110.90
1	M	120	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	M	232	VAL	CA-CB-CG2	6.01	119.92	110.90
1	O	110	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	O	516	ALA	N-CA-CB	-6.01	101.69	110.10
1	G	440	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	N	129	THR	CA-CB-CG2	-6.01	103.99	112.40
1	Q	183	ASP	CB-CG-OD2	6.01	123.70	118.30
1	Q	490	TYR	CA-CB-CG	-6.00	102.00	113.40
1	I	399	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	E	261	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	E	510	MET	CG-SD-CE	-5.99	90.62	100.20
1	M	311	TYR	CG-CD1-CE1	-5.99	116.51	121.30
1	R	59	LEU	O-C-N	5.99	132.28	122.70
1	H	263	GLU	O-C-N	-5.98	113.13	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	462	ALA	N-CA-CB	5.98	118.48	110.10
1	G	232	VAL	CA-CB-CG2	5.98	119.88	110.90
1	G	321	ARG	CD-NE-CZ	5.98	131.98	123.60
1	I	177	ALA	N-CA-CB	-5.98	101.72	110.10
1	L	485	TYR	CB-CG-CD1	5.98	124.59	121.00
1	S	384	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	E	229	ASP	O-C-N	-5.97	113.15	122.70
1	P	320	VAL	CG1-CB-CG2	-5.97	101.35	110.90
1	G	433	ALA	CA-C-N	5.97	133.81	117.10
1	P	135	TYR	CB-CG-CD2	5.97	124.58	121.00
1	S	150	ALA	N-CA-CB	5.97	118.46	110.10
1	C	275	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	F	265	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	G	338	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	I	488	ASP	CB-CG-OD1	5.96	123.67	118.30
1	L	525	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	K	425	ILE	O-C-N	-5.96	113.17	122.70
1	H	90	VAL	CG1-CB-CG2	5.95	120.42	110.90
1	I	421	VAL	CA-CB-CG2	-5.95	101.98	110.90
1	N	46	LEU	CB-CG-CD2	5.95	121.11	111.00
1	S	237	MET	CG-SD-CE	-5.95	90.69	100.20
1	E	322	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	H	305	ASP	CB-CG-OD1	5.95	123.65	118.30
1	L	274	LYS	CA-C-O	5.94	132.57	120.10
1	P	480	GLU	CG-CD-OE2	-5.94	106.42	118.30
1	G	224	TYR	CB-CG-CD2	5.94	124.56	121.00
1	E	462	ALA	CB-CA-C	-5.93	101.20	110.10
1	I	432	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	L	121	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	Q	265	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	R	391	VAL	CA-CB-CG2	-5.93	102.01	110.90
1	E	157	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	E	373	ALA	CB-CA-C	5.92	118.98	110.10
1	G	310	SER	N-CA-CB	5.92	119.38	110.50
1	I	240	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	G	194	GLU	OE1-CD-OE2	-5.92	116.20	123.30
1	H	360	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	K	33	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	Q	198	ASP	CB-CG-OD1	5.92	123.63	118.30
1	H	265	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
1	O	485	TYR	CB-CG-CD2	5.91	124.55	121.00
1	A	295	ALA	N-CA-CB	-5.91	101.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	384	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	Q	512	ALA	CB-CA-C	5.90	118.95	110.10
1	O	265	ARG	CD-NE-CZ	5.90	131.86	123.60
1	E	33	ARG	CG-CD-NE	-5.89	99.42	111.80
1	H	478	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	O	175	ALA	CA-C-N	5.89	127.99	116.20
1	N	48	SER	O-C-N	-5.89	113.27	122.70
1	F	123	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	D	77	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	F	293	THR	CA-CB-OG1	5.89	121.36	109.00
1	D	414	ALA	O-C-N	-5.88	113.29	122.70
1	G	432	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	S	56	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	Q	53	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	R	255	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	L	322	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	N	219	ASP	CA-CB-CG	-5.88	100.47	113.40
1	N	120	ASP	O-C-N	-5.88	113.30	122.70
1	I	311	TYR	CB-CG-CD1	5.88	124.53	121.00
1	K	102	ASP	CB-CG-OD1	5.88	123.59	118.30
1	S	471	MET	CG-SD-CE	-5.88	90.80	100.20
1	M	317	VAL	CA-CB-CG2	-5.87	102.09	110.90
1	O	367	MET	CG-SD-CE	-5.87	90.80	100.20
1	G	272	MET	CG-SD-CE	-5.87	90.81	100.20
1	I	247	ALA	C-N-CA	5.87	136.38	121.70
1	O	204	LEU	O-C-N	-5.87	113.31	122.70
1	Q	389	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	E	396	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	F	157	ASP	CB-CG-OD1	5.86	123.57	118.30
1	S	396	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	S	453	SER	N-CA-CB	-5.85	101.72	110.50
1	R	247	ALA	CB-CA-C	-5.85	101.32	110.10
1	E	436	VAL	CA-CB-CG2	5.85	119.67	110.90
1	K	265	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	L	341	SER	N-CA-CB	5.85	119.27	110.50
1	O	473	LEU	CA-CB-CG	5.85	128.75	115.30
1	S	455	VAL	CA-CB-CG1	-5.85	102.13	110.90
1	B	474	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	H	527	ASP	CB-CG-OD2	5.84	123.56	118.30
1	S	272	MET	CG-SD-CE	-5.84	90.85	100.20
1	S	228	VAL	CA-CB-CG1	-5.84	102.14	110.90
1	R	50	TYR	CZ-CE2-CD2	5.84	125.06	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	K	180	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	S	117	LYS	O-C-N	-5.84	113.36	122.70
1	M	231	GLU	N-CA-CB	-5.83	100.10	110.60
1	A	180	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	S	322	ARG	CD-NE-CZ	5.83	131.76	123.60
1	H	512	ALA	C-N-CA	5.83	136.27	121.70
1	P	141	VAL	CA-CB-CG2	-5.83	102.16	110.90
1	B	319	ALA	CB-CA-C	-5.83	101.36	110.10
1	D	429	LEU	CB-CG-CD1	5.83	120.91	111.00
1	H	470	LEU	CB-CG-CD2	-5.82	101.10	111.00
1	E	331	LEU	O-C-N	-5.82	113.39	122.70
1	L	110	PHE	CB-CG-CD1	-5.82	116.73	120.80
1	P	192	VAL	CA-CB-CG2	-5.82	102.18	110.90
1	D	474	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	E	285	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	A	119	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	A	329	GLU	O-C-N	-5.81	113.41	122.70
1	I	149	LEU	O-C-N	-5.81	113.40	122.70
1	K	320	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	O	525	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	Q	475	SER	N-CA-CB	5.81	119.21	110.50
1	C	220	THR	O-C-N	-5.81	113.41	122.70
1	F	33	ARG	CG-CD-NE	-5.81	99.60	111.80
1	G	484	TRP	CB-CG-CD2	5.81	134.15	126.60
1	C	222	LEU	CB-CG-CD2	5.81	120.87	111.00
1	D	338	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	B	392	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	270	THR	O-C-N	-5.79	113.43	122.70
1	E	45	ALA	N-CA-CB	-5.79	101.99	110.10
1	H	123	TYR	CZ-CE2-CD2	5.79	125.01	119.80
1	L	447	TYR	CG-CD1-CE1	-5.79	116.67	121.30
1	L	195	LEU	O-C-N	-5.79	113.44	122.70
1	A	505	PRO	N-CA-CB	5.79	110.24	103.30
1	H	338	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	S	378	SER	CB-CA-C	-5.78	99.12	110.10
1	L	174	VAL	CG1-CB-CG2	-5.78	101.66	110.90
1	B	430	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	R	107	ALA	CB-CA-C	5.77	118.76	110.10
1	R	43	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	C	39	VAL	CA-CB-CG2	-5.77	102.25	110.90
1	K	525	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	237	MET	CG-SD-CE	-5.76	90.98	100.20
1	O	480	GLU	O-C-N	-5.76	113.48	122.70
1	R	413	ARG	CG-CD-NE	-5.76	99.71	111.80
1	Q	530	VAL	O-C-N	-5.75	113.50	122.70
1	N	389	ARG	CG-CD-NE	-5.75	99.73	111.80
1	S	59	LEU	CB-CG-CD2	5.75	120.77	111.00
1	D	123	TYR	CG-CD2-CE2	-5.75	116.70	121.30
1	H	80	ASP	N-CA-CB	-5.74	100.26	110.60
1	O	123	TYR	CG-CD1-CE1	-5.74	116.71	121.30
1	D	370	VAL	CA-CB-CG2	-5.74	102.30	110.90
1	P	369	PHE	CB-CG-CD1	-5.74	116.78	120.80
1	R	151	GLN	CG-CD-OE1	5.73	133.06	121.60
1	C	501	GLY	O-C-N	-5.73	113.53	122.70
1	M	496	ASP	CB-CG-OD2	5.73	123.45	118.30
1	Q	470	LEU	CB-CG-CD2	5.73	120.73	111.00
1	R	318	LEU	CB-CG-CD2	5.73	120.73	111.00
1	P	265	ARG	CG-CD-NE	-5.72	99.78	111.80
1	E	450	ALA	CB-CA-C	5.72	118.68	110.10
1	B	369	PHE	CB-CG-CD1	5.72	124.81	120.80
1	C	407	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	510	MET	CG-SD-CE	-5.72	91.05	100.20
1	L	384	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	H	229	ASP	CB-CG-OD2	5.71	123.44	118.30
1	H	162	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	Q	104	THR	N-CA-CB	5.71	121.15	110.30
1	Q	185	VAL	CA-CB-CG2	-5.71	102.33	110.90
1	L	125	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	D	382	LEU	CB-CG-CD1	5.71	120.70	111.00
1	G	265	ARG	CG-CD-NE	-5.71	99.81	111.80
1	I	227	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	G	311	TYR	CB-CG-CD2	5.70	124.42	121.00
1	R	305	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	O	334	ALA	CB-CA-C	-5.70	101.55	110.10
1	G	180	TYR	CG-CD2-CE2	-5.70	116.74	121.30
1	S	469	LEU	CB-CG-CD2	5.70	120.68	111.00
1	B	79	MET	CA-CB-CG	5.69	122.98	113.30
1	B	259	GLU	O-C-N	-5.69	113.59	122.70
1	H	178	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	E	297	VAL	CB-CA-C	5.69	122.20	111.40
1	P	178	ARG	NH1-CZ-NH2	-5.69	113.15	119.40
1	E	333	ARG	CD-NE-CZ	5.68	131.56	123.60
1	F	76	LEU	N-CA-CB	-5.68	99.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	198	ASP	CB-CA-C	5.68	121.77	110.40
1	E	365	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	D	351	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	G	334	ALA	CB-CA-C	-5.67	101.59	110.10
1	N	33	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	C	30	GLU	N-CA-C	5.67	126.30	111.00
1	D	365	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	205	ASP	CB-CG-OD2	5.66	123.39	118.30
1	H	432	TYR	CB-CG-CD2	5.66	124.40	121.00
1	K	224	TYR	CA-CB-CG	-5.66	102.66	113.40
1	R	496	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	422	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	G	338	ARG	CA-CB-CG	5.65	125.82	113.40
1	H	102	ASP	CB-CG-OD2	5.65	123.38	118.30
1	I	445	GLU	O-C-N	-5.65	113.66	122.70
1	P	259	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	R	426	ALA	O-C-N	-5.65	113.67	122.70
1	E	70	ASN	O-C-N	-5.64	113.67	122.70
1	G	432	TYR	CG-CD2-CE2	5.64	125.81	121.30
1	A	220	THR	CA-CB-CG2	-5.64	104.51	112.40
1	E	360	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	S	311	TYR	CG-CD2-CE2	-5.64	116.79	121.30
1	C	350	ASP	CB-CG-OD2	5.63	123.37	118.30
1	L	248	LEU	CB-CG-CD2	5.63	120.58	111.00
1	E	358	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	O	304	ILE	O-C-N	-5.63	113.70	122.70
1	H	327	ASP	CB-CG-OD1	5.62	123.36	118.30
1	G	407	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	F	201	TYR	CD1-CE1-CZ	5.62	124.85	119.80
1	S	345	GLU	O-C-N	-5.61	113.72	122.70
1	M	180	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	B	327	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	B	432	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	N	370	VAL	O-C-N	-5.61	113.73	122.70
1	S	389	ARG	CG-CD-NE	-5.61	100.03	111.80
1	I	525	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	F	318	LEU	CB-CG-CD2	5.60	120.52	111.00
1	K	413	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	S	362	VAL	CG1-CB-CG2	-5.59	101.95	110.90
1	F	427	LYS	N-CA-CB	-5.59	100.54	110.60
1	R	416	ALA	N-CA-CB	5.59	117.92	110.10
1	D	353	TYR	CG-CD2-CE2	-5.59	116.83	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	391	VAL	CA-CB-CG1	5.58	119.28	110.90
1	D	528	ASP	CB-CG-OD1	5.58	123.33	118.30
1	L	123	TYR	CB-CG-CD2	5.58	124.35	121.00
1	B	350	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	C	242	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	S	527	ASP	N-CA-CB	-5.58	100.56	110.60
1	R	430	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	R	194	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	R	498	TRP	CB-CG-CD1	5.58	134.25	127.00
1	M	430	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	365	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	F	250	ASP	CB-CG-OD2	5.57	123.31	118.30
1	N	440	GLU	O-C-N	-5.57	113.80	122.70
1	I	384	ARG	N-CA-C	-5.56	95.98	111.00
1	I	333	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	M	65	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	F	490	TYR	CA-CB-CG	-5.55	102.85	113.40
1	N	185	VAL	CA-CB-CG1	5.55	119.23	110.90
1	N	327	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	287	VAL	CG1-CB-CG2	-5.55	102.02	110.90
1	C	175	ALA	O-C-N	-5.55	113.76	123.20
1	N	328	LEU	CB-CG-CD2	5.55	120.43	111.00
1	R	74	THR	O-C-N	-5.55	113.82	122.70
1	F	44	GLU	O-C-N	-5.55	113.83	122.70
1	I	50	TYR	CD1-CG-CD2	5.55	124.00	117.90
1	K	79	MET	CG-SD-CE	-5.54	91.33	100.20
1	A	353	TYR	CG-CD1-CE1	5.54	125.73	121.30
1	A	523	VAL	CA-CB-CG2	-5.54	102.58	110.90
1	C	80	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	148	GLU	CA-C-O	5.54	131.74	120.10
1	D	391	VAL	C-N-CA	5.54	135.56	121.70
1	P	115	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	Q	320	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	K	139	GLU	CB-CA-C	5.54	121.48	110.40
1	E	360	ARG	O-C-N	-5.54	113.84	122.70
1	L	49	THR	CA-CB-OG1	5.54	120.63	109.00
1	H	272	MET	CG-SD-CE	-5.54	91.34	100.20
1	R	526	ILE	O-C-N	-5.54	113.84	122.70
1	H	277	ASP	CB-CG-OD2	5.53	123.28	118.30
1	M	484	TRP	CH2-CZ2-CE2	5.53	122.93	117.40
1	A	465	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	K	322	ARG	NE-CZ-NH2	-5.53	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	426	ALA	CB-CA-C	5.53	118.39	110.10
1	S	350	ASP	CB-CG-OD1	5.53	123.28	118.30
1	E	208	GLN	O-C-N	-5.53	113.86	122.70
1	E	433	ALA	CA-C-O	-5.53	108.50	120.10
1	A	275	PHE	CB-CG-CD1	-5.52	116.93	120.80
1	N	305	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	R	119	GLU	OE1-CD-OE2	-5.52	116.67	123.30
1	D	78	LYS	O-C-N	-5.52	113.86	122.70
1	M	529	VAL	CA-CB-CG1	-5.52	102.62	110.90
1	P	49	THR	CA-CB-CG2	-5.52	104.67	112.40
1	C	451	LEU	CB-CA-C	-5.51	99.72	110.20
1	R	153	VAL	CA-CB-CG2	-5.51	102.63	110.90
1	Q	382	LEU	CB-CG-CD1	5.51	120.37	111.00
1	P	425	ILE	CA-CB-CG1	5.51	121.47	111.00
1	P	474	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	R	275	PHE	CB-CG-CD1	5.51	124.66	120.80
1	N	101	ALA	O-C-N	-5.51	113.89	122.70
1	A	180	TYR	CD1-CE1-CZ	5.51	124.76	119.80
1	Q	333	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	L	389	ARG	CG-CD-NE	-5.50	100.24	111.80
1	B	219	ASP	CB-CG-OD1	5.50	123.25	118.30
1	G	474	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	S	411	ASP	CB-CA-C	5.50	121.41	110.40
1	P	413	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	C	490	TYR	CG-CD2-CE2	-5.50	116.90	121.30
1	B	502	VAL	CA-CB-CG2	-5.50	102.65	110.90
1	E	341	SER	N-CA-CB	5.50	118.75	110.50
1	B	360	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	H	57	LYS	N-CA-CB	5.50	120.50	110.60
1	S	174	VAL	O-C-N	-5.50	113.91	122.70
1	B	205	ASP	CB-CG-OD2	5.50	123.25	118.30
1	R	244	ALA	N-CA-CB	-5.49	102.41	110.10
1	A	317	VAL	O-C-N	-5.49	113.92	122.70
1	H	429	LEU	CB-CG-CD1	5.49	120.33	111.00
1	Q	50	TYR	CG-CD2-CE2	-5.49	116.91	121.30
1	K	484	TRP	CB-CG-CD1	-5.49	119.87	127.00
1	P	240	ARG	NH1-CZ-NH2	-5.49	113.37	119.40
1	D	456	SER	N-CA-CB	5.48	118.72	110.50
1	R	242	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	A	389	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	F	434	PRO	N-CA-CB	5.48	109.88	103.30
1	G	101	ALA	CB-CA-C	5.48	118.32	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	153	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	C	250	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	495	VAL	CA-CB-CG1	-5.47	102.69	110.90
1	C	460	GLU	OE1-CD-OE2	5.47	129.87	123.30
1	H	180	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	K	222	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	O	432	TYR	CG-CD1-CE1	-5.47	116.92	121.30
1	B	468	ASP	CB-CG-OD1	5.47	123.22	118.30
1	R	288	ASP	O-C-N	-5.47	113.95	122.70
1	G	351	LEU	O-C-N	-5.47	113.91	123.20
1	G	389	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	411	ASP	CB-CG-OD1	5.46	123.22	118.30
1	H	167	THR	O-C-N	-5.46	113.96	122.70
1	H	392	ASP	CB-CG-OD1	5.46	123.22	118.30
1	K	121	LEU	O-C-N	-5.46	113.96	122.70
1	N	525	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	O	411	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	79	MET	CG-SD-CE	-5.46	91.47	100.20
1	G	487	ILE	CA-CB-CG1	5.46	121.37	111.00
1	R	50	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	A	82	GLN	O-C-N	-5.46	113.97	122.70
1	N	338	ARG	CD-NE-CZ	5.45	131.23	123.60
1	L	389	ARG	CB-CG-CD	5.45	125.77	111.60
1	I	413	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	G	211	LYS	CA-CB-CG	5.45	125.38	113.40
1	P	504	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	H	178	ARG	CD-NE-CZ	5.45	131.22	123.60
1	L	98	GLU	O-C-N	-5.45	113.99	122.70
1	B	220	THR	CA-CB-CG2	-5.44	104.78	112.40
1	I	311	TYR	CG-CD2-CE2	-5.44	116.94	121.30
1	Q	512	ALA	N-CA-CB	-5.44	102.48	110.10
1	D	494	PRO	N-CA-CB	5.44	109.83	103.30
1	E	447	TYR	CB-CG-CD1	5.44	124.27	121.00
1	P	157	ASP	CB-CG-OD1	5.44	123.20	118.30
1	D	305	ASP	CB-CG-OD1	5.44	123.19	118.30
1	L	125	ASP	CB-CG-OD2	5.44	123.19	118.30
1	P	392	ASP	CB-CG-OD1	5.44	123.19	118.30
1	E	484	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	A	470	LEU	CB-CG-CD1	5.43	120.24	111.00
1	C	90	VAL	CA-CB-CG1	-5.43	102.75	110.90
1	C	522	LEU	CB-CG-CD1	5.43	120.24	111.00
1	D	349	GLN	CG-CD-OE1	-5.43	110.73	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	ASP	CB-CA-C	5.43	121.27	110.40
1	B	331	LEU	N-CA-CB	-5.43	99.53	110.40
1	H	255	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	P	304	ILE	CA-CB-CG2	-5.43	100.03	110.90
1	E	481	ASN	CA-CB-CG	-5.43	101.45	113.40
1	I	415	ILE	O-C-N	-5.43	114.01	122.70
1	D	160	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	B	55	MET	CG-SD-CE	-5.42	91.52	100.20
1	I	39	VAL	CA-CB-CG2	-5.41	102.78	110.90
1	K	317	VAL	CA-CB-CG1	-5.41	102.78	110.90
1	L	333	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	M	261	ASP	CB-CG-OD1	5.41	123.17	118.30
1	M	291	LEU	C-N-CA	5.41	135.22	121.70
1	P	516	ALA	N-CA-C	5.41	125.61	111.00
1	H	129	THR	CA-CB-CG2	-5.41	104.83	112.40
1	N	186	VAL	CB-CA-C	-5.41	101.13	111.40
1	C	229	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	528	ASP	CA-C-N	-5.40	105.31	117.20
1	D	406	ALA	N-CA-CB	-5.40	102.53	110.10
1	R	485	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	N	71	ASP	CB-CG-OD2	5.40	123.16	118.30
1	P	514	LYS	N-CA-CB	5.40	120.32	110.60
1	H	354	ALA	N-CA-CB	5.40	117.66	110.10
1	I	322	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	S	215	GLY	O-C-N	-5.40	114.06	122.70
1	B	108	VAL	CA-CB-CG1	5.40	119.00	110.90
1	F	384	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	L	525	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	R	279	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	S	292	ALA	N-CA-CB	5.39	117.65	110.10
1	D	484	TRP	CH2-CZ2-CE2	5.39	122.79	117.40
1	L	384	ARG	CD-NE-CZ	5.39	131.15	123.60
1	I	400	ASP	CB-CG-OD2	5.39	123.15	118.30
1	I	432	TYR	CB-CG-CD2	5.39	124.23	121.00
1	M	369	PHE	CB-CG-CD2	5.39	124.57	120.80
1	N	432	TYR	CG-CD2-CE2	-5.39	116.99	121.30
1	R	305	ASP	O-C-N	-5.39	114.08	122.70
1	F	475	SER	C-N-CA	5.38	135.16	121.70
1	C	389	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	G	279	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	B	296	ASN	O-C-N	-5.38	114.09	122.70
1	G	401	ALA	CB-CA-C	5.38	118.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	100	THR	CA-CB-CG2	-5.38	104.87	112.40
1	R	353	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	N	162	ARG	CD-NE-CZ	5.38	131.13	123.60
1	G	201	TYR	CZ-CE2-CD2	5.37	124.64	119.80
1	O	224	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	P	203	ASP	CA-CB-CG	5.37	125.21	113.40
1	K	506	ALA	CB-CA-C	5.36	118.14	110.10
1	F	506	ALA	O-C-N	-5.36	114.12	122.70
1	G	327	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	S	46	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	C	256	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	D	301	GLN	O-C-N	-5.36	114.13	122.70
1	E	430	ARG	CD-NE-CZ	-5.36	116.10	123.60
1	K	489	LEU	CB-CG-CD2	5.36	120.10	111.00
1	G	236	GLY	O-C-N	-5.35	114.14	122.70
1	M	135	TYR	CD1-CE1-CZ	-5.35	114.98	119.80
1	A	272	MET	CG-SD-CE	-5.35	91.64	100.20
1	M	224	TYR	CD1-CE1-CZ	-5.35	114.98	119.80
1	H	50	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	C	424	GLU	O-C-N	-5.34	114.15	122.70
1	O	280	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	F	287	VAL	CA-CB-CG2	5.34	118.91	110.90
1	L	399	ARG	CG-CD-NE	-5.34	100.58	111.80
1	C	277	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	F	247	ALA	C-N-CA	5.34	135.05	121.70
1	C	510	MET	CG-SD-CE	-5.34	91.66	100.20
1	D	466	PRO	N-CA-C	5.33	125.97	112.10
1	I	42	VAL	CA-CB-CG2	-5.33	102.90	110.90
1	S	219	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	279	GLU	CA-CB-CG	5.33	125.13	113.40
1	D	222	LEU	CB-CA-C	5.33	120.32	110.20
1	E	344	ASP	CB-CG-OD2	5.33	123.09	118.30
1	O	122	LEU	O-C-N	-5.33	114.18	122.70
1	S	244	ALA	N-CA-CB	-5.33	102.64	110.10
1	E	505	PRO	N-CD-CG	5.33	111.19	103.20
1	K	208	GLN	CA-CB-CG	5.33	125.12	113.40
1	E	219	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	E	527	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	F	120	ASP	CB-CG-OD1	5.33	123.09	118.30
1	F	298	ILE	O-C-N	-5.33	114.18	122.70
1	O	275	PHE	CG-CD2-CE2	-5.33	114.94	120.80
1	D	485	TYR	CB-CG-CD1	5.32	124.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	147	GLN	O-C-N	-5.32	114.19	122.70
1	P	219	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	N	353	TYR	CD1-CG-CD2	5.32	123.75	117.90
1	D	396	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Q	277	ASP	CB-CG-OD2	5.32	123.08	118.30
1	P	55	MET	CA-CB-CG	5.32	122.34	113.30
1	C	476	THR	C-N-CA	5.31	134.98	121.70
1	D	241	LEU	CB-CG-CD1	5.31	120.03	111.00
1	F	65	ASP	CB-CG-OD1	5.31	123.08	118.30
1	G	190	THR	O-C-N	-5.31	114.20	122.70
1	L	136	LYS	O-C-N	-5.31	114.20	122.70
1	A	233	VAL	O-C-N	-5.31	114.21	122.70
1	C	340	VAL	CA-CB-CG2	-5.31	102.94	110.90
1	S	448	ALA	O-C-N	-5.31	114.21	122.70
1	D	224	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	H	384	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	265	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	P	438	GLY	CA-C-O	5.30	130.15	120.60
1	D	31	ALA	CB-CA-C	5.30	118.05	110.10
1	N	310	SER	O-C-N	-5.30	114.22	122.70
1	Q	50	TYR	CB-CG-CD1	5.30	124.18	121.00
1	R	100	THR	O-C-N	-5.29	114.23	122.70
1	G	473	LEU	CB-CG-CD2	5.29	119.99	111.00
1	K	430	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	L	74	THR	O-C-N	-5.29	114.24	122.70
1	L	263	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	D	108	VAL	CG1-CB-CG2	-5.29	102.44	110.90
1	R	332	ALA	CB-CA-C	5.29	118.03	110.10
1	H	223	VAL	O-C-N	-5.29	114.24	122.70
1	E	278	GLU	N-CA-CB	-5.28	101.09	110.60
1	M	368	VAL	CA-CB-CG2	-5.28	102.97	110.90
1	D	150	ALA	O-C-N	-5.28	114.25	122.70
1	C	528	ASP	CB-CG-OD1	5.28	123.05	118.30
1	I	122	LEU	CB-CG-CD2	5.28	119.97	111.00
1	S	232	VAL	CA-CB-CG1	5.28	118.81	110.90
1	B	301	GLN	N-CA-CB	-5.27	101.11	110.60
1	Q	262	ALA	N-CA-CB	5.27	117.48	110.10
1	B	305	ASP	OD1-CG-OD2	-5.27	113.29	123.30
1	C	305	ASP	O-C-N	-5.27	114.27	122.70
1	M	189	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	P	265	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	S	359	GLU	OE1-CD-OE2	-5.27	116.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	443	ALA	N-CA-CB	5.26	117.47	110.10
1	C	125	ASP	CB-CG-OD2	5.26	123.04	118.30
1	O	232	VAL	O-C-N	-5.26	114.28	122.70
1	B	215	GLY	O-C-N	-5.26	114.28	122.70
1	B	485	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	D	523	VAL	O-C-N	-5.26	114.28	122.70
1	I	344	ASP	CB-CA-C	-5.26	99.88	110.40
1	I	355	SER	CB-CA-C	-5.26	100.11	110.10
1	M	224	TYR	CG-CD2-CE2	-5.26	117.09	121.30
1	A	354	ALA	O-C-N	-5.26	114.29	122.70
1	O	32	VAL	CA-CB-CG2	-5.26	103.01	110.90
1	H	344	ASP	CB-CG-OD2	5.26	123.03	118.30
1	N	32	VAL	CA-CB-CG2	-5.25	103.02	110.90
1	S	411	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	B	203	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	B	384	ARG	O-C-N	-5.25	114.27	123.20
1	E	392	ASP	CB-CG-OD2	5.25	123.03	118.30
1	E	305	ASP	CB-CA-C	-5.25	99.90	110.40
1	F	421	VAL	C-N-CA	5.25	134.83	121.70
1	G	423	ILE	O-C-N	-5.25	114.30	122.70
1	O	220	THR	CA-CB-OG1	5.25	120.03	109.00
1	S	203	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	D	477	HIS	CA-CB-CG	5.25	122.52	113.60
1	E	224	TYR	O-C-N	-5.25	114.28	123.20
1	N	165	ALA	O-C-N	-5.25	114.30	122.70
1	E	83	HIS	CA-CB-CG	5.25	122.52	113.60
1	H	185	VAL	O-C-N	-5.25	114.31	122.70
1	I	77	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	O	413	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	E	389	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	N	224	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	R	391	VAL	CA-CB-CG1	5.24	118.77	110.90
1	S	384	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	392	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	S	339	VAL	CB-CA-C	-5.24	101.45	111.40
1	O	416	ALA	CA-C-N	5.24	126.67	116.20
1	E	408	VAL	CA-CB-CG2	-5.23	103.05	110.90
1	N	135	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	R	80	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	S	359	GLU	O-C-N	-5.23	114.33	122.70
1	I	347	SER	N-CA-CB	5.23	118.34	110.50
1	K	71	ASP	CB-CG-OD2	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	257	LYS	CB-CA-C	-5.23	99.94	110.40
1	N	232	VAL	CA-CB-CG2	5.22	118.74	110.90
1	R	407	ASP	OD1-CG-OD2	-5.22	113.37	123.30
1	C	296	ASN	CB-CG-OD1	5.22	132.05	121.60
1	D	465	ASP	CB-CG-OD1	5.22	123.00	118.30
1	F	443	ALA	N-CA-CB	5.22	117.41	110.10
1	G	370	VAL	CG1-CB-CG2	-5.22	102.55	110.90
1	P	55	MET	CG-SD-CE	-5.22	91.85	100.20
1	P	484	TRP	CA-CB-CG	5.22	123.61	113.70
1	B	422	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	K	196	ARG	CD-NE-CZ	5.21	130.90	123.60
1	P	399	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	E	403	GLY	O-C-N	-5.21	114.36	122.70
1	L	369	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	O	317	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	141	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	B	250	ASP	CB-CG-OD1	5.20	122.98	118.30
1	M	63	LEU	CB-CG-CD2	5.20	119.85	111.00
1	N	474	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	P	53	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	M	178	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	166	MET	CA-CB-CG	5.20	122.14	113.30
1	B	285	GLU	N-CA-CB	5.20	119.96	110.60
1	D	503	ILE	CA-CB-CG1	5.20	120.88	111.00
1	K	474	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	C	432	TYR	CD1-CG-CD2	5.20	123.62	117.90
1	L	295	ALA	O-C-N	-5.20	114.39	122.70
1	I	389	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	R	507	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	K	347	SER	N-CA-CB	5.19	118.29	110.50
1	N	397	ALA	N-CA-CB	-5.19	102.83	110.10
1	P	53	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	B	219	ASP	O-C-N	-5.19	114.40	122.70
1	D	524	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	O	107	ALA	O-C-N	-5.19	114.40	122.70
1	C	55	MET	N-CA-CB	-5.19	101.26	110.60
1	H	49	THR	CA-CB-OG1	5.18	119.88	109.00
1	S	108	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	B	157	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	196	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	H	50	TYR	C-N-CA	5.18	133.17	122.30
1	H	339	VAL	CB-CA-C	-5.17	101.57	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	192	VAL	CA-CB-CG1	5.17	118.66	110.90
1	N	322	ARG	O-C-N	-5.17	114.43	122.70
1	L	159	ASP	CB-CG-OD1	5.17	122.95	118.30
1	E	447	TYR	CA-C-O	5.17	130.96	120.10
1	H	348	GLU	CA-CB-CG	5.17	124.77	113.40
1	M	292	ALA	CB-CA-C	-5.17	102.35	110.10
1	N	240	ARG	CG-CD-NE	-5.17	100.94	111.80
1	O	389	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	D	258	PRO	N-CA-C	5.17	125.53	112.10
1	E	321	ARG	CG-CD-NE	-5.17	100.95	111.80
1	I	356	LEU	O-C-N	-5.17	114.44	122.70
1	C	77	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	Q	471	MET	CG-SD-CE	-5.16	91.94	100.20
1	H	152	THR	CA-CB-CG2	-5.16	105.17	112.40
1	M	458	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	E	237	MET	CG-SD-CE	-5.16	91.95	100.20
1	E	498	TRP	CB-CG-CD1	5.16	133.71	127.00
1	H	201	TYR	CZ-CE2-CD2	-5.16	115.16	119.80
1	L	250	ASP	N-CA-CB	-5.16	101.32	110.60
1	M	50	TYR	CB-CG-CD1	5.16	124.09	121.00
1	M	469	LEU	CB-CG-CD1	5.16	119.77	111.00
1	E	277	ASP	N-CA-CB	-5.16	101.32	110.60
1	C	196	ARG	CA-C-N	5.15	126.51	116.20
1	S	256	GLU	N-CA-CB	-5.15	101.32	110.60
1	F	125	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	L	71	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	L	523	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	S	447	TYR	CG-CD1-CE1	-5.15	117.18	121.30
1	E	379	ILE	CA-CB-CG1	5.15	120.78	111.00
1	S	413	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	E	128	PRO	CA-N-CD	5.15	118.91	111.70
1	H	101	ALA	N-CA-CB	-5.15	102.89	110.10
1	K	468	ASP	O-C-N	-5.15	114.46	122.70
1	K	185	VAL	CA-CB-CG1	5.15	118.62	110.90
1	C	162	ARG	CG-CD-NE	-5.14	101.00	111.80
1	M	178	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
1	O	162	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	Q	484	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	C	428	LYS	CA-CB-CG	5.14	124.71	113.40
1	B	521	THR	CA-CB-CG2	-5.14	105.20	112.40
1	A	149	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	S	329	GLU	OE1-CD-OE2	-5.14	117.14	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	227	VAL	CA-CB-CG2	-5.13	103.20	110.90
1	H	220	THR	CA-CB-CG2	-5.13	105.21	112.40
1	H	321	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	P	203	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	O	474	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	S	58	MET	CG-SD-CE	-5.13	91.99	100.20
1	K	322	ARG	CD-NE-CZ	5.13	130.78	123.60
1	P	233	VAL	O-C-N	-5.13	114.49	122.70
1	I	230	LYS	CA-C-O	5.13	130.87	120.10
1	L	135	TYR	CG-CD2-CE2	-5.13	117.20	121.30
1	L	224	TYR	CZ-CE2-CD2	5.13	124.42	119.80
1	M	97	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	L	399	ARG	NH1-CZ-NH2	5.12	125.04	119.40
1	C	431	LYS	N-CA-CB	-5.12	101.38	110.60
1	C	512	ALA	CB-CA-C	-5.12	102.42	110.10
1	A	35	ASN	CB-CG-OD1	5.12	131.84	121.60
1	A	490	TYR	CG-CD2-CE2	-5.12	117.21	121.30
1	E	220	THR	CA-CB-CG2	-5.12	105.23	112.40
1	F	317	VAL	CA-CB-CG1	5.12	118.58	110.90
1	G	248	LEU	CB-CG-CD1	5.12	119.70	111.00
1	G	288	ASP	CB-CG-OD1	-5.12	113.70	118.30
1	M	224	TYR	CB-CG-CD2	5.12	124.07	121.00
1	S	338	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	F	340	VAL	CA-CB-CG2	-5.11	103.23	110.90
1	D	420	ALA	N-CA-CB	-5.11	102.95	110.10
1	F	102	ASP	CB-CG-OD1	5.11	122.90	118.30
1	M	143	LEU	O-C-N	-5.11	114.53	122.70
1	Q	126	VAL	CA-CB-CG1	-5.11	103.23	110.90
1	A	384	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	R	202	VAL	O-C-N	-5.11	114.53	122.70
1	C	288	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	E	319	ALA	N-CA-CB	-5.11	102.95	110.10
1	B	174	VAL	CA-CB-CG1	-5.10	103.25	110.90
1	F	353	TYR	CG-CD2-CE2	5.10	125.38	121.30
1	P	198	ASP	O-C-N	-5.10	114.53	122.70
1	R	474	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	G	220	THR	CA-CB-CG2	-5.10	105.26	112.40
1	M	469	LEU	O-C-N	-5.10	114.54	122.70
1	M	525	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	E	141	VAL	CA-CB-CG1	5.09	118.54	110.90
1	G	317	VAL	CA-CB-CG2	-5.09	103.26	110.90
1	H	396	ARG	NH1-CZ-NH2	-5.09	113.80	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	508	VAL	CG1-CB-CG2	5.09	119.05	110.90
1	I	109	ILE	CB-CA-C	-5.09	101.41	111.60
1	K	341	SER	CB-CA-C	-5.09	100.42	110.10
1	P	399	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	F	436	VAL	CA-CB-CG1	5.09	118.53	110.90
1	G	433	ALA	CA-C-O	-5.09	109.41	120.10
1	M	462	ALA	C-N-CA	5.09	132.99	122.30
1	O	461	ASN	CA-CB-CG	-5.09	102.20	113.40
1	A	162	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	R	139	GLU	C-N-CA	5.09	134.42	121.70
1	C	384	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	E	447	TYR	O-C-N	-5.08	114.56	122.70
1	H	413	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	462	ALA	N-CA-CB	5.08	117.22	110.10
1	F	427	LYS	CB-CA-C	5.08	120.57	110.40
1	G	414	ALA	CB-CA-C	-5.08	102.47	110.10
1	K	488	ASP	O-C-N	-5.08	114.56	122.70
1	L	50	TYR	CZ-CE2-CD2	5.08	124.38	119.80
1	O	207	ILE	N-CA-C	-5.08	97.27	111.00
1	Q	490	TYR	CB-CG-CD2	5.08	124.05	121.00
1	H	471	MET	CG-SD-CE	5.08	108.33	100.20
1	K	229	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	77	ASP	CB-CG-OD1	5.08	122.87	118.30
1	G	528	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	33	ARG	CD-NE-CZ	5.07	130.70	123.60
1	B	471	MET	CG-SD-CE	-5.07	92.09	100.20
1	I	485	TYR	CB-CG-CD2	5.07	124.04	121.00
1	L	297	VAL	CA-CB-CG2	5.07	118.50	110.90
1	Q	430	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	R	392	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	333	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	E	403	GLY	C-N-CA	5.07	134.37	121.70
1	A	317	VAL	C-N-CA	5.07	134.37	121.70
1	F	116	LYS	CA-CB-CG	5.07	124.54	113.40
1	M	234	HIS	CA-CB-CG	5.07	122.21	113.60
1	S	110	PHE	CB-CA-C	5.07	120.53	110.40
1	C	228	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	L	414	ALA	O-C-N	-5.06	114.60	122.70
1	B	427	LYS	CA-CB-CG	5.05	124.52	113.40
1	C	392	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	325	LYS	C-N-CA	5.05	134.32	121.70
1	M	325	LYS	C-N-CA	5.05	134.32	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	464	PHE	CZ-CE2-CD2	5.05	126.16	120.10
1	E	398	LEU	CB-CG-CD2	5.05	119.58	111.00
1	H	114	LEU	CB-CG-CD2	5.05	119.58	111.00
1	R	436	VAL	CG1-CB-CG2	-5.04	102.83	110.90
1	B	146	ILE	CA-CB-CG1	-5.04	101.42	111.00
1	B	288	ASP	CB-CA-C	5.04	120.49	110.40
1	D	261	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	393	GLU	CG-CD-OE2	5.04	128.38	118.30
1	M	289	LYS	N-CA-CB	-5.04	101.52	110.60
1	O	360	ARG	N-CA-CB	5.04	119.67	110.60
1	I	525	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	32	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	M	201	TYR	CD1-CG-CD2	5.04	123.44	117.90
1	H	372	GLY	O-C-N	-5.04	114.64	122.70
1	M	383	ILE	CG1-CB-CG2	-5.04	100.32	111.40
1	R	102	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	P	277	ASP	CA-C-O	5.03	130.67	120.10
1	O	340	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	R	65	ASP	O-C-N	-5.03	114.65	122.70
1	I	159	ASP	CB-CG-OD1	5.03	122.83	118.30
1	L	426	ALA	CA-C-N	5.03	128.26	117.20
1	S	290	ILE	O-C-N	-5.03	114.66	122.70
1	F	389	ARG	CB-CA-C	-5.02	100.36	110.40
1	G	396	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	K	400	ASP	N-CA-CB	-5.02	101.56	110.60
1	C	135	TYR	CG-CD1-CE1	-5.02	117.28	121.30
1	D	360	ARG	NH1-CZ-NH2	5.02	124.92	119.40
1	M	115	VAL	CA-CB-CG2	-5.02	103.37	110.90
1	P	340	VAL	O-C-N	-5.02	114.67	122.70
1	F	240	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	N	274	LYS	O-C-N	-5.02	114.67	122.70
1	G	303	GLY	O-C-N	5.01	130.72	122.70
1	I	159	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	N	265	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	H	245	LYS	O-C-N	-5.01	114.68	122.70
1	R	472	LYS	CD-CE-NZ	-5.01	100.17	111.70
1	A	353	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
1	R	365	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	180	TYR	CB-CG-CD1	5.01	124.00	121.00
1	M	311	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	A	521	THR	O-C-N	-5.00	114.69	122.70
1	I	384	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	490	TYR	CD1-CE1-CZ	-5.00	115.30	119.80
1	K	97	ASP	CA-C-O	5.00	130.61	120.10
1	H	120	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (185) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	PHE	Sidechain
1	A	135	TYR	Sidechain
1	A	162	ARG	Sidechain
1	A	201	TYR	Sidechain
1	A	224	TYR	Sidechain
1	A	240	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	360	ARG	Sidechain
1	A	399	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	525	ARG	Sidechain
1	B	123	TYR	Sidechain
1	B	135	TYR	Sidechain
1	B	178	ARG	Sidechain
1	B	196	ARG	Sidechain
1	B	224	TYR	Sidechain
1	B	240	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	353	TYR	Sidechain
1	B	399	ARG	Sidechain
1	B	432	TYR	Sidechain
1	B	447	TYR	Sidechain
1	B	474	ARG	Sidechain
1	B	490	TYR	Sidechain
1	B	50	TYR	Sidechain
1	B	53	ARG	Sidechain
1	C	333	ARG	Sidechain
1	C	353	TYR	Sidechain
1	C	389	ARG	Sidechain
1	C	399	ARG	Sidechain
1	C	474	ARG	Sidechain
1	D	162	ARG	Sidechain
1	D	275	PHE	Sidechain
1	D	311	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	321	ARG	Sidechain
1	D	322	ARG	Sidechain
1	D	338	ARG	Sidechain
1	D	353	TYR	Sidechain
1	D	360	ARG	Sidechain
1	D	430	ARG	Sidechain
1	D	490	TYR	Sidechain
1	D	53	ARG	Sidechain
1	E	123	TYR	Sidechain
1	E	162	ARG	Sidechain
1	E	240	ARG	Sidechain
1	E	33	ARG	Sidechain
1	E	333	ARG	Mainchain
1	E	360	ARG	Sidechain
1	E	396	ARG	Sidechain
1	E	430	ARG	Sidechain
1	E	447	TYR	Sidechain
1	E	525	ARG	Sidechain
1	F	196	ARG	Sidechain
1	F	224	TYR	Sidechain
1	F	322	ARG	Sidechain
1	F	353	TYR	Sidechain
1	F	360	ARG	Sidechain
1	F	389	ARG	Sidechain
1	F	399	ARG	Sidechain
1	F	413	ARG	Sidechain
1	F	447	TYR	Sidechain
1	F	50	TYR	Sidechain
1	G	110	PHE	Sidechain
1	G	178	ARG	Sidechain
1	G	180	TYR	Sidechain
1	G	196	ARG	Sidechain
1	G	224	TYR	Sidechain
1	G	240	ARG	Sidechain
1	G	321	ARG	Sidechain
1	G	353	TYR	Sidechain
1	G	413	ARG	Sidechain
1	G	430	ARG	Sidechain
1	G	525	ARG	Sidechain
1	H	224	TYR	Sidechain
1	H	265	ARG	Sidechain
1	H	275	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	H	311	TYR	Sidechain
1	H	333	ARG	Sidechain
1	H	360	ARG	Sidechain
1	H	389	ARG	Sidechain
1	H	474	ARG	Sidechain
1	I	162	ARG	Sidechain
1	I	180	TYR	Sidechain
1	I	311	TYR	Sidechain
1	I	321	ARG	Sidechain
1	I	322	ARG	Sidechain
1	I	430	ARG	Sidechain
1	I	50	TYR	Sidechain
1	I	525	ARG	Sidechain
1	K	127	HIS	Sidechain
1	K	135	TYR	Sidechain
1	K	224	TYR	Sidechain
1	K	234	HIS	Sidechain
1	K	311	TYR	Sidechain
1	K	322	ARG	Sidechain
1	K	360	ARG	Sidechain
1	K	399	ARG	Sidechain
1	K	447	TYR	Sidechain
1	K	464	PHE	Sidechain
1	K	474	ARG	Sidechain
1	K	53	ARG	Sidechain
1	L	180	TYR	Sidechain
1	L	240	ARG	Sidechain
1	L	265	ARG	Sidechain
1	L	322	ARG	Sidechain
1	L	474	ARG	Sidechain
1	L	485	TYR	Sidechain
1	L	490	TYR	Sidechain
1	L	525	ARG	Sidechain
1	M	110	PHE	Sidechain
1	M	309	GLN	Mainchain
1	M	311	TYR	Sidechain
1	M	384	ARG	Sidechain
1	M	389	ARG	Sidechain
1	M	399	ARG	Sidechain
1	M	430	ARG	Sidechain
1	M	447	TYR	Sidechain
1	M	474	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	490	TYR	Sidechain
1	N	110	PHE	Sidechain
1	N	123	TYR	Sidechain
1	N	178	ARG	Sidechain
1	N	196	ARG	Sidechain
1	N	201	TYR	Sidechain
1	N	224	TYR	Sidechain
1	N	240	ARG	Sidechain
1	N	311	TYR	Sidechain
1	N	321	ARG	Sidechain
1	N	333	ARG	Sidechain
1	N	360	ARG	Sidechain
1	N	389	ARG	Sidechain
1	N	396	ARG	Sidechain
1	N	447	TYR	Sidechain
1	N	525	ARG	Sidechain
1	O	178	ARG	Sidechain
1	O	180	TYR	Sidechain
1	O	33	ARG	Sidechain
1	O	396	ARG	Sidechain
1	O	432	TYR	Sidechain
1	O	447	TYR	Sidechain
1	O	525	ARG	Sidechain
1	P	123	TYR	Sidechain
1	P	135	TYR	Sidechain
1	P	162	ARG	Sidechain
1	P	224	TYR	Sidechain
1	P	265	ARG	Sidechain
1	P	333	ARG	Sidechain
1	P	384	ARG	Sidechain
1	P	474	ARG	Sidechain
1	P	480	GLU	Sidechain
1	Q	123	TYR	Sidechain
1	Q	135	TYR	Sidechain
1	Q	162	ARG	Sidechain
1	Q	29	LYS	Mainchain
1	Q	33	ARG	Sidechain
1	Q	333	ARG	Sidechain
1	Q	353	TYR	Sidechain
1	Q	432	TYR	Sidechain
1	Q	447	TYR	Sidechain
1	Q	464	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	Q	477	HIS	Sidechain
1	Q	490	TYR	Sidechain
1	Q	50	TYR	Sidechain
1	Q	525	ARG	Sidechain
1	R	135	TYR	Sidechain
1	R	162	ARG	Sidechain
1	R	201	TYR	Sidechain
1	R	240	ARG	Sidechain
1	R	265	ARG	Sidechain
1	R	333	ARG	Sidechain
1	R	338	ARG	Sidechain
1	R	389	ARG	Sidechain
1	R	399	ARG	Sidechain
1	R	432	TYR	Sidechain
1	S	135	TYR	Sidechain
1	S	162	ARG	Sidechain
1	S	178	ARG	Sidechain
1	S	224	TYR	Sidechain
1	S	311	TYR	Sidechain
1	S	389	ARG	Sidechain
1	S	399	ARG	Sidechain
1	S	432	TYR	Sidechain
1	S	474	ARG	Sidechain
1	S	50	TYR	Sidechain
1	S	53	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3849	0	3995	14	0
1	B	3849	0	3995	17	0
1	C	3849	0	3995	17	0
1	D	3849	0	3995	14	0
1	E	3849	0	3995	6	0
1	F	3849	0	3995	14	0
1	G	3849	0	3995	19	0
1	H	3849	0	3995	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3849	0	3995	12	0
1	K	3849	0	3995	13	0
1	L	3849	0	3995	18	0
1	M	3849	0	3995	21	0
1	N	3849	0	3995	7	0
1	O	3849	0	3995	12	0
1	P	3849	0	3995	28	0
1	Q	3849	0	3995	13	0
1	R	3849	0	3995	9	0
1	S	3849	0	3995	17	0
All	All	69282	0	71910	259	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 (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:415:ILE:HD12	1:G:421:VAL:HG21	1.72	0.71
1:D:89:LEU:HD12	1:D:519:ALA:HB1	1.73	0.71
1:G:246:ILE:HD12	1:G:246:ILE:H	1.53	0.71
1:M:153:VAL:HG22	1:M:160:LEU:HD23	1.76	0.67
1:P:474:ARG:HE	1:P:477:HIS:CE1	2.13	0.66
1:B:127:HIS:CD2	1:C:463:GLY:HA2	2.34	0.63
1:H:507:LEU:HD23	1:H:507:LEU:H	1.64	0.63
1:F:246:ILE:HA	1:F:297:VAL:HG13	1.82	0.62
1:G:191:GLN:HG2	1:G:379:ILE:HD13	1.82	0.61
1:S:167:THR:HG22	1:S:167:THR:O	2.00	0.61
1:S:297:VAL:HG21	1:S:357:ILE:HD13	1.83	0.60
1:G:100:THR:HG21	1:G:508:VAL:HG13	1.84	0.59
1:K:244:ALA:HB2	1:K:357:ILE:HG22	1.84	0.58
1:R:246:ILE:H	1:R:246:ILE:HD12	1.67	0.58
1:F:155:ILE:HG13	1:F:190:THR:HG22	1.86	0.57
1:G:486:GLY:O	1:G:494:PRO:HA	2.05	0.57
1:A:164:ILE:HG21	1:A:408:VAL:HG21	1.87	0.57
1:L:30:GLU:CD	1:L:30:GLU:H	2.08	0.57
1:I:246:ILE:HA	1:I:297:VAL:HG13	1.87	0.56
1:C:423:ILE:HD13	1:C:473:LEU:HD13	1.87	0.56
1:M:220:THR:HG22	1:M:384:ARG:H	1.70	0.56
1:Q:290:ILE:HA	1:Q:346:ILE:HG21	1.88	0.56
1:D:442:LEU:H	1:D:442:LEU:HD12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:153:VAL:HG22	1:P:160:LEU:CD2	2.37	0.55
1:M:153:VAL:HG22	1:M:160:LEU:CD2	2.36	0.55
1:H:164:ILE:HG21	1:H:408:VAL:HG21	1.89	0.54
1:R:480:GLU:H	1:R:480:GLU:CD	2.11	0.54
1:L:423:ILE:HD13	1:L:473:LEU:HD13	1.90	0.54
1:S:430:ARG:HH21	1:S:452:GLU:CD	2.12	0.53
1:A:290:ILE:HA	1:A:346:ILE:HG21	1.90	0.53
1:L:297:VAL:HG21	1:L:357:ILE:HD13	1.90	0.53
1:E:246:ILE:HA	1:E:297:VAL:HG13	1.89	0.53
1:M:452:GLU:CD	1:M:474:ARG:HH22	2.11	0.53
1:L:474:ARG:HA	1:L:477:HIS:CD2	2.43	0.52
1:O:425:ILE:HG22	1:O:451:LEU:HD13	1.92	0.52
1:P:153:VAL:HG22	1:P:160:LEU:HD23	1.90	0.52
1:Q:220:THR:HG22	1:Q:383:ILE:HA	1.90	0.52
1:K:234:HIS:CD2	1:K:236:GLY:H	2.28	0.52
1:H:477:HIS:CG	1:H:477:HIS:O	2.63	0.52
1:B:246:ILE:HD12	1:B:246:ILE:H	1.74	0.52
1:K:127:HIS:CG	1:L:463:GLY:HA2	2.45	0.52
1:M:192:VAL:HG13	1:M:206:ASN:HB2	1.92	0.52
1:I:246:ILE:HD12	1:I:246:ILE:H	1.74	0.51
1:S:404:THR:O	1:S:408:VAL:HG23	2.10	0.51
1:B:532:ALA:HB3	1:C:61:ASP:HA	1.92	0.51
1:F:383:ILE:N	1:F:383:ILE:HD12	2.26	0.51
1:I:244:ALA:HB2	1:I:357:ILE:HG22	1.93	0.51
1:R:238:PRO:HB2	1:R:241:LEU:HD21	1.93	0.51
1:B:283:ILE:HG23	1:B:308:ALA:HB2	1.93	0.50
1:E:421:VAL:O	1:E:425:ILE:HG13	2.11	0.50
1:B:526:ILE:HD11	1:C:68:ILE:HD13	1.93	0.50
1:L:244:ALA:HB2	1:L:357:ILE:HG22	1.93	0.50
1:P:505:PRO:HB2	1:P:508:VAL:HG12	1.93	0.50
1:E:473:LEU:HD13	1:E:473:LEU:C	2.31	0.50
1:I:312:LEU:HD22	1:I:317:VAL:HG11	1.93	0.50
1:G:312:LEU:HD22	1:G:317:VAL:HG11	1.94	0.49
1:S:383:ILE:CD1	1:S:395:GLU:HA	2.42	0.49
1:G:220:THR:HG22	1:G:383:ILE:HA	1.94	0.49
1:S:121:LEU:HB2	1:S:131:ILE:HD11	1.93	0.49
1:I:185:VAL:HG13	1:I:402:LEU:HA	1.95	0.49
1:P:227:VAL:HG22	1:P:369:PHE:CD1	2.48	0.49
1:H:89:LEU:HD11	1:H:111:SER:HB3	1.95	0.49
1:P:213:ALA:HA	1:P:391:VAL:HG11	1.93	0.49
1:O:249:ILE:HG22	1:O:251:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HH21	1:A:452:GLU:CD	2.16	0.49
1:E:498:TRP:CZ3	1:E:503:ILE:HG23	2.48	0.49
1:K:164:ILE:HG21	1:K:408:VAL:HG21	1.95	0.49
1:C:423:ILE:HD12	1:C:477:HIS:CD2	2.47	0.48
1:F:483:LYS:HE2	1:F:484:TRP:CE2	2.48	0.48
1:L:474:ARG:HG3	1:L:477:HIS:CE1	2.48	0.48
1:D:415:ILE:HB	1:D:421:VAL:HG21	1.95	0.48
1:G:227:VAL:HG22	1:G:369:PHE:CD1	2.49	0.48
1:B:161:LEU:HD22	1:B:405:VAL:HG13	1.95	0.48
1:F:312:LEU:HD22	1:F:317:VAL:HG11	1.95	0.48
1:M:149:LEU:HD21	1:M:421:VAL:HG12	1.96	0.48
1:R:164:ILE:HG21	1:R:408:VAL:HG21	1.96	0.48
1:S:298:ILE:CG2	1:S:319:ALA:HB2	2.44	0.48
1:I:178:ARG:NE	1:I:178:ARG:H	2.12	0.48
1:R:455:VAL:O	1:R:459:ILE:HG12	2.14	0.48
1:F:527:ASP:HB2	1:G:55:MET:HB3	1.95	0.47
1:D:129:THR:HG23	1:D:130:ILE:HD13	1.95	0.47
1:P:268:ASP:HB2	1:P:271:GLN:HE21	1.79	0.47
1:R:158:THR:HB	1:R:186:VAL:HG11	1.95	0.47
1:B:459:ILE:HD13	1:B:469:LEU:HB2	1.96	0.47
1:O:226:ILE:HG13	1:O:334:ALA:CB	2.45	0.47
1:P:255:VAL:HG12	1:P:279:GLU:HG3	1.96	0.47
1:K:459:ILE:HG21	1:K:466:PRO:HA	1.97	0.47
1:P:248:LEU:H	1:P:248:LEU:HD12	1.79	0.47
1:B:497:MET:HB3	1:B:502:VAL:HB	1.97	0.47
1:K:253:LEU:HD11	1:K:298:ILE:HD11	1.96	0.47
1:L:88:LEU:CD1	1:M:68:ILE:HD11	2.44	0.47
1:B:248:LEU:H	1:B:248:LEU:HD22	1.80	0.47
1:A:453:SER:O	1:A:456:SER:HB2	2.15	0.47
1:H:220:THR:HG22	1:H:384:ARG:H	1.80	0.47
1:P:387:LEU:HD23	1:P:389:ARG:H	1.80	0.47
1:I:485:TYR:CE1	1:I:496:ASP:HB2	2.50	0.46
1:K:192:VAL:HG13	1:K:206:ASN:HD22	1.81	0.46
1:D:504:GLU:HB2	1:D:505:PRO:HD2	1.98	0.46
1:C:291:LEU:HD11	1:C:312:LEU:HD23	1.97	0.46
1:F:408:VAL:HG22	1:F:505:PRO:HG3	1.98	0.46
1:S:310:SER:O	1:S:314:LYS:HE2	2.15	0.46
1:A:106:THR:HG23	1:A:454:LEU:HD21	1.98	0.46
1:N:404:THR:O	1:N:408:VAL:HG23	2.15	0.46
1:A:225:GLY:HA3	1:A:371:GLU:HA	1.98	0.46
1:B:114:LEU:HD11	1:B:447:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:340:VAL:HG21	1:K:346:ILE:HD13	1.97	0.46
1:G:423:ILE:HG23	1:G:477:HIS:CD2	2.51	0.46
1:H:217:ILE:H	1:H:217:ILE:HD12	1.81	0.46
1:N:477:HIS:CD2	1:N:477:HIS:O	2.69	0.46
1:O:226:ILE:HG13	1:O:334:ALA:HB2	1.98	0.46
1:M:233:VAL:HG12	1:M:319:ALA:O	2.16	0.45
1:B:242:GLU:CD	1:B:242:GLU:H	2.19	0.45
1:L:248:LEU:H	1:L:248:LEU:HD22	1.81	0.45
1:C:246:ILE:HA	1:C:297:VAL:HG13	1.97	0.45
1:I:469:LEU:HD13	1:I:487:ILE:HD11	1.98	0.45
1:P:465:ASP:HA	1:P:466:PRO:HD2	1.86	0.45
1:N:248:LEU:HD12	1:N:248:LEU:H	1.81	0.45
1:R:430:ARG:HH21	1:R:452:GLU:CD	2.18	0.45
1:L:46:LEU:HD12	1:L:108:VAL:HG11	1.97	0.45
1:F:299:ILE:HA	1:F:320:VAL:HB	1.99	0.45
1:Q:204:LEU:O	1:Q:204:LEU:HD13	2.17	0.45
1:A:38:ALA:O	1:A:41:ALA:HB3	2.17	0.45
1:L:458:LEU:HG	1:L:489:LEU:HD11	1.98	0.45
1:M:415:ILE:HD12	1:M:415:ILE:O	2.16	0.45
1:Q:297:VAL:HG21	1:Q:357:ILE:HG21	1.98	0.45
1:Q:415:ILE:O	1:Q:503:ILE:HG23	2.16	0.45
1:Q:488:ASP:HB3	1:Q:491:ALA:HB3	1.99	0.45
1:S:252:SER:HB2	1:S:302:LYS:HD3	1.98	0.45
1:C:477:HIS:CG	1:C:477:HIS:O	2.69	0.45
1:H:192:VAL:HG21	1:H:207:ILE:CG1	2.47	0.45
1:H:241:LEU:HD23	1:H:318:LEU:HB2	1.99	0.45
1:G:232:VAL:HG12	1:G:318:LEU:HD21	1.99	0.44
1:N:312:LEU:HD22	1:N:317:VAL:HG11	1.99	0.44
1:B:290:ILE:HG21	1:B:298:ILE:HD12	1.98	0.44
1:H:383:ILE:HD13	1:H:395:GLU:HA	1.99	0.44
1:P:357:ILE:HD11	1:P:370:VAL:HG13	1.98	0.44
1:P:517:THR:O	1:P:517:THR:HG22	2.18	0.44
1:M:459:ILE:HD13	1:M:469:LEU:HB2	2.00	0.44
1:O:430:ARG:HH21	1:O:452:GLU:CD	2.21	0.44
1:P:149:LEU:HG	1:P:483:LYS:HD2	2.00	0.44
1:F:459:ILE:O	1:F:462:ALA:HB3	2.17	0.44
1:K:38:ALA:O	1:K:41:ALA:HB3	2.17	0.44
1:O:250:ASP:OD1	1:O:302:LYS:NZ	2.50	0.44
1:B:127:HIS:CD2	1:C:463:GLY:CA	3.01	0.44
1:N:234:HIS:CD2	1:N:236:GLY:H	2.36	0.44
1:Q:383:ILE:HD11	1:Q:398:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:ILE:HD11	1:G:343:ILE:HG22	1.99	0.44
1:P:153:VAL:CG2	1:P:160:LEU:HD23	2.48	0.44
1:Q:283:ILE:HD13	1:Q:286:LYS:HD2	2.00	0.44
1:B:340:VAL:HG21	1:B:346:ILE:HD12	2.00	0.44
1:K:423:ILE:HD12	1:K:477:HIS:CG	2.52	0.44
1:M:522:LEU:HD11	1:N:68:ILE:HD13	1.99	0.44
1:P:98:GLU:HG2	1:P:508:VAL:HB	2.00	0.44
1:E:141:VAL:HA	1:E:144:GLN:HG2	2.00	0.43
1:O:425:ILE:HG22	1:O:451:LEU:CD1	2.47	0.43
1:D:254:GLU:CD	1:D:321:ARG:HH12	2.22	0.43
1:H:232:VAL:HG13	1:H:319:ALA:O	2.17	0.43
1:L:233:VAL:HG23	1:L:321:ARG:HG2	1.99	0.43
1:M:335:THR:HB	1:M:353:TYR:H	1.83	0.43
1:O:244:ALA:O	1:O:353:TYR:HA	2.18	0.43
1:R:153:VAL:HG21	1:R:414:ALA:HB3	2.00	0.43
1:A:164:ILE:HG23	1:A:505:PRO:HD3	2.01	0.43
1:H:164:ILE:H	1:H:164:ILE:HG13	1.63	0.43
1:S:127:HIS:O	1:S:130:ILE:HB	2.19	0.43
1:C:433:ALA:HB1	1:C:441:GLN:HG3	2.01	0.43
1:G:246:ILE:H	1:G:246:ILE:CD1	2.25	0.43
1:O:195:LEU:HD23	1:O:200:TRP:HA	2.01	0.43
1:P:451:LEU:HD13	1:P:451:LEU:HA	1.85	0.43
1:Q:188:ALA:O	1:Q:192:VAL:HG23	2.19	0.43
1:C:526:ILE:HD12	1:D:58:MET:HB2	2.01	0.43
1:M:241:LEU:HD12	1:M:318:LEU:HB2	2.01	0.43
1:G:106:THR:HG23	1:G:454:LEU:HD21	2.01	0.43
1:H:244:ALA:HB2	1:H:357:ILE:HG22	2.00	0.43
1:D:99:GLU:O	1:D:100:THR:HB	2.19	0.43
1:H:297:VAL:HG11	1:H:357:ILE:HG21	2.01	0.43
1:I:462:ALA:HB2	1:I:489:LEU:HD22	1.99	0.43
1:K:425:ILE:O	1:K:429:LEU:HD13	2.19	0.43
1:L:88:LEU:HD11	1:M:68:ILE:HD11	1.99	0.43
1:O:473:LEU:HD12	1:O:487:ILE:HG13	2.01	0.42
1:R:291:LEU:HD11	1:R:312:LEU:HD23	2.01	0.42
1:C:161:LEU:HA	1:C:164:ILE:HG22	2.02	0.42
1:F:89:LEU:HD11	1:F:111:SER:OG	2.19	0.42
1:S:195:LEU:HD13	1:S:200:TRP:CE2	2.54	0.42
1:B:39:VAL:HG21	1:B:523:VAL:HG21	2.01	0.42
1:C:233:VAL:HG12	1:C:319:ALA:O	2.20	0.42
1:F:527:ASP:HB2	1:G:55:MET:CB	2.49	0.42
1:H:364:GLU:CD	1:H:384:ARG:HH22	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:287:VAL:HG13	1:Q:312:LEU:HD21	2.00	0.42
1:H:462:ALA:HB2	1:H:489:LEU:HD22	2.01	0.42
1:P:427:LYS:HE3	1:P:477:HIS:CE1	2.55	0.42
1:S:312:LEU:HD22	1:S:317:VAL:HG11	2.02	0.42
1:M:226:ILE:HD11	1:M:378:SER:HB3	2.01	0.42
1:O:226:ILE:HD11	1:O:378:SER:HB3	2.00	0.42
1:P:226:ILE:HD11	1:P:378:SER:HB3	2.01	0.42
1:A:100:THR:HG22	1:A:103:GLY:H	1.84	0.42
1:K:383:ILE:HD13	1:K:383:ILE:HG21	1.92	0.42
1:L:185:VAL:HG13	1:L:402:LEU:HA	2.01	0.42
1:O:222:LEU:HD21	1:O:379:ILE:HD12	2.01	0.42
1:A:381:ILE:HD12	1:A:402:LEU:HD11	2.01	0.42
1:B:340:VAL:HG21	1:B:346:ILE:CD1	2.49	0.42
1:D:193:ALA:HA	1:D:201:TYR:O	2.20	0.42
1:H:226:ILE:HD13	1:H:226:ILE:HA	1.88	0.42
1:A:173:ALA:HB3	1:A:393:GLU:HG2	2.00	0.42
1:C:505:PRO:HG2	1:C:508:VAL:HB	2.02	0.42
1:D:81:LEU:HD12	1:D:81:LEU:HA	1.92	0.42
1:D:110:PHE:CD2	1:D:454:LEU:HD22	2.55	0.42
1:F:31:ALA:O	1:F:34:ALA:HB3	2.20	0.42
1:S:298:ILE:HG23	1:S:319:ALA:HB2	2.00	0.42
1:I:477:HIS:O	1:I:477:HIS:CG	2.73	0.41
1:S:282:LEU:O	1:S:285:GLU:HB3	2.20	0.41
1:M:415:ILE:HD12	1:M:415:ILE:C	2.40	0.41
1:P:423:ILE:HD13	1:P:473:LEU:HD13	2.02	0.41
1:F:343:ILE:O	1:F:346:ILE:HG22	2.20	0.41
1:G:160:LEU:HD21	1:G:498:TRP:CZ2	2.55	0.41
1:D:245:LYS:HB3	1:D:351:LEU:HD23	2.03	0.41
1:H:430:ARG:HH11	1:H:430:ARG:HG2	1.86	0.41
1:M:234:HIS:HA	1:M:235:PRO:HD3	1.79	0.41
1:S:181:ILE:HG23	1:S:398:LEU:HD12	2.03	0.41
1:S:361:LYS:HA	1:S:366:LYS:HA	2.01	0.41
1:A:312:LEU:HD13	1:A:319:ALA:HB2	2.02	0.41
1:M:145:THR:HG22	1:M:145:THR:O	2.19	0.41
1:A:28:GLY:N	1:A:30:GLU:OE1	2.53	0.41
1:C:144:GLN:O	1:C:148:GLU:HG2	2.20	0.41
1:M:232:VAL:HG12	1:M:318:LEU:HD21	2.03	0.41
1:M:312:LEU:HD13	1:M:319:ALA:HB2	2.02	0.41
1:D:440:GLU:O	1:D:443:ALA:HB3	2.21	0.41
1:I:430:ARG:HH21	1:I:452:GLU:CD	2.24	0.41
1:K:167:THR:O	1:K:167:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:226:ILE:HD11	1:L:378:SER:HB3	2.03	0.41
1:P:473:LEU:HB2	1:P:487:ILE:HD11	2.02	0.41
1:D:51:GLY:HA3	1:D:458:LEU:HD12	2.02	0.41
1:G:469:LEU:HD13	1:G:469:LEU:HA	1.88	0.41
1:H:107:ALA:HA	1:H:516:ALA:HB2	2.03	0.41
1:I:487:ILE:O	1:I:487:ILE:HG23	2.20	0.41
1:L:143:LEU:CD2	1:L:510:MET:HG3	2.50	0.41
1:P:290:ILE:HD11	1:P:343:ILE:HG22	2.03	0.41
1:Q:39:VAL:HG11	1:Q:115:VAL:HG21	2.03	0.41
1:F:290:ILE:CG1	1:F:343:ILE:HG23	2.51	0.41
1:M:361:LYS:HA	1:M:366:LYS:HA	2.03	0.41
1:P:415:ILE:HD12	1:P:421:VAL:HG21	2.03	0.41
1:P:521:THR:HA	1:P:524:LEU:HD12	2.02	0.41
1:P:529:VAL:HG22	1:Q:58:MET:HE2	2.02	0.41
1:B:222:LEU:HD23	1:B:223:VAL:N	2.35	0.41
1:G:46:LEU:HD21	1:G:76:LEU:HD13	2.03	0.41
1:N:299:ILE:HD13	1:N:299:ILE:HG21	1.88	0.41
1:C:423:ILE:HD12	1:C:477:HIS:CG	2.57	0.40
1:P:305:ASP:O	1:P:309:GLN:HG3	2.21	0.40
1:S:304:ILE:HG21	1:S:304:ILE:HD13	1.86	0.40
1:G:93:ALA:HB1	1:G:108:VAL:HG22	2.03	0.40
1:H:161:LEU:HD11	1:H:409:ILE:HD11	2.03	0.40
1:L:249:ILE:O	1:L:300:CYS:HA	2.21	0.40
1:L:331:LEU:HA	1:L:331:LEU:HD12	1.89	0.40
1:P:30:GLU:CD	1:P:30:GLU:H	2.25	0.40
1:A:304:ILE:H	1:A:321:ARG:HD3	1.86	0.40
1:E:84:PRO:O	1:E:88:LEU:HG	2.21	0.40
1:H:246:ILE:H	1:H:246:ILE:HG13	1.61	0.40
1:P:451:LEU:HD13	1:P:454:LEU:HD12	2.04	0.40
1:Q:329:GLU:O	1:Q:332:ALA:HB3	2.21	0.40
1:C:346:ILE:HG13	1:C:350:ASP:HB2	2.04	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	503/553 (91%)	455 (90%)	40 (8%)	8 (2%)	9 44
1	B	503/553 (91%)	453 (90%)	42 (8%)	8 (2%)	9 44
1	C	503/553 (91%)	458 (91%)	42 (8%)	3 (1%)	25 66
1	D	503/553 (91%)	451 (90%)	47 (9%)	5 (1%)	15 55
1	E	503/553 (91%)	451 (90%)	49 (10%)	3 (1%)	25 66
1	F	503/553 (91%)	456 (91%)	41 (8%)	6 (1%)	13 50
1	G	503/553 (91%)	444 (88%)	50 (10%)	9 (2%)	8 40
1	H	503/553 (91%)	450 (90%)	47 (9%)	6 (1%)	13 50
1	I	503/553 (91%)	457 (91%)	41 (8%)	5 (1%)	15 55
1	K	503/553 (91%)	452 (90%)	45 (9%)	6 (1%)	13 50
1	L	503/553 (91%)	454 (90%)	44 (9%)	5 (1%)	15 55
1	M	503/553 (91%)	458 (91%)	42 (8%)	3 (1%)	25 66
1	N	503/553 (91%)	455 (90%)	41 (8%)	7 (1%)	11 46
1	O	503/553 (91%)	449 (89%)	46 (9%)	8 (2%)	9 44
1	P	503/553 (91%)	456 (91%)	41 (8%)	6 (1%)	13 50
1	Q	503/553 (91%)	454 (90%)	44 (9%)	5 (1%)	15 55
1	R	503/553 (91%)	455 (90%)	42 (8%)	6 (1%)	13 50
1	S	503/553 (91%)	450 (90%)	49 (10%)	4 (1%)	19 60
All	All	9054/9954 (91%)	8158 (90%)	793 (9%)	103 (1%)	18 52

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	387	LEU
1	M	387	LEU
1	N	387	LEU
1	O	264	ILE
1	R	387	LEU
1	A	30	GLU
1	D	30	GLU
1	D	100	THR
1	E	30	GLU
1	F	30	GLU
1	G	30	GLU

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Mol	Chain	Res	Type
1	G	100	THR
1	H	95	GLY
1	K	30	GLU
1	K	386	GLY
1	K	387	LEU
1	K	438	GLY
1	O	30	GLU
1	O	240	ARG
1	Q	385	GLY
1	S	438	GLY
1	A	100	THR
1	A	385	GLY
1	A	387	LEU
1	B	30	GLU
1	B	385	GLY
1	C	30	GLU
1	C	438	GLY
1	E	438	GLY
1	F	438	GLY
1	G	387	LEU
1	H	30	GLU
1	I	30	GLU
1	L	30	GLU
1	L	385	GLY
1	L	438	GLY
1	M	30	GLU
1	N	30	GLU
1	N	149	LEU
1	N	258	PRO
1	N	385	GLY
1	O	305	ASP
1	P	30	GLU
1	P	259	GLU
1	P	385	GLY
1	Q	30	GLU
1	Q	387	LEU
1	Q	438	GLY
1	S	30	GLU
1	B	148	GLU
1	B	149	LEU
1	B	438	GLY
1	D	385	GLY

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Mol	Chain	Res	Type
1	D	438	GLY
1	E	266	ILE
1	F	149	LEU
1	G	61	ASP
1	H	149	LEU
1	I	149	LEU
1	I	387	LEU
1	L	149	LEU
1	M	438	GLY
1	O	385	GLY
1	O	438	GLY
1	O	499	GLN
1	P	438	GLY
1	R	322	ARG
1	R	385	GLY
1	A	149	LEU
1	A	438	GLY
1	B	258	PRO
1	B	387	LEU
1	C	149	LEU
1	D	258	PRO
1	F	47	LYS
1	G	149	LEU
1	G	363	GLY
1	H	438	GLY
1	I	438	GLY
1	K	149	LEU
1	L	148	GLU
1	N	438	GLY
1	O	149	LEU
1	P	47	LYS
1	P	149	LEU
1	Q	149	LEU
1	R	30	GLU
1	R	149	LEU
1	R	438	GLY
1	S	373	ALA
1	A	363	GLY
1	F	259	GLU
1	G	438	GLY
1	H	148	GLU
1	K	499	GLN

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Mol	Chain	Res	Type
1	S	149	LEU
1	F	174	VAL
1	G	266	ILE
1	G	385	GLY
1	I	385	GLY
1	N	376	PRO
1	B	215	GLY
1	A	434	PRO

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	410/447 (92%)	396 (97%)	14 (3%)	37	60
1	B	410/447 (92%)	393 (96%)	17 (4%)	30	55
1	C	410/447 (92%)	397 (97%)	13 (3%)	39	61
1	D	410/447 (92%)	394 (96%)	16 (4%)	32	56
1	E	410/447 (92%)	402 (98%)	8 (2%)	55	74
1	F	410/447 (92%)	396 (97%)	14 (3%)	37	60
1	G	410/447 (92%)	400 (98%)	10 (2%)	49	69
1	H	410/447 (92%)	402 (98%)	8 (2%)	55	74
1	I	410/447 (92%)	399 (97%)	11 (3%)	44	65
1	K	410/447 (92%)	403 (98%)	7 (2%)	60	78
1	L	410/447 (92%)	395 (96%)	15 (4%)	34	58
1	M	410/447 (92%)	399 (97%)	11 (3%)	44	65
1	N	410/447 (92%)	395 (96%)	15 (4%)	34	58
1	O	410/447 (92%)	391 (95%)	19 (5%)	27	52
1	P	410/447 (92%)	401 (98%)	9 (2%)	52	71
1	Q	410/447 (92%)	401 (98%)	9 (2%)	52	71
1	R	410/447 (92%)	401 (98%)	9 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	S	410/447 (92%)	394 (96%)	16 (4%)	32 56
All	All	7380/8046 (92%)	7159 (97%)	221 (3%)	44 63

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LYS
1	A	144	GLN
1	A	167	THR
1	A	269	PRO
1	A	297	VAL
1	A	301	GLN
1	A	305	ASP
1	A	343	ILE
1	A	367	MET
1	A	369	PHE
1	A	370	VAL
1	A	422	GLU
1	A	423	ILE
1	A	473	LEU
1	B	56	ASP
1	B	76	LEU
1	B	80	ASP
1	B	83	HIS
1	B	149	LEU
1	B	242	GLU
1	B	248	LEU
1	B	273	GLN
1	B	297	VAL
1	B	331	LEU
1	B	356	LEU
1	B	367	MET
1	B	392	ASP
1	B	398	LEU
1	B	473	LEU
1	B	477	HIS
1	B	509	LYS
1	C	76	LEU
1	C	89	LEU
1	C	128	PRO
1	C	164	ILE
1	C	167	THR

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Mol	Chain	Res	Type
1	C	241	LEU
1	C	288	ASP
1	C	301	GLN
1	C	367	MET
1	C	453	SER
1	C	473	LEU
1	C	509	LYS
1	C	522	LEU
1	D	82	GLN
1	D	139	GLU
1	D	144	GLN
1	D	152	THR
1	D	159	ASP
1	D	203	ASP
1	D	204	LEU
1	D	241	LEU
1	D	288	ASP
1	D	297	VAL
1	D	301	GLN
1	D	341	SER
1	D	365	ASP
1	D	453	SER
1	D	470	LEU
1	D	477	HIS
1	E	76	LEU
1	E	153	VAL
1	E	246	ILE
1	E	273	GLN
1	E	288	ASP
1	E	297	VAL
1	E	305	ASP
1	E	365	ASP
1	F	84	PRO
1	F	160	LEU
1	F	167	THR
1	F	169	LEU
1	F	210	VAL
1	F	211	LYS
1	F	297	VAL
1	F	301	GLN
1	F	367	MET
1	F	436	VAL

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Mol	Chain	Res	Type
1	F	473	LEU
1	F	476	THR
1	F	477	HIS
1	F	485	TYR
1	G	61	ASP
1	G	198	ASP
1	G	211	LYS
1	G	231	GLU
1	G	232	VAL
1	G	246	ILE
1	G	254	GLU
1	G	297	VAL
1	G	301	GLN
1	G	351	LEU
1	H	100	THR
1	H	241	LEU
1	H	297	VAL
1	H	301	GLN
1	H	356	LEU
1	H	422	GLU
1	H	441	GLN
1	H	473	LEU
1	I	33	ARG
1	I	47	LYS
1	I	62	SER
1	I	123	TYR
1	I	127	HIS
1	I	178	ARG
1	I	238	PRO
1	I	297	VAL
1	I	429	LEU
1	I	480	GLU
1	I	484	TRP
1	K	59	LEU
1	K	97	ASP
1	K	100	THR
1	K	297	VAL
1	K	434	PRO
1	K	473	LEU
1	K	484	TRP
1	L	30	GLU
1	L	47	LYS

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Mol	Chain	Res	Type
1	L	56	ASP
1	L	129	THR
1	L	144	GLN
1	L	248	LEU
1	L	288	ASP
1	L	297	VAL
1	L	301	GLN
1	L	331	LEU
1	L	356	LEU
1	L	367	MET
1	L	391	VAL
1	L	392	ASP
1	L	477	HIS
1	M	56	ASP
1	M	82	GLN
1	M	167	THR
1	M	263	GLU
1	M	297	VAL
1	M	298	ILE
1	M	301	GLN
1	M	329	GLU
1	M	356	LEU
1	M	376	PRO
1	M	379	ILE
1	N	30	GLU
1	N	66	ILE
1	N	76	LEU
1	N	99	GLU
1	N	139	GLU
1	N	167	THR
1	N	297	VAL
1	N	301	GLN
1	N	305	ASP
1	N	329	GLU
1	N	367	MET
1	N	453	SER
1	N	473	LEU
1	N	484	TRP
1	N	517	THR
1	O	30	GLU
1	O	63	LEU
1	O	77	ASP

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Mol	Chain	Res	Type
1	O	144	GLN
1	O	222	LEU
1	O	231	GLU
1	O	242	GLU
1	O	283	ILE
1	O	297	VAL
1	O	305	ASP
1	O	312	LEU
1	O	326	SER
1	O	329	GLU
1	O	343	ILE
1	O	356	LEU
1	O	367	MET
1	O	473	LEU
1	O	484	TRP
1	O	487	ILE
1	P	167	THR
1	P	211	LYS
1	P	241	LEU
1	P	269	PRO
1	P	367	MET
1	P	451	LEU
1	P	473	LEU
1	P	477	HIS
1	P	484	TRP
1	Q	29	LYS
1	Q	74	THR
1	Q	167	THR
1	Q	204	LEU
1	Q	208	GLN
1	Q	210	VAL
1	Q	273	GLN
1	Q	398	LEU
1	Q	510	MET
1	R	42	VAL
1	R	168	SER
1	R	297	VAL
1	R	301	GLN
1	R	322	ARG
1	R	367	MET
1	R	376	PRO
1	R	453	SER

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Mol	Chain	Res	Type
1	R	473	LEU
1	S	33	ARG
1	S	43	GLU
1	S	82	GLN
1	S	84	PRO
1	S	144	GLN
1	S	231	GLU
1	S	258	PRO
1	S	283	ILE
1	S	288	ASP
1	S	297	VAL
1	S	301	GLN
1	S	333	ARG
1	S	366	LYS
1	S	473	LEU
1	S	528	ASP
1	S	530	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	GLN
1	B	127	HIS
1	B	147	GLN
1	C	70	ASN
1	D	96	GLN
1	E	127	HIS
1	F	82	GLN
1	F	127	HIS
1	F	221	GLN
1	F	267	ASN
1	G	441	GLN
1	G	477	HIS
1	H	441	GLN
1	I	83	HIS
1	K	127	HIS
1	K	144	GLN
1	K	151	GLN
1	K	206	ASN
1	L	218	ASN
1	M	83	HIS
1	M	221	GLN

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Mol	Chain	Res	Type
1	N	234	HIS
1	N	482	ASN
1	O	441	GLN
1	O	477	HIS
1	P	127	HIS
1	P	271	GLN
1	P	441	GLN
1	S	144	GLN
1	S	234	HIS
1	S	479	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

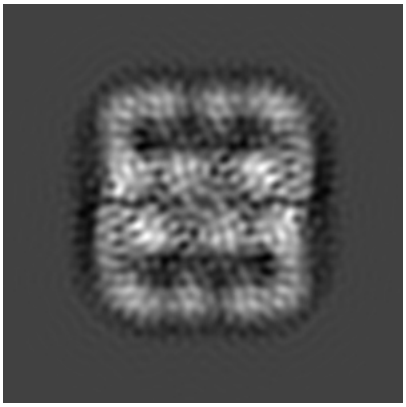
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5395. These allow visual inspection of the internal detail of the map and identification of artifacts.

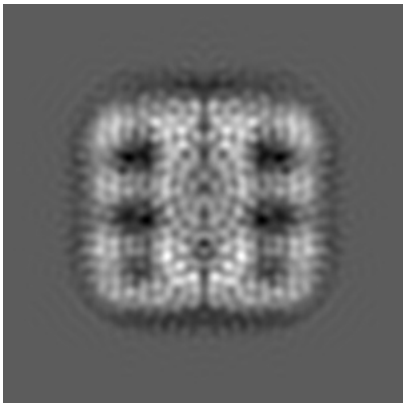
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

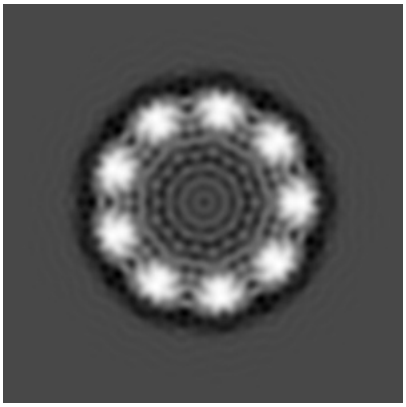
6.1.1 Primary map



X



Y

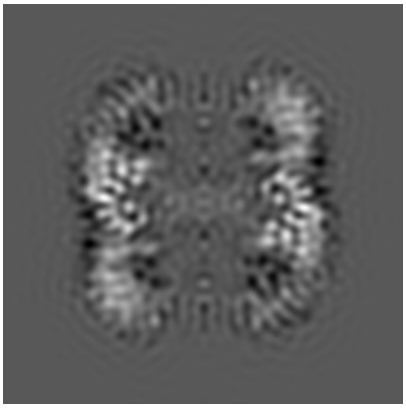


Z

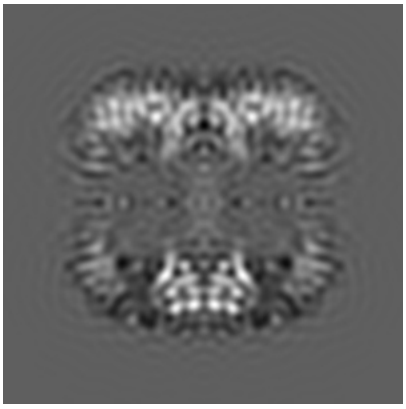
The images above show the map projected in three orthogonal directions.

6.2 Central slices

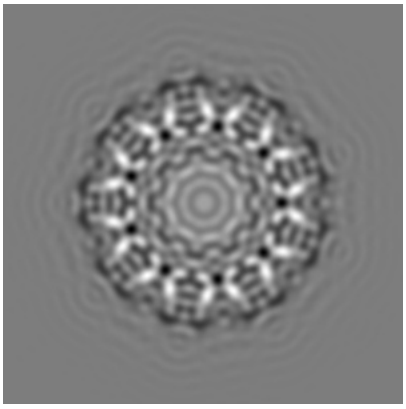
6.2.1 Primary map



X Index: 80



Y Index: 80

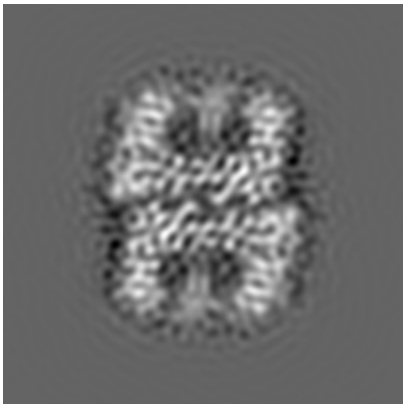


Z Index: 80

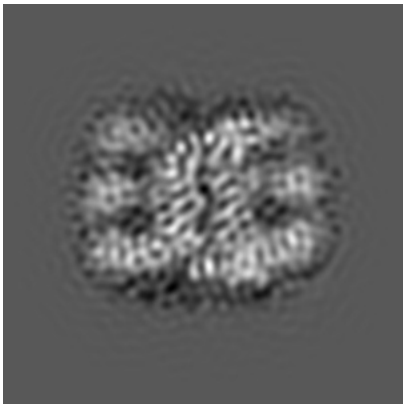
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 109



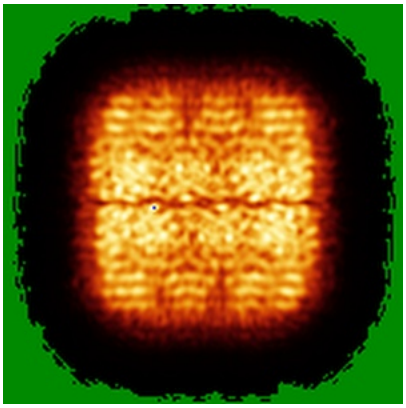
Y Index: 49

Z Index: 65

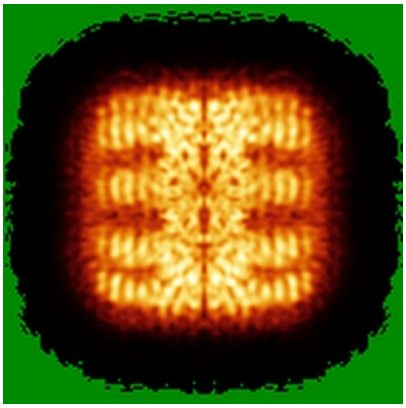
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

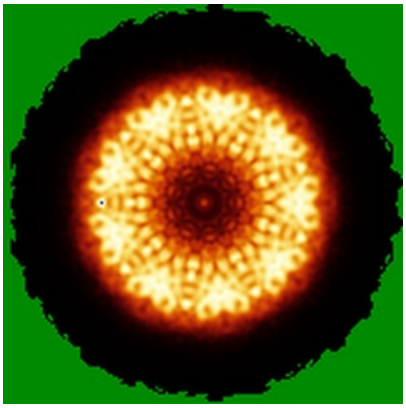
6.4.1 Primary map



X



Y

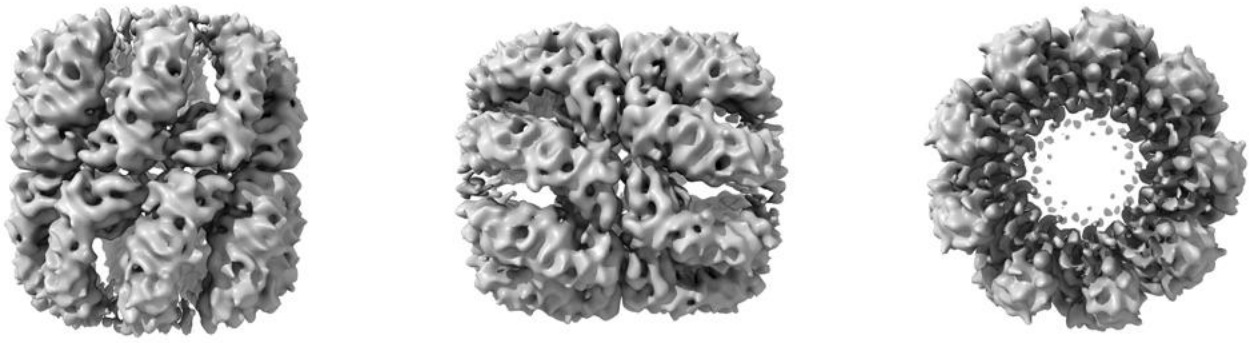


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

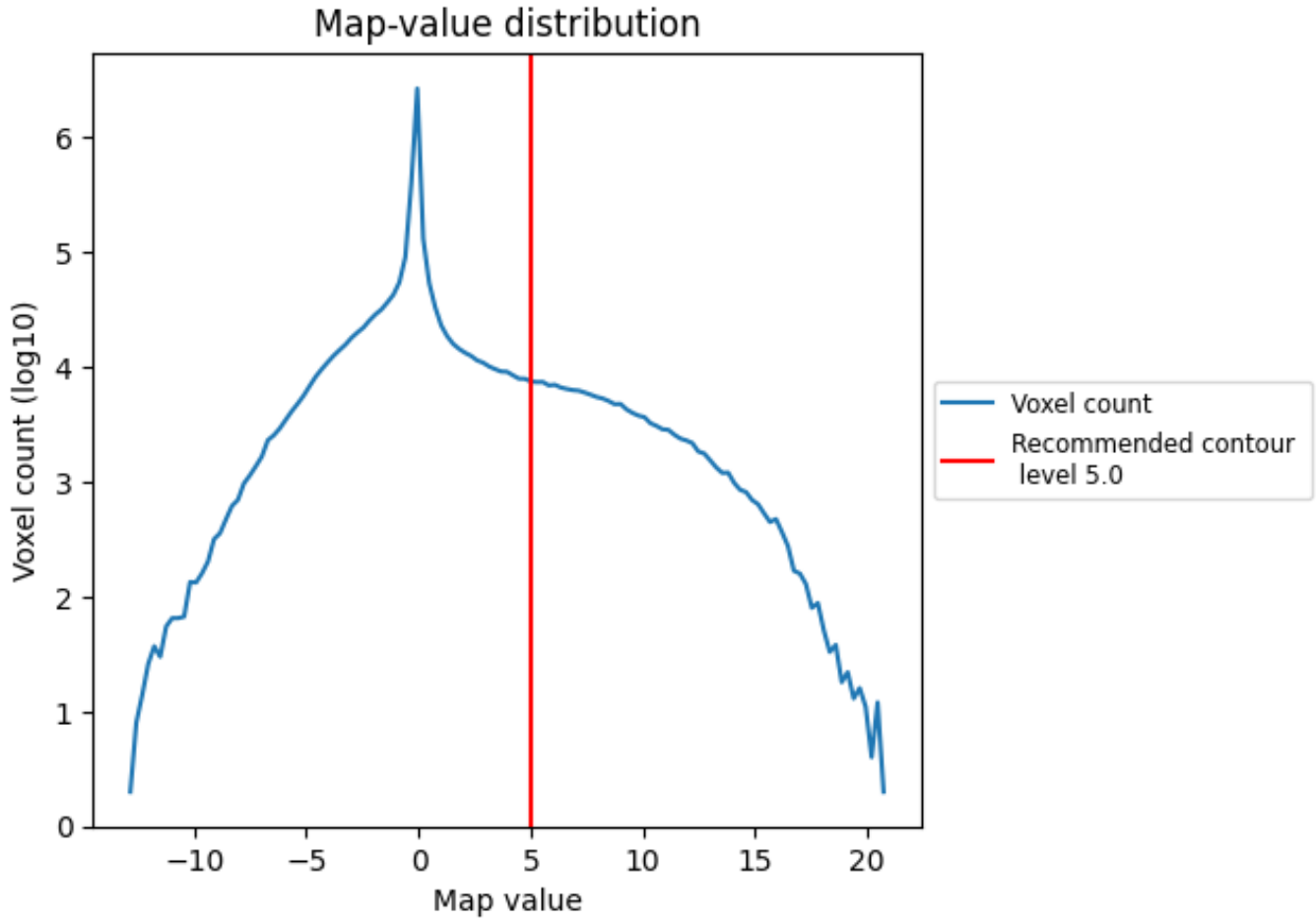
6.6 Mask visualisation (i)

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

7 Map analysis

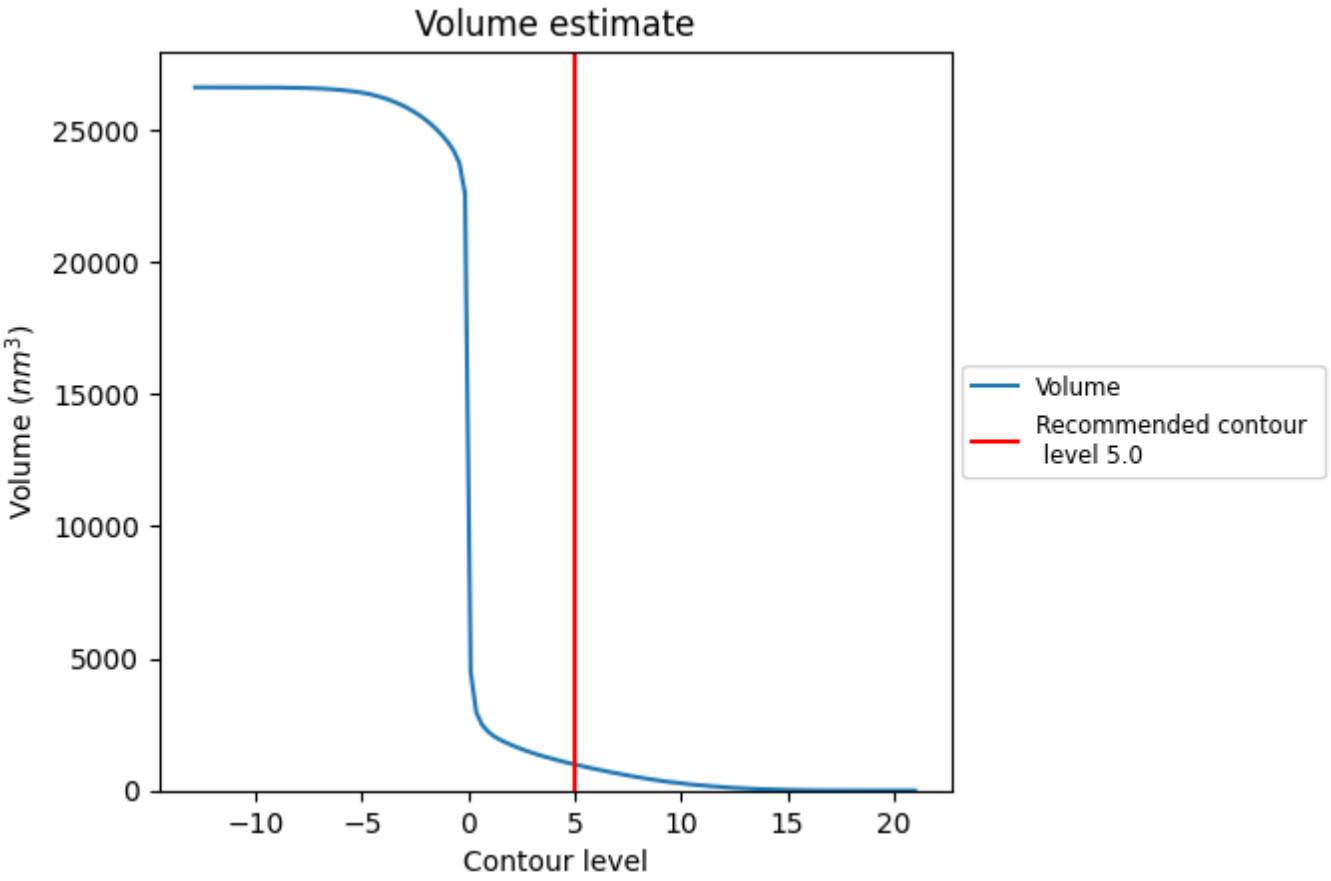
This section contains the results of statistical analysis of the map.

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.

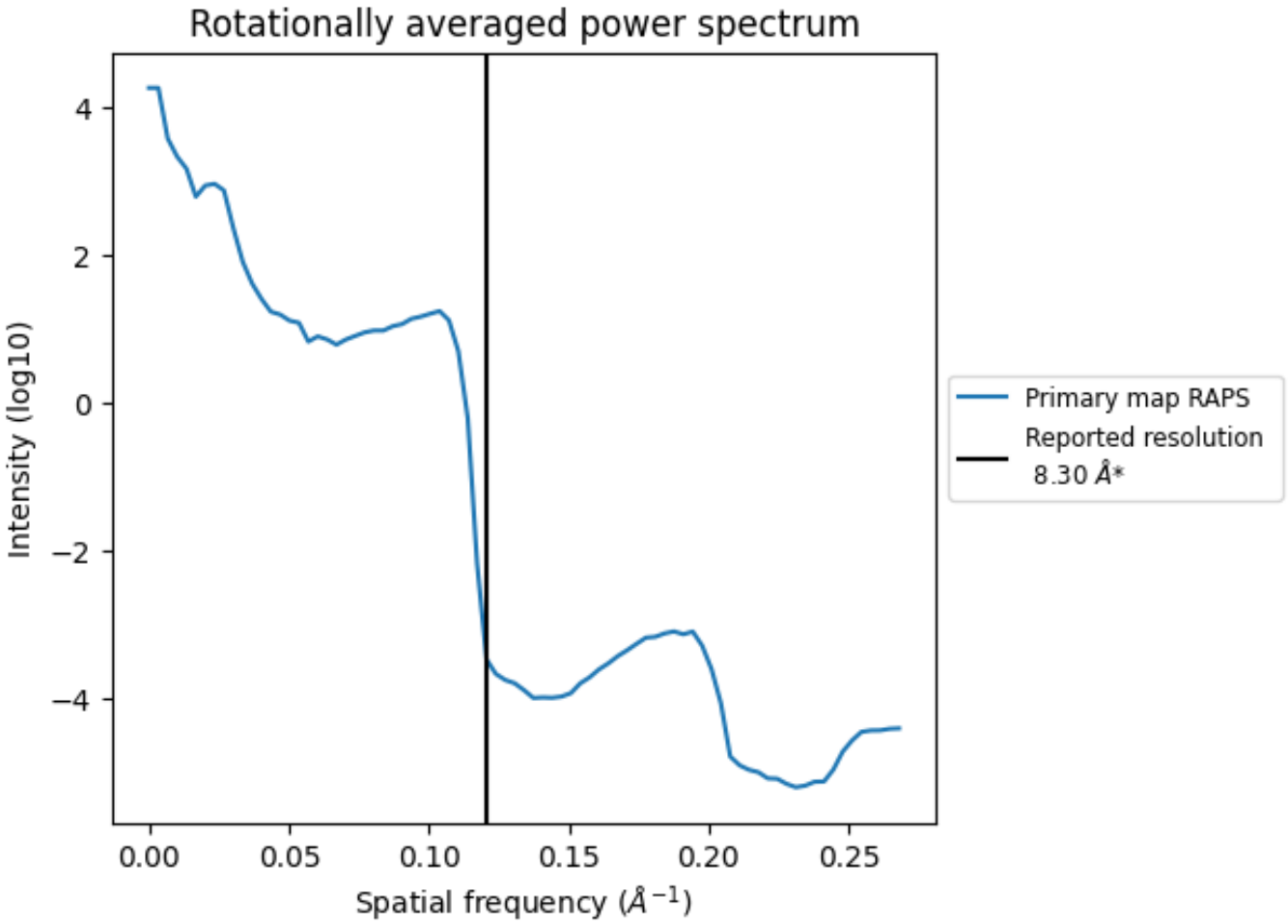
7.2 Volume estimate



The volume at the recommended contour level is 989 nm^3; this corresponds to an approximate mass of 893 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 0.120 Å^{-1}

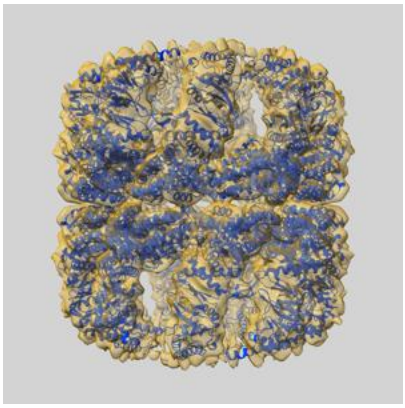
8 Fourier-Shell correlation (i)

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

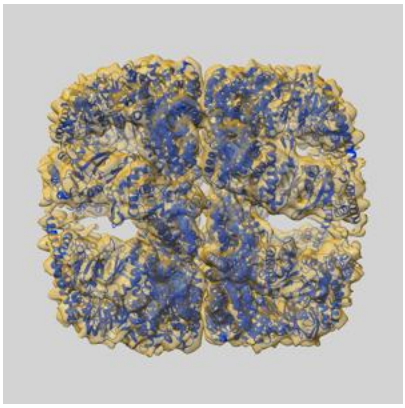
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-5395 and PDB model 3J1E. Per-residue inclusion information can be found in section 3 on page 6.

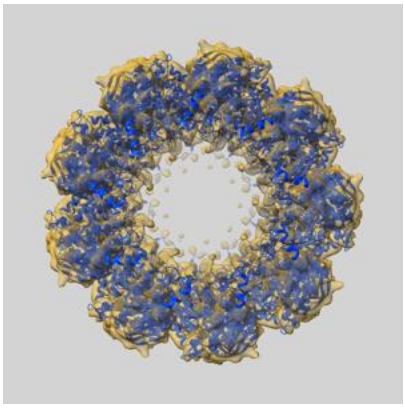
9.1 Map-model overlay



X



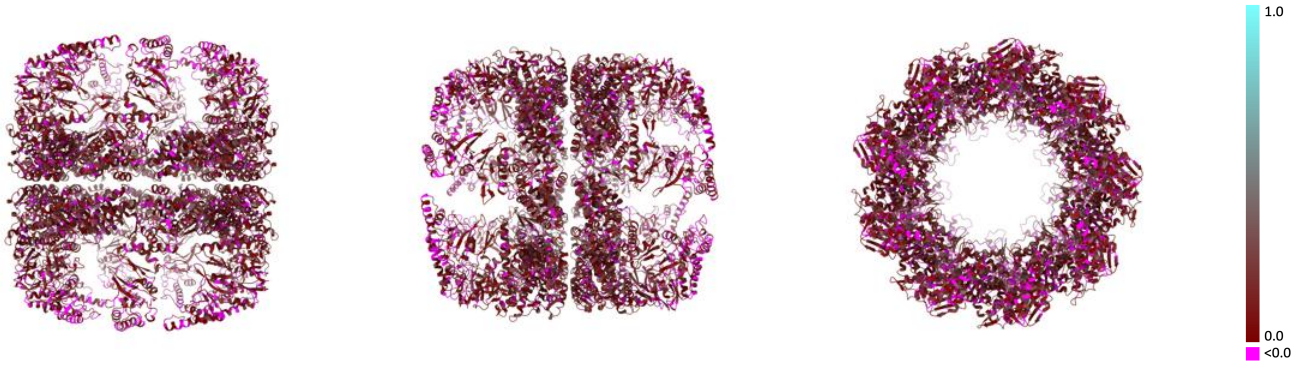
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

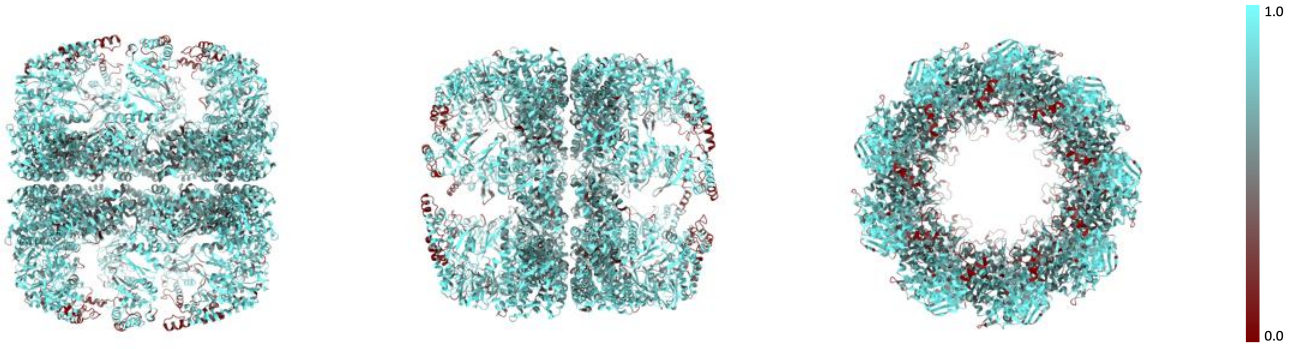
9.2 Q-score mapped to coordinate model (i)



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.

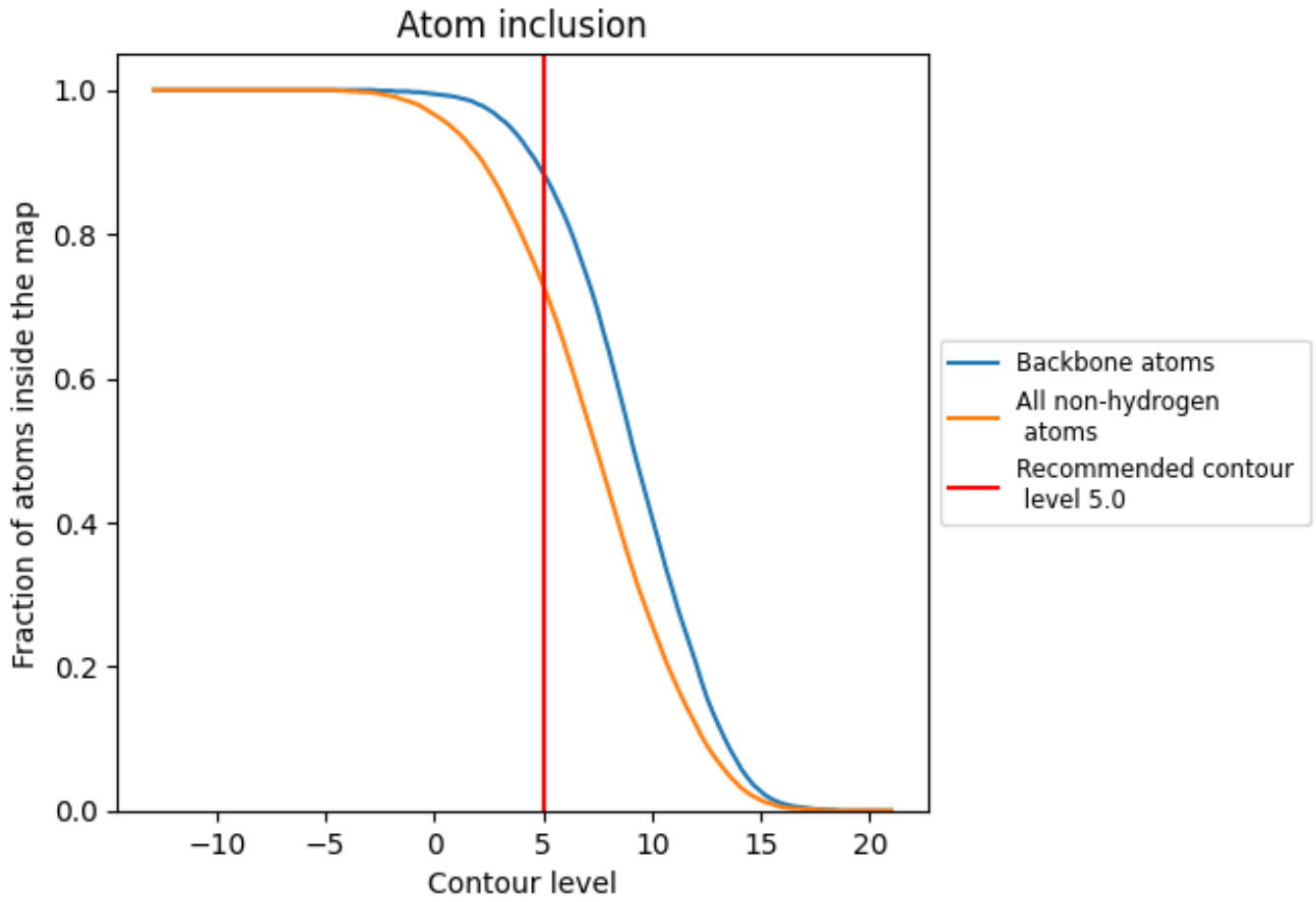
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 73% 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 (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	0.1130
A	0.7260	0.1160
B	0.7330	0.1150
C	0.7290	0.1140
D	0.7290	0.1120
E	0.7310	0.1160
F	0.7320	0.1150
G	0.7300	0.1120
H	0.7280	0.1110
I	0.7290	0.1140
K	0.7320	0.1140
L	0.7350	0.1120
M	0.7320	0.1110
N	0.7310	0.1130
O	0.7360	0.1140
P	0.7270	0.1130
Q	0.7300	0.1130
R	0.7270	0.1110
S	0.7260	0.1160