Full wwPDB EM Validation Report

Nov 22, 2022 – 02:40 PM EST

PDB ID	:	7N84
EMDB ID	:	EMD-24231
Title	:	Double nuclear outer ring from the isolated yeast NPC
Authors	:	Akey, C.W.; Rout, M.P.; Ouch, C.; Echevarria, I.; Fernandez-Martinez, J.; Nudelman, I.
Deposited on	:	2021-06-13
Resolution	:	11.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

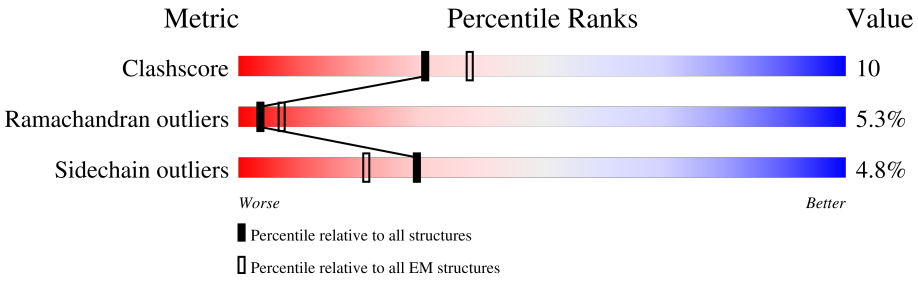
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 11.60 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	X	1655	6% 44% 18% 6% • 31%
2	Y	63	100%
2	Z	63	100%
3	a	1037	66% 25% 5% • •
3	l	1037	68% 24% 5% •
4	b	744	64% 23% • 9%
4	m	744	62% 22% 6% 10%
5	c	712	56% 19% • 21%

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Mol	Chain	Length	Quality of chain
5	n	712	
6	d	297	
6	o	297	
7	e	349	
7	p	349	
8	f	726	
8	q	726	
9	g	1157	
9	r	1157	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 83142 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 Nucleoporin NUP188.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	1137	Total	C	N	O	S	0	0
			9208	6035	1455	1700	18		

- Molecule 2 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Y	63	Total	C	N	O	0	0
			315	189	63	63		
2	Z	63	Total	C	N	O	0	0
			315	189	63	63		

- Molecule 3 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	1006	Total	C	N	O	S	0	0
			8279	5346	1334	1566	33		
3	l	1006	Total	C	N	O	S	0	0
			8279	5346	1334	1566	33		

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	675	Total	C	N	O	S	0	0
			5424	3493	863	1038	30		
4	m	670	Total	C	N	O	S	0	0
			5384	3468	857	1031	28		

- Molecule 5 is a protein called Nucleoporin 145c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	559	Total	C	N	O	S	0	0
			4520	2884	750	869	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	n	557	Total 4505	C 2873	N 748	O 867	S 17	0	0

- Molecule 6 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	274	Total 2160	C 1379	N 369	O 409	S 3	0	0
6	o	274	Total 2160	C 1379	N 369	O 409	S 3	0	0

- Molecule 7 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	307	Total 2438	C 1543	N 422	O 462	S 11	0	0
7	p	307	Total 2438	C 1543	N 422	O 462	S 11	0	0

- Molecule 8 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	649	Total 5261	C 3370	N 866	O 1011	S 14	0	0
8	q	648	Total 5254	C 3365	N 865	O 1010	S 14	0	0

- Molecule 9 is a protein called Nucleoporin NUP133.

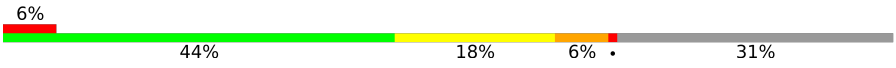
Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	1062	Total 8627	C 5541	N 1393	O 1664	S 29	0	0
9	r	1056	Total 8575	C 5511	N 1381	O 1654	S 29	0	0

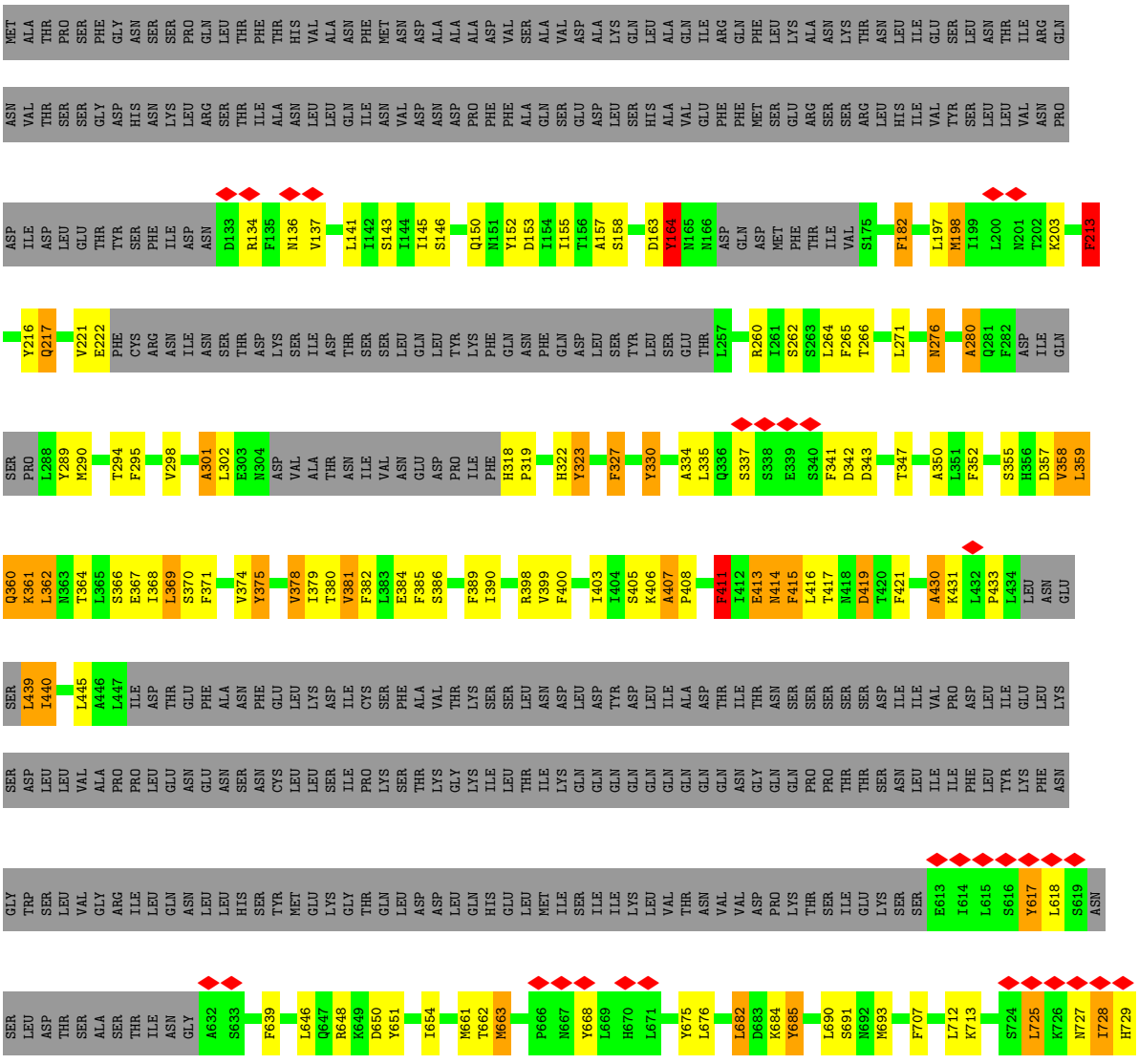
3 Residue-property plots (i)

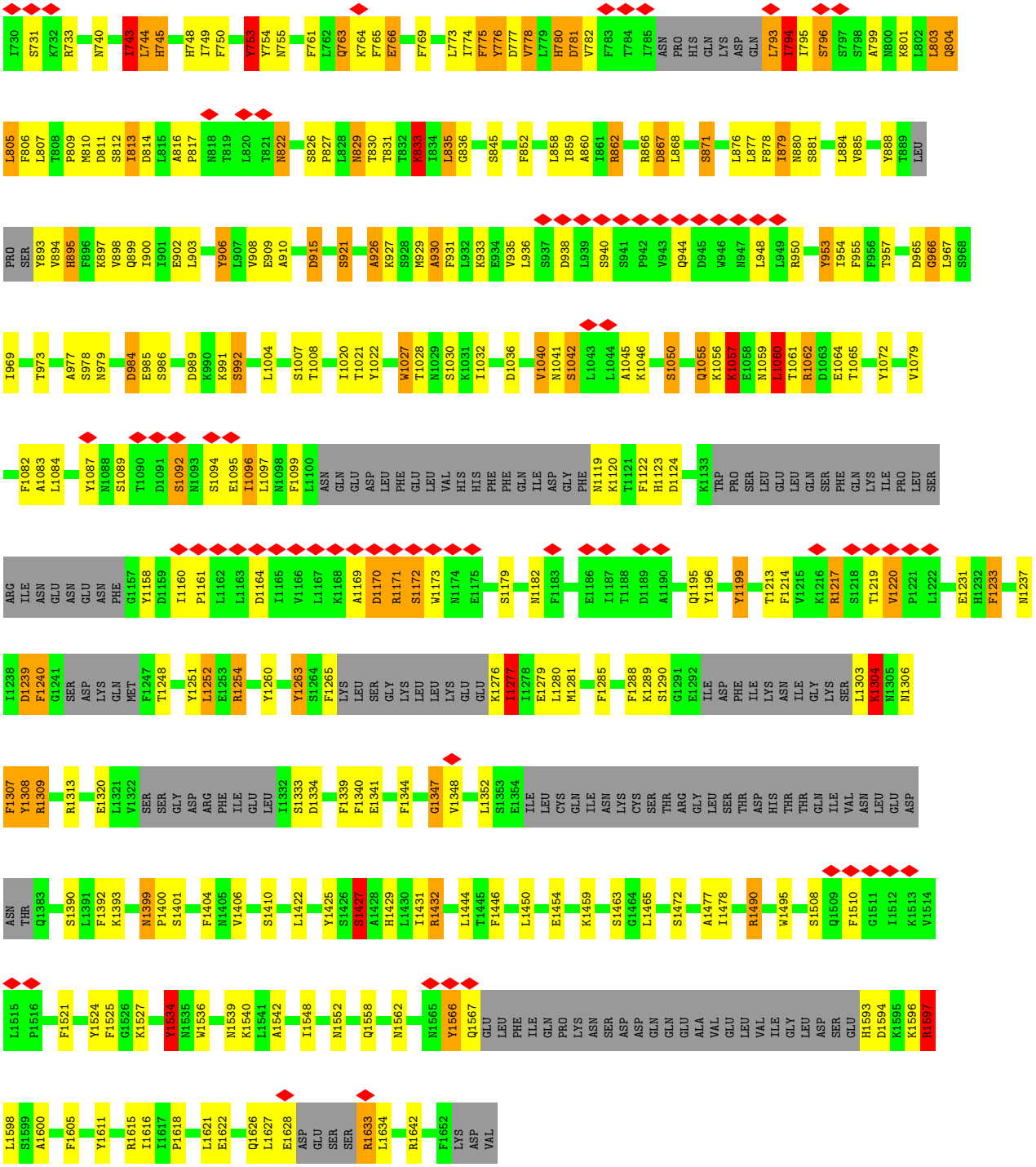
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Nucleoporin NUP188

Chain X:

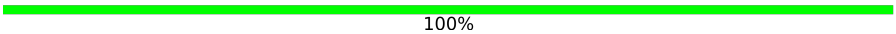






• Molecule 2: unknown

Chain Y:



There are no outlier residues recorded for this chain.

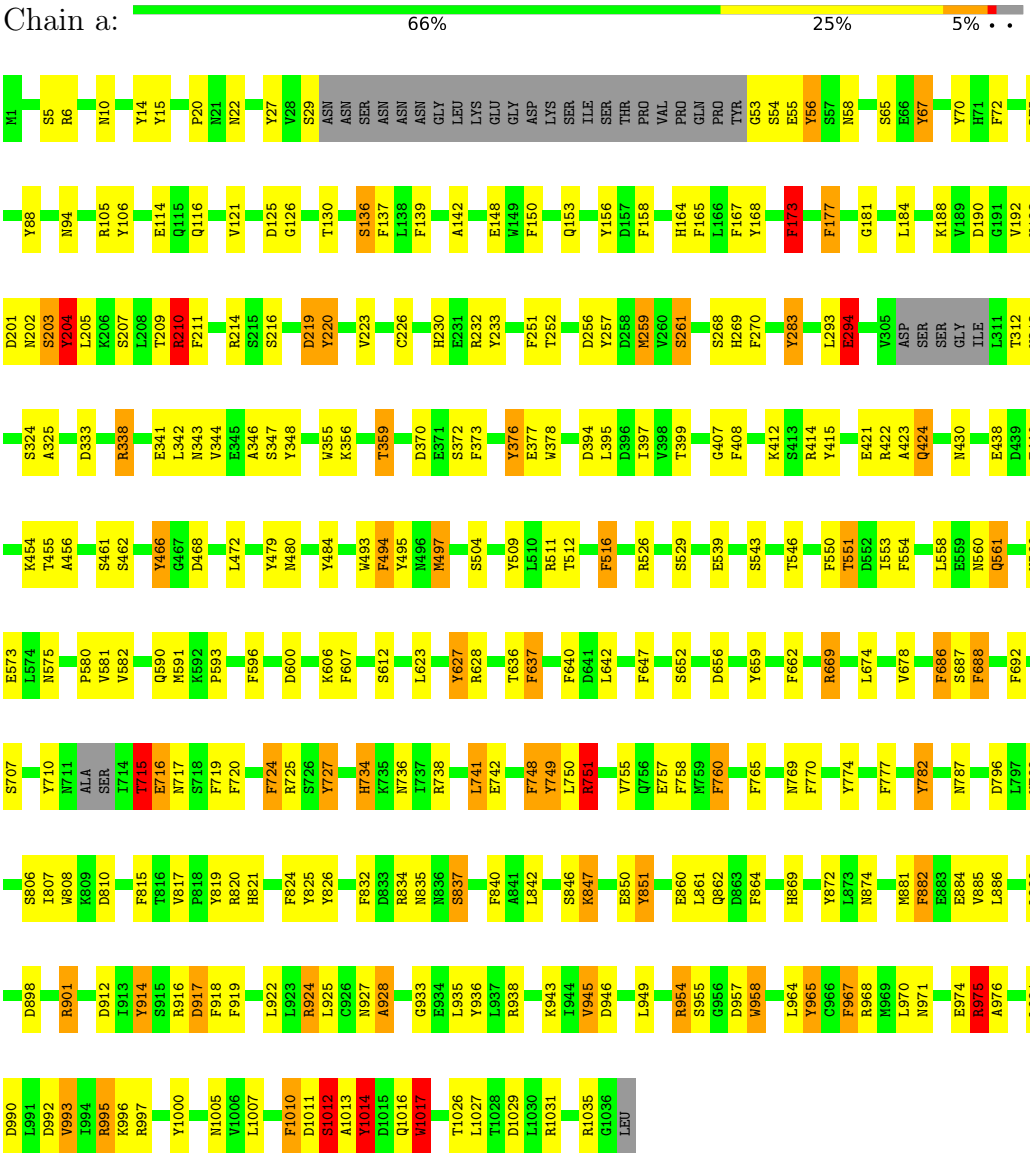
• Molecule 2: unknown

Chain Z:

There are no outlier residues recorded for this chain.

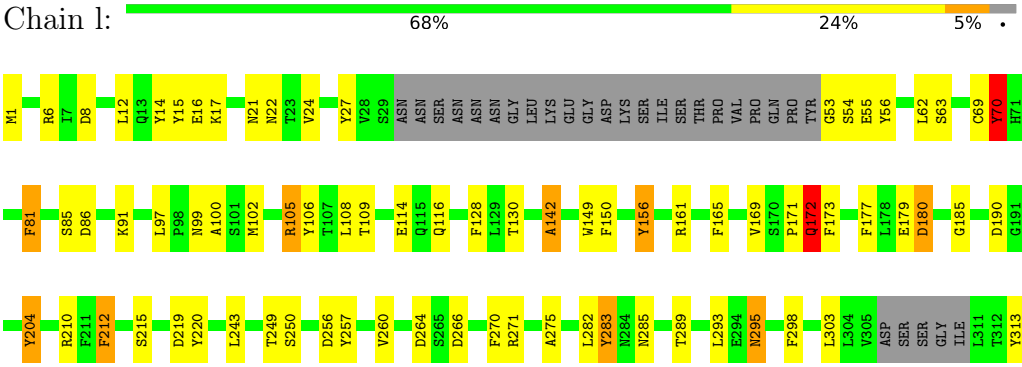
• Molecule 3: Nucleoporin NUP120

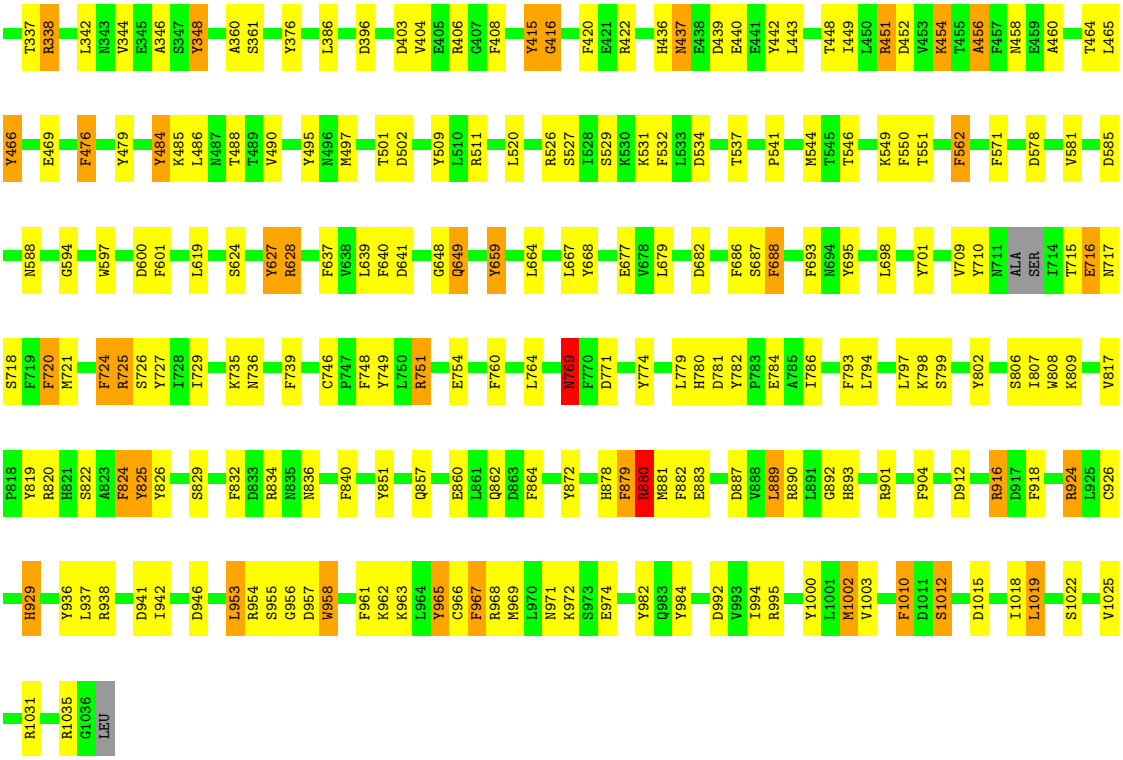
Chain a:



• Molecule 3: Nucleoporin NUP120

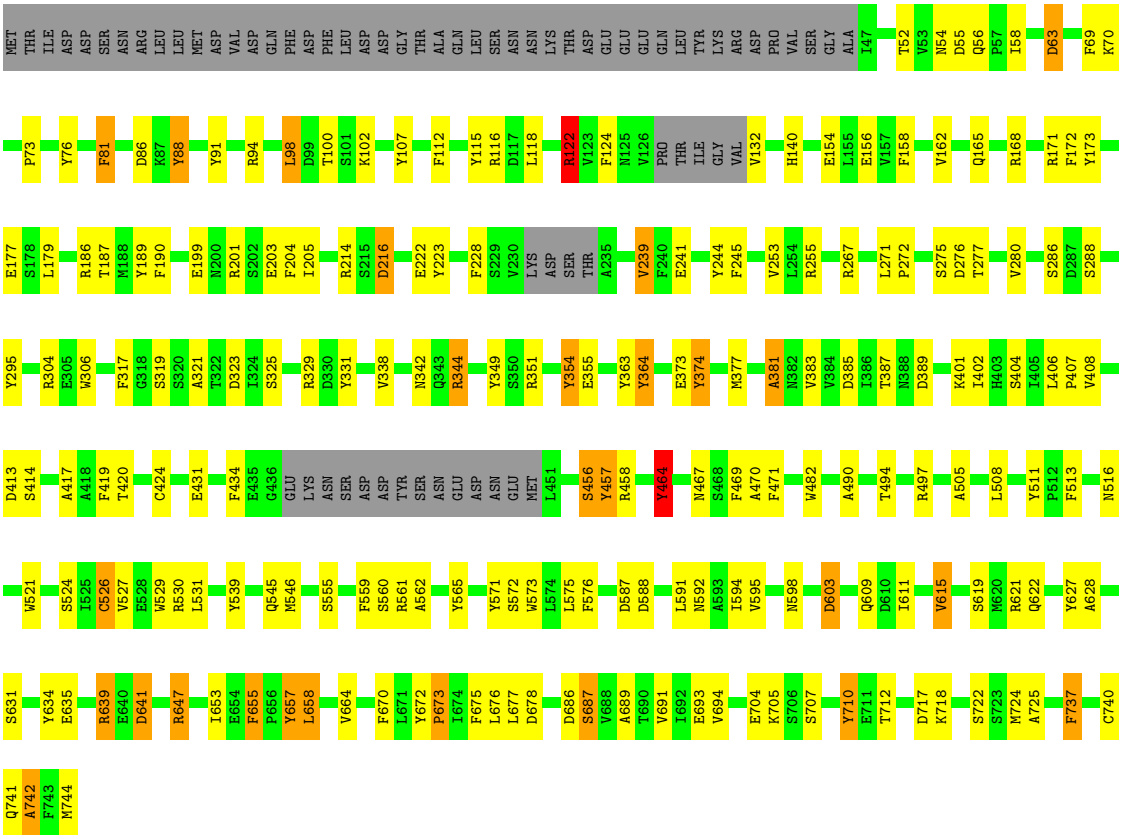
Chain l:





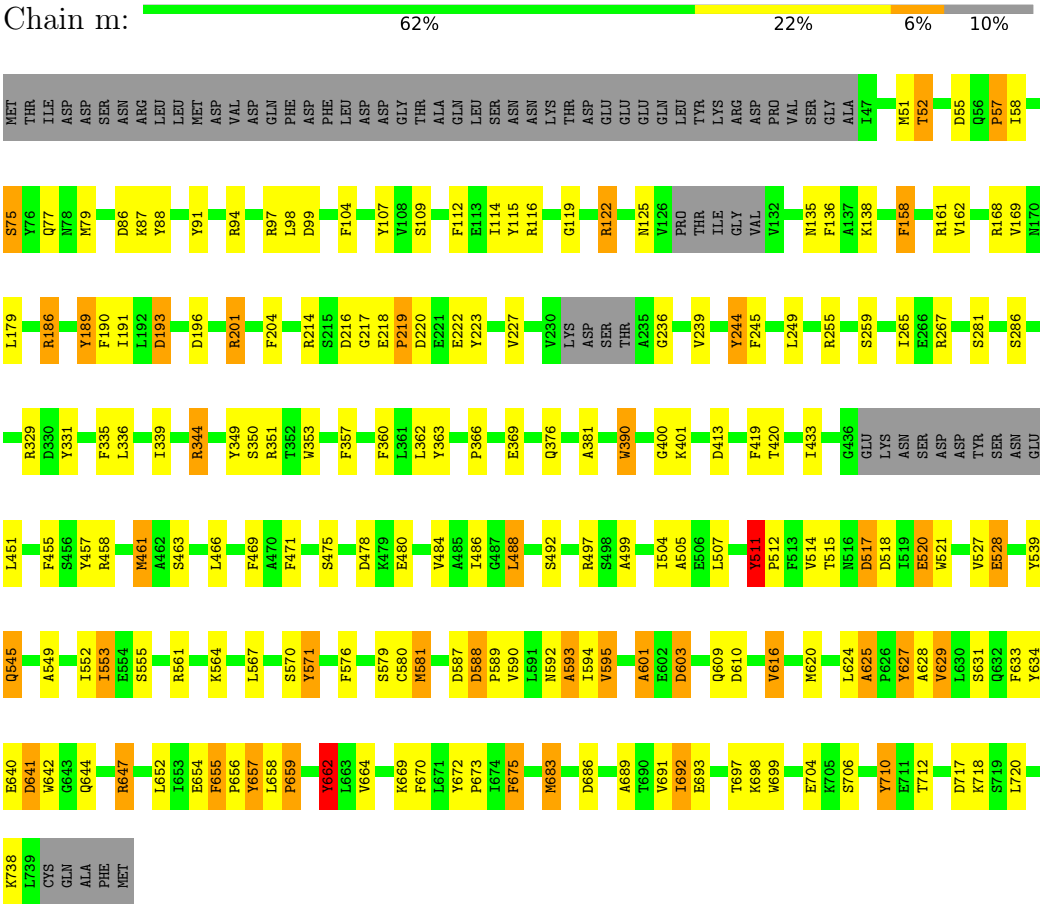
• Molecule 4: Nucleoporin NUP85

Chain b:



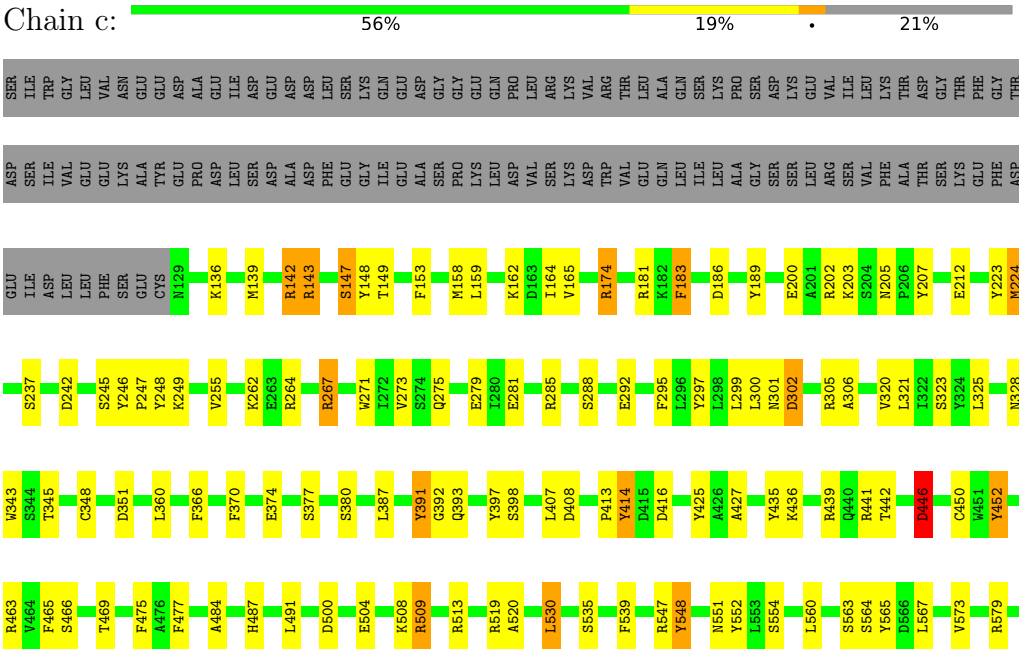
• Molecule 4: Nucleoporin NUP85

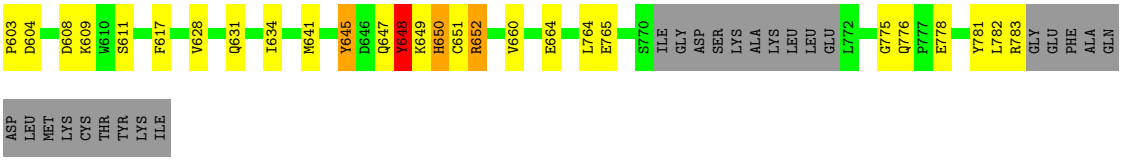
Chain m:



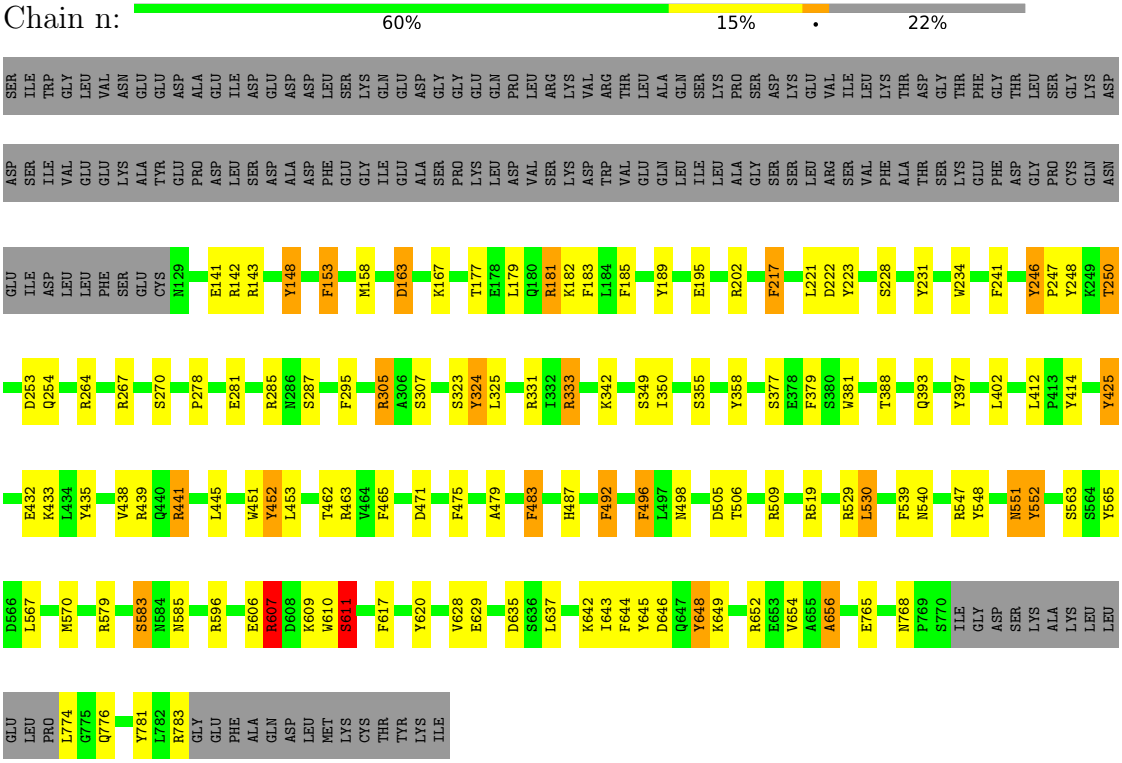
• Molecule 5: Nucleoporin 145c

Chain c:

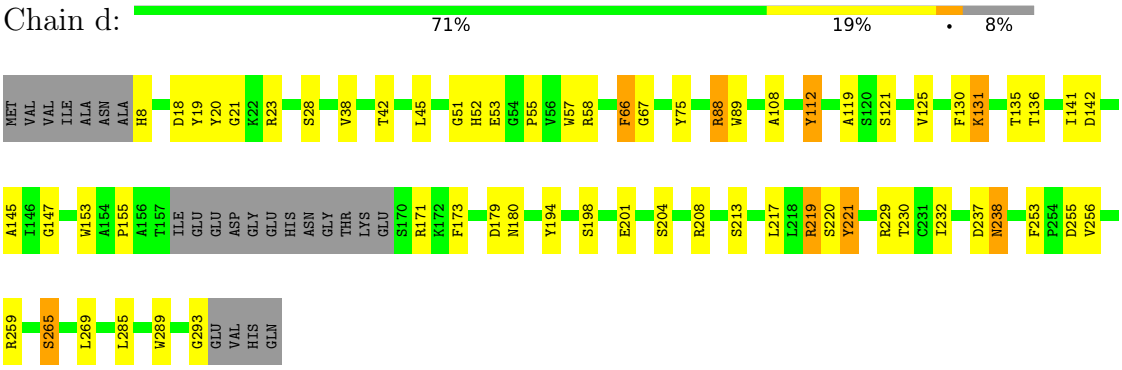




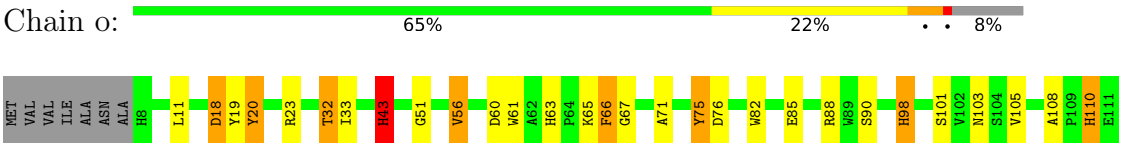
• Molecule 5: Nucleoporin 145c

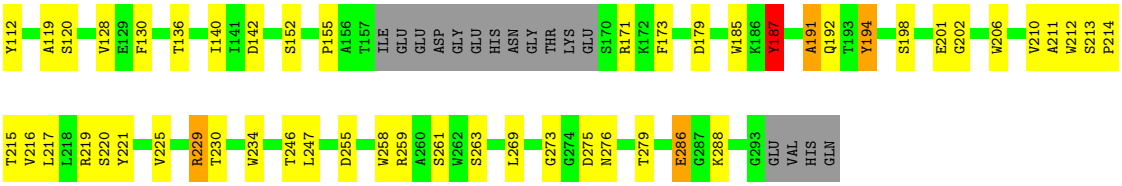


• Molecule 6: Protein transport protein SEC13



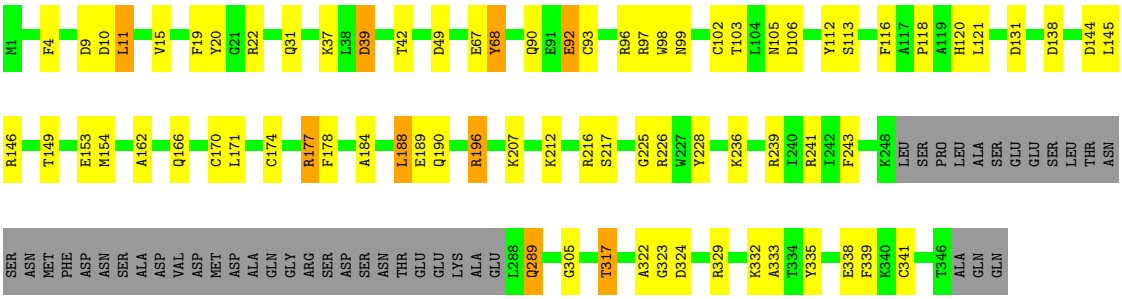
• Molecule 6: Protein transport protein SEC13





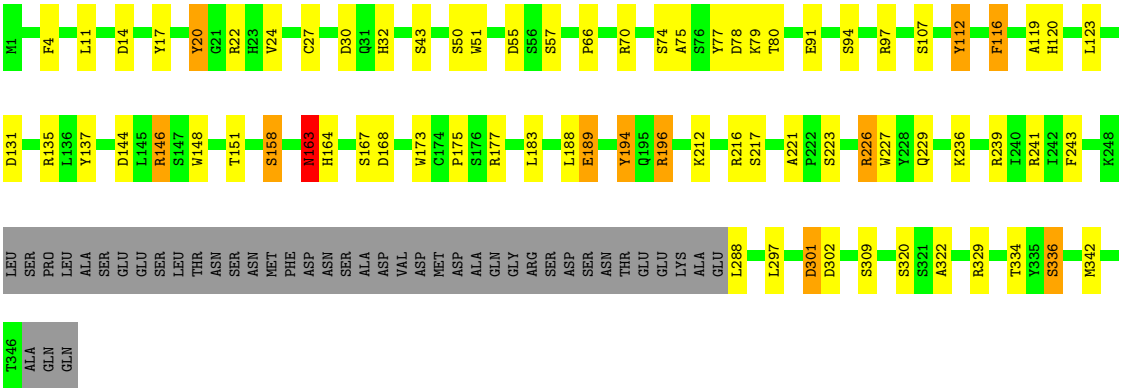
• Molecule 7: Nucleoporin SEH1

Chain e:



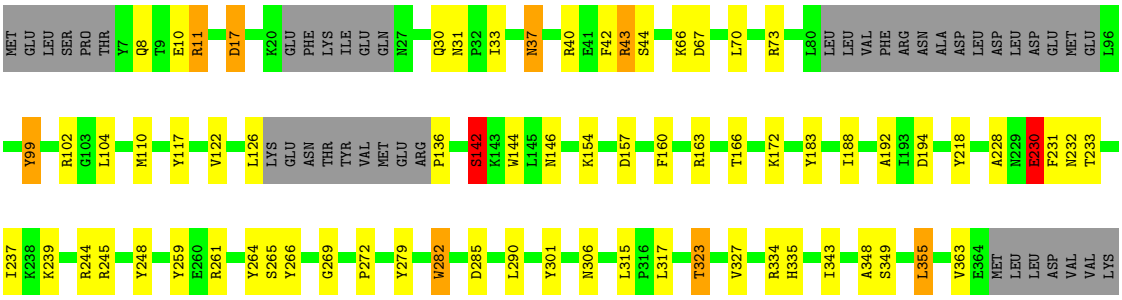
• Molecule 7: Nucleoporin SEH1

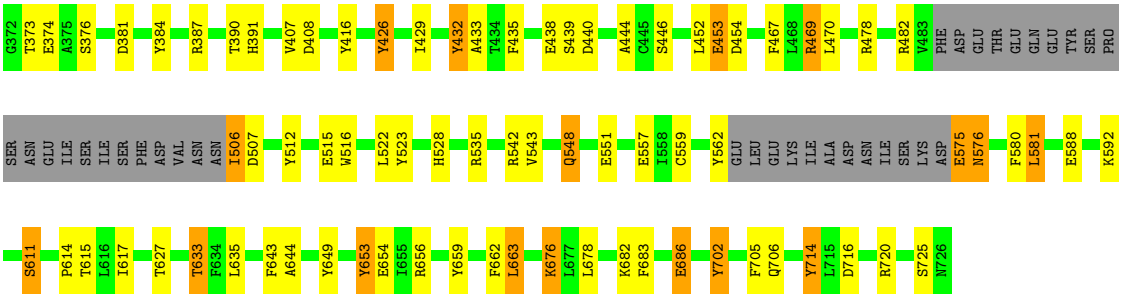
Chain p:



• Molecule 8: Nucleoporin NUP84

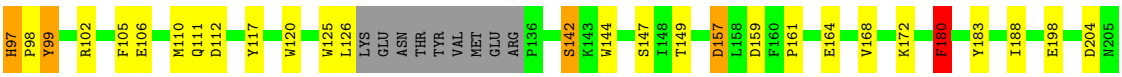
Chain f:

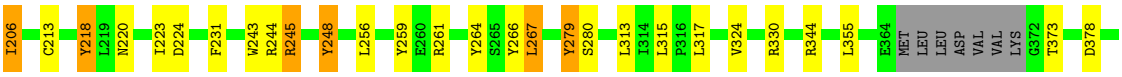


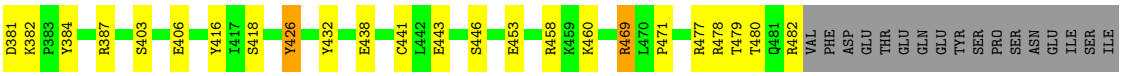


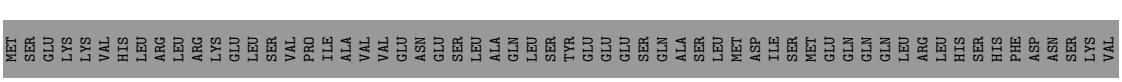
• Molecule 8: Nucleoporin NUP84

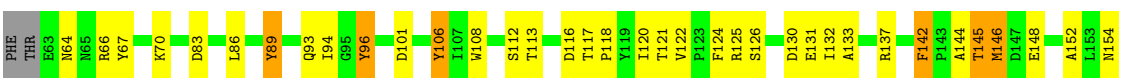
Chain q:

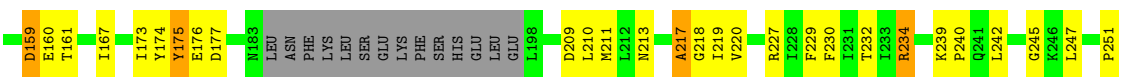






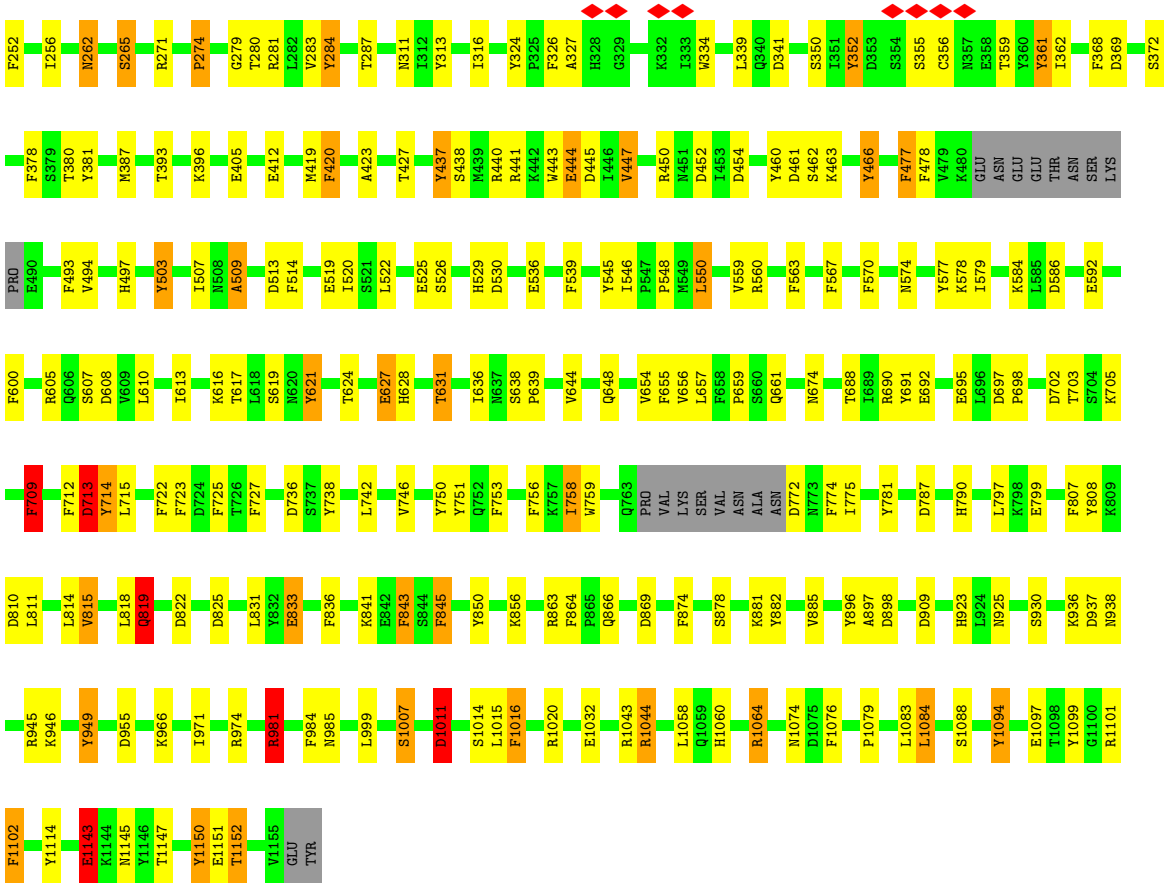






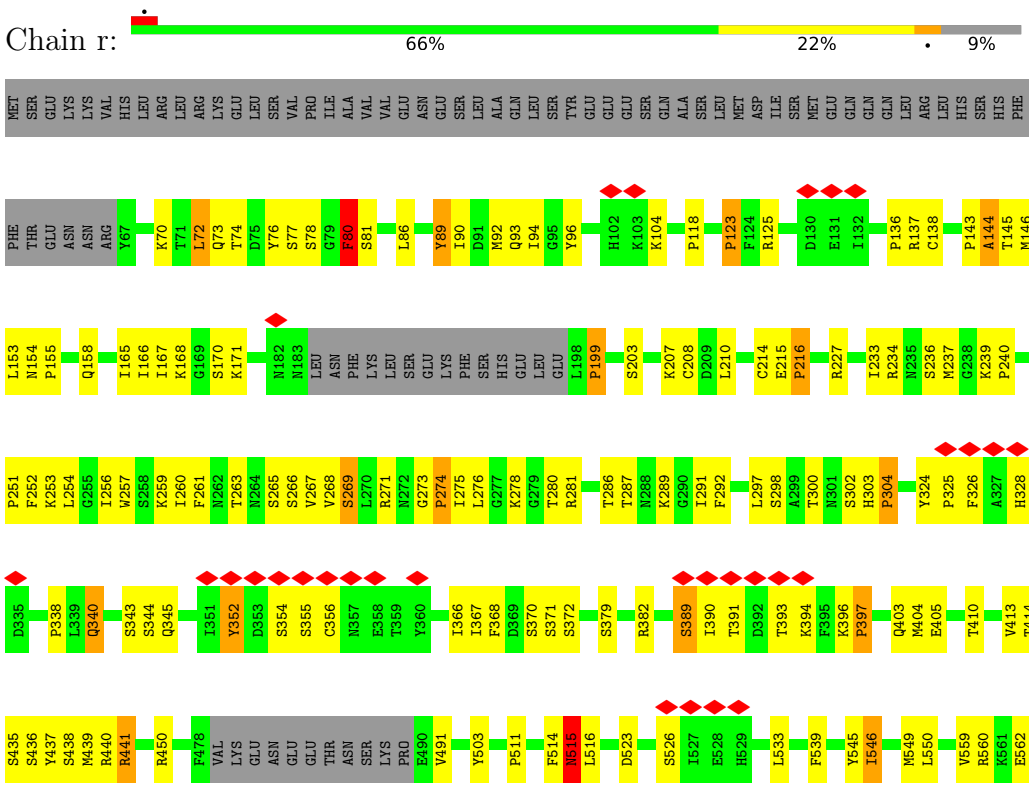
• Molecule 9: Nucleoporin NUP133

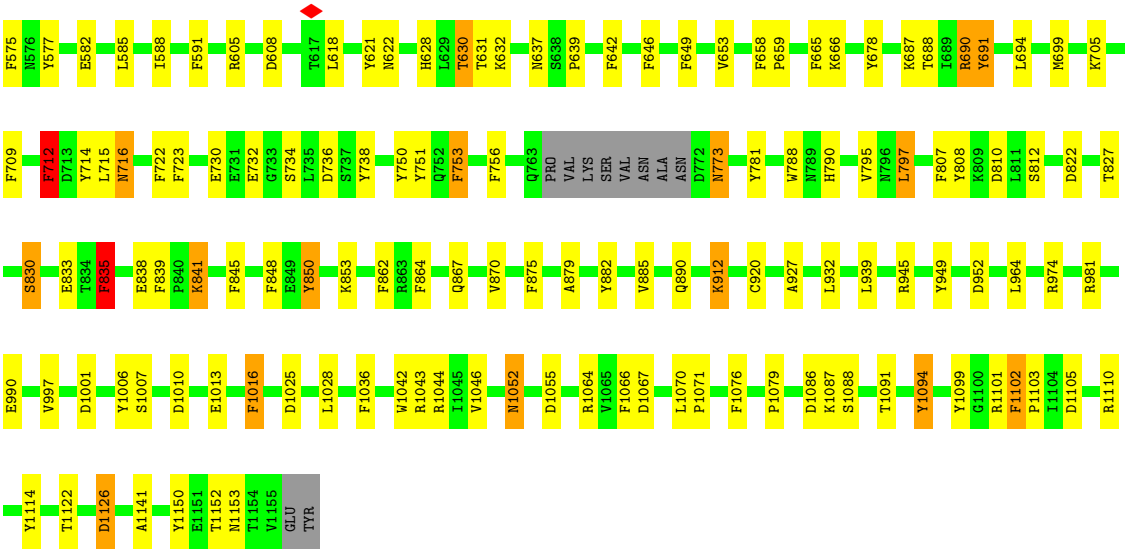
Chain g:



• Molecule 9: Nucleoporin NUP133

Chain r:




F575 N576 Y577 E582 L585 I588 F591 R605 D608 T617 L618 Y621 N622 H628 L629 T630 T631 K632 N637 S638 P639 F642 F646 F649 V653 F658 P659 F665 K666 Y678 K687 T688 I689 R690 Y691 L694 M699 K705
F709 F712 D713 Y714 L715 N716 F722 F723 E730 E731 E732 G733 S734 L735 D736 S737 Y738 Y750 Y751 Q752 F753 F756 Q763 PRO VAL LYS SER VAL ASN ALA ASN D772 N773 Y781 W788 N789 H790 V795 N796 L797 F807 Y808 K809 D810 L811 S812 D822 T827
S830 E833 T834 F835 E838 F839 P840 K841 F845 F848 E849 Y850 K853 F862 R863 F864 Q867 V870 F875 A879 Y882 V885 Q890 K912 C920 A927 L932 L939 R945 Y949 D962 L964 R974 R981
E990 V997 D1001 Y1006 S1007 D1010 E1013 F1016 D1025 L1028 F1036 W1042 R1043 R1044 I1045 V1046 N1052 D1055 R1064 V1065 F1066 D1067 L1070 P1071 F1076 P1079 D1086 K1087 S1088 T1091 Y1094 Y1099 G1100 R1101 F1102 P1103 I1104 D1105 R1110
Y1114 T1122 D1126 A1141 Y1150 E1151 T1152 N1153 T1154 V1155 GLU TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	37651	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	1276.8, 1276.8, 1276.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	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	X	1.68	65/9370 (0.7%)	2.00	242/12670 (1.9%)
3	a	1.73	82/8464 (1.0%)	2.03	250/11469 (2.2%)
3	l	1.75	82/8461 (1.0%)	2.03	235/11460 (2.1%)
4	b	1.71	48/5533 (0.9%)	2.00	149/7493 (2.0%)
4	m	1.73	42/5492 (0.8%)	1.97	149/7440 (2.0%)
5	c	1.72	40/4600 (0.9%)	1.95	107/6211 (1.7%)
5	n	1.70	30/4584 (0.7%)	1.93	95/6188 (1.5%)
6	d	1.75	22/2220 (1.0%)	1.91	46/3028 (1.5%)
6	o	1.72	16/2220 (0.7%)	2.04	73/3028 (2.4%)
7	e	1.71	19/2499 (0.8%)	2.01	70/3388 (2.1%)
7	p	1.66	14/2499 (0.6%)	1.95	60/3388 (1.8%)
8	f	1.64	22/5359 (0.4%)	1.90	115/7258 (1.6%)
8	q	1.69	39/5352 (0.7%)	1.92	139/7248 (1.9%)
9	g	1.69	58/8806 (0.7%)	1.97	210/11936 (1.8%)
9	r	3.94	53/8755 (0.6%)	2.91	392/11870 (3.3%)
All	All	2.05	632/84214 (0.8%)	2.09	2332/114075 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	7	51
3	a	0	71
3	l	1	50
4	b	0	30
4	m	0	29
5	c	0	27
5	n	0	28
6	d	0	5
6	o	0	11
7	e	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	p	0	12
8	f	1	15
8	q	1	19
9	g	0	54
9	r	0	33
All	All	10	444

All (632) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	251	PRO	N-CD	123.85	3.21	1.47
9	r	150	PRO	N-CD	123.31	3.20	1.47
9	r	155	PRO	N-CD	122.44	3.19	1.47
9	r	325	PRO	N-CD	121.60	3.18	1.47
9	r	304	PRO	N-CD	119.21	3.14	1.47
9	r	274	PRO	N-CD	118.78	3.14	1.47
9	r	199	PRO	N-CD	58.09	2.29	1.47
9	r	118	PRO	N-CD	56.72	2.27	1.47
9	r	143	PRO	N-CD	53.40	2.22	1.47
9	r	240	PRO	N-CD	53.19	2.22	1.47
9	r	421	PRO	N-CD	52.89	2.21	1.47
9	r	136	PRO	N-CD	52.67	2.21	1.47
9	r	397	PRO	N-CD	49.70	2.17	1.47
9	r	123	PRO	N-CD	49.49	2.17	1.47
9	r	216	PRO	N-CD	43.63	2.08	1.47
9	r	338	PRO	N-CD	43.42	2.08	1.47
3	l	416	GLY	CA-C	-31.26	1.01	1.51
9	r	138	CYS	CB-SG	-23.44	1.42	1.82
9	r	356	CYS	CB-SG	-23.44	1.42	1.82
9	r	214	CYS	CB-SG	-23.42	1.42	1.82
9	r	208	CYS	CB-SG	-23.33	1.42	1.82
1	X	1059	ASN	N-CA	-20.20	1.05	1.46
1	X	794	ILE	CA-CB	-19.48	1.10	1.54
3	l	415	TYR	CA-CB	-19.35	1.11	1.53
1	X	1304	LYS	CA-CB	-18.86	1.12	1.53
1	X	1060	LEU	CA-CB	-17.53	1.13	1.53
1	X	1277	ILE	CA-CB	-13.35	1.24	1.54
8	q	482	ARG	N-CA	-13.33	1.19	1.46
8	f	576	ASN	CA-CB	-12.95	1.19	1.53
1	X	1303	LEU	N-CA	-12.53	1.21	1.46
1	X	793	LEU	N-CA	-12.06	1.22	1.46
6	d	28	SER	CA-CB	10.16	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1276	LYS	N-CA	-9.51	1.27	1.46
7	p	77	TYR	CZ-OH	9.04	1.53	1.37
3	l	784	GLU	CB-CG	8.69	1.68	1.52
5	n	377	SER	CA-CB	8.52	1.65	1.52
6	d	21	GLY	CA-C	-8.43	1.38	1.51
3	a	136	SER	CA-CB	8.42	1.65	1.52
5	n	652	ARG	NE-CZ	8.29	1.43	1.33
3	l	479	TYR	CG-CD2	8.14	1.49	1.39
4	m	627	TYR	CB-CG	-8.12	1.39	1.51
5	n	432	GLU	CG-CD	8.10	1.64	1.51
6	o	185	TRP	CD2-CE2	-7.91	1.31	1.41
3	l	774	TYR	CG-CD2	7.85	1.49	1.39
4	m	457	TYR	CE2-CZ	7.84	1.48	1.38
5	c	245	SER	CA-CB	7.80	1.64	1.52
9	g	462	SER	CA-CB	7.76	1.64	1.52
7	e	177	ARG	CZ-NH2	7.70	1.43	1.33
1	X	158	SER	CA-CB	7.67	1.64	1.52
8	q	36	PHE	CG-CD1	7.66	1.50	1.38
5	n	606	GLU	CD-OE1	7.66	1.34	1.25
3	l	361	SER	CA-CB	7.64	1.64	1.52
8	f	725	SER	CA-CB	7.64	1.64	1.52
6	d	204	SER	CA-CB	7.57	1.64	1.52
4	m	259	SER	CB-OG	7.56	1.52	1.42
7	p	194	TYR	CZ-OH	7.49	1.50	1.37
8	q	245	ARG	CZ-NH1	7.49	1.42	1.33
4	m	267	ARG	NE-CZ	7.41	1.42	1.33
1	X	1622	GLU	CG-CD	7.39	1.63	1.51
9	g	234	ARG	NE-CZ	7.39	1.42	1.33
7	e	335	TYR	CG-CD2	7.39	1.48	1.39
7	p	20	TYR	CE1-CZ	7.37	1.48	1.38
1	X	1495	TRP	CD2-CE2	7.36	1.50	1.41
8	q	576	ASN	CA-CB	-7.35	1.34	1.53
3	l	313	TYR	CG-CD1	7.32	1.48	1.39
3	a	652	SER	CA-CB	7.28	1.63	1.52
5	n	333	ARG	NE-CZ	7.24	1.42	1.33
3	l	701	TYR	CE1-CZ	7.22	1.48	1.38
4	b	471	PHE	CG-CD2	7.18	1.49	1.38
5	n	452	TYR	CZ-OH	7.16	1.50	1.37
3	l	106	TYR	CE2-CZ	7.14	1.47	1.38
4	m	400	GLY	CA-C	-7.12	1.40	1.51
3	a	422	ARG	CZ-NH1	7.11	1.42	1.33
3	l	1000	TYR	CE2-CZ	-7.10	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	112	TYR	CE1-CZ	7.08	1.47	1.38
3	a	495	TYR	CG-CD2	7.07	1.48	1.39
3	a	802	TYR	CG-CD1	7.07	1.48	1.39
3	l	215	SER	CA-CB	7.07	1.63	1.52
4	b	524	SER	CA-CB	7.04	1.63	1.52
4	b	431	GLU	CG-CD	7.01	1.62	1.51
5	c	466	SER	CA-CB	7.01	1.63	1.52
3	a	724	PHE	CG-CD1	7.00	1.49	1.38
4	b	171	ARG	CD-NE	6.99	1.58	1.46
8	q	418	SER	CA-CB	6.97	1.63	1.52
8	f	426	TYR	CG-CD2	6.96	1.48	1.39
6	o	258	TRP	NE1-CE2	6.96	1.46	1.37
3	a	627	TYR	CG-CD2	6.94	1.48	1.39
1	X	1390	SER	CA-CB	6.92	1.63	1.52
8	q	330	ARG	NE-CZ	6.89	1.42	1.33
6	d	142	ASP	CB-CG	6.89	1.66	1.51
5	n	246	TYR	CE2-CZ	6.87	1.47	1.38
9	g	850	TYR	CZ-OH	6.85	1.49	1.37
3	a	233	TYR	CE1-CZ	6.83	1.47	1.38
8	f	659	TYR	CE1-CZ	6.81	1.47	1.38
3	l	70	TYR	CB-CG	-6.80	1.41	1.51
1	X	978	SER	CA-CB	6.75	1.63	1.52
4	m	571	TYR	CD1-CE1	6.75	1.49	1.39
9	g	466	TYR	CG-CD2	6.75	1.48	1.39
9	g	949	TYR	CD1-CE1	6.71	1.49	1.39
1	X	1059	ASN	CA-CB	6.70	1.70	1.53
4	m	109	SER	CA-CB	6.67	1.62	1.52
8	f	439	SER	CA-CB	6.67	1.62	1.52
7	e	92	GLU	CD-OE2	6.66	1.32	1.25
9	r	1141	ALA	CA-CB	6.66	1.66	1.52
7	p	22	ARG	NE-CZ	6.64	1.41	1.33
4	b	275	SER	CA-CB	6.61	1.62	1.52
4	m	236	GLY	N-CA	6.61	1.55	1.46
9	g	1088	SER	CA-CB	6.61	1.62	1.52
5	c	374	GLU	CD-OE2	6.60	1.32	1.25
4	b	571	TYR	CE2-CZ	6.60	1.47	1.38
3	a	749	TYR	CG-CD1	6.57	1.47	1.39
9	g	444	GLU	CG-CD	6.57	1.61	1.51
9	r	738	TYR	CG-CD2	6.56	1.47	1.39
3	a	377	GLU	CG-CD	6.55	1.61	1.51
9	r	1001	ASP	CB-CG	6.55	1.65	1.51
9	g	619	SER	CA-CB	6.54	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	1007	SER	CA-CB	6.54	1.62	1.52
3	a	105	ARG	CZ-NH1	6.51	1.41	1.33
6	d	171	ARG	NE-CZ	6.50	1.41	1.33
3	l	408	PHE	CG-CD1	6.49	1.48	1.38
3	a	313	TYR	CG-CD1	6.49	1.47	1.39
6	d	19	TYR	CB-CG	-6.47	1.42	1.51
9	r	723	PHE	CE1-CZ	6.46	1.49	1.37
4	b	565	TYR	CG-CD2	6.44	1.47	1.39
6	d	67	GLY	N-CA	-6.44	1.36	1.46
5	c	664	GLU	CG-CD	6.43	1.61	1.51
8	q	243	TRP	CZ2-CH2	6.43	1.49	1.37
6	d	265	SER	CA-CB	6.42	1.62	1.52
7	p	137	TYR	CE2-CZ	-6.40	1.30	1.38
8	q	446	SER	CA-CB	6.39	1.62	1.52
1	X	953	TYR	CE2-CZ	6.39	1.46	1.38
1	X	1454	GLU	CG-CD	6.37	1.61	1.51
6	d	221	TYR	CE1-CZ	6.37	1.46	1.38
4	b	115	TYR	CE2-CZ	6.37	1.46	1.38
3	l	760	PHE	CG-CD2	6.37	1.48	1.38
5	c	519	ARG	NE-CZ	6.37	1.41	1.33
3	l	527	SER	CA-CB	6.35	1.62	1.52
9	r	1042	TRP	CG-CD1	6.33	1.45	1.36
3	a	734	HIS	CA-C	-6.32	1.36	1.52
9	r	781	TYR	CE1-CZ	6.32	1.46	1.38
4	b	228	PHE	CG-CD2	6.31	1.48	1.38
3	a	29	SER	CA-CB	6.31	1.62	1.52
3	l	479	TYR	CE2-CZ	6.31	1.46	1.38
3	l	72	PHE	CG-CD1	6.30	1.48	1.38
4	m	457	TYR	CE1-CZ	6.30	1.46	1.38
3	a	984	TYR	CD2-CE2	6.28	1.48	1.39
1	X	733	ARG	NE-CZ	6.28	1.41	1.33
1	X	386	SER	CA-CB	6.28	1.62	1.52
9	g	174	TYR	CD1-CE1	6.27	1.48	1.39
3	l	53	GLY	N-CA	6.26	1.55	1.46
7	e	189	GLU	CD-OE2	6.24	1.32	1.25
7	e	196	ARG	NE-CZ	6.24	1.41	1.33
9	g	536	GLU	CD-OE2	6.24	1.32	1.25
3	a	495	TYR	CE2-CZ	6.22	1.46	1.38
1	X	1508	SER	CA-CB	6.22	1.62	1.52
9	g	981	ARG	NE-CZ	6.20	1.41	1.33
9	g	1151	GLU	CG-CD	6.20	1.61	1.51
3	a	56	TYR	CZ-OH	6.20	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	348	TYR	CB-CG	6.20	1.60	1.51
9	g	1043	ARG	CZ-NH1	6.19	1.41	1.33
9	g	131	GLU	CD-OE2	-6.19	1.18	1.25
8	q	512	TYR	CE1-CZ	6.18	1.46	1.38
1	X	731	SER	CA-CB	6.17	1.62	1.52
5	n	287	SER	CA-CB	6.17	1.62	1.52
8	q	587	TYR	CE2-CZ	6.16	1.46	1.38
8	q	416	TYR	CZ-OH	6.15	1.48	1.37
1	X	337	SER	CA-CB	6.15	1.62	1.52
3	l	106	TYR	CG-CD1	6.15	1.47	1.39
4	m	480	GLU	CD-OE1	6.14	1.32	1.25
4	m	528	GLU	CD-OE1	6.14	1.32	1.25
1	X	1231	GLU	CD-OE1	6.14	1.32	1.25
3	a	554	PHE	CG-CD2	6.14	1.48	1.38
3	l	1035	ARG	CZ-NH1	6.14	1.41	1.33
3	l	15	TYR	CZ-OH	6.13	1.48	1.37
5	c	564	SER	CA-CB	6.13	1.62	1.52
5	c	465	PHE	N-CA	-6.12	1.34	1.46
4	b	245	PHE	CG-CD1	6.12	1.48	1.38
1	X	685	TYR	CE1-CZ	6.11	1.46	1.38
8	q	575	GLU	N-CA	6.11	1.58	1.46
3	l	376	TYR	CG-CD1	6.10	1.47	1.39
4	b	464	TYR	CG-CD2	6.09	1.47	1.39
3	a	850	GLU	CG-CD	6.08	1.61	1.51
9	g	896	TYR	CG-CD1	6.08	1.47	1.39
4	b	286	SER	CA-CB	6.08	1.62	1.52
6	d	20	TYR	CG-CD1	6.08	1.47	1.39
9	g	807	PHE	CG-CD2	6.07	1.47	1.38
1	X	966	GLY	CA-C	-6.06	1.42	1.51
9	g	1101	ARG	CD-NE	6.06	1.56	1.46
5	n	610	TRP	CD2-CE3	-6.06	1.31	1.40
6	o	101	SER	CA-CB	6.05	1.62	1.52
5	n	451	TRP	CG-CD1	6.05	1.45	1.36
3	l	624	SER	CA-CB	6.05	1.62	1.52
3	l	834	ARG	CZ-NH2	6.05	1.41	1.33
3	a	860	GLU	CD-OE2	6.05	1.32	1.25
1	X	1313	ARG	CZ-NH2	6.04	1.41	1.33
1	X	1341	GLU	CD-OE1	6.03	1.32	1.25
5	n	432	GLU	CD-OE1	-6.03	1.19	1.25
3	a	526	ARG	CD-NE	6.03	1.56	1.46
3	a	88	TYR	CG-CD2	6.02	1.47	1.39
8	q	180	PHE	CG-CD1	6.02	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	91	GLU	CB-CG	6.02	1.63	1.52
4	m	620	MET	CG-SD	6.01	1.96	1.81
1	X	931	PHE	CG-CD1	6.00	1.47	1.38
8	q	536	ARG	CD-NE	6.00	1.56	1.46
4	b	214	ARG	CZ-NH2	5.99	1.40	1.33
1	X	221	VAL	CB-CG1	5.99	1.65	1.52
3	l	271	ARG	CZ-NH1	5.99	1.40	1.33
7	e	11	LEU	CA-CB	5.98	1.67	1.53
4	b	295	TYR	CD2-CE2	5.97	1.48	1.39
3	l	15	TYR	CE2-CZ	5.97	1.46	1.38
4	m	620	MET	C-N	5.96	1.47	1.34
8	q	244	ARG	CZ-NH2	5.96	1.40	1.33
6	d	220	SER	CB-OG	-5.95	1.34	1.42
4	m	173	TYR	CG-CD1	5.95	1.46	1.39
5	c	547	ARG	CD-NE	5.95	1.56	1.46
3	l	185	GLY	CA-C	-5.95	1.42	1.51
1	X	1087	TYR	CZ-OH	5.94	1.48	1.37
8	q	618	GLU	CD-OE2	5.94	1.32	1.25
9	g	64	ASN	N-CA	-5.93	1.34	1.46
3	a	716	GLU	N-CA	-5.93	1.34	1.46
3	a	992	ASP	N-CA	-5.93	1.34	1.46
4	b	325	SER	CB-OG	5.93	1.50	1.42
9	g	211	MET	CA-C	-5.93	1.37	1.52
4	m	640	GLU	CG-CD	5.92	1.60	1.51
5	n	281	GLU	CD-OE1	5.92	1.32	1.25
8	f	720	ARG	CZ-NH2	5.91	1.40	1.33
5	n	781	TYR	CZ-OH	5.91	1.47	1.37
4	b	122	ARG	CZ-NH2	5.91	1.40	1.33
3	a	851	TYR	CE1-CZ	5.90	1.46	1.38
6	d	293	GLY	CA-C	5.90	1.61	1.51
3	a	261	SER	CA-CB	5.89	1.61	1.52
9	g	1094	TYR	CZ-OH	5.89	1.47	1.37
1	X	367	GLU	CD-OE1	5.89	1.32	1.25
4	b	349	TYR	CE1-CZ	5.88	1.46	1.38
4	b	545	GLN	CA-CB	5.88	1.66	1.53
9	r	850	TYR	CB-CG	5.88	1.60	1.51
3	l	313	TYR	CE2-CZ	5.87	1.46	1.38
8	q	384	TYR	CG-CD1	5.87	1.46	1.39
6	o	75	TYR	CZ-OH	5.87	1.47	1.37
3	a	607	PHE	CG-CD1	5.86	1.47	1.38
3	l	936	TYR	CG-CD1	5.86	1.46	1.39
5	n	596	ARG	NE-CZ	5.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1593	HIS	N-CA	5.86	1.58	1.46
6	o	198	SER	CA-CB	5.86	1.61	1.52
7	p	175	PRO	CA-C	-5.85	1.41	1.52
1	X	1628	GLU	CG-CD	5.85	1.60	1.51
3	a	820	ARG	CZ-NH1	5.83	1.40	1.33
3	a	748	PHE	CG-CD1	5.83	1.47	1.38
5	c	142	ARG	CD-NE	5.83	1.56	1.46
3	a	324	SER	CA-CB	5.83	1.61	1.52
9	g	1007	SER	CB-OG	-5.82	1.34	1.42
8	q	707	SER	CA-CB	5.82	1.61	1.52
9	g	850	TYR	CG-CD2	5.81	1.46	1.39
9	g	1143	GLU	CD-OE1	5.81	1.32	1.25
4	b	414	SER	CA-CB	5.81	1.61	1.52
1	X	1092	SER	CA-CB	5.80	1.61	1.52
3	a	407	GLY	N-CA	-5.80	1.37	1.46
3	a	967	PHE	CB-CG	5.80	1.61	1.51
8	q	75	TRP	CZ2-CH2	5.80	1.48	1.37
6	d	112	TYR	CG-CD1	5.80	1.46	1.39
6	o	185	TRP	NE1-CE2	5.79	1.45	1.37
4	m	486	ILE	C-N	5.79	1.43	1.33
3	l	802	TYR	CG-CD2	5.79	1.46	1.39
7	e	118	PRO	CA-CB	5.79	1.65	1.53
5	c	463	ARG	CZ-NH1	5.79	1.40	1.33
1	X	375	TYR	CE2-CZ	5.79	1.46	1.38
8	q	378	ASP	CA-CB	5.79	1.66	1.53
8	q	628	PHE	CG-CD2	5.78	1.47	1.38
4	m	672	TYR	CG-CD1	5.78	1.46	1.39
9	r	1016	PHE	CA-CB	5.78	1.66	1.53
4	b	560	SER	CA-CB	5.77	1.61	1.52
5	n	548	TYR	CZ-OH	5.76	1.47	1.37
9	r	570	PHE	CG-CD2	5.76	1.47	1.38
3	a	421	GLU	CD-OE1	5.75	1.31	1.25
3	l	179	GLU	N-CA	-5.75	1.34	1.46
8	q	446	SER	CB-OG	5.75	1.49	1.42
5	c	648	TYR	CG-CD1	5.75	1.46	1.39
7	e	339	PHE	CA-CB	5.74	1.66	1.53
7	e	96	ARG	NE-CZ	5.74	1.40	1.33
5	c	285	ARG	CZ-NH2	5.74	1.40	1.33
8	q	261	ARG	CZ-NH2	5.74	1.40	1.33
5	c	212	GLU	CG-CD	-5.74	1.43	1.51
6	d	213	SER	C-N	-5.73	1.23	1.34
5	c	764	LEU	CA-CB	5.73	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	653	TYR	CZ-OH	5.72	1.47	1.37
1	X	1231	GLU	CA-C	-5.72	1.38	1.52
7	e	322	ALA	CA-CB	5.72	1.64	1.52
5	n	324	TYR	CE2-CZ	5.72	1.46	1.38
7	p	50	SER	CA-CB	5.72	1.61	1.52
8	q	552	ARG	NE-CZ	5.71	1.40	1.33
5	n	189	TYR	CB-CG	-5.71	1.43	1.51
3	a	581	VAL	N-CA	-5.71	1.34	1.46
3	a	834	ARG	CD-NE	5.71	1.56	1.46
8	f	17	ASP	CA-CB	5.70	1.66	1.53
9	g	252	PHE	CG-CD1	5.70	1.47	1.38
9	g	781	TYR	CE1-CZ	5.69	1.46	1.38
5	n	307	SER	CA-CB	5.69	1.61	1.52
3	a	313	TYR	CB-CG	5.69	1.60	1.51
4	b	201	ARG	CZ-NH2	5.69	1.40	1.33
7	p	107	SER	CA-CB	5.68	1.61	1.52
1	X	950	ARG	CZ-NH1	5.68	1.40	1.33
3	l	466	TYR	CG-CD2	5.68	1.46	1.39
3	l	550	PHE	CG-CD1	5.67	1.47	1.38
3	l	406	ARG	NE-CZ	5.66	1.40	1.33
5	c	554	SER	CA-CB	5.66	1.61	1.52
3	l	422	ARG	CZ-NH1	5.65	1.40	1.33
3	l	938	ARG	NE-CZ	5.65	1.40	1.33
3	a	561	GLN	CA-CB	5.65	1.66	1.53
3	a	688	PHE	CG-CD1	5.64	1.47	1.38
9	g	690	ARG	CZ-NH2	5.64	1.40	1.33
6	o	85	GLU	CB-CG	5.64	1.62	1.52
4	b	73	PRO	N-CD	-5.64	1.40	1.47
5	c	477	PHE	CE2-CZ	5.64	1.48	1.37
3	l	156	TYR	CE2-CZ	5.64	1.45	1.38
7	e	4	PHE	CA-CB	5.63	1.66	1.53
9	g	381	TYR	CD1-CE1	5.63	1.47	1.39
9	r	1153	ASN	C-N	5.63	1.47	1.34
9	g	230	PHE	CE2-CZ	5.63	1.48	1.37
3	l	822	SER	CA-CB	5.63	1.61	1.52
3	l	890	ARG	CD-NE	5.63	1.56	1.46
4	m	662	TYR	CE2-CZ	5.62	1.45	1.38
7	p	223	SER	CA-CB	5.62	1.61	1.52
1	X	366	SER	CA-CB	5.62	1.61	1.52
9	g	567	PHE	CE1-CZ	5.62	1.48	1.37
8	f	384	TYR	CG-CD1	5.62	1.46	1.39
3	l	716	GLU	CD-OE2	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	97	ARG	NE-CZ	5.61	1.40	1.33
9	r	949	TYR	CG-CD1	5.61	1.46	1.39
5	c	563	SER	CA-CB	5.59	1.61	1.52
3	l	415	TYR	N-CA	5.58	1.57	1.46
9	g	229	PHE	CG-CD2	5.58	1.47	1.38
1	X	1199	TYR	CE1-CZ	5.58	1.45	1.38
9	g	220	VAL	CB-CG1	5.57	1.64	1.52
9	g	66	ARG	NE-CZ	5.57	1.40	1.33
5	c	343	TRP	CD2-CE2	5.57	1.48	1.41
5	c	279	GLU	CB-CG	5.57	1.62	1.52
1	X	992	SER	N-CA	-5.56	1.35	1.46
4	b	539	TYR	CZ-OH	5.56	1.47	1.37
1	X	421	PHE	CG-CD1	5.55	1.47	1.38
3	l	342	LEU	N-CA	-5.55	1.35	1.46
9	g	1007	SER	CA-CB	5.55	1.61	1.52
4	b	408	VAL	CB-CG1	5.54	1.64	1.52
5	c	292	GLU	CD-OE1	5.54	1.31	1.25
3	l	955	SER	C-N	5.54	1.43	1.33
8	f	349	SER	CA-CB	5.54	1.61	1.52
5	c	617	PHE	CG-CD2	5.54	1.47	1.38
4	b	319	SER	CA-CB	5.53	1.61	1.52
4	b	177	GLU	CD-OE1	5.53	1.31	1.25
4	m	627	TYR	CE2-CZ	5.52	1.45	1.38
1	X	1611	TYR	CZ-OH	5.52	1.47	1.37
4	b	76	TYR	CZ-OH	5.52	1.47	1.37
9	g	352	TYR	CG-CD2	-5.52	1.31	1.39
8	f	265	SER	CA-CB	5.52	1.61	1.52
3	l	531	LYS	CD-CE	5.51	1.65	1.51
7	e	170	CYS	CB-SG	5.50	1.91	1.82
3	a	484	TYR	CE1-CZ	5.50	1.45	1.38
4	m	657	TYR	CG-CD2	5.50	1.46	1.39
5	c	781	TYR	CE1-CZ	5.50	1.45	1.38
3	l	782	TYR	CE1-CZ	5.50	1.45	1.38
5	c	583	SER	CA-CB	5.49	1.61	1.52
1	X	355	SER	CA-CB	5.49	1.61	1.52
3	a	355	TRP	CD2-CE2	5.49	1.48	1.41
9	r	691	TYR	CE1-CZ	5.49	1.45	1.38
3	a	268	SER	CA-CB	5.48	1.61	1.52
9	r	659	PRO	N-CD	5.48	1.55	1.47
1	X	909	GLU	CB-CG	5.47	1.62	1.52
5	n	358	TYR	CZ-OH	5.47	1.47	1.37
6	o	187	TYR	CZ-OH	5.46	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	918	PHE	CE1-CZ	5.46	1.47	1.37
8	f	714	TYR	CZ-OH	5.46	1.47	1.37
3	l	199	PHE	C-N	5.46	1.46	1.34
4	m	570	SER	CA-CB	5.46	1.61	1.52
8	q	105	PHE	CG-CD1	5.45	1.47	1.38
5	c	281	GLU	CG-CD	5.45	1.60	1.51
3	a	914	TYR	CB-CG	5.44	1.59	1.51
8	f	506	ILE	CB-CG1	5.44	1.69	1.54
6	o	206	TRP	CG-CD2	5.43	1.52	1.43
5	n	438	VAL	CB-CG1	5.42	1.64	1.52
4	b	562	ALA	CA-CB	5.42	1.63	1.52
7	e	329	ARG	CD-NE	5.42	1.55	1.46
9	g	262	ASN	CA-CB	5.42	1.67	1.53
1	X	1087	TYR	CD2-CE2	5.42	1.47	1.39
1	X	1401	SER	CA-CB	5.42	1.61	1.52
3	a	27	TYR	CD1-CE1	5.42	1.47	1.39
3	l	686	PHE	CG-CD2	5.42	1.46	1.38
4	m	589	PRO	N-CD	-5.41	1.40	1.47
1	X	827	PRO	N-CA	-5.41	1.38	1.47
5	c	366	PHE	CG-CD1	5.41	1.46	1.38
4	b	572	SER	CA-CB	5.40	1.61	1.52
9	r	788	TRP	NE1-CE2	5.40	1.44	1.37
3	l	820	ARG	CZ-NH1	5.40	1.40	1.33
5	c	645	TYR	CG-CD1	5.40	1.46	1.39
9	r	1071	PRO	N-CD	-5.40	1.40	1.47
3	a	647	PHE	CG-CD2	5.40	1.46	1.38
6	d	269	LEU	CA-C	-5.39	1.39	1.52
4	b	331	TYR	CE2-CZ	5.39	1.45	1.38
3	a	56	TYR	CB-CG	5.39	1.59	1.51
3	a	958	TRP	NE1-CE2	-5.39	1.30	1.37
3	a	826	TYR	CB-CG	5.38	1.59	1.51
5	c	435	TYR	CZ-OH	5.38	1.47	1.37
1	X	1605	PHE	CG-CD2	5.38	1.46	1.38
3	l	727	TYR	CE1-CZ	5.38	1.45	1.38
4	b	693	GLU	CD-OE1	5.38	1.31	1.25
3	a	216	SER	CA-CB	5.37	1.61	1.52
3	l	754	GLU	CG-CD	5.37	1.60	1.51
5	c	450	CYS	CB-SG	5.37	1.91	1.82
3	a	214	ARG	CZ-NH2	5.37	1.40	1.33
8	f	659	TYR	CZ-OH	5.37	1.47	1.37
9	g	106	TYR	CZ-OH	5.37	1.47	1.37
9	g	227	ARG	NE-CZ	5.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	m	104	PHE	CG-CD1	5.36	1.46	1.38
4	b	189	TYR	CG-CD2	5.36	1.46	1.39
3	l	668	TYR	CZ-OH	5.36	1.47	1.37
4	m	463	SER	CA-CB	5.36	1.60	1.52
3	a	707	SER	CA-CB	5.36	1.60	1.52
3	l	640	PHE	CB-CG	5.36	1.60	1.51
3	l	968	ARG	NE-CZ	5.36	1.40	1.33
3	l	832	PHE	CE1-CZ	5.35	1.47	1.37
4	m	306	TRP	CE3-CZ3	5.35	1.47	1.38
6	o	211	ALA	CA-C	-5.35	1.39	1.52
9	g	946	LYS	CD-CE	5.35	1.64	1.51
3	a	782	TYR	CB-CG	-5.35	1.43	1.51
3	l	892	GLY	N-CA	-5.35	1.38	1.46
3	a	53	GLY	N-CA	5.35	1.54	1.46
5	n	231	TYR	CE1-CZ	5.35	1.45	1.38
5	c	487	HIS	N-CA	-5.34	1.35	1.46
9	g	592	GLU	CD-OE1	5.34	1.31	1.25
5	n	295	PHE	CE2-CZ	5.34	1.47	1.37
8	q	516	TRP	CG-CD1	5.34	1.44	1.36
5	c	143	ARG	CZ-NH2	5.34	1.40	1.33
4	m	732	ARG	NE-CZ	5.34	1.40	1.33
9	g	341	ASP	CB-CG	5.34	1.62	1.51
3	l	173	PHE	CB-CG	5.33	1.60	1.51
3	l	926	CYS	CB-SG	-5.33	1.73	1.81
8	q	609	SER	CA-CB	5.33	1.60	1.52
1	X	413	GLU	CD-OE1	5.33	1.31	1.25
8	q	406	GLU	CD-OE2	5.33	1.31	1.25
1	X	921	SER	CA-CB	5.33	1.60	1.52
1	X	888	TYR	CG-CD2	5.32	1.46	1.39
9	g	923	HIS	CA-CB	5.32	1.65	1.53
8	q	709	GLY	N-CA	-5.32	1.38	1.46
3	a	158	PHE	CG-CD2	5.32	1.46	1.38
3	a	181	GLY	CA-C	-5.32	1.43	1.51
3	a	968	ARG	NE-CZ	5.32	1.40	1.33
9	r	838	GLU	N-CA	-5.32	1.35	1.46
3	a	628	ARG	NE-CZ	5.31	1.40	1.33
6	d	89	TRP	CG-CD1	5.31	1.44	1.36
3	a	872	TYR	CE2-CZ	5.31	1.45	1.38
5	c	603	PRO	N-CD	-5.31	1.40	1.47
3	l	422	ARG	NE-CZ	5.31	1.40	1.33
3	a	835	ASN	N-CA	-5.31	1.35	1.46
8	q	259	TYR	CG-CD2	5.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	243	LEU	CA-CB	5.30	1.66	1.53
9	g	313	TYR	CE1-CZ	5.30	1.45	1.38
9	g	545	TYR	CE2-CZ	5.30	1.45	1.38
6	o	152	SER	CA-CB	5.30	1.60	1.52
3	l	677	GLU	CD-OE2	5.29	1.31	1.25
5	c	519	ARG	CA-CB	5.29	1.65	1.53
5	c	602	PHE	CD1-CE1	5.29	1.49	1.39
4	m	520	GLU	CD-OE2	5.29	1.31	1.25
4	m	219	PRO	N-CD	-5.29	1.40	1.47
1	X	871	SER	CA-CB	5.29	1.60	1.52
8	f	279	TYR	CE2-CZ	5.29	1.45	1.38
9	g	1097	GLU	CB-CG	5.28	1.62	1.52
3	a	612	SER	CA-CB	5.28	1.60	1.52
9	g	545	TYR	CG-CD2	5.28	1.46	1.39
6	o	171	ARG	CD-NE	5.28	1.55	1.46
1	X	400	PHE	CG-CD2	5.28	1.46	1.38
3	a	173	PHE	CG-CD2	5.28	1.46	1.38
3	a	494	PHE	CA-CB	5.28	1.65	1.53
4	m	704	GLU	CG-CD	5.28	1.59	1.51
3	l	165	PHE	CA-CB	5.28	1.65	1.53
8	q	120	TRP	NE1-CE2	-5.28	1.30	1.37
8	q	587	TYR	CG-CD2	5.27	1.46	1.39
9	r	658	PHE	CE2-CZ	5.27	1.47	1.37
3	a	918	PHE	CE2-CZ	5.27	1.47	1.37
7	e	217	SER	CA-CB	5.27	1.60	1.52
3	a	758	PHE	N-CA	-5.27	1.35	1.46
3	a	692	PHE	CA-CB	5.26	1.65	1.53
5	c	535	SER	CB-OG	5.26	1.49	1.42
9	g	1079	PRO	CA-C	-5.26	1.42	1.52
1	X	1072	TYR	CE1-CZ	5.26	1.45	1.38
3	a	220	TYR	CG-CD2	5.25	1.46	1.39
5	n	355	SER	CA-CB	5.25	1.60	1.52
9	r	1088	SER	CA-CB	5.25	1.60	1.52
4	m	122	ARG	NE-CZ	5.25	1.39	1.33
6	d	253	PHE	CE1-CZ	5.25	1.47	1.37
7	p	43	SER	CB-OG	5.25	1.49	1.42
9	r	1101	ARG	CZ-NH1	5.25	1.39	1.33
3	a	765	PHE	CG-CD2	5.24	1.46	1.38
3	l	75	ARG	CA-CB	5.24	1.65	1.53
3	l	893	HIS	C-N	5.24	1.46	1.34
4	m	710	TYR	CG-CD2	5.24	1.46	1.39
9	g	966	LYS	CD-CE	5.24	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	214	ARG	CZ-NH1	5.24	1.39	1.33
5	n	195	GLU	CG-CD	5.23	1.59	1.51
3	a	874	ASN	CB-CG	5.23	1.63	1.51
5	n	540	ASN	CA-CB	5.22	1.66	1.53
1	X	833	LYS	N-CA	-5.22	1.35	1.46
1	X	685	TYR	CE2-CZ	5.22	1.45	1.38
3	l	266	ASP	C-N	5.22	1.44	1.34
9	r	1043	ARG	NE-CZ	5.21	1.39	1.33
9	r	526	SER	CA-CB	5.21	1.60	1.52
9	r	751	TYR	CB-CG	5.21	1.59	1.51
1	X	1279	GLU	CB-CG	5.21	1.62	1.52
1	X	766	GLU	CB-CG	5.20	1.62	1.52
7	e	4	PHE	CD2-CE2	5.20	1.49	1.39
3	l	210	ARG	NE-CZ	5.20	1.39	1.33
6	o	261	SER	CA-CB	5.20	1.60	1.52
4	m	339	ILE	C-N	5.20	1.42	1.33
5	c	305	ARG	CZ-NH1	5.20	1.39	1.33
3	l	724	PHE	CG-CD1	5.20	1.46	1.38
9	r	875	PHE	CG-CD2	5.20	1.46	1.38
8	q	685	SER	CB-OG	5.19	1.49	1.42
3	a	283	TYR	CE1-CZ	5.19	1.45	1.38
8	q	142	SER	CA-CB	5.19	1.60	1.52
5	c	329	ASP	C-N	-5.18	1.24	1.34
3	a	710	TYR	CG-CD2	5.18	1.45	1.39
3	l	720	PHE	CB-CG	-5.18	1.42	1.51
3	l	779	LEU	N-CA	-5.18	1.35	1.46
8	f	535	ARG	CZ-NH1	5.18	1.39	1.33
4	m	692	ILE	N-CA	-5.17	1.36	1.46
9	g	981	ARG	CZ-NH2	5.17	1.39	1.33
8	f	43	ARG	CZ-NH1	5.17	1.39	1.33
9	g	627	GLU	CD-OE1	5.16	1.31	1.25
4	m	281	SER	CA-CB	5.16	1.60	1.52
5	n	607	ARG	NE-CZ	5.16	1.39	1.33
8	q	426	TYR	CG-CD2	5.16	1.45	1.39
9	r	1102	PHE	CG-CD2	5.16	1.46	1.38
4	b	223	TYR	CE1-CZ	5.15	1.45	1.38
5	c	142	ARG	CZ-NH2	5.15	1.39	1.33
6	o	103	ASN	CB-CG	5.15	1.62	1.51
7	p	227	TRP	CD2-CE2	5.15	1.47	1.41
3	a	637	PHE	CE2-CZ	5.15	1.47	1.37
3	l	829	SER	CA-CB	5.15	1.60	1.52
4	b	529	TRP	N-CA	-5.14	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	392	GLY	C-N	5.14	1.45	1.34
7	e	67	GLU	CG-CD	5.14	1.59	1.51
4	b	571	TYR	CE1-CZ	-5.14	1.31	1.38
3	l	204	TYR	CZ-OH	5.14	1.46	1.37
4	b	621	ARG	CZ-NH2	5.14	1.39	1.33
9	g	450	ARG	NE-CZ	5.14	1.39	1.33
3	l	640	PHE	CG-CD2	5.14	1.46	1.38
9	r	730	GLU	CD-OE1	5.14	1.31	1.25
3	a	341	GLU	CD-OE2	5.14	1.31	1.25
3	l	860	GLU	CG-CD	5.14	1.59	1.51
6	d	52	HIS	CB-CG	5.13	1.59	1.50
3	a	493	TRP	NE1-CE2	-5.13	1.30	1.37
9	g	356	CYS	CB-SG	5.13	1.91	1.82
5	n	439	ARG	CZ-NH2	5.13	1.39	1.33
8	q	692	SER	CA-CB	5.13	1.60	1.52
9	r	990	GLU	CB-CG	5.13	1.61	1.52
3	a	914	TYR	CE2-CZ	5.13	1.45	1.38
5	n	463	ARG	CZ-NH2	5.13	1.39	1.33
3	a	1000	TYR	CG-CD1	5.12	1.45	1.39
4	b	88	TYR	CE1-CZ	5.12	1.45	1.38
3	l	479	TYR	CZ-OH	5.12	1.46	1.37
3	l	695	TYR	CZ-OH	5.12	1.46	1.37
1	X	301	ALA	CA-CB	5.12	1.63	1.52
3	l	85	SER	CB-OG	5.11	1.48	1.42
3	l	594	GLY	CA-C	5.11	1.60	1.51
3	l	628	ARG	CZ-NH1	5.11	1.39	1.33
9	g	896	TYR	CE2-CZ	5.11	1.45	1.38
1	X	280	ALA	CA-CB	5.11	1.63	1.52
3	l	1018	ILE	N-CA	5.11	1.56	1.46
6	o	128	VAL	CA-CB	-5.10	1.44	1.54
8	f	384	TYR	CE1-CZ	5.10	1.45	1.38
3	a	438	GLU	CG-CD	5.10	1.59	1.51
8	f	244	ARG	NE-CZ	5.10	1.39	1.33
4	b	363	TYR	CE2-CZ	5.09	1.45	1.38
3	l	529	SER	N-CA	-5.09	1.36	1.46
8	q	125	TRP	CD2-CE3	-5.09	1.32	1.40
3	l	81	PHE	CG-CD1	5.09	1.46	1.38
1	X	295	PHE	CG-CD2	5.08	1.46	1.38
4	b	707	SER	CA-CB	5.08	1.60	1.52
3	a	662	PHE	CG-CD2	5.08	1.46	1.38
4	m	475	SER	CA-CB	5.08	1.60	1.52
1	X	1220	VAL	CB-CG2	5.08	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	355	GLU	CB-CG	5.08	1.61	1.52
4	m	119	GLY	N-CA	-5.08	1.38	1.46
4	b	140	HIS	CB-CG	5.08	1.59	1.50
5	c	297	TYR	CE1-CZ	5.08	1.45	1.38
8	f	611	SER	CB-OG	5.08	1.48	1.42
9	r	511	PRO	CA-C	-5.08	1.42	1.52
4	m	627	TYR	CE1-CZ	-5.07	1.31	1.38
4	m	335	PHE	CA-CB	5.07	1.65	1.53
5	n	765	GLU	N-CA	-5.07	1.36	1.46
7	e	145	LEU	N-CA	-5.07	1.36	1.46
9	g	863	ARG	CZ-NH1	5.07	1.39	1.33
1	X	754	TYR	CZ-OH	5.06	1.46	1.37
9	g	695	GLU	CG-CD	5.06	1.59	1.51
9	r	952	ASP	CA-CB	5.06	1.65	1.53
3	a	738	ARG	CZ-NH2	5.06	1.39	1.33
4	m	168	ARG	CZ-NH2	5.06	1.39	1.33
9	r	920	CYS	CB-SG	5.06	1.90	1.82
6	d	238	ASN	CA-CB	5.05	1.66	1.53
9	g	461	ASP	N-CA	-5.05	1.36	1.46
3	l	69	CYS	CB-SG	-5.05	1.73	1.81
9	r	545	TYR	CG-CD2	-5.05	1.32	1.39
6	o	110	HIS	CB-CG	5.05	1.59	1.50
3	a	372	SER	N-CA	-5.05	1.36	1.46
4	b	712	THR	C-N	5.05	1.45	1.34
6	d	147	GLY	CA-C	-5.05	1.43	1.51
5	c	275	GLN	C-O	5.05	1.32	1.23
7	e	184	ALA	CA-C	-5.05	1.39	1.52
6	d	232	ILE	N-CA	-5.04	1.36	1.46
1	X	902	GLU	CG-CD	5.04	1.59	1.51
1	X	986	SER	CB-OG	5.04	1.48	1.42
4	b	675	PHE	CG-CD2	5.04	1.46	1.38
8	q	443	GLU	CD-OE1	5.04	1.31	1.25
7	p	158	SER	CA-CB	5.04	1.60	1.52
4	b	214	ARG	CD-NE	5.03	1.55	1.46
4	m	595	VAL	CB-CG2	5.03	1.63	1.52
9	g	621	TYR	CE1-CZ	5.03	1.45	1.38
4	m	555	SER	CA-CB	5.02	1.60	1.52
3	a	210	ARG	NE-CZ	5.02	1.39	1.33
9	r	1064	ARG	CZ-NH1	5.02	1.39	1.33
9	g	283	VAL	CB-CG1	5.02	1.63	1.52
4	b	154	GLU	CB-CG	5.02	1.61	1.52
8	f	588	GLU	CD-OE1	5.01	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1285	PHE	CG-CD1	5.01	1.46	1.38
7	e	90	GLN	CA-CB	5.01	1.65	1.53
9	g	324	TYR	CZ-OH	5.01	1.46	1.37
4	m	579	SER	CA-CB	5.01	1.60	1.52
3	a	710	TYR	CZ-OH	5.01	1.46	1.37
4	b	203	GLU	CD-OE1	5.01	1.31	1.25
4	b	573	TRP	CA-CB	5.01	1.65	1.53
9	r	562	GLU	CB-CG	5.01	1.61	1.52
3	a	742	GLU	CD-OE1	5.00	1.31	1.25
8	q	512	TYR	CG-CD2	5.00	1.45	1.39
5	n	768	ASN	CB-CG	5.00	1.62	1.51
8	f	702	TYR	CB-CG	-5.00	1.44	1.51

All (2332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	72	LEU	O-C-N	-62.08	23.37	122.70
9	r	431	SER	O-C-N	-49.50	43.50	122.70
9	r	215	GLU	C-N-CD	-43.53	24.84	120.60
9	r	274	PRO	N-CA-CB	38.04	148.95	103.30
9	r	150	PRO	N-CA-CB	37.90	148.78	103.30
9	r	304	PRO	N-CA-CB	37.87	148.74	103.30
9	r	155	PRO	N-CA-CB	37.79	148.65	103.30
9	r	325	PRO	N-CA-CB	37.73	148.57	103.30
9	r	251	PRO	N-CA-CB	37.72	148.57	103.30
9	r	155	PRO	CA-N-CD	-33.14	65.11	111.50
9	r	325	PRO	CA-N-CD	-33.02	65.27	111.50
9	r	150	PRO	CA-N-CD	-33.01	65.29	111.50
9	r	251	PRO	CA-N-CD	-32.95	65.37	111.50
9	r	304	PRO	CA-N-CD	-32.50	66.00	111.50
9	r	274	PRO	CA-N-CD	-32.47	66.04	111.50
9	r	271	ARG	NE-CZ-NH2	-25.27	107.66	120.30
9	r	125	ARG	NE-CZ-NH1	-25.27	107.67	120.30
9	r	382	ARG	NE-CZ-NH2	-25.24	107.68	120.30
9	r	450	ARG	NE-CZ-NH1	-25.23	107.68	120.30
9	r	281	ARG	NE-CZ-NH1	-25.19	107.70	120.30
9	r	137	ARG	NE-CZ-NH1	-25.16	107.72	120.30
9	r	227	ARG	NE-CZ-NH1	-25.15	107.72	120.30
9	r	281	ARG	NE-CZ-NH2	-25.15	107.72	120.30
9	r	234	ARG	NE-CZ-NH1	-25.14	107.73	120.30
9	r	234	ARG	NE-CZ-NH2	-25.13	107.73	120.30
9	r	441	ARG	NE-CZ-NH2	-25.13	107.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	440	ARG	NE-CZ-NH2	-25.10	107.75	120.30
9	r	125	ARG	NE-CZ-NH2	-25.09	107.75	120.30
9	r	271	ARG	NE-CZ-NH1	-25.09	107.75	120.30
9	r	450	ARG	NE-CZ-NH2	-25.09	107.76	120.30
9	r	227	ARG	NE-CZ-NH2	-25.07	107.76	120.30
9	r	440	ARG	NE-CZ-NH1	-25.04	107.78	120.30
9	r	441	ARG	NE-CZ-NH1	-25.04	107.78	120.30
9	r	137	ARG	NE-CZ-NH2	-25.04	107.78	120.30
9	r	382	ARG	NE-CZ-NH1	-24.96	107.82	120.30
9	r	286	THR	N-CA-CB	24.25	156.38	110.30
9	r	280	THR	N-CA-CB	24.24	156.35	110.30
9	r	145	THR	N-CA-CB	24.13	156.15	110.30
9	r	391	THR	N-CA-CB	24.11	156.10	110.30
9	r	410	THR	N-CA-CB	24.07	156.04	110.30
9	r	414	THR	N-CA-CB	24.07	156.04	110.30
9	r	74	THR	N-CA-CB	23.98	155.86	110.30
9	r	393	THR	N-CA-CB	23.97	155.83	110.30
9	r	300	THR	N-CA-CB	23.94	155.79	110.30
9	r	287	THR	N-CA-CB	23.80	155.52	110.30
9	r	263	THR	N-CA-CB	23.74	155.41	110.30
9	r	396	LYS	C-N-CD	-23.05	69.90	120.60
9	r	271	ARG	NH1-CZ-NH2	22.89	144.58	119.40
9	r	125	ARG	NH1-CZ-NH2	22.89	144.58	119.40
9	r	281	ARG	NH1-CZ-NH2	22.89	144.57	119.40
9	r	450	ARG	NH1-CZ-NH2	22.87	144.56	119.40
1	X	794	ILE	N-CA-CB	22.85	163.36	110.80
9	r	234	ARG	NH1-CZ-NH2	22.85	144.53	119.40
9	r	227	ARG	NH1-CZ-NH2	22.83	144.51	119.40
9	r	382	ARG	NH1-CZ-NH2	22.82	144.50	119.40
9	r	137	ARG	NH1-CZ-NH2	22.81	144.50	119.40
9	r	441	ARG	NH1-CZ-NH2	22.80	144.48	119.40
9	r	440	ARG	NH1-CZ-NH2	22.79	144.47	119.40
1	X	1304	LYS	N-CA-CB	21.17	148.70	110.60
9	r	154	ASN	C-N-CD	19.52	169.40	128.40
5	c	297	TYR	CB-CG-CD2	-18.89	109.67	121.00
9	r	149	SER	C-N-CD	17.95	166.09	128.40
9	r	273	GLY	C-N-CD	17.95	166.09	128.40
9	r	324	TYR	C-N-CD	17.89	165.97	128.40
8	f	384	TYR	CB-CG-CD2	-17.88	110.27	121.00
9	g	605	ARG	NE-CZ-NH2	-17.59	111.51	120.30
1	X	794	ILE	N-CA-C	-17.48	63.79	111.00
3	a	105	ARG	NE-CZ-NH1	17.46	129.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	503	TYR	CB-CG-CD2	-17.46	110.53	121.00
3	l	416	GLY	N-CA-C	17.15	155.97	113.10
1	X	1633	ARG	NE-CZ-NH2	-17.08	111.76	120.30
5	n	607	ARG	NE-CZ-NH2	-16.87	111.87	120.30
3	l	954	ARG	NE-CZ-NH2	-16.62	111.99	120.30
9	r	1101	ARG	NE-CZ-NH1	16.28	128.44	120.30
3	a	826	TYR	CB-CG-CD2	-16.28	111.23	121.00
8	q	482	ARG	N-CA-CB	16.14	139.65	110.60
5	c	202	ARG	NE-CZ-NH1	16.12	128.36	120.30
3	a	414	ARG	NE-CZ-NH2	-16.08	112.26	120.30
1	X	216	TYR	CB-CG-CD1	-15.94	111.44	121.00
3	l	511	ARG	NE-CZ-NH1	15.93	128.26	120.30
4	b	116	ARG	NE-CZ-NH1	15.90	128.25	120.30
9	r	250	LYS	C-N-CD	15.86	161.70	128.40
5	c	648	TYR	CB-CG-CD1	15.85	130.51	121.00
9	g	605	ARG	NE-CZ-NH1	15.82	128.21	120.30
3	l	415	TYR	N-CA-CB	15.80	139.04	110.60
7	p	146	ARG	NE-CZ-NH1	15.79	128.20	120.30
1	X	1263	TYR	CB-CG-CD1	-15.71	111.58	121.00
3	l	901	ARG	NE-CZ-NH2	-15.70	112.45	120.30
1	X	323	TYR	CB-CG-CD2	-15.68	111.59	121.00
7	e	239	ARG	NE-CZ-NH2	15.57	128.09	120.30
3	l	957	ASP	CB-CG-OD1	15.43	132.19	118.30
1	X	1059	ASN	CB-CA-C	-15.35	79.70	110.40
9	g	252	PHE	CB-CG-CD1	15.33	131.53	120.80
5	n	565	TYR	CB-CG-CD2	-15.23	111.86	121.00
5	n	241	PHE	CB-CG-CD1	15.22	131.45	120.80
1	X	1263	TYR	CB-CG-CD2	15.15	130.09	121.00
5	c	285	ARG	NE-CZ-NH2	-15.13	112.73	120.30
4	b	530	ARG	NE-CZ-NH2	15.11	127.85	120.30
8	q	102	ARG	NE-CZ-NH2	-15.05	112.78	120.30
4	m	360	PHE	CB-CG-CD1	-14.97	110.32	120.80
1	X	342	ASP	CB-CG-OD2	-14.82	104.96	118.30
9	r	325	PRO	CB-CA-C	-14.82	74.95	112.00
3	l	982	TYR	CB-CG-CD1	-14.72	112.17	121.00
5	n	202	ARG	NE-CZ-NH1	14.71	127.65	120.30
3	a	451	ARG	NE-CZ-NH2	-14.66	112.97	120.30
8	q	535	ARG	NE-CZ-NH2	-14.61	113.00	120.30
9	r	155	PRO	CB-CA-C	-14.59	75.52	112.00
4	b	214	ARG	NE-CZ-NH1	14.56	127.58	120.30
9	r	267	VAL	CB-CA-C	-14.56	83.73	111.40
9	r	251	PRO	CB-CA-C	-14.54	75.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	o	23	ARG	NE-CZ-NH1	14.41	127.50	120.30
9	r	304	PRO	CB-CA-C	-14.35	76.14	112.00
5	n	241	PHE	CB-CG-CD2	-14.29	110.80	120.80
9	g	577	TYR	CB-CG-CD2	-14.26	112.45	121.00
9	r	150	PRO	CB-CA-C	-14.21	76.47	112.00
9	r	413	VAL	CB-CA-C	-14.17	84.48	111.40
1	X	134	ARG	NE-CZ-NH2	-14.14	113.23	120.30
4	b	737	PHE	CB-CG-CD2	-14.09	110.94	120.80
9	r	268	VAL	CB-CA-C	-14.02	84.77	111.40
9	r	413	VAL	N-CA-CB	14.00	142.30	111.50
9	r	268	VAL	N-CA-CB	13.98	142.25	111.50
3	a	832	PHE	CB-CG-CD2	-13.95	111.04	120.80
5	c	648	TYR	CB-CG-CD2	-13.88	112.67	121.00
9	r	267	VAL	N-CA-CB	13.88	142.03	111.50
4	m	161	ARG	NE-CZ-NH2	-13.86	113.37	120.30
9	r	80	PHE	O-C-N	-13.84	100.56	122.70
4	b	172	PHE	CB-CG-CD1	-13.81	111.13	120.80
9	r	274	PRO	CB-CA-C	-13.81	77.47	112.00
4	b	223	TYR	CB-CG-CD2	-13.75	112.75	121.00
3	a	105	ARG	NE-CZ-NH2	-13.71	113.44	120.30
7	p	22	ARG	NE-CZ-NH1	-13.71	113.45	120.30
5	n	565	TYR	CB-CG-CD1	13.69	129.21	121.00
1	X	1304	LYS	N-CA-C	-13.66	74.13	111.00
5	n	548	TYR	CB-CG-CD1	13.64	129.19	121.00
9	r	649	PHE	CB-CG-CD1	13.63	130.34	120.80
3	a	210	ARG	NE-CZ-NH2	-13.61	113.50	120.30
3	l	957	ASP	CB-CG-OD2	-13.60	106.06	118.30
9	r	1150	TYR	CB-CG-CD1	13.59	129.16	121.00
5	c	333	ARG	NE-CZ-NH2	-13.55	113.52	120.30
3	a	995	ARG	NE-CZ-NH2	-13.52	113.54	120.30
3	l	562	PHE	CB-CG-CD1	13.49	130.24	120.80
4	b	657	TYR	CB-CG-CD1	13.43	129.06	121.00
9	g	1044	ARG	NE-CZ-NH1	-13.42	113.59	120.30
1	X	1060	LEU	CB-CA-C	13.41	135.68	110.20
9	g	142	PHE	CB-CG-CD1	13.34	130.14	120.80
8	q	656	ARG	NE-CZ-NH2	-13.31	113.64	120.30
3	l	415	TYR	CB-CA-C	13.29	136.97	110.40
9	r	263	THR	CB-CA-C	-13.21	75.93	111.60
4	m	360	PHE	CB-CG-CD2	13.17	130.02	120.80
3	a	414	ARG	NE-CZ-NH1	13.13	126.87	120.30
3	a	1000	TYR	CB-CG-CD2	-13.12	113.13	121.00
9	r	864	PHE	CB-CG-CD1	-13.05	111.67	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	874	PHE	CB-CG-CD2	-13.02	111.69	120.80
9	r	287	THR	CB-CA-C	-13.01	76.47	111.60
5	c	183	PHE	CB-CG-CD1	12.98	129.89	120.80
5	c	183	PHE	CB-CG-CD2	-12.96	111.72	120.80
5	n	439	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	X	216	TYR	CB-CG-CD2	12.91	128.74	121.00
4	m	351	ARG	NE-CZ-NH2	-12.89	113.86	120.30
8	q	426	TYR	CB-CG-CD1	-12.89	113.27	121.00
8	q	575	GLU	N-CA-C	-12.88	76.22	111.00
5	c	297	TYR	CB-CG-CD1	12.84	128.71	121.00
9	r	300	THR	CB-CA-C	-12.83	76.97	111.60
1	X	1615	ARG	NE-CZ-NH1	-12.79	113.90	120.30
3	a	338	ARG	NE-CZ-NH2	12.74	126.67	120.30
9	r	74	THR	CB-CA-C	-12.73	77.24	111.60
3	a	70	TYR	CB-CG-CD2	-12.72	113.37	121.00
4	m	344	ARG	NE-CZ-NH2	-12.66	113.97	120.30
9	r	393	THR	CB-CA-C	-12.66	77.43	111.60
8	f	478	ARG	NE-CZ-NH1	12.56	126.58	120.30
4	b	122	ARG	NE-CZ-NH1	12.54	126.57	120.30
5	n	548	TYR	CB-CG-CD2	-12.48	113.51	121.00
9	r	414	THR	CB-CA-C	-12.45	77.98	111.60
1	X	1022	TYR	CB-CG-CD1	12.41	128.45	121.00
3	a	313	TYR	CB-CG-CD1	12.40	128.44	121.00
3	l	820	ARG	NE-CZ-NH2	12.39	126.49	120.30
9	r	391	THR	CB-CA-C	-12.36	78.22	111.60
3	l	376	TYR	CB-CG-CD1	-12.35	113.59	121.00
3	a	637	PHE	CB-CG-CD1	-12.34	112.16	120.80
9	r	410	THR	CB-CA-C	-12.33	78.30	111.60
9	r	145	THR	CB-CA-C	-12.31	78.37	111.60
8	q	478	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	X	323	TYR	CB-CG-CD1	12.27	128.36	121.00
3	a	257	TYR	CB-CG-CD1	-12.27	113.64	121.00
5	c	513	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	X	1304	LYS	CB-CA-C	12.08	134.56	110.40
4	b	172	PHE	CB-CG-CD2	12.08	129.26	120.80
4	m	561	ARG	NE-CZ-NH2	-12.01	114.29	120.30
8	f	575	GLU	CB-CA-C	-11.99	86.42	110.40
1	X	793	LEU	CB-CA-C	-11.98	87.44	110.20
1	X	342	ASP	CB-CG-OD1	11.97	129.07	118.30
9	g	825	ASP	CB-CG-OD2	-11.94	107.55	118.30
9	r	286	THR	CB-CA-C	-11.93	79.38	111.60
5	c	231	TYR	CB-CG-CD1	-11.92	113.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	102	ARG	NE-CZ-NH1	11.91	126.25	120.30
9	r	280	THR	CB-CA-C	-11.91	79.45	111.60
4	b	657	TYR	CB-CG-CD2	-11.86	113.88	121.00
5	c	285	ARG	NE-CZ-NH1	11.83	126.22	120.30
6	d	58	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	X	1059	ASN	N-CA-C	11.81	142.89	111.00
4	m	637	ARG	NE-CZ-NH2	-11.79	114.41	120.30
9	r	1114	TYR	CB-CG-CD1	-11.77	113.94	121.00
9	g	560	ARG	NE-CZ-NH2	-11.77	114.42	120.30
4	m	168	ARG	NE-CZ-NH1	11.73	126.17	120.30
8	q	266	TYR	CB-CG-CD1	11.70	128.02	121.00
3	a	315	PHE	CB-CG-CD1	-11.70	112.61	120.80
7	e	241	ARG	NE-CZ-NH2	-11.70	114.45	120.30
9	g	843	PHE	CB-CG-CD2	11.66	128.96	120.80
4	m	186	ARG	NE-CZ-NH2	-11.66	114.47	120.30
9	r	649	PHE	CB-CG-CD2	-11.65	112.64	120.80
9	g	690	ARG	NE-CZ-NH1	11.65	126.12	120.30
8	f	99	TYR	CB-CG-CD1	11.62	127.97	121.00
9	g	738	TYR	CB-CG-CD1	-11.56	114.06	121.00
4	b	168	ARG	NE-CZ-NH1	11.56	126.08	120.30
9	r	298	SER	N-CA-CB	11.54	127.81	110.50
3	a	82	TYR	CB-CG-CD1	-11.51	114.09	121.00
6	o	88	ARG	NE-CZ-NH1	-11.49	114.56	120.30
5	c	519	ARG	NE-CZ-NH2	-11.47	114.56	120.30
9	r	269	SER	N-CA-CB	11.46	127.68	110.50
3	l	820	ARG	NE-CZ-NH1	-11.43	114.59	120.30
9	g	1114	TYR	CB-CG-CD2	-11.42	114.15	121.00
1	X	1277	ILE	CB-CA-C	11.41	134.42	111.60
7	e	4	PHE	CB-CG-CD2	11.39	128.78	120.80
1	X	1022	TYR	CB-CG-CD2	-11.35	114.19	121.00
4	b	374	TYR	CB-CG-CD1	11.31	127.78	121.00
7	e	216	ARG	NE-CZ-NH1	11.29	125.95	120.30
3	l	1010	PHE	CB-CG-CD1	11.27	128.69	120.80
9	g	751	TYR	CB-CG-CD1	-11.26	114.24	121.00
8	q	266	TYR	CB-CG-CD2	-11.25	114.25	121.00
9	g	478	PHE	CB-CG-CD2	11.22	128.66	120.80
3	a	982	TYR	CB-CG-CD1	11.21	127.72	121.00
7	e	241	ARG	NE-CZ-NH1	11.20	125.90	120.30
9	r	415	SER	N-CA-CB	11.20	127.30	110.50
9	r	435	SER	N-CA-CB	11.19	127.28	110.50
9	r	545	TYR	CB-CG-CD2	-11.19	114.29	121.00
4	b	561	ARG	NE-CZ-NH2	11.15	125.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	754	TYR	CB-CG-CD2	11.14	127.69	121.00
7	p	329	ARG	NE-CZ-NH1	11.14	125.87	120.30
9	r	1036	PHE	CB-CG-CD2	-11.14	113.00	120.80
4	b	497	ARG	NE-CZ-NH1	11.10	125.85	120.30
9	r	149	SER	N-CA-CB	11.10	127.15	110.50
1	X	1309	ARG	NE-CZ-NH2	-11.10	114.75	120.30
3	l	936	TYR	CB-CG-CD1	-11.07	114.36	121.00
7	p	137	TYR	CB-CG-CD1	-11.05	114.37	121.00
1	X	1633	ARG	NE-CZ-NH1	11.03	125.82	120.30
9	r	81	SER	N-CA-CB	11.02	127.03	110.50
9	g	723	PHE	CB-CG-CD1	11.00	128.50	120.80
9	r	170	SER	N-CA-CB	11.00	127.00	110.50
4	m	710	TYR	CB-CG-CD2	10.93	127.56	121.00
3	l	526	ARG	NE-CZ-NH1	10.92	125.76	120.30
8	f	523	TYR	CB-CG-CD2	-10.91	114.45	121.00
1	X	793	LEU	N-CA-CB	10.91	132.21	110.40
3	a	67	TYR	CB-CG-CD1	10.89	127.54	121.00
3	l	6	ARG	NE-CZ-NH1	-10.89	114.85	120.30
3	a	82	TYR	CB-CG-CD2	10.89	127.53	121.00
1	X	793	LEU	N-CA-C	10.87	140.34	111.00
9	r	302	SER	N-CA-CB	10.84	126.75	110.50
9	g	437	TYR	CB-CG-CD1	-10.84	114.50	121.00
9	r	436	SER	N-CA-CB	10.83	126.74	110.50
3	l	27	TYR	CB-CG-CD1	-10.82	114.51	121.00
9	r	78	SER	N-CA-CB	10.80	126.71	110.50
1	X	289	TYR	CB-CG-CD2	-10.79	114.53	121.00
9	r	344	SER	N-CA-CB	10.78	126.67	110.50
8	q	714	TYR	CB-CG-CD1	-10.78	114.53	121.00
8	q	432	TYR	CB-CG-CD1	10.77	127.46	121.00
8	q	264	TYR	CB-CG-CD2	-10.74	114.56	121.00
3	a	67	TYR	CB-CG-CD2	-10.73	114.56	121.00
9	r	251	PRO	N-CD-CG	-10.73	87.11	103.20
5	c	143	ARG	NE-CZ-NH1	10.72	125.66	120.30
8	q	575	GLU	CB-CA-C	-10.69	89.01	110.40
9	r	390	ILE	CB-CA-C	-10.67	90.26	111.60
3	l	727	TYR	CB-CG-CD1	10.66	127.40	121.00
4	b	471	PHE	CB-CG-CD2	-10.65	113.35	120.80
3	l	338	ARG	NE-CZ-NH1	10.63	125.61	120.30
8	q	17	ASP	CB-CG-OD2	-10.62	108.75	118.30
9	r	94	ILE	CB-CA-C	-10.61	90.37	111.60
9	g	450	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	X	1276	LYS	N-CA-CB	10.57	129.63	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	354	SER	N-CA-CB	10.57	126.35	110.50
9	r	712	PHE	CB-CG-CD1	-10.57	113.40	120.80
4	b	497	ARG	NE-CZ-NH2	-10.56	115.02	120.30
9	r	371	SER	N-CA-CB	10.56	126.33	110.50
3	a	56	TYR	CB-CG-CD2	-10.53	114.68	121.00
4	m	136	PHE	CB-CG-CD1	-10.53	113.43	120.80
1	X	754	TYR	CB-CG-CD1	-10.53	114.68	121.00
8	q	720	ARG	NE-CZ-NH1	10.53	125.56	120.30
9	r	355	SER	N-CA-CB	10.53	126.29	110.50
5	c	147	SER	N-CA-CB	10.52	126.28	110.50
9	g	898	ASP	CB-CG-OD2	-10.51	108.84	118.30
4	b	655	PHE	CB-CG-CD1	-10.51	113.45	120.80
4	m	511	TYR	CB-CG-CD1	-10.49	114.71	121.00
9	r	372	SER	N-CA-CB	10.49	126.23	110.50
9	r	642	PHE	CB-CG-CD1	10.48	128.14	120.80
1	X	1303	LEU	N-CA-CB	10.46	131.33	110.40
4	m	116	ARG	NE-CZ-NH2	-10.46	115.07	120.30
9	g	1064	ARG	NE-CZ-NH2	-10.46	115.07	120.30
4	m	662	TYR	CB-CG-CD2	-10.45	114.73	121.00
9	r	438	SER	N-CA-CB	10.43	126.14	110.50
8	f	183	TYR	CB-CG-CD2	-10.42	114.75	121.00
9	r	150	PRO	N-CD-CG	-10.41	87.58	103.20
4	m	329	ARG	NE-CZ-NH2	-10.40	115.10	120.30
3	a	832	PHE	CB-CG-CD1	10.40	128.08	120.80
8	f	575	GLU	N-CA-C	-10.40	82.93	111.00
9	r	77	SER	N-CA-CB	10.39	126.08	110.50
9	r	236	SER	N-CA-CB	10.39	126.08	110.50
9	r	370	SER	N-CA-CB	10.38	126.08	110.50
1	X	794	ILE	CB-CA-C	10.38	132.36	111.60
8	f	248	TYR	CB-CG-CD2	-10.38	114.77	121.00
9	r	167	ILE	CB-CA-C	-10.36	90.88	111.60
3	a	168	TYR	CB-CG-CD1	10.35	127.21	121.00
7	e	39	ASP	CB-CG-OD2	-10.34	109.00	118.30
9	r	165	ILE	CB-CA-C	-10.34	90.92	111.60
5	n	509	ARG	NE-CZ-NH1	10.33	125.46	120.30
9	r	266	SER	N-CA-CB	10.30	125.94	110.50
8	f	576	ASN	CB-CA-C	10.27	130.94	110.40
3	l	659	TYR	CB-CG-CD2	10.27	127.16	121.00
3	l	532	PHE	CB-CG-CD1	-10.26	113.62	120.80
6	d	88	ARG	NE-CZ-NH2	-10.25	115.17	120.30
9	g	461	ASP	CB-CG-OD2	-10.23	109.09	118.30
9	r	260	ILE	CB-CA-C	-10.22	91.15	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	535	ARG	NE-CZ-NH1	10.21	125.41	120.30
3	l	585	ASP	CB-CG-OD2	-10.19	109.13	118.30
7	e	335	TYR	CB-CG-CD1	-10.18	114.89	121.00
3	l	415	TYR	N-CA-C	-10.17	83.55	111.00
4	b	471	PHE	CB-CG-CD1	10.15	127.91	120.80
3	l	995	ARG	NE-CZ-NH1	10.12	125.36	120.30
9	r	343	SER	N-CA-CB	10.12	125.68	110.50
4	m	458	ARG	NE-CZ-NH2	-10.12	115.24	120.30
9	g	874	PHE	CB-CG-CD1	10.08	127.86	120.80
4	b	295	TYR	CB-CG-CD2	10.04	127.02	121.00
6	o	130	PHE	CB-CG-CD2	-10.04	113.77	120.80
3	a	1000	TYR	CB-CG-CD1	10.03	127.02	121.00
6	o	259	ARG	NE-CZ-NH1	10.03	125.31	120.30
9	r	503	TYR	CB-CG-CD1	10.02	127.01	121.00
8	q	183	TYR	CB-CG-CD1	-9.99	115.01	121.00
9	r	233	ILE	CB-CA-C	-9.98	91.64	111.60
1	X	852	PHE	CB-CG-CD2	-9.97	113.82	120.80
3	a	1031	ARG	NE-CZ-NH2	-9.97	115.31	120.30
8	q	426	TYR	CB-CG-CD2	9.94	126.97	121.00
3	a	1010	PHE	CB-CG-CD1	-9.92	113.85	120.80
8	f	67	ASP	CB-CG-OD2	-9.92	109.38	118.30
5	n	547	ARG	NE-CZ-NH1	9.92	125.26	120.30
9	g	234	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	X	1217	ARG	NE-CZ-NH2	9.89	125.25	120.30
9	r	807	PHE	CB-CG-CD1	9.87	127.71	120.80
3	a	75	ARG	NE-CZ-NH1	9.86	125.23	120.30
9	g	252	PHE	CB-CG-CD2	-9.86	113.90	120.80
9	r	265	SER	N-CA-CB	9.83	125.24	110.50
3	a	251	PHE	CB-CG-CD2	-9.82	113.92	120.80
4	b	457	TYR	CG-CD1-CE1	9.82	129.16	121.30
3	a	315	PHE	CB-CG-CD2	9.81	127.67	120.80
6	d	20	TYR	CB-CG-CD2	-9.80	115.12	121.00
3	a	70	TYR	CB-CG-CD1	9.78	126.87	121.00
9	r	712	PHE	CB-CG-CD2	9.78	127.65	120.80
9	g	570	PHE	CB-CG-CD1	-9.77	113.96	120.80
9	r	291	ILE	CB-CA-C	-9.76	92.07	111.60
5	c	509	ARG	NE-CZ-NH1	9.76	125.18	120.30
9	g	174	TYR	CB-CG-CD1	9.75	126.85	121.00
9	r	256	ILE	CB-CA-C	-9.75	92.10	111.60
9	r	90	ILE	CB-CA-C	-9.74	92.13	111.60
9	r	155	PRO	N-CD-CG	-9.73	88.60	103.20
3	a	1014	TYR	CB-CG-CD2	9.72	126.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	675	TYR	CB-CG-CD1	-9.72	115.17	121.00
6	o	20	TYR	CB-CG-CD1	-9.72	115.17	121.00
8	q	523	TYR	CB-CG-CD1	-9.72	115.17	121.00
5	n	783	ARG	NE-CZ-NH1	9.71	125.15	120.30
8	f	218	TYR	CB-CG-CD1	9.70	126.82	121.00
9	r	1150	TYR	CB-CG-CD2	-9.65	115.21	121.00
7	e	335	TYR	CB-CG-CD2	9.65	126.79	121.00
4	m	267	ARG	NE-CZ-NH1	-9.64	115.48	120.30
3	a	936	TYR	CB-CG-CD2	-9.62	115.22	121.00
9	g	137	ARG	NE-CZ-NH1	9.62	125.11	120.30
3	l	562	PHE	CB-CG-CD2	-9.62	114.06	120.80
1	X	1092	SER	N-CA-CB	9.61	124.92	110.50
7	e	178	PHE	CB-CG-CD2	-9.61	114.08	120.80
3	l	210	ARG	NE-CZ-NH1	-9.60	115.50	120.30
8	q	477	ARG	NE-CZ-NH1	9.60	125.10	120.30
7	p	177	ARG	NE-CZ-NH2	9.60	125.10	120.30
3	a	975	ARG	NE-CZ-NH1	9.59	125.09	120.30
8	f	384	TYR	CB-CG-CD1	9.59	126.75	121.00
9	r	144	ALA	O-C-N	-9.59	107.36	122.70
3	a	204	TYR	CB-CG-CD1	9.58	126.75	121.00
7	e	146	ARG	NE-CZ-NH1	9.56	125.08	120.30
3	a	725	ARG	NE-CZ-NH2	-9.55	115.53	120.30
9	r	199	PRO	CA-N-CD	-9.54	98.15	111.50
6	d	19	TYR	CB-CG-CD1	-9.53	115.28	121.00
1	X	862	ARG	NE-CZ-NH2	-9.52	115.54	120.30
3	a	394	ASP	CB-CG-OD2	9.52	126.87	118.30
1	X	648	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	X	415	PHE	CB-CG-CD2	-9.50	114.15	120.80
8	q	469	ARG	NE-CZ-NH1	9.49	125.05	120.30
8	f	615	THR	CA-CB-CG2	-9.49	99.12	112.40
4	b	329	ARG	NE-CZ-NH1	-9.47	115.56	120.30
3	l	416	GLY	CA-C-O	9.47	137.64	120.60
4	m	204	PHE	CB-CG-CD1	9.46	127.42	120.80
9	r	690	ARG	NE-CZ-NH1	9.46	125.03	120.30
4	b	655	PHE	CB-CG-CD2	9.44	127.41	120.80
9	r	325	PRO	N-CD-CG	-9.42	89.08	103.20
4	b	603	ASP	N-CA-CB	9.40	127.53	110.60
6	o	187	TYR	CB-CG-CD1	-9.40	115.36	121.00
3	l	106	TYR	CB-CG-CD2	-9.39	115.36	121.00
8	f	432	TYR	CB-CG-CD1	-9.37	115.38	121.00
4	b	223	TYR	CB-CG-CD1	9.32	126.59	121.00
4	m	214	ARG	NE-CZ-NH1	9.31	124.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	400	PHE	CB-CG-CD2	9.28	127.29	120.80
3	a	512	THR	CA-CB-CG2	-9.27	99.42	112.40
9	r	416	ILE	CB-CA-C	-9.27	93.06	111.60
9	r	304	PRO	N-CD-CG	-9.26	89.31	103.20
6	o	173	PHE	CB-CG-CD1	9.26	127.28	120.80
9	r	265	SER	CB-CA-C	-9.26	92.51	110.10
4	b	204	PHE	CB-CG-CD2	-9.25	114.32	120.80
9	r	367	ILE	CB-CA-C	-9.25	93.10	111.60
8	f	542	ARG	NE-CZ-NH1	9.25	124.92	120.30
8	f	117	TYR	CG-CD1-CE1	-9.24	113.91	121.30
6	d	23	ARG	NE-CZ-NH2	-9.24	115.68	120.30
9	r	340	GLN	O-C-N	-9.23	107.93	122.70
9	r	166	ILE	CB-CA-C	-9.22	93.15	111.60
3	l	415	TYR	CB-CG-CD1	-9.20	115.48	121.00
3	l	484	TYR	CB-CG-CD2	-9.20	115.48	121.00
9	r	274	PRO	N-CD-CG	-9.19	89.42	103.20
9	r	367	ILE	N-CA-CB	9.19	131.93	110.80
4	m	88	TYR	CB-CG-CD2	-9.19	115.49	121.00
9	r	366	ILE	CB-CA-C	-9.18	93.23	111.60
9	r	366	ILE	N-CA-CB	9.18	131.91	110.80
3	l	14	TYR	CB-CG-CD2	-9.18	115.49	121.00
3	l	936	TYR	CB-CG-CD2	9.18	126.50	121.00
8	f	478	ARG	NE-CZ-NH2	-9.17	115.72	120.30
3	a	313	TYR	CB-CG-CD2	-9.17	115.50	121.00
1	X	1276	LYS	N-CA-C	9.16	135.75	111.00
5	c	509	ARG	NE-CZ-NH2	-9.16	115.72	120.30
9	r	275	ILE	N-CA-CB	9.16	131.88	110.80
9	r	275	ILE	CB-CA-C	-9.15	93.30	111.60
9	r	166	ILE	N-CA-CB	9.14	131.83	110.80
9	r	416	ILE	N-CA-CB	9.14	131.82	110.80
4	m	672	TYR	CB-CG-CD1	-9.13	115.52	121.00
7	e	9	ASP	CB-CG-OD1	9.13	126.52	118.30
4	b	69	PHE	CB-CG-CD1	9.11	127.18	120.80
9	g	600	PHE	CB-CG-CD1	9.11	127.17	120.80
3	l	912	ASP	CB-CG-OD2	9.10	126.49	118.30
4	m	710	TYR	CB-CG-CD1	-9.10	115.54	121.00
6	o	75	TYR	CB-CG-CD1	-9.10	115.54	121.00
1	X	213	PHE	CB-CG-CD1	9.10	127.17	120.80
3	l	1015	ASP	CB-CG-OD2	-9.10	110.11	118.30
3	a	758	PHE	CB-CG-CD2	9.08	127.16	120.80
3	l	995	ARG	NE-CZ-NH2	-9.07	115.77	120.30
7	p	146	ARG	NE-CZ-NH2	-9.06	115.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	270	PHE	CB-CG-CD2	-9.05	114.47	120.80
5	n	305	ARG	NE-CZ-NH1	9.04	124.82	120.30
4	b	737	PHE	CB-CG-CD1	9.02	127.11	120.80
4	m	107	TYR	CG-CD2-CE2	-9.02	114.08	121.30
6	o	171	ARG	NE-CZ-NH2	-9.01	115.80	120.30
8	q	482	ARG	CB-CA-C	-9.01	92.39	110.40
4	m	204	PHE	CB-CG-CD2	-8.99	114.50	120.80
3	a	442	TYR	CB-CG-CD2	-8.99	115.61	121.00
1	X	1597	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	X	651	TYR	CB-CG-CD2	-8.98	115.61	121.00
8	f	523	TYR	CB-CG-CD1	8.97	126.39	121.00
4	b	321	ALA	N-CA-CB	8.97	122.66	110.10
8	q	248	TYR	CB-CG-CD1	-8.97	115.62	121.00
5	n	153	PHE	CB-CG-CD1	-8.96	114.53	120.80
9	r	90	ILE	N-CA-CB	8.96	131.40	110.80
6	d	20	TYR	CB-CG-CD1	8.96	126.37	121.00
8	f	183	TYR	CB-CG-CD1	8.95	126.37	121.00
4	b	214	ARG	NE-CZ-NH2	-8.93	115.83	120.30
3	l	880	ARG	NE-CZ-NH2	-8.93	115.84	120.30
9	r	343	SER	CB-CA-C	-8.92	93.15	110.10
9	g	1101	ARG	NE-CZ-NH1	8.92	124.76	120.30
9	r	291	ILE	N-CA-CB	8.91	131.30	110.80
3	a	924	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	X	1615	ARG	NE-CZ-NH2	8.89	124.75	120.30
9	r	256	ILE	N-CA-CB	8.88	131.22	110.80
1	X	1050	SER	N-CA-CB	8.87	123.81	110.50
3	l	283	TYR	CB-CG-CD2	8.85	126.31	121.00
9	r	437	TYR	N-CA-CB	8.85	126.52	110.60
1	X	675	TYR	CB-CG-CD2	8.84	126.31	121.00
8	f	576	ASN	CA-C-O	-8.84	101.54	120.10
5	n	583	SER	N-CA-CB	8.83	123.75	110.50
3	l	403	ASP	CB-CG-OD1	8.82	126.24	118.30
1	X	1199	TYR	CB-CG-CD1	8.82	126.29	121.00
6	d	208	ARG	NE-CZ-NH1	8.77	124.69	120.30
9	r	233	ILE	N-CA-CB	8.77	130.97	110.80
6	o	187	TYR	CB-CG-CD2	8.76	126.25	121.00
3	l	376	TYR	CG-CD1-CE1	-8.72	114.32	121.30
8	f	67	ASP	CB-CG-OD1	8.72	126.15	118.30
9	r	118	PRO	CA-N-CD	-8.71	99.30	111.50
1	X	1060	LEU	N-CA-CB	8.71	127.82	110.40
1	X	1340	PHE	CB-CG-CD1	-8.71	114.70	120.80
3	l	8	ASP	CB-CG-OD2	-8.70	110.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	266	SER	CB-CA-C	-8.70	93.57	110.10
9	r	236	SER	CB-CA-C	-8.70	93.57	110.10
3	l	826	TYR	CB-CG-CD1	8.69	126.21	121.00
4	m	295	TYR	CB-CG-CD2	-8.69	115.79	121.00
9	r	260	ILE	N-CA-CB	8.68	130.77	110.80
7	p	4	PHE	CB-CG-CD2	-8.68	114.72	120.80
1	X	1277	ILE	CA-C-N	-8.68	98.11	117.20
9	g	106	TYR	CB-CG-CD1	-8.66	115.80	121.00
5	n	645	TYR	CB-CG-CD2	8.65	126.19	121.00
9	r	324	TYR	N-CA-CB	8.65	126.16	110.60
5	c	267	ARG	NE-CZ-NH1	8.64	124.62	120.30
9	r	77	SER	CB-CA-C	-8.64	93.68	110.10
9	r	438	SER	CB-CA-C	-8.64	93.68	110.10
3	l	682	ASP	CB-CG-OD2	-8.63	110.53	118.30
9	r	165	ILE	N-CA-CB	8.63	130.66	110.80
3	a	751	ARG	NE-CZ-NH2	-8.63	115.98	120.30
8	f	387	ARG	NE-CZ-NH1	-8.62	115.99	120.30
4	m	672	TYR	CB-CG-CD2	8.62	126.17	121.00
7	e	96	ARG	NE-CZ-NH1	8.61	124.61	120.30
3	a	982	TYR	CB-CG-CD2	-8.59	115.84	121.00
9	r	136	PRO	N-CD-CG	-8.59	90.31	103.20
9	r	370	SER	CB-CA-C	-8.58	93.79	110.10
9	r	167	ILE	N-CA-CB	8.58	130.53	110.80
9	g	909	ASP	CB-CG-OD2	-8.58	110.58	118.30
8	q	231	PHE	CB-CG-CD1	-8.58	114.80	120.80
3	a	15	TYR	CB-CG-CD2	-8.57	115.86	121.00
1	X	1059	ASN	N-CA-CB	8.57	126.03	110.60
3	l	1035	ARG	NE-CZ-NH1	8.57	124.59	120.30
3	l	128	PHE	CB-CG-CD2	8.56	126.80	120.80
4	m	732	ARG	NE-CZ-NH1	-8.56	116.02	120.30
7	e	97	ARG	NE-CZ-NH2	-8.55	116.02	120.30
9	g	217	ALA	N-CA-CB	8.55	122.07	110.10
3	l	484	TYR	CB-CG-CD1	8.55	126.13	121.00
7	e	339	PHE	CB-CG-CD1	8.51	126.76	120.80
6	o	221	TYR	CB-CG-CD2	8.51	126.11	121.00
5	n	264	ARG	NE-CZ-NH2	-8.50	116.05	120.30
3	l	749	TYR	CB-CG-CD2	-8.50	115.90	121.00
4	b	158	PHE	CB-CG-CD1	-8.50	114.85	120.80
9	r	356	CYS	N-CA-CB	8.50	125.89	110.60
1	X	1288	PHE	CB-CG-CD2	-8.49	114.86	120.80
9	r	94	ILE	N-CA-CB	8.49	130.32	110.80
3	a	232	ARG	NE-CZ-NH1	8.49	124.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	714	TYR	CB-CG-CD2	8.47	126.08	121.00
7	p	168	ASP	CB-CG-OD2	-8.47	110.68	118.30
9	r	390	ILE	N-CA-CB	8.46	130.26	110.80
9	r	355	SER	CB-CA-C	-8.45	94.05	110.10
3	a	204	TYR	CB-CG-CD2	-8.45	115.93	121.00
3	a	662	PHE	CB-CG-CD1	-8.45	114.89	120.80
8	f	11	ARG	NE-CZ-NH1	8.44	124.52	120.30
3	a	173	PHE	CB-CG-CD1	-8.44	114.89	120.80
9	r	372	SER	CB-CA-C	-8.43	94.09	110.10
3	l	751	ARG	NE-CZ-NH2	8.42	124.51	120.30
8	q	576	ASN	CB-CA-C	8.41	127.22	110.40
4	m	381	ALA	N-CA-CB	8.40	121.85	110.10
7	p	173	TRP	CB-CG-CD2	-8.39	115.69	126.60
3	a	686	PHE	CB-CG-CD2	8.38	126.67	120.80
9	r	371	SER	CB-CA-C	-8.36	94.21	110.10
7	e	39	ASP	CB-CG-OD1	8.36	125.82	118.30
9	r	208	CYS	N-CA-CB	8.36	125.64	110.60
9	g	759	TRP	CB-CG-CD2	-8.35	115.74	126.60
3	a	15	TYR	CB-CG-CD1	8.35	126.01	121.00
7	p	173	TRP	CB-CG-CD1	8.35	137.85	127.00
9	g	1020	ARG	NE-CZ-NH1	-8.34	116.13	120.30
3	a	872	TYR	CB-CG-CD2	8.34	126.00	121.00
9	r	354	SER	CB-CA-C	-8.34	94.25	110.10
4	m	641	ASP	CB-CG-OD1	8.33	125.80	118.30
4	b	710	TYR	CB-CG-CD2	-8.32	116.01	121.00
1	X	1062	ARG	NE-CZ-NH1	8.30	124.45	120.30
6	d	18	ASP	CB-CG-OD2	-8.31	110.82	118.30
8	f	576	ASN	CA-C-N	8.29	135.43	117.20
9	g	1094	TYR	CB-CG-CD2	-8.27	116.04	121.00
5	n	519	ARG	NE-CZ-NH1	8.26	124.43	120.30
9	r	1122	THR	CA-CB-CG2	-8.26	100.84	112.40
8	q	144	TRP	CB-CG-CD1	-8.26	116.27	127.00
9	r	885	VAL	CA-CB-CG2	8.25	123.27	110.90
7	e	329	ARG	NE-CZ-NH2	-8.24	116.18	120.30
3	a	1017	TRP	N-CA-CB	8.23	125.42	110.60
3	a	669	ARG	NE-CZ-NH2	-8.23	116.19	120.30
5	c	459	PHE	CB-CG-CD2	-8.23	115.04	120.80
9	r	96	TYR	N-CA-CB	8.22	125.39	110.60
1	X	330	TYR	CB-CG-CD1	8.21	125.92	121.00
4	b	186	ARG	NE-CZ-NH1	8.20	124.40	120.30
4	m	214	ARG	NE-CZ-NH2	-8.20	116.20	120.30
6	o	60	ASP	CB-CG-OD1	8.19	125.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	375	TYR	CZ-CE2-CD2	-8.19	112.43	119.80
8	q	536	ARG	NE-CZ-NH1	8.19	124.39	120.30
4	m	112	PHE	CB-CG-CD1	-8.18	115.07	120.80
3	a	725	ARG	NE-CZ-NH1	8.18	124.39	120.30
9	g	67	TYR	CB-CG-CD1	-8.18	116.09	121.00
9	r	344	SER	CB-CA-C	-8.18	94.57	110.10
8	f	381	ASP	CB-CG-OD1	8.17	125.65	118.30
5	n	607	ARG	NE-CZ-NH1	8.17	124.38	120.30
4	b	571	TYR	CB-CG-CD2	-8.17	116.10	121.00
3	l	509	TYR	CB-CG-CD1	-8.17	116.10	121.00
5	c	552	TYR	CB-CG-CD2	-8.16	116.10	121.00
7	e	20	TYR	CB-CG-CD2	-8.16	116.11	121.00
5	n	285	ARG	NE-CZ-NH2	8.15	124.38	120.30
3	a	348	TYR	CZ-CE2-CD2	-8.15	112.46	119.80
9	g	560	ARG	NE-CZ-NH1	8.14	124.37	120.30
8	f	285	ASP	CB-CG-OD2	-8.14	110.97	118.30
8	f	264	TYR	CB-CG-CD2	-8.13	116.12	121.00
4	b	81	PHE	CB-CG-CD1	-8.13	115.11	120.80
3	l	257	TYR	CB-CG-CD1	-8.13	116.12	121.00
8	f	142	SER	N-CA-CB	8.12	122.68	110.50
4	m	173	TYR	CB-CG-CD2	8.12	125.87	121.00
9	r	78	SER	CB-CA-C	-8.12	94.67	110.10
9	g	326	PHE	CB-CG-CD1	-8.11	115.12	120.80
8	f	285	ASP	CB-CG-OD1	8.11	125.59	118.30
8	f	261	ARG	NE-CZ-NH1	8.10	124.35	120.30
9	g	108	TRP	CB-CG-CD1	8.10	137.53	127.00
4	b	331	TYR	CB-CG-CD1	-8.09	116.15	121.00
3	l	965	TYR	CB-CG-CD2	-8.08	116.15	121.00
9	r	240	PRO	CA-N-CD	-8.08	100.18	111.50
9	r	237	MET	CB-CA-C	-8.07	94.25	110.40
9	g	230	PHE	CB-CG-CD1	8.07	126.45	120.80
8	q	634	PHE	CB-CG-CD1	8.06	126.45	120.80
9	r	436	SER	CB-CA-C	-8.06	94.78	110.10
9	g	882	TYR	CB-CG-CD2	-8.06	116.16	121.00
9	r	76	TYR	N-CA-CB	8.06	125.10	110.60
9	r	397	PRO	N-CD-CG	-8.05	91.12	103.20
4	m	641	ASP	CB-CG-OD2	-8.05	111.05	118.30
9	r	503	TYR	CG-CD2-CE2	-8.04	114.86	121.30
9	g	265	SER	N-CA-CB	8.04	122.56	110.50
5	n	414	TYR	CB-CG-CD1	8.03	125.82	121.00
3	a	27	TYR	CB-CG-CD1	-8.02	116.19	121.00
3	l	6	ARG	NE-CZ-NH2	8.02	124.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	751	TYR	CB-CG-CD2	8.02	125.81	121.00
9	r	208	CYS	CB-CA-C	-8.02	94.36	110.40
9	r	302	SER	CB-CA-C	-8.02	94.87	110.10
9	g	443	TRP	CB-CG-CD2	-8.01	116.19	126.60
9	g	372	SER	N-CA-CB	8.00	122.49	110.50
3	l	864	PHE	CB-CG-CD1	7.99	126.40	120.80
8	q	218	TYR	CG-CD1-CE1	-7.99	114.91	121.30
6	d	219	ARG	NE-CZ-NH2	7.99	124.30	120.30
4	b	317	PHE	CB-CG-CD1	-7.98	115.21	120.80
5	c	439	ARG	NE-CZ-NH1	7.98	124.29	120.30
8	f	245	ARG	NE-CZ-NH1	7.97	124.29	120.30
3	l	194	TYR	CB-CG-CD2	7.96	125.78	121.00
4	b	717	ASP	CB-CG-OD2	-7.96	111.13	118.30
9	r	1101	ARG	NE-CZ-NH2	-7.96	116.32	120.30
8	q	11	ARG	NE-CZ-NH2	-7.95	116.32	120.30
9	g	712	PHE	CB-CG-CD2	-7.95	115.23	120.80
9	r	199	PRO	N-CA-CB	7.95	112.83	103.30
3	l	695	TYR	CB-CG-CD1	-7.94	116.23	121.00
3	l	415	TYR	CA-CB-CG	7.94	128.49	113.40
1	X	415	PHE	CB-CG-CD1	7.94	126.36	120.80
8	q	183	TYR	CB-CG-CD2	7.94	125.76	121.00
1	X	1276	LYS	CB-CA-C	-7.93	94.53	110.40
3	l	1031	ARG	NE-CZ-NH1	-7.93	116.34	120.30
3	l	748	PHE	CB-CG-CD1	7.92	126.35	120.80
5	n	620	TYR	CB-CG-CD1	-7.92	116.25	121.00
3	l	27	TYR	CB-CG-CD2	7.91	125.75	121.00
4	m	189	TYR	CG-CD1-CE1	-7.91	114.97	121.30
9	g	334	TRP	CA-CB-CG	7.91	128.73	113.70
9	r	216	PRO	N-CD-CG	-7.91	91.34	103.20
3	a	719	PHE	CB-CG-CD2	-7.90	115.27	120.80
4	b	280	VAL	CA-CB-CG1	-7.89	99.06	110.90
9	r	1025	ASP	CB-CG-OD2	-7.89	111.19	118.30
9	g	577	TYR	CB-CG-CD1	7.89	125.73	121.00
7	p	75	ALA	N-CA-CB	7.88	121.14	110.10
9	r	146	MET	N-CA-CB	7.88	124.78	110.60
5	c	548	TYR	CB-CG-CD2	7.88	125.72	121.00
8	q	248	TYR	CB-CG-CD2	7.87	125.72	121.00
9	r	170	SER	CB-CA-C	-7.87	95.15	110.10
9	g	909	ASP	CB-CG-OD1	7.87	125.38	118.30
3	l	270	PHE	CB-CG-CD1	-7.87	115.29	120.80
3	l	442	TYR	CB-CG-CD2	7.85	125.71	121.00
9	r	143	PRO	N-CD-CG	-7.85	91.42	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	720	ARG	NE-CZ-NH1	7.85	124.22	120.30
9	r	356	CYS	CB-CA-C	-7.85	94.71	110.40
4	m	107	TYR	CB-CG-CD1	-7.84	116.29	121.00
4	m	455	PHE	CB-CG-CD1	7.84	126.29	120.80
9	r	421	PRO	CA-N-CD	-7.84	100.52	111.50
1	X	1171	ARG	NE-CZ-NH1	7.84	124.22	120.30
4	b	571	TYR	CB-CG-CD1	7.83	125.70	121.00
8	q	117	TYR	CB-CG-CD2	-7.83	116.30	121.00
3	a	758	PHE	CB-CG-CD1	-7.83	115.32	120.80
6	o	23	ARG	NE-CZ-NH2	-7.83	116.38	120.30
4	b	678	ASP	CB-CG-OD1	7.83	125.35	118.30
1	X	1217	ARG	NE-CZ-NH1	-7.83	116.39	120.30
3	l	793	PHE	CB-CG-CD2	-7.82	115.33	120.80
3	a	214	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	X	1277	ILE	CA-C-O	7.80	136.49	120.10
3	l	550	PHE	CB-CG-CD1	7.80	126.26	120.80
9	r	864	PHE	CB-CG-CD2	7.80	126.26	120.80
8	f	656	ARG	NE-CZ-NH2	-7.79	116.40	120.30
5	c	143	ARG	NE-CZ-NH2	-7.78	116.41	120.30
9	r	81	SER	CB-CA-C	-7.78	95.31	110.10
4	m	161	ARG	NE-CZ-NH1	7.77	124.19	120.30
8	q	62	VAL	CA-CB-CG1	7.77	122.55	110.90
3	l	840	PHE	CB-CG-CD1	-7.75	115.37	120.80
8	f	218	TYR	CB-CG-CD2	-7.75	116.35	121.00
9	g	736	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	X	385	PHE	CB-CG-CD1	7.74	126.22	120.80
9	r	404	MET	N-CA-CB	7.74	124.53	110.60
4	m	539	TYR	CB-CG-CD1	7.73	125.64	121.00
8	q	36	PHE	CB-CG-CD1	-7.73	115.39	120.80
3	a	422	ARG	NE-CZ-NH2	-7.73	116.44	120.30
9	r	1044	ARG	NE-CZ-NH1	7.72	124.16	120.30
4	m	638	ASP	CB-CG-OD2	-7.72	111.35	118.30
3	l	637	PHE	CB-CG-CD1	-7.72	115.40	120.80
3	a	757	GLU	OE1-CD-OE2	7.70	132.54	123.30
3	a	724	PHE	CB-CG-CD1	7.70	126.19	120.80
5	n	479	ALA	CB-CA-C	-7.70	98.56	110.10
7	p	57	SER	O-C-N	7.68	134.98	122.70
9	r	1006	TYR	CB-CG-CD1	-7.67	116.40	121.00
6	o	66	PHE	CB-CG-CD2	7.67	126.17	120.80
9	r	714	TYR	CB-CG-CD1	-7.67	116.40	121.00
9	r	404	MET	CB-CA-C	-7.67	95.06	110.40
9	r	149	SER	CB-CA-C	-7.67	95.53	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	223	TYR	CB-CG-CD2	7.66	125.60	121.00
7	p	216	ARG	NE-CZ-NH2	-7.65	116.47	120.30
3	l	338	ARG	NE-CZ-NH2	-7.65	116.47	120.30
9	g	563	PHE	CB-CG-CD1	7.64	126.15	120.80
8	f	301	TYR	CB-CG-CD2	-7.64	116.42	121.00
8	q	535	ARG	NE-CZ-NH1	7.63	124.12	120.30
9	r	92	MET	CB-CA-C	-7.63	95.13	110.40
3	l	771	ASP	CB-CG-OD1	7.63	125.17	118.30
3	l	1031	ARG	NE-CZ-NH2	-7.63	116.48	120.30
9	r	92	MET	N-CA-CB	7.63	124.33	110.60
9	r	158	GLN	N-CA-CB	7.63	124.33	110.60
9	g	759	TRP	CB-CG-CD1	7.62	136.91	127.00
5	c	414	TYR	CB-CG-CD1	-7.62	116.43	121.00
4	m	419	PHE	CB-CG-CD1	-7.62	115.47	120.80
9	g	709	PHE	CB-CG-CD1	-7.61	115.47	120.80
6	d	142	ASP	CB-CG-OD2	-7.61	111.45	118.30
5	n	783	ARG	NE-CZ-NH2	-7.60	116.50	120.30
5	c	414	TYR	CG-CD2-CE2	-7.60	115.22	121.30
3	a	984	TYR	CB-CG-CD2	-7.60	116.44	121.00
9	r	415	SER	CB-CA-C	-7.59	95.68	110.10
3	a	965	TYR	CB-CG-CD2	-7.59	116.45	121.00
4	m	478	ASP	CB-CG-OD2	-7.59	111.47	118.30
7	p	116	PHE	CB-CG-CD1	7.59	126.11	120.80
9	g	125	ARG	NE-CZ-NH2	-7.59	116.51	120.30
7	e	19	PHE	CB-CG-CD2	7.58	126.11	120.80
4	b	374	TYR	CB-CG-CD2	-7.58	116.45	121.00
8	q	432	TYR	CB-CG-CD2	-7.57	116.46	121.00
9	r	723	PHE	CB-CG-CD1	-7.57	115.50	120.80
9	r	1110	ARG	NE-CZ-NH1	7.56	124.08	120.30
3	l	938	ARG	NE-CZ-NH1	7.54	124.07	120.30
9	g	723	PHE	CB-CG-CD2	-7.54	115.52	120.80
3	l	502	ASP	CB-CG-OD1	7.53	125.08	118.30
5	n	483	PHE	CB-CG-CD2	-7.53	115.53	120.80
1	X	1233	PHE	CB-CG-CD2	-7.52	115.53	120.80
3	l	882	PHE	CB-CG-CD1	-7.52	115.53	120.80
4	m	223	TYR	CG-CD1-CE1	7.52	127.32	121.30
9	r	240	PRO	N-CD-CG	-7.52	91.92	103.20
5	n	529	ARG	NE-CZ-NH2	-7.52	116.54	120.30
8	q	64	SER	N-CA-CB	7.52	121.78	110.50
7	e	97	ARG	NE-CZ-NH1	7.51	124.06	120.30
9	r	240	PRO	N-CA-CB	7.49	112.29	103.30
7	p	51	TRP	CA-CB-CG	7.48	127.92	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	608	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	X	1642	ARG	NE-CZ-NH1	-7.47	116.56	120.30
6	o	18	ASP	CB-CG-OD2	-7.47	111.58	118.30
6	o	76	ASP	CB-CG-OD1	7.47	125.02	118.30
4	m	136	PHE	CB-CG-CD2	7.46	126.03	120.80
9	r	118	PRO	N-CD-CG	-7.46	92.00	103.20
9	r	981	ARG	NE-CZ-NH1	7.46	124.03	120.30
3	l	982	TYR	CB-CG-CD2	7.46	125.48	121.00
1	X	1072	TYR	CB-CG-CD2	-7.46	116.53	121.00
9	r	435	SER	CB-CA-C	-7.46	95.94	110.10
3	l	578	ASP	CB-CG-OD1	7.45	125.01	118.30
7	e	339	PHE	CB-CG-CD2	-7.44	115.59	120.80
8	f	653	TYR	CB-CG-CD2	-7.43	116.54	121.00
5	c	645	TYR	CB-CG-CD2	7.43	125.46	121.00
1	X	411	PHE	CD1-CE1-CZ	-7.42	111.19	120.10
8	q	99	TYR	CB-CG-CD1	7.42	125.45	121.00
4	m	471	PHE	CB-CG-CD2	-7.42	115.61	120.80
8	q	99	TYR	CB-CG-CD2	-7.41	116.56	121.00
1	X	650	ASP	CB-CG-OD2	7.40	124.96	118.30
6	o	88	ARG	NE-CZ-NH2	7.40	124.00	120.30
9	r	237	MET	N-CA-CB	7.40	123.92	110.60
5	c	142	ARG	NE-CZ-NH1	7.39	124.00	120.30
9	r	722	PHE	CB-CG-CD2	-7.39	115.63	120.80
7	p	112	TYR	CB-CG-CD1	-7.39	116.57	121.00
3	l	502	ASP	CB-CG-OD2	-7.38	111.66	118.30
9	r	549	MET	CG-SD-CE	-7.37	88.41	100.20
5	c	427	ALA	N-CA-CB	7.36	120.41	110.10
9	r	146	MET	CB-CA-C	-7.35	95.69	110.40
9	r	835	PHE	N-CA-CB	7.35	123.84	110.60
4	b	304	ARG	NE-CZ-NH1	-7.35	116.63	120.30
3	l	1010	PHE	CB-CG-CD2	-7.35	115.66	120.80
6	d	88	ARG	NE-CZ-NH1	7.34	123.97	120.30
9	g	447	VAL	CG1-CB-CG2	7.34	122.64	110.90
5	c	142	ARG	NE-CZ-NH2	7.33	123.97	120.30
9	g	845	PHE	CB-CG-CD1	7.33	125.93	120.80
5	c	202	ARG	NH1-CZ-NH2	-7.33	111.34	119.40
8	q	180	PHE	CB-CG-CD2	-7.33	115.67	120.80
8	q	656	ARG	NE-CZ-NH1	7.33	123.96	120.30
5	c	565	TYR	CB-CG-CD2	7.32	125.39	121.00
9	g	89	TYR	CB-CG-CD2	-7.32	116.61	121.00
8	q	224	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	X	1084	LEU	CB-CG-CD2	7.31	123.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	984	TYR	CB-CG-CD1	7.31	125.39	121.00
8	f	576	ASN	N-CA-CB	7.31	123.76	110.60
3	l	194	TYR	CB-CG-CD1	-7.31	116.61	121.00
6	o	75	TYR	CB-CG-CD2	7.31	125.39	121.00
4	b	349	TYR	CB-CG-CD1	7.31	125.39	121.00
5	n	774	LEU	CB-CG-CD1	7.30	123.42	111.00
6	d	58	ARG	NE-CZ-NH2	-7.30	116.65	120.30
3	l	918	PHE	CB-CG-CD2	-7.30	115.69	120.80
1	X	1082	PHE	CB-CG-CD1	7.29	125.90	120.80
3	l	724	PHE	CB-CG-CD2	-7.29	115.70	120.80
1	X	712	LEU	CB-CG-CD2	7.28	123.38	111.00
9	r	199	PRO	N-CD-CG	-7.28	92.28	103.20
9	r	123	PRO	CA-N-CD	-7.28	101.31	111.50
3	l	271	ARG	NE-CZ-NH1	7.27	123.94	120.30
9	r	143	PRO	CA-N-CD	-7.27	101.32	111.50
9	g	116	ASP	CB-CG-OD2	-7.27	111.75	118.30
5	c	174	ARG	NE-CZ-NH1	7.27	123.94	120.30
9	r	421	PRO	N-CD-CG	-7.26	92.30	103.20
3	a	834	ARG	NE-CZ-NH2	-7.26	116.67	120.30
4	b	88	TYR	CB-CG-CD1	7.26	125.36	121.00
1	X	152	TYR	CB-CG-CD1	-7.26	116.65	121.00
5	n	441	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	a	177	PHE	CB-CG-CD1	7.25	125.88	120.80
4	m	244	TYR	CB-CG-CD1	-7.25	116.65	121.00
4	m	662	TYR	CB-CG-CD1	7.25	125.35	121.00
3	l	551	THR	CA-CB-CG2	-7.24	102.27	112.40
8	f	117	TYR	CB-CG-CD2	-7.24	116.66	121.00
4	b	639	ARG	NE-CZ-NH1	7.23	123.92	120.30
4	m	75	SER	N-CA-CB	7.23	121.34	110.50
6	o	76	ASP	CB-CG-OD2	-7.22	111.80	118.30
7	e	189	GLU	N-CA-CB	7.21	123.58	110.60
9	g	124	PHE	CB-CG-CD1	7.21	125.85	120.80
9	g	981	ARG	NE-CZ-NH1	-7.21	116.70	120.30
6	o	259	ARG	NH1-CZ-NH2	-7.21	111.47	119.40
3	a	199	PHE	CB-CG-CD1	7.20	125.84	120.80
4	b	456	SER	N-CA-CB	7.20	121.31	110.50
1	X	650	ASP	CB-CG-OD1	-7.20	111.82	118.30
9	r	269	SER	CB-CA-C	-7.20	96.42	110.10
9	r	753	PHE	CG-CD1-CE1	-7.20	112.88	120.80
1	X	364	THR	CA-CB-CG2	-7.20	102.33	112.40
8	f	194	ASP	CB-CG-OD1	7.20	124.78	118.30
1	X	1404	PHE	CB-CG-CD1	-7.19	115.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	455	PHE	CB-CG-CD2	-7.19	115.77	120.80
1	X	1303	LEU	N-CA-C	7.18	130.40	111.00
9	r	234	ARG	N-CA-CB	7.18	123.53	110.60
3	l	14	TYR	N-CA-C	-7.18	91.61	111.00
4	m	223	TYR	CD1-CE1-CZ	-7.18	113.33	119.80
3	a	139	PHE	CB-CG-CD2	-7.18	115.77	120.80
8	q	545	ALA	N-CA-CB	7.18	120.15	110.10
3	a	219	ASP	N-CA-CB	7.18	123.52	110.60
9	r	736	ASP	CB-CG-OD1	7.16	124.75	118.30
9	g	808	TYR	CG-CD2-CE2	7.16	127.03	121.30
3	l	825	TYR	CB-CG-CD2	-7.16	116.71	121.00
9	g	284	TYR	CB-CG-CD2	7.15	125.29	121.00
1	X	639	PHE	CB-CG-CD1	7.14	125.80	120.80
9	g	715	LEU	CB-CG-CD2	7.14	123.14	111.00
9	g	981	ARG	NE-CZ-NH2	-7.14	116.73	120.30
9	g	608	ASP	CB-CG-OD1	7.14	124.72	118.30
1	X	289	TYR	CB-CG-CD1	7.13	125.28	121.00
9	g	229	PHE	CB-CG-CD1	-7.13	115.81	120.80
9	g	1094	TYR	CG-CD2-CE2	-7.13	115.60	121.30
9	r	136	PRO	N-CA-CB	7.13	111.85	103.30
9	r	699	MET	CG-SD-CE	-7.13	88.80	100.20
3	a	376	TYR	CB-CG-CD2	-7.12	116.73	121.00
5	c	408	ASP	CB-CG-OD2	-7.12	111.90	118.30
1	X	375	TYR	CB-CG-CD1	-7.11	116.73	121.00
9	g	420	PHE	CB-CG-CD1	-7.10	115.83	120.80
9	g	145	THR	CA-CB-CG2	-7.10	102.46	112.40
9	r	1043	ARG	NE-CZ-NH2	-7.10	116.75	120.30
7	e	68	TYR	CB-CG-CD1	-7.10	116.74	121.00
9	r	338	PRO	N-CD-CG	-7.09	92.56	103.20
3	l	456	ALA	N-CA-CB	7.08	120.01	110.10
8	q	11	ARG	NE-CZ-NH1	7.08	123.84	120.30
8	q	477	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	X	343	ASP	CB-CG-OD2	7.08	124.67	118.30
4	b	190	PHE	N-CA-CB	7.07	123.33	110.60
8	q	542	ARG	N-CA-CB	7.07	123.33	110.60
3	l	534	ASP	CB-CG-OD2	-7.07	111.94	118.30
9	g	825	ASP	CB-CG-OD1	7.07	124.66	118.30
1	X	1251	TYR	CB-CG-CD2	-7.06	116.76	121.00
3	a	571	PHE	CG-CD1-CE1	7.06	128.57	120.80
3	l	260	VAL	CA-CB-CG1	7.06	121.49	110.90
3	l	501	THR	CA-CB-CG2	-7.06	102.52	112.40
7	e	228	TYR	CG-CD1-CE1	7.05	126.94	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	167	PHE	CB-CG-CD1	-7.04	115.87	120.80
9	r	298	SER	CB-CA-C	-7.04	96.72	110.10
3	a	359	THR	CA-CB-CG2	-7.04	102.55	112.40
9	g	1044	ARG	NH1-CZ-NH2	7.04	127.14	119.40
4	b	329	ARG	NH1-CZ-NH2	7.04	127.14	119.40
4	m	521	TRP	CG-CD1-NE1	-7.03	103.07	110.10
9	r	352	TYR	O-C-N	-7.02	111.46	122.70
6	d	45	LEU	CB-CG-CD1	7.02	122.93	111.00
8	q	180	PHE	CB-CG-CD1	7.02	125.71	120.80
9	g	925	ASN	N-CA-CB	7.01	123.22	110.60
4	b	295	TYR	CB-CG-CD1	-7.01	116.79	121.00
3	l	219	ASP	N-CA-CB	7.01	123.22	110.60
8	f	702	TYR	CG-CD2-CE2	-7.01	115.69	121.30
4	b	94	ARG	NE-CZ-NH2	-7.01	116.80	120.30
5	c	264	ARG	NE-CZ-NH1	7.00	123.80	120.30
8	f	144	TRP	CB-CG-CD2	7.00	135.70	126.60
3	l	1019	LEU	N-CA-CB	7.00	124.41	110.40
3	a	378	TRP	CB-CG-CD2	-7.00	117.50	126.60
1	X	1285	PHE	CB-CG-CD2	6.99	125.69	120.80
8	f	301	TYR	CB-CG-CD1	6.98	125.19	121.00
1	X	334	ALA	N-CA-CB	6.97	119.86	110.10
8	f	231	PHE	N-CA-CB	6.97	123.15	110.60
1	X	419	ASP	CB-CG-OD2	6.97	124.57	118.30
7	e	144	ASP	CB-CG-OD2	-6.97	112.03	118.30
3	a	968	ARG	NE-CZ-NH2	6.96	123.78	120.30
9	r	303	HIS	C-N-CD	6.96	143.02	128.40
9	g	124	PHE	CB-CG-CD2	-6.96	115.93	120.80
1	X	143	SER	N-CA-CB	6.96	120.93	110.50
4	b	381	ALA	N-CA-CB	6.96	119.84	110.10
8	q	384	TYR	CG-CD1-CE1	-6.96	115.73	121.30
6	o	276	ASN	N-CA-CB	6.95	123.11	110.60
3	l	782	TYR	CB-CG-CD1	-6.95	116.83	121.00
5	c	267	ARG	NE-CZ-NH2	-6.94	116.83	120.30
4	m	249	LEU	CB-CG-CD2	6.94	122.80	111.00
1	X	685	TYR	N-CA-CB	6.94	123.09	110.60
9	r	76	TYR	CB-CA-C	-6.94	96.52	110.40
4	m	353	TRP	CD1-NE1-CE2	-6.94	102.76	109.00
1	X	1265	PHE	CB-CG-CD1	-6.93	115.95	120.80
1	X	1233	PHE	CB-CG-CD1	6.93	125.65	120.80
3	l	106	TYR	CB-CG-CD1	6.93	125.16	121.00
3	l	454	LYS	CB-CA-C	6.93	124.25	110.40
9	r	912	LYS	N-CA-CB	6.93	123.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	p	239	ARG	NE-CZ-NH2	-6.92	116.84	120.30
8	f	192	ALA	N-CA-CB	6.92	119.79	110.10
4	b	385	ASP	CB-CG-OD1	6.92	124.53	118.30
5	n	505	ASP	CB-CG-OD1	6.92	124.52	118.30
3	l	14	TYR	CA-CB-CG	-6.91	100.27	113.40
4	b	511	TYR	CD1-CE1-CZ	6.91	126.02	119.80
3	l	824	PHE	CB-CG-CD1	6.91	125.64	120.80
7	e	116	PHE	CB-CG-CD1	-6.91	115.96	120.80
6	o	71	ALA	N-CA-CB	6.90	119.76	110.10
9	g	466	TYR	CB-CG-CD1	6.89	125.14	121.00
3	a	566	ASN	N-CA-CB	6.89	123.00	110.60
6	d	237	ASP	CB-CG-OD2	-6.89	112.10	118.30
7	e	15	VAL	CA-CB-CG2	-6.89	100.57	110.90
4	m	627	TYR	CB-CG-CD1	6.88	125.13	121.00
5	c	305	ARG	NE-CZ-NH1	6.88	123.74	120.30
4	b	91	TYR	CB-CG-CD2	-6.88	116.87	121.00
5	n	435	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	X	852	PHE	CB-CG-CD1	6.88	125.61	120.80
9	g	808	TYR	CZ-CE2-CD2	-6.88	113.61	119.80
9	g	753	PHE	CB-CG-CD1	-6.87	115.99	120.80
3	l	637	PHE	CG-CD1-CE1	-6.87	113.25	120.80
9	r	257	TRP	N-CA-CB	6.87	122.96	110.60
6	o	20	TYR	CB-CG-CD2	6.86	125.12	121.00
4	b	389	ASP	CB-CG-OD1	6.86	124.47	118.30
3	a	928	ALA	CB-CA-C	-6.86	99.81	110.10
4	b	124	PHE	CB-CG-CD1	-6.86	116.00	120.80
4	m	576	PHE	CB-CG-CD1	-6.85	116.00	120.80
3	l	106	TYR	CD1-CE1-CZ	6.85	125.97	119.80
9	r	136	PRO	CA-N-CD	-6.85	101.91	111.50
4	b	464	TYR	CB-CG-CD1	-6.85	116.89	121.00
9	r	753	PHE	CD1-CE1-CZ	6.85	128.32	120.10
6	o	279	THR	CA-CB-CG2	-6.85	102.81	112.40
6	d	153	TRP	CB-CG-CD2	-6.84	117.70	126.60
4	m	521	TRP	CD1-NE1-CE2	6.84	115.16	109.00
9	r	73	GLN	N-CA-CB	6.83	122.90	110.60
6	o	82	TRP	CB-CG-CD2	6.83	135.48	126.60
6	d	153	TRP	CB-CG-CD1	6.82	135.87	127.00
3	l	668	TYR	CB-CG-CD2	-6.82	116.91	121.00
4	m	466	LEU	CB-CA-C	-6.82	97.25	110.20
8	q	648	ASP	CB-CG-OD2	-6.82	112.17	118.30
5	c	660	VAL	CA-CB-CG2	-6.81	100.68	110.90
3	a	955	SER	N-CA-CB	6.81	120.71	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	777	PHE	CB-CG-CD2	6.80	125.56	120.80
6	o	219	ARG	NE-CZ-NH1	6.80	123.70	120.30
5	n	143	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	X	862	ARG	NE-CZ-NH1	6.79	123.70	120.30
8	f	580	PHE	CB-CG-CD2	-6.79	116.05	120.80
3	a	882	PHE	CB-CG-CD1	-6.79	116.05	120.80
8	f	705	PHE	CB-CG-CD2	-6.79	116.05	120.80
3	a	257	TYR	CB-CG-CD2	6.79	125.07	121.00
4	m	471	PHE	CB-CG-CD1	6.78	125.55	120.80
6	d	38	VAL	CA-CB-CG2	-6.78	100.73	110.90
9	r	665	PHE	CB-CG-CD1	6.78	125.55	120.80
3	a	373	PHE	CB-CG-CD1	6.77	125.54	120.80
4	m	51	MET	CG-SD-CE	-6.77	89.37	100.20
7	p	14	ASP	CB-CG-OD1	6.77	124.39	118.30
5	c	360	LEU	CB-CG-CD1	6.76	122.49	111.00
9	g	787	ASP	CB-CG-OD1	6.76	124.38	118.30
3	a	997	ARG	NE-CZ-NH1	6.76	123.68	120.30
3	a	627	TYR	CB-CG-CD2	6.75	125.05	121.00
5	n	547	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
8	q	112	ASP	CB-CG-OD1	6.75	124.38	118.30
4	b	744	MET	CG-SD-CE	-6.75	89.41	100.20
4	b	304	ARG	NE-CZ-NH2	-6.74	116.93	120.30
3	l	212	PHE	CB-CG-CD2	-6.74	116.08	120.80
5	c	142	ARG	NH1-CZ-NH2	-6.74	111.99	119.40
6	o	171	ARG	NE-CZ-NH1	6.74	123.67	120.30
9	r	781	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	X	769	PHE	CB-CG-CD2	6.73	125.51	120.80
4	b	587	ASP	CB-CG-OD2	-6.73	112.24	118.30
4	m	561	ARG	NE-CZ-NH1	6.73	123.66	120.30
8	f	562	TYR	CB-CG-CD1	-6.71	116.97	121.00
1	X	289	TYR	N-CA-CB	6.71	122.68	110.60
8	q	157	ASP	CB-CG-OD1	6.71	124.34	118.30
3	l	808	TRP	CH2-CZ2-CE2	6.71	124.11	117.40
9	r	830	SER	N-CA-CB	6.71	120.57	110.50
3	a	710	TYR	CB-CG-CD2	-6.71	116.97	121.00
8	q	259	TYR	CB-CG-CD1	-6.71	116.98	121.00
8	f	435	PHE	CB-CG-CD2	6.70	125.49	120.80
3	l	70	TYR	N-CA-CB	6.70	122.67	110.60
9	r	1028	LEU	CB-CG-CD2	6.70	122.39	111.00
9	r	123	PRO	N-CD-CG	-6.70	93.15	103.20
3	a	995	ARG	NH1-CZ-NH2	6.70	126.77	119.40
9	r	96	TYR	CB-CA-C	-6.69	97.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	727	TYR	CG-CD2-CE2	6.69	126.65	121.30
4	m	655	PHE	CB-CG-CD1	-6.69	116.12	120.80
3	l	190	ASP	CB-CG-OD2	-6.68	112.28	118.30
3	l	809	LYS	CA-CB-CG	6.68	128.10	113.40
9	r	292	PHE	N-CA-CB	6.68	122.63	110.60
3	l	965	TYR	CB-CG-CD1	6.68	125.01	121.00
4	m	363	TYR	N-CA-CB	6.68	122.62	110.60
1	X	1425	TYR	CB-CG-CD1	-6.67	117.00	121.00
5	n	648	TYR	CG-CD1-CE1	-6.67	115.96	121.30
7	p	167	SER	N-CA-CB	6.67	120.51	110.50
1	X	1099	PHE	CB-CG-CD2	-6.67	116.13	120.80
9	r	246	LYS	N-CA-CB	6.66	122.58	110.60
3	a	825	TYR	CB-CG-CD2	-6.66	117.01	121.00
4	b	222	GLU	OE1-CD-OE2	6.66	131.29	123.30
3	l	802	TYR	CB-CG-CD1	6.65	124.99	121.00
6	d	108	ALA	CB-CA-C	-6.65	100.12	110.10
4	m	642	TRP	CD1-NE1-CE2	6.65	114.99	109.00
3	a	765	PHE	CB-CG-CD1	-6.65	116.15	120.80
1	X	1277	ILE	N-CA-CB	6.65	126.09	110.80
9	r	93	GLN	N-CA-CB	6.64	122.56	110.60
8	q	600	TRP	CB-CG-CD1	-6.64	118.37	127.00
4	m	457	TYR	CB-CG-CD2	-6.64	117.02	121.00
4	m	641	ASP	N-CA-CB	6.64	122.55	110.60
4	b	505	ALA	N-CA-CB	6.63	119.39	110.10
7	e	239	ARG	NH1-CZ-NH2	-6.63	112.10	119.40
3	l	739	PHE	CB-CG-CD2	6.63	125.44	120.80
3	l	415	TYR	CG-CD1-CE1	-6.63	116.00	121.30
4	m	539	TYR	CB-CG-CD2	-6.63	117.02	121.00
3	a	826	TYR	CB-CG-CD1	6.63	124.98	121.00
9	g	674	ASN	N-CA-CB	6.63	122.53	110.60
5	n	393	GLN	N-CA-CB	6.62	122.52	110.60
9	g	106	TYR	CB-CG-CD2	6.62	124.97	121.00
1	X	341	PHE	CB-CG-CD2	6.61	125.43	120.80
4	b	63	ASP	CB-CG-OD2	-6.61	112.35	118.30
3	a	210	ARG	NE-CZ-NH1	6.61	123.61	120.30
8	q	259	TYR	CG-CD2-CE2	-6.61	116.01	121.30
1	X	685	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	X	835	LEU	CB-CG-CD1	-6.61	99.77	111.00
9	r	1001	ASP	CB-CG-OD2	-6.61	112.35	118.30
3	a	686	PHE	CB-CG-CD1	-6.60	116.18	120.80
9	r	261	PHE	N-CA-CB	6.60	122.48	110.60
1	X	1099	PHE	CB-CG-CD1	6.60	125.42	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	575	PHE	CB-CG-CD1	-6.60	116.18	120.80
9	r	1103	PRO	N-CD-CG	6.60	113.10	103.20
9	g	638	SER	N-CA-CB	6.60	120.39	110.50
9	g	738	TYR	CB-CG-CD2	6.60	124.96	121.00
9	r	1006	TYR	CG-CD1-CE1	-6.59	116.03	121.30
9	r	89	TYR	O-C-N	-6.59	112.16	122.70
4	b	63	ASP	N-CA-CB	6.59	122.46	110.60
9	r	421	PRO	N-CA-CB	6.59	111.20	103.30
9	g	142	PHE	CB-CG-CD2	-6.58	116.19	120.80
9	g	126	SER	N-CA-CB	6.58	120.37	110.50
5	c	560	LEU	CB-CG-CD1	6.58	122.18	111.00
9	r	714	TYR	CB-CG-CD2	6.58	124.95	121.00
7	e	226	ARG	NE-CZ-NH2	-6.57	117.01	120.30
8	f	99	TYR	CG-CD1-CE1	6.57	126.56	121.30
3	a	466	TYR	CB-CG-CD2	6.57	124.94	121.00
4	m	201	ARG	NE-CZ-NH1	6.57	123.58	120.30
3	a	553	ILE	CA-CB-CG1	-6.56	98.53	111.00
7	e	4	PHE	CB-CG-CD1	-6.56	116.21	120.80
3	a	949	LEU	CB-CG-CD1	-6.56	99.85	111.00
3	l	924	ARG	NE-CZ-NH1	6.56	123.58	120.30
9	g	461	ASP	CB-CG-OD1	6.56	124.20	118.30
4	m	223	TYR	CB-CG-CD2	6.56	124.93	121.00
8	f	702	TYR	CD1-CG-CD2	6.55	125.11	117.90
3	a	824	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	X	1427	SER	N-CA-CB	6.54	120.31	110.50
4	b	288	SER	N-CA-CB	6.54	120.31	110.50
8	q	533	LEU	CB-CG-CD1	6.54	122.12	111.00
4	b	116	ARG	NE-CZ-NH2	-6.54	117.03	120.30
8	f	633	THR	N-CA-CB	6.53	122.71	110.30
4	m	295	TYR	CB-CG-CD1	6.52	124.92	121.00
1	X	685	TYR	CD1-CE1-CZ	-6.52	113.93	119.80
4	b	190	PHE	CB-CG-CD1	6.52	125.36	120.80
9	g	108	TRP	CB-CG-CD2	-6.52	118.13	126.60
3	l	739	PHE	CB-CG-CD1	-6.52	116.24	120.80
9	g	324	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	X	1525	PHE	CB-CG-CD1	-6.51	116.24	120.80
3	l	840	PHE	CB-CG-CD2	6.51	125.36	120.80
9	r	1114	TYR	CG-CD2-CE2	-6.51	116.09	121.30
3	a	917	ASP	CB-CG-OD1	6.50	124.15	118.30
8	f	42	PHE	CB-CG-CD1	-6.50	116.25	120.80
3	l	194	TYR	CG-CD2-CE2	6.50	126.50	121.30
7	p	336	SER	N-CA-CB	6.50	120.25	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	691	TYR	CB-CG-CD1	-6.50	117.10	121.00
3	l	204	TYR	CB-CG-CD1	-6.49	117.10	121.00
3	l	695	TYR	CD1-CE1-CZ	-6.49	113.95	119.80
5	n	492	PHE	CB-CG-CD2	-6.49	116.25	120.80
8	f	714	TYR	CB-CG-CD1	-6.49	117.11	121.00
4	m	683	MET	CG-SD-CE	6.49	110.58	100.20
5	n	628	VAL	CA-CB-CG1	6.49	120.63	110.90
6	o	98	HIS	N-CA-CB	6.49	122.27	110.60
5	c	500	ASP	CB-CG-OD1	-6.48	112.47	118.30
9	r	345	GLN	N-CA-CB	6.48	122.26	110.60
4	m	349	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	X	164	TYR	CG-CD2-CE2	-6.48	116.12	121.30
8	q	595	ARG	NE-CZ-NH1	6.47	123.54	120.30
9	r	875	PHE	CB-CG-CD1	-6.47	116.27	120.80
1	X	198	MET	CG-SD-CE	-6.47	89.84	100.20
4	b	658	LEU	N-CA-CB	6.47	123.34	110.40
9	r	118	PRO	N-CA-CB	6.46	111.06	103.30
8	q	231	PHE	CB-CG-CD2	6.46	125.32	120.80
4	b	122	ARG	NH1-CZ-NH2	-6.46	112.29	119.40
5	c	231	TYR	CB-CG-CD2	6.46	124.88	121.00
9	g	339	LEU	CB-CG-CD2	6.46	121.98	111.00
8	q	144	TRP	CB-CG-CD2	6.46	135.00	126.60
9	g	712	PHE	CB-CG-CD1	6.45	125.32	120.80
8	q	576	ASN	N-CA-CB	6.45	122.22	110.60
7	e	166	GLN	N-CA-C	-6.45	93.58	111.00
5	n	519	ARG	NE-CZ-NH2	-6.45	117.07	120.30
9	r	642	PHE	CB-CG-CD2	-6.45	116.29	120.80
9	g	287	THR	CA-CB-CG2	-6.44	103.38	112.40
5	n	425	TYR	CB-CG-CD2	6.44	124.87	121.00
4	b	317	PHE	CB-CG-CD2	6.44	125.31	120.80
7	p	137	TYR	CG-CD1-CE1	-6.44	116.15	121.30
1	X	153	ASP	CB-CG-OD1	6.44	124.09	118.30
3	a	158	PHE	CB-CG-CD1	6.44	125.31	120.80
1	X	1410	SER	N-CA-CB	6.43	120.15	110.50
3	l	14	TYR	CB-CG-CD1	6.43	124.86	121.00
8	f	266	TYR	CB-CG-CD1	-6.43	117.14	121.00
5	n	217	PHE	CB-CG-CD2	6.43	125.30	120.80
8	q	67	ASP	N-CA-CB	6.42	122.16	110.60
4	b	419	PHE	O-C-N	-6.42	112.43	122.70
5	n	453	LEU	CB-CG-CD1	6.42	121.91	111.00
3	a	898	ASP	CB-CG-OD1	6.42	124.08	118.30
3	a	774	TYR	CZ-CE2-CD2	6.42	125.57	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	436	LYS	CB-CA-C	-6.41	97.58	110.40
6	o	61	TRP	CB-CG-CD1	6.40	135.32	127.00
4	b	559	PHE	CB-CG-CD2	6.40	125.28	120.80
1	X	1169	ALA	N-CA-CB	6.40	119.06	110.10
9	r	691	TYR	CG-CD2-CE2	-6.40	116.18	121.30
8	f	44	SER	N-CA-CB	6.40	120.10	110.50
5	c	641	MET	CG-SD-CE	-6.40	89.97	100.20
4	m	511	TYR	CB-CG-CD2	6.39	124.83	121.00
1	X	137	VAL	CA-CB-CG1	-6.39	101.32	110.90
3	l	257	TYR	CG-CD1-CE1	-6.39	116.19	121.30
3	l	916	ARG	NE-CZ-NH1	6.39	123.49	120.30
3	a	701	TYR	CG-CD1-CE1	-6.39	116.19	121.30
1	X	260	ARG	NE-CZ-NH2	-6.38	117.11	120.30
9	g	819	GLN	N-CA-CB	6.38	122.09	110.60
9	r	1102	PHE	CB-CG-CD2	6.38	125.27	120.80
5	n	509	ARG	NE-CZ-NH2	-6.38	117.11	120.30
8	q	653	TYR	CG-CD1-CE1	6.38	126.41	121.30
8	q	562	TYR	CB-CG-CD1	-6.38	117.17	121.00
9	g	1152	THR	CA-CB-CG2	-6.38	103.47	112.40
5	n	579	ARG	NE-CZ-NH2	-6.38	117.11	120.30
3	a	338	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
3	a	738	ARG	NE-CZ-NH1	6.37	123.49	120.30
6	d	57	TRP	CD1-NE1-CE2	6.37	114.74	109.00
6	o	66	PHE	CD1-CG-CD2	-6.37	110.01	118.30
3	l	142	ALA	N-CA-CB	6.37	119.02	110.10
8	q	264	TYR	CB-CG-CD1	6.37	124.82	121.00
8	q	561	ASN	C-N-CA	6.37	137.63	121.70
7	e	10	ASP	CB-CG-OD2	6.37	124.03	118.30
7	p	131	ASP	CB-CG-OD1	6.37	124.03	118.30
4	b	565	TYR	CG-CD2-CE2	-6.37	116.21	121.30
7	e	121	LEU	N-CA-CB	6.37	123.13	110.40
4	b	304	ARG	NH1-CZ-NH2	6.36	126.40	119.40
3	l	386	LEU	CA-CB-CG	6.36	129.93	115.30
8	f	643	PHE	CB-CG-CD1	-6.36	116.35	120.80
3	a	914	TYR	CZ-CE2-CD2	-6.35	114.08	119.80
8	f	716	ASP	CB-CG-OD2	-6.35	112.58	118.30
9	g	1014	SER	N-CA-CB	6.35	120.03	110.50
8	f	512	TYR	CZ-CE2-CD2	-6.35	114.08	119.80
6	d	23	ARG	NE-CZ-NH1	6.35	123.47	120.30
8	q	159	ASP	CB-CG-OD2	-6.35	112.59	118.30
8	q	469	ARG	NE-CZ-NH2	-6.35	117.13	120.30
3	a	294	GLU	N-CA-CB	6.34	122.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	345	GLN	CB-CA-C	-6.34	97.71	110.40
4	b	694	VAL	O-C-N	-6.34	112.56	122.70
1	X	1303	LEU	CB-CA-C	-6.34	98.16	110.20
5	n	202	ARG	NE-CZ-NH2	-6.34	117.13	120.30
5	n	552	TYR	CB-CG-CD1	-6.34	117.20	121.00
9	g	781	TYR	CB-CG-CD2	6.33	124.80	121.00
4	m	633	PHE	CB-CG-CD1	6.33	125.23	120.80
1	X	921	SER	N-CA-CB	6.33	119.99	110.50
8	q	144	TRP	CD1-NE1-CE2	6.33	114.69	109.00
3	l	70	TYR	CB-CG-CD2	-6.33	117.20	121.00
8	q	381	ASP	CB-CG-OD2	6.33	123.99	118.30
1	X	1308	TYR	CD1-CE1-CZ	6.32	125.49	119.80
3	a	116	GLN	N-CA-CB	6.32	121.98	110.60
3	l	1031	ARG	NH1-CZ-NH2	6.31	126.34	119.40
9	g	818	LEU	CB-CG-CD1	6.31	121.72	111.00
9	g	930	SER	N-CA-CB	6.31	119.96	110.50
3	a	466	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	X	182	PHE	CB-CG-CD1	6.30	125.21	120.80
9	r	328	HIS	CB-CA-C	-6.30	97.81	110.40
7	e	243	PHE	CB-CG-CD2	6.29	125.21	120.80
7	e	99	ASN	CB-CG-OD1	-6.29	109.02	121.60
1	X	1062	ARG	NE-CZ-NH2	-6.29	117.16	120.30
9	g	133	ALA	CB-CA-C	-6.29	100.67	110.10
4	m	97	ARG	NE-CZ-NH2	-6.29	117.16	120.30
3	l	422	ARG	NE-CZ-NH1	-6.28	117.16	120.30
4	m	484	VAL	CA-CB-CG2	-6.28	101.48	110.90
9	g	833	GLU	N-CA-CB	6.28	121.90	110.60
6	o	212	TRP	CB-CG-CD2	6.28	134.76	126.60
1	X	421	PHE	CB-CG-CD2	-6.27	116.41	120.80
9	r	368	PHE	CB-CA-C	-6.27	97.86	110.40
9	g	130	ASP	CB-CG-OD1	-6.27	112.66	118.30
3	l	825	TYR	CB-CG-CD1	6.27	124.76	121.00
8	q	111	GLN	N-CA-CB	6.27	121.88	110.60
8	q	482	ARG	N-CA-C	6.27	127.92	111.00
4	m	505	ALA	N-CA-CB	6.26	118.87	110.10
9	r	326	PHE	N-CA-CB	6.26	121.88	110.60
4	b	351	ARG	NE-CZ-NH2	-6.26	117.17	120.30
3	a	656	ASP	CB-CG-OD1	6.26	123.93	118.30
5	n	435	TYR	CB-CG-CD1	6.26	124.75	121.00
3	a	199	PHE	CB-CG-CD2	-6.26	116.42	120.80
1	X	1251	TYR	CB-CG-CD1	6.25	124.75	121.00
4	b	156	GLU	N-CA-CB	6.25	121.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	15	TYR	CZ-CE2-CD2	-6.25	114.17	119.80
5	c	181	ARG	NE-CZ-NH1	6.25	123.42	120.30
8	q	324	VAL	CA-CB-CG2	-6.25	101.53	110.90
8	f	144	TRP	CB-CG-CD1	-6.24	118.88	127.00
9	g	281	ARG	NE-CZ-NH1	6.24	123.42	120.30
9	r	405	GLU	CB-CA-C	-6.24	97.92	110.40
1	X	888	TYR	CB-CG-CD1	6.24	124.74	121.00
4	b	672	TYR	CD1-CE1-CZ	-6.24	114.18	119.80
3	a	837	SER	N-CA-CB	6.24	119.86	110.50
9	r	250	LYS	N-CA-CB	6.24	121.83	110.60
3	l	210	ARG	NE-CZ-NH2	6.24	123.42	120.30
3	l	293	LEU	N-CA-C	-6.24	94.16	111.00
9	g	727	PHE	CB-CG-CD1	-6.23	116.44	120.80
9	g	177	ASP	CB-CG-OD2	-6.23	112.69	118.30
5	c	181	ARG	N-CA-CB	6.23	121.81	110.60
9	g	478	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	X	1254	ARG	NE-CZ-NH2	-6.23	117.19	120.30
3	l	161	ARG	N-CA-C	-6.23	94.19	111.00
9	r	1091	THR	N-CA-C	-6.23	94.19	111.00
1	X	1626	GLN	N-CA-CB	6.22	121.81	110.60
3	l	771	ASP	CB-CG-OD2	-6.22	112.70	118.30
9	r	1064	ARG	NE-CZ-NH2	6.22	123.41	120.30
7	e	188	LEU	N-CA-CB	6.22	122.84	110.40
1	X	1340	PHE	CB-CG-CD2	6.22	125.15	120.80
3	l	799	SER	N-CA-CB	6.22	119.83	110.50
8	q	523	TYR	CG-CD1-CE1	-6.22	116.33	121.30
8	f	653	TYR	CG-CD2-CE2	-6.21	116.33	121.30
3	l	376	TYR	CB-CG-CD2	6.21	124.73	121.00
1	X	1281	MET	CG-SD-CE	-6.21	90.26	100.20
3	a	283	TYR	CZ-CE2-CD2	6.21	125.39	119.80
6	o	61	TRP	CB-CG-CD2	-6.21	118.53	126.60
7	p	20	TYR	CB-CG-CD2	-6.20	117.28	121.00
9	r	691	TYR	CG-CD1-CE1	-6.20	116.34	121.30
5	c	446	ASP	CB-CG-OD2	-6.19	112.72	118.30
7	p	30	ASP	C-N-CA	6.19	137.19	121.70
3	a	1010	PHE	CZ-CE2-CD2	-6.19	112.67	120.10
3	a	56	TYR	CB-CG-CD1	6.19	124.71	121.00
9	g	691	TYR	CB-CG-CD2	-6.19	117.28	121.00
7	p	78	ASP	CB-CG-OD1	6.19	123.87	118.30
9	r	1102	PHE	CB-CG-CD1	-6.19	116.47	120.80
1	X	407	ALA	CB-CA-C	-6.19	100.82	110.10
6	o	194	TYR	CB-CG-CD2	-6.19	117.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	1105	ASP	CB-CG-OD2	-6.19	112.73	118.30
9	g	974	ARG	NE-CZ-NH2	6.19	123.39	120.30
5	n	183	PHE	CB-CG-CD1	-6.18	116.47	120.80
5	n	185	PHE	CB-CG-CD1	-6.18	116.47	120.80
4	b	457	TYR	CB-CG-CD2	6.18	124.71	121.00
4	m	331	TYR	CG-CD1-CE1	-6.18	116.35	121.30
3	a	997	ARG	N-CA-CB	-6.18	99.47	110.60
6	d	119	ALA	N-CA-CB	6.18	118.75	110.10
9	r	252	PHE	CB-CA-C	-6.18	98.04	110.40
9	g	450	ARG	NE-CZ-NH2	-6.18	117.21	120.30
9	r	750	TYR	CZ-CE2-CD2	6.18	125.36	119.80
9	r	756	PHE	CB-CG-CD2	-6.18	116.48	120.80
3	a	840	PHE	CB-CG-CD1	-6.17	116.48	120.80
3	l	824	PHE	CB-CG-CD2	-6.17	116.48	120.80
4	m	517	ASP	CB-CG-OD2	-6.17	112.74	118.30
9	g	530	ASP	CB-CG-OD1	6.17	123.85	118.30
1	X	1334	ASP	CB-CG-OD2	-6.17	112.75	118.30
3	a	751	ARG	NH1-CZ-NH2	6.17	126.18	119.40
3	l	532	PHE	CB-CG-CD2	6.17	125.12	120.80
9	r	432	LYS	CB-CA-C	-6.16	98.08	110.40
3	l	476	PHE	CB-CG-CD2	6.16	125.11	120.80
6	o	286	GLU	N-CA-CB	6.15	121.68	110.60
1	X	663	MET	O-C-N	6.15	132.53	122.70
3	a	919	PHE	CB-CG-CD1	-6.15	116.50	120.80
3	l	864	PHE	CB-CG-CD2	-6.15	116.50	120.80
6	o	234	TRP	CG-CD1-NE1	-6.14	103.95	110.10
9	r	807	PHE	CB-CG-CD2	-6.14	116.50	120.80
3	a	511	ARG	NE-CZ-NH2	-6.14	117.23	120.30
7	e	19	PHE	CB-CG-CD1	-6.14	116.50	120.80
5	c	608	ASP	CB-CG-OD2	-6.14	112.78	118.30
7	p	57	SER	N-CA-CB	6.13	119.70	110.50
3	a	509	TYR	CB-CG-CD1	-6.13	117.32	121.00
9	r	1105	ASP	CB-CG-OD1	6.13	123.82	118.30
9	g	878	SER	N-CA-CB	6.13	119.69	110.50
3	l	668	TYR	CB-CG-CD1	6.12	124.67	121.00
6	o	179	ASP	CB-CG-OD1	6.12	123.81	118.30
7	p	301	ASP	CB-CG-OD1	6.12	123.80	118.30
9	r	171	LYS	N-CA-CB	6.12	121.61	110.60
9	r	324	TYR	CB-CA-C	-6.12	98.17	110.40
3	a	256	ASP	CB-CG-OD2	-6.11	112.80	118.30
9	g	1102	PHE	CB-CG-CD1	-6.11	116.52	120.80
8	q	649	TYR	CB-CG-CD2	-6.11	117.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	146	SER	CB-CA-C	-6.11	98.50	110.10
6	d	130	PHE	CB-CG-CD2	-6.11	116.53	120.80
3	l	150	PHE	CB-CG-CD1	-6.10	116.53	120.80
3	l	180	ASP	CB-CG-OD2	-6.10	112.81	118.30
9	r	93	GLN	CB-CA-C	-6.10	98.20	110.40
1	X	1179	SER	N-CA-CB	6.10	119.64	110.50
5	c	328	ASN	N-CA-CB	6.09	121.56	110.60
9	g	525	GLU	N-CA-CB	6.09	121.56	110.60
4	b	244	TYR	CB-CG-CD1	6.09	124.65	121.00
1	X	302	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	X	1254	ARG	NE-CZ-NH1	6.09	123.34	120.30
6	d	42	THR	N-CA-CB	6.08	121.86	110.30
5	n	645	TYR	CB-CG-CD1	-6.08	117.35	121.00
4	b	527	VAL	CA-CB-CG1	-6.08	101.78	110.90
9	g	159	ASP	CB-CG-OD2	6.08	123.77	118.30
3	l	693	PHE	CB-CG-CD1	-6.08	116.54	120.80
5	c	484	ALA	N-CA-CB	6.08	118.61	110.10
4	m	647	ARG	NE-CZ-NH1	-6.08	117.26	120.30
5	n	148	TYR	CB-CG-CD1	6.08	124.65	121.00
3	l	968	ARG	NE-CZ-NH1	6.07	123.34	120.30
4	m	634	TYR	CA-CB-CG	6.07	124.93	113.40
3	a	715	THR	CA-CB-CG2	-6.06	103.91	112.40
5	c	652	ARG	NE-CZ-NH2	-6.06	117.27	120.30
9	r	1126	ASP	N-CA-CB	6.06	121.52	110.60
5	c	186	ASP	CB-CG-OD1	6.06	123.75	118.30
8	f	444	ALA	N-CA-CB	6.05	118.58	110.10
9	g	981	ARG	NH1-CZ-NH2	6.05	126.06	119.40
3	l	415	TYR	CB-CG-CD2	-6.05	117.37	121.00
3	l	872	TYR	CA-CB-CG	6.05	124.90	113.40
6	o	19	TYR	CG-CD1-CE1	-6.05	116.46	121.30
6	d	259	ARG	N-CA-CB	6.05	121.49	110.60
8	f	432	TYR	CB-CG-CD2	6.05	124.63	121.00
5	c	273	VAL	CA-CB-CG2	-6.05	101.83	110.90
9	g	175	TYR	CB-CG-CD1	6.05	124.63	121.00
4	b	329	ARG	NE-CZ-NH2	-6.05	117.28	120.30
5	c	271	TRP	CG-CD2-CE3	-6.05	128.46	133.90
4	m	357	PHE	CZ-CE2-CD2	-6.05	112.84	120.10
6	d	75	TYR	CB-CG-CD1	-6.04	117.37	121.00
8	f	702	TYR	CB-CG-CD1	-6.04	117.38	121.00
8	f	644	ALA	N-CA-CB	6.04	118.56	110.10
3	l	581	VAL	CA-CB-CG2	-6.03	101.85	110.90
4	m	590	VAL	CA-CB-CG1	-6.03	101.85	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	434	PHE	CB-CG-CD1	-6.03	116.58	120.80
3	l	75	ARG	C-N-CA	6.03	136.77	121.70
8	q	403	SER	N-CA-CB	6.03	119.55	110.50
4	m	305	GLU	OE1-CD-OE2	-6.03	116.06	123.30
3	a	990	ASP	CB-CG-OD2	-6.03	112.88	118.30
9	r	1086	ASP	CB-CG-OD2	-6.03	112.88	118.30
8	f	535	ARG	NH1-CZ-NH2	-6.02	112.77	119.40
5	c	645	TYR	CB-CG-CD1	-6.02	117.39	121.00
9	r	810	ASP	CB-CG-OD2	-6.02	112.88	118.30
3	a	468	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	X	1432	ARG	NE-CZ-NH2	6.02	123.31	120.30
3	a	659	TYR	CB-CG-CD2	6.02	124.61	121.00
3	l	511	ARG	NH1-CZ-NH2	-6.02	112.78	119.40
9	r	715	LEU	C-N-CA	6.02	136.75	121.70
1	X	182	PHE	CB-CG-CD2	-6.02	116.59	120.80
5	n	475	PHE	CB-CG-CD1	-6.02	116.59	120.80
8	f	136	PRO	O-C-N	-6.01	113.08	122.70
8	q	702	TYR	CG-CD1-CE1	-6.01	116.49	121.30
3	a	847	LYS	N-CA-CB	6.01	121.41	110.60
4	m	57	PRO	N-CD-CG	6.01	112.21	103.20
7	p	226	ARG	NE-CZ-NH2	6.01	123.30	120.30
3	l	834	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	a	808	TRP	CE2-CD2-CG	-6.00	102.50	107.30
4	b	725	ALA	N-CA-CB	6.00	118.50	110.10
3	a	958	TRP	CD1-NE1-CE2	6.00	114.40	109.00
1	X	775	PHE	CB-CG-CD1	-6.00	116.60	120.80
4	b	216	ASP	CB-CG-OD2	-5.99	112.91	118.30
3	a	203	SER	N-CA-CB	5.98	119.47	110.50
3	l	526	ARG	NE-CZ-NH2	-5.98	117.31	120.30
9	r	207	LYS	CB-CA-C	-5.98	98.44	110.40
1	X	1392	PHE	CB-CG-CD1	-5.98	116.62	120.80
3	a	551	THR	CA-CB-CG2	-5.97	104.04	112.40
3	a	990	ASP	CB-CG-OD1	5.97	123.67	118.30
3	a	529	SER	N-CA-CB	5.97	119.46	110.50
9	g	697	ASP	CB-CG-OD1	5.97	123.67	118.30
6	o	33	ILE	CA-CB-CG1	5.97	122.34	111.00
4	m	220	ASP	N-CA-CB	5.97	121.34	110.60
9	r	276	LEU	N-CA-CB	5.97	122.33	110.40
3	a	872	TYR	CB-CG-CD1	-5.96	117.42	121.00
4	b	214	ARG	O-C-N	-5.96	113.16	122.70
3	l	746	CYS	CB-CA-C	-5.96	98.48	110.40
3	l	749	TYR	CA-CB-CG	-5.96	102.08	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	252	PHE	N-CA-CB	5.96	121.33	110.60
9	g	174	TYR	CG-CD1-CE1	5.96	126.07	121.30
9	g	175	TYR	CB-CG-CD2	-5.96	117.43	121.00
8	f	662	PHE	CB-CG-CD1	-5.96	116.63	120.80
1	X	654	ILE	O-C-N	-5.95	113.17	122.70
3	l	24	VAL	CA-CB-CG1	5.95	119.83	110.90
1	X	617	TYR	CB-CG-CD2	5.95	124.57	121.00
9	r	368	PHE	N-CA-CB	5.95	121.31	110.60
9	g	841	LYS	N-CA-CB	5.95	121.31	110.60
7	p	221	ALA	N-CA-CB	5.94	118.42	110.10
5	c	560	LEU	CA-CB-CG	5.94	128.97	115.30
7	p	119	ALA	CB-CA-C	-5.94	101.19	110.10
1	X	1597	ARG	NH1-CZ-NH2	5.94	125.94	119.40
3	a	727	TYR	N-CA-CB	5.94	121.29	110.60
6	o	173	PHE	CB-CG-CD2	-5.94	116.64	120.80
9	r	839	PHE	CD1-CE1-CZ	-5.93	112.98	120.10
7	e	177	ARG	NE-CZ-NH2	-5.93	117.33	120.30
9	g	822	ASP	CB-CG-OD1	5.93	123.64	118.30
1	X	262	SER	C-N-CA	5.93	136.52	121.70
8	q	147	SER	N-CA-CB	5.93	119.40	110.50
3	l	709	VAL	CA-CB-CG2	-5.93	102.01	110.90
4	m	52	THR	CA-CB-CG2	-5.93	104.10	112.40
8	q	575	GLU	CA-CB-CG	-5.93	100.36	113.40
9	r	945	ARG	NE-CZ-NH1	5.93	123.26	120.30
9	g	559	VAL	CA-CB-CG2	-5.92	102.01	110.90
9	r	239	LYS	N-CA-CB	5.92	121.26	110.60
1	X	1280	LEU	CB-CG-CD1	5.92	121.06	111.00
4	b	55	ASP	N-CA-CB	5.92	121.25	110.60
4	m	699	TRP	CA-CB-CG	5.92	124.95	113.70
9	g	656	VAL	N-CA-C	-5.92	95.02	111.00
9	g	722	PHE	CB-CG-CD2	5.92	124.94	120.80
5	n	278	PRO	N-CA-CB	5.92	110.40	103.30
8	f	720	ARG	NE-CZ-NH2	-5.91	117.34	120.30
9	g	96	TYR	N-CA-CB	5.91	121.24	110.60
9	g	420	PHE	CB-CG-CD2	5.91	124.94	120.80
3	a	819	TYR	CA-CB-CG	-5.91	102.17	113.40
9	r	515	ASN	N-CA-CB	5.91	121.24	110.60
1	X	761	PHE	CB-CG-CD1	-5.91	116.66	120.80
3	l	721	MET	CG-SD-CE	-5.91	90.75	100.20
5	n	635	ASP	CB-CG-OD1	5.91	123.62	118.30
9	r	808	TYR	CD1-CE1-CZ	-5.91	114.48	119.80
8	f	686	GLU	N-CA-CB	5.91	121.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	156	TYR	CG-CD1-CE1	-5.91	116.58	121.30
4	m	363	TYR	CB-CG-CD1	-5.91	117.46	121.00
5	c	242	ASP	N-CA-C	-5.90	95.06	111.00
1	X	1170	ASP	CB-CG-OD2	-5.90	112.99	118.30
4	b	389	ASP	CB-CG-OD2	-5.90	112.99	118.30
8	f	290	LEU	CB-CG-CD1	5.90	121.03	111.00
9	g	1007	SER	N-CA-CB	5.90	119.35	110.50
3	l	954	ARG	NE-CZ-NH1	5.90	123.25	120.30
9	r	168	LYS	CB-CA-C	-5.90	98.61	110.40
7	p	189	GLU	N-CA-CB	5.90	121.21	110.60
1	X	352	PHE	CB-CG-CD1	-5.89	116.68	120.80
1	X	1172	SER	CA-C-O	-5.89	107.73	120.10
8	q	636	VAL	CA-CB-CG2	5.89	119.74	110.90
3	l	749	TYR	CB-CG-CD1	5.89	124.53	121.00
5	c	608	ASP	CB-CG-OD1	5.89	123.60	118.30
3	a	975	ARG	NE-CZ-NH2	-5.89	117.36	120.30
5	c	159	LEU	CB-CA-C	-5.88	99.02	110.20
5	c	329	ASP	N-CA-C	-5.88	95.11	111.00
9	r	73	GLN	CB-CA-C	-5.88	98.63	110.40
8	f	387	ARG	NH1-CZ-NH2	5.88	125.87	119.40
9	g	503	TYR	CB-CG-CD1	-5.88	117.47	121.00
4	m	331	TYR	CB-CG-CD1	-5.88	117.47	121.00
3	a	153	GLN	N-CA-CB	5.88	121.18	110.60
9	g	1114	TYR	CB-CG-CD1	5.87	124.52	121.00
3	l	969	MET	CG-SD-CE	-5.87	90.80	100.20
1	X	1036	ASP	CB-CG-OD1	5.87	123.58	118.30
5	c	435	TYR	CZ-CE2-CD2	5.87	125.08	119.80
3	a	659	TYR	CB-CG-CD1	-5.87	117.48	121.00
3	l	77	THR	CA-CB-CG2	-5.87	104.19	112.40
9	g	807	PHE	CZ-CE2-CD2	-5.87	113.06	120.10
3	a	715	THR	N-CA-C	-5.87	95.16	111.00
8	q	612	ASN	N-CA-CB	5.86	121.16	110.60
7	e	196	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	X	398	ARG	NE-CZ-NH1	5.86	123.23	120.30
5	c	387	LEU	CB-CG-CD2	5.86	120.96	111.00
9	r	253	LYS	CB-CA-C	-5.86	98.69	110.40
9	r	278	LYS	N-CA-CB	5.86	121.14	110.60
3	a	741	LEU	CB-CG-CD2	5.85	120.94	111.00
9	r	709	PHE	CZ-CE2-CD2	-5.85	113.08	120.10
1	X	936	LEU	CB-CG-CD2	-5.85	101.06	111.00
9	g	624	THR	CA-CB-CG2	-5.85	104.21	112.40
3	a	209	THR	CA-CB-CG2	-5.84	104.22	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	117	TYR	CD1-CE1-CZ	5.84	125.06	119.80
3	a	946	ASP	CB-CG-OD2	5.84	123.56	118.30
4	b	571	TYR	CD1-CE1-CZ	5.84	125.06	119.80
3	a	582	VAL	O-C-N	-5.84	113.35	122.70
4	b	647	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	a	539	GLU	OE1-CD-OE2	5.84	130.31	123.30
3	a	958	TRP	CG-CD1-NE1	-5.84	104.26	110.10
3	l	537	THR	CA-CB-OG1	5.84	121.25	109.00
5	n	253	ASP	CB-CG-OD2	5.84	123.55	118.30
8	q	623	PHE	CG-CD1-CE1	-5.84	114.38	120.80
8	q	645	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	X	753	TYR	CA-CB-CG	5.83	124.48	113.40
1	X	1598	LEU	CB-CG-CD1	-5.83	101.08	111.00
4	b	588	ASP	CB-CG-OD1	5.83	123.55	118.30
8	q	542	ARG	NE-CZ-NH1	-5.83	117.39	120.30
8	f	160	PHE	CB-CG-CD1	5.83	124.88	120.80
6	o	259	ARG	NE-CZ-NH2	5.83	123.21	120.30
8	q	637	ASP	N-CA-CB	5.83	121.09	110.60
1	X	1566	TYR	N-CA-CB	5.83	121.09	110.60
3	a	220	TYR	CB-CG-CD2	5.82	124.49	121.00
1	X	1313	ARG	NE-CZ-NH2	5.82	123.21	120.30
4	b	63	ASP	CB-CG-OD1	5.82	123.54	118.30
9	r	437	TYR	CB-CA-C	-5.82	98.77	110.40
3	a	251	PHE	CG-CD2-CE2	-5.81	114.41	120.80
4	b	91	TYR	CB-CG-CD1	5.81	124.49	121.00
4	b	628	ALA	N-CA-CB	5.81	118.24	110.10
3	a	1014	TYR	CG-CD2-CE2	5.81	125.95	121.30
9	g	608	ASP	CB-CA-C	-5.81	98.78	110.40
3	a	976	ALA	N-CA-CB	5.81	118.23	110.10
8	f	702	TYR	CB-CG-CD2	-5.81	117.52	121.00
7	e	149	THR	CA-CB-CG2	-5.81	104.27	112.40
3	l	958	TRP	CE2-CD2-CG	-5.81	102.66	107.30
5	c	153	PHE	CG-CD1-CE1	5.80	127.18	120.80
4	m	517	ASP	CB-CG-OD1	5.80	123.52	118.30
5	c	295	PHE	CB-CG-CD2	5.80	124.86	120.80
9	r	289	LYS	N-CA-CB	5.80	121.04	110.60
9	r	649	PHE	CG-CD2-CE2	5.80	127.18	120.80
9	g	843	PHE	CB-CG-CD1	-5.80	116.74	120.80
4	m	193	ASP	N-CA-CB	5.80	121.03	110.60
1	X	876	LEU	CB-CG-CD1	5.79	120.85	111.00
4	m	179	LEU	CB-CG-CD1	5.79	120.85	111.00
1	X	407	ALA	N-CA-CB	5.79	118.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	461	SER	N-CA-CB	5.79	119.19	110.50
9	g	393	THR	CA-CB-CG2	-5.79	104.30	112.40
4	m	511	TYR	CG-CD1-CE1	-5.79	116.67	121.30
8	q	507	ASP	CB-CG-OD2	5.79	123.51	118.30
9	g	503	TYR	CG-CD2-CE2	-5.79	116.67	121.30
9	g	738	TYR	N-CA-CB	-5.79	100.19	110.60
4	m	99	ASP	N-CA-C	-5.78	95.39	111.00
6	o	60	ASP	CB-CG-OD2	-5.78	113.10	118.30
8	q	580	PHE	CB-CG-CD2	-5.78	116.75	120.80
6	o	112	TYR	CB-CA-C	-5.77	98.86	110.40
3	a	916	ARG	NE-CZ-NH2	-5.77	117.42	120.30
9	r	254	LEU	CB-CA-C	-5.77	99.24	110.20
6	o	215	THR	CA-CB-CG2	-5.77	104.33	112.40
4	m	616	VAL	CA-CB-CG2	-5.76	102.25	110.90
9	g	725	PHE	CB-CG-CD2	5.76	124.83	120.80
9	g	419	MET	N-CA-CB	5.76	120.97	110.60
6	o	20	TYR	CZ-CE2-CD2	5.76	124.98	119.80
7	p	22	ARG	NH1-CZ-NH2	5.76	125.73	119.40
3	a	270	PHE	CB-CG-CD1	5.76	124.83	120.80
4	b	546	MET	CG-SD-CE	-5.76	90.99	100.20
9	g	898	ASP	CB-CG-OD1	5.76	123.48	118.30
3	a	312	THR	CA-CB-CG2	-5.75	104.34	112.40
3	a	497	MET	CG-SD-CE	-5.75	90.99	100.20
3	a	560	ASN	N-CA-CB	5.75	120.96	110.60
8	f	334	ARG	NE-CZ-NH1	5.75	123.18	120.30
8	q	378	ASP	CB-CG-OD2	-5.75	113.12	118.30
9	r	326	PHE	CB-CA-C	-5.75	98.90	110.40
5	n	642	LYS	N-CA-CB	5.75	120.95	110.60
9	g	452	ASP	CB-CA-C	5.75	121.89	110.40
5	c	539	PHE	CB-CG-CD2	-5.74	116.78	120.80
3	a	325	ALA	N-CA-CB	5.74	118.14	110.10
9	g	311	ASN	N-CA-CB	5.74	120.93	110.60
1	X	713	LYS	N-CA-CB	5.74	120.93	110.60
6	d	255	ASP	CB-CG-OD2	5.74	123.47	118.30
9	g	923	HIS	CA-CB-CG	5.74	123.36	113.60
3	l	416	GLY	CA-C-N	-5.74	104.57	117.20
7	p	97	ARG	NE-CZ-NH2	-5.74	117.43	120.30
4	b	675	PHE	CB-CG-CD2	-5.74	116.78	120.80
7	p	135	ARG	NE-CZ-NH2	-5.74	117.43	120.30
7	e	190	GLN	N-CA-CB	5.74	120.92	110.60
3	l	774	TYR	CB-CG-CD1	-5.74	117.56	121.00
4	m	609	GLN	CG-CD-OE1	-5.73	110.13	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	100	THR	CA-CB-CG2	-5.73	104.37	112.40
5	c	552	TYR	CG-CD2-CE2	-5.73	116.72	121.30
5	n	379	PHE	CB-CG-CD1	5.73	124.81	120.80
9	r	143	PRO	N-CA-CB	5.73	110.18	103.30
9	r	248	LEU	N-CA-CB	5.73	121.86	110.40
5	c	765	GLU	N-CA-CB	5.73	120.91	110.60
6	o	214	PRO	N-CD-CG	5.73	111.80	103.20
3	a	377	GLU	OE1-CD-OE2	5.73	130.17	123.30
3	l	754	GLU	OE1-CD-OE2	5.73	130.17	123.30
4	m	363	TYR	CB-CG-CD2	5.73	124.44	121.00
3	a	259	MET	CA-CB-CG	5.72	123.03	113.30
1	X	134	ARG	NE-CZ-NH1	5.72	123.16	120.30
3	a	623	LEU	CB-CA-C	-5.72	99.33	110.20
9	r	845	PHE	CB-CG-CD1	-5.72	116.80	120.80
7	e	171	LEU	CB-CG-CD2	5.72	120.72	111.00
9	g	545	TYR	CB-CG-CD1	-5.72	117.57	121.00
3	l	688	PHE	CZ-CE2-CD2	5.72	126.96	120.10
9	g	691	TYR	CD1-CE1-CZ	-5.71	114.66	119.80
4	b	216	ASP	N-CA-CB	5.71	120.88	110.60
4	b	505	ALA	CB-CA-C	-5.71	101.53	110.10
8	f	122	VAL	CA-CB-CG2	-5.71	102.33	110.90
6	d	66	PHE	CB-CG-CD2	-5.71	116.80	120.80
7	p	329	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
1	X	352	PHE	CB-CG-CD2	5.71	124.80	120.80
1	X	1083	ALA	N-CA-CB	5.71	118.09	110.10
9	r	397	PRO	CA-N-CD	-5.71	103.51	111.50
8	f	157	ASP	CB-CG-OD2	-5.71	113.17	118.30
9	g	327	ALA	O-C-N	-5.71	113.57	122.70
6	o	90	SER	N-CA-CB	5.71	119.06	110.50
9	g	274	PRO	N-CA-CB	5.71	110.15	103.30
9	r	86	LEU	N-CA-CB	5.70	121.81	110.40
9	r	582	GLU	CB-CA-C	-5.70	99.00	110.40
7	e	96	ARG	NE-CZ-NH2	-5.70	117.45	120.30
5	n	231	TYR	CZ-CE2-CD2	5.70	124.93	119.80
6	o	216	VAL	CG1-CB-CG2	5.70	120.01	110.90
1	X	1425	TYR	CB-CG-CD2	5.69	124.42	121.00
3	l	597	TRP	CB-CG-CD2	-5.69	119.20	126.60
9	r	1094	TYR	CB-CG-CD1	-5.69	117.58	121.00
1	X	1622	GLU	OE1-CD-OE2	5.69	130.13	123.30
9	r	939	LEU	CB-CG-CD2	-5.69	101.33	111.00
5	n	462	THR	CA-CB-CG2	-5.68	104.44	112.40
7	p	243	PHE	CB-CG-CD1	-5.68	116.82	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	639	ARG	CB-CG-CD	5.68	126.37	111.60
3	a	346	ALA	N-CA-CB	5.68	118.05	110.10
3	a	864	PHE	CB-CG-CD2	5.68	124.77	120.80
5	c	302	ASP	N-CA-C	-5.68	95.67	111.00
8	f	230	GLU	N-CA-CB	5.68	120.82	110.60
9	g	577	TYR	CZ-CE2-CD2	-5.68	114.69	119.80
9	r	649	PHE	CZ-CE2-CD2	-5.68	113.29	120.10
3	a	748	PHE	CB-CG-CD1	-5.67	116.83	120.80
5	c	604	ASP	CB-CG-OD1	5.67	123.41	118.30
7	p	239	ARG	NH1-CZ-NH2	5.67	125.64	119.40
9	r	303	HIS	N-CA-CB	5.67	120.81	110.60
4	m	107	TYR	CZ-CE2-CD2	5.67	124.91	119.80
9	r	491	VAL	CA-CB-CG2	-5.67	102.39	110.90
3	l	396	ASP	N-CA-CB	5.67	120.81	110.60
8	q	578	ASP	O-C-N	-5.67	113.63	122.70
5	c	435	TYR	CG-CD2-CE2	-5.67	116.77	121.30
9	g	232	THR	CA-CB-CG2	-5.67	104.46	112.40
1	X	1596	LYS	CB-CA-C	-5.67	99.07	110.40
4	b	189	TYR	CB-CG-CD1	-5.67	117.60	121.00
8	f	654	GLU	N-CA-CB	5.67	120.80	110.60
8	q	106	GLU	OE1-CD-OE2	5.67	130.10	123.30
8	f	323	THR	N-CA-C	-5.66	95.71	111.00
3	l	1012	SER	N-CA-CB	5.66	119.00	110.50
6	o	210	VAL	CA-CB-CG1	-5.66	102.40	110.90
4	b	686	ASP	CB-CG-OD1	5.66	123.40	118.30
9	g	514	PHE	CB-CG-CD2	-5.66	116.84	120.80
9	g	440	ARG	NE-CZ-NH2	5.66	123.13	120.30
4	m	697	THR	CA-CB-CG2	-5.66	104.48	112.40
9	g	284	TYR	CB-CG-CD1	-5.65	117.61	121.00
9	g	361	TYR	CG-CD1-CE1	-5.65	116.78	121.30
3	l	546	THR	CA-CB-CG2	-5.65	104.49	112.40
8	f	469	ARG	NE-CZ-NH1	5.65	123.12	120.30
3	l	585	ASP	CB-CG-OD1	5.65	123.38	118.30
5	n	254	GLN	N-CA-CB	5.64	120.76	110.60
8	q	587	TYR	CG-CD2-CE2	-5.64	116.79	121.30
9	r	247	LEU	CB-CA-C	-5.64	99.48	110.20
1	X	1164	ASP	CB-CG-OD1	5.64	123.37	118.30
1	X	944	GLN	N-CA-CB	5.64	120.75	110.60
5	c	459	PHE	CB-CG-CD1	5.64	124.75	120.80
9	r	123	PRO	N-CA-CB	5.64	110.06	103.30
8	q	706	GLN	N-CA-CB	5.63	120.74	110.60
6	d	173	PHE	CB-CG-CD2	-5.63	116.86	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	o	43	HIS	N-CA-CB	5.63	120.73	110.60
8	f	516	TRP	CD2-CE2-CZ2	-5.63	115.55	122.30
7	p	78	ASP	CB-CG-OD2	-5.63	113.23	118.30
8	q	599	GLU	OE1-CD-OE2	-5.63	116.55	123.30
4	m	353	TRP	NE1-CE2-CD2	5.63	112.93	107.30
6	o	142	ASP	N-CA-CB	5.63	120.73	110.60
9	g	648	GLN	N-CA-CB	5.62	120.72	110.60
4	b	385	ASP	CB-CG-OD2	-5.62	113.24	118.30
8	f	282	TRP	O-C-N	-5.62	113.70	122.70
9	r	1114	TYR	CG-CD1-CE1	-5.62	116.80	121.30
5	c	149	THR	CA-CB-CG2	-5.62	104.53	112.40
3	l	337	THR	CA-CB-CG2	-5.62	104.53	112.40
9	g	1043	ARG	CD-NE-CZ	5.62	131.47	123.60
3	a	65	SER	N-CA-CB	5.62	118.93	110.50
3	l	878	HIS	CA-CB-CG	-5.62	104.05	113.60
4	m	629	VAL	N-CA-C	-5.62	95.83	111.00
9	r	151	LEU	N-CA-CB	5.62	121.64	110.40
1	X	926	ALA	N-CA-CB	5.62	117.96	110.10
5	c	414	TYR	CZ-CE2-CD2	5.62	124.85	119.80
6	o	32	THR	CA-CB-CG2	-5.62	104.54	112.40
1	X	1045	ALA	N-CA-CB	5.61	117.96	110.10
6	o	194	TYR	CB-CG-CD1	5.61	124.37	121.00
6	o	56	VAL	CG1-CB-CG2	5.61	119.87	110.90
8	q	168	VAL	CA-CB-CG1	-5.61	102.49	110.90
5	c	233	LEU	CB-CG-CD2	5.61	120.53	111.00
4	b	190	PHE	CB-CG-CD2	-5.60	116.88	120.80
3	l	764	LEU	CB-CG-CD1	-5.60	101.47	111.00
3	a	252	THR	CA-CB-CG2	-5.60	104.56	112.40
3	a	72	PHE	CB-CG-CD2	-5.60	116.88	120.80
5	n	246	TYR	CB-CG-CD1	-5.60	117.64	121.00
9	g	279	GLY	O-C-N	5.60	131.66	122.70
9	r	550	LEU	CB-CA-C	-5.60	99.56	110.20
9	r	691	TYR	CD1-CG-CD2	5.60	124.06	117.90
4	b	539	TYR	CB-CG-CD1	-5.60	117.64	121.00
9	g	519	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	X	867	ASP	CB-CG-OD1	-5.59	113.27	118.30
3	a	997	ARG	NE-CZ-NH2	-5.59	117.50	120.30
8	q	204	ASP	CB-CG-OD2	-5.59	113.26	118.30
3	l	956	GLY	N-CA-C	-5.59	99.12	113.10
1	X	433	PRO	N-CA-CB	5.59	110.01	103.30
4	m	189	TYR	CD1-CE1-CZ	5.59	124.83	119.80
8	q	576	ASN	CA-CB-CG	-5.59	101.10	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	906	TYR	CB-CG-CD2	-5.59	117.65	121.00
3	a	840	PHE	CB-CG-CD2	5.59	124.71	120.80
4	b	186	ARG	NE-CZ-NH2	-5.59	117.51	120.30
4	b	239	VAL	CG1-CB-CG2	5.59	119.84	110.90
4	m	549	ALA	CB-CA-C	-5.59	101.72	110.10
1	X	682	LEU	N-CA-CB	5.58	121.57	110.40
8	f	562	TYR	CB-CG-CD2	5.58	124.35	121.00
4	b	81	PHE	CB-CG-CD2	5.58	124.71	120.80
4	b	627	TYR	CB-CG-CD2	-5.58	117.65	121.00
4	m	664	VAL	CA-CB-CG1	5.58	119.27	110.90
1	X	1339	PHE	CB-CG-CD1	5.58	124.70	120.80
5	n	158	MET	CG-SD-CE	-5.58	91.27	100.20
3	a	192	VAL	CA-CB-CG2	-5.58	102.53	110.90
9	g	644	VAL	CA-CB-CG2	-5.58	102.54	110.90
5	c	475	PHE	CB-CG-CD1	5.57	124.70	120.80
8	q	355	LEU	CB-CG-CD2	5.57	120.47	111.00
3	l	961	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	X	871	SER	N-CA-CB	5.57	118.85	110.50
3	a	933	GLY	N-CA-C	-5.57	99.18	113.10
4	b	722	SER	N-CA-CB	5.57	118.85	110.50
8	f	384	TYR	CG-CD1-CE1	-5.57	116.84	121.30
5	n	563	SER	N-CA-CB	5.57	118.85	110.50
7	p	239	ARG	NE-CZ-NH1	-5.57	117.52	120.30
4	b	511	TYR	CG-CD1-CE1	-5.56	116.85	121.30
8	f	444	ALA	CB-CA-C	-5.56	101.75	110.10
7	e	322	ALA	N-CA-CB	5.56	117.89	110.10
8	q	458	ARG	NE-CZ-NH2	-5.56	117.52	120.30
9	r	153	LEU	N-CA-CB	5.56	121.53	110.40
9	r	822	ASP	CB-CG-OD2	-5.56	113.29	118.30
7	e	10	ASP	CB-CG-OD1	-5.56	113.30	118.30
9	g	350	SER	CB-CA-C	5.56	120.66	110.10
4	m	366	PRO	N-CA-CB	5.56	109.97	103.30
8	q	42	PHE	N-CA-CB	5.56	120.61	110.60
3	a	121	VAL	CA-CB-CG2	5.56	119.23	110.90
5	c	650	HIS	CA-CB-CG	5.56	123.05	113.60
9	g	713	ASP	CB-CG-OD2	-5.56	113.30	118.30
3	l	760	PHE	CB-CG-CD1	-5.56	116.91	120.80
7	e	37	LYS	N-CA-CB	5.55	120.59	110.60
9	g	1150	TYR	CB-CG-CD2	5.55	124.33	121.00
1	X	1020	ILE	CA-CB-CG1	5.55	121.54	111.00
4	m	189	TYR	CB-CG-CD1	-5.55	117.67	121.00
4	b	69	PHE	CB-CG-CD2	-5.55	116.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	968	ARG	NE-CZ-NH2	-5.55	117.53	120.30
3	a	526	ARG	NE-CZ-NH1	5.54	123.07	120.30
6	o	275	ASP	CB-CG-OD1	5.54	123.29	118.30
9	r	151	LEU	CB-CA-C	-5.54	99.67	110.20
3	l	628	ARG	NE-CZ-NH1	5.54	123.07	120.30
5	n	611	SER	N-CA-CB	5.54	118.81	110.50
4	m	91	TYR	CZ-CE2-CD2	-5.54	114.82	119.80
9	r	433	LEU	N-CA-CB	5.54	121.48	110.40
1	X	1422	LEU	CB-CG-CD2	5.54	120.41	111.00
5	c	452	TYR	CB-CG-CD1	5.54	124.32	121.00
9	g	67	TYR	N-CA-CB	5.54	120.56	110.60
8	q	149	THR	CA-CB-CG2	-5.53	104.65	112.40
8	f	327	VAL	CG1-CB-CG2	5.53	119.74	110.90
9	g	999	LEU	CB-CA-C	-5.53	99.70	110.20
3	l	165	PHE	CB-CG-CD1	-5.53	116.93	120.80
9	r	253	LYS	N-CA-CB	5.53	120.55	110.60
1	X	330	TYR	CB-CG-CD2	-5.53	117.68	121.00
4	b	670	PHE	CB-CG-CD1	5.53	124.67	120.80
5	c	416	ASP	CB-CG-OD1	-5.53	113.33	118.30
9	r	716	ASN	N-CA-CB	5.52	120.54	110.60
9	g	808	TYR	CG-CD1-CE1	-5.52	116.89	121.30
1	X	1082	PHE	CD1-CG-CD2	-5.52	111.13	118.30
1	X	1308	TYR	CG-CD2-CE2	5.51	125.71	121.30
9	g	1011	ASP	CA-CB-CG	5.51	125.53	113.40
1	X	1446	PHE	CG-CD2-CE2	-5.51	114.73	120.80
9	g	477	PHE	CB-CG-CD2	-5.51	116.94	120.80
4	m	545	GLN	CG-CD-OE1	-5.51	110.58	121.60
3	a	982	TYR	CG-CD1-CE1	5.50	125.70	121.30
3	a	678	VAL	CA-CB-CG1	-5.50	102.65	110.90
3	l	793	PHE	CB-CG-CD1	5.50	124.65	120.80
8	q	587	TYR	CB-CG-CD1	-5.50	117.70	121.00
9	r	433	LEU	CB-CA-C	-5.50	99.75	110.20
1	X	1199	TYR	CB-CG-CD2	-5.50	117.70	121.00
9	g	570	PHE	CB-CG-CD2	5.50	124.65	120.80
7	p	55	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	X	1060	LEU	N-CA-C	-5.50	96.16	111.00
4	b	694	VAL	CA-CB-CG2	5.50	119.15	110.90
3	l	451	ARG	NE-CZ-NH1	-5.50	117.55	120.30
6	o	105	VAL	CB-CA-C	5.50	121.84	111.40
3	l	880	ARG	C-N-CA	5.49	135.43	121.70
5	c	513	ARG	NE-CZ-NH2	-5.49	117.56	120.30
9	r	546	ILE	N-CA-CB	5.49	123.43	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	267	ARG	C-N-CA	5.49	135.42	121.70
6	d	75	TYR	CB-CG-CD2	5.49	124.29	121.00
9	g	362	ILE	N-CA-C	-5.49	96.19	111.00
8	q	649	TYR	CB-CG-CD1	5.49	124.29	121.00
8	q	552	ARG	NE-CZ-NH1	5.48	123.04	120.30
9	r	289	LYS	CB-CA-C	-5.48	99.43	110.40
5	c	174	ARG	O-C-N	5.48	131.47	122.70
9	g	636	ILE	CB-CA-C	5.48	122.56	111.60
1	X	668	TYR	CB-CG-CD2	-5.48	117.71	121.00
9	g	252	PHE	CG-CD2-CE2	5.48	126.83	120.80
3	l	439	ASP	CB-CG-OD2	-5.48	113.37	118.30
3	l	102	MET	CG-SD-CE	-5.48	91.43	100.20
3	a	14	TYR	CB-CG-CD1	5.48	124.28	121.00
8	f	653	TYR	CZ-CE2-CD2	5.48	124.73	119.80
7	p	322	ALA	N-CA-CB	5.48	117.77	110.10
5	c	370	PHE	CG-CD2-CE2	-5.47	114.78	120.80
9	g	83	ASP	N-CA-CB	5.47	120.45	110.60
9	g	742	LEU	O-C-N	5.47	131.46	122.70
9	r	153	LEU	CB-CA-C	-5.47	99.80	110.20
3	a	590	GLN	N-CA-CB	5.47	120.45	110.60
4	b	691	VAL	CG1-CB-CG2	5.47	119.66	110.90
4	m	162	VAL	CA-CB-CG2	-5.47	102.69	110.90
7	p	196	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	X	294	THR	CA-CB-CG2	-5.47	104.74	112.40
9	g	256	ILE	CA-CB-CG2	-5.47	99.96	110.90
3	l	520	LEU	O-C-N	5.47	131.45	122.70
3	l	448	THR	CA-CB-CG2	-5.47	104.75	112.40
3	l	452	ASP	CB-CG-OD1	5.47	123.22	118.30
3	l	715	THR	N-CA-CB	5.47	120.69	110.30
5	c	551	ASN	CB-CA-C	5.46	121.33	110.40
6	d	18	ASP	CB-CG-OD1	5.46	123.22	118.30
3	l	256	ASP	CB-CG-OD2	-5.46	113.38	118.30
9	r	247	LEU	N-CA-CB	5.46	121.32	110.40
3	a	796	ASP	CB-CG-OD2	-5.46	113.39	118.30
3	a	825	TYR	CB-CG-CD1	5.46	124.28	121.00
9	r	949	TYR	CB-CG-CD1	5.46	124.28	121.00
7	p	148	TRP	CB-CG-CD1	-5.46	119.91	127.00
3	a	440	GLU	OE1-CD-OE2	5.46	129.85	123.30
3	l	460	ALA	N-CA-CB	5.45	117.73	110.10
7	e	49	ASP	CB-CA-C	-5.45	99.50	110.40
6	d	220	SER	N-CA-CB	5.45	118.67	110.50
3	a	1029	ASP	CB-CG-OD1	-5.45	113.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	339	LEU	CB-CA-C	-5.45	99.85	110.20
3	l	376	TYR	CD1-CE1-CZ	5.45	124.70	119.80
3	a	695	TYR	CB-CG-CD1	5.45	124.27	121.00
7	e	42	THR	CA-CB-OG1	5.45	120.44	109.00
4	m	552	ILE	C-N-CA	5.45	135.31	121.70
7	p	151	THR	O-C-N	-5.45	113.99	122.70
9	r	168	LYS	N-CA-CB	5.45	120.40	110.60
7	e	105	ASN	N-CA-C	-5.44	96.30	111.00
3	l	360	ALA	N-CA-CB	5.44	117.72	110.10
3	l	14	TYR	N-CA-CB	5.44	120.39	110.60
3	l	511	ARG	NE-CZ-NH2	-5.44	117.58	120.30
4	b	530	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
9	g	536	GLU	OE1-CD-OE2	-5.43	116.78	123.30
9	r	278	LYS	CB-CA-C	-5.43	99.53	110.40
7	p	241	ARG	NE-CZ-NH1	5.43	123.02	120.30
3	l	748	PHE	CB-CG-CD2	-5.43	117.00	120.80
5	n	142	ARG	NE-CZ-NH1	5.43	123.01	120.30
8	q	699	ASP	CB-CG-OD2	-5.43	113.41	118.30
7	e	22	ARG	NE-CZ-NH1	5.43	123.01	120.30
4	m	686	ASP	N-CA-CB	5.43	120.37	110.60
1	X	725	LEU	N-CA-CB	5.42	121.25	110.40
4	m	158	PHE	CB-CG-CD2	-5.42	117.00	120.80
1	X	439	LEU	CB-CG-CD2	5.42	120.22	111.00
5	c	573	VAL	CA-CB-CG1	5.42	119.03	110.90
7	p	123	LEU	CB-CG-CD1	5.42	120.22	111.00
3	a	198	LEU	CB-CG-CD1	5.42	120.22	111.00
3	a	727	TYR	CB-CA-C	-5.42	99.56	110.40
8	f	653	TYR	CG-CD1-CE1	-5.42	116.96	121.30
5	n	492	PHE	CB-CG-CD1	5.42	124.59	120.80
1	X	265	PHE	CA-CB-CG	5.42	126.91	113.90
1	X	1060	LEU	CA-CB-CG	5.42	127.76	115.30
3	l	946	ASP	CB-CG-OD1	5.42	123.18	118.30
4	m	115	TYR	CA-CB-CG	5.42	123.69	113.40
1	X	1427	SER	N-CA-C	-5.42	96.38	111.00
4	b	306	TRP	CE2-CD2-CE3	5.42	125.20	118.70
8	f	315	LEU	N-CA-CB	5.42	121.23	110.40
8	f	507	ASP	O-C-N	5.42	131.37	122.70
4	m	169	VAL	CA-CB-CG1	-5.42	102.78	110.90
3	l	17	LYS	N-CA-C	-5.42	96.38	111.00
9	r	254	LEU	N-CA-CB	5.42	121.23	110.40
8	f	416	TYR	CG-CD2-CE2	-5.41	116.97	121.30
3	l	961	PHE	N-CA-CB	5.41	120.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	470	ALA	CB-CA-C	-5.41	101.98	110.10
5	c	491	LEU	CB-CG-CD2	5.41	120.20	111.00
3	l	912	ASP	CB-CG-OD1	-5.41	113.43	118.30
9	g	864	PHE	CB-CA-C	-5.41	99.58	110.40
1	X	1534	TYR	CB-CG-CD2	-5.41	117.76	121.00
4	b	742	ALA	N-CA-CB	5.41	117.67	110.10
3	l	769	ASN	CB-CG-OD1	-5.41	110.79	121.60
7	p	163	ASN	N-CA-CB	5.41	120.33	110.60
8	f	390	THR	CA-CB-CG2	-5.40	104.83	112.40
5	n	540	ASN	N-CA-CB	5.40	120.33	110.60
4	b	187	THR	CA-CB-CG2	-5.40	104.84	112.40
9	r	875	PHE	CB-CG-CD2	5.40	124.58	120.80
5	c	285	ARG	CG-CD-NE	-5.40	100.46	111.80
7	e	131	ASP	CB-CG-OD2	-5.40	113.44	118.30
9	g	443	TRP	CD1-CG-CD2	5.40	110.62	106.30
9	r	207	LYS	N-CA-CB	5.40	120.32	110.60
9	r	646	PHE	CB-CG-CD2	-5.40	117.02	120.80
6	d	131	LYS	CA-CB-CG	5.40	125.27	113.40
3	l	303	LEU	O-C-N	5.40	131.33	122.70
3	l	725	ARG	NE-CZ-NH1	5.40	123.00	120.30
8	f	233	THR	CA-CB-CG2	5.39	119.95	112.40
4	b	56	GLN	CG-CD-OE1	-5.39	110.82	121.60
4	m	420	THR	N-CA-CB	5.39	120.54	110.30
4	m	691	VAL	N-CA-C	-5.39	96.45	111.00
3	l	904	PHE	CB-CG-CD2	-5.38	117.03	120.80
8	f	653	TYR	CD1-CE1-CZ	5.38	124.64	119.80
5	n	181	ARG	NE-CZ-NH1	5.38	122.99	120.30
4	b	413	ASP	CB-CG-OD2	-5.38	113.46	118.30
4	b	635	GLU	OE1-CD-OE2	-5.38	116.85	123.30
9	g	513	ASP	CB-CG-OD1	-5.38	113.46	118.30
5	c	255	VAL	CA-CB-CG2	-5.38	102.83	110.90
5	n	221	LEU	N-CA-CB	5.38	121.15	110.40
6	o	194	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
8	q	267	LEU	CB-CG-CD2	-5.37	101.86	111.00
1	X	374	VAL	CA-CB-CG1	-5.37	102.84	110.90
3	a	10	ASN	N-CA-C	-5.37	96.50	111.00
8	q	157	ASP	N-CA-CB	5.37	120.27	110.60
4	b	647	ARG	CB-CA-C	-5.37	99.67	110.40
3	a	1010	PHE	CB-CG-CD2	5.37	124.56	120.80
4	b	88	TYR	CB-CG-CD2	-5.37	117.78	121.00
5	c	333	ARG	NE-CZ-NH1	5.36	122.98	120.30
9	g	845	PHE	CA-CB-CG	-5.36	101.03	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	142	SER	N-CA-CB	5.36	118.54	110.50
9	r	261	PHE	CB-CA-C	-5.36	99.67	110.40
3	a	936	TYR	CB-CG-CD1	5.36	124.22	121.00
9	r	1070	LEU	CB-CG-CD2	5.36	120.11	111.00
4	b	615	VAL	CG1-CB-CG2	5.36	119.47	110.90
4	m	631	SER	N-CA-CB	-5.36	102.47	110.50
4	m	633	PHE	CB-CG-CD2	-5.36	117.05	120.80
8	q	552	ARG	CG-CD-NE	-5.35	100.56	111.80
9	r	379	SER	CB-CA-C	-5.35	99.93	110.10
9	r	738	TYR	CB-CG-CD2	5.35	124.21	121.00
9	r	1046	VAL	CB-CA-C	5.35	121.57	111.40
7	e	178	PHE	CG-CD2-CE2	-5.35	114.92	120.80
6	o	206	TRP	CD1-CG-CD2	-5.35	102.02	106.30
8	f	266	TYR	CG-CD2-CE2	-5.35	117.02	121.30
9	g	600	PHE	CB-CG-CD2	-5.35	117.06	120.80
3	l	128	PHE	N-CA-C	-5.35	96.56	111.00
3	l	735	LYS	N-CA-CB	5.35	120.23	110.60
7	p	144	ASP	CB-CG-OD1	5.35	123.11	118.30
7	p	302	ASP	CB-CG-OD2	5.35	123.11	118.30
1	X	1308	TYR	CG-CD1-CE1	-5.34	117.03	121.30
1	X	323	TYR	C-N-CA	5.34	135.05	121.70
1	X	369	LEU	CB-CG-CD1	5.34	120.08	111.00
3	l	639	LEU	CB-CG-CD2	5.34	120.08	111.00
4	m	581	MET	N-CA-CB	5.34	120.21	110.60
6	o	269	LEU	CB-CG-CD2	-5.34	101.92	111.00
7	e	11	LEU	N-CA-CB	5.34	121.08	110.40
7	p	148	TRP	CE3-CZ3-CH2	-5.34	115.33	121.20
5	c	271	TRP	CE3-CZ3-CH2	5.34	127.07	121.20
3	l	879	PHE	CB-CG-CD1	5.34	124.54	120.80
5	n	250	THR	N-CA-CB	5.34	120.44	110.30
1	X	754	TYR	CG-CD1-CE1	-5.33	117.03	121.30
1	X	1213	THR	CA-CB-CG2	-5.33	104.93	112.40
9	g	836	PHE	CZ-CE2-CD2	-5.33	113.70	120.10
4	m	610	ASP	CB-CA-C	5.33	121.07	110.40
9	r	1066	PHE	CZ-CE2-CD2	-5.33	113.70	120.10
1	X	989	ASP	CB-CG-OD1	5.33	123.10	118.30
3	a	573	GLU	N-CA-CB	5.33	120.20	110.60
5	n	656	ALA	CB-CA-C	-5.33	102.10	110.10
1	X	327	PHE	CB-CG-CD1	5.33	124.53	120.80
7	e	98	TRP	CH2-CZ2-CE2	5.33	122.73	117.40
8	f	467	PHE	CB-CG-CD1	-5.33	117.07	120.80
4	m	712	THR	CA-CB-OG1	5.33	120.18	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	335	LEU	CB-CA-C	-5.32	100.08	110.20
3	l	597	TRP	CB-CG-CD1	5.32	133.92	127.00
5	c	306	ALA	CB-CA-C	-5.32	102.12	110.10
4	b	276	ASP	CB-CG-OD2	5.32	123.09	118.30
4	b	228	PHE	CB-CG-CD2	5.32	124.52	120.80
3	l	404	VAL	CA-CB-CG1	5.32	118.88	110.90
8	q	157	ASP	CB-CG-OD2	-5.32	113.52	118.30
4	b	331	TYR	CB-CA-C	-5.32	99.77	110.40
6	o	263	SER	CB-CA-C	-5.32	100.00	110.10
1	X	375	TYR	CG-CD2-CE2	5.31	125.55	121.30
3	l	56	TYR	CB-CG-CD1	5.31	124.19	121.00
6	o	119	ALA	N-CA-CB	5.31	117.54	110.10
7	p	74	SER	N-CA-CB	5.31	118.47	110.50
9	r	753	PHE	CZ-CE2-CD2	-5.31	113.72	120.10
3	a	348	TYR	CB-CG-CD1	-5.31	117.81	121.00
9	g	368	PHE	CB-CG-CD2	5.31	124.52	120.80
3	l	526	ARG	CG-CD-NE	-5.31	100.65	111.80
1	X	639	PHE	CB-CG-CD2	-5.31	117.09	120.80
9	r	248	LEU	CB-CA-C	-5.30	100.12	110.20
7	e	225	GLY	CA-C-O	-5.30	111.06	120.60
3	a	751	ARG	CG-CD-NE	-5.30	100.68	111.80
4	b	70	LYS	O-C-N	5.30	131.18	122.70
4	b	689	ALA	N-CA-CB	5.30	117.52	110.10
3	a	378	TRP	CD1-CG-CD2	5.29	110.54	106.30
3	a	755	VAL	CA-CB-CG1	-5.29	102.96	110.90
4	b	98	LEU	N-CA-C	-5.29	96.71	111.00
4	m	732	ARG	NH1-CZ-NH2	5.29	125.22	119.40
8	q	279	TYR	C-N-CA	5.29	134.93	121.70
9	r	1067	ASP	CB-CG-OD2	-5.29	113.54	118.30
9	r	389	SER	N-CA-CB	-5.29	102.56	110.50
3	a	810	ASP	N-CA-CB	5.29	120.12	110.60
5	c	320	VAL	N-CA-C	-5.29	96.72	111.00
7	p	70	ARG	NE-CZ-NH1	-5.29	117.66	120.30
9	r	573	LYS	N-CA-CB	5.29	120.12	110.60
1	X	893	TYR	CB-CG-CD2	-5.29	117.83	121.00
9	g	756	PHE	CB-CG-CD1	5.29	124.50	120.80
5	c	237	SER	N-CA-CB	5.29	118.43	110.50
3	l	695	TYR	CA-CB-CG	-5.29	103.36	113.40
3	a	130	THR	N-CA-CB	5.28	120.34	110.30
1	X	1392	PHE	CB-CG-CD2	5.28	124.50	120.80
7	e	15	VAL	O-C-N	5.28	131.15	122.70
3	l	130	THR	N-CA-C	-5.28	96.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	404	SER	N-CA-CB	-5.28	102.58	110.50
9	g	232	THR	CA-CB-OG1	5.28	120.08	109.00
7	e	166	GLN	N-CA-CB	5.28	120.09	110.60
8	q	676	LYS	N-CA-C	-5.27	96.76	111.00
3	a	210	ARG	CA-CB-CG	5.27	125.00	113.40
6	d	20	TYR	CZ-CE2-CD2	5.27	124.55	119.80
9	g	586	ASP	CB-CG-OD2	-5.27	113.55	118.30
4	m	351	ARG	NE-CZ-NH1	5.27	122.94	120.30
4	m	64	LYS	CB-CA-C	-5.27	99.86	110.40
6	o	32	THR	N-CA-CB	5.27	120.31	110.30
1	X	753	TYR	CB-CG-CD1	5.27	124.16	121.00
3	a	727	TYR	CB-CG-CD2	-5.27	117.84	121.00
9	g	405	GLU	N-CA-C	-5.27	96.77	111.00
9	g	712	PHE	N-CA-CB	-5.27	101.11	110.60
4	m	77	GLN	N-CA-CB	5.27	120.08	110.60
6	o	225	VAL	CA-CB-CG1	-5.27	103.00	110.90
6	o	229	ARG	CG-CD-NE	-5.27	100.74	111.80
6	o	234	TRP	CD1-CG-CD2	5.27	110.51	106.30
9	r	795	VAL	CA-CB-CG1	5.27	118.80	110.90
4	m	376	GLN	N-CA-CB	5.27	120.08	110.60
3	l	953	LEU	N-CA-CB	5.26	120.93	110.40
8	f	355	LEU	CB-CA-C	-5.26	100.20	110.20
5	n	141	GLU	OE1-CD-OE2	-5.26	116.99	123.30
6	d	38	VAL	CB-CA-C	-5.25	101.42	111.40
3	l	27	TYR	CG-CD1-CE1	-5.25	117.10	121.30
4	m	138	LYS	CB-CA-C	-5.25	99.89	110.40
8	q	20	LYS	N-CA-CB	5.25	120.05	110.60
1	X	1004	LEU	CB-CG-CD2	5.25	119.92	111.00
3	a	333	ASP	CB-CG-OD1	5.25	123.02	118.30
6	d	121	SER	CB-CA-C	5.25	120.07	110.10
3	l	966	CYS	CA-CB-SG	-5.25	104.55	114.00
3	l	544	MET	CB-CA-C	-5.25	99.91	110.40
8	q	126	LEU	CB-CG-CD1	-5.25	102.08	111.00
6	o	82	TRP	CB-CG-CD1	-5.24	120.18	127.00
6	o	258	TRP	CG-CD2-CE3	-5.24	129.18	133.90
4	m	457	TYR	CG-CD1-CE1	-5.24	117.11	121.30
5	c	246	TYR	CB-CG-CD2	5.24	124.14	121.00
6	d	125	VAL	N-CA-C	-5.24	96.85	111.00
5	n	644	PHE	CG-CD1-CE1	-5.24	115.04	120.80
8	q	519	GLU	C-N-CA	5.24	133.31	122.30
7	e	207	LYS	N-CA-C	-5.24	96.86	111.00
9	g	381	TYR	CG-CD1-CE1	-5.24	117.11	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	539	PHE	CB-CG-CD1	-5.24	117.13	120.80
9	g	122	VAL	CA-CB-CG1	-5.24	103.05	110.90
8	f	102	ARG	NE-CZ-NH1	5.23	122.92	120.30
9	r	1076	PHE	CB-CG-CD1	-5.23	117.14	120.80
4	b	641	ASP	CB-CG-OD1	-5.23	113.59	118.30
5	c	442	THR	CA-CB-CG2	-5.23	105.07	112.40
5	n	412	LEU	N-CA-C	-5.23	96.87	111.00
8	q	482	ARG	NE-CZ-NH2	-5.23	117.68	120.30
4	b	526	CYS	N-CA-CB	5.23	120.02	110.60
8	f	581	LEU	CB-CG-CD2	5.23	119.89	111.00
9	g	722	PHE	CG-CD2-CE2	5.23	126.55	120.80
9	r	949	TYR	CB-CG-CD2	-5.23	117.86	121.00
4	b	417	ALA	N-CA-CB	5.22	117.42	110.10
4	b	513	PHE	CZ-CE2-CD2	5.22	126.37	120.10
4	m	336	LEU	CB-CG-CD1	5.22	119.88	111.00
3	a	494	PHE	CB-CG-CD1	5.22	124.46	120.80
4	b	52	THR	CA-CB-CG2	5.22	119.71	112.40
4	b	338	VAL	CA-CB-CG2	-5.22	103.07	110.90
5	c	530	LEU	CB-CA-C	5.22	120.12	110.20
7	e	317	THR	CA-CB-CG2	-5.22	105.09	112.40
3	l	177	PHE	CB-CG-CD1	-5.22	117.14	120.80
4	m	601	ALA	N-CA-CB	5.22	117.41	110.10
8	q	17	ASP	CB-CG-OD1	5.22	123.00	118.30
8	q	685	SER	CB-CA-C	-5.22	100.17	110.10
9	r	239	LYS	CB-CA-C	-5.22	99.95	110.40
3	a	88	TYR	CG-CD2-CE2	-5.22	117.12	121.30
3	a	774	TYR	CG-CD2-CE2	-5.22	117.12	121.30
9	r	86	LEU	CB-CA-C	-5.22	100.28	110.20
3	a	640	PHE	CB-CG-CD2	-5.22	117.15	120.80
3	l	275	ALA	CB-CA-C	-5.22	102.27	110.10
4	m	451	LEU	CB-CG-CD1	5.22	119.87	111.00
9	r	292	PHE	CB-CA-C	-5.22	99.97	110.40
3	a	344	VAL	CA-CB-CG1	-5.21	103.08	110.90
3	a	1027	LEU	CB-CG-CD2	5.21	119.86	111.00
9	g	64	ASN	N-CA-CB	5.21	119.98	110.60
8	q	480	THR	CA-CB-CG2	-5.21	105.10	112.40
3	a	965	TYR	CB-CG-CD1	5.21	124.13	121.00
9	g	466	TYR	CG-CD1-CE1	5.21	125.47	121.30
5	n	539	PHE	CB-CG-CD1	5.21	124.45	120.80
7	p	297	LEU	O-C-N	-5.21	114.36	122.70
1	X	899	GLN	CG-CD-OE1	-5.21	111.18	121.60
5	c	647	GLN	N-CA-CB	5.21	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	578	ASP	CB-CG-OD1	5.21	122.99	118.30
9	r	432	LYS	N-CA-CB	5.21	119.97	110.60
1	X	1539	ASN	N-CA-C	-5.21	96.94	111.00
7	e	228	TYR	CB-CG-CD1	5.21	124.12	121.00
8	f	146	ASN	CB-CG-OD1	-5.21	111.19	121.60
1	X	881	SER	C-N-CA	5.21	134.71	121.70
3	a	898	ASP	CB-CG-OD2	-5.21	113.61	118.30
3	a	184	LEU	CB-CA-C	-5.20	100.31	110.20
6	d	219	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
9	r	1042	TRP	CG-CD2-CE3	5.20	138.58	133.90
3	a	571	PHE	CD1-CE1-CZ	-5.20	113.86	120.10
4	m	553	ILE	CA-CB-CG2	-5.20	100.50	110.90
8	q	416	TYR	CG-CD2-CE2	-5.20	117.14	121.30
4	b	434	PHE	CB-CG-CD2	-5.20	117.16	120.80
3	l	458	ASN	N-CA-CB	5.20	119.96	110.60
9	g	177	ASP	N-CA-CB	5.20	119.95	110.60
4	m	488	LEU	CB-CG-CD2	5.19	119.83	111.00
7	p	79	LYS	CA-CB-CG	5.19	124.83	113.40
1	X	1122	PHE	N-CA-CB	5.19	119.95	110.60
1	X	1621	LEU	CB-CA-C	-5.19	100.33	110.20
9	r	630	THR	N-CA-CB	5.19	120.17	110.30
9	r	797	LEU	CB-CG-CD2	5.19	119.83	111.00
1	X	1347	GLY	C-N-CA	5.19	134.68	121.70
1	X	1510	PHE	N-CA-CB	5.19	119.94	110.60
1	X	1169	ALA	CB-CA-C	-5.19	102.32	110.10
1	X	775	PHE	CB-CG-CD2	5.18	124.43	120.80
1	X	1248	THR	CA-CB-CG2	-5.18	105.14	112.40
5	c	782	LEU	CB-CG-CD1	-5.18	102.19	111.00
3	l	937	LEU	CB-CA-C	-5.18	100.35	110.20
6	o	229	ARG	NE-CZ-NH2	-5.18	117.71	120.30
5	c	142	ARG	CB-CA-C	-5.18	100.03	110.40
7	p	14	ASP	CB-CG-OD2	-5.18	113.64	118.30
4	m	603	ASP	N-CA-CB	5.18	119.93	110.60
6	d	179	ASP	CB-CG-OD1	5.18	122.96	118.30
7	e	138	ASP	CB-CG-OD2	5.18	122.96	118.30
7	e	226	ARG	N-CA-C	-5.18	97.02	111.00
5	n	189	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	X	366	SER	O-C-N	5.18	130.98	122.70
3	a	938	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	a	751	ARG	NE-CZ-NH1	-5.17	117.71	120.30
5	c	504	GLU	OE1-CD-OE2	5.17	129.51	123.30
9	g	713	ASP	CB-CG-OD1	5.17	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	267	ARG	CD-NE-CZ	5.17	130.84	123.60
9	g	121	THR	N-CA-CB	5.17	120.13	110.30
3	a	283	TYR	CB-CG-CD2	-5.17	117.90	121.00
3	a	954	ARG	NE-CZ-NH2	-5.17	117.72	120.30
9	r	997	VAL	N-CA-C	-5.17	97.05	111.00
5	n	189	TYR	CD1-CE1-CZ	-5.17	115.15	119.80
1	X	950	ARG	NE-CZ-NH1	-5.16	117.72	120.30
3	l	298	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	X	877	LEU	N-CA-CB	5.16	120.72	110.40
1	X	1219	THR	CA-CB-CG2	-5.16	105.17	112.40
3	l	963	LYS	CD-CE-NZ	-5.16	99.83	111.70
9	r	1126	ASP	CB-CG-OD2	-5.16	113.66	118.30
5	c	351	ASP	CB-CG-OD1	5.16	122.94	118.30
3	a	5	SER	CB-CA-C	-5.16	100.30	110.10
3	a	927	ASN	CA-CB-CG	-5.16	102.06	113.40
9	r	841	LYS	N-CA-CB	5.16	119.88	110.60
1	X	290	MET	CB-CA-C	-5.15	100.09	110.40
4	m	461	MET	CG-SD-CE	-5.15	91.95	100.20
6	o	191	ALA	N-CA-CB	5.15	117.31	110.10
9	r	781	TYR	CB-CG-CD1	5.15	124.09	121.00
8	q	715	LEU	CB-CG-CD2	5.15	119.76	111.00
9	r	870	VAL	CG1-CB-CG2	5.15	119.14	110.90
5	n	163	ASP	CB-CG-OD1	5.15	122.93	118.30
5	n	539	PHE	CB-CG-CD2	-5.15	117.19	120.80
3	a	397	ILE	CA-CB-CG1	5.15	120.78	111.00
3	l	97	LEU	CB-CG-CD2	5.15	119.75	111.00
4	m	499	ALA	N-CA-CB	5.15	117.31	110.10
8	q	542	ARG	CA-CB-CG	5.15	124.73	113.40
1	X	915	ASP	CB-CA-C	5.15	120.69	110.40
3	a	201	ASP	CB-CG-OD2	-5.15	113.67	118.30
4	m	267	ARG	NH1-CZ-NH2	5.14	125.06	119.40
5	n	247	PRO	N-CA-CB	5.14	109.47	103.30
1	X	1171	ARG	CG-CD-NE	-5.14	101.00	111.80
4	b	255	ARG	NE-CZ-NH2	-5.14	117.73	120.30
9	r	653	VAL	CB-CA-C	-5.14	101.63	111.40
8	f	706	GLN	N-CA-CB	5.14	119.85	110.60
4	b	469	PHE	CB-CG-CD2	5.14	124.40	120.80
4	m	640	GLU	CA-CB-CG	5.14	124.71	113.40
3	a	943	LYS	N-CA-CB	-5.14	101.35	110.60
7	p	288	LEU	CB-CG-CD1	5.14	119.73	111.00
1	X	675	TYR	CG-CD2-CE2	5.14	125.41	121.30
5	c	408	ASP	O-C-N	-5.13	114.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	306	ASN	N-CA-CB	5.13	119.84	110.60
3	l	627	TYR	CB-CA-C	5.13	120.67	110.40
4	m	173	TYR	CA-CB-CG	5.13	123.15	113.40
7	p	236	LYS	CA-CB-CG	5.13	124.70	113.40
9	r	148	GLU	N-CA-CB	5.13	119.84	110.60
1	X	893	TYR	O-C-N	5.13	130.91	122.70
9	g	1076	PHE	CB-CG-CD2	-5.13	117.21	120.80
5	n	350	ILE	N-CA-C	-5.13	97.14	111.00
9	r	1110	ARG	NE-CZ-NH2	-5.13	117.73	120.30
8	f	575	GLU	N-CA-CB	-5.13	101.36	110.60
7	p	216	ARG	NH1-CZ-NH2	5.13	125.04	119.40
8	q	98	PRO	N-CA-CB	5.13	109.46	103.30
6	o	234	TRP	CD1-NE1-CE2	5.13	113.62	109.00
1	X	868	LEU	CB-CG-CD2	5.13	119.72	111.00
9	r	533	LEU	CA-CB-CG	-5.13	103.51	115.30
3	a	715	THR	N-CA-CB	5.13	120.04	110.30
3	a	719	PHE	O-C-N	-5.13	114.50	122.70
7	e	153	GLU	OE1-CD-OE2	5.13	129.45	123.30
4	m	79	MET	N-CA-CB	5.13	119.83	110.60
3	a	760	PHE	CB-CG-CD2	-5.12	117.21	120.80
3	a	226	CYS	CB-CA-C	-5.12	100.15	110.40
9	r	1010	ASP	N-CA-C	-5.12	97.17	111.00
3	a	637	PHE	CD1-CG-CD2	5.12	124.96	118.30
9	r	688	THR	CA-CB-OG1	5.12	119.75	109.00
1	X	1600	ALA	N-CA-CB	5.12	117.27	110.10
3	a	504	SER	N-CA-CB	-5.12	102.83	110.50
4	m	350	SER	N-CA-CB	5.12	118.17	110.50
5	n	234	TRP	CE3-CZ3-CH2	-5.12	115.57	121.20
5	n	617	PHE	CB-CG-CD2	5.12	124.38	120.80
8	q	46	ALA	CB-CA-C	-5.12	102.43	110.10
8	f	543	VAL	CA-CB-CG1	-5.11	103.23	110.90
9	g	610	LEU	CB-CG-CD2	5.11	119.69	111.00
4	b	253	VAL	N-CA-C	-5.11	97.20	111.00
8	f	663	LEU	C-N-CA	5.11	134.48	121.70
8	q	198	GLU	N-CA-CB	5.11	119.80	110.60
9	r	691	TYR	CZ-CE2-CD2	5.11	124.40	119.80
9	r	1036	PHE	CB-CG-CD1	5.11	124.38	120.80
8	q	550	MET	CG-SD-CE	-5.11	92.03	100.20
3	a	993	VAL	CA-CB-CG1	5.11	118.56	110.90
5	c	139	MET	CG-SD-CE	-5.11	92.03	100.20
4	m	86	ASP	CB-CG-OD1	5.11	122.90	118.30
3	a	399	THR	CA-CB-CG2	-5.11	105.25	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	465	PHE	N-CA-C	-5.11	97.21	111.00
5	n	496	PHE	CB-CG-CD1	-5.11	117.23	120.80
3	l	172	GLN	N-CA-CB	5.10	119.79	110.60
3	l	819	TYR	CB-CG-CD1	5.10	124.06	121.00
7	e	154	MET	O-C-N	-5.10	114.54	122.70
4	m	469	PHE	CB-CG-CD1	-5.10	117.23	120.80
3	a	824	PHE	CB-CG-CD1	5.10	124.37	120.80
4	b	531	LEU	N-CA-C	-5.10	97.23	111.00
5	n	643	ILE	CA-CB-CG1	-5.10	101.31	111.00
1	X	796	SER	N-CA-C	-5.10	97.23	111.00
3	a	85	SER	N-CA-C	-5.10	97.23	111.00
8	q	256	LEU	N-CA-CB	5.10	120.60	110.40
8	q	315	LEU	CB-CG-CD2	5.10	119.67	111.00
3	a	106	TYR	CA-CB-CG	-5.10	103.72	113.40
9	g	509	ALA	CB-CA-C	-5.10	102.45	110.10
3	a	214	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
4	m	644	GLN	N-CA-CB	5.09	119.77	110.60
5	n	381	TRP	CH2-CZ2-CE2	-5.09	112.31	117.40
3	a	925	LEU	N-CA-C	-5.09	97.25	111.00
6	d	198	SER	C-N-CA	5.09	134.43	121.70
4	m	527	VAL	CA-CB-CG1	-5.09	103.26	110.90
1	X	1239	ASP	N-CA-C	-5.09	97.25	111.00
6	o	120	SER	N-CA-C	-5.09	97.25	111.00
3	a	965	TYR	CA-CB-CG	5.09	123.07	113.40
3	l	106	TYR	CG-CD1-CE1	-5.09	117.23	121.30
7	p	24	VAL	CG1-CB-CG2	-5.09	102.76	110.90
3	a	636	THR	CA-CB-OG1	5.09	119.68	109.00
5	c	380	SER	N-CA-CB	5.09	118.13	110.50
7	e	178	PHE	CB-CG-CD1	5.09	124.36	120.80
4	m	699	TRP	N-CA-CB	5.09	119.75	110.60
5	n	646	ASP	N-CA-CB	5.09	119.76	110.60
1	X	950	ARG	CB-CG-CD	5.08	124.82	111.60
7	e	226	ARG	N-CA-CB	5.08	119.75	110.60
1	X	845	SER	N-CA-CB	5.08	118.12	110.50
7	e	226	ARG	CB-CA-C	-5.08	100.24	110.40
4	m	286	SER	N-CA-CB	5.08	118.12	110.50
9	r	927	ALA	N-CA-CB	5.08	117.21	110.10
1	X	1022	TYR	CD1-CE1-CZ	-5.08	115.23	119.80
3	a	1007	LEU	CA-CB-CG	-5.08	103.62	115.30
4	b	363	TYR	O-C-N	-5.08	114.57	122.70
4	b	364	TYR	N-CA-CB	5.08	119.74	110.60
8	q	592	LYS	N-CA-CB	5.08	119.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	142	ALA	CA-C-O	5.08	130.76	120.10
9	g	240	PRO	C-N-CA	5.08	134.39	121.70
9	g	690	ARG	NE-CZ-NH2	-5.08	117.76	120.30
3	l	100	ALA	CB-CA-C	-5.08	102.49	110.10
1	X	389	PHE	CB-CG-CD2	-5.07	117.25	120.80
3	a	981	LEU	CB-CG-CD2	5.07	119.62	111.00
6	d	53	GLU	CA-C-O	5.07	130.75	120.10
6	d	285	LEU	C-N-CA	5.07	134.38	121.70
9	g	691	TYR	CB-CG-CD1	5.07	124.04	121.00
5	n	506	THR	CA-CB-CG2	-5.07	105.30	112.40
7	e	20	TYR	CB-CG-CD1	5.07	124.04	121.00
3	l	1035	ARG	CD-NE-CZ	5.07	130.70	123.60
9	g	369	ASP	CB-CG-OD2	-5.07	113.74	118.30
5	c	466	SER	N-CA-CB	5.07	118.10	110.50
9	g	230	PHE	CB-CG-CD2	-5.07	117.25	120.80
3	l	641	ASP	CB-CG-OD1	5.07	122.86	118.30
3	l	832	PHE	CG-CD1-CE1	-5.07	115.23	120.80
4	m	567	LEU	CB-CG-CD2	5.07	119.61	111.00
1	X	298	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	X	1289	LYS	C-N-CA	5.07	134.37	121.70
3	a	912	ASP	CB-CG-OD1	5.07	122.86	118.30
9	g	897	ALA	N-CA-CB	5.07	117.19	110.10
3	a	922	LEU	CB-CG-CD2	5.06	119.61	111.00
4	b	168	ARG	N-CA-C	-5.06	97.33	111.00
4	b	470	ALA	N-CA-CB	5.06	117.19	110.10
1	X	1348	VAL	CG1-CB-CG2	5.06	119.00	110.90
4	b	513	PHE	CG-CD2-CE2	-5.06	115.23	120.80
3	l	967	PHE	CD1-CE1-CZ	5.06	126.17	120.10
4	m	114	ILE	CG1-CB-CG2	-5.06	100.27	111.40
7	p	177	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
3	a	580	PRO	N-CD-CG	5.06	110.78	103.20
3	a	662	PHE	CG-CD2-CE2	-5.06	115.24	120.80
5	n	234	TRP	N-CA-CB	5.06	119.70	110.60
8	q	722	ALA	CB-CA-C	-5.06	102.52	110.10
3	a	165	PHE	CB-CG-CD2	-5.05	117.26	120.80
1	X	1465	LEU	O-C-N	5.05	130.78	122.70
6	d	136	THR	CA-CB-CG2	-5.05	105.33	112.40
8	f	37	ASN	C-N-CA	5.05	134.33	121.70
9	g	539	PHE	CB-CG-CD2	5.05	124.34	120.80
8	q	659	TYR	CB-CG-CD2	5.05	124.03	121.00
1	X	930	ALA	N-CA-CB	5.05	117.17	110.10
3	a	516	PHE	CB-CG-CD1	-5.05	117.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	d	145	ALA	CB-CA-C	-5.05	102.52	110.10
5	n	402	LEU	CB-CG-CD1	5.05	119.59	111.00
5	c	391	TYR	CB-CG-CD2	-5.05	117.97	121.00
9	g	955	ASP	CB-CG-OD2	-5.05	113.75	118.30
9	r	405	GLU	N-CA-C	5.05	124.63	111.00
3	a	916	ARG	NE-CZ-NH1	5.05	122.82	120.30
9	g	713	ASP	C-N-CA	5.05	134.31	121.70
3	l	1025	VAL	CA-CB-CG2	5.05	118.47	110.90
6	o	212	TRP	CG-CD2-CE3	-5.05	129.36	133.90
8	q	611	SER	C-N-CA	5.05	134.32	121.70
1	X	400	PHE	CB-CG-CD1	-5.04	117.27	120.80
1	X	1079	VAL	CG1-CB-CG2	5.04	118.97	110.90
3	l	588	ASN	CB-CG-OD1	-5.04	111.51	121.60
8	f	446	SER	O-C-N	-5.04	114.63	122.70
5	n	635	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	X	157	ALA	CB-CA-C	-5.04	102.54	110.10
3	a	378	TRP	CG-CD1-NE1	-5.04	105.06	110.10
6	d	19	TYR	CD1-CG-CD2	5.04	123.44	117.90
3	l	541	PRO	N-CD-CG	5.04	110.76	103.20
9	r	171	LYS	CB-CA-C	-5.04	100.32	110.40
9	r	1052	ASN	N-CA-C	-5.04	97.40	111.00
8	f	438	GLU	OE1-CD-OE2	5.04	129.34	123.30
9	g	493	PHE	CG-CD2-CE2	-5.04	115.26	120.80
3	l	627	TYR	CB-CG-CD2	-5.04	117.98	121.00
5	c	224	MET	N-CA-CB	5.04	119.66	110.60
4	m	171	ARG	NE-CZ-NH2	-5.04	117.78	120.30
6	o	213	SER	CB-CA-C	-5.04	100.53	110.10
1	X	1182	ASN	CB-CA-C	-5.03	100.34	110.40
8	f	432	TYR	N-CA-C	-5.03	97.42	111.00
9	r	605	ARG	NE-CZ-NH1	5.03	122.81	120.30
7	e	333	ALA	N-CA-CB	5.03	117.14	110.10
9	r	523	ASP	N-CA-CB	5.03	119.65	110.60
9	r	559	VAL	CB-CA-C	-5.03	101.84	111.40
9	g	810	ASP	CB-CG-OD2	-5.03	113.78	118.30
5	n	471	ASP	CB-CG-OD2	5.03	122.83	118.30
8	q	691	THR	CA-CB-CG2	-5.03	105.36	112.40
1	X	763	GLN	C-N-CA	5.03	134.27	121.70
1	X	948	LEU	N-CA-CB	5.03	120.45	110.40
3	a	156	TYR	CB-CG-CD2	-5.03	117.98	121.00
8	f	70	LEU	C-N-CA	5.03	134.26	121.70
8	q	117	TYR	CD1-CE1-CZ	5.03	124.32	119.80
8	q	576	ASN	CA-C-N	5.03	128.26	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	757	GLU	CG-CD-OE1	-5.02	108.25	118.30
9	r	303	HIS	CB-CA-C	-5.02	100.35	110.40
3	a	94	ASN	O-C-N	-5.02	114.67	122.70
3	a	1014	TYR	CD1-CG-CD2	-5.02	112.38	117.90
3	l	549	LYS	O-C-N	5.02	130.74	122.70
5	n	530	LEU	CA-CB-CG	5.02	126.85	115.30
7	e	103	THR	CA-CB-CG2	-5.02	105.37	112.40
1	X	754	TYR	N-CA-CB	5.02	119.64	110.60
3	a	526	ARG	CA-CB-CG	5.02	124.44	113.40
8	f	614	PRO	N-CA-CB	5.02	109.32	103.30
3	l	726	SER	N-CA-CB	5.02	118.03	110.50
9	r	694	LEU	CB-CG-CD2	5.02	119.53	111.00
1	X	693	MET	CG-SD-CE	-5.02	92.17	100.20
1	X	1022	TYR	C-N-CA	5.02	134.24	121.70
3	a	607	PHE	CB-CG-CD2	5.02	124.31	120.80
3	a	918	PHE	CB-CG-CD2	-5.02	117.29	120.80
6	o	201	GLU	CB-CA-C	-5.02	100.36	110.40
1	X	661	MET	CA-CB-CG	5.02	121.83	113.30
9	g	445	ASP	N-CA-CB	5.01	119.62	110.60
1	X	1444	LEU	CB-CG-CD2	5.01	119.52	111.00
1	X	1534	TYR	C-N-CA	5.01	134.23	121.70
8	q	218	TYR	CD1-CE1-CZ	5.01	124.31	119.80
9	g	210	LEU	CB-CG-CD1	5.01	119.52	111.00
8	q	102	ARG	CG-CD-NE	-5.01	101.28	111.80
3	l	720	PHE	CB-CG-CD2	5.01	124.31	120.80
6	d	194	TYR	CG-CD1-CE1	-5.01	117.29	121.30
3	l	466	TYR	CB-CG-CD1	5.01	124.00	121.00
8	q	479	THR	CA-CB-CG2	-5.01	105.39	112.40
5	c	223	TYR	CZ-CE2-CD2	-5.01	115.29	119.80
3	a	949	LEU	CB-CG-CD2	5.00	119.51	111.00
6	d	57	TRP	CG-CD1-NE1	-5.00	105.09	110.10
9	g	869	ASP	CB-CG-OD1	-5.00	113.80	118.30
5	n	270	SER	N-CA-CB	5.00	118.01	110.50
8	f	348	ALA	CB-CA-C	-5.00	102.59	110.10
8	q	628	PHE	CB-CG-CD1	5.00	124.30	120.80
7	e	243	PHE	CG-CD2-CE2	5.00	126.30	120.80
8	f	649	TYR	CB-CG-CD1	-5.00	118.00	121.00
9	g	702	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (10) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
1	X	793	LEU	CA
1	X	794	ILE	CA
1	X	1060	LEU	CA
1	X	1276	LYS	CA
1	X	1277	ILE	CA
1	X	1303	LEU	CA
1	X	1304	LYS	CA
8	f	576	ASN	CA
3	l	415	TYR	CA
8	q	482	ARG	CA

All (444) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1008	THR	Peptide
1	X	1042	SER	Peptide
1	X	1060	LEU	Mainchain
1	X	1062	ARG	Sidechain
1	X	1170	ASP	Peptide
1	X	1196	TYR	Sidechain
1	X	1199	TYR	Sidechain
1	X	1233	PHE	Sidechain
1	X	1240	PHE	Sidechain
1	X	1260	TYR	Sidechain
1	X	1263	TYR	Sidechain
1	X	1304	LYS	Mainchain
1	X	1307	PHE	Sidechain
1	X	1308	TYR	Sidechain
1	X	1399	ASN	Peptide
1	X	1463	SER	Peptide
1	X	1490	ARG	Sidechain
1	X	150	GLN	Peptide
1	X	1524	TYR	Sidechain
1	X	1534	TYR	Sidechain
1	X	1536	TRP	Peptide
1	X	1566	TYR	Sidechain
1	X	1597	ARG	Sidechain
1	X	164	TYR	Sidechain
1	X	182	PHE	Sidechain
1	X	213	PHE	Peptide
1	X	322	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	X	327	PHE	Sidechain
1	X	330	TYR	Sidechain
1	X	369	LEU	Peptide
1	X	371	PHE	Sidechain
1	X	382	PHE	Sidechain
1	X	411	PHE	Sidechain
1	X	413	GLU	Peptide
1	X	430	ALA	Peptide
1	X	439	LEU	Peptide
1	X	440	ILE	Peptide
1	X	617	TYR	Sidechain
1	X	727	ASN	Peptide
1	X	728	ILE	Peptide
1	X	753	TYR	Sidechain
1	X	776	TYR	Sidechain
1	X	833	LYS	Peptide
1	X	835	LEU	Peptide
1	X	879	ILE	Peptide
1	X	884	LEU	Peptide
1	X	894	VAL	Peptide
1	X	906	TYR	Sidechain
1	X	927	LYS	Peptide
1	X	953	TYR	Sidechain
1	X	984	ASP	Peptide
3	a	1005	ASN	Peptide
3	a	1010	PHE	Sidechain,Peptide
3	a	1012	SER	Peptide
3	a	1014	TYR	Sidechain
3	a	1017	TRP	Peptide
3	a	1035	ARG	Peptide
3	a	173	PHE	Sidechain
3	a	177	PHE	Sidechain
3	a	193	HIS	Sidechain
3	a	204	TYR	Sidechain
3	a	220	TYR	Sidechain
3	a	223	VAL	Peptide
3	a	294	GLU	Peptide
3	a	342	LEU	Peptide
3	a	408	PHE	Sidechain
3	a	415	TYR	Sidechain
3	a	442	TYR	Sidechain
3	a	456	ALA	Peptide

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Mol	Chain	Res	Type	Group
3	a	466	TYR	Sidechain
3	a	479	TYR	Sidechain
3	a	516	PHE	Peptide
3	a	54	SER	Peptide
3	a	550	PHE	Sidechain
3	a	56	TYR	Sidechain
3	a	561	GLN	Peptide
3	a	591	MET	Peptide
3	a	593	PRO	Peptide
3	a	596	PHE	Peptide
3	a	6	ARG	Peptide
3	a	627	TYR	Sidechain
3	a	637	PHE	Peptide
3	a	642	LEU	Peptide
3	a	67	TYR	Sidechain
3	a	674	LEU	Peptide
3	a	686	PHE	Sidechain
3	a	688	PHE	Sidechain
3	a	695	TYR	Sidechain
3	a	701	TYR	Sidechain
3	a	717	ASN	Peptide
3	a	720	PHE	Peptide
3	a	727	TYR	Sidechain
3	a	734	HIS	Sidechain
3	a	748	PHE	Peptide
3	a	749	TYR	Peptide
3	a	751	ARG	Sidechain
3	a	760	PHE	Sidechain
3	a	769	ASN	Peptide
3	a	770	PHE	Sidechain
3	a	782	TYR	Sidechain,Peptide
3	a	806	SER	Peptide
3	a	815	PHE	Sidechain
3	a	821	HIS	Peptide
3	a	846	SER	Peptide
3	a	851	TYR	Peptide
3	a	862	GLN	Peptide
3	a	869	HIS	Sidechain
3	a	889	LEU	Peptide
3	a	892	GLY	Peptide
3	a	901	ARG	Sidechain
3	a	914	TYR	Peptide

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Mol	Chain	Res	Type	Group
3	a	945	VAL	Peptide
3	a	954	ARG	Sidechain
3	a	957	ASP	Peptide
3	a	958	TRP	Peptide
3	a	964	LEU	Peptide
3	a	970	LEU	Peptide
3	a	971	ASN	Peptide
3	a	975	ARG	Peptide
3	a	995	ARG	Sidechain
4	b	102	LYS	Peptide
4	b	173	TYR	Sidechain
4	b	179	LEU	Peptide
4	b	267	ARG	Sidechain
4	b	271	LEU	Peptide
4	b	344	ARG	Sidechain
4	b	354	TYR	Sidechain
4	b	364	TYR	Sidechain
4	b	374	TYR	Sidechain
4	b	406	LEU	Peptide
4	b	464	TYR	Sidechain
4	b	482	TRP	Peptide
4	b	490	ALA	Peptide
4	b	54	ASN	Peptide
4	b	576	PHE	Sidechain
4	b	619	SER	Mainchain
4	b	634	TYR	Sidechain
4	b	639	ARG	Sidechain
4	b	641	ASP	Peptide
4	b	647	ARG	Sidechain
4	b	655	PHE	Sidechain,Peptide
4	b	657	TYR	Peptide
4	b	673	PRO	Peptide
4	b	676	LEU	Peptide
4	b	687	SER	Peptide
4	b	704	GLU	Peptide
4	b	737	PHE	Peptide
4	b	81	PHE	Sidechain
4	b	88	TYR	Sidechain
5	c	142	ARG	Sidechain
5	c	143	ARG	Sidechain
5	c	148	TYR	Sidechain
5	c	189	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	c	200	GLU	Peptide
5	c	207	TYR	Peptide
5	c	225	GLU	Peptide
5	c	248	TYR	Sidechain
5	c	267	ARG	Sidechain
5	c	300	LEU	Peptide
5	c	391	TYR	Sidechain
5	c	397	TYR	Sidechain
5	c	414	TYR	Sidechain
5	c	425	TYR	Sidechain
5	c	446	ASP	Peptide
5	c	456	THR	Peptide
5	c	459	PHE	Sidechain
5	c	509	ARG	Sidechain
5	c	548	TYR	Sidechain
5	c	579	ARG	Sidechain
5	c	583	SER	Peptide
5	c	634	ILE	Peptide
5	c	645	TYR	Peptide
5	c	648	TYR	Peptide
5	c	649	LYS	Peptide
5	c	650	HIS	Peptide
5	c	783	ARG	Sidechain
6	d	112	TYR	Sidechain
6	d	131	LYS	Peptide
6	d	221	TYR	Sidechain
6	d	229	ARG	Sidechain
6	d	8	HIS	Sidechain
7	e	112	TYR	Sidechain
7	e	113	SER	Peptide
7	e	174	CYS	Peptide
7	e	196	ARG	Sidechain
7	e	305	GLY	Peptide
7	e	323	GLY	Peptide
7	e	324	ASP	Peptide
7	e	332	LYS	Peptide
7	e	68	TYR	Peptide
8	f	163	ARG	Sidechain
8	f	259	TYR	Sidechain
8	f	269	GLY	Peptide
8	f	335	HIS	Sidechain
8	f	391	HIS	Sidechain

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Mol	Chain	Res	Type	Group
8	f	432	TYR	Sidechain
8	f	482	ARG	Sidechain,Peptide
8	f	653	TYR	Sidechain
8	f	676	LYS	Peptide
8	f	683	PHE	Sidechain
8	f	686	GLU	Peptide
8	f	714	TYR	Sidechain
8	f	73	ARG	Sidechain
8	f	99	TYR	Sidechain
9	g	1044	ARG	Sidechain
9	g	106	TYR	Sidechain
9	g	1060	HIS	Sidechain
9	g	1094	TYR	Sidechain
9	g	1099	TYR	Sidechain
9	g	1102	PHE	Sidechain
9	g	112	SER	Peptide
9	g	113	THR	Peptide
9	g	118	PRO	Peptide
9	g	120	ILE	Peptide
9	g	142	PHE	Peptide
9	g	145	THR	Peptide
9	g	146	MET	Peptide
9	g	175	TYR	Sidechain
9	g	234	ARG	Sidechain
9	g	271	ARG	Sidechain
9	g	284	TYR	Sidechain
9	g	316	ILE	Peptide
9	g	352	TYR	Sidechain
9	g	361	TYR	Sidechain
9	g	378	PHE	Peptide
9	g	380	THR	Peptide
9	g	420	PHE	Peptide
9	g	437	TYR	Sidechain
9	g	441	ARG	Sidechain
9	g	447	VAL	Peptide
9	g	466	TYR	Sidechain
9	g	477	PHE	Sidechain
9	g	497	HIS	Peptide
9	g	503	TYR	Sidechain
9	g	526	SER	Peptide
9	g	574	ASN	Peptide
9	g	579	ILE	Peptide

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Mol	Chain	Res	Type	Group
9	g	621	TYR	Peptide
9	g	627	GLU	Peptide
9	g	628	HIS	Peptide
9	g	654	VAL	Peptide
9	g	659	PRO	Peptide
9	g	692	GLU	Peptide
9	g	709	PHE	Sidechain
9	g	713	ASP	Peptide
9	g	714	TYR	Sidechain
9	g	750	TYR	Sidechain
9	g	790	HIS	Peptide
9	g	797	LEU	Peptide
9	g	843	PHE	Sidechain
9	g	845	PHE	Sidechain
9	g	881	LYS	Peptide
9	g	89	TYR	Sidechain
9	g	936	LYS	Peptide
9	g	945	ARG	Sidechain
9	g	949	TYR	Sidechain
9	g	96	TYR	Sidechain
9	g	981	ARG	Sidechain
3	l	1	MET	Peptide
3	l	1010	PHE	Sidechain
3	l	156	TYR	Sidechain
3	l	199	PHE	Peptide
3	l	204	TYR	Sidechain
3	l	212	PHE	Sidechain
3	l	264	ASP	Peptide
3	l	283	TYR	Sidechain
3	l	295	ASN	Peptide
3	l	338	ARG	Peptide
3	l	348	TYR	Sidechain
3	l	415	TYR	Sidechain
3	l	466	TYR	Sidechain
3	l	484	TYR	Sidechain
3	l	485	LYS	Peptide
3	l	490	VAL	Mainchain
3	l	495	TYR	Sidechain
3	l	571	PHE	Sidechain
3	l	601	PHE	Sidechain
3	l	627	TYR	Sidechain
3	l	628	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	l	659	TYR	Sidechain
3	l	688	PHE	Sidechain
3	l	698	LEU	Peptide
3	l	70	TYR	Sidechain
3	l	710	TYR	Sidechain
3	l	72	PHE	Sidechain
3	l	720	PHE	Sidechain,Peptide
3	l	724	PHE	Sidechain
3	l	725	ARG	Sidechain
3	l	75	ARG	Sidechain
3	l	751	ARG	Sidechain
3	l	769	ASN	Peptide
3	l	798	LYS	Peptide
3	l	81	PHE	Sidechain
3	l	824	PHE	Sidechain
3	l	825	TYR	Sidechain
3	l	851	TYR	Peptide
3	l	862	GLN	Peptide
3	l	880	ARG	Peptide
3	l	883	GLU	Peptide
3	l	887	ASP	Peptide
3	l	916	ARG	Sidechain
3	l	924	ARG	Peptide
3	l	929	HIS	Sidechain
3	l	941	ASP	Peptide
3	l	965	TYR	Peptide
3	l	984	TYR	Sidechain
3	l	992	ASP	Peptide
4	m	158	PHE	Sidechain
4	m	189	TYR	Sidechain
4	m	190	PHE	Peptide
4	m	218	GLU	Peptide
4	m	239	VAL	Peptide
4	m	244	TYR	Sidechain
4	m	245	PHE	Sidechain
4	m	255	ARG	Sidechain
4	m	265	ILE	Peptide
4	m	344	ARG	Sidechain
4	m	362	LEU	Peptide
4	m	511	TYR	Peptide
4	m	528	GLU	Peptide
4	m	545	GLN	Peptide

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Mol	Chain	Res	Type	Group
4	m	564	LYS	Peptide
4	m	571	TYR	Sidechain
4	m	593	ALA	Peptide
4	m	625	ALA	Peptide
4	m	629	VAL	Mainchain
4	m	652	LEU	Peptide
4	m	655	PHE	Peptide
4	m	657	TYR	Peptide
4	m	658	LEU	Peptide
4	m	659	PRO	Peptide
4	m	662	TYR	Peptide
4	m	675	PHE	Peptide
4	m	69	PHE	Sidechain
4	m	717	ASP	Peptide
4	m	87	LYS	Peptide
5	n	148	TYR	Sidechain
5	n	153	PHE	Sidechain
5	n	163	ASP	Peptide
5	n	181	ARG	Sidechain
5	n	217	PHE	Sidechain
5	n	246	TYR	Sidechain
5	n	248	TYR	Sidechain
5	n	250	THR	Peptide
5	n	305	ARG	Sidechain
5	n	323	SER	Peptide
5	n	324	TYR	Sidechain
5	n	325	LEU	Peptide
5	n	333	ARG	Sidechain
5	n	397	TYR	Sidechain
5	n	425	TYR	Sidechain
5	n	441	ARG	Sidechain
5	n	483	PHE	Sidechain
5	n	492	PHE	Sidechain
5	n	496	PHE	Sidechain,Peptide
5	n	498	ASN	Peptide
5	n	551	ASN	Peptide
5	n	552	TYR	Sidechain
5	n	607	ARG	Sidechain
5	n	611	SER	Peptide
5	n	629	GLU	Peptide
5	n	648	TYR	Peptide
5	n	649	LYS	Peptide

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Mol	Chain	Res	Type	Group
6	o	108	ALA	Peptide
6	o	110	HIS	Peptide
6	o	140	ILE	Peptide
6	o	187	TYR	Sidechain,Peptide
6	o	194	TYR	Sidechain
6	o	20	TYR	Sidechain
6	o	273	GLY	Peptide
6	o	288	LYS	Peptide
6	o	67	GLY	Peptide
6	o	75	TYR	Sidechain
7	p	112	TYR	Sidechain
7	p	116	PHE	Sidechain
7	p	120	HIS	Sidechain
7	p	164	HIS	Sidechain
7	p	17	TYR	Sidechain
7	p	194	TYR	Sidechain
7	p	196	ARG	Sidechain
7	p	20	TYR	Sidechain
7	p	226	ARG	Sidechain
7	p	27	CYS	Peptide
7	p	309	SER	Peptide
7	p	32	HIS	Sidechain
8	q	11	ARG	Sidechain
8	q	180	PHE	Sidechain
8	q	248	TYR	Sidechain
8	q	279	TYR	Peptide
8	q	344	ARG	Sidechain
8	q	387	ARG	Sidechain
8	q	42	PHE	Sidechain
8	q	426	TYR	Sidechain
8	q	453	GLU	Peptide
8	q	469	ARG	Sidechain
8	q	506	ILE	Peptide
8	q	576	ASN	Mainchain
8	q	587	TYR	Sidechain
8	q	597	TYR	Sidechain
8	q	604	VAL	Peptide
8	q	623	PHE	Sidechain
8	q	73	ARG	Sidechain
8	q	97	HIS	Peptide
8	q	99	TYR	Sidechain
9	r	1094	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	r	1099	TYR	Sidechain
9	r	1102	PHE	Sidechain
9	r	144	ALA	Mainchain
9	r	203	SER	Mainchain
9	r	259	LYS	Mainchain
9	r	297	LEU	Mainchain
9	r	340	GLN	Mainchain
9	r	352	TYR	Mainchain
9	r	389	SER	Mainchain
9	r	403	GLN	Mainchain
9	r	431	SER	Mainchain
9	r	539	PHE	Sidechain
9	r	570	PHE	Sidechain
9	r	577	TYR	Sidechain
9	r	621	TYR	Sidechain
9	r	678	TYR	Sidechain
9	r	690	ARG	Sidechain
9	r	691	TYR	Sidechain
9	r	712	PHE	Sidechain
9	r	72	LEU	Mainchain
9	r	732	GLU	Peptide
9	r	753	PHE	Sidechain
9	r	790	HIS	Sidechain
9	r	80	PHE	Mainchain
9	r	835	PHE	Peptide
9	r	850	TYR	Peptide
9	r	853	LYS	Peptide
9	r	862	PHE	Peptide
9	r	867	GLN	Peptide
9	r	882	TYR	Sidechain
9	r	89	TYR	Mainchain
9	r	890	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	9208	0	9538	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	315	0	65	0	0
2	Z	315	0	65	0	0
3	a	8279	0	8125	0	0
3	l	8279	0	8121	0	0
4	b	5424	0	5397	0	0
4	m	5384	0	5361	0	0
5	c	4520	0	4539	0	0
5	n	4505	0	4521	0	0
6	d	2160	0	2096	0	0
6	o	2160	0	2096	0	0
7	e	2438	0	2378	0	0
7	p	2438	0	2378	0	0
8	f	5261	0	5261	0	0
8	q	5254	0	5252	0	0
9	g	8627	0	8539	0	0
9	r	8575	0	8469	0	0
All	All	83142	0	82201	148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (148) 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:X:745:HIS:CE1	1:X:749:ILE:HG22	1.41	1.50
1:X:319:PRO:HD2	1:X:357:ASP:OD2	1.22	1.32
1:X:775:PHE:CE2	1:X:811:ASP:O	1.88	1.26
1:X:745:HIS:CE1	1:X:749:ILE:CG2	2.32	1.13
1:X:813:ILE:HG23	1:X:816:ALA:HB3	1.14	1.12
1:X:323:TYR:OH	1:X:359:LEU:HB3	1.51	1.10
1:X:813:ILE:HG23	1:X:816:ALA:CB	1.82	1.09
1:X:813:ILE:CG2	1:X:816:ALA:HB3	1.83	1.09
1:X:319:PRO:HD2	1:X:357:ASP:CG	1.74	1.07
1:X:684:LYS:CG	1:X:744:LEU:HB2	1.83	1.07
1:X:745:HIS:ND1	1:X:749:ILE:HG22	1.76	1.00
1:X:380:THR:HG22	1:X:411:PHE:O	1.61	0.99
1:X:684:LYS:HG2	1:X:744:LEU:HB2	1.43	0.95
1:X:318:HIS:HB3	1:X:357:ASP:OD2	1.69	0.93
1:X:380:THR:CG2	1:X:411:PHE:O	2.18	0.92
1:X:684:LYS:HG3	1:X:744:LEU:HB2	1.52	0.92
1:X:775:PHE:HE2	1:X:811:ASP:O	1.45	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:745:HIS:HE1	1:X:749:ILE:HG22	1.33	0.91
1:X:319:PRO:CD	1:X:357:ASP:OD2	2.16	0.89
1:X:380:THR:CB	1:X:411:PHE:HB3	2.05	0.86
1:X:1096:ILE:HG23	1:X:1097:LEU:HD22	1.58	0.85
1:X:743:ILE:HG12	1:X:805:LEU:HB2	1.59	0.84
1:X:745:HIS:ND1	1:X:749:ILE:CG2	2.36	0.84
1:X:776:TYR:O	1:X:781:ASP:HB2	1.79	0.82
1:X:319:PRO:CD	1:X:357:ASP:CG	2.49	0.81
1:X:1096:ILE:HD11	1:X:1214:PHE:HE1	1.44	0.81
1:X:745:HIS:HA	1:X:749:ILE:HB	1.63	0.81
1:X:684:LYS:CG	1:X:744:LEU:CB	2.59	0.79
1:X:222:GLU:OE2	1:X:361:LYS:CG	2.32	0.78
1:X:684:LYS:HG2	1:X:744:LEU:CB	2.16	0.76
1:X:1057:LYS:NZ	1:X:1158:TYR:OH	2.19	0.76
1:X:375:TYR:O	1:X:378:VAL:HG12	1.88	0.73
1:X:318:HIS:HA	1:X:357:ASP:OD1	1.89	0.72
1:X:690:LEU:HG	1:X:745:HIS:HE1	1.56	0.70
1:X:319:PRO:HG3	1:X:358:VAL:O	1.92	0.70
1:X:774:ILE:HB	1:X:806:PHE:CE1	2.27	0.70
1:X:318:HIS:CB	1:X:357:ASP:OD2	2.41	0.69
1:X:380:THR:HG21	1:X:411:PHE:CB	2.24	0.69
1:X:380:THR:HG21	1:X:411:PHE:HB3	1.75	0.69
1:X:381:VAL:O	1:X:384:GLU:OE1	2.12	0.67
1:X:684:LYS:HG3	1:X:744:LEU:CB	2.21	0.67
1:X:908:VAL:HG21	1:X:967:LEU:HD11	1.77	0.66
1:X:380:THR:HB	1:X:411:PHE:HB3	1.77	0.66
1:X:380:THR:CG2	1:X:411:PHE:HB3	2.24	0.66
1:X:323:TYR:HE1	1:X:359:LEU:HG	1.61	0.65
1:X:1097:LEU:HD22	1:X:1097:LEU:H	1.61	0.65
1:X:740:ASN:O	1:X:743:ILE:HB	1.97	0.64
1:X:743:ILE:HA	1:X:805:LEU:HD12	1.80	0.63
1:X:1095:GLU:O	1:X:1119:ASN:ND2	2.31	0.63
1:X:1057:LYS:CE	1:X:1158:TYR:OH	2.47	0.63
1:X:966:GLY:H	1:X:969:ILE:HG22	1.62	0.63
1:X:801:LYS:O	1:X:804:GLN:HB2	2.01	0.61
1:X:318:HIS:CD2	1:X:357:ASP:OD1	2.53	0.61
1:X:775:PHE:CZ	1:X:812:SER:HA	2.35	0.61
1:X:1095:GLU:OE2	1:X:1095:GLU:HA	2.00	0.61
1:X:1548:ILE:HD11	1:X:1616:ILE:HD13	1.82	0.60
1:X:740:ASN:HA	1:X:743:ILE:HD12	1.83	0.60
1:X:777:ASP:HA	1:X:781:ASP:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:690:LEU:HG	1:X:745:HIS:CE1	2.37	0.59
1:X:323:TYR:CE1	1:X:359:LEU:HG	2.38	0.59
1:X:813:ILE:O	1:X:813:ILE:HG22	2.02	0.59
1:X:813:ILE:HG22	1:X:817:PRO:HD3	1.85	0.59
1:X:859:ILE:HD13	1:X:910:ALA:HB2	1.85	0.58
1:X:1160:ILE:HB	1:X:1161:PRO:HD3	1.86	0.58
1:X:222:GLU:OE2	1:X:361:LYS:HD3	2.04	0.58
1:X:222:GLU:OE2	1:X:361:LYS:HG2	2.03	0.57
1:X:803:LEU:O	1:X:803:LEU:HG	2.03	0.57
1:X:775:PHE:CD2	1:X:811:ASP:O	2.55	0.57
1:X:1007:SER:HA	1:X:1195:GLN:HE22	1.69	0.57
1:X:360:GLN:HE21	1:X:399:VAL:HG21	1.69	0.56
1:X:1096:ILE:HG21	1:X:1217:ARG:CZ	2.35	0.56
1:X:813:ILE:CG2	1:X:817:PRO:HD3	2.35	0.56
1:X:1057:LYS:HE2	1:X:1158:TYR:OH	2.06	0.55
1:X:1096:ILE:HG21	1:X:1217:ARG:NH1	2.22	0.55
1:X:1304:LYS:HD2	1:X:1306:ASN:HD22	1.72	0.55
1:X:813:ILE:HG23	1:X:816:ALA:HB2	1.85	0.54
1:X:745:HIS:HD1	1:X:749:ILE:CG2	2.16	0.54
1:X:360:GLN:NE2	1:X:399:VAL:HG21	2.23	0.53
1:X:1096:ILE:HD11	1:X:1214:PHE:CE1	2.34	0.53
1:X:829:ASN:HD22	1:X:830:THR:H	1.55	0.52
1:X:1089:SER:HA	1:X:1217:ARG:HH21	1.74	0.52
1:X:213:PHE:CD2	1:X:301:ALA:HB3	2.45	0.52
1:X:222:GLU:OE2	1:X:361:LYS:CD	2.58	0.52
1:X:793:LEU:HD23	1:X:794:ILE:H	1.75	0.52
1:X:1633:ARG:HE	1:X:1634:LEU:H	1.57	0.52
1:X:1160:ILE:N	1:X:1161:PRO:CD	2.73	0.51
1:X:777:ASP:HA	1:X:781:ASP:CB	2.39	0.51
1:X:685:TYR:HE1	1:X:744:LEU:HG	1.76	0.51
1:X:774:ILE:HB	1:X:806:PHE:CD1	2.46	0.50
1:X:318:HIS:CD2	1:X:357:ASP:CG	2.85	0.50
1:X:1055:GLN:HG2	1:X:1064:GLU:HB3	1.93	0.50
1:X:806:PHE:HA	1:X:811:ASP:CB	2.41	0.50
1:X:357:ASP:OD1	1:X:357:ASP:N	2.44	0.49
1:X:1160:ILE:H	1:X:1161:PRO:CD	2.25	0.49
1:X:319:PRO:HG3	1:X:358:VAL:C	2.32	0.49
1:X:380:THR:HG22	1:X:380:THR:O	2.11	0.49
1:X:1096:ILE:CG2	1:X:1217:ARG:NH1	2.76	0.49
1:X:360:GLN:C	1:X:362:LEU:H	2.16	0.48
1:X:774:ILE:CB	1:X:806:PHE:CE1	2.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:360:GLN:HE21	1:X:399:VAL:CG2	2.25	0.48
1:X:935:VAL:HG11	1:X:955:PHE:HB2	1.95	0.48
1:X:803:LEU:HD12	1:X:807:LEU:HD23	1.95	0.48
1:X:318:HIS:HD2	1:X:357:ASP:CG	2.17	0.47
1:X:271:LEU:HD13	1:X:378:VAL:HA	1.97	0.47
1:X:390:ILE:HD12	1:X:390:ILE:H	1.80	0.47
1:X:403:ILE:O	1:X:403:ILE:HG22	2.15	0.46
1:X:359:LEU:N	1:X:359:LEU:HD13	2.30	0.46
1:X:745:HIS:CD2	1:X:750:PHE:HA	2.49	0.46
1:X:743:ILE:O	1:X:743:ILE:HG23	2.15	0.46
1:X:900:ILE:HG22	1:X:929:MET:HG2	1.98	0.46
1:X:954:ILE:HD12	1:X:957:THR:HB	1.97	0.46
1:X:685:TYR:CE1	1:X:744:LEU:HG	2.52	0.45
1:X:368:ILE:HG22	1:X:368:ILE:O	2.17	0.45
1:X:1160:ILE:CB	1:X:1161:PRO:HD3	2.45	0.45
1:X:793:LEU:CD2	1:X:794:ILE:H	2.29	0.45
1:X:271:LEU:HD22	1:X:378:VAL:HB	1.99	0.45
1:X:813:ILE:HD12	1:X:816:ALA:HB2	1.98	0.45
1:X:1057:LYS:HA	1:X:1057:LYS:HD2	1.57	0.44
1:X:222:GLU:OE2	1:X:361:LYS:HG3	2.15	0.44
1:X:740:ASN:CA	1:X:743:ILE:HD12	2.48	0.44
1:X:908:VAL:HG21	1:X:967:LEU:CD1	2.46	0.43
1:X:780:HIS:CG	1:X:780:HIS:O	2.71	0.43
1:X:684:LYS:HE2	1:X:744:LEU:HB3	1.99	0.43
1:X:380:THR:HG21	1:X:411:PHE:HB2	1.99	0.43
1:X:813:ILE:HG22	1:X:817:PRO:CD	2.48	0.43
1:X:1558:GLN:HE21	1:X:1562:ASN:HD21	1.67	0.43
1:X:380:THR:HG21	1:X:411:PHE:O	2.11	0.43
1:X:381:VAL:HA	1:X:414:ASN:CB	2.49	0.42
1:X:799:ALA:O	1:X:803:LEU:HB3	2.19	0.42
1:X:860:ALA:HB2	1:X:957:THR:HG21	2.02	0.42
1:X:347:THR:O	1:X:350:ALA:HB3	2.20	0.42
1:X:900:ILE:H	1:X:900:ILE:HD12	1.83	0.42
1:X:1594:ASP:HB2	1:X:1597:ARG:HE	1.84	0.42
1:X:213:PHE:CE2	1:X:301:ALA:HB3	2.55	0.42
1:X:740:ASN:CB	1:X:743:ILE:HD12	2.50	0.42
1:X:774:ILE:CG2	1:X:806:PHE:CE1	3.03	0.42
1:X:803:LEU:HA	1:X:807:LEU:HB2	2.00	0.42
1:X:1450:LEU:HD23	1:X:1450:LEU:HA	1.93	0.42
1:X:618:LEU:HD23	1:X:618:LEU:HA	1.96	0.41
1:X:319:PRO:CG	1:X:358:VAL:O	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:858:LEU:HD12	1:X:867:ASP:H	1.84	0.41
1:X:965:ASP:HB2	1:X:979:ASN:H	1.84	0.41
1:X:264:LEU:HD22	1:X:375:TYR:CZ	2.56	0.41
1:X:774:ILE:HB	1:X:806:PHE:HE1	1.80	0.41
1:X:833:LYS:HA	1:X:895:HIS:CE1	2.56	0.41
1:X:782:VAL:HG23	1:X:782:VAL:O	2.20	0.40
1:X:1344:PHE:H	1:X:1347:GLY:HA3	1.86	0.40
1:X:1618:PRO:HG3	1:X:1627:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	1099/1655 (66%)	839 (76%)	171 (16%)	89 (8%)	1	12
3	a	996/1037 (96%)	825 (83%)	114 (11%)	57 (6%)	1	18
3	l	991/1037 (96%)	809 (82%)	115 (12%)	67 (7%)	1	15
4	b	667/744 (90%)	545 (82%)	80 (12%)	42 (6%)	1	17
4	m	662/744 (89%)	531 (80%)	81 (12%)	50 (8%)	1	13
5	c	551/712 (77%)	474 (86%)	53 (10%)	24 (4%)	2	22
5	n	549/712 (77%)	488 (89%)	48 (9%)	13 (2%)	6	33
6	d	270/297 (91%)	229 (85%)	35 (13%)	6 (2%)	6	35
6	o	270/297 (91%)	231 (86%)	28 (10%)	11 (4%)	3	23
7	e	303/349 (87%)	263 (87%)	30 (10%)	10 (3%)	4	26
7	p	303/349 (87%)	265 (88%)	30 (10%)	8 (3%)	5	31
8	f	635/726 (88%)	554 (87%)	55 (9%)	26 (4%)	3	23
8	q	634/726 (87%)	546 (86%)	66 (10%)	22 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	g	1052/1157 (91%)	847 (80%)	137 (13%)	68 (6%)	1 16
9	r	1048/1157 (91%)	917 (88%)	88 (8%)	43 (4%)	3 23
All	All	10030/11699 (86%)	8363 (83%)	1131 (11%)	536 (5%)	3 19

All (536) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	136	ASN
1	X	217	GLN
1	X	370	SER
1	X	408	PRO
1	X	430	ALA
1	X	431	LYS
1	X	440	ILE
1	X	728	ILE
1	X	748	HIS
1	X	764	LYS
1	X	794	ILE
1	X	826	SER
1	X	871	SER
1	X	878	PHE
1	X	930	ALA
1	X	1030	SER
1	X	1042	SER
1	X	1046	LYS
1	X	1050	SER
1	X	1057	LYS
1	X	1171	ARG
1	X	1239	ASP
1	X	1240	PHE
1	X	1252	LEU
1	X	1304	LYS
1	X	1429	HIS
3	a	207	SER
3	a	230	HIS
3	a	294	GLU
3	a	424	GLN
3	a	543	SER
3	a	750	LEU
3	a	798	LYS
3	a	881	MET

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Mol	Chain	Res	Type
3	a	886	LEU
3	a	993	VAL
4	b	199	GLU
4	b	216	ASP
4	b	344	ARG
4	b	424	CYS
4	b	457	TYR
4	b	615	VAL
4	b	677	LEU
4	b	687	SER
4	b	741	GLN
5	c	147	SER
5	c	323	SER
5	c	377	SER
5	c	398	SER
5	c	520	ALA
5	c	628	VAL
5	c	648	TYR
8	f	228	ALA
8	f	440	ASP
8	f	551	GLU
8	f	557	GLU
8	f	559	CYS
8	f	611	SER
8	f	633	THR
9	g	94	ILE
9	g	117	THR
9	g	146	MET
9	g	154	ASN
9	g	159	ASP
9	g	265	SER
9	g	280	THR
9	g	578	LYS
9	g	688	THR
9	g	705	LYS
9	g	713	ASP
9	g	714	TYR
9	g	1011	ASP
9	g	1015	LEU
9	g	1083	LEU
3	l	55	GLU
3	l	105	ARG

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Mol	Chain	Res	Type
3	l	142	ALA
3	l	180	ASP
3	l	346	ALA
3	l	416	GLY
3	l	456	ALA
3	l	476	PHE
3	l	600	ASP
3	l	716	GLU
3	l	729	ILE
3	l	769	ASN
3	l	806	SER
3	l	994	ILE
3	l	1003	VAL
3	l	1012	SER
3	l	1019	LEU
4	m	227	VAL
4	m	369	GLU
4	m	401	LYS
4	m	492	SER
4	m	507	LEU
4	m	553	ILE
4	m	580	CYS
4	m	587	ASP
4	m	625	ALA
4	m	669	LYS
4	m	710	TYR
4	m	718	LYS
5	n	179	LEU
5	n	228	SER
5	n	530	LEU
5	n	583	SER
5	n	609	LYS
5	n	611	SER
6	o	98	HIS
6	o	286	GLU
7	p	189	GLU
7	p	336	SER
8	q	142	SER
8	q	542	ARG
8	q	612	ASN
8	q	645	ASP
9	r	210	LEU

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Mol	Chain	Res	Type
9	r	216	PRO
9	r	304	PRO
9	r	394	LYS
9	r	397	PRO
9	r	421	PRO
9	r	439	MET
9	r	515	ASN
9	r	628	HIS
9	r	630	THR
9	r	631	THR
9	r	712	PHE
9	r	716	ASN
9	r	734	SER
9	r	797	LEU
9	r	830	SER
9	r	841	LYS
9	r	879	ALA
9	r	912	LYS
9	r	1013	GLU
9	r	1126	ASP
1	X	163	ASP
1	X	164	TYR
1	X	276	ASN
1	X	381	VAL
1	X	405	SER
1	X	417	THR
1	X	445	LEU
1	X	729	HIS
1	X	755	ASN
1	X	810	MET
1	X	862	ARG
1	X	880	ASN
1	X	897	LYS
1	X	898	VAL
1	X	921	SER
1	X	926	ALA
1	X	938	ASP
1	X	940	SER
1	X	977	ALA
1	X	984	ASP
1	X	985	GLU
1	X	992	SER

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Mol	Chain	Res	Type
1	X	1032	ILE
1	X	1040	VAL
1	X	1060	LEU
1	X	1061	THR
1	X	1092	SER
1	X	1173	TRP
1	X	1277	ILE
1	X	1307	PHE
1	X	1399	ASN
1	X	1427	SER
1	X	1478	ILE
1	X	1542	ALA
3	a	55	GLU
3	a	210	ARG
3	a	211	PHE
3	a	219	ASP
3	a	261	SER
3	a	347	SER
3	a	359	THR
3	a	494	PHE
3	a	497	MET
3	a	600	ASP
3	a	715	THR
3	a	736	ASN
3	a	751	ARG
3	a	837	SER
3	a	882	PHE
3	a	884	GLU
3	a	885	VAL
3	a	917	ASP
3	a	975	ARG
3	a	1011	ASP
3	a	1013	ALA
4	b	86	ASP
4	b	98	LEU
4	b	118	LEU
4	b	122	ARG
4	b	165	GLN
4	b	323	ASP
4	b	377	MET
4	b	381	ALA
4	b	516	ASN

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Mol	Chain	Res	Type
4	b	526	CYS
4	b	591	LEU
4	b	595	VAL
4	b	603	ASP
4	b	710	TYR
4	b	740	CYS
5	c	224	MET
5	c	345	THR
5	c	348	CYS
5	c	530	LEU
5	c	651	CYS
6	d	219	ARG
7	e	92	GLU
7	e	106	ASP
7	e	162	ALA
7	e	338	GLU
8	f	232	ASN
8	f	515	GLU
8	f	627	THR
8	f	635	LEU
8	f	702	TYR
9	g	152	ALA
9	g	218	GLY
9	g	550	LEU
9	g	661	GLN
9	g	799	GLU
9	g	811	LEU
9	g	819	GLN
9	g	856	LYS
9	g	885	VAL
9	g	938	ASN
9	g	1007	SER
9	g	1084	LEU
9	g	1143	GLU
9	g	1150	TYR
3	l	12	LEU
3	l	21	ASN
3	l	63	SER
3	l	86	ASP
3	l	116	GLN
3	l	250	SER
3	l	328	ILE

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Mol	Chain	Res	Type
3	l	454	LYS
3	l	794	LEU
3	l	836	ASN
3	l	881	MET
3	l	889	LEU
3	l	929	HIS
3	l	953	LEU
3	l	962	LYS
3	l	974	GLU
3	l	1002	MET
4	m	222	GLU
4	m	413	ASP
4	m	542	LEU
4	m	601	ALA
4	m	628	ALA
4	m	641	ASP
4	m	654	GLU
4	m	670	PHE
4	m	692	ILE
4	m	693	GLU
4	m	698	LYS
4	m	706	SER
4	m	738	LYS
5	n	222	ASP
5	n	567	LEU
5	n	607	ARG
6	o	11	LEU
6	o	65	LYS
6	o	191	ALA
7	p	301	ASP
8	q	55	ASN
8	q	157	ASP
8	q	280	SER
8	q	471	PRO
8	q	557	GLU
8	q	576	ASN
8	q	632	LYS
8	q	638	LEU
9	r	80	PHE
9	r	269	SER
9	r	514	PHE
9	r	637	ASN

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Mol	Chain	Res	Type
9	r	705	LYS
9	r	827	THR
9	r	835	PHE
9	r	932	LEU
9	r	974	ARG
9	r	1016	PHE
9	r	1055	ASP
1	X	280	ALA
1	X	419	ASP
1	X	662	THR
1	X	796	SER
1	X	809	PRO
1	X	866	ARG
1	X	1027	TRP
1	X	1041	ASN
1	X	1124	ASP
1	X	1172	SER
1	X	1320	GLU
1	X	1477	ALA
3	a	20	PRO
3	a	283	TYR
3	a	370	ASP
3	a	423	ALA
3	a	454	LYS
3	a	606	LYS
3	a	687	SER
3	a	861	LEU
3	a	1012	SER
4	b	272	PRO
4	b	387	THR
4	b	456	SER
4	b	464	TYR
4	b	594	ILE
4	b	718	LYS
5	c	302	ASP
5	c	393	GLN
5	c	609	LYS
6	d	51	GLY
7	e	39	ASP
7	e	93	CYS
8	f	142	SER
8	f	426	TYR

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Mol	Chain	Res	Type
8	f	433	ALA
8	f	469	ARG
9	g	70	LYS
9	g	160	GLU
9	g	209	ASP
9	g	239	LYS
9	g	412	GLU
9	g	423	ALA
9	g	438	SER
9	g	494	VAL
9	g	607	SER
9	g	631	THR
9	g	655	PHE
9	g	709	PHE
9	g	866	GLN
3	l	16	GLU
3	l	22	ASN
3	l	54	SER
3	l	62	LEU
3	l	172	GLN
3	l	295	ASN
3	l	420	PHE
3	l	436	HIS
3	l	443	LEU
3	l	649	GLN
3	l	717	ASN
3	l	736	ASN
3	l	797	LEU
3	l	857	GLN
3	l	880	ARG
3	l	967	PHE
3	l	971	ASN
4	m	55	ASP
4	m	98	LEU
4	m	511	TYR
4	m	517	ASP
4	m	518	ASP
4	m	544	ASN
4	m	656	PRO
4	m	689	ALA
4	m	720	LEU
5	n	349	SER

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Mol	Chain	Res	Type
5	n	656	ALA
6	o	43	HIS
6	o	187	TYR
6	o	192	GLN
7	p	158	SER
8	q	97	HIS
8	q	206	ILE
8	q	373	THR
8	q	578	ASP
8	q	683	PHE
8	q	699	ASP
9	r	199	PRO
9	r	622	ASN
9	r	773	ASN
9	r	833	GLU
9	r	1052	ASN
1	X	416	LEU
1	X	646	LEU
1	X	765	PHE
1	X	822	ASN
1	X	836	GLY
1	X	1028	THR
1	X	1120	LYS
1	X	1290	SER
1	X	1540	LYS
3	a	114	GLU
3	a	126	GLY
3	a	173	PHE
3	a	269	HIS
3	a	395	LEU
3	a	716	GLU
3	a	817	VAL
3	a	847	LYS
3	a	928	ALA
3	a	967	PHE
3	a	996	LYS
3	a	1017	TRP
4	b	555	SER
4	b	592	ASN
4	b	658	LEU
4	b	664	VAL
4	b	742	ALA

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Mol	Chain	Res	Type
5	c	288	SER
5	c	301	ASN
5	c	778	GLU
6	d	201	GLU
7	e	120	HIS
8	f	230	GLU
8	f	272	PRO
8	f	522	LEU
8	f	548	GLN
8	f	678	LEU
9	g	144	ALA
9	g	454	ASP
9	g	546	ILE
9	g	937	ASP
9	g	1016	PHE
3	l	437	ASN
3	l	440	GLU
3	l	687	SER
3	l	781	ASP
3	l	879	PHE
3	l	958	TRP
4	m	193	ASP
4	m	581	MET
5	n	551	ASN
6	o	255	ASP
7	p	163	ASN
7	p	217	SER
1	X	991	LYS
3	a	190	ASP
3	a	1026	THR
4	b	63	ASP
4	b	342	ASN
4	b	383	VAL
4	b	521	TRP
5	c	247	PRO
5	c	321	LEU
5	c	413	PRO
5	c	611	SER
6	d	55	PRO
6	d	289	TRP
7	e	31	GLN
7	e	188	LEU

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Mol	Chain	Res	Type
7	e	289	GLN
8	f	154	LYS
8	f	429	ILE
8	f	453	GLU
9	g	86	LEU
9	g	93	GLN
9	g	148	GLU
9	g	161	THR
9	g	217	ALA
9	g	247	LEU
9	g	251	PRO
9	g	444	GLU
9	g	509	ALA
9	g	833	GLU
9	g	1032	GLU
3	l	114	GLU
3	l	327	ALA
3	l	786	ILE
4	m	593	ALA
4	m	675	PHE
7	p	66	PRO
7	p	94	SER
8	q	164	GLU
8	q	441	CYS
9	r	123	PRO
9	r	431	SER
9	r	1079	PRO
1	X	407	ALA
1	X	691	SER
1	X	780	HIS
1	X	1472	SER
3	a	203	SER
3	a	894	GLU
3	a	945	VAL
8	f	33	ILE
9	g	245	GLY
9	g	355	SER
9	g	639	PRO
3	l	149	TRP
4	m	57	PRO
4	m	75	SER
4	m	191	ILE

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Mol	Chain	Res	Type
4	m	390	TRP
4	m	588	ASP
4	m	594	ILE
4	m	627	TYR
4	m	659	PRO
8	q	628	PHE
9	r	687	LYS
1	X	743	ILE
5	c	775	GLY
9	g	274	PRO
4	m	219	PRO
4	m	512	PRO
5	n	654	VAL
6	o	51	GLY
6	o	202	GLY
9	r	546	ILE
9	g	396	LYS
9	g	548	PRO
3	l	648	GLY
4	b	402	ILE
5	c	776	GLN
8	f	470	LEU
9	g	758	ILE
3	l	192	VAL
4	m	595	VAL
1	X	778	VAL
1	X	813	ILE
4	b	673	PRO
9	g	132	ILE
9	g	815	VAL
3	l	807	ILE
3	l	817	VAL
8	q	520	GLY
9	r	274	PRO
4	b	653	ILE
6	d	155	PRO
9	g	613	ILE
3	l	169	VAL
3	l	171	PRO
4	m	217	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	1072/1557 (69%)	990 (92%)	82 (8%)	13	37
3	a	945/972 (97%)	897 (95%)	48 (5%)	24	48
3	l	945/972 (97%)	908 (96%)	37 (4%)	32	56
4	b	606/670 (90%)	579 (96%)	27 (4%)	27	52
4	m	602/670 (90%)	572 (95%)	30 (5%)	24	49
5	c	513/646 (79%)	487 (95%)	26 (5%)	24	48
5	n	511/646 (79%)	497 (97%)	14 (3%)	44	65
6	d	233/252 (92%)	223 (96%)	10 (4%)	29	53
6	o	233/252 (92%)	219 (94%)	14 (6%)	19	44
7	e	269/305 (88%)	261 (97%)	8 (3%)	41	63
7	p	269/305 (88%)	258 (96%)	11 (4%)	30	55
8	f	594/669 (89%)	549 (92%)	45 (8%)	13	37
8	q	593/669 (89%)	566 (95%)	27 (5%)	27	52
9	g	997/1088 (92%)	949 (95%)	48 (5%)	25	51
9	r	991/1088 (91%)	971 (98%)	20 (2%)	55	74
All	All	9373/10761 (87%)	8926 (95%)	447 (5%)	29	51

All (447) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	141	LEU
1	X	145	ILE
1	X	155	ILE
1	X	197	LEU
1	X	198	MET
1	X	203	LYS
1	X	217	GLN
1	X	266	THR
1	X	276	ASN
1	X	358	VAL

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Mol	Chain	Res	Type
1	X	359	LEU
1	X	360	GLN
1	X	361	LYS
1	X	362	LEU
1	X	378	VAL
1	X	379	ILE
1	X	406	LYS
1	X	414	ASN
1	X	415	PHE
1	X	663	MET
1	X	676	LEU
1	X	682	LEU
1	X	707	PHE
1	X	725	LEU
1	X	743	ILE
1	X	744	LEU
1	X	745	HIS
1	X	753	TYR
1	X	763	GLN
1	X	766	GLU
1	X	773	LEU
1	X	778	VAL
1	X	781	ASP
1	X	794	ILE
1	X	795	ILE
1	X	803	LEU
1	X	804	GLN
1	X	805	LEU
1	X	814	ASP
1	X	822	ASN
1	X	829	ASN
1	X	831	THR
1	X	833	LYS
1	X	879	ILE
1	X	885	VAL
1	X	895	HIS
1	X	903	LEU
1	X	915	ASP
1	X	933	LYS
1	X	973	THR
1	X	1021	THR
1	X	1027	TRP

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Mol	Chain	Res	Type
1	X	1040	VAL
1	X	1055	GLN
1	X	1056	LYS
1	X	1057	LYS
1	X	1060	LEU
1	X	1065	THR
1	X	1094	SER
1	X	1096	ILE
1	X	1123	HIS
1	X	1220	VAL
1	X	1237	ASN
1	X	1252	LEU
1	X	1254	ARG
1	X	1277	ILE
1	X	1309	ARG
1	X	1333	SER
1	X	1352	LEU
1	X	1393	LYS
1	X	1400	PRO
1	X	1406	VAL
1	X	1427	SER
1	X	1431	ILE
1	X	1432	ARG
1	X	1459	LYS
1	X	1490	ARG
1	X	1521	PHE
1	X	1527	LYS
1	X	1534	TYR
1	X	1552	ASN
1	X	1567	GLN
3	a	22	ASN
3	a	58	ASN
3	a	125	ASP
3	a	136	SER
3	a	137	PHE
3	a	148	GLU
3	a	150	PHE
3	a	164	HIS
3	a	188	LYS
3	a	202	ASN
3	a	204	TYR
3	a	205	LEU

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Mol	Chain	Res	Type
3	a	210	ARG
3	a	259	MET
3	a	293	LEU
3	a	319	ILE
3	a	338	ARG
3	a	343	ASN
3	a	356	LYS
3	a	376	TYR
3	a	412	LYS
3	a	424	GLN
3	a	430	ASN
3	a	455	THR
3	a	462	SER
3	a	472	LEU
3	a	480	ASN
3	a	546	THR
3	a	551	THR
3	a	558	LEU
3	a	567	LEU
3	a	575	ASN
3	a	669	ARG
3	a	715	THR
3	a	724	PHE
3	a	741	LEU
3	a	787	ASN
3	a	800	GLU
3	a	807	ILE
3	a	842	LEU
3	a	901	ARG
3	a	924	ARG
3	a	935	LEU
3	a	965	TYR
3	a	974	GLU
3	a	1012	SER
3	a	1014	TYR
3	a	1016	GLN
4	b	58	ILE
4	b	107	TYR
4	b	112	PHE
4	b	122	ARG
4	b	132	VAL
4	b	162	VAL

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Mol	Chain	Res	Type
4	b	205	ILE
4	b	239	VAL
4	b	241	GLU
4	b	277	THR
4	b	354	TYR
4	b	373	GLU
4	b	401	LYS
4	b	407	PRO
4	b	420	THR
4	b	458	ARG
4	b	467	ASN
4	b	494	THR
4	b	508	LEU
4	b	575	LEU
4	b	598	ASN
4	b	609	GLN
4	b	611	ILE
4	b	622	GLN
4	b	631	SER
4	b	705	LYS
4	b	724	MET
5	c	136	LYS
5	c	158	MET
5	c	162	LYS
5	c	164	ILE
5	c	165	VAL
5	c	174	ARG
5	c	183	PHE
5	c	203	LYS
5	c	205	ASN
5	c	233	LEU
5	c	249	LYS
5	c	262	LYS
5	c	299	LEU
5	c	325	LEU
5	c	332	ILE
5	c	407	LEU
5	c	441	ARG
5	c	446	ASP
5	c	452	TYR
5	c	458	ARG
5	c	469	THR

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Mol	Chain	Res	Type
5	c	508	LYS
5	c	567	LEU
5	c	596	ARG
5	c	631	GLN
5	c	652	ARG
6	d	66	PHE
6	d	88	ARG
6	d	135	THR
6	d	141	ILE
6	d	180	ASN
6	d	217	LEU
6	d	230	THR
6	d	238	ASN
6	d	256	VAL
6	d	265	SER
7	e	11	LEU
7	e	102	CYS
7	e	177	ARG
7	e	212	LYS
7	e	236	LYS
7	e	289	GLN
7	e	317	THR
7	e	341	CYS
8	f	8	GLN
8	f	10	GLU
8	f	11	ARG
8	f	17	ASP
8	f	30	GLN
8	f	31	ASN
8	f	37	ASN
8	f	40	ARG
8	f	43	ARG
8	f	66	LYS
8	f	104	LEU
8	f	110	MET
8	f	126	LEU
8	f	142	SER
8	f	166	THR
8	f	172	LYS
8	f	188	ILE
8	f	230	GLU
8	f	237	ILE

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Mol	Chain	Res	Type
8	f	239	LYS
8	f	282	TRP
8	f	317	LEU
8	f	323	THR
8	f	343	ILE
8	f	355	LEU
8	f	363	VAL
8	f	373	THR
8	f	374	GLU
8	f	376	SER
8	f	407	VAL
8	f	408	ASP
8	f	452	LEU
8	f	453	GLU
8	f	454	ASP
8	f	506	ILE
8	f	528	HIS
8	f	548	GLN
8	f	575	GLU
8	f	576	ASN
8	f	581	LEU
8	f	592	LYS
8	f	617	ILE
8	f	663	LEU
8	f	676	LYS
8	f	682	LYS
9	g	101	ASP
9	g	167	ILE
9	g	173	ILE
9	g	176	GLU
9	g	213	ASN
9	g	219	ILE
9	g	242	LEU
9	g	262	ASN
9	g	359	THR
9	g	387	MET
9	g	427	THR
9	g	460	TYR
9	g	463	LYS
9	g	507	ILE
9	g	520	ILE
9	g	522	LEU

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Mol	Chain	Res	Type
9	g	529	HIS
9	g	550	LEU
9	g	584	LYS
9	g	616	LYS
9	g	617	THR
9	g	631	THR
9	g	657	LEU
9	g	698	PRO
9	g	703	THR
9	g	746	VAL
9	g	758	ILE
9	g	772	ASP
9	g	774	PHE
9	g	775	ILE
9	g	814	LEU
9	g	815	VAL
9	g	819	GLN
9	g	831	LEU
9	g	971	ILE
9	g	981	ARG
9	g	984	PHE
9	g	985	ASN
9	g	1011	ASP
9	g	1016	PHE
9	g	1058	LEU
9	g	1064	ARG
9	g	1074	ASN
9	g	1084	LEU
9	g	1143	GLU
9	g	1145	ASN
9	g	1147	THR
9	g	1152	THR
3	l	70	TYR
3	l	77	THR
3	l	91	LYS
3	l	99	ASN
3	l	105	ARG
3	l	108	LEU
3	l	109	THR
3	l	172	GLN
3	l	220	TYR
3	l	249	THR

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Mol	Chain	Res	Type
3	l	282	LEU
3	l	285	ASN
3	l	289	THR
3	l	315	PHE
3	l	344	VAL
3	l	437	ASN
3	l	449	ILE
3	l	451	ARG
3	l	464	THR
3	l	465	LEU
3	l	469	GLU
3	l	486	LEU
3	l	488	THR
3	l	497	MET
3	l	562	PHE
3	l	619	LEU
3	l	649	GLN
3	l	664	LEU
3	l	667	LEU
3	l	679	LEU
3	l	718	SER
3	l	780	HIS
3	l	889	LEU
3	l	942	ILE
3	l	972	LYS
3	l	1002	MET
3	l	1022	SER
4	m	52	THR
4	m	58	ILE
4	m	94	ARG
4	m	122	ARG
4	m	125	ASN
4	m	135	ASN
4	m	186	ARG
4	m	196	ASP
4	m	201	ARG
4	m	216	ASP
4	m	390	TRP
4	m	433	ILE
4	m	461	MET
4	m	488	LEU
4	m	497	ARG

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Mol	Chain	Res	Type
4	m	504	ILE
4	m	514	VAL
4	m	515	THR
4	m	520	GLU
4	m	542	LEU
4	m	588	ASP
4	m	592	ASN
4	m	603	ASP
4	m	616	VAL
4	m	624	LEU
4	m	647	ARG
4	m	662	TYR
4	m	673	PRO
4	m	683	MET
4	m	730	ASN
5	n	167	LYS
5	n	177	THR
5	n	182	LYS
5	n	331	ARG
5	n	342	LYS
5	n	388	THR
5	n	433	LYS
5	n	445	LEU
5	n	452	TYR
5	n	487	HIS
5	n	570	MET
5	n	585	ASN
5	n	637	LEU
5	n	776	GLN
6	o	18	ASP
6	o	32	THR
6	o	43	HIS
6	o	56	VAL
6	o	63	HIS
6	o	66	PHE
6	o	136	THR
6	o	155	PRO
6	o	217	LEU
6	o	220	SER
6	o	229	ARG
6	o	230	THR
6	o	246	THR

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Mol	Chain	Res	Type
6	o	247	LEU
7	p	11	LEU
7	p	80	THR
7	p	146	ARG
7	p	163	ASN
7	p	183	LEU
7	p	188	LEU
7	p	212	LYS
7	p	229	GLN
7	p	320	SER
7	p	334	THR
7	p	342	MET
8	q	7	TYR
8	q	8	GLN
8	q	27	ASN
8	q	31	ASN
8	q	66	LYS
8	q	110	MET
8	q	161	PRO
8	q	172	LYS
8	q	180	PHE
8	q	188	ILE
8	q	206	ILE
8	q	213	CYS
8	q	218	TYR
8	q	220	ASN
8	q	223	ILE
8	q	245	ARG
8	q	267	LEU
8	q	313	LEU
8	q	317	LEU
8	q	382	LYS
8	q	438	GLU
8	q	460	LYS
8	q	523	TYR
8	q	603	SER
8	q	619	LYS
8	q	633	THR
8	q	679	LYS
9	r	70	LYS
9	r	104	LYS
9	r	441	ARG

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Mol	Chain	Res	Type
9	r	515	ASN
9	r	516	LEU
9	r	560	ARG
9	r	569	THR
9	r	585	LEU
9	r	588	ILE
9	r	591	PHE
9	r	618	LEU
9	r	632	LYS
9	r	639	PRO
9	r	666	LYS
9	r	773	ASN
9	r	812	SER
9	r	848	PHE
9	r	964	LEU
9	r	1087	LYS
9	r	1152	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	318	HIS
1	X	322	HIS
1	X	360	GLN
1	X	414	ASN
1	X	692	ASN
1	X	740	ASN
1	X	780	HIS
1	X	804	GLN
1	X	829	ASN
1	X	849	ASN
1	X	1055	GLN
1	X	1093	ASN
1	X	1195	GLN
1	X	1249	GLN
1	X	1306	ASN
1	X	1558	GLN
3	a	132	GLN
3	a	269	HIS
3	a	343	ASN
3	a	369	ASN
3	a	393	HIS

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Mol	Chain	Res	Type
3	a	418	GLN
3	a	430	ASN
3	a	584	ASN
3	a	756	GLN
3	a	780	HIS
3	a	903	ASN
3	a	929	HIS
3	a	952	ASN
4	b	54	ASN
4	b	77	GLN
4	b	141	ASN
4	b	153	ASN
4	b	226	GLN
4	b	467	ASN
4	b	545	GLN
4	b	550	HIS
4	b	632	GLN
5	c	265	HIS
5	c	293	GLN
5	c	328	ASN
5	c	341	GLN
5	c	480	GLN
5	c	489	HIS
5	c	631	GLN
6	d	103	ASN
6	d	110	HIS
6	d	144	HIS
6	d	192	GLN
6	d	276	ASN
7	e	300	HIS
8	f	8	GLN
8	f	31	ASN
8	f	61	ASN
8	f	220	ASN
8	f	240	HIS
8	f	273	ASN
8	f	274	GLN
8	f	300	ASN
8	f	305	ASN
8	f	428	ASN
8	f	466	ASN
8	f	586	GLN

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Mol	Chain	Res	Type
8	f	589	HIS
9	g	158	GLN
9	g	241	GLN
9	g	262	ASN
9	g	422	ASN
9	g	555	GLN
9	g	628	HIS
9	g	663	GLN
9	g	761	ASN
9	g	854	HIS
9	g	948	GLN
9	g	962	ASN
9	g	1027	ASN
9	g	1134	HIS
3	l	21	ASN
3	l	22	ASN
3	l	58	ASN
3	l	200	ASN
3	l	481	HIS
3	l	492	ASN
3	l	658	HIS
3	l	780	HIS
3	l	871	HIS
4	m	61	ASN
5	n	252	ASN
5	n	289	ASN
5	n	317	HIS
5	n	339	GLN
5	n	406	HIS
5	n	428	ASN
5	n	443	ASN
5	n	487	HIS
5	n	523	ASN
5	n	525	HIS
6	o	98	HIS
6	o	144	HIS
7	p	23	HIS
7	p	32	HIS
7	p	211	HIS
7	p	289	GLN
8	q	8	GLN
8	q	27	ASN

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Mol	Chain	Res	Type
8	q	240	HIS
8	q	509	HIS
8	q	528	HIS
8	q	553	ASN
8	q	586	GLN
8	q	668	HIS
9	r	100	ASN
9	r	111	HIS
9	r	249	ASN
9	r	321	GLN
9	r	428	GLN
9	r	451	ASN
9	r	497	HIS
9	r	508	ASN
9	r	510	ASN
9	r	515	ASN
9	r	625	GLN
9	r	637	ASN
9	r	668	ASN
9	r	752	GLN
9	r	761	ASN
9	r	773	ASN
9	r	785	HIS
9	r	789	ASN
9	r	790	HIS
9	r	796	ASN
9	r	854	HIS
9	r	858	ASN
9	r	873	GLN
9	r	889	GLN
9	r	1027	ASN
9	r	1060	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	l	4
5	c	2
5	n	2
9	r	1
3	a	1
9	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	877:GLU	C	878:SER	N	16.07
1	l	207:SER	C	208:LEU	N	14.63
1	l	206:LYS	C	207:SER	N	13.72
1	a	486:LEU	C	487:ASN	N	6.43
1	c	533:PRO	C	535:SER	N	5.54
1	g	807:PHE	C	808:TYR	N	5.07
1	n	665:ILE	C	760:VAL	N	4.73
1	l	486:LEU	C	487:ASN	N	4.13
1	n	533:PRO	C	535:SER	N	4.10
1	l	460:ALA	C	461:SER	N	4.03
1	c	665:ILE	C	760:VAL	N	3.49

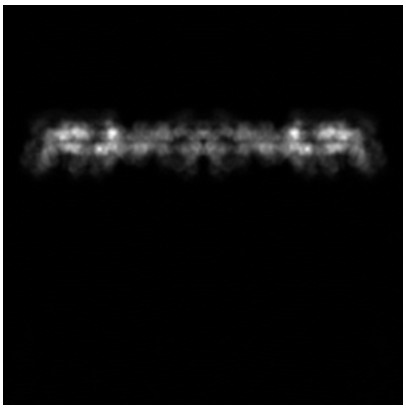
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24231. These allow visual inspection of the internal detail of the map and identification of artifacts.

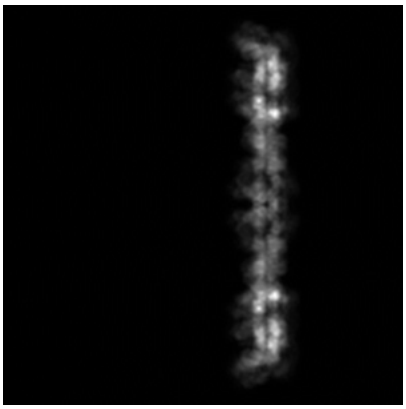
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

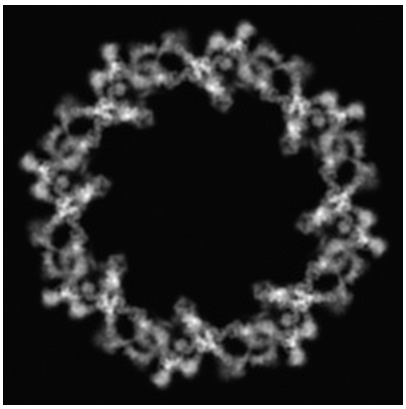
6.1.1 Primary map



X

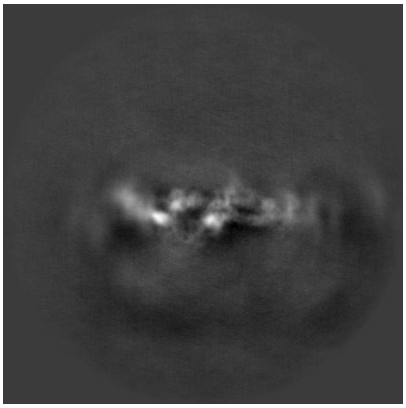


Y

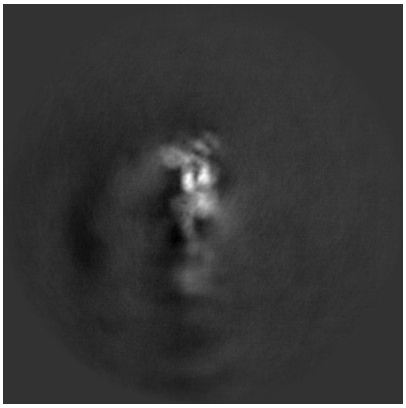


Z

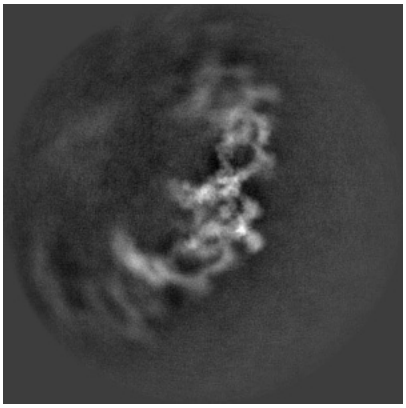
6.1.2 Raw map



X



Y



Z

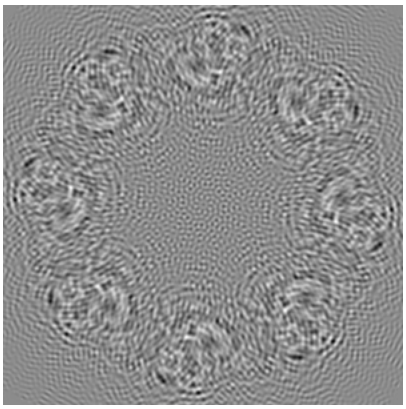
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

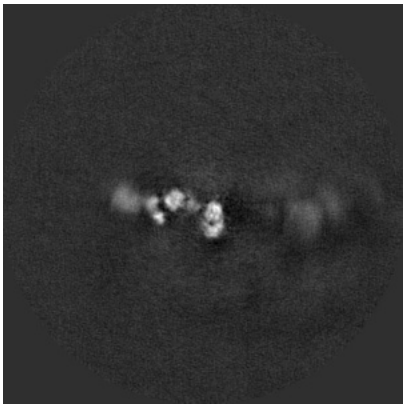
X Index: 240

Y Index: 240

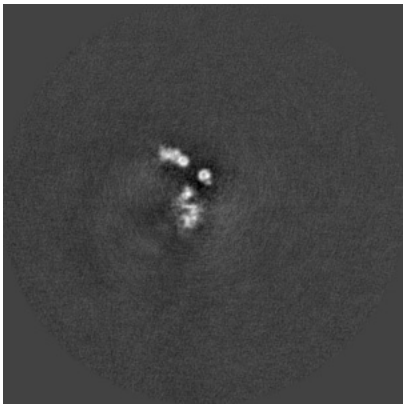


Z Index: 240

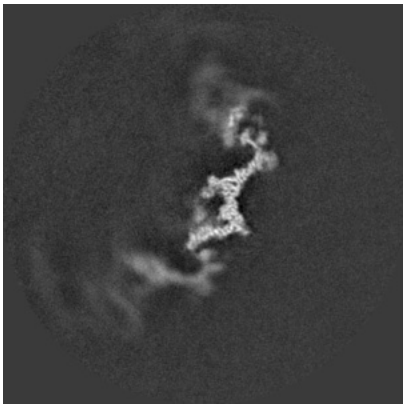
6.2.2 Raw map



X Index: 150



Y Index: 150

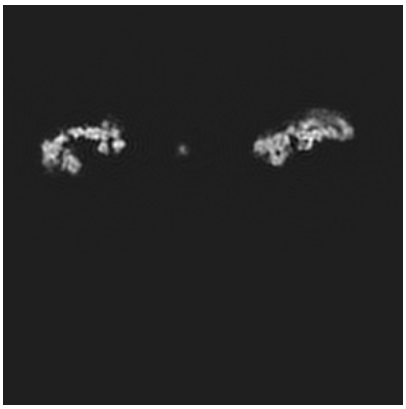


Z Index: 150

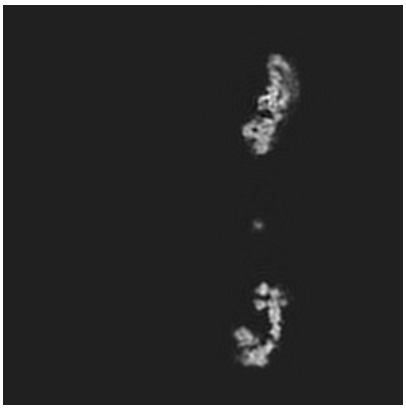
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

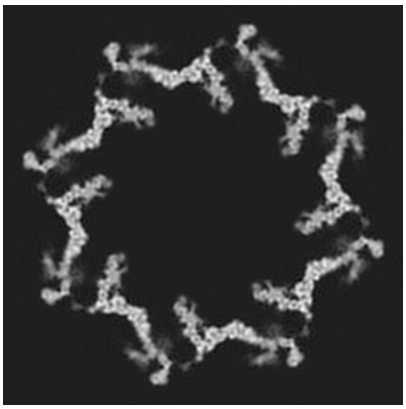
6.3.1 Primary map



X Index: 351

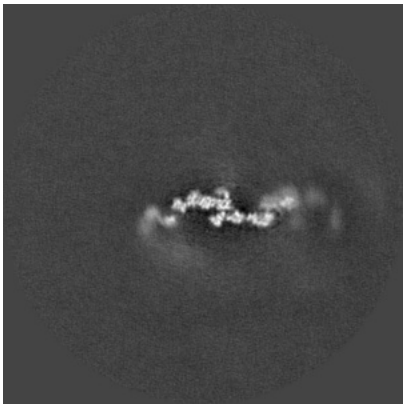


Y Index: 129

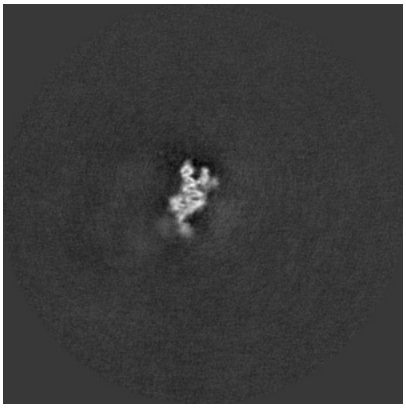


Z Index: 309

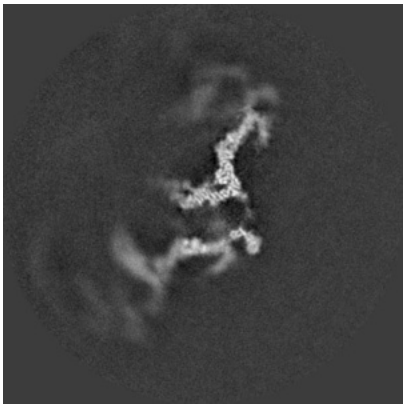
6.3.2 Raw map



X Index: 170



Y Index: 158

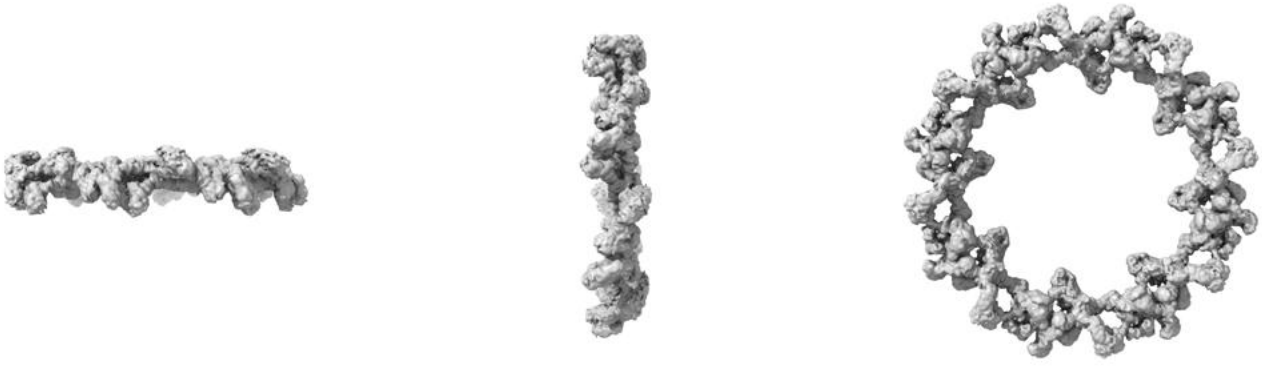


Z Index: 140

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

6.4 Orthogonal surface views (i)

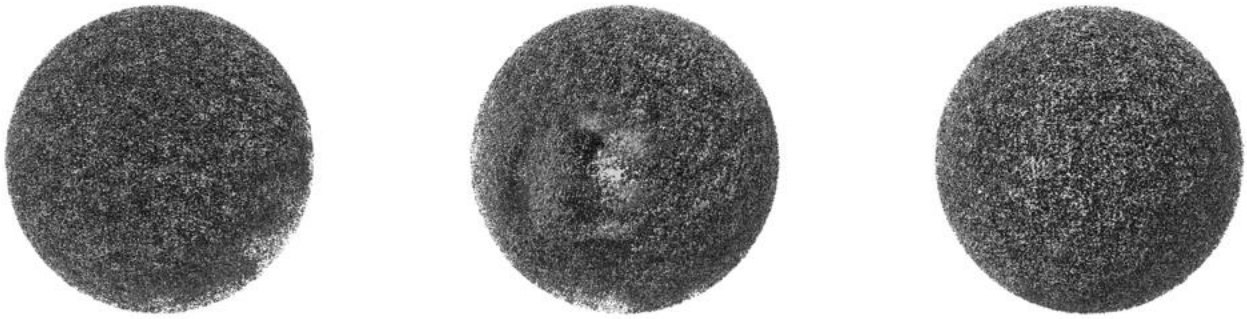
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

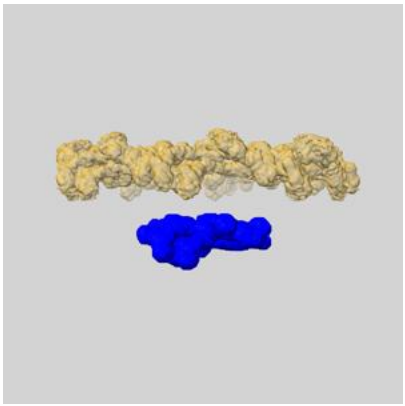
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

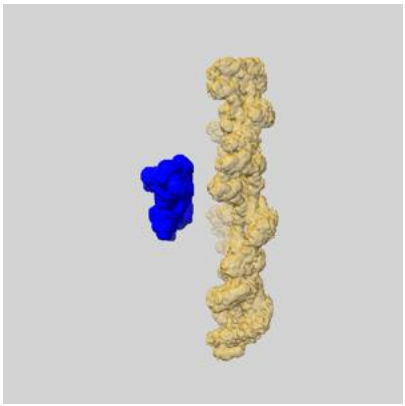
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

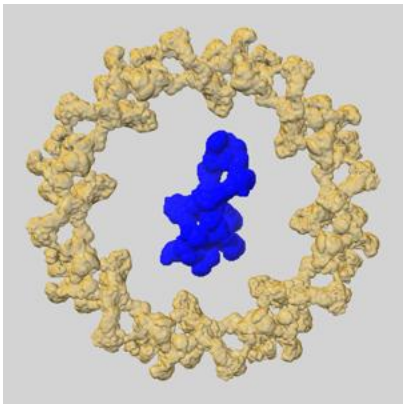
6.5.1 emd_24231_msk_1.map (i)



X



Y

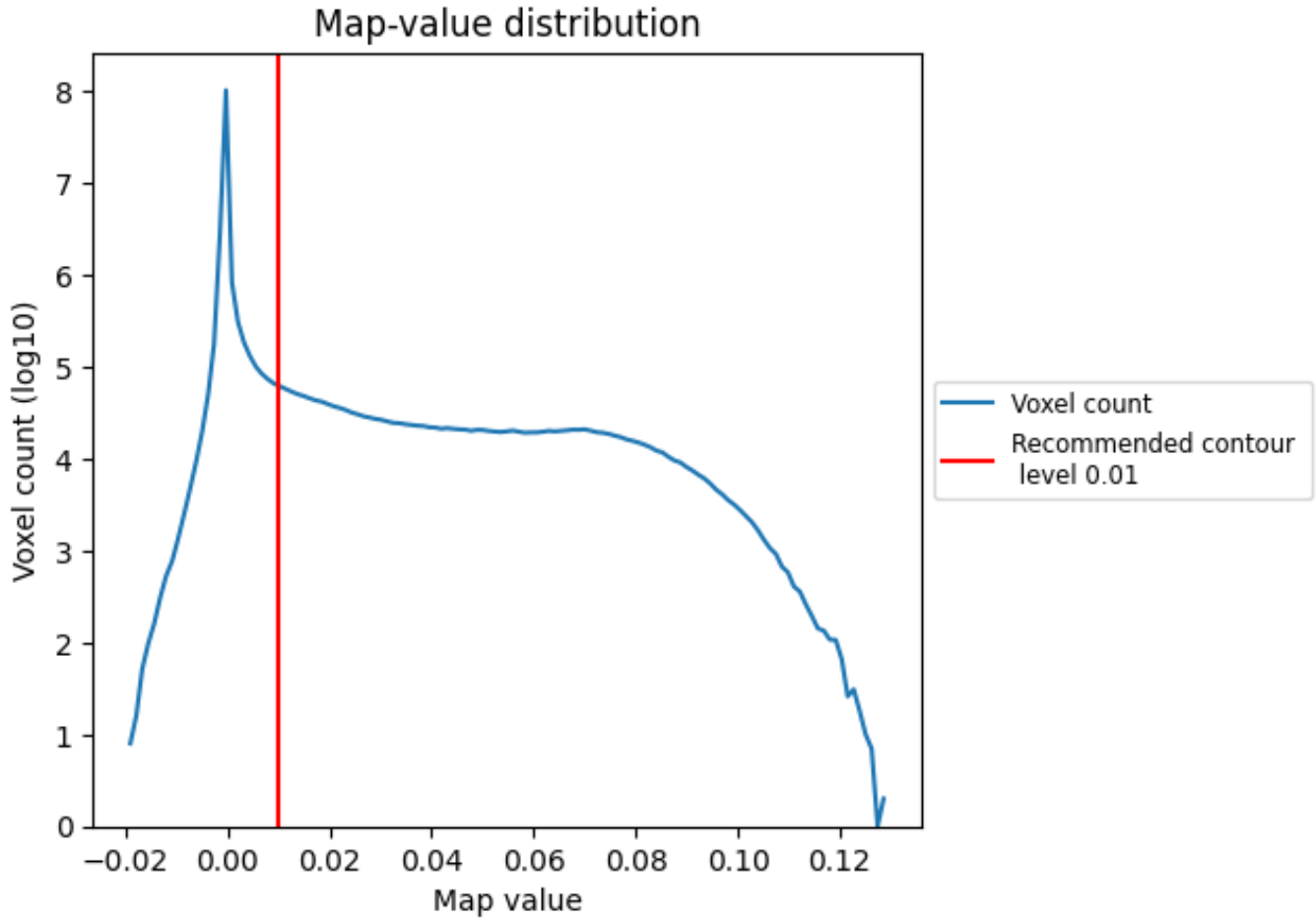


Z

7 Map analysis

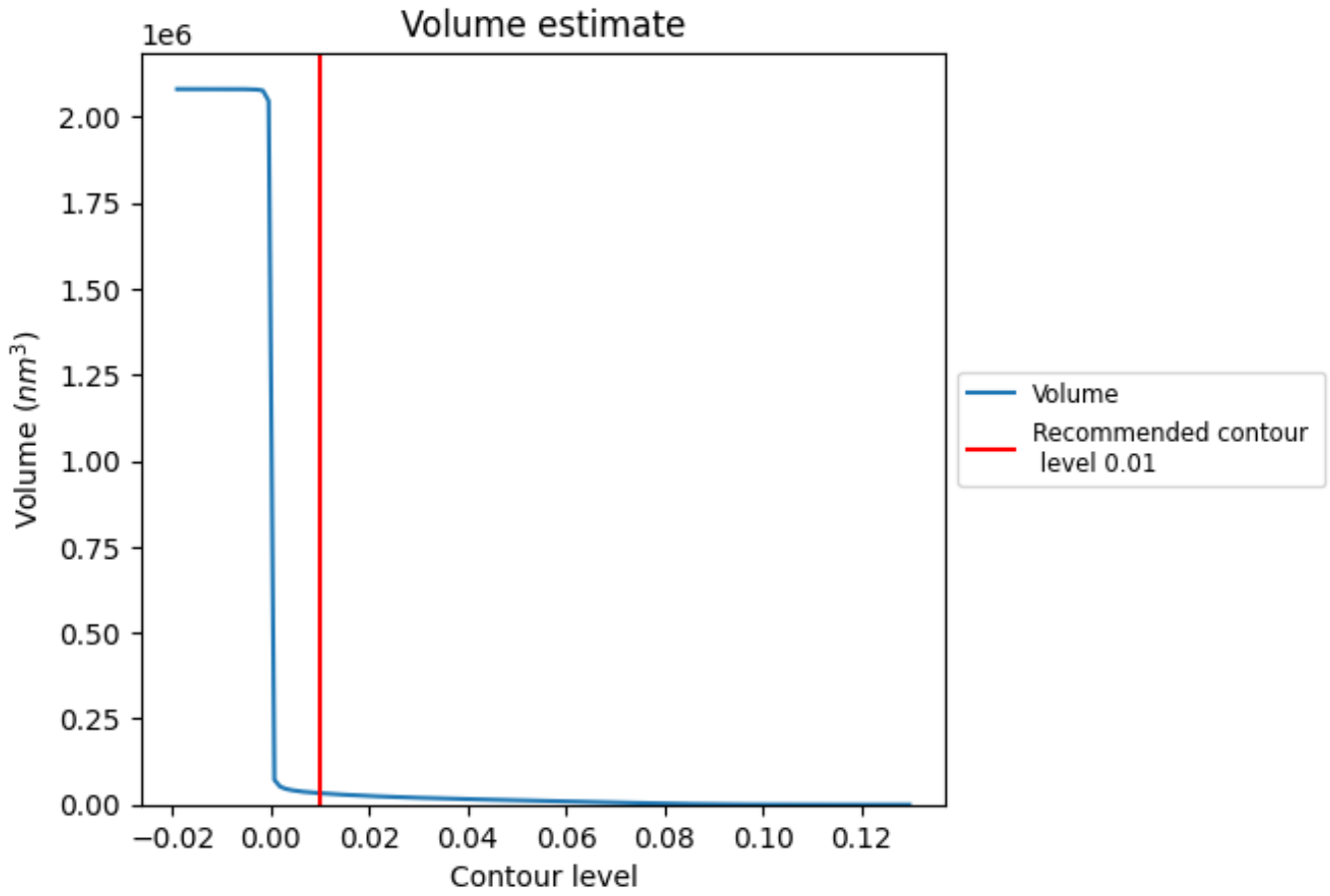
This section contains the results of statistical analysis of the map.

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.

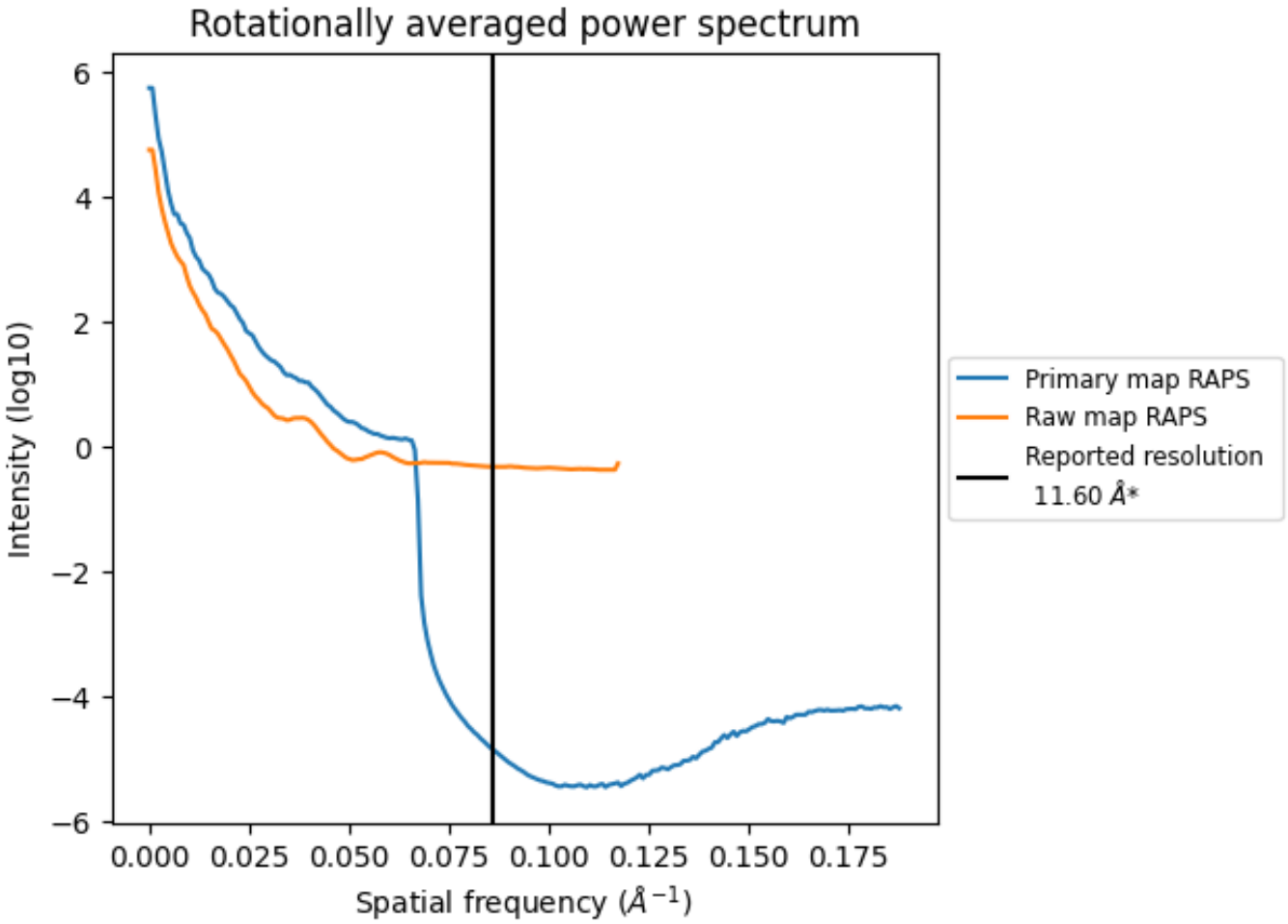
7.2 Volume estimate



The volume at the recommended contour level is 33303 nm^3; this corresponds to an approximate mass of 30083 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)

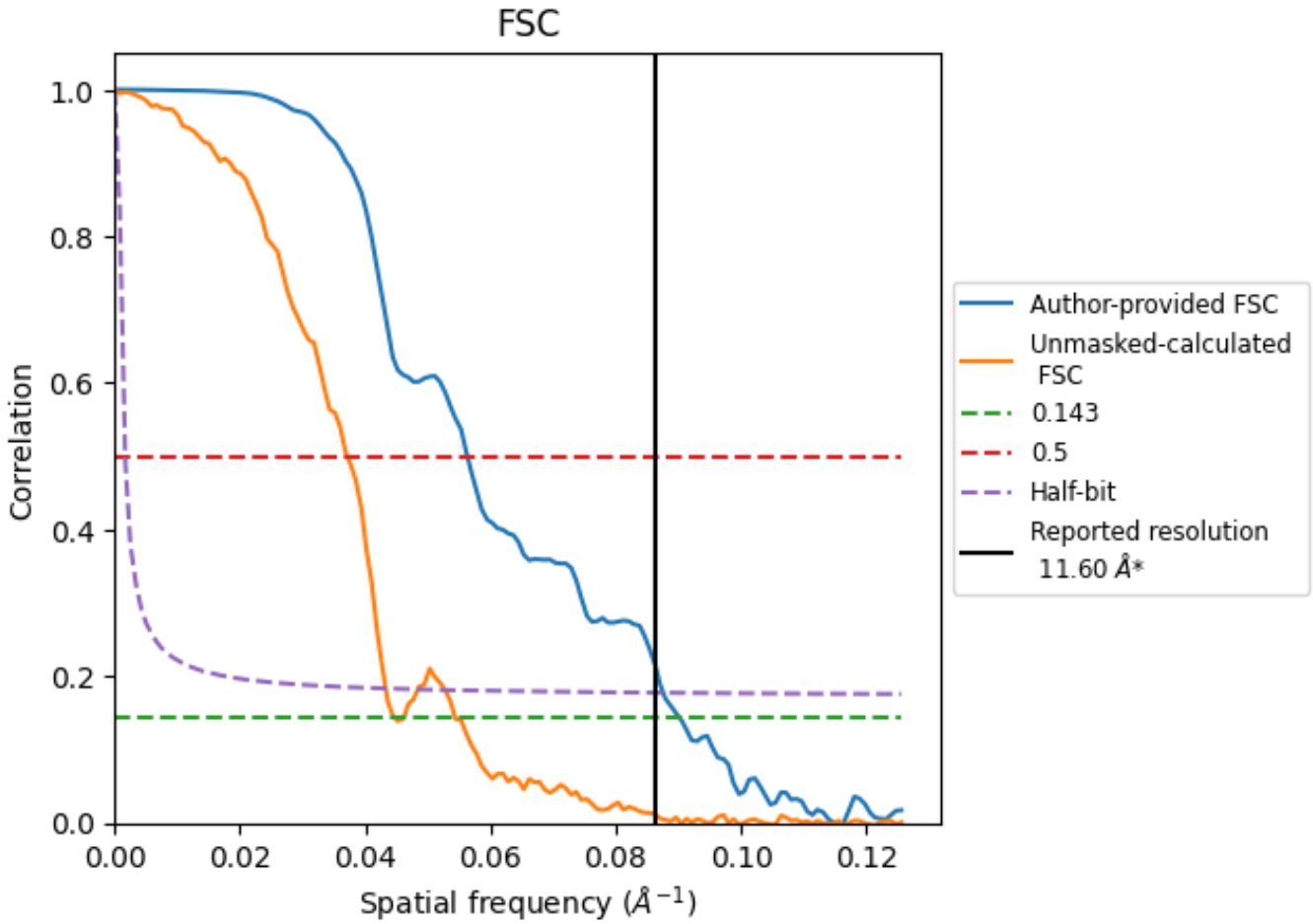


*Reported resolution corresponds to spatial frequency of 0.086 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.086 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.60	-	-
Author-provided FSC curve	11.09	17.76	11.42
Unmasked-calculated*	22.37	26.95	23.15

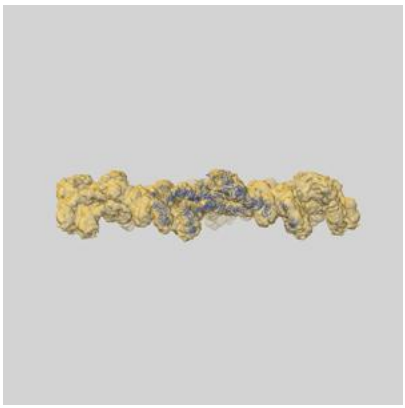
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 22.37 differs from the reported value 11.6 by more than 10 %

9 Map-model fit

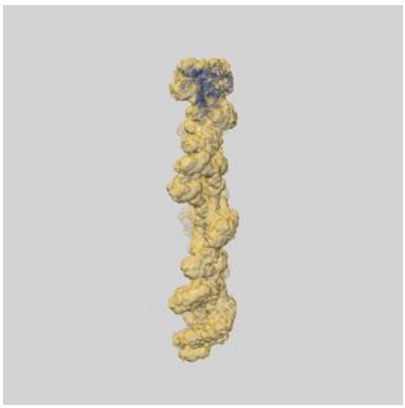
This section contains information regarding the fit between EMDB map EMD-24231 and PDB model 7N84. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

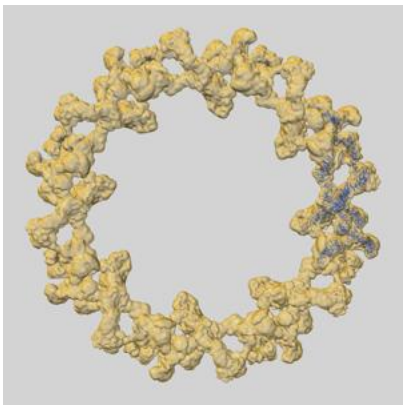
9.1.1 Map-model overlay



X

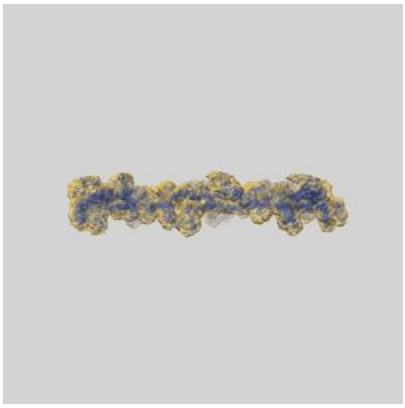


Y

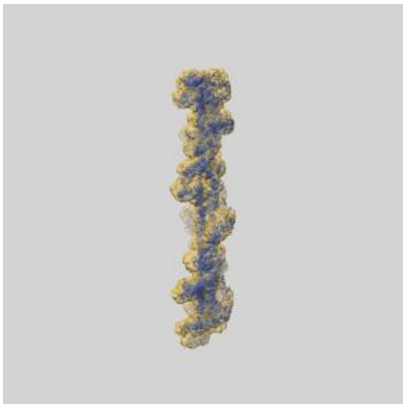


Z

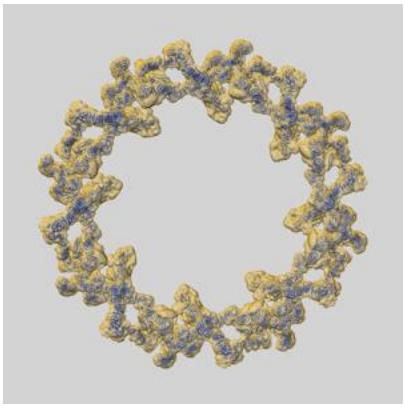
9.1.2 Map-model assembly overlay



X



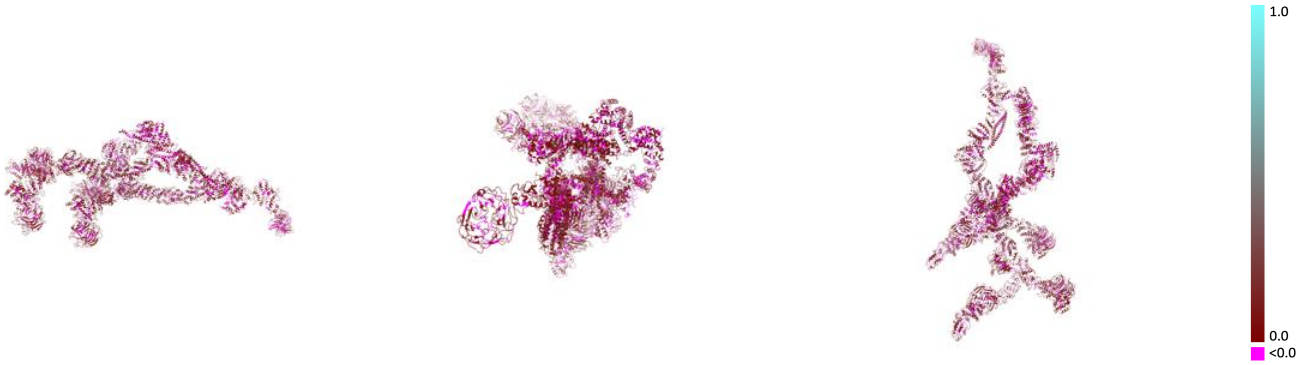
Y



Z

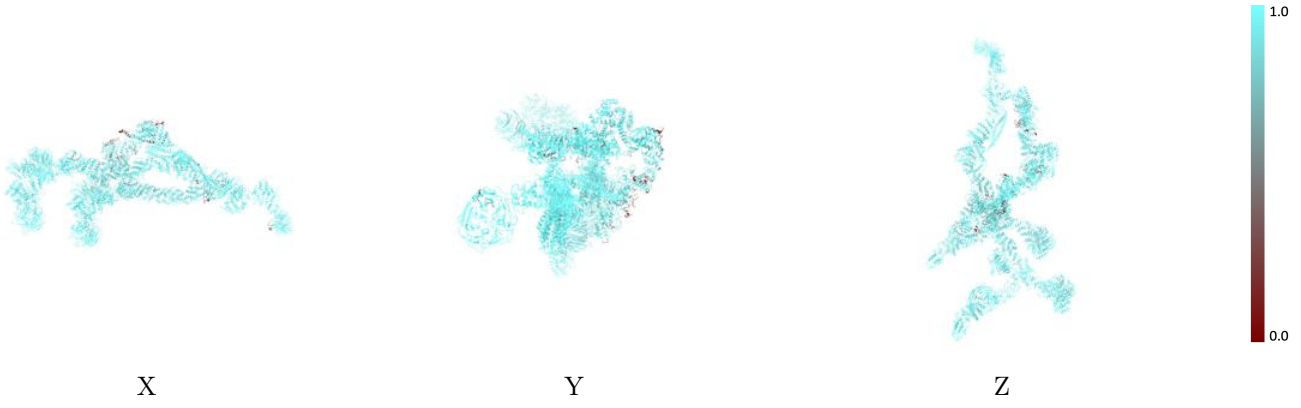
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



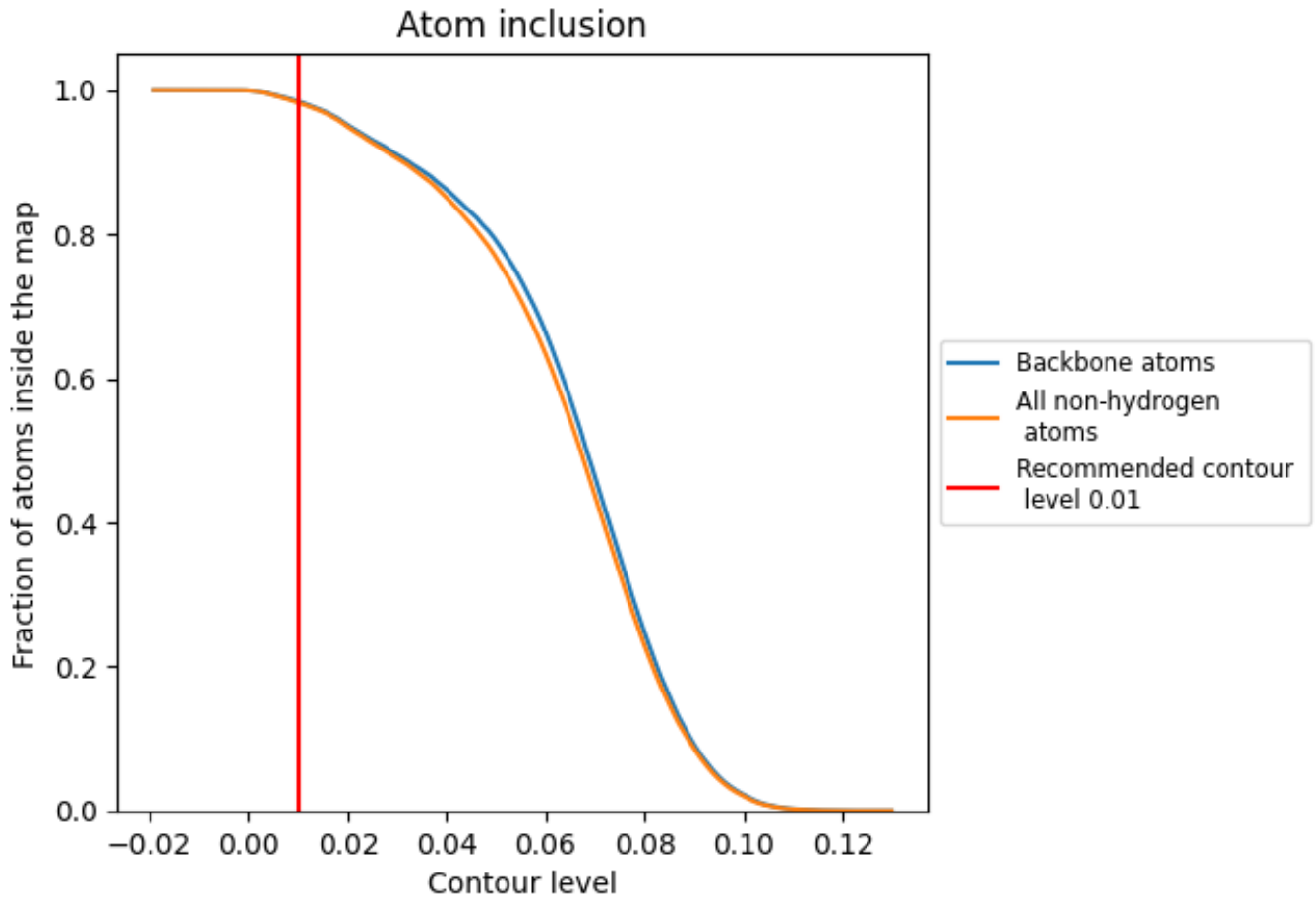
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9824	0.0630
X	0.8873	0.0340
Y	0.9873	0.0690
Z	1.0000	0.0680
a	0.9999	0.0700
b	1.0000	0.0610
c	1.0000	0.0820
d	1.0000	0.0660
e	1.0000	0.0680
f	1.0000	0.0760
g	0.9913	0.0490
l	1.0000	0.0700
m	1.0000	0.0700
n	1.0000	0.0860
o	1.0000	0.0690
p	1.0000	0.0620
q	1.0000	0.0770
r	0.9607	0.0520