



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:50 AM UTC

PDB ID : 7N85 / pdb_00007n85
EMDB ID : EMD-24232
Title : Inner ring spoke from the isolated yeast NPC
Authors : Akey, C.W.; Rout, M.P.; Ouch, C.; Echeverria, I.; Fernandez-Martinez, J.;
Nudelman, I.
Deposited on : 2021-06-13
Resolution : 7.60 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:

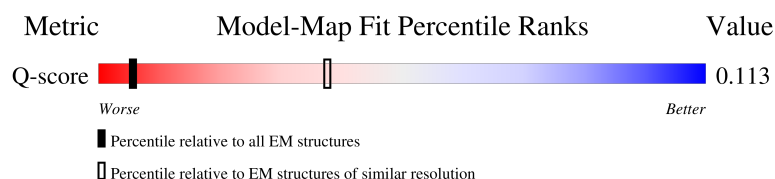
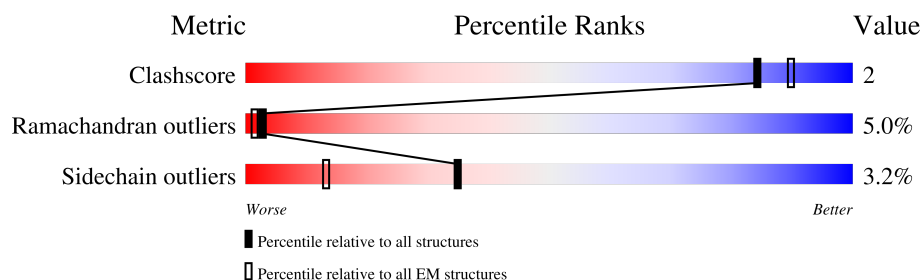
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 7.60 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.



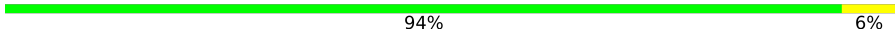
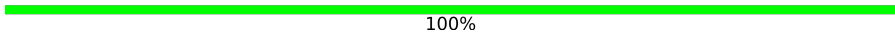
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	389 (7.10 - 8.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	1502	
1	Y	1502	
2	1	1391	
2	Z	1391	

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Mol	Chain	Length	Quality of chain
3	5	36	 94% 6%
3	6	36	 100%
4	A	823	 18% 80%
4	D	823	 18% 80%
4	G	823	 18% 80%
4	J	823	 18% 80%
5	B	541	 6% 34% 5% 60%
5	E	541	 35% 5% 60%
5	H	541	 35% 5% 60%
5	K	541	 35% 5% 60%
6	C	472	 5% 32% 65%
6	F	472	 33% 65%
6	I	472	 33% 65%
6	L	472	 34% 65%
7	M	1683	 78% 11% 10%
7	O	1683	 78% 11% 10%
8	N	1655	 66% 13% 18%
8	P	1655	 64% 15% 18%
9	Q	839	 11% 74% 7% 18%
9	R	839	 76% 7% 16%
9	S	839	 10% 74% 7% 18%
9	T	839	 76% 8% 16%
10	U	475	 16% 80%
10	W	475	 17% 80%
11	V	528	 15% 83%

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Mol	Chain	Length	Quality of chain
11	X	528	16% . 82%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 123117 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 NUP170.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	1102	Total	C	N	O	S	0	0
			8890	5753	1449	1659	29		
1	Y	1084	Total	C	N	O	S	0	0
			8747	5663	1422	1632	30		

- Molecule 2 is a protein called Nucleoporin NUP157.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	1111	Total	C	N	O	S	0	0
			8903	5707	1477	1691	28		
2	Z	1108	Total	C	N	O	S	0	0
			8883	5695	1474	1686	28		

- Molecule 3 is a protein called Unknown connectors.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	5	36	Total	C	N	O	0	0
			181	108	36	37		
3	6	36	Total	C	N	O	0	0
			181	108	36	37		

- Molecule 4 is a protein called Nucleoporin NSP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	163	Total	C	N	O	S	0	0
			1315	814	220	280	1		
4	D	163	Total	C	N	O	S	0	0
			1315	814	220	280	1		
4	G	164	Total	C	N	O	S	0	0
			1321	817	221	282	1		
4	J	163	Total	C	N	O	S	0	0
			1315	814	220	280	1		

- Molecule 5 is a protein called Nucleoporin NUP57.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		
5	E	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		
5	H	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		
5	K	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		

- Molecule 6 is a protein called Nucleoporin NUP49/NSP49.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	166	Total	C	N	O	S	0	0
			1347	863	217	265	2		
6	F	167	Total	C	N	O	S	0	0
			1351	865	218	266	2		
6	I	166	Total	C	N	O	S	0	0
			1347	863	217	265	2		
6	L	167	Total	C	N	O	S	0	0
			1351	865	218	266	2		

- Molecule 7 is a protein called Nucleoporin NUP192.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	1520	Total	C	N	O	S	0	0
			11905	7692	1942	2240	31		
7	O	1521	Total	C	N	O	S	0	0
			11909	7694	1943	2241	31		

- Molecule 8 is a protein called Nucleoporin NUP188.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	1358	Total	C	N	O	S	0	0
			10955	7154	1742	2034	25		
8	P	1358	Total	C	N	O	S	0	0
			10955	7153	1743	2035	24		

- Molecule 9 is a protein called Nucleoporin NIC96.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	689	Total	C	N	O	S	0	0
			5192	3300	895	980	17		
9	R	707	Total	C	N	O	S	0	0
			5279	3351	913	998	17		
9	S	689	Total	C	N	O	S	0	0
			5189	3297	895	980	17		
9	T	707	Total	C	N	O	S	0	0
			5279	3351	913	998	17		

- Molecule 10 is a protein called Nucleoporin NUP53.

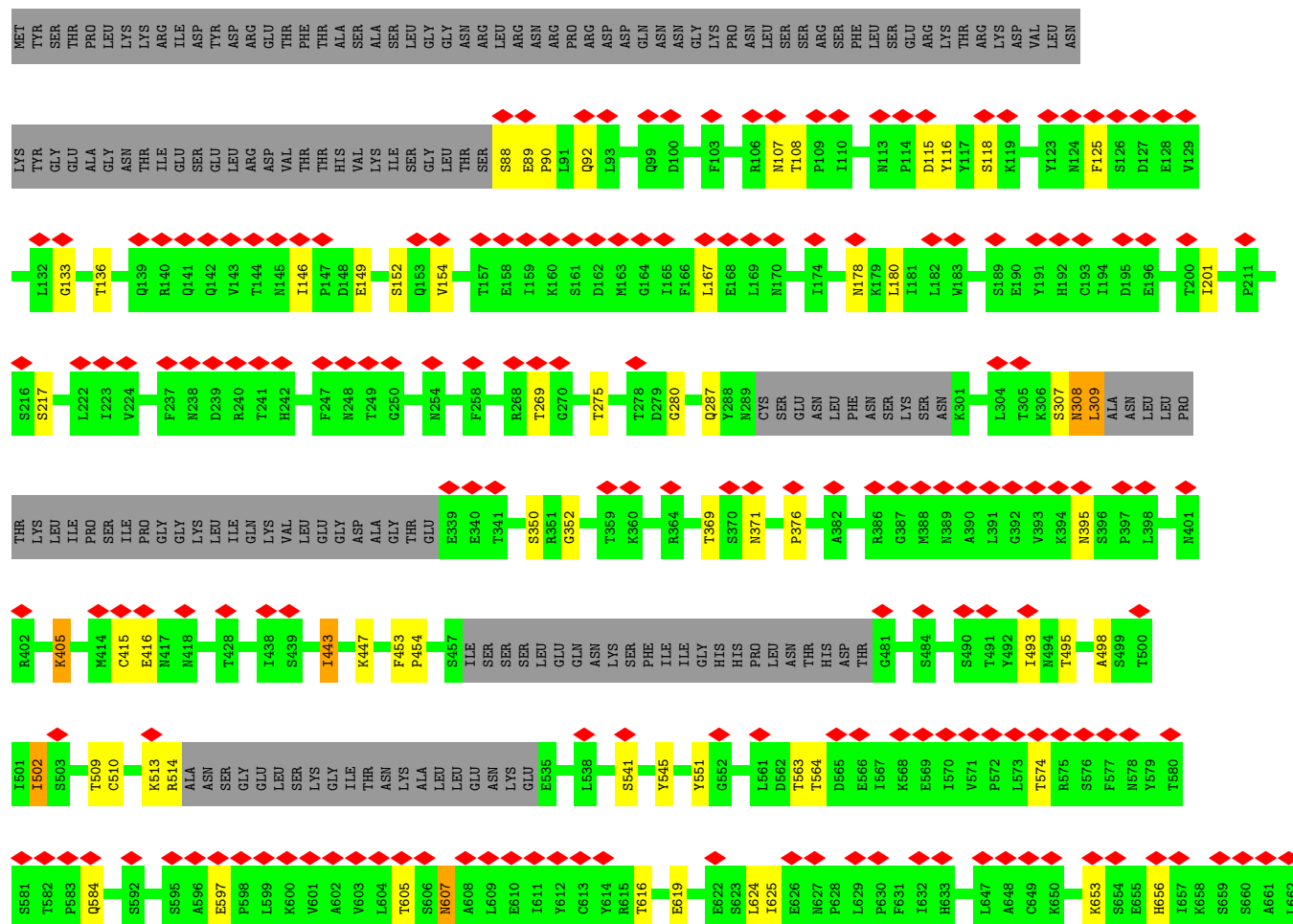
Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	93	Total	C	N	O	S	0	0
			736	480	118	136	2		
10	W	93	Total	C	N	O	S	0	0
			736	480	118	136	2		

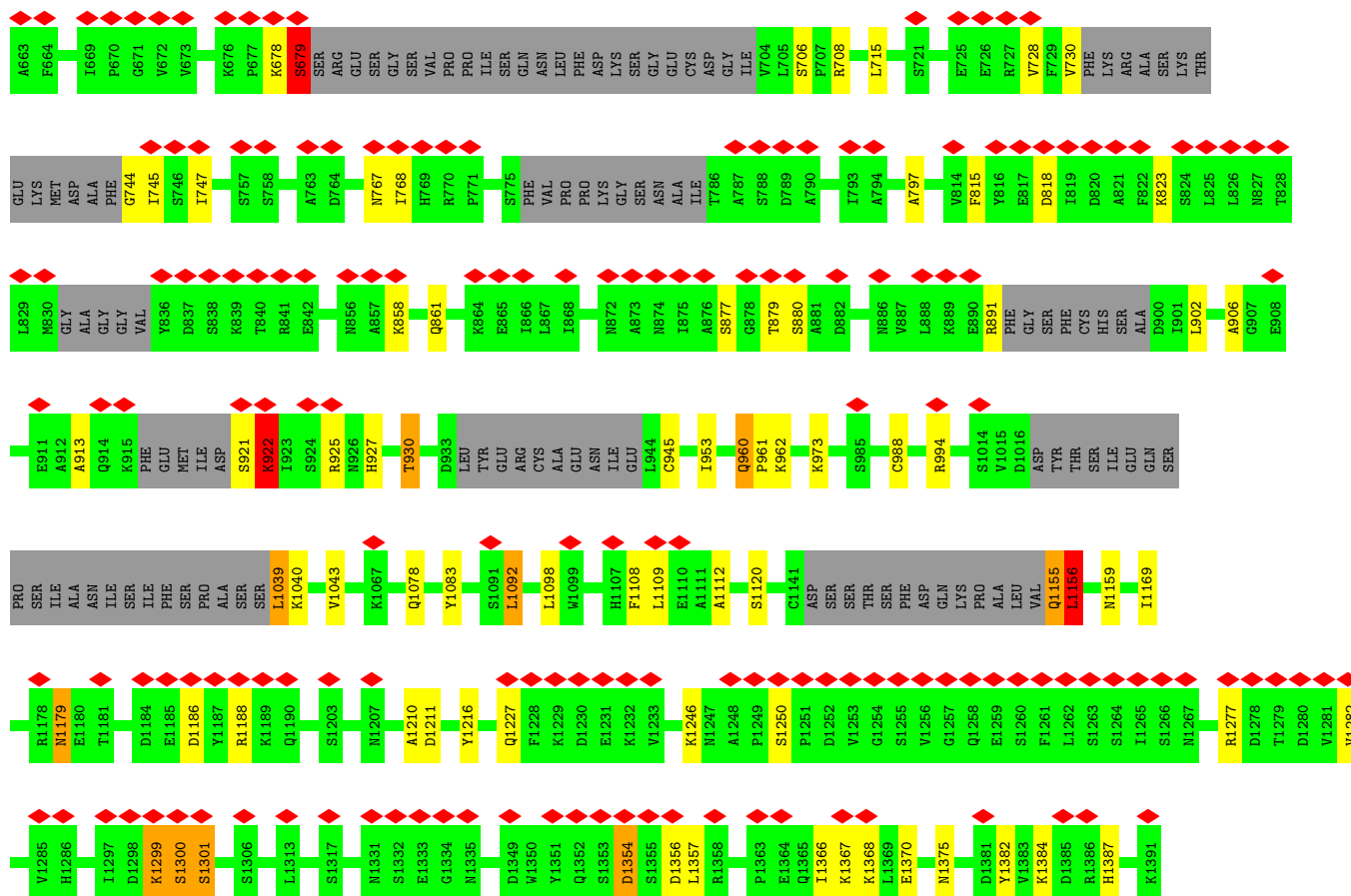
- Molecule 11 is a protein called Nucleoporin ASM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	92	Total	C	N	O	S	0	0
			720	465	116	136	3		
11	X	93	Total	C	N	O	S	0	0
			731	471	120	137	3		

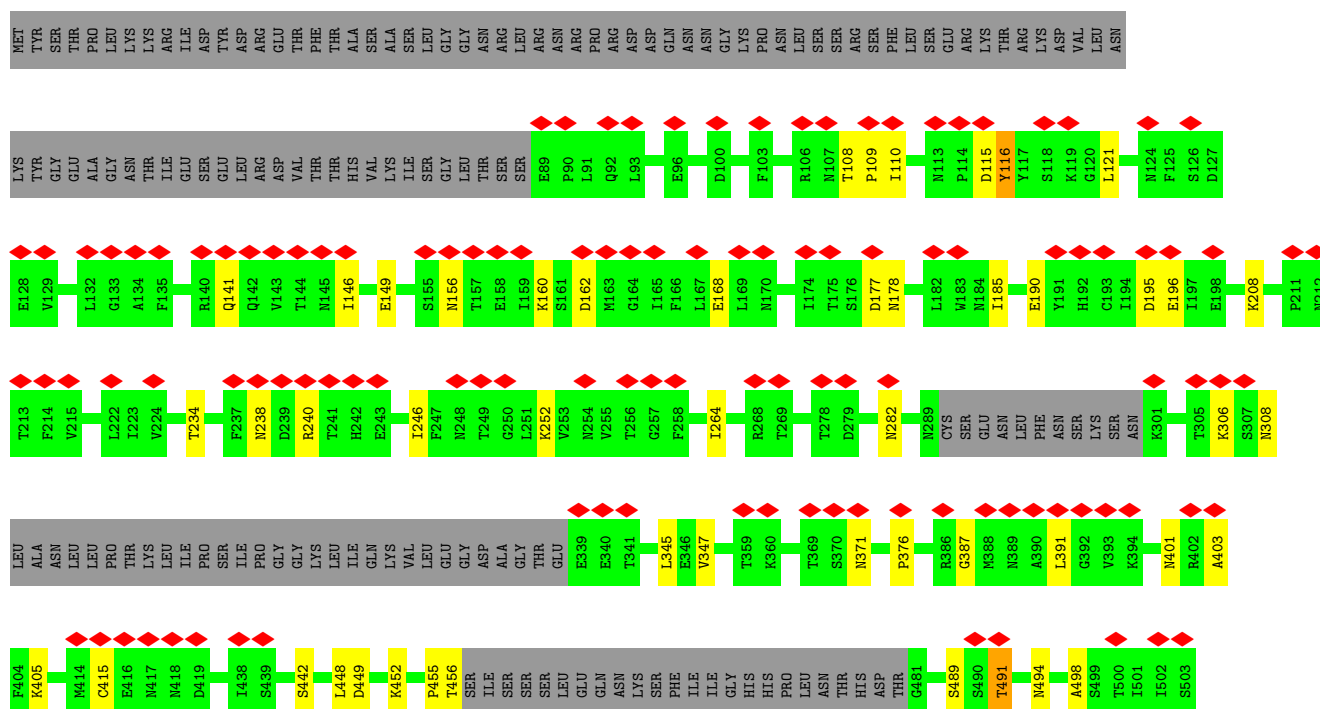


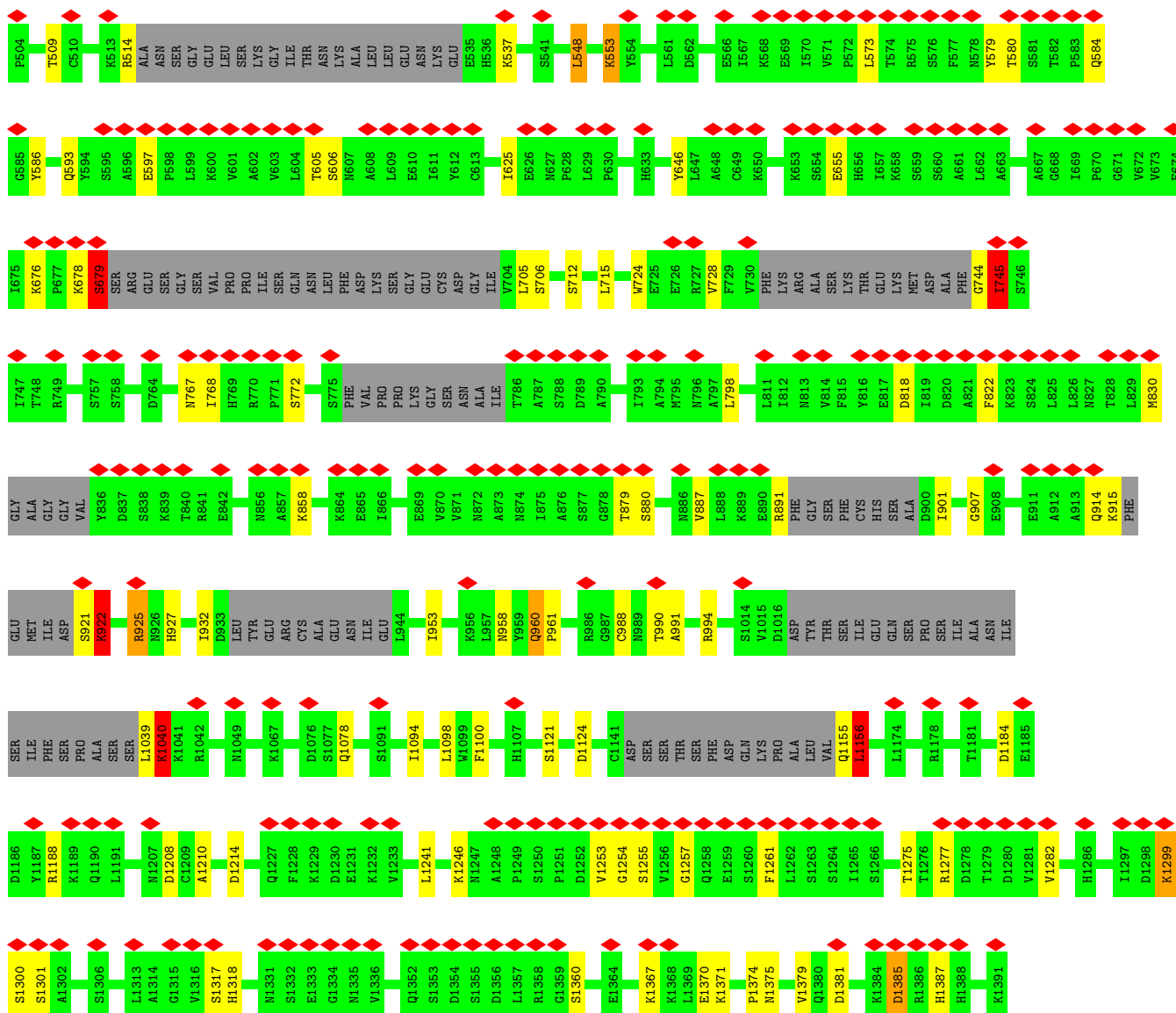
- Molecule 2: Nucleoporin NUP157





• Molecule 2: Nucleoporin NUP157





- Molecule 3: Unknown connectors

Chain 5: 94% 6%



- Molecule 3: Unknown connectors

Chain 6: 100%

There are no outlier residues recorded for this chain.

- Molecule 4: Nucleoporin NSP1

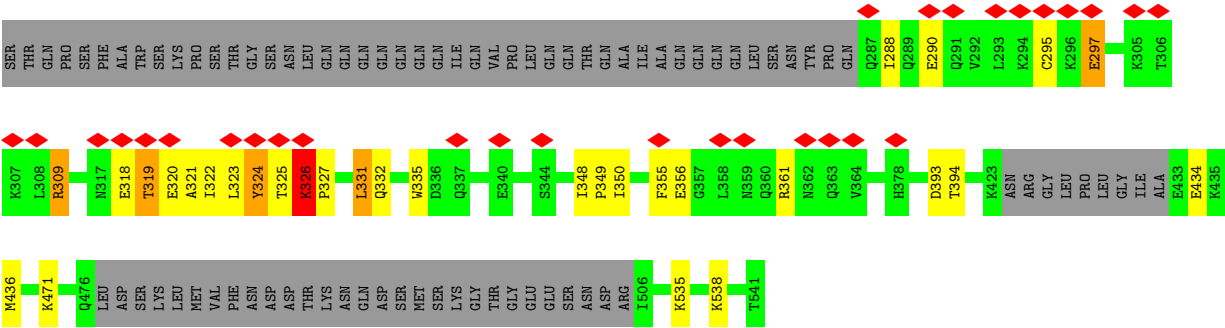
Chain A: 18% 80%

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- Molecule 4: Nucleoporin NSP1

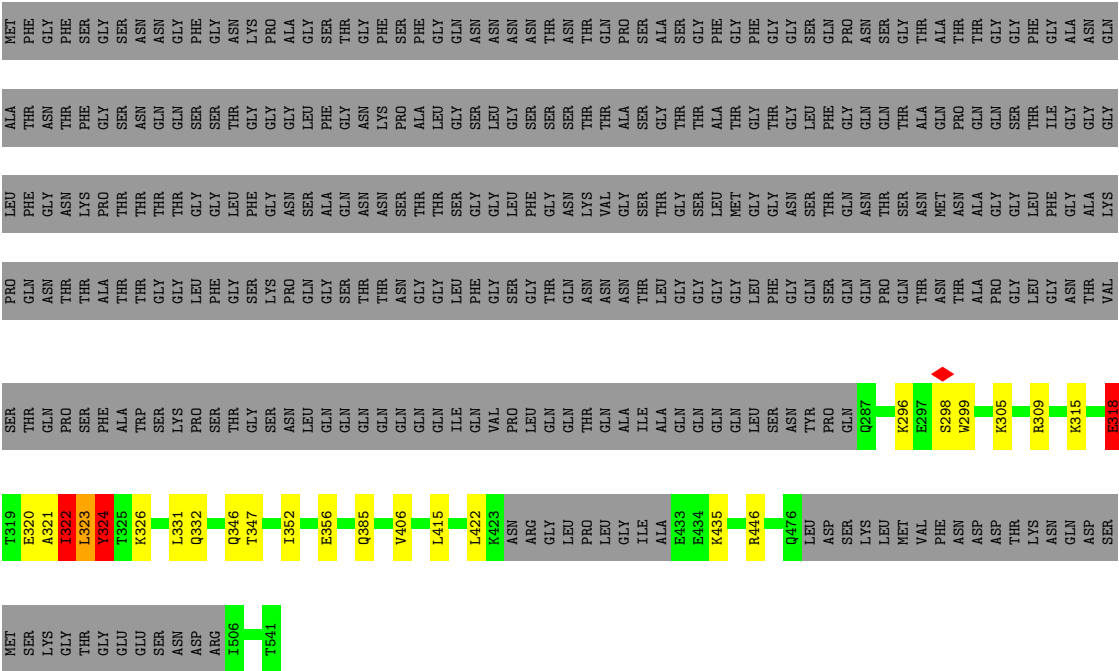


V725	GLU	LYS	ASP	ALA	SER	PRO	SER	PHE	GLY	ASN	THR	MET
V726	GLU	GLU	GLY	LYS	SER	PHE	GLY	ALA	THR	PRO	ASN	THR
S727	SER	SER	LYS	LYS	SER	ALA	GLY	SER	ALA	PHE	THR	PHE
THR	SER	GLU	ASP	GLY	ASN	ALA	GLY	THR	GLY	GLY	GLY	GLY
SER	GLY	SER	SER	ASP	ASP	SER	SER	ALA	ALA	SER	SER	SER
GLY	LYS	LYS	ASP	LYS	LYS	ALA	GLY	ALA	ASN	ASN	GLN	GLN
ALA	SER	SER	SER	GLN	SER	GLY	GLY	PRO	ASN	GLN	ASN	ASN
ALA	SER	ALA	SER	ASP	GLY	GLY	GLY	GLY	LYS	THR	LYS	LYS
ASN	ASP	SER	PRO	THR	THR	ALA	ASP	GLY	ALA	THR	ASN	THR
ASN	VAL	PHE	ALA	ALA	GLY	LYS	GLY	GLY	PRO	THR	THR	PRO
ASN	LYS	GLY	PHE	LYS	ASP	LYS	ASP	PRO	GLU	ALA	PHE	PHE
GLN	SER	SER	SER	PRO	ALA	ASP	ALA	ASP	GLY	ASN	SER	SER
GLN	SER	LYS	PHE	ALA	SER	GLY	SER	GLY	GLY	GLY	PHE	PHE
LYS	ASP	PRO	GLY	PHE	LYS	ASN	PRO	LYS	PRO	ASN	GLY	ASN
ARG	SER	THR	THR	SER	SER	PRO	SER	THR	ALA	SER	THR	THR
Q742	LEU	GLY	LYS	PHE	ALA	ALA	PHE	ALA	THR	THR	ALA	THR
Q743	LYS	LYS	SER	GLY	GLY	GLY	PHE	GLY	GLY	ASN	ASN	ASN
K744	LEU	GLU	ASN	GLY	ALA	SER	PHE	GLY	PHE	PRO	THR	THR
	ASN	GLU	ASN	GLY	LYS	LYS	SER	ALA	ALA	ASN	GLN	GLN
D752	LEU	GLY	GLY	GLY	LYS	PHE	GLY	ALA	ALA	ASN	ASN	ASN
E753	SER	GLY	LYS	LYS	GLY	PHE	GLY	ALA	SER	PHE	ASN	ASN
N754	LYS	ASP	LYS	ALA	ALA	LYS	LYS	ALA	SER	GLY	VAL	ASN
L755	PRO	GLY	ASP	GLY	GLY	LYS	LYS	PHE	VAL	GLY	PHE	THR
N756	VAL	ALA	SER	SER	LYS	PRO	GLY	PRO	ALA	GLY	LEU	GLY
	LEU	LYS	GLY	GLY	ASN	ASP	GLY	ALA	ALA	THR	GLY	THR
K778	LEU	ALA	SER	ALA	GLY	GLY	GLY	GLY	LYS	PHE	ASN	GLN
THR	PRO	ILE	LYS	GLY	THR	GLY	GLY	THR	GLY	GLY	GLY	THR
THR	VAL	SER	PRO	LYS	SER	ALA	ALA	ALA	ALA	THR	GLY	THR
ASN	SER	PHE	GLY	LYS	LYS	LYS	LYS	LYS	GLN	ASN	ASN	THR
ILE	LEU	GLY	PHE	LYS	LYS	ALA	PHE	ALA	ALA	ASN	GLY	GLY
ASP	ASN	ALA	SER	PRO	PRO	THR	THR	SER	THR	THR	THR	ALA
ILE	ASN	LYS	PHE	ALA	ALA	ALA	SER	ASP	THR	THR	THR	PHE
ASN	THR	PRO	GLY	PHE	LYS	LYS	LYS	ASN	THR	PRO	GLY	GLY
ASN	LYS	GLY	ALA	SER	SER	PRO	PRO	THR	GLY	SER	SER	ALA
GLU	L637	GLU	LYS	ALA	PHE	ALA	ALA	ALA	GLY	GLY	GLY	PHE
	D638	GLN	PRO	GLY	PHE	ALA	PHE	ALA	THR	THR	GLY	GLY
E789	D639	LYS	ASP	ALA	SER	SER	PHE	ALA	THR	THR	GLY	GLY
	L640	SER	GLY	LYS	PHE	LYS	PHE	ALA	THR	THR	GLY	GLY
L797	V641	SER	LYS	ASP	GLY	ASP	GLY	GLY	GLY	ALA	ASN	ALA
	T642	THR	ASN	GLY	GLY	GLY	LYS	LYS	PRO	GLN	ASN	THR
D808	K643	SER	ASP	LYS	LYS	PRO	GLY	GLY	PHE	LEU	THR	PHE
K823	W644	LYS	GLY	LYS	GLY	ALA	GLY	GLY	GLY	ASN	GLY	GLY
	T645	ALA	SER	VAL	ASP	GLY	GLY	GLY	PHE	LYS	LEU	GLY
	W646	PHE	LYS	LYS	GLY	ASP	ASP	ALA	THR	VAL	PHE	GLY
	T649	THR	PRO	ALA	ALA	ASP	ALA	GLY	LYS	VAL	GLY	GLY
		PHE	PHE	ALA	SER	ASP	LYS	LYS	ASN	ASN	ALA	ALA
	Y658	ALA	SER	PRO	LYS	PRO	ALA	GLY	GLY	GLY	GLY	GLY
	K671	GLN	PHE	ALA	PHE	ALA	PHE	ALA	LYS	LYS	ALA	ALA
G672		LYS	GLY	ALA	SER	PRO	PRO	ALA	LYS	PRO	ASN	ASN
		ASN	LYS	PHE	ALA	SER	PHE	ALA	GLY	GLY	GLY	ALA
Q695		GLU	ALA	GLY	PHE	GLY	PHE	GLY	ALA	THR	THR	ALA
		LYS	ASN	LYS	ALA	ALA	SER	THR	GLY	ALA	ALA	SER
		THR	LYS	THR	SER	GLY	PHE	GLY	LYS	PHE	GLY	THR
	R702	LYS	LYS	LYS	THR	SER	GLY	ALA	THR	THR	THR	THR



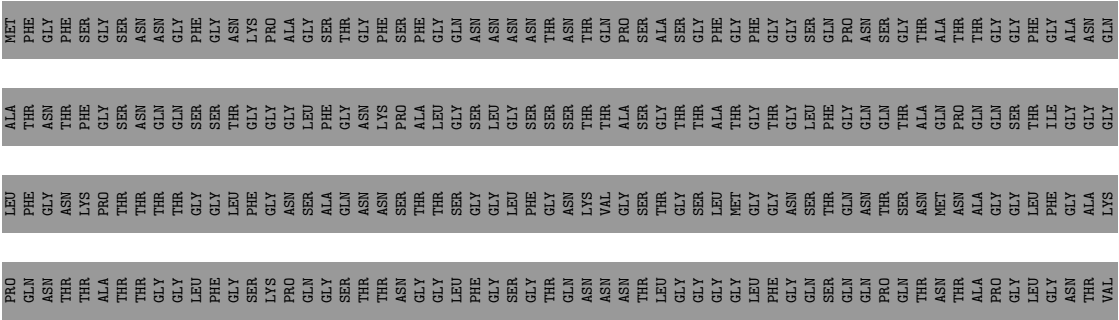
• Molecule 5: Nucleoporin NUP57

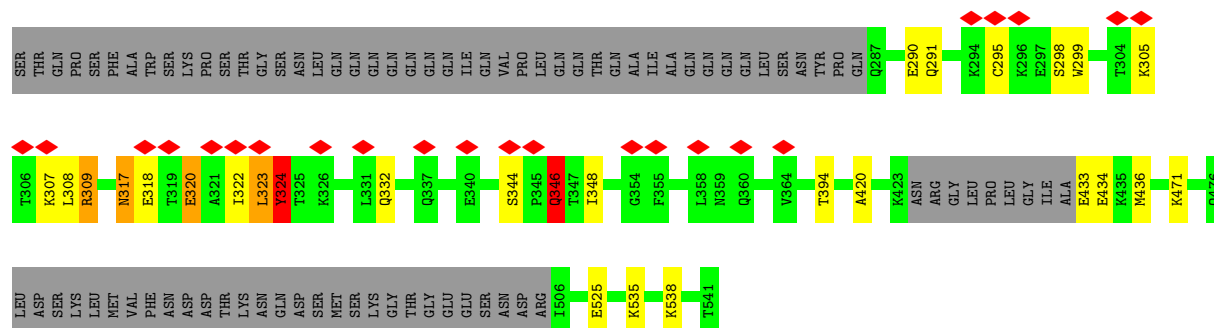
Chain E: 35% 60%



• Molecule 5: Nucleoporin NUP57

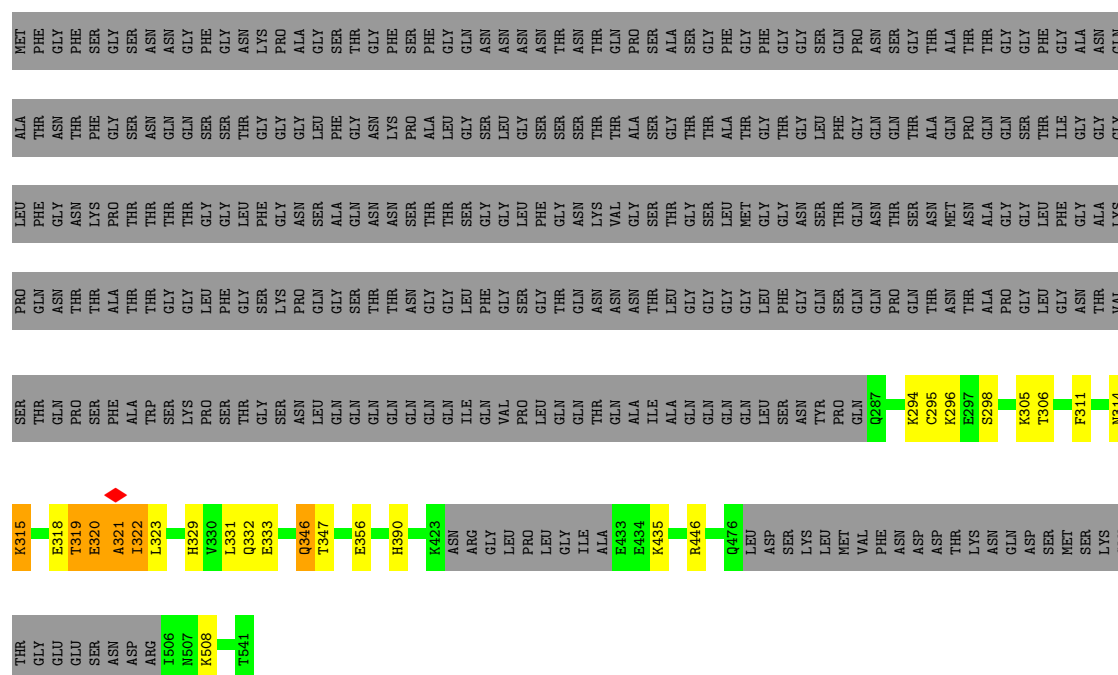
Chain H: 35% 60%





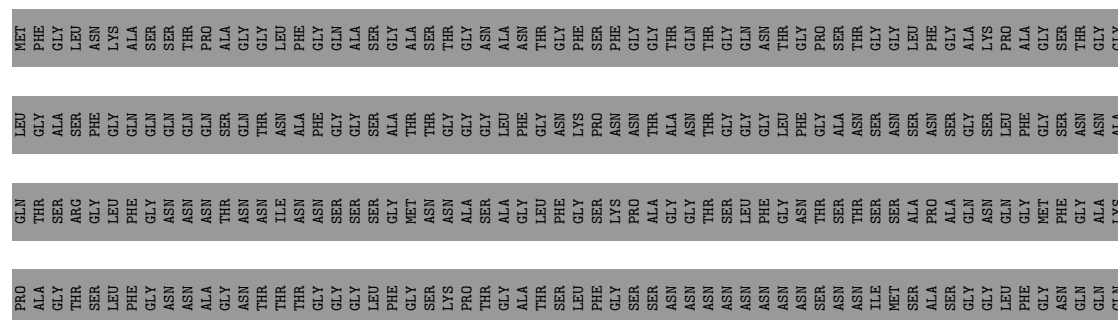
• Molecule 5: Nucleoporin NUP57

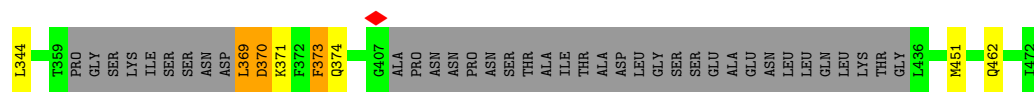
Chain K: 35% 60%



• Molecule 6: Nucleoporin NUP49/NSP49

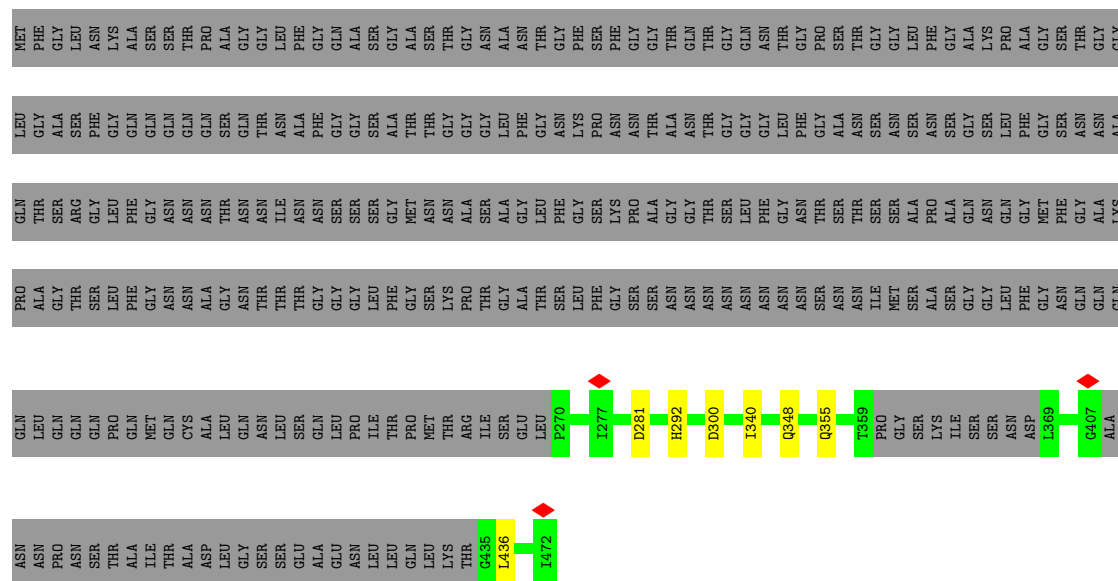
Chain C: 5% 32% 65%





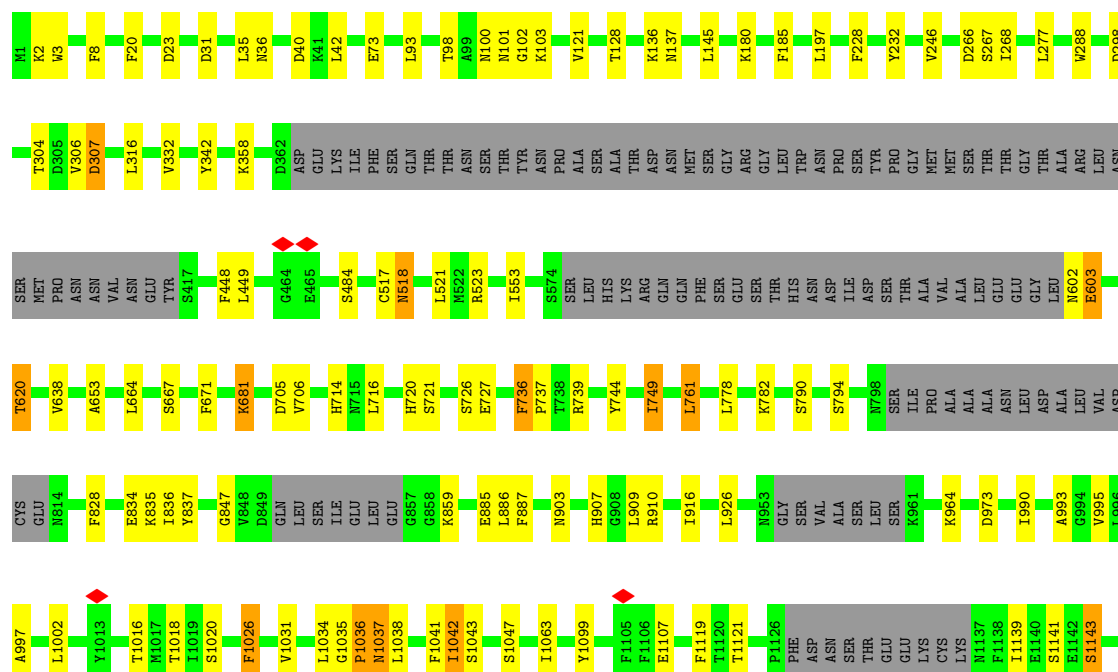
• Molecule 6: Nucleoporin NUP49/NSP49

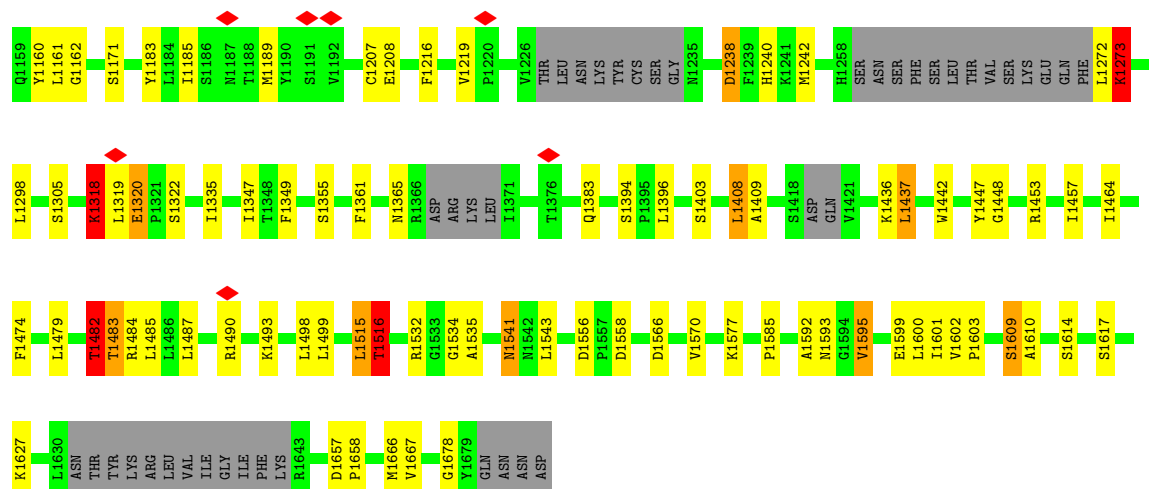
Chain L: 34% 65%



• Molecule 7: Nucleoporin NUP192

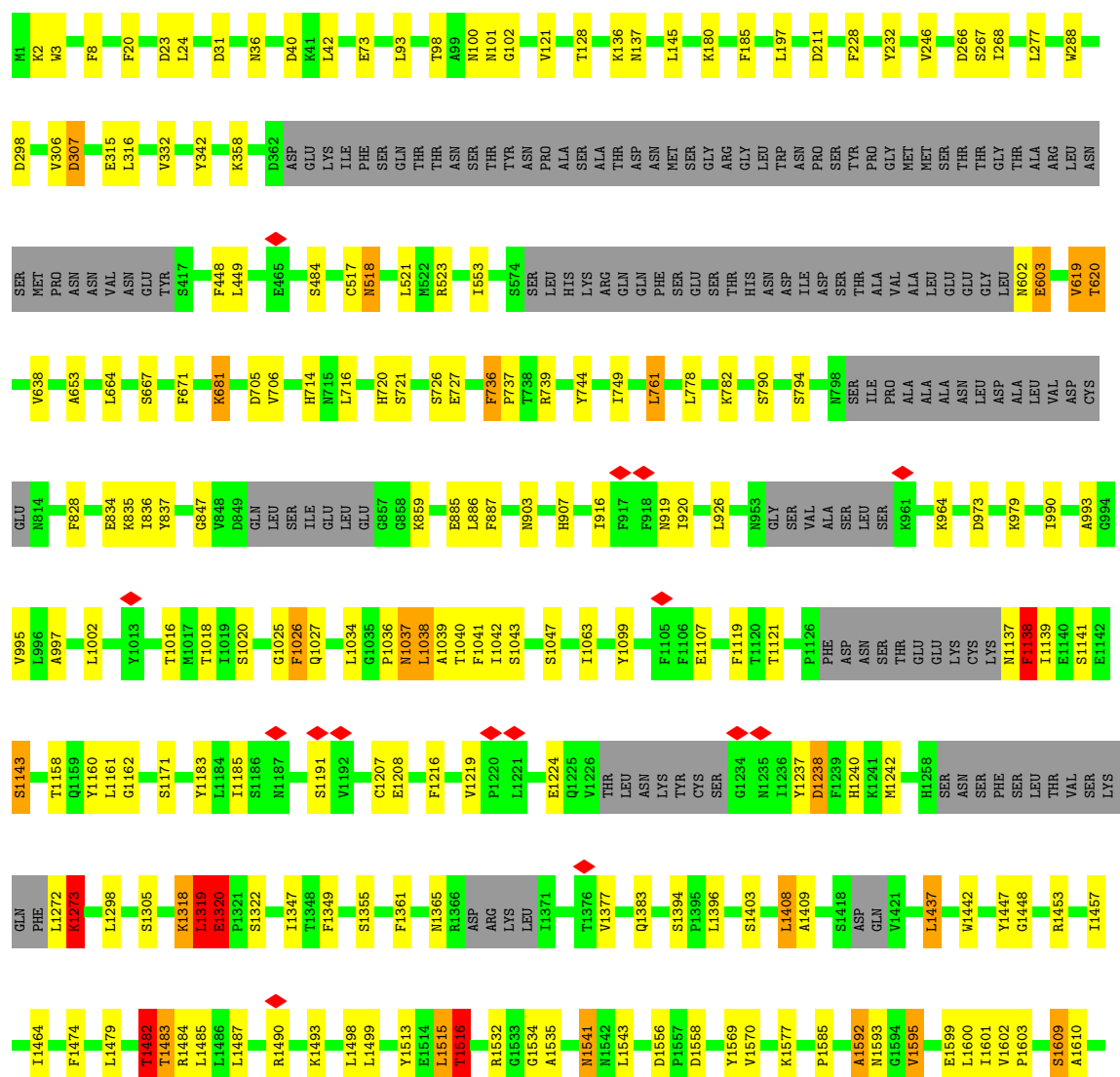
Chain M: 78% 11% 10%





• Molecule 7: Nucleoporin NUP192

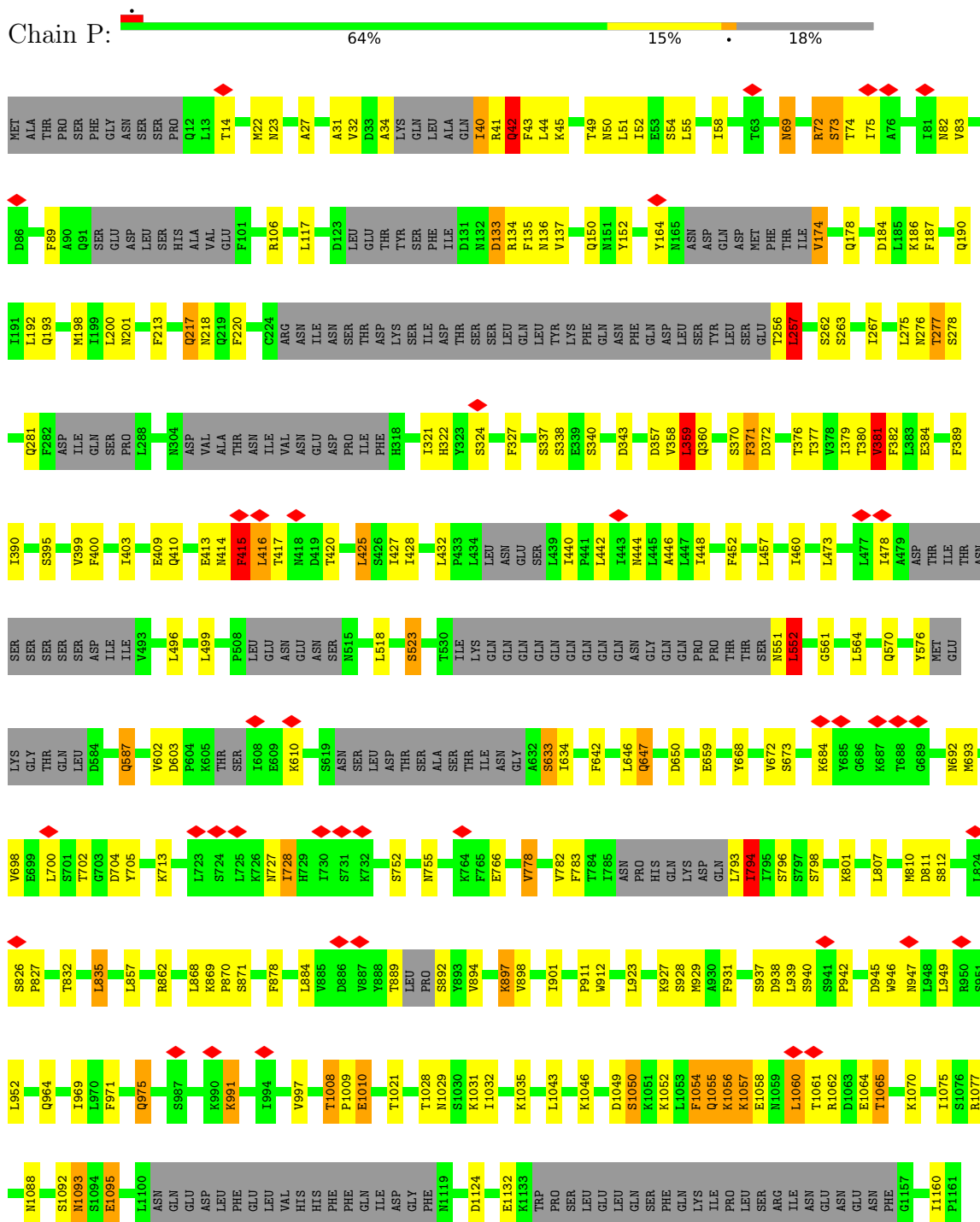
Chain O: 78% 11% 10%

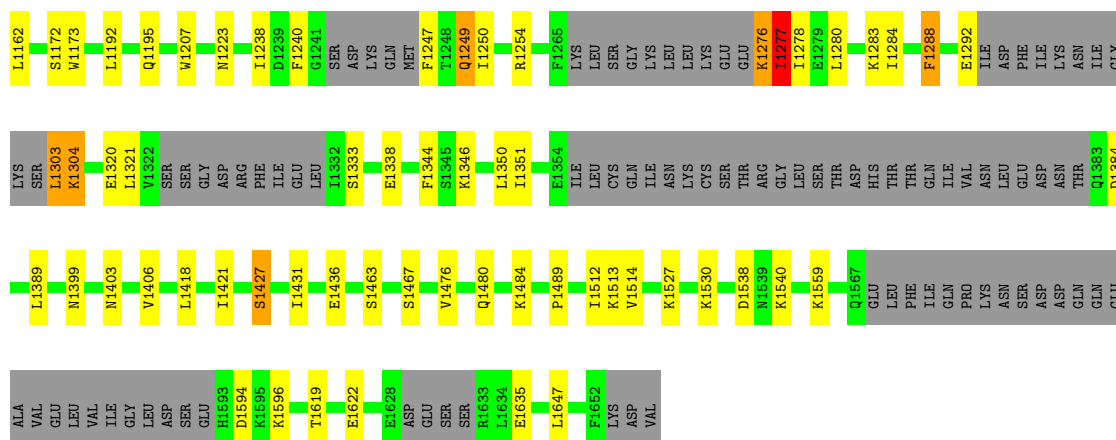


Chain N: 66% 13% 18%

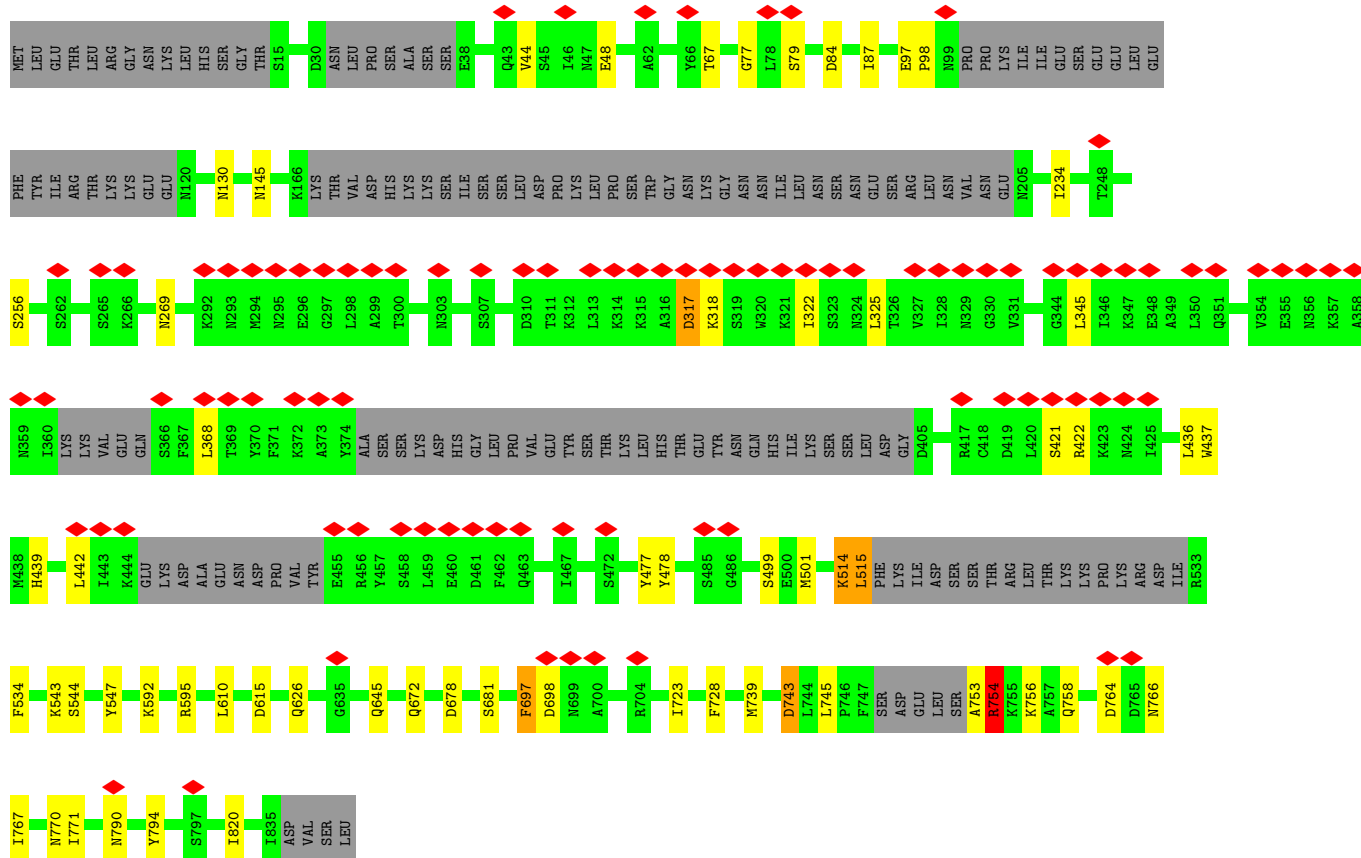
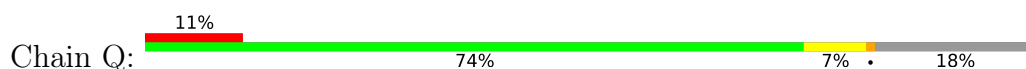


- Molecule 8: Nucleoporin NUP188

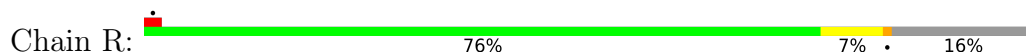


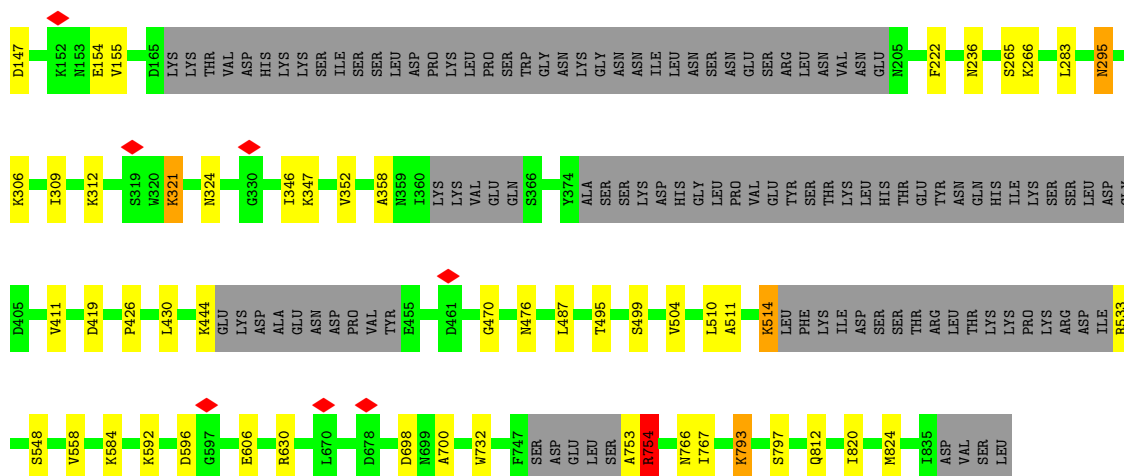


• Molecule 9: Nucleoporin NIC96

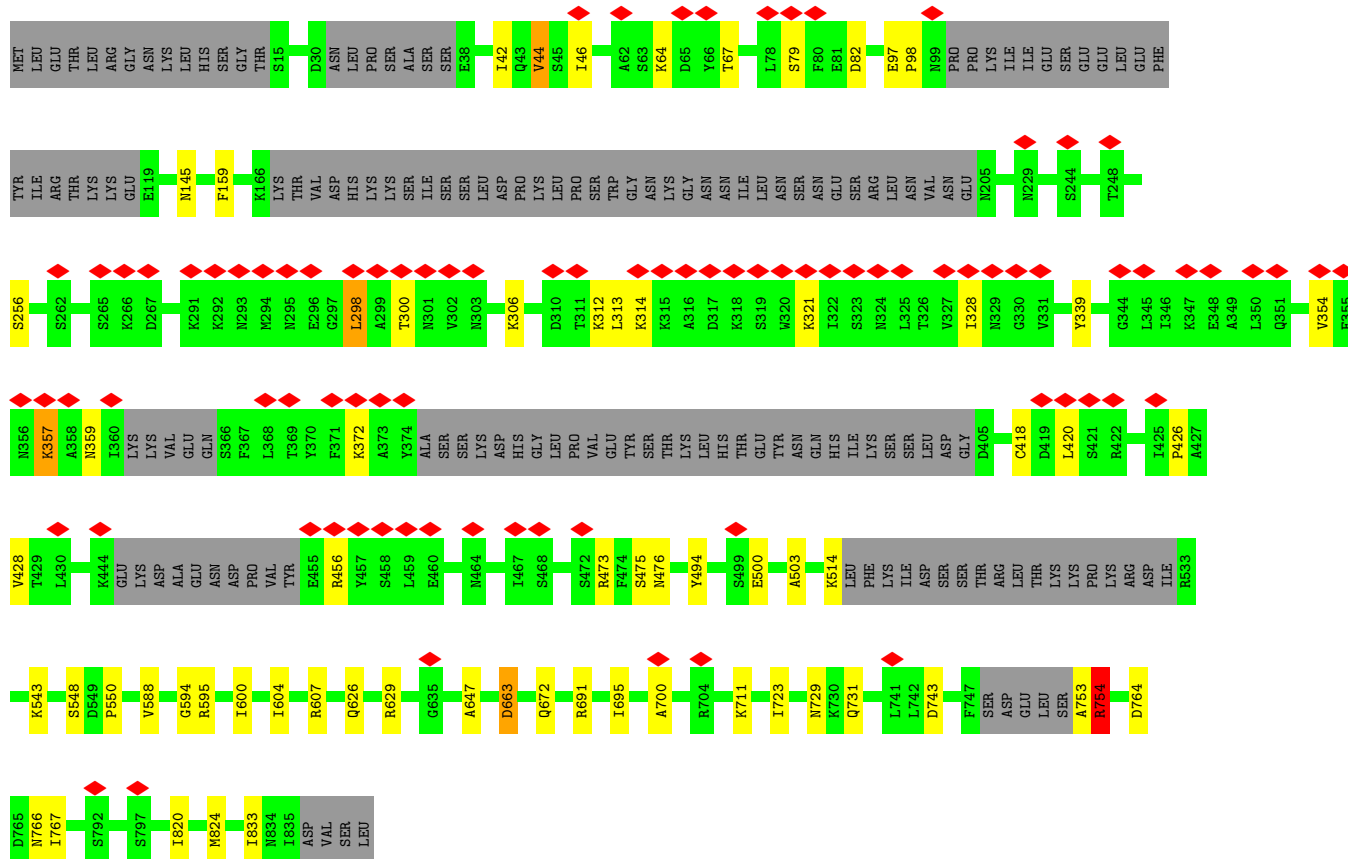
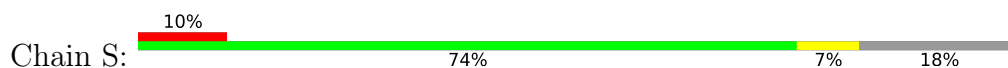


• Molecule 9: Nucleoporin NIC96

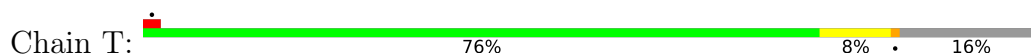


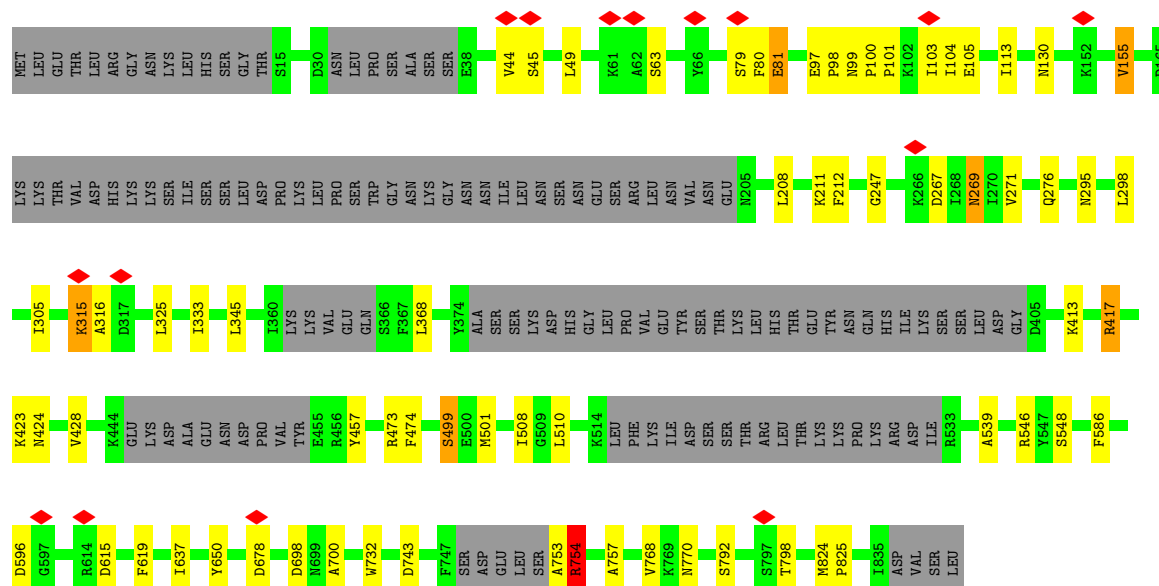


• Molecule 9: Nucleoporin NIC96



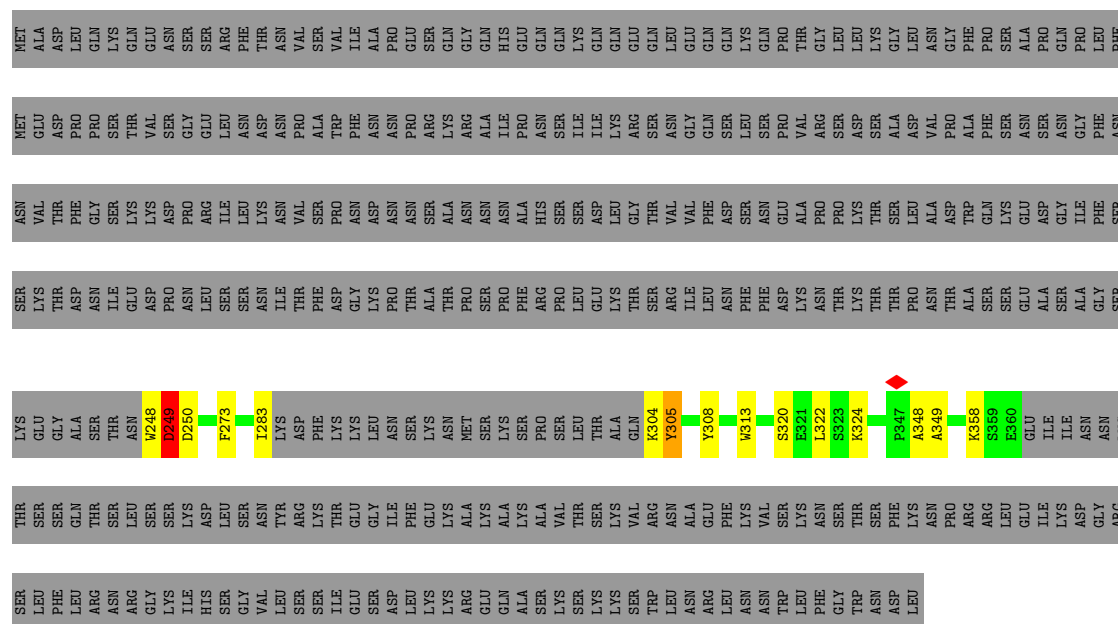
• Molecule 9: Nucleoporin NIC96



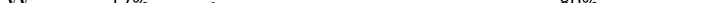


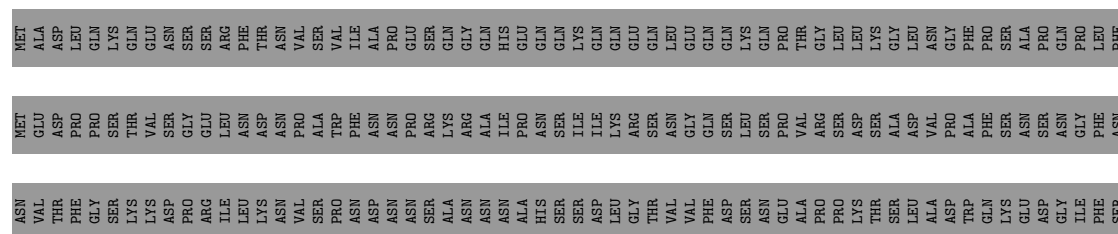
- Molecule 10: Nucleoporin NUP53

Chain U: 16% 80%



- Molecule 10: Nucleoporin NUP53

Chain W:  17% 80%





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145000	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 ($e^-/\text{\AA}^2$)	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	4.327	Depositor
Minimum map value	0.000	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.595	Depositor
Map size ($\text{\AA}$)	1276.8, 1276.8, 1276.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	O	1.27	13/9065 (0.1%)	1.58	100/12247 (0.8%)
1	Y	1.19	8/8920 (0.1%)	1.55	96/12052 (0.8%)
2	1	1.28	13/9072 (0.1%)	1.58	95/12276 (0.8%)
2	Z	1.35	20/9052 (0.2%)	1.67	102/12249 (0.8%)
4	A	1.14	2/1327 (0.2%)	1.52	11/1788 (0.6%)
4	D	1.14	2/1328 (0.2%)	1.47	7/1791 (0.4%)
4	G	1.37	2/1334 (0.1%)	1.69	19/1799 (1.1%)
4	J	1.15	2/1328 (0.2%)	1.46	4/1791 (0.2%)
5	B	1.13	0/1793	1.45	12/2411 (0.5%)
5	E	1.34	3/1793 (0.2%)	1.60	12/2411 (0.5%)
5	H	1.38	2/1793 (0.1%)	1.52	14/2411 (0.6%)
5	K	1.12	0/1793	1.42	9/2411 (0.4%)
6	C	1.09	0/1364	1.41	0/1837
6	F	1.27	2/1368 (0.1%)	1.63	13/1842 (0.7%)
6	I	1.11	0/1364	1.42	2/1837 (0.1%)
6	L	1.11	0/1368	1.42	3/1842 (0.2%)
7	M	1.17	7/12128 (0.1%)	1.67	142/16436 (0.9%)
7	O	1.22	15/12132 (0.1%)	1.70	147/16441 (0.9%)
8	N	1.26	21/11142 (0.2%)	1.69	157/15068 (1.0%)
8	P	1.22	13/11142 (0.1%)	1.67	162/15069 (1.1%)
9	Q	1.24	6/5265 (0.1%)	1.61	42/7137 (0.6%)
9	R	1.21	4/5353 (0.1%)	1.68	63/7262 (0.9%)
9	S	1.21	3/5262 (0.1%)	1.56	52/7133 (0.7%)
9	T	1.20	2/5353 (0.0%)	1.66	62/7262 (0.9%)
10	U	1.77	6/752 (0.8%)	2.16	20/1016 (2.0%)
10	W	1.55	3/752 (0.4%)	1.81	17/1016 (1.7%)
11	V	1.37	2/737 (0.3%)	1.70	12/996 (1.2%)
11	X	1.45	2/748 (0.3%)	1.81	9/1010 (0.9%)
All	All	1.24	153/124828 (0.1%)	1.63	1384/168841 (0.8%)

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	0	7	6
1	Y	4	8
2	1	8	1
2	Z	14	1
4	A	1	0
4	D	1	0
4	G	2	1
4	J	1	0
5	E	2	3
5	H	2	0
6	F	2	0
7	M	3	14
7	O	7	14
8	N	13	23
8	P	10	21
9	Q	4	0
9	R	3	1
9	S	3	1
9	T	2	0
10	U	5	1
10	W	3	2
11	V	2	0
11	X	2	0
All	All	101	97

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	470	SER	N-CA	-28.64	1.10	1.45
8	N	1059	ASN	N-CA	-26.19	1.11	1.45
10	W	305	TYR	CA-CB	-24.32	1.15	1.53
4	G	726	VAL	N-CA	-23.60	1.16	1.46
2	Z	745	ILE	CA-CB	-23.36	1.22	1.54
5	H	323	LEU	N-CA	-22.91	1.16	1.46
5	H	324	TYR	CA-CB	-22.86	1.14	1.53
9	Q	754	ARG	CA-CB	-22.81	1.15	1.53
2	Z	678	LYS	N-CA	-22.71	1.19	1.46
2	Z	744	GLY	N-CA	-22.16	1.10	1.45
10	U	305	TYR	CA-CB	-22.00	1.18	1.53
8	P	794	ILE	CA-CB	-21.89	1.24	1.54
2	Z	922	LYS	CA-CB	-21.87	1.16	1.53
10	U	249	ASP	CA-CB	-21.77	1.16	1.53
2	Z	679	SER	CA-CB	-21.50	1.17	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	1156	LEU	CA-CB	-21.41	1.17	1.53
9	S	754	ARG	CA-CB	-21.41	1.17	1.53
2	Z	1040	LYS	CA-CB	-21.36	1.17	1.53
1	0	1258	LEU	CA-CB	-21.30	1.17	1.53
2	1	1301	SER	CA-C	-21.17	1.24	1.52
2	1	678	LYS	CA-CB	-20.92	1.24	1.53
9	T	754	ARG	CA-CB	-20.90	1.18	1.53
2	1	308	ASN	N-CA	-20.77	1.19	1.46
5	E	324	TYR	CA-CB	-20.44	1.19	1.53
5	E	323	LEU	CA-CB	-20.43	1.22	1.53
2	1	922	LYS	CA-CB	-20.35	1.19	1.53
8	P	257	LEU	CA-CB	-20.01	1.19	1.53
6	F	370	ASP	CA-CB	-19.66	1.20	1.53
1	0	885	ALA	CA-CB	-19.54	1.20	1.53
8	N	257	LEU	CA-CB	-19.44	1.20	1.53
11	X	302	ARG	CA-CB	-19.32	1.14	1.53
1	Y	991	ARG	CA-CB	-19.32	1.20	1.53
8	P	358	VAL	N-CA	-19.20	1.19	1.46
1	0	991	ARG	CA-CB	-18.85	1.21	1.53
8	P	552	LEU	CA-CB	-18.84	1.21	1.53
8	P	359	LEU	CA-C	-18.79	1.27	1.52
2	1	309	LEU	CA-CB	-18.48	1.16	1.53
7	O	1138	PHE	CA-CB	-18.41	1.22	1.53
4	G	727	SER	CA-CB	-17.96	1.17	1.53
8	N	552	LEU	CA-CB	-17.67	1.23	1.53
9	R	754	ARG	CA-CB	-17.47	1.24	1.53
2	1	679	SER	CA-CB	-17.37	1.24	1.53
8	N	794	ILE	CA-C	-17.15	1.30	1.52
7	O	1137	ASN	N-CA	-17.14	1.13	1.46
8	N	1060	LEU	CA-CB	-17.01	1.24	1.53
9	T	753	ALA	N-CA	-16.96	1.14	1.46
8	N	41	ARG	CA-C	-16.54	1.30	1.52
9	Q	514	LYS	CA-CB	-16.49	1.25	1.53
7	O	1319	LEU	N-CA	-16.46	1.25	1.46
11	V	401	ASP	N-CA	-16.25	1.15	1.46
9	R	753	ALA	N-CA	-16.11	1.15	1.46
7	O	1273	LYS	CA-CB	-15.84	1.26	1.53
7	M	1273	LYS	CA-CB	-15.81	1.26	1.53
8	N	1055	GLN	CA-CB	-15.45	1.27	1.53
7	O	1320	GLU	CA-CB	-15.43	1.29	1.53
8	P	174	VAL	CA-CB	-15.42	1.12	1.54
8	N	41	ARG	CA-CB	-15.34	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	603	GLU	CA-CB	-15.29	1.27	1.53
7	M	603	GLU	CA-CB	-15.27	1.27	1.53
8	P	551	ASN	N-CA	-15.16	1.17	1.46
1	0	1257	GLN	N-CA	-14.89	1.18	1.46
8	N	551	ASN	CA-CB	-14.79	1.23	1.53
2	Z	1039	LEU	N-CA	-14.19	1.19	1.46
9	Q	515	LEU	CA-C	-14.18	1.23	1.52
10	U	248	TRP	N-CA	-14.10	1.19	1.46
7	O	1320	GLU	CA-C	-13.98	1.35	1.52
9	S	514	LYS	N-CA	-13.91	1.19	1.46
8	N	577	MET	CA-CB	-13.47	1.26	1.53
10	U	304	LYS	N-CA	-13.33	1.21	1.46
7	O	603	GLU	CA-C	-13.32	1.34	1.52
7	M	603	GLU	CA-C	-13.30	1.34	1.52
10	W	304	LYS	N-CA	-13.29	1.21	1.46
1	Y	992	CYS	CA-CB	-13.03	1.27	1.53
8	P	256	THR	N-CA	-12.99	1.21	1.46
11	X	301	LEU	CA-CB	-12.91	1.25	1.53
2	Z	921	SER	N-CA	-12.76	1.22	1.46
8	P	576	TYR	N-CA	-12.76	1.22	1.46
1	0	992	CYS	CA-CB	-12.68	1.28	1.53
2	1	514	ARG	N-CA	-12.68	1.22	1.46
2	1	1300	SER	N-CA	-12.53	1.30	1.46
6	F	369	LEU	N-CA	-12.48	1.22	1.46
8	N	1055	GLN	CA-C	-12.37	1.36	1.52
1	0	471	SER	CA-CB	-12.32	1.28	1.53
8	N	794	ILE	CA-CB	-12.20	1.37	1.54
11	V	301	LEU	CA-CB	-12.11	1.29	1.53
7	O	602	ASN	CA-CB	-12.08	1.29	1.53
7	M	602	ASN	CA-CB	-12.06	1.29	1.53
8	N	256	THR	N-CA	-12.03	1.23	1.46
2	Z	915	LYS	N-CA	-12.02	1.23	1.46
9	S	753	ALA	N-CA	-11.73	1.24	1.46
1	Y	790	PHE	CA-CB	-11.54	1.37	1.52
8	N	40	ILE	N-CA	-11.48	1.24	1.46
8	P	359	LEU	CA-CB	-11.48	1.34	1.53
1	Y	790	PHE	N-CA	-11.48	1.32	1.46
2	1	921	SER	N-CA	-11.41	1.24	1.46
9	R	514	LYS	N-CA	-11.35	1.24	1.46
1	Y	791	MET	CA-C	-11.30	1.29	1.52
10	W	283	ILE	N-CA	-11.17	1.25	1.46
2	Z	308	ASN	N-CA	-11.17	1.25	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	514	ARG	N-CA	-10.94	1.25	1.46
2	Z	456	THR	N-CA	-10.69	1.25	1.46
2	1	678	LYS	N-CA	10.62	1.61	1.46
1	Y	991	ARG	N-CA	10.39	1.59	1.46
9	Q	753	ALA	CA-CB	-10.22	1.18	1.52
8	N	1054	PHE	CA-CB	-10.16	1.23	1.53
1	0	991	ARG	N-CA	9.87	1.58	1.46
10	U	283	ILE	N-CA	-9.75	1.27	1.46
9	R	754	ARG	CA-C	-9.44	1.40	1.52
2	Z	745	ILE	CA-C	-9.39	1.40	1.52
8	N	793	LEU	CA-CB	-9.30	1.34	1.53
2	1	1300	SER	CA-CB	-8.89	1.38	1.53
1	0	884	VAL	N-CA	-8.81	1.29	1.46
7	O	1137	ASN	CA-CB	8.66	1.70	1.53
4	A	726	VAL	N-CA	-8.57	1.29	1.46
8	N	1059	ASN	CA-CB	8.21	1.67	1.53
9	Q	753	ALA	N-CA	7.83	1.61	1.46
2	1	1301	SER	CA-CB	-7.74	1.40	1.53
8	N	576	TYR	CA-CB	-7.49	1.28	1.54
2	Z	1155	GLN	N-CA	-7.43	1.32	1.46
7	O	1272	LEU	CA-CB	7.36	1.68	1.53
7	M	1272	LEU	CA-CB	7.33	1.68	1.53
7	O	1138	PHE	CA-C	-7.28	1.43	1.52
2	Z	891	ARG	CA-CB	-7.10	1.39	1.53
2	1	891	ARG	CA-CB	7.07	1.67	1.53
8	P	793	LEU	CA-CB	-7.01	1.39	1.53
5	E	324	TYR	CA-C	-6.96	1.43	1.52
4	D	726	VAL	CA-CB	-6.96	1.35	1.54
4	J	726	VAL	CA-CB	-6.90	1.35	1.54
1	Y	791	MET	CA-CB	-6.61	1.40	1.53
1	0	885	ALA	CA-C	-6.58	1.44	1.52
8	P	552	LEU	CA-C	-6.53	1.44	1.52
2	Z	891	ARG	N-CA	-6.45	1.34	1.46
4	J	726	VAL	N-CA	-6.36	1.34	1.46
8	N	1060	LEU	CA-C	-6.22	1.44	1.52
7	M	1272	LEU	N-CA	6.13	1.57	1.46
7	O	1319	LEU	CA-CB	-6.12	1.45	1.52
7	O	1272	LEU	N-CA	6.11	1.57	1.46
7	O	1273	LYS	CA-C	-6.10	1.44	1.52
7	M	1273	LYS	CA-C	-6.08	1.44	1.52
2	Z	1155	GLN	CA-CB	-5.97	1.41	1.53
8	P	793	LEU	N-CA	-5.96	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	552	LEU	CA-C	-5.76	1.45	1.52
9	Q	514	LYS	N-CA	5.76	1.53	1.46
1	O	470	SER	CA-CB	5.70	1.64	1.53
2	Z	1156	LEU	CA-C	5.63	1.60	1.52
1	O	471	SER	CA-C	-5.60	1.41	1.52
4	D	726	VAL	N-CA	-5.33	1.36	1.46
1	O	992	CYS	CA-C	-5.31	1.41	1.52
2	Z	456	THR	CA-CB	-5.31	1.40	1.54
1	Y	992	CYS	CA-C	-5.22	1.42	1.52
4	A	726	VAL	CA-CB	-5.19	1.40	1.54
10	U	283	ILE	CA-CB	-5.16	1.40	1.54
8	N	40	ILE	CA-CB	-5.00	1.41	1.54

All (1384) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	1156	LEU	N-CA-CB	30.45	161.94	110.49
2	Z	1040	LYS	N-CA-CB	27.76	157.41	110.49
9	Q	753	ALA	CB-CA-C	25.30	148.44	110.50
8	P	359	LEU	N-CA-CB	-24.67	68.80	110.49
10	U	249	ASP	N-CA-CB	23.79	150.70	110.49
2	1	678	LYS	N-CA-C	-22.69	81.84	110.88
2	1	678	LYS	CB-CA-C	22.29	149.79	111.45
8	N	41	ARG	CB-CA-C	21.61	153.43	110.42
2	1	309	LEU	N-CA-CB	21.53	147.10	110.50
2	Z	922	LYS	N-CA-CB	21.37	146.61	110.49
8	N	1059	ASN	N-CA-C	20.93	141.83	109.81
5	E	323	LEU	N-CA-CB	20.54	133.36	110.35
7	O	1319	LEU	N-CA-CB	20.46	139.91	110.24
1	O	470	SER	N-CA-C	20.40	141.02	108.99
2	Z	745	ILE	CB-CA-C	20.34	144.65	111.29
11	X	302	ARG	N-CA-CB	20.12	144.70	110.50
8	P	358	VAL	N-CA-CB	19.82	136.87	111.90
2	Z	1156	LEU	N-CA-C	-19.73	68.76	110.80
2	Z	679	SER	N-CA-CB	19.64	143.69	110.49
2	Z	1040	LYS	N-CA-C	-19.27	69.75	110.80
4	G	727	SER	N-CA-CB	19.04	142.88	110.50
7	O	1320	GLU	CB-CA-C	18.76	147.13	110.17
2	Z	308	ASN	N-CA-CB	18.30	141.61	110.50
8	N	1055	GLN	CB-CA-C	18.12	146.49	110.42
5	E	323	LEU	CB-CA-C	18.02	138.74	112.07
1	Y	991	ARG	CB-CA-C	18.00	146.24	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	359	LEU	CB-CA-C	17.94	146.13	110.42
1	O	1258	LEU	N-CA-CB	17.71	140.41	110.49
6	F	370	ASP	N-CA-CB	17.66	140.33	110.49
10	U	249	ASP	N-CA-C	-17.44	73.65	110.80
7	O	1138	PHE	CB-CA-C	17.44	145.12	110.42
1	O	991	ARG	CB-CA-C	17.39	145.02	110.42
1	Y	790	PHE	N-CA-CB	17.35	136.17	110.49
9	S	754	ARG	N-CA-CB	17.19	139.53	110.49
7	O	603	GLU	CB-CA-C	17.15	144.55	110.42
8	P	257	LEU	N-CA-CB	17.11	139.41	110.49
7	M	603	GLU	CB-CA-C	17.10	144.46	110.42
9	T	753	ALA	CB-CA-C	-17.04	84.94	110.50
8	N	551	ASN	CB-CA-C	16.91	142.22	110.10
2	1	1301	SER	CB-CA-C	16.88	144.02	110.42
2	Z	678	LYS	N-CA-CB	16.85	137.28	110.65
5	E	323	LEU	N-CA-C	-16.81	86.01	109.71
10	W	283	ILE	N-CA-CB	16.79	140.04	111.50
1	O	885	ALA	N-CA-CB	16.59	138.52	110.49
1	O	471	SER	CB-CA-C	16.51	141.46	110.10
1	Y	791	MET	CB-CA-C	16.44	141.34	110.10
11	X	301	LEU	CB-CA-C	16.43	136.00	111.85
8	N	40	ILE	N-CA-CB	16.30	139.21	111.50
9	R	753	ALA	CB-CA-C	-16.28	86.08	110.50
1	Y	992	CYS	CB-CA-C	16.25	140.98	110.10
1	O	992	CYS	CB-CA-C	16.11	140.70	110.10
10	U	283	ILE	N-CA-CB	16.09	138.86	111.50
8	N	1054	PHE	CB-CA-C	16.08	136.32	111.72
2	1	1301	SER	N-CA-CB	-15.92	83.58	110.49
2	Z	456	THR	N-CA-CB	15.82	138.39	111.50
8	P	359	LEU	N-CA-C	15.72	144.28	110.80
8	P	794	ILE	CB-CA-C	15.63	136.92	111.29
10	U	305	TYR	N-CA-CB	15.61	138.15	110.37
9	Q	754	ARG	N-CA-CB	15.51	136.70	110.49
8	P	174	VAL	CB-CA-C	15.44	140.73	111.40
9	R	514	LYS	N-CA-CB	15.44	136.74	110.50
8	N	577	MET	CB-CA-C	15.43	139.41	110.10
8	N	41	ARG	CA-C-O	15.36	142.48	120.51
2	1	1300	SER	N-CA-CB	15.36	136.44	110.49
8	N	257	LEU	N-CA-CB	15.35	136.43	110.49
8	N	1054	PHE	N-CA-CB	15.17	133.93	110.11
2	1	922	LYS	N-CA-CB	15.10	136.01	110.49
8	N	1054	PHE	N-CA-C	-15.05	87.73	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	754	ARG	CB-CA-C	15.00	140.27	110.42
7	O	1137	ASN	CB-CA-C	-14.89	81.81	110.10
8	N	1059	ASN	CB-CA-C	-14.82	82.38	110.24
2	1	308	ASN	N-CA-CB	14.76	135.43	110.49
8	N	794	ILE	CB-CA-C	14.75	135.48	111.29
2	Z	891	ARG	N-CA-CB	14.71	135.51	110.50
8	N	552	LEU	CB-CA-C	14.68	139.62	110.42
9	Q	515	LEU	CB-CA-C	14.65	137.94	110.10
4	G	727	SER	CB-CA-C	14.55	137.75	110.10
2	Z	514	ARG	N-CA-CB	14.54	135.22	110.50
10	W	305	TYR	N-CA-CB	14.46	136.10	110.37
2	Z	922	LYS	N-CA-C	-14.44	80.05	110.80
5	E	324	TYR	CB-CA-C	14.39	139.06	110.42
8	N	576	TYR	N-CA-CB	14.37	136.47	110.60
1	0	885	ALA	CB-CA-C	14.31	138.91	110.42
9	S	514	LYS	N-CA-CB	14.31	134.82	110.50
7	O	1137	ASN	N-CA-C	14.30	151.04	111.00
2	Z	744	GLY	N-CA-C	14.25	154.62	113.30
9	S	753	ALA	N-CA-CB	14.05	131.48	110.40
8	P	552	LEU	CB-CA-C	14.05	138.38	110.42
8	P	576	TYR	N-CA-CB	13.96	134.23	110.50
7	O	1320	GLU	N-CA-CB	-13.92	85.60	110.37
4	G	726	VAL	N-CA-CB	13.82	134.03	111.23
1	Y	791	MET	N-CA-CB	-13.80	87.04	110.50
2	1	922	LYS	CB-CA-C	13.79	137.86	110.42
11	X	301	LEU	N-CA-CB	13.75	132.27	111.23
7	O	1320	GLU	CA-C-O	-13.73	101.35	120.16
11	V	301	LEU	N-CA-CB	13.67	133.73	110.50
9	Q	514	LYS	CB-CA-C	13.63	137.53	110.42
1	0	884	VAL	N-CA-CB	13.46	134.38	111.50
8	N	577	MET	N-CA-CB	13.44	133.34	110.50
2	Z	915	LYS	N-CA-CB	13.37	133.22	110.50
2	Z	679	SER	N-CA-C	-13.32	82.43	110.80
11	V	401	ASP	N-CA-CB	13.32	133.14	110.50
4	J	726	VAL	N-CA-CB	13.31	134.13	111.50
1	0	885	ALA	N-CA-C	-13.25	82.57	110.80
4	D	726	VAL	N-CA-CB	13.25	134.02	111.50
1	0	470	SER	CB-CA-C	-13.24	81.75	109.94
9	T	754	ARG	CB-CA-C	13.23	136.75	110.42
6	F	369	LEU	N-CA-CB	13.18	132.90	110.50
2	Z	921	SER	N-CA-CB	13.12	132.80	110.50
10	U	248	TRP	N-CA-CB	13.12	132.80	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	726	VAL	CB-CA-C	-13.08	89.84	111.29
9	R	753	ALA	N-CA-CB	13.03	129.94	110.40
2	Z	1155	GLN	N-CA-CB	13.00	132.60	110.50
2	1	514	ARG	N-CA-CB	12.99	132.58	110.50
8	N	1060	LEU	CB-CA-C	12.92	136.14	110.42
4	G	726	VAL	N-CA-C	12.84	136.05	109.34
9	T	754	ARG	N-CA-CB	12.84	132.19	110.49
8	P	256	THR	N-CA-CB	12.83	133.31	111.50
8	P	552	LEU	N-CA-CB	12.81	132.15	110.49
5	H	323	LEU	N-CA-C	12.74	137.93	110.80
2	1	309	LEU	CB-CA-C	12.72	134.27	110.10
5	H	324	TYR	CB-CA-C	12.68	135.66	110.42
4	A	726	VAL	N-CA-CB	12.68	133.05	111.50
5	H	323	LEU	N-CA-CB	12.67	131.90	110.49
7	M	1272	LEU	CB-CA-C	-12.62	86.12	110.10
7	O	1272	LEU	CB-CA-C	-12.61	86.13	110.10
8	N	793	LEU	N-CA-CB	12.61	131.93	110.50
10	U	249	ASP	CB-CA-C	12.60	135.49	110.42
6	F	370	ASP	N-CA-C	-12.48	84.22	110.80
8	N	256	THR	N-CA-CB	12.46	132.69	111.50
6	F	370	ASP	CB-CA-C	12.46	135.21	110.42
2	1	679	SER	N-CA-CB	12.45	131.53	110.49
2	1	921	SER	N-CA-CB	12.41	131.60	110.50
8	P	552	LEU	CA-C-O	-12.41	102.76	120.51
8	P	551	ASN	N-CA-CB	12.38	131.54	110.50
9	T	753	ALA	N-CA-C	12.35	145.59	111.00
8	P	257	LEU	CB-CA-C	12.32	134.94	110.42
7	O	602	ASN	N-CA-CB	12.30	131.41	110.50
8	P	793	LEU	N-CA-CB	12.29	131.39	110.50
1	Y	991	ARG	N-CA-C	-12.27	84.67	110.80
7	M	602	ASN	N-CA-CB	12.23	131.29	110.50
6	F	370	ASP	CA-C-O	-12.20	103.07	120.51
10	W	304	LYS	N-CA-CB	12.13	131.12	110.50
2	1	679	SER	CB-CA-C	12.08	134.47	110.42
8	N	257	LEU	CA-C-O	-12.05	103.27	120.51
8	P	551	ASN	CB-CA-C	-12.05	87.21	110.10
9	Q	515	LEU	N-CA-CB	-12.02	90.06	110.50
8	N	257	LEU	CB-CA-C	11.99	134.29	110.42
8	P	257	LEU	N-CA-C	-11.89	85.47	110.80
2	Z	1039	LEU	N-CA-CB	11.87	130.67	110.50
9	T	753	ALA	N-CA-CB	11.86	128.19	110.40
1	0	1258	LEU	N-CA-C	-11.84	85.59	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	794	ILE	CA-C-O	-11.77	106.07	120.78
1	0	1258	LEU	CB-CA-C	11.71	133.72	110.42
8	P	358	VAL	N-CA-C	11.69	125.86	107.28
1	0	991	ARG	N-CA-C	-11.66	85.96	110.80
8	P	257	LEU	CA-C-O	-11.64	103.87	120.51
2	Z	679	SER	CB-CA-C	11.61	133.52	110.42
7	M	1273	LYS	CB-CA-C	11.60	133.50	110.42
2	1	309	LEU	N-CA-C	-11.59	78.55	111.00
2	1	922	LYS	N-CA-C	-11.59	86.12	110.80
7	O	1273	LYS	CB-CA-C	11.58	133.47	110.42
9	Q	514	LYS	N-CA-CB	11.54	129.99	110.49
8	P	358	VAL	CB-CA-C	-11.54	96.00	110.99
9	Q	754	ARG	CB-CA-C	11.52	133.34	110.42
9	R	753	ALA	N-CA-C	11.51	143.23	111.00
1	0	885	ALA	CA-C-O	-11.48	104.09	120.51
10	W	305	TYR	CB-CA-C	11.47	132.77	110.17
10	U	304	LYS	N-CA-CB	11.40	129.88	110.50
1	0	1257	GLN	N-CA-CB	11.39	129.86	110.50
4	G	727	SER	N-CA-C	-11.37	79.17	111.00
2	Z	922	LYS	CB-CA-C	11.36	133.02	110.42
7	M	1273	LYS	CA-C-O	-11.35	104.28	120.51
11	X	301	LEU	N-CA-C	-11.33	89.80	108.49
7	O	1273	LYS	CA-C-O	-11.30	104.35	120.51
9	S	754	ARG	CB-CA-C	11.22	132.75	110.42
10	U	248	TRP	CB-CA-C	-11.18	88.86	110.10
10	U	305	TYR	CB-CA-C	11.18	132.19	110.17
11	X	302	ARG	CB-CA-C	11.11	131.21	110.10
5	H	324	TYR	N-CA-CB	11.07	129.21	110.49
11	V	401	ASP	CB-CA-C	-11.02	89.16	110.10
9	S	514	LYS	CB-CA-C	-10.94	89.32	110.10
9	S	754	ARG	N-CA-C	-10.90	87.58	110.80
2	Z	922	LYS	CA-C-O	-10.87	104.96	120.51
9	R	99	ASN	CA-C-N	10.82	131.53	120.38
9	R	99	ASN	C-N-CA	10.82	131.53	120.38
2	Z	679	SER	CA-C-O	-10.82	105.04	120.51
2	1	922	LYS	CA-C-O	-10.73	105.17	120.51
8	N	41	ARG	CA-CB-CG	10.71	135.52	114.10
1	Y	991	ARG	N-CA-CB	10.71	128.59	110.49
2	Z	1040	LYS	CB-CA-C	10.63	131.57	110.42
7	O	1272	LEU	N-CA-C	-10.58	81.39	111.00
7	M	1272	LEU	N-CA-C	-10.57	81.40	111.00
10	U	249	ASP	CA-CB-CG	10.56	123.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	551	ASN	N-CA-C	10.55	140.54	111.00
9	S	754	ARG	CA-C-O	-10.53	105.46	120.51
2	Z	678	LYS	N-CA-C	10.49	126.38	108.02
7	M	602	ASN	CB-CA-C	10.42	129.90	110.10
7	O	1138	PHE	CA-C-O	-10.39	105.64	120.51
7	O	602	ASN	CB-CA-C	10.37	129.80	110.10
1	0	470	SER	N-CA-CB	10.34	130.75	111.52
2	Z	1039	LEU	CB-CA-C	-10.28	90.56	110.10
8	N	1055	GLN	N-CA-CB	-10.26	93.15	110.49
5	H	323	LEU	CB-CA-C	-10.24	90.04	110.42
8	N	257	LEU	N-CA-C	-10.21	89.06	110.80
9	T	81	GLU	N-CA-CB	10.18	127.69	110.49
9	R	100	PRO	N-CA-CB	10.16	112.94	103.08
7	M	836	ILE	N-CA-C	-10.10	103.63	112.12
1	0	991	ARG	N-CA-CB	10.07	127.51	110.49
2	1	679	SER	CA-C-O	-10.06	106.13	120.51
8	P	552	LEU	N-CA-C	-10.05	89.38	110.80
1	0	1257	GLN	CB-CA-C	-10.03	91.05	110.10
7	O	1273	LYS	N-CA-CB	10.02	127.42	110.49
7	M	1273	LYS	N-CA-CB	10.02	127.42	110.49
7	O	836	ILE	N-CA-C	-10.02	103.70	112.12
9	T	101	PRO	N-CA-CB	9.95	112.71	103.46
2	Z	1156	LEU	CA-C-O	-9.94	106.30	120.51
7	O	603	GLU	N-CA-CB	-9.92	93.73	110.49
1	0	1257	GLN	N-CA-C	9.89	138.68	111.00
2	1	1301	SER	N-CA-C	9.85	131.79	110.80
7	M	603	GLU	N-CA-CB	-9.84	93.87	110.49
9	Q	754	ARG	N-CA-C	-9.82	89.88	110.80
9	Q	754	ARG	CA-C-O	-9.81	106.48	120.51
11	X	302	ARG	N-CA-C	-9.73	83.77	111.00
2	1	308	ASN	N-CA-C	9.72	131.51	110.80
10	U	248	TRP	N-CA-C	9.72	138.22	111.00
6	F	370	ASP	CA-CB-CG	9.66	122.26	112.60
2	Z	1039	LEU	N-CA-C	9.66	138.04	111.00
10	U	304	LYS	CB-CA-C	-9.62	91.82	110.10
8	N	40	ILE	CA-CB-CG1	-9.61	94.07	110.40
9	T	754	ARG	N-CA-C	-9.59	90.37	110.80
7	O	602	ASN	CA-CB-CG	9.54	122.14	112.60
10	U	304	LYS	N-CA-C	9.54	137.71	111.00
9	T	98	PRO	N-CA-CB	9.51	113.79	103.33
9	Q	753	ALA	N-CA-C	-9.50	84.39	111.00
5	B	326	LYS	CA-C-N	9.49	129.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	326	LYS	C-N-CA	9.49	129.58	119.90
11	V	401	ASP	N-CA-C	9.48	137.54	111.00
7	M	602	ASN	CA-CB-CG	9.44	122.04	112.60
10	U	305	TYR	N-CA-C	-9.42	89.00	109.81
9	S	44	VAL	N-CA-CB	9.40	126.75	111.23
2	Z	745	ILE	CA-CB-CG1	9.35	126.29	110.40
2	Z	1040	LYS	CA-C-O	-9.28	107.24	120.51
8	P	807	LEU	N-CA-C	-9.28	104.04	114.62
8	N	551	ASN	N-CA-CB	9.26	126.24	110.50
9	S	753	ALA	CB-CA-C	-9.23	96.66	110.50
2	Z	678	LYS	CB-CA-C	-9.20	95.93	110.74
9	Q	514	LYS	N-CA-C	-9.12	91.38	110.80
8	N	576	TYR	CB-CA-C	9.07	125.13	111.70
8	N	794	ILE	CA-CB-CG1	9.06	125.81	110.40
9	R	98	PRO	N-CA-CB	9.04	113.28	103.33
2	1	269	THR	N-CA-C	-8.92	104.45	114.62
8	P	794	ILE	CA-CB-CG1	8.90	125.54	110.40
2	Z	1156	LEU	CB-CA-C	8.89	128.12	110.42
10	W	304	LYS	CB-CA-C	-8.83	93.32	110.10
9	Q	753	ALA	N-CA-CB	8.80	123.60	110.40
11	V	301	LEU	CB-CA-C	8.79	126.81	110.10
2	1	308	ASN	CB-CA-C	-8.78	92.95	110.42
2	Z	921	SER	CB-CA-C	-8.77	93.43	110.10
9	S	514	LYS	N-CA-C	8.73	135.46	111.00
10	W	304	LYS	N-CA-C	8.71	135.40	111.00
8	P	256	THR	N-CA-C	8.63	135.16	111.00
8	N	552	LEU	N-CA-CB	8.60	125.03	110.49
9	S	695	ILE	N-CA-C	-8.50	105.64	113.71
8	N	577	MET	N-CA-C	-8.49	87.21	111.00
10	W	305	TYR	N-CA-C	-8.48	91.07	109.81
2	1	679	SER	N-CA-C	-8.44	92.81	110.80
8	P	794	ILE	N-CA-CB	8.39	125.08	111.23
6	F	369	LEU	CB-CA-C	-8.36	94.22	110.10
8	N	1059	ASN	CA-CB-CG	-8.26	104.34	112.60
1	Y	1199	ILE	N-CA-C	-8.22	105.31	113.20
8	N	1165	ILE	N-CA-C	-8.21	104.75	112.96
2	1	1299	LYS	CA-C-N	8.20	137.21	121.54
2	1	1299	LYS	C-N-CA	8.20	137.21	121.54
5	K	306	THR	N-CA-C	-8.18	104.44	114.75
2	Z	745	ILE	CA-CB-CG2	-8.16	96.63	110.50
2	1	1282	VAL	N-CA-C	-8.14	105.20	113.10
8	N	794	ILE	N-CA-CB	-8.14	97.80	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	576	TYR	N-CA-C	-8.08	97.15	108.54
1	O	1001	ILE	N-CA-C	-8.08	105.24	111.62
1	O	1046	LYS	N-CA-C	-8.06	102.92	114.12
2	Z	921	SER	N-CA-C	8.03	133.48	111.00
8	P	256	THR	CB-CA-C	-8.01	91.47	109.10
8	N	671	LEU	N-CA-C	-8.00	105.50	114.62
2	Z	915	LYS	CB-CA-C	-7.99	94.91	110.10
2	Z	1370	GLU	N-CA-C	-7.99	104.13	114.04
9	R	514	LYS	CB-CA-C	-7.99	94.92	110.10
1	Y	1304	THR	N-CA-C	-7.99	104.69	114.75
9	T	100	PRO	N-CA-CB	7.96	110.80	103.08
8	N	256	THR	N-CA-C	7.96	133.28	111.00
7	M	1320	GLU	N-CA-C	7.94	127.36	109.81
9	R	312	LYS	N-CA-C	-7.92	105.59	114.62
8	N	794	ILE	CA-CB-CG2	-7.92	97.04	110.50
1	Y	1007	ILE	N-CA-C	-7.91	105.48	112.12
7	O	1320	GLU	N-CA-C	7.86	127.19	109.81
6	F	369	LEU	N-CA-C	7.78	132.79	111.00
9	Q	770	ASN	CA-C-N	7.78	125.14	120.24
9	Q	770	ASN	C-N-CA	7.78	125.14	120.24
7	M	603	GLU	CA-C-O	-7.78	109.39	120.51
7	O	603	GLU	CA-C-O	-7.75	109.42	120.51
1	O	884	VAL	CA-CB-CG1	7.72	123.52	110.40
7	M	1658	PRO	N-CA-CB	7.70	111.80	103.33
9	R	101	PRO	N-CA-CB	7.69	111.33	103.25
8	P	997	VAL	N-CA-C	-7.68	106.00	113.53
7	M	1603	PRO	N-CA-CB	7.68	111.78	103.33
8	P	136	ASN	N-CA-C	-7.66	104.36	112.93
7	O	1658	PRO	N-CA-CB	7.64	111.73	103.33
1	O	1258	LEU	CA-C-O	-7.63	109.60	120.51
7	O	1603	PRO	N-CA-CB	7.62	111.71	103.33
9	R	820	ILE	N-CA-C	-7.60	103.82	111.88
11	V	400	ILE	CA-C-N	7.60	135.38	121.70
11	V	400	ILE	C-N-CA	7.60	135.38	121.70
9	Q	98	PRO	N-CA-CB	7.57	111.92	103.44
9	S	98	PRO	N-CA-CB	7.57	111.91	103.44
8	P	58	ILE	N-CA-C	-7.56	103.87	111.88
8	P	201	ASN	N-CA-C	-7.55	106.01	114.62
2	1	678	LYS	N-CA-CB	7.54	122.67	111.51
8	N	794	ILE	N-CA-C	7.52	124.98	109.34
8	N	552	LEU	N-CA-C	-7.45	94.94	110.80
7	M	1365	ASN	N-CA-C	-7.44	105.38	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	327	PHE	CA-CB-CG	-7.38	106.42	113.80
7	O	100	ASN	N-CA-C	-7.38	104.89	114.04
7	M	100	ASN	N-CA-C	-7.37	104.90	114.04
5	H	324	TYR	N-CA-C	-7.37	95.11	110.80
9	S	753	ALA	N-CA-C	7.37	131.63	111.00
7	O	1365	ASN	N-CA-C	-7.36	105.48	114.75
7	M	1541	ASN	CA-CB-CG	-7.36	105.24	112.60
9	T	824	MET	N-CA-C	-7.34	101.61	108.22
1	Y	128	ASN	N-CA-C	-7.33	104.19	113.43
9	R	548	SER	N-CA-C	-7.33	106.27	114.62
1	Y	1166	VAL	N-CA-C	-7.33	105.87	112.90
1	Y	791	MET	N-CA-C	7.32	131.49	111.00
5	H	394	THR	N-CA-C	-7.31	104.22	113.43
8	P	174	VAL	CA-CB-CG2	7.31	122.83	110.40
9	S	767	ILE	N-CA-C	-7.31	105.46	113.43
9	T	770	ASN	CA-C-N	7.28	124.83	120.24
9	T	770	ASN	C-N-CA	7.28	124.83	120.24
8	N	551	ASN	N-CA-C	-7.27	90.64	111.00
7	O	1541	ASN	CA-CB-CG	-7.27	105.33	112.60
9	Q	515	LEU	N-CA-C	7.26	131.32	111.00
7	O	1614	SER	N-CA-C	-7.25	104.41	113.55
8	P	1351	ILE	N-CA-C	-7.25	106.42	113.53
7	M	1320	GLU	CA-C-N	-7.23	113.37	120.52
7	M	1320	GLU	C-N-CA	-7.23	113.37	120.52
7	M	1614	SER	N-CA-C	-7.23	104.44	113.55
7	O	1137	ASN	N-CA-CB	7.23	122.78	110.50
8	P	794	ILE	CA-CB-CG2	-7.18	98.29	110.50
8	P	570	GLN	N-CA-C	-7.17	104.56	113.38
7	O	926	LEU	CA-C-N	7.16	128.08	119.99
7	O	926	LEU	C-N-CA	7.16	128.08	119.99
2	1	921	SER	CA-CB-OG	7.14	125.38	111.10
7	M	926	LEU	CA-C-N	7.14	128.06	119.99
7	M	926	LEU	C-N-CA	7.14	128.06	119.99
1	Y	970	ILE	N-CA-C	-7.14	106.53	113.53
9	Q	767	ILE	N-CA-C	-7.12	105.67	113.43
7	O	1593	ASN	N-CA-C	7.12	120.86	111.75
7	O	1318	LYS	CA-C-N	7.10	133.67	122.17
7	O	1318	LYS	C-N-CA	7.10	133.67	122.17
4	G	808	ASP	CA-CB-CG	7.08	119.68	112.60
8	P	1431	ILE	N-CA-C	-7.07	106.24	113.10
2	1	953	ILE	N-CA-C	-7.05	105.75	111.81
8	N	756	TRP	N-CA-CB	7.04	116.69	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	808	ASP	CA-CB-CG	7.02	119.62	112.60
2	Z	456	THR	CA-CB-CG2	7.01	122.42	110.50
2	1	513	LYS	CA-C-N	7.01	134.32	121.70
2	1	513	LYS	C-N-CA	7.01	134.32	121.70
7	M	1593	ASN	N-CA-C	7.00	120.70	111.75
7	M	268	ILE	N-CA-C	-6.98	105.92	112.83
8	P	576	TYR	CA-CB-CG	6.97	126.45	113.90
2	1	416	GLU	N-CA-C	-6.96	106.68	114.62
2	Z	745	ILE	N-CA-C	-6.94	94.91	109.34
8	P	389	PHE	N-CA-C	-6.94	106.71	114.62
9	Q	610	LEU	N-CA-C	-6.93	103.50	113.21
5	K	322	ILE	N-CA-C	-6.93	106.25	112.90
8	N	794	ILE	CA-C-O	-6.92	112.13	120.78
9	S	723	ILE	N-CA-C	-6.91	104.25	111.58
11	V	401	ASP	CA-CB-CG	-6.91	105.69	112.60
8	N	256	THR	CB-CA-C	-6.90	93.92	109.10
2	1	1188	ARG	N-CA-C	-6.88	104.88	113.55
8	N	1420	VAL	N-CA-C	-6.88	105.37	113.42
7	O	268	ILE	N-CA-C	-6.88	106.02	112.83
1	0	615	PHE	N-CA-C	-6.87	104.21	112.59
9	T	345	LEU	CA-C-N	6.87	130.21	120.53
9	T	345	LEU	C-N-CA	6.87	130.21	120.53
2	Z	308	ASN	CB-CA-C	-6.87	97.06	110.10
4	G	725	VAL	CA-C-N	6.86	134.33	121.97
4	G	725	VAL	C-N-CA	6.86	134.33	121.97
1	Y	1359	ASP	CA-CB-CG	6.86	119.46	112.60
9	S	663	ASP	CA-CB-CG	6.85	119.45	112.60
8	P	1238	ILE	N-CA-C	-6.83	106.06	112.83
1	0	1205	SER	CA-C-N	6.82	129.72	120.38
1	0	1205	SER	C-N-CA	6.82	129.72	120.38
9	Q	743	ASP	CA-CB-CG	6.82	119.42	112.60
2	Z	990	THR	N-CA-C	-6.82	106.16	114.75
9	T	97	GLU	CA-C-N	6.81	126.61	119.05
9	T	97	GLU	C-N-CA	6.81	126.61	119.05
2	Z	915	LYS	N-CA-C	6.81	130.06	111.00
9	T	99	ASN	CA-C-N	6.81	127.39	120.38
9	T	99	ASN	C-N-CA	6.81	127.39	120.38
8	N	895	HIS	N-CA-C	-6.79	105.94	114.56
8	N	62	VAL	N-CA-C	-6.77	106.20	112.43
8	N	1478	ILE	N-CA-C	-6.77	105.74	112.17
2	Z	728	VAL	N-CA-C	-6.76	106.54	113.10
9	T	305	ILE	N-CA-C	-6.74	105.27	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	449	ASP	N-CA-C	-6.73	105.07	113.55
9	T	650	TYR	N-CA-C	-6.72	106.02	114.56
9	S	743	ASP	CA-CB-CG	6.72	119.32	112.60
9	R	430	LEU	N-CA-C	-6.70	105.39	113.97
2	1	768	ILE	N-CA-C	-6.69	106.14	113.43
1	Y	609	ILE	N-CA-C	-6.68	101.46	109.01
9	R	700	ALA	CA-C-N	6.64	127.47	120.03
9	R	700	ALA	C-N-CA	6.64	127.47	120.03
2	1	307	SER	CA-C-N	6.63	134.20	121.54
2	1	307	SER	C-N-CA	6.63	134.20	121.54
8	N	41	ARG	N-CA-CB	-6.62	99.30	110.49
8	N	967	LEU	N-CA-C	-6.60	106.43	114.75
6	F	344	LEU	N-CA-C	-6.59	105.13	113.43
9	Q	256	SER	N-CA-C	-6.59	104.89	113.12
1	0	980	SER	N-CA-C	-6.58	105.14	113.43
2	Z	772	SER	N-CA-C	-6.58	105.88	114.04
2	Z	1188	ARG	N-CA-C	-6.55	105.17	113.43
1	Y	1383	PHE	N-CA-C	-6.55	102.72	111.96
1	Y	1219	ARG	N-CA-C	-6.54	105.27	112.72
7	M	1609	SER	CA-C-N	6.54	134.02	121.54
7	M	1609	SER	C-N-CA	6.54	134.02	121.54
7	M	1185	ILE	N-CA-C	-6.53	106.77	113.10
8	N	577	MET	CA-CB-CG	6.51	127.13	114.10
7	M	1349	PHE	CA-CB-CG	-6.51	107.29	113.80
8	N	704	ASP	N-CA-C	-6.50	103.40	112.12
7	O	1609	SER	CA-C-N	6.50	133.97	121.54
7	O	1609	SER	C-N-CA	6.50	133.97	121.54
2	1	154	VAL	N-CA-C	-6.49	105.00	111.88
8	N	1060	LEU	CA-C-O	-6.48	111.24	120.51
8	P	1436	GLU	N-CA-C	-6.48	102.30	108.07
7	O	1349	PHE	CA-CB-CG	-6.48	107.32	113.80
9	Q	368	LEU	N-CA-C	-6.47	106.59	114.75
2	1	921	SER	N-CA-C	6.47	129.12	111.00
7	O	1595	VAL	N-CA-CB	6.47	121.90	111.23
1	Y	406	THR	N-CA-CB	6.47	121.42	110.49
5	E	352	ILE	N-CA-C	-6.46	98.82	108.12
2	1	1366	ILE	N-CA-C	-6.45	105.88	113.42
8	P	427	ILE	CA-C-N	6.44	129.21	120.77
8	P	427	ILE	C-N-CA	6.44	129.21	120.77
8	P	1043	LEU	N-CA-C	-6.44	107.28	114.62
10	W	308	TYR	N-CA-C	-6.43	102.82	110.41
1	0	846	ILE	N-CA-C	-6.43	107.60	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	1298	LEU	N-CA-C	-6.43	106.06	114.04
7	M	1318	LYS	N-CA-C	6.43	118.62	110.33
8	P	263	SER	CA-C-N	6.43	128.80	120.44
8	P	263	SER	C-N-CA	6.43	128.80	120.44
7	O	1585	PRO	N-CA-CB	6.42	110.10	103.23
8	N	322	HIS	N-CA-C	6.42	118.28	111.28
7	M	1298	LEU	N-CA-C	-6.42	106.08	114.04
4	J	726	VAL	CA-CB-CG1	6.41	121.30	110.40
7	O	246	VAL	N-CA-C	-6.41	105.92	113.42
8	P	704	ASP	N-CA-C	-6.41	103.35	112.13
5	E	322	ILE	CA-C-N	6.40	130.96	122.06
5	E	322	ILE	C-N-CA	6.40	130.96	122.06
8	P	971	PHE	N-CA-C	-6.39	107.33	114.62
2	Z	1208	ASP	N-CA-C	-6.39	106.12	114.04
7	M	246	VAL	N-CA-C	-6.39	105.95	113.42
2	1	616	THR	CA-C-N	6.38	126.07	119.56
2	1	616	THR	C-N-CA	6.38	126.07	119.56
4	A	726	VAL	CA-CB-CG2	6.38	121.24	110.40
9	T	743	ASP	CA-CB-CG	6.37	118.97	112.60
4	A	694	ASP	CA-CB-CG	6.36	118.96	112.60
10	W	283	ILE	CA-CB-CG2	6.35	121.30	110.50
7	O	1273	LYS	CA-CB-CG	6.34	126.79	114.10
1	Y	1102	ILE	N-CA-C	-6.34	106.60	112.43
7	M	1273	LYS	CA-CB-CG	6.33	126.77	114.10
9	T	271	VAL	N-CA-C	-6.31	106.04	113.42
1	Y	663	ILE	N-CA-C	-6.31	106.55	113.43
11	X	302	ARG	CA-C-O	6.29	131.49	120.80
5	B	538	LYS	N-CA-C	-6.28	105.25	113.17
10	U	283	ILE	CA-CB-CG2	6.28	121.17	110.50
2	Z	914	GLN	CA-C-N	6.28	133.00	121.70
2	Z	914	GLN	C-N-CA	6.28	133.00	121.70
1	0	467	PHE	CA-C-N	6.27	124.24	119.66
1	0	467	PHE	C-N-CA	6.27	124.24	119.66
8	N	950	ARG	CA-C-N	6.26	130.70	120.63
8	N	950	ARG	C-N-CA	6.26	130.70	120.63
1	0	170	LYS	N-CA-CB	6.25	121.06	110.49
9	T	45	SER	N-CA-CB	6.25	119.43	110.06
7	M	1595	VAL	N-CA-CB	6.24	121.52	111.23
8	N	1385	LEU	CA-C-N	6.23	128.88	120.65
8	N	1385	LEU	C-N-CA	6.23	128.88	120.65
5	H	538	LYS	N-CA-C	-6.22	105.33	113.17
1	0	1294	ILE	N-CA-C	-6.21	105.29	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	298	SER	N-CA-C	-6.21	105.60	113.43
1	Y	654	THR	CA-C-N	6.21	126.39	119.32
1	Y	654	THR	C-N-CA	6.21	126.39	119.32
7	M	1585	PRO	N-CA-CB	6.21	109.87	103.23
7	O	101	ASN	CA-C-N	6.20	126.99	119.99
7	O	101	ASN	C-N-CA	6.20	126.99	119.99
8	P	812	SER	N-CA-C	-6.19	106.95	114.75
8	P	1173	TRP	CA-C-N	6.18	128.47	120.44
8	P	1173	TRP	C-N-CA	6.18	128.47	120.44
8	P	1384	ASP	N-CA-C	-6.17	105.06	112.59
8	N	292	THR	N-CA-C	-6.15	106.41	114.04
4	G	726	VAL	CA-CB-CG2	-6.14	99.96	110.40
5	H	322	ILE	CA-C-N	6.14	133.27	121.54
5	H	322	ILE	C-N-CA	6.14	133.27	121.54
8	P	602	VAL	N-CA-C	-6.14	105.37	111.88
8	P	672	VAL	CA-C-N	6.14	128.42	120.44
8	P	672	VAL	C-N-CA	6.14	128.42	120.44
9	Q	269	ASN	N-CA-CB	6.13	115.76	109.51
8	N	1224	ASP	N-CA-C	-6.13	106.41	114.31
8	N	199	ILE	N-CA-C	-6.12	106.77	112.83
1	Y	577	PHE	CA-CB-CG	6.12	119.92	113.80
8	N	1053	LEU	N-CA-C	-6.11	105.87	113.38
8	N	1059	ASN	N-CA-CB	6.11	120.21	111.05
1	O	1166	VAL	N-CA-C	-6.10	107.00	112.12
8	N	1334	ASP	N-CA-C	-6.09	107.07	114.75
2	1	133	GLY	N-CA-C	-6.09	106.53	115.72
8	P	262	SER	CA-C-N	6.09	129.27	120.38
8	P	262	SER	C-N-CA	6.09	129.27	120.38
1	O	654	THR	CA-C-N	6.09	126.26	119.32
1	O	654	THR	C-N-CA	6.09	126.26	119.32
9	Q	478	TYR	CA-C-N	6.08	128.43	120.28
9	Q	478	TYR	C-N-CA	6.08	128.43	120.28
8	P	360	GLN	CA-C-N	6.08	128.71	120.38
8	P	360	GLN	C-N-CA	6.08	128.71	120.38
1	Y	980	SER	N-CA-C	-6.08	105.77	113.43
8	P	417	THR	N-CA-C	-6.08	104.51	112.41
9	T	81	GLU	CB-CA-C	6.07	122.50	110.42
7	M	761	LEU	N-CA-CB	6.06	120.74	110.49
2	Z	1379	VAL	N-CA-C	-6.06	106.83	112.83
9	T	333	ILE	N-CA-C	6.04	116.78	110.62
7	O	761	LEU	N-CA-CB	6.03	120.68	110.49
2	Z	1282	VAL	N-CA-C	-6.03	105.49	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	1538	ASP	N-CA-C	-6.02	106.92	114.56
1	0	1339	LYS	N-CA-C	-6.01	104.06	112.12
5	E	318	GLU	N-CA-C	6.01	123.61	110.80
1	0	617	ALA	N-CA-C	-6.01	106.10	113.50
4	D	640	LEU	N-CA-C	-6.01	106.58	114.04
1	0	390	PRO	N-CA-C	-6.00	106.22	114.98
7	M	101	ASN	CA-C-N	6.00	126.77	119.99
7	M	101	ASN	C-N-CA	6.00	126.77	119.99
9	S	711	LYS	N-CA-C	-6.00	105.88	113.43
7	M	1242	MET	CA-C-N	5.99	129.13	120.38
7	M	1242	MET	C-N-CA	5.99	129.13	120.38
9	R	130	ASN	CA-C-N	5.98	126.73	120.03
9	R	130	ASN	C-N-CA	5.98	126.73	120.03
8	P	975	GLN	N-CA-CB	5.98	120.59	110.49
9	T	345	LEU	N-CA-C	-5.98	103.27	110.44
7	M	706	VAL	N-CA-C	-5.98	106.59	111.91
7	O	1119	PHE	N-CA-C	-5.97	106.03	113.38
2	1	1384	LYS	N-CA-C	5.97	117.46	111.07
9	S	604	ILE	N-CA-C	-5.97	107.17	112.90
11	V	362	SER	CA-C-N	5.97	125.68	119.05
11	V	362	SER	C-N-CA	5.97	125.68	119.05
2	Z	880	SER	N-CA-C	-5.97	105.08	112.72
1	Y	1339	LYS	N-CA-C	-5.97	105.24	113.18
5	K	296	LYS	N-CA-C	-5.96	105.19	112.88
7	M	1119	PHE	N-CA-C	-5.96	106.05	113.38
7	O	1185	ILE	N-CA-C	-5.96	107.18	112.90
8	P	673	SER	CA-C-N	5.96	128.59	120.54
8	P	673	SER	C-N-CA	5.96	128.59	120.54
1	0	1202	VAL	N-CA-C	-5.95	106.94	112.83
7	M	31	ASP	CA-C-N	5.95	128.18	120.44
7	M	31	ASP	C-N-CA	5.95	128.18	120.44
10	W	320	SER	N-CA-CB	5.95	120.54	110.49
7	O	31	ASP	CA-C-N	5.94	128.16	120.44
7	O	31	ASP	C-N-CA	5.94	128.16	120.44
9	T	130	ASN	CA-C-N	5.94	126.68	120.03
9	T	130	ASN	C-N-CA	5.94	126.68	120.03
7	O	1242	MET	CA-C-N	5.94	129.05	120.38
7	O	1242	MET	C-N-CA	5.94	129.05	120.38
11	X	280	ILE	N-CA-C	-5.94	106.96	113.43
8	P	794	ILE	N-CA-C	-5.93	97.00	109.34
9	S	588	VAL	N-CA-C	-5.93	106.54	112.17
8	P	416	LEU	N-CA-CB	5.92	120.50	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	369	THR	N-CA-C	-5.92	100.25	109.72
9	Q	754	ARG	CA-CB-CG	5.92	125.94	114.10
2	1	1382	TYR	N-CA-C	-5.92	105.37	112.59
9	R	606	GLU	N-CA-C	-5.91	106.04	113.72
1	0	1222	THR	N-CA-C	-5.91	98.22	110.80
1	0	1024	LEU	CA-C-N	5.90	132.82	121.54
1	0	1024	LEU	C-N-CA	5.90	132.82	121.54
8	P	174	VAL	CA-CB-CG1	-5.89	100.39	110.40
7	M	1556	ASP	CA-CB-CG	5.88	118.48	112.60
9	S	256	SER	N-CA-C	-5.88	104.85	112.68
9	Q	97	GLU	CA-C-N	5.88	125.26	118.85
9	Q	97	GLU	C-N-CA	5.88	125.26	118.85
1	Y	1059	TYR	N-CA-CB	5.88	120.43	110.49
7	O	706	VAL	N-CA-C	-5.88	106.68	111.91
1	Y	462	LEU	N-CA-C	5.88	117.69	111.28
7	M	1020	SER	CA-C-N	5.88	128.43	120.38
7	M	1020	SER	C-N-CA	5.88	128.43	120.38
2	Z	455	PRO	CA-C-N	5.87	132.27	121.70
2	Z	455	PRO	C-N-CA	5.87	132.27	121.70
1	0	1479	ILE	CA-C-N	5.86	128.41	120.38
1	0	1479	ILE	C-N-CA	5.86	128.41	120.38
7	O	1020	SER	CA-C-N	5.86	128.41	120.38
7	O	1020	SER	C-N-CA	5.86	128.41	120.38
8	P	1338	GLU	CA-C-N	5.86	128.14	120.28
8	P	1338	GLU	C-N-CA	5.86	128.14	120.28
5	B	355	PHE	N-CA-C	-5.85	104.36	112.03
8	P	1594	ASP	CA-C-N	5.85	128.93	120.38
8	P	1594	ASP	C-N-CA	5.85	128.93	120.38
1	Y	251	THR	N-CA-CB	5.85	120.38	110.49
8	N	1437	PRO	CA-C-N	5.85	128.47	120.46
8	N	1437	PRO	C-N-CA	5.85	128.47	120.46
8	N	56	ASN	N-CA-CB	5.84	120.37	110.49
1	0	1441	ASN	CA-C-N	5.84	128.38	120.38
1	0	1441	ASN	C-N-CA	5.84	128.38	120.38
9	S	97	GLU	CA-C-N	5.84	125.22	118.85
9	S	97	GLU	C-N-CA	5.84	125.22	118.85
8	N	1007	SER	N-CA-C	-5.84	106.78	114.31
7	O	1556	ASP	CA-CB-CG	5.84	118.44	112.60
9	R	793	LYS	N-CA-C	-5.84	103.59	112.99
2	Z	678	LYS	CA-CB-CG	-5.84	102.43	114.10
8	N	449	ASP	N-CA-C	-5.83	103.15	108.75
8	N	1404	PHE	CA-C-N	5.83	128.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	1404	PHE	C-N-CA	5.83	128.09	120.28
9	Q	77	GLY	N-CA-C	-5.82	99.38	113.18
1	Y	790	PHE	CA-CB-CG	-5.82	107.98	113.80
6	F	436	LEU	N-CA-C	-5.82	106.10	113.43
5	K	311	PHE	CA-CB-CG	-5.82	107.98	113.80
7	M	1532	ARG	N-CA-C	5.82	118.12	111.02
1	Y	630	THR	N-CA-C	-5.81	105.84	113.17
1	O	531	PHE	CA-CB-CG	-5.81	107.99	113.80
2	Z	573	LEU	N-CA-C	-5.81	106.11	113.43
9	S	494	TYR	N-CA-C	-5.80	105.21	112.93
7	O	1216	PHE	CA-CB-CG	-5.80	108.00	113.80
1	Y	1155	ARG	N-CA-C	-5.80	105.40	112.88
1	O	603	GLY	CA-C-N	5.80	127.08	119.84
1	O	603	GLY	C-N-CA	5.80	127.08	119.84
2	1	1216	TYR	N-CA-C	-5.80	105.52	112.59
7	O	828	PHE	CA-CB-CG	-5.80	108.00	113.80
8	N	759	ASN	N-CA-C	-5.79	105.41	112.88
9	R	767	ILE	N-CA-C	-5.79	107.34	112.90
2	Z	1100	PHE	N-CA-C	5.78	117.58	111.28
1	Y	523	SER	N-CA-CB	5.78	120.26	110.49
7	M	1627	LYS	CA-C-N	5.78	126.36	119.94
7	M	1627	LYS	C-N-CA	5.78	126.36	119.94
7	M	1099	TYR	CA-C-N	5.78	128.82	120.38
7	M	1099	TYR	C-N-CA	5.78	128.82	120.38
2	1	921	SER	CB-CA-C	-5.78	99.13	110.10
4	G	671	LYS	CA-C-N	5.78	126.35	120.00
4	G	671	LYS	C-N-CA	5.78	126.35	120.00
8	P	1029	ASN	N-CA-C	-5.77	103.40	110.61
5	B	355	PHE	CA-CB-CG	-5.77	108.03	113.80
8	N	722	SER	N-CA-C	-5.77	106.29	113.38
1	O	1447	GLU	CA-C-N	5.76	128.32	120.54
1	O	1447	GLU	C-N-CA	5.76	128.32	120.54
8	P	428	ILE	CA-C-N	5.76	128.32	120.54
8	P	428	ILE	C-N-CA	5.76	128.32	120.54
2	Z	282	ASN	N-CA-C	-5.76	103.61	110.41
1	O	1387	ILE	N-CA-C	-5.76	107.52	113.10
6	L	436	LEU	N-CA-C	-5.75	106.18	113.43
7	O	1482	THR	CA-C-N	5.75	132.52	121.54
7	O	1482	THR	C-N-CA	5.75	132.52	121.54
7	O	1516	THR	N-CA-C	-5.75	98.55	110.80
7	O	1099	TYR	CA-C-N	5.74	128.76	120.38
7	O	1099	TYR	C-N-CA	5.74	128.76	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	356	GLU	N-CA-C	-5.74	105.94	113.12
7	M	1216	PHE	CA-CB-CG	-5.74	108.06	113.80
8	N	298	VAL	CA-C-N	5.74	127.97	120.28
8	N	298	VAL	C-N-CA	5.74	127.97	120.28
1	O	693	GLU	N-CA-CB	5.74	120.19	110.49
7	M	828	PHE	CA-CB-CG	-5.74	108.06	113.80
7	M	1162	GLY	CA-C-N	5.74	128.54	120.28
7	M	1162	GLY	C-N-CA	5.74	128.54	120.28
7	M	1273	LYS	N-CA-C	-5.74	98.58	110.80
7	O	1442	TRP	CA-C-N	5.74	128.75	120.38
7	O	1442	TRP	C-N-CA	5.74	128.75	120.38
8	P	698	VAL	N-CA-C	-5.74	107.39	112.90
2	1	280	GLY	CA-C-N	5.73	128.31	120.46
2	1	280	GLY	C-N-CA	5.73	128.31	120.46
8	P	801	LYS	CA-C-N	5.73	128.27	120.54
8	P	801	LYS	C-N-CA	5.73	128.27	120.54
5	B	356	GLU	N-CA-C	-5.72	106.94	114.04
7	M	1437	LEU	CA-C-N	5.72	127.86	120.70
7	M	1437	LEU	C-N-CA	5.72	127.86	120.70
9	T	548	SER	N-CA-C	-5.72	107.54	114.75
7	O	1627	LYS	CA-C-N	5.72	126.29	119.94
7	O	1627	LYS	C-N-CA	5.72	126.29	119.94
8	N	1021	THR	CA-C-N	5.72	128.26	120.54
8	N	1021	THR	C-N-CA	5.72	128.26	120.54
7	O	1273	LYS	N-CA-C	-5.72	98.62	110.80
10	W	305	TYR	CA-C-N	5.72	126.99	119.84
10	W	305	TYR	C-N-CA	5.72	126.99	119.84
1	O	156	ILE	N-CA-C	-5.72	101.48	107.60
1	Y	140	ASN	N-CA-CB	5.72	120.15	110.49
8	N	1437	PRO	N-CA-C	-5.72	106.23	114.18
7	O	1592	ALA	N-CA-C	5.72	118.28	111.71
7	O	267	SER	N-CA-C	-5.71	105.51	112.88
7	O	1657	ASP	CA-C-N	5.71	125.39	119.05
7	O	1657	ASP	C-N-CA	5.71	125.39	119.05
7	M	267	SER	N-CA-C	-5.71	105.52	112.88
4	J	700	ILE	N-CA-C	-5.70	107.43	112.90
1	O	1335	VAL	N-CA-C	-5.69	106.76	113.42
2	1	453	PHE	CA-C-N	5.69	126.24	120.38
2	1	453	PHE	C-N-CA	5.69	126.24	120.38
9	S	300	THR	N-CA-C	-5.69	101.60	110.42
10	U	305	TYR	CA-C-N	5.69	125.71	119.90
10	U	305	TYR	C-N-CA	5.69	125.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	531	PHE	CA-CB-CG	-5.69	108.11	113.80
9	R	144	LEU	CA-C-N	5.68	127.82	120.44
9	R	144	LEU	C-N-CA	5.68	127.82	120.44
9	R	824	MET	N-CA-C	-5.68	97.27	109.81
9	S	475	SER	N-CA-C	-5.68	105.67	112.59
2	Z	109	PRO	CA-C-N	5.68	128.24	120.35
2	Z	109	PRO	C-N-CA	5.68	128.24	120.35
2	Z	553	LYS	N-CA-CB	5.68	120.08	110.49
8	N	1595	LYS	CA-C-N	5.67	128.15	120.38
8	N	1595	LYS	C-N-CA	5.67	128.15	120.38
7	O	1532	ARG	N-CA-C	5.67	117.94	111.02
7	M	1657	ASP	CA-C-N	5.67	125.34	119.05
7	M	1657	ASP	C-N-CA	5.67	125.34	119.05
7	O	1063	ILE	N-CA-C	-5.67	106.25	113.22
9	R	147	ASP	CA-C-N	5.67	128.15	120.44
9	R	147	ASP	C-N-CA	5.67	128.15	120.44
1	Y	1066	PHE	CA-CB-CG	-5.66	108.14	113.80
8	P	1476	VAL	N-CA-C	-5.66	107.22	112.43
1	Y	1224	ASN	N-CA-C	-5.66	105.12	113.61
7	O	1162	GLY	CA-C-N	5.66	128.43	120.28
7	O	1162	GLY	C-N-CA	5.66	128.43	120.28
8	P	1132	GLU	N-CA-C	-5.66	104.00	112.54
7	M	73	GLU	N-CA-C	-5.65	105.16	112.68
1	0	468	PRO	CA-C-O	-5.65	116.83	120.90
2	1	545	TYR	N-CA-C	5.65	117.89	111.11
9	R	52	ARG	CA-C-N	5.65	127.89	120.60
9	R	52	ARG	C-N-CA	5.65	127.89	120.60
8	N	969	ILE	N-CA-C	-5.65	107.28	113.43
1	0	1198	ASN	N-CA-CB	5.64	120.03	110.49
1	Y	791	MET	CA-C-O	5.64	130.39	120.80
4	J	776	PHE	CA-CB-CG	5.64	119.44	113.80
7	O	73	GLU	N-CA-C	-5.64	105.18	112.68
1	Y	632	TYR	N-CA-C	-5.63	106.45	113.38
7	M	1063	ILE	N-CA-C	-5.63	106.29	113.22
7	M	1002	LEU	N-CA-C	-5.63	106.08	113.12
2	1	502	ILE	CA-C-N	5.63	127.13	120.09
2	1	502	ILE	C-N-CA	5.63	127.13	120.09
9	R	487	LEU	CA-C-N	5.63	128.08	120.65
9	R	487	LEU	C-N-CA	5.63	128.08	120.65
1	0	583	TYR	CA-C-N	5.62	126.18	119.94
1	0	583	TYR	C-N-CA	5.62	126.18	119.94
7	O	1437	LEU	CA-C-N	5.62	127.72	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	1437	LEU	C-N-CA	5.62	127.72	120.70
1	Y	1361	MET	N-CA-C	-5.62	105.77	113.30
9	Q	317	ASP	CA-CB-CG	5.62	118.22	112.60
1	Y	402	ILE	N-CA-CB	5.62	118.18	110.54
8	P	755	ASN	N-CA-C	-5.61	104.67	112.30
8	P	782	VAL	N-CA-C	-5.61	106.31	113.22
8	P	939	LEU	N-CA-C	-5.61	107.08	114.04
8	P	1195	GLN	CA-C-N	5.61	128.12	120.54
8	P	1195	GLN	C-N-CA	5.61	128.12	120.54
2	Z	579	TYR	N-CA-C	-5.61	105.03	112.94
2	Z	953	ILE	N-CA-C	-5.61	106.99	111.81
8	N	59	ARG	N-CA-CB	5.61	119.96	110.49
9	R	346	ILE	CA-C-N	5.60	127.79	120.28
9	R	346	ILE	C-N-CA	5.60	127.79	120.28
9	S	456	ARG	N-CA-C	-5.60	106.49	113.38
2	Z	149	GLU	N-CA-C	-5.60	107.45	114.56
8	P	561	GLY	CA-C-N	5.60	127.78	120.28
8	P	561	GLY	C-N-CA	5.60	127.78	120.28
8	P	646	LEU	N-CA-C	-5.60	106.13	114.64
9	T	474	PHE	N-CA-C	-5.60	102.06	110.06
8	P	901	ILE	CA-C-N	5.59	128.09	120.54
8	P	901	ILE	C-N-CA	5.59	128.09	120.54
9	S	731	GLN	CA-C-N	5.59	128.04	120.44
9	S	731	GLN	C-N-CA	5.59	128.04	120.44
7	O	1002	LEU	N-CA-C	-5.59	106.14	113.12
2	I	308	ASN	CA-CB-CG	-5.59	107.01	112.60
8	P	267	ILE	CA-C-N	5.59	128.08	120.54
8	P	267	ILE	C-N-CA	5.59	128.08	120.54
9	S	700	ALA	CA-C-N	5.59	126.18	119.98
9	S	700	ALA	C-N-CA	5.59	126.18	119.98
7	M	358	LYS	N-CA-C	-5.58	107.71	114.75
2	Z	915	LYS	CA-CB-CG	-5.58	102.93	114.10
8	P	1338	GLU	N-CA-C	-5.58	104.59	111.40
7	M	1442	TRP	CA-C-N	5.58	128.53	120.38
7	M	1442	TRP	C-N-CA	5.58	128.53	120.38
7	M	1464	ILE	N-CA-CB	5.58	117.08	110.55
7	O	1121	THR	N-CA-C	-5.58	100.69	109.50
8	P	184	ASP	CA-C-N	5.58	127.75	120.28
8	P	184	ASP	C-N-CA	5.58	127.75	120.28
2	Z	1318	HIS	CA-C-N	5.58	127.75	120.28
2	Z	1318	HIS	C-N-CA	5.58	127.75	120.28
9	S	298	LEU	N-CA-CB	5.58	119.91	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	1464	ILE	N-CA-CB	5.57	117.07	110.55
2	Z	745	ILE	N-CA-CB	5.57	120.43	111.23
2	Z	1246	LYS	N-CA-C	-5.57	107.48	114.56
7	O	664	LEU	CA-C-N	5.57	127.75	120.28
7	O	664	LEU	C-N-CA	5.57	127.75	120.28
1	0	1067	LEU	CA-C-N	5.57	128.51	120.38
1	0	1067	LEU	C-N-CA	5.57	128.51	120.38
8	N	559	PHE	N-CA-C	-5.57	100.27	108.79
8	P	395	SER	CA-C-N	5.57	128.51	120.38
8	P	395	SER	C-N-CA	5.57	128.51	120.38
7	M	1121	THR	N-CA-C	-5.57	100.70	109.50
8	N	577	MET	CA-C-O	5.57	130.26	120.80
9	T	368	LEU	N-CA-C	-5.57	106.53	113.38
7	M	1602	VAL	CA-C-N	5.56	125.23	119.05
7	M	1602	VAL	C-N-CA	5.56	125.23	119.05
7	M	1601	ILE	CA-C-N	5.56	124.78	120.33
7	M	1601	ILE	C-N-CA	5.56	124.78	120.33
1	0	1422	SER	CA-C-N	5.56	129.16	120.82
1	0	1422	SER	C-N-CA	5.56	129.16	120.82
7	M	664	LEU	CA-C-N	5.56	127.73	120.28
7	M	664	LEU	C-N-CA	5.56	127.73	120.28
9	T	792	SER	N-CA-C	-5.56	106.39	112.72
8	N	1513	LYS	N-CA-C	-5.55	106.40	114.12
7	O	358	LYS	N-CA-C	-5.55	107.75	114.75
8	N	1062	ARG	CA-C-N	5.55	128.49	120.38
8	N	1062	ARG	C-N-CA	5.55	128.49	120.38
4	A	706	GLU	N-CA-C	-5.55	107.15	114.31
5	B	297	GLU	N-CA-CB	5.55	119.87	110.49
9	R	558	VAL	CA-C-N	5.55	128.27	120.28
9	R	558	VAL	C-N-CA	5.55	128.27	120.28
9	T	825	PRO	CA-C-N	5.54	127.65	120.44
9	T	825	PRO	C-N-CA	5.54	127.65	120.44
2	1	514	ARG	N-CA-C	5.54	126.51	111.00
8	N	40	ILE	CB-CA-C	-5.54	100.53	111.60
7	M	1026	PHE	CA-CB-CG	-5.53	108.27	113.80
7	M	1516	THR	N-CA-C	-5.53	99.02	110.80
7	O	316	LEU	N-CA-C	-5.53	106.53	113.72
10	U	308	TYR	N-CA-C	-5.53	104.19	112.54
5	K	390	HIS	N-CA-C	-5.53	105.15	112.94
7	M	40	ASP	N-CA-C	-5.53	106.12	112.92
1	Y	401	ILE	N-CA-CB	5.53	117.02	110.55
4	G	640	LEU	N-CA-C	-5.53	106.47	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	64	LYS	CB-CA-C	-5.53	103.87	110.94
9	R	514	LYS	N-CA-C	5.53	126.47	111.00
8	P	277	THR	N-CA-CB	5.52	119.83	110.49
5	B	290	GLU	N-CA-C	-5.52	107.80	114.75
7	M	316	LEU	N-CA-C	-5.52	106.55	113.72
2	Z	822	PHE	N-CA-C	-5.52	105.34	112.68
9	T	619	PHE	CA-CB-CG	-5.51	108.28	113.80
7	O	1143	SER	N-CA-C	-5.51	99.06	110.80
7	O	484	SER	CA-C-N	5.51	127.50	120.56
7	O	484	SER	C-N-CA	5.51	127.50	120.56
9	R	495	THR	CA-C-N	5.51	127.93	120.38
9	R	495	THR	C-N-CA	5.51	127.93	120.38
8	N	824	LEU	N-CA-CB	5.50	119.79	110.49
7	O	1602	VAL	CA-C-N	5.50	125.16	119.05
7	O	1602	VAL	C-N-CA	5.50	125.16	119.05
8	N	1235	LYS	N-CA-C	-5.50	106.24	113.17
9	T	770	ASN	N-CA-C	-5.49	107.13	113.88
7	M	1143	SER	N-CA-C	-5.49	99.12	110.80
9	R	510	LEU	CA-C-N	5.48	127.94	120.54
9	R	510	LEU	C-N-CA	5.48	127.94	120.54
8	N	1055	GLN	CA-C-O	5.48	128.34	120.51
7	O	1601	ILE	CA-C-N	5.48	124.71	120.33
7	O	1601	ILE	C-N-CA	5.48	124.71	120.33
7	M	484	SER	CA-C-N	5.47	127.46	120.56
7	M	484	SER	C-N-CA	5.47	127.46	120.56
7	M	1483	THR	N-CA-C	5.47	122.45	110.80
9	T	798	THR	CA-C-N	5.47	127.61	120.28
9	T	798	THR	C-N-CA	5.47	127.61	120.28
5	E	326	LYS	CA-C-N	5.47	125.47	119.89
5	E	326	LYS	C-N-CA	5.47	125.47	119.89
1	Y	905	GLU	CA-C-N	5.47	126.01	120.00
1	Y	905	GLU	C-N-CA	5.47	126.01	120.00
8	P	1513	LYS	N-CA-C	-5.46	105.98	113.30
9	Q	745	LEU	CA-C-N	5.46	126.67	119.84
9	Q	745	LEU	C-N-CA	5.46	126.67	119.84
7	O	40	ASP	N-CA-C	-5.46	106.20	112.92
2	Z	676	LYS	N-CA-C	-5.46	103.30	108.22
8	N	845	SER	CA-C-N	5.46	128.35	120.38
8	N	845	SER	C-N-CA	5.46	128.35	120.38
8	N	1608	HIS	CA-C-N	5.46	124.98	119.19
8	N	1608	HIS	C-N-CA	5.46	124.98	119.19
7	O	24	LEU	N-CA-C	-5.46	106.53	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	909	LEU	CA-C-N	5.46	127.53	120.44
7	M	909	LEU	C-N-CA	5.46	127.53	120.44
4	A	752	ASP	CA-CB-CG	5.45	118.05	112.60
1	O	423	ILE	N-CA-C	-5.44	100.64	108.42
7	M	1482	THR	CA-C-N	5.44	131.93	121.54
7	M	1482	THR	C-N-CA	5.44	131.93	121.54
8	N	901	ILE	CA-C-N	5.44	127.88	120.54
8	N	901	ILE	C-N-CA	5.44	127.88	120.54
9	R	584	LYS	N-CA-C	-5.44	105.96	112.59
1	Y	1281	THR	N-CA-C	-5.44	106.32	113.17
7	M	671	PHE	CA-C-N	5.44	127.88	120.54
7	M	671	PHE	C-N-CA	5.44	127.88	120.54
7	M	1161	LEU	CA-C-N	5.43	125.97	119.94
7	M	1161	LEU	C-N-CA	5.43	125.97	119.94
2	Z	401	ASN	N-CA-C	-5.43	104.53	113.50
7	M	307	ASP	N-CA-CB	5.43	119.67	110.49
7	O	307	ASP	N-CA-CB	5.43	119.67	110.49
1	Y	1260	SER	N-CA-C	5.43	117.20	111.28
2	Z	306	LYS	N-CA-C	-5.43	102.29	110.06
8	N	935	VAL	N-CA-C	-5.43	107.50	111.90
1	Y	407	ALA	N-CA-CB	5.43	119.67	110.49
8	N	387	LEU	N-CA-C	-5.43	107.31	114.04
9	S	418	CYS	N-CA-C	-5.43	105.47	113.61
1	Y	951	ASP	N-CA-C	-5.43	107.67	114.56
1	Y	1046	LYS	N-CA-C	-5.43	106.70	113.38
7	M	128	THR	CA-C-N	5.42	128.30	120.38
7	M	128	THR	C-N-CA	5.42	128.30	120.38
7	O	521	LEU	N-CA-C	-5.42	105.97	113.18
7	O	671	PHE	CA-C-N	5.42	127.86	120.54
7	O	671	PHE	C-N-CA	5.42	127.86	120.54
1	Y	452	MET	CA-C-N	5.42	126.94	121.35
1	Y	452	MET	C-N-CA	5.42	126.94	121.35
5	B	288	ILE	N-CA-C	-5.42	107.46	112.83
1	O	1222	THR	N-CA-CB	5.42	119.65	110.49
9	T	247	GLY	CA-C-N	5.42	127.54	120.28
9	T	247	GLY	C-N-CA	5.42	127.54	120.28
2	Z	146	ILE	CA-C-N	5.42	125.41	119.89
2	Z	146	ILE	C-N-CA	5.42	125.41	119.89
8	N	650	ASP	CA-C-N	5.42	128.29	120.38
8	N	650	ASP	C-N-CA	5.42	128.29	120.38
7	M	8	PHE	CA-CB-CG	-5.41	108.39	113.80
9	R	295	ASN	N-CA-CB	5.41	119.64	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	992	CYS	CA-CB-SG	-5.41	101.96	114.40
8	P	370	SER	CA-C-N	5.41	131.88	121.54
8	P	370	SER	C-N-CA	5.41	131.88	121.54
1	Y	134	ASN	N-CA-C	-5.41	106.45	112.57
1	Y	1160	HIS	CA-C-N	5.41	127.53	120.28
1	Y	1160	HIS	C-N-CA	5.41	127.53	120.28
7	O	1161	LEU	CA-C-N	5.41	125.94	119.94
7	O	1161	LEU	C-N-CA	5.41	125.94	119.94
2	Z	1381	ASP	N-CA-C	-5.41	105.99	112.59
1	Y	365	ARG	N-CA-C	-5.41	107.94	114.75
2	1	574	THR	CA-C-N	5.40	129.36	121.31
2	1	574	THR	C-N-CA	5.40	129.36	121.31
8	N	992	SER	N-CA-C	-5.40	106.69	113.28
7	O	1139	ILE	N-CA-C	-5.40	107.04	112.17
8	N	986	SER	N-CA-CB	5.40	119.62	110.49
2	Z	345	LEU	N-CA-C	-5.40	99.30	108.26
8	P	390	ILE	CA-C-N	5.40	126.59	119.84
8	P	390	ILE	C-N-CA	5.40	126.59	119.84
9	S	754	ARG	CA-CB-CG	5.40	124.89	114.10
7	O	8	PHE	CA-CB-CG	-5.39	108.41	113.80
7	O	306	VAL	N-CA-C	-5.39	100.71	108.42
7	O	128	THR	CA-C-N	5.39	128.25	120.38
7	O	128	THR	C-N-CA	5.39	128.25	120.38
6	F	281	ASP	CA-CB-CG	5.39	117.99	112.60
7	O	1377	VAL	CA-C-N	5.39	127.50	120.28
7	O	1377	VAL	C-N-CA	5.39	127.50	120.28
9	T	499	SER	N-CA-CB	5.39	119.60	110.49
7	O	1305	SER	CA-C-N	5.39	127.76	120.38
7	O	1305	SER	C-N-CA	5.39	127.76	120.38
7	O	1487	LEU	N-CA-C	5.39	116.83	111.07
8	P	358	VAL	CA-CB-CG2	-5.39	101.24	110.40
8	P	633	SER	CA-C-N	5.38	129.45	120.62
8	P	633	SER	C-N-CA	5.38	129.45	120.62
2	Z	391	LEU	N-CA-C	-5.38	105.77	112.93
2	1	1301	SER	CA-CB-OG	-5.38	100.34	111.10
8	P	1249	GLN	N-CA-C	-5.38	105.68	113.21
1	0	1096	GLN	CA-C-N	5.38	127.75	120.65
1	0	1096	GLN	C-N-CA	5.38	127.75	120.65
8	N	1060	LEU	N-CA-CB	5.38	119.58	110.49
2	Z	1317	SER	CA-C-N	5.38	127.48	120.28
2	Z	1317	SER	C-N-CA	5.38	127.48	120.28
7	M	306	VAL	N-CA-C	-5.37	100.74	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1305	SER	CA-C-N	5.37	127.74	120.38
7	M	1305	SER	C-N-CA	5.37	127.74	120.38
8	N	1401	SER	N-CA-C	-5.37	104.07	110.41
7	O	1026	PHE	CA-CB-CG	-5.37	108.43	113.80
8	P	55	LEU	N-CA-C	-5.37	105.43	112.41
5	B	394	THR	N-CA-C	-5.37	106.04	113.18
7	M	521	LEU	N-CA-C	-5.37	106.04	113.18
9	Q	820	ILE	CB-CA-C	5.37	120.10	111.29
1	O	1305	SER	N-CA-CB	5.37	119.56	110.49
1	Y	631	GLN	N-CA-C	-5.37	106.50	113.16
8	N	263	SER	CA-C-N	5.37	127.42	120.44
8	N	263	SER	C-N-CA	5.37	127.42	120.44
8	P	106	ARG	CA-C-N	5.37	127.78	120.54
8	P	106	ARG	C-N-CA	5.37	127.78	120.54
1	Y	1279	VAL	N-CA-C	-5.37	107.49	112.43
9	S	428	VAL	N-CA-C	-5.36	107.52	112.83
1	Y	1154	ASP	N-CA-CB	5.36	119.55	110.49
9	T	615	ASP	CA-C-N	5.36	127.72	120.38
9	T	615	ASP	C-N-CA	5.36	127.72	120.38
2	Z	1385	ASP	N-CA-CB	5.36	119.55	110.49
2	1	922	LYS	CA-C-N	5.36	127.31	120.56
2	1	922	LYS	C-N-CA	5.36	127.31	120.56
8	N	389	PHE	N-CA-C	-5.36	108.51	114.62
1	Y	386	SER	N-CA-CB	5.36	119.54	110.49
2	1	747	ILE	N-CA-C	-5.36	100.14	108.81
8	P	752	SER	N-CA-C	5.36	117.12	111.28
9	S	820	ILE	N-CA-C	-5.36	107.26	112.29
1	O	1265	ALA	N-CA-C	-5.35	107.76	114.56
5	B	309	ARG	N-CA-CB	5.35	119.53	110.49
6	L	281	ASP	CA-CB-CG	5.35	117.95	112.60
8	P	192	LEU	CA-C-N	5.35	127.71	120.38
8	P	192	LEU	C-N-CA	5.35	127.71	120.38
9	R	352	VAL	N-CA-C	-5.35	107.09	112.17
9	S	306	LYS	N-CA-C	5.35	117.11	111.28
7	M	1139	ILE	N-CA-C	-5.35	107.09	112.17
2	Z	108	THR	CA-C-N	5.35	126.52	119.84
2	Z	108	THR	C-N-CA	5.35	126.52	119.84
1	O	1429	ILE	CA-C-N	5.34	127.44	120.28
1	O	1429	ILE	C-N-CA	5.34	127.44	120.28
2	1	597	GLU	CA-C-N	5.34	126.52	119.84
2	1	597	GLU	C-N-CA	5.34	126.52	119.84
2	1	309	LEU	CA-C-O	5.34	129.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	1284	ILE	CA-C-N	5.33	128.17	120.38
8	P	1284	ILE	C-N-CA	5.33	128.17	120.38
7	O	448	PHE	CA-CB-CG	-5.33	108.47	113.80
2	1	1368	LYS	N-CA-C	-5.33	106.46	113.17
7	M	1543	LEU	CA-C-N	5.33	127.42	120.28
7	M	1543	LEU	C-N-CA	5.33	127.42	120.28
2	1	880	SER	N-CA-C	-5.33	104.98	112.12
7	M	1403	SER	CA-C-N	5.33	127.42	120.28
7	M	1403	SER	C-N-CA	5.33	127.42	120.28
1	Y	1471	ILE	CA-C-N	5.32	127.47	120.60
1	Y	1471	ILE	C-N-CA	5.32	127.47	120.60
7	M	448	PHE	CA-CB-CG	-5.32	108.48	113.80
1	Y	1262	ILE	N-CA-C	-5.32	107.59	111.90
1	0	1102	ILE	N-CA-C	-5.32	106.24	111.88
2	1	107	ASN	CA-CB-CG	5.32	117.92	112.60
2	1	514	ARG	CB-CA-C	-5.32	100.00	110.10
9	R	309	ILE	N-CA-C	-5.32	107.80	112.90
1	Y	1311	PHE	N-CA-C	-5.32	99.47	110.80
4	G	752	ASP	CA-CB-CG	5.31	117.91	112.60
8	N	183	SER	CA-C-N	5.31	127.71	120.54
8	N	183	SER	C-N-CA	5.31	127.71	120.54
7	O	1403	SER	CA-C-N	5.31	127.39	120.28
7	O	1403	SER	C-N-CA	5.31	127.39	120.28
8	P	425	LEU	N-CA-CB	5.31	119.46	110.49
8	N	493	VAL	CA-C-N	5.31	125.30	119.89
8	N	493	VAL	C-N-CA	5.31	125.30	119.89
1	0	1409	SER	CA-C-N	5.30	125.87	119.98
1	0	1409	SER	C-N-CA	5.30	125.87	119.98
8	N	290	MET	N-CA-C	-5.30	106.49	113.17
2	1	1083	TYR	CA-C-N	5.30	127.65	120.65
2	1	1083	TYR	C-N-CA	5.30	127.65	120.65
9	T	508	ILE	CA-C-N	5.30	125.83	120.00
9	T	508	ILE	C-N-CA	5.30	125.83	120.00
9	T	510	LEU	CA-C-N	5.30	127.92	120.28
9	T	510	LEU	C-N-CA	5.30	127.92	120.28
8	N	1334	ASP	CA-CB-CG	5.30	117.90	112.60
8	P	415	PHE	N-CA-CB	5.30	119.45	110.49
2	1	146	ILE	CA-C-N	5.30	126.46	119.84
2	1	146	ILE	C-N-CA	5.30	126.46	119.84
5	E	356	GLU	N-CA-C	-5.30	106.95	113.41
1	Y	290	GLY	N-CA-C	-5.29	106.44	112.79
7	O	185	PHE	CA-CB-CG	-5.29	108.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	732	TRP	N-CA-C	-5.29	107.19	113.97
4	A	715	GLU	CA-C-N	5.29	127.63	120.38
4	A	715	GLU	C-N-CA	5.29	127.63	120.38
8	P	1635	GLU	CA-C-N	5.29	128.75	120.82
8	P	1635	GLU	C-N-CA	5.29	128.75	120.82
6	I	373	PHE	CA-CB-CG	-5.29	108.51	113.80
8	P	478	ILE	N-CA-C	-5.29	107.59	112.83
9	Q	728	PHE	N-CA-C	-5.28	106.51	113.17
1	Y	453	GLY	N-CA-C	-5.28	103.09	110.96
8	N	675	TYR	CA-C-N	5.28	127.62	120.38
8	N	675	TYR	C-N-CA	5.28	127.62	120.38
7	O	1543	LEU	CA-C-N	5.28	127.36	120.28
7	O	1543	LEU	C-N-CA	5.28	127.36	120.28
2	Z	994	ARG	CA-C-N	5.28	128.09	120.38
2	Z	994	ARG	C-N-CA	5.28	128.09	120.38
7	O	721	SER	N-CA-C	-5.28	106.15	112.59
8	P	1467	SER	CA-C-N	5.28	128.81	120.47
8	P	1467	SER	C-N-CA	5.28	128.81	120.47
7	M	721	SER	N-CA-C	-5.27	106.16	112.59
8	N	86	ASP	CA-CB-CG	5.27	117.87	112.60
5	H	346	GLN	N-CA-CB	5.27	119.40	110.49
8	P	783	PHE	CA-CB-CG	-5.27	108.53	113.80
9	Q	771	ILE	N-CA-CB	5.27	113.82	110.50
7	M	1448	GLY	N-CA-C	-5.27	107.95	115.64
2	1	1370	GLU	N-CA-C	-5.26	105.72	113.61
7	O	885	GLU	CA-C-N	5.26	131.58	121.54
7	O	885	GLU	C-N-CA	5.26	131.58	121.54
8	P	945	ASP	CA-CB-CG	5.26	117.86	112.60
1	0	522	ALA	N-CA-CB	5.26	119.37	110.49
1	0	1308	PHE	N-CA-C	-5.26	106.55	113.17
7	M	885	GLU	CA-C-N	5.26	131.58	121.54
7	M	885	GLU	C-N-CA	5.26	131.58	121.54
10	W	330	GLU	CA-C-N	5.26	127.32	120.28
10	W	330	GLU	C-N-CA	5.26	127.32	120.28
8	N	1166	VAL	CA-C-N	5.25	127.32	120.28
8	N	1166	VAL	C-N-CA	5.25	127.32	120.28
2	Z	208	LYS	CA-C-N	5.25	125.26	119.90
2	Z	208	LYS	C-N-CA	5.25	125.26	119.90
1	Y	1285	ILE	N-CA-C	-5.25	100.56	108.12
6	F	356	GLN	N-CA-C	-5.25	104.22	110.41
8	N	1175	GLU	CA-C-N	5.25	125.30	119.32
8	N	1175	GLU	C-N-CA	5.25	125.30	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	164	TYR	N-CA-C	-5.25	106.92	113.38
8	P	1427	SER	N-CA-CB	5.25	119.36	110.49
1	Y	1205	SER	CA-C-N	5.25	127.84	120.28
1	Y	1205	SER	C-N-CA	5.25	127.84	120.28
5	H	535	LYS	N-CA-C	-5.25	106.56	113.12
8	P	1288	PHE	N-CA-C	5.25	118.47	111.75
5	K	333	GLU	CA-C-N	5.24	127.31	120.28
5	K	333	GLU	C-N-CA	5.24	127.31	120.28
8	N	390	ILE	CA-C-N	5.24	126.39	119.84
8	N	390	ILE	C-N-CA	5.24	126.39	119.84
9	R	470	GLY	CA-C-N	5.24	124.91	119.56
9	R	470	GLY	C-N-CA	5.24	124.91	119.56
7	M	1272	LEU	N-CA-CB	-5.24	101.59	110.50
1	Y	789	VAL	CA-C-N	5.24	130.72	122.34
1	Y	789	VAL	C-N-CA	5.24	130.72	122.34
8	N	650	ASP	N-CA-CB	5.23	119.33	110.49
8	N	1054	PHE	CA-CB-CG	-5.23	108.57	113.80
8	P	1489	PRO	CA-C-N	5.23	127.56	120.65
8	P	1489	PRO	C-N-CA	5.23	127.56	120.65
9	T	754	ARG	CA-C-O	-5.23	113.03	120.51
7	M	185	PHE	CA-CB-CG	-5.23	108.57	113.80
8	P	399	VAL	N-CA-C	5.23	115.45	110.53
9	R	143	ASN	CA-C-N	5.23	127.24	120.44
9	R	143	ASN	C-N-CA	5.23	127.24	120.44
5	B	535	LYS	N-CA-C	-5.23	106.59	113.12
4	G	789	GLU	N-CA-C	-5.23	106.95	113.38
1	Y	992	CYS	CA-CB-SG	-5.23	102.38	114.40
9	T	637	ILE	CA-C-N	5.23	127.74	120.63
9	T	637	ILE	C-N-CA	5.23	127.74	120.63
7	O	20	PHE	CA-CB-CG	-5.22	108.58	113.80
1	0	1217	LEU	N-CA-C	-5.22	105.58	112.94
2	1	405	LYS	N-CA-CB	5.22	119.31	110.49
8	P	452	PHE	CA-CB-CG	-5.22	108.58	113.80
9	R	630	ARG	CA-C-N	5.22	127.53	120.38
9	R	630	ARG	C-N-CA	5.22	127.53	120.38
1	Y	626	ASN	N-CA-C	-5.22	99.68	110.80
1	Y	1062	LYS	N-CA-C	-5.22	108.18	114.75
9	R	57	ARG	CA-C-N	5.21	127.99	120.38
9	R	57	ARG	C-N-CA	5.21	127.99	120.38
9	S	159	PHE	CA-C-N	5.21	125.73	119.94
9	S	159	PHE	C-N-CA	5.21	125.73	119.94
9	R	510	LEU	N-CA-C	-5.21	106.98	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1238	ASP	N-CA-CB	5.21	119.30	110.49
8	P	634	ILE	CA-C-N	5.21	127.60	120.77
8	P	634	ILE	C-N-CA	5.21	127.60	120.77
9	S	500	GLU	N-CA-C	-5.21	106.61	113.17
1	O	632	TYR	N-CA-C	-5.21	106.99	113.55
7	O	1272	LEU	N-CA-CB	-5.21	101.64	110.50
1	Y	1385	PHE	CA-C-N	5.21	125.20	119.89
1	Y	1385	PHE	C-N-CA	5.21	125.20	119.89
7	M	778	LEU	CA-C-N	5.21	124.83	119.05
7	M	778	LEU	C-N-CA	5.21	124.83	119.05
8	N	878	PHE	CA-C-N	5.21	127.59	120.46
8	N	878	PHE	C-N-CA	5.21	127.59	120.46
8	P	610	LYS	N-CA-C	-5.21	106.88	114.12
9	S	600	ILE	CA-C-N	5.21	126.35	119.84
9	S	600	ILE	C-N-CA	5.21	126.35	119.84
7	O	1208	GLU	CA-C-N	5.21	125.20	119.89
7	O	1208	GLU	C-N-CA	5.21	125.20	119.89
8	N	1538	ASP	N-CA-C	-5.20	106.33	113.30
1	Y	118	THR	CA-C-N	5.20	126.34	119.84
1	Y	118	THR	C-N-CA	5.20	126.34	119.84
7	M	102	GLY	CA-C-N	5.20	128.02	120.79
7	M	102	GLY	C-N-CA	5.20	128.02	120.79
7	M	1208	GLU	CA-C-N	5.20	125.19	119.89
7	M	1208	GLU	C-N-CA	5.20	125.19	119.89
8	N	1053	LEU	CA-C-N	5.20	129.75	122.79
8	N	1053	LEU	C-N-CA	5.20	129.75	122.79
9	Q	477	TYR	N-CA-C	-5.20	106.62	113.17
4	D	672	GLY	CA-C-N	5.20	125.75	119.98
4	D	672	GLY	C-N-CA	5.20	125.75	119.98
1	Y	1218	TYR	N-CA-C	-5.20	105.65	112.41
8	P	1288	PHE	CA-CB-CG	5.20	119.00	113.80
2	Z	887	VAL	CA-C-N	5.20	127.50	120.44
2	Z	887	VAL	C-N-CA	5.20	127.50	120.44
8	P	152	TYR	N-CA-C	-5.19	106.75	114.64
2	1	1120	SER	N-CA-C	-5.19	104.75	111.71
8	N	495	ASP	N-CA-CB	5.19	119.27	110.49
7	O	93	LEU	N-CA-C	-5.19	106.97	113.72
7	O	1238	ASP	N-CA-CB	5.19	119.27	110.49
1	Y	1280	TYR	N-CA-C	-5.19	106.63	113.17
7	M	20	PHE	CA-CB-CG	-5.18	108.61	113.80
7	M	93	LEU	N-CA-C	-5.18	106.98	113.72
7	O	1448	GLY	N-CA-C	-5.18	108.07	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	324	TYR	CA-CB-CG	5.17	123.21	113.90
4	D	726	VAL	CA-CB-CG1	5.17	119.19	110.40
8	N	634	ILE	CA-C-N	5.17	127.55	120.77
8	N	634	ILE	C-N-CA	5.17	127.55	120.77
10	W	258	TYR	CA-C-N	5.17	125.17	119.89
10	W	258	TYR	C-N-CA	5.17	125.17	119.89
8	N	651	TYR	CA-C-N	5.17	128.57	120.82
8	N	651	TYR	C-N-CA	5.17	128.57	120.82
1	Y	1201	TRP	N-CA-C	-5.17	106.29	112.59
2	1	564	THR	N-CA-C	-5.16	105.66	112.94
4	A	789	GLU	N-CA-C	-5.16	107.03	113.38
6	L	355	GLN	N-CA-C	-5.16	106.66	113.17
2	Z	1184	ASP	CA-C-N	5.16	129.00	121.31
2	Z	1184	ASP	C-N-CA	5.16	129.00	121.31
1	0	1444	PHE	CA-CB-CG	-5.16	108.64	113.80
8	P	1223	ASN	N-CA-C	-5.16	105.45	112.26
9	T	155	VAL	CA-C-N	5.16	127.15	120.44
9	T	155	VAL	C-N-CA	5.16	127.15	120.44
9	R	236	ASN	CA-C-N	5.16	127.91	120.38
9	R	236	ASN	C-N-CA	5.16	127.91	120.38
6	F	292	HIS	CA-CB-CG	5.16	118.96	113.80
2	1	447	LYS	CA-C-N	5.16	128.19	120.87
2	1	447	LYS	C-N-CA	5.16	128.19	120.87
7	M	1322	SER	N-CA-C	-5.16	106.77	113.16
8	N	1050	SER	N-CA-CB	5.16	119.20	110.49
9	Q	790	ASN	N-CA-C	-5.16	106.23	112.88
1	0	835	SER	N-CA-C	-5.15	102.27	109.69
7	M	103	LYS	CA-C-N	5.15	127.25	120.60
7	M	103	LYS	C-N-CA	5.15	127.25	120.60
1	0	838	CYS	CA-C-N	5.15	127.52	120.46
1	0	838	CYS	C-N-CA	5.15	127.52	120.46
2	1	679	SER	CA-CB-OG	-5.15	100.80	111.10
7	O	1383	GLN	CA-C-N	5.15	127.49	120.54
7	O	1383	GLN	C-N-CA	5.15	127.49	120.54
9	T	269	ASN	N-CA-CB	5.15	119.19	110.49
10	W	313	TRP	N-CA-C	-5.15	106.31	112.59
1	Y	914	TYR	N-CA-C	-5.15	106.24	112.88
8	P	642	PHE	N-CA-C	-5.15	107.67	114.31
1	0	374	LYS	N-CA-C	-5.15	107.05	113.38
5	H	344	SER	CA-C-N	5.15	125.14	119.89
5	H	344	SER	C-N-CA	5.15	125.14	119.89
9	S	354	VAL	N-CA-C	-5.14	107.70	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	700	ALA	CA-C-N	5.14	125.65	119.94
9	T	700	ALA	C-N-CA	5.14	125.65	119.94
9	R	797	SER	N-CA-C	-5.14	106.94	114.39
8	N	767	ILE	CA-C-N	5.14	127.17	120.28
8	N	767	ILE	C-N-CA	5.14	127.17	120.28
9	T	615	ASP	CA-CB-CG	5.14	117.74	112.60
8	P	587	GLN	N-CA-CB	5.14	119.17	110.49
1	Y	1109	PHE	CA-CB-CG	-5.14	108.66	113.80
8	N	801	LYS	CA-C-N	5.13	127.47	120.54
8	N	801	LYS	C-N-CA	5.13	127.47	120.54
4	G	672	GLY	CA-C-N	5.13	125.65	120.00
4	G	672	GLY	C-N-CA	5.13	125.65	120.00
2	Z	907	GLY	CA-C-N	5.13	127.11	120.44
2	Z	907	GLY	C-N-CA	5.13	127.11	120.44
2	1	1179	ASN	N-CA-CB	5.13	119.16	110.49
1	Y	509	PHE	N-CA-C	-5.13	106.71	113.17
2	1	454	PRO	N-CA-C	5.12	116.95	110.70
9	R	49	LEU	CA-C-N	5.12	127.46	120.54
9	R	49	LEU	C-N-CA	5.12	127.46	120.54
1	0	394	GLU	CA-C-N	5.12	124.92	119.28
1	0	394	GLU	C-N-CA	5.12	124.92	119.28
8	N	207	ASP	CA-CB-CG	5.12	117.72	112.60
8	N	1433	ILE	N-CA-C	-5.12	99.14	107.28
8	P	186	LYS	CA-C-N	5.12	127.65	120.28
8	P	186	LYS	C-N-CA	5.12	127.65	120.28
9	S	420	LEU	N-CA-C	-5.12	106.35	112.59
7	M	749	ILE	CA-C-N	5.11	127.33	120.58
7	M	749	ILE	C-N-CA	5.11	127.33	120.58
2	1	551	TYR	N-CA-C	-5.11	108.31	114.75
1	Y	1357	LYS	N-CA-C	-5.11	107.08	113.72
1	Y	710	VAL	CA-C-N	5.11	131.17	121.97
1	Y	710	VAL	C-N-CA	5.11	131.17	121.97
1	0	1076	LYS	CA-C-N	5.10	126.00	120.44
1	0	1076	LYS	C-N-CA	5.10	126.00	120.44
7	O	1322	SER	N-CA-C	-5.10	106.83	113.16
9	R	511	ALA	CA-C-N	5.10	127.37	120.38
9	R	511	ALA	C-N-CA	5.10	127.37	120.38
9	S	357	LYS	N-CA-CB	5.10	119.11	110.49
11	X	290	HIS	N-CA-C	-5.10	106.74	113.17
1	Y	711	VAL	N-CA-CB	5.10	119.65	111.23
1	0	618	THR	N-CA-C	-5.10	98.94	108.02
1	0	664	ASP	N-CA-C	-5.10	105.96	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	653	SER	CA-C-N	5.10	127.44	120.46
8	N	653	SER	C-N-CA	5.10	127.44	120.46
1	O	767	SER	CA-C-N	5.10	125.13	119.32
1	O	767	SER	C-N-CA	5.10	125.13	119.32
8	P	713	LYS	N-CA-CB	5.10	117.40	110.01
4	D	694	ASP	CA-CB-CG	5.09	117.69	112.60
7	O	603	GLU	N-CA-C	5.09	121.65	110.80
7	O	1617	SER	CA-C-N	5.09	127.06	120.44
7	O	1617	SER	C-N-CA	5.09	127.06	120.44
9	Q	130	ASN	CA-C-N	5.09	125.60	119.94
9	Q	130	ASN	C-N-CA	5.09	125.60	119.94
10	U	305	TYR	CA-C-O	5.09	127.14	120.16
8	P	969	ILE	N-CA-C	-5.09	108.01	112.90
1	Y	1220	LEU	N-CA-C	-5.09	106.75	113.17
7	M	1617	SER	CA-C-N	5.09	127.06	120.44
7	M	1617	SER	C-N-CA	5.09	127.06	120.44
1	Y	641	VAL	N-CA-C	-5.09	100.42	107.80
2	1	607	ASN	N-CA-CB	5.09	119.09	110.49
2	1	1354	ASP	N-CA-CB	5.09	119.09	110.49
7	O	778	LEU	CA-C-N	5.09	124.70	119.05
7	O	778	LEU	C-N-CA	5.09	124.70	119.05
2	Z	597	GLU	CA-C-N	5.09	126.20	119.84
2	Z	597	GLU	C-N-CA	5.09	126.20	119.84
1	O	1157	PHE	N-CA-C	-5.08	105.44	111.69
2	1	1092	LEU	N-CA-CB	5.08	119.08	110.49
8	P	1124	ASP	CA-CB-CG	5.08	117.69	112.60
2	1	1108	PHE	CA-CB-CG	-5.08	108.72	113.80
2	1	728	VAL	N-CA-C	-5.08	108.02	112.90
8	N	1033	PHE	CA-CB-CG	-5.08	108.72	113.80
8	N	798	SER	CA-C-N	5.08	127.59	120.28
8	N	798	SER	C-N-CA	5.08	127.59	120.28
7	M	603	GLU	N-CA-C	5.08	121.61	110.80
2	Z	818	ASP	CA-CB-CG	5.08	117.67	112.60
8	N	262	SER	CA-C-N	5.07	127.79	120.38
8	N	262	SER	C-N-CA	5.07	127.79	120.38
7	O	102	GLY	CA-C-N	5.07	127.84	120.79
7	O	102	GLY	C-N-CA	5.07	127.84	120.79
8	P	321	ILE	N-CA-C	-5.07	106.98	113.22
9	Q	345	LEU	N-CA-C	-5.07	104.35	110.44
8	N	447	LEU	N-CA-C	-5.07	101.03	108.79
8	N	672	VAL	CA-C-N	5.07	127.33	120.38
8	N	672	VAL	C-N-CA	5.07	127.33	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	1594	ASP	CA-C-N	5.07	127.78	120.38
8	N	1594	ASP	C-N-CA	5.07	127.78	120.38
7	O	1143	SER	N-CA-CB	5.07	119.06	110.49
9	Q	697	PHE	N-CA-CB	5.07	119.06	110.49
4	G	702	ARG	N-CA-C	-5.07	107.14	113.72
8	P	14	THR	CA-C-N	5.07	127.77	120.38
8	P	14	THR	C-N-CA	5.07	127.77	120.38
4	D	789	GLU	N-CA-C	-5.06	107.78	114.31
7	M	653	ALA	CA-C-N	5.06	127.37	120.54
7	M	653	ALA	C-N-CA	5.06	127.37	120.54
8	P	1062	ARG	CA-C-N	5.06	127.77	120.38
8	P	1062	ARG	C-N-CA	5.06	127.77	120.38
4	G	727	SER	CA-C-O	5.06	129.40	120.80
11	V	285	ILE	CA-C-N	5.06	127.06	120.28
11	V	285	ILE	C-N-CA	5.06	127.06	120.28
7	M	1355	SER	CA-C-N	5.05	127.36	120.54
7	M	1355	SER	C-N-CA	5.05	127.36	120.54
7	O	211	ASP	CA-C-N	5.05	127.36	120.54
7	O	211	ASP	C-N-CA	5.05	127.36	120.54
8	P	187	PHE	CA-C-N	5.05	127.66	120.53
8	P	187	PHE	C-N-CA	5.05	127.66	120.53
8	P	798	SER	CA-C-N	5.05	127.76	120.38
8	P	798	SER	C-N-CA	5.05	127.76	120.38
2	Z	606	SER	N-CA-C	5.05	116.48	111.07
1	0	922	PHE	CA-CB-CG	-5.05	108.75	113.80
1	0	1218	TYR	N-CA-C	-5.05	104.86	112.99
2	1	510	CYS	CA-C-N	5.05	127.27	120.50
2	1	510	CYS	C-N-CA	5.05	127.27	120.50
8	N	47	ASN	N-CA-CB	5.05	119.02	110.49
9	S	313	LEU	N-CA-C	-5.05	106.37	112.88
7	M	1335	ILE	CA-C-N	5.05	124.37	120.33
7	M	1335	ILE	C-N-CA	5.05	124.37	120.33
8	P	940	SER	N-CA-C	-5.05	107.29	113.50
9	T	417	ARG	N-CA-CB	5.04	119.02	110.49
2	Z	196	GLU	N-CA-C	-5.04	106.54	113.30
8	N	1039	PHE	CA-CB-CG	-5.04	108.76	113.80
9	R	504	VAL	N-CA-CB	5.04	116.45	110.55
1	Y	419	LYS	N-CA-C	-5.04	99.41	108.48
9	T	757	ALA	N-CA-C	-5.04	107.27	113.41
1	0	1239	ALA	N-CA-C	-5.03	106.99	113.23
7	M	1383	GLN	CA-C-N	5.03	127.33	120.54
7	M	1383	GLN	C-N-CA	5.03	127.33	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	1341	ASP	CA-CB-CG	5.03	117.63	112.60
9	S	824	MET	CA-C-N	5.03	126.13	119.84
9	S	824	MET	C-N-CA	5.03	126.13	119.84
7	O	653	ALA	CA-C-N	5.03	127.33	120.54
7	O	653	ALA	C-N-CA	5.03	127.33	120.54
8	P	1622	GLU	CA-C-N	5.03	127.02	120.28
8	P	1622	GLU	C-N-CA	5.03	127.02	120.28
1	O	938	LEU	CA-C-N	5.03	127.72	120.38
1	O	938	LEU	C-N-CA	5.03	127.72	120.38
8	N	993	SER	N-CA-C	-5.03	100.10	110.80
8	P	931	PHE	CA-CB-CG	-5.03	108.78	113.80
9	T	732	TRP	N-CA-C	-5.03	105.21	113.50
7	O	720	HIS	N-CA-C	-5.02	104.90	112.99
2	1	108	THR	CA-C-N	5.02	126.12	119.84
2	1	108	THR	C-N-CA	5.02	126.12	119.84
4	A	672	GLY	CA-C-N	5.02	125.53	120.00
4	A	672	GLY	C-N-CA	5.02	125.53	120.00
7	M	1143	SER	N-CA-CB	5.02	118.98	110.49
8	P	1010	GLU	N-CA-CB	5.02	118.98	110.49
8	P	343	ASP	CA-CB-CG	5.02	117.62	112.60
9	T	539	ALA	CA-C-N	5.02	127.51	120.28
9	T	539	ALA	C-N-CA	5.02	127.51	120.28
1	Y	134	ASN	CA-C-N	5.02	131.13	121.54
1	Y	134	ASN	C-N-CA	5.02	131.13	121.54
1	Y	1106	ASP	N-CA-C	-5.02	99.09	108.02
2	Z	1275	THR	N-CA-C	-5.02	107.10	113.43
2	1	619	GLU	N-CA-C	-5.02	107.33	113.50
8	N	1346	LYS	N-CA-C	-5.02	107.55	113.97
7	O	315	GLU	N-CA-C	-5.01	107.20	113.72
7	M	304	THR	N-CA-C	-5.01	106.51	113.18
7	M	720	HIS	N-CA-C	-5.01	104.92	112.99
8	P	857	LEU	CA-C-N	5.01	127.00	120.28
8	P	857	LEU	C-N-CA	5.01	127.00	120.28
10	U	273	PHE	N-CA-C	-5.01	105.87	112.94
7	M	35	LEU	CA-C-N	5.01	131.11	121.54
7	M	35	LEU	C-N-CA	5.01	131.11	121.54
7	O	1355	SER	CA-C-N	5.01	127.30	120.54
7	O	1355	SER	C-N-CA	5.01	127.30	120.54
8	P	1514	VAL	N-CA-C	-5.01	107.58	112.29
9	S	503	ALA	CA-C-N	5.01	126.87	120.56
9	S	503	ALA	C-N-CA	5.01	126.87	120.56
1	Y	664	ASP	N-CA-C	-5.01	107.22	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1288	ALA	N-CA-C	5.01	117.39	111.33
6	I	344	LEU	N-CA-C	-5.01	106.52	113.18
7	O	1483	THR	N-CA-C	5.01	121.46	110.80
9	Q	87	ILE	CA-C-N	5.01	126.95	120.44
9	Q	87	ILE	C-N-CA	5.01	126.95	120.44
9	S	647	ALA	CA-C-N	5.01	129.52	122.46
9	S	647	ALA	C-N-CA	5.01	129.52	122.46
2	1	962	LYS	N-CA-C	-5.00	105.49	112.45
1	Y	1370	VAL	N-CA-C	-5.00	108.62	113.53
1	0	1279	VAL	N-CA-C	-5.00	107.46	111.91
2	1	902	LEU	N-CA-C	-5.00	106.59	113.30
2	Z	185	ILE	N-CA-C	-5.00	107.88	112.83
2	Z	712	SER	CA-C-N	5.00	126.98	120.28
2	Z	712	SER	C-N-CA	5.00	126.98	120.28

All (101) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	471	SER	CA
1	0	884	VAL	CA
1	0	885	ALA	CA
1	0	991	ARG	CA
1	0	992	CYS	CA
1	0	1257	GLN	CA
1	0	1258	LEU	CA
2	1	308	ASN	CA
2	1	309	LEU	CA
2	1	514	ARG	CA
2	1	679	SER	CA
2	1	921	SER	CA
2	1	922	LYS	CA
2	1	1300	SER	CA
2	1	1301	SER	CA
4	A	726	VAL	CA
4	D	726	VAL	CA
5	E	323	LEU	CA
5	E	324	TYR	CA
6	F	369	LEU	CA
6	F	370	ASP	CA
4	G	726	VAL	CA
4	G	727	SER	CA
5	H	323	LEU	CA

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Mol	Chain	Res	Type	Atom
5	H	324	TYR	CA
4	J	726	VAL	CA
7	M	602	ASN	CA
7	M	603	GLU	CA
7	M	1273	LYS	CA
8	N	40	ILE	CA
8	N	41	ARG	CA
8	N	256	THR	CA
8	N	257	LEU	CA
8	N	551	ASN	CA
8	N	552	LEU	CA
8	N	576	TYR	CA
8	N	577	MET	CA
8	N	793	LEU	CA
8	N	794	ILE	CA
8	N	1054	PHE	CA
8	N	1055	GLN	CA
8	N	1060	LEU	CA
7	O	602	ASN	CA
7	O	603	GLU	CA
7	O	1137	ASN	CA
7	O	1138	PHE	CA
7	O	1273	LYS	CA
7	O	1319	LEU	CA
7	O	1320	GLU	CA
8	P	174	VAL	CA
8	P	256	THR	CA
8	P	257	LEU	CA
8	P	358	VAL	CA
8	P	359	LEU	CA
8	P	551	ASN	CA
8	P	552	LEU	CA
8	P	576	TYR	CA
8	P	793	LEU	CA
8	P	794	ILE	CA
9	Q	514	LYS	CA
9	Q	515	LEU	CA
9	Q	753	ALA	CA
9	Q	754	ARG	CA
9	R	514	LYS	CA
9	R	753	ALA	CA
9	R	754	ARG	CA

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Mol	Chain	Res	Type	Atom
9	S	514	LYS	CA
9	S	753	ALA	CA
9	S	754	ARG	CA
9	T	753	ALA	CA
9	T	754	ARG	CA
10	U	248	TRP	CA
10	U	249	ASP	CA
10	U	283	ILE	CA
10	U	304	LYS	CA
10	U	305	TYR	CA
11	V	301	LEU	CA
11	V	401	ASP	CA
10	W	283	ILE	CA
10	W	304	LYS	CA
10	W	305	TYR	CA
11	X	301	LEU	CA
11	X	302	ARG	CA
1	Y	790	PHE	CA
1	Y	791	MET	CA
1	Y	991	ARG	CA
1	Y	992	CYS	CA
2	Z	308	ASN	CA
2	Z	456	THR	CA
2	Z	514	ARG	CA
2	Z	678	LYS	CA
2	Z	679	SER	CA
2	Z	745	ILE	CA
2	Z	891	ARG	CA
2	Z	915	LYS	CA
2	Z	921	SER	CA
2	Z	922	LYS	CA
2	Z	1039	LEU	CA
2	Z	1040	LYS	CA
2	Z	1155	GLN	CA
2	Z	1156	LEU	CA

All (97) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1208	SER	Peptide
1	0	1299	GLY	Peptide
1	0	1421	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	0	186	ILE	Peptide
1	0	523	SER	Peptide
1	0	782	ARG	Peptide
2	1	1098	LEU	Peptide
5	E	315	LYS	Peptide
5	E	324	TYR	Mainchain
5	E	385	GLN	Peptide
4	G	658	TYR	Sidechain
7	M	1160	TYR	Sidechain
7	M	1219	VAL	Peptide
7	M	1361	PHE	Peptide
7	M	1394	SER	Peptide
7	M	1453	ARG	Sidechain
7	M	1515	LEU	Peptide
7	M	1534	GLY	Peptide
7	M	1592	ALA	Mainchain
7	M	232	TYR	Sidechain
7	M	619	VAL	Peptide
7	M	620	THR	Peptide
7	M	744	TYR	Peptide
7	M	834	GLU	Peptide
7	M	993	ALA	Peptide
8	N	1008	THR	Peptide
8	N	1060	LEU	Mainchain
8	N	1162	LEU	Peptide
8	N	1399	ASN	Peptide
8	N	1463	SER	Peptide
8	N	210	ASN	Peptide
8	N	213	PHE	Peptide
8	N	333	ARG	Sidechain
8	N	369	LEU	Peptide
8	N	413	GLU	Peptide
8	N	432	LEU	Peptide
8	N	440	ILE	Peptide
8	N	552	LEU	Mainchain
8	N	727	ASN	Peptide
8	N	728	ILE	Peptide
8	N	806	PHE	Peptide
8	N	810	MET	Peptide
8	N	811	ASP	Peptide
8	N	835	LEU	Peptide
8	N	879	ILE	Peptide

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Mol	Chain	Res	Type	Group
8	N	894	VAL	Peptide
8	N	927	LYS	Peptide
8	N	937	SER	Peptide
7	O	1160	TYR	Sidechain
7	O	1219	VAL	Peptide
7	O	1361	PHE	Peptide
7	O	1394	SER	Peptide
7	O	1453	ARG	Sidechain
7	O	1515	LEU	Peptide
7	O	1534	GLY	Peptide
7	O	1592	ALA	Mainchain
7	O	232	TYR	Sidechain
7	O	619	VAL	Peptide
7	O	620	THR	Peptide
7	O	744	TYR	Peptide
7	O	834	GLU	Peptide
7	O	993	ALA	Peptide
8	P	1008	THR	Peptide
8	P	1162	LEU	Peptide
8	P	1399	ASN	Peptide
8	P	1463	SER	Peptide
8	P	150	GLN	Peptide
8	P	213	PHE	Peptide
8	P	371	PHE	Peptide
8	P	432	LEU	Peptide
8	P	693	MET	Peptide
8	P	727	ASN	Peptide
8	P	728	ILE	Peptide
8	P	778	VAL	Peptide
8	P	810	MET	Peptide
8	P	811	ASP	Peptide
8	P	826	SER	Peptide
8	P	835	LEU	Peptide
8	P	894	VAL	Peptide
8	P	912	TRP	Peptide
8	P	927	LYS	Peptide
8	P	937	SER	Peptide
8	P	991	LYS	Peptide
9	R	754	ARG	Mainchain
9	S	339	TYR	Sidechain
10	U	249	ASP	Mainchain
10	W	305	TYR	Mainchain

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Mol	Chain	Res	Type	Group
10	W	318	TYR	Sidechain
1	Y	1045	GLU	Peptide
1	Y	1060	TYR	Peptide
1	Y	1208	SER	Peptide
1	Y	1299	GLY	Peptide
1	Y	133	TYR	Sidechain
1	Y	292	ASN	Peptide
1	Y	523	SER	Peptide
1	Y	782	ARG	Peptide
2	Z	1098	LEU	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	0	8890	0	8960	9	0
1	Y	8747	0	8800	41	0
2	1	8903	0	8919	38	0
2	Z	8883	0	8898	31	0
3	5	181	0	37	3	0
3	6	181	0	38	0	0
4	A	1315	0	1274	0	0
4	D	1315	0	1275	0	0
4	G	1321	0	1280	1	0
4	J	1315	0	1275	8	0
5	B	1771	0	1832	29	0
5	E	1771	0	1832	15	0
5	H	1771	0	1832	5	0
5	K	1771	0	1831	31	0
6	C	1347	0	1376	8	0
6	F	1351	0	1379	1	0
6	I	1347	0	1376	5	0
6	L	1351	0	1379	0	0
7	M	11905	0	11614	30	0
7	O	11909	0	11617	47	0
8	N	10955	0	11304	99	0
8	P	10955	0	11301	142	0
9	Q	5192	0	4911	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	R	5279	0	4937	0	0
9	S	5189	0	4902	14	0
9	T	5279	0	4937	11	0
10	U	736	0	739	10	0
10	W	736	0	739	13	0
11	V	720	0	703	0	0
11	X	731	0	716	1	0
All	All	123117	0	122013	570	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (570) 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)
8:N:1277:ILE:HD11	8:N:1280:LEU:CG	1.25	1.65
2:1:745:ILE:HG21	2:1:815:PHE:CZ	1.22	1.61
8:P:1277:ILE:CD1	8:P:1280:LEU:HB2	1.22	1.61
2:1:745:ILE:CG2	2:1:815:PHE:CZ	1.82	1.57
2:1:745:ILE:HG22	2:1:815:PHE:CE2	1.36	1.56
8:P:1050:SER:HA	8:P:1054:PHE:CD2	1.40	1.55
1:Y:832:VAL:HG11	1:Y:914:TYR:CD1	1.39	1.54
8:N:1277:ILE:CD1	8:N:1280:LEU:HG	1.17	1.54
8:P:1050:SER:CA	8:P:1054:PHE:HD2	1.27	1.48
7:O:1027:GLN:CG	7:O:1039:ALA:HB3	1.48	1.44
1:Y:832:VAL:CG1	1:Y:914:TYR:CD1	2.06	1.38
8:P:1292:GLU:HB3	8:P:1304:LYS:CG	1.53	1.38
2:Z:1253:VAL:HG12	2:Z:1300:SER:OG	1.21	1.36
8:N:12:GLN:NE2	8:N:73:SER:CB	1.89	1.36
8:P:380:THR:OG1	8:P:400:PHE:CZ	1.79	1.35
8:P:1060:LEU:CB	8:P:1065:THR:HG21	1.60	1.32
1:Y:832:VAL:HG21	1:Y:914:TYR:CZ	1.62	1.32
7:O:1027:GLN:NE2	7:O:1039:ALA:O	1.63	1.32
7:O:1027:GLN:HG2	7:O:1039:ALA:CB	1.61	1.30
1:Y:832:VAL:HG11	1:Y:914:TYR:CE1	1.65	1.30
8:N:12:GLN:NE2	8:N:73:SER:HB2	1.42	1.30
8:P:1292:GLU:OE2	8:P:1304:LYS:HB3	1.31	1.29
5:K:320:GLU:HB3	5:K:323:LEU:CG	1.60	1.29
8:P:1277:ILE:CD1	8:P:1280:LEU:CB	2.11	1.27
2:1:745:ILE:HG21	2:1:815:PHE:CE1	1.72	1.24
8:P:1277:ILE:HD13	8:P:1280:LEU:CD1	1.66	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:979:LYS:NZ	7:O:1040:THR:CG2	2.02	1.20
8:P:376:THR:O	8:P:379:ILE:HG12	1.03	1.19
7:M:1041:PHE:CE2	7:M:1042:ILE:HG12	1.75	1.18
7:O:1027:GLN:CD	7:O:1039:ALA:O	1.85	1.18
8:P:379:ILE:HG22	8:P:400:PHE:HE1	1.07	1.18
8:P:379:ILE:CG2	8:P:400:PHE:HE1	1.56	1.17
2:1:745:ILE:CG2	2:1:815:PHE:CE2	2.06	1.16
1:Y:832:VAL:HG11	1:Y:914:TYR:CG	1.80	1.16
7:O:979:LYS:HZ1	7:O:1040:THR:HG23	1.07	1.16
8:N:12:GLN:NE2	8:N:73:SER:OG	1.76	1.15
1:Y:832:VAL:CG1	1:Y:914:TYR:CE1	2.27	1.15
7:O:979:LYS:NZ	7:O:1040:THR:HG21	1.58	1.14
8:P:42:GLN:HA	8:P:45:LYS:HD3	1.23	1.14
8:P:379:ILE:HG22	8:P:400:PHE:CE1	1.81	1.14
7:O:979:LYS:HZ1	7:O:1040:THR:CG2	1.56	1.13
8:P:376:THR:O	8:P:379:ILE:CG1	1.96	1.12
9:S:594:GLY:HA3	10:W:322:LEU:CD2	1.78	1.12
2:Z:1253:VAL:CG1	2:Z:1300:SER:OG	1.97	1.11
2:1:730:VAL:HG13	2:1:744:GLY:HA3	1.32	1.11
4:J:670:VAL:HG12	5:K:315:LYS:HB2	1.33	1.10
1:Y:832:VAL:HG21	1:Y:914:TYR:CE1	1.85	1.10
5:B:324:TYR:O	5:B:349:PRO:CG	1.98	1.10
8:P:134:ARG:O	8:P:198:MET:HE2	1.50	1.10
5:K:320:GLU:HG2	5:K:323:LEU:HD21	1.26	1.09
8:N:1277:ILE:CG1	8:N:1280:LEU:HG	1.81	1.09
8:P:1050:SER:CB	8:P:1054:PHE:HD2	1.64	1.08
9:S:594:GLY:CA	10:W:322:LEU:HD21	1.83	1.08
9:T:208:LEU:HD12	9:T:211:LYS:HE2	1.30	1.08
8:P:1060:LEU:HB2	8:P:1065:THR:CG2	1.83	1.08
8:P:1277:ILE:HD13	8:P:1280:LEU:HD12	1.20	1.07
9:T:208:LEU:HD12	9:T:211:LYS:CE	1.83	1.07
8:P:1049:ASP:O	8:P:1054:PHE:HE2	1.39	1.06
8:P:1050:SER:CB	8:P:1054:PHE:CD2	2.39	1.06
8:N:380:THR:HG21	8:N:414:ASN:HD22	1.12	1.06
2:1:960:GLN:HG3	2:1:1039:LEU:HD21	1.39	1.05
9:S:691:ARG:HH21	10:W:322:LEU:CD1	1.68	1.05
5:K:320:GLU:HB3	5:K:323:LEU:HG	1.21	1.04
8:P:1277:ILE:HD13	8:P:1280:LEU:CG	1.87	1.04
9:Q:595:ARG:HD2	10:U:322:LEU:HD21	1.34	1.04
5:K:320:GLU:CG	5:K:323:LEU:HD21	1.87	1.04
7:M:1041:PHE:CE2	7:M:1042:ILE:CG1	2.41	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:832:VAL:CG2	1:Y:914:TYR:CE1	2.41	1.04
7:O:979:LYS:HZ3	7:O:1040:THR:HG21	1.03	1.03
1:Y:832:VAL:HG21	1:Y:914:TYR:OH	1.57	1.03
8:P:1304:LYS:HE3	8:P:1304:LYS:HA	1.41	1.02
8:P:1277:ILE:HD13	8:P:1280:LEU:HB2	1.32	1.02
7:M:1041:PHE:CD2	7:M:1042:ILE:HG12	1.94	1.02
8:N:275:LEU:HD23	8:N:381:VAL:O	1.58	1.02
8:P:73:SER:HB2	8:P:83:VAL:O	1.58	1.01
9:Q:681:SER:CB	10:U:322:LEU:HD11	1.90	1.01
2:Z:1253:VAL:HG12	2:Z:1300:SER:HG	1.19	1.01
8:P:1292:GLU:CB	8:P:1304:LYS:HG3	1.91	1.01
5:B:325:THR:HA	5:B:335:TRP:CH2	1.97	1.00
5:H:317:ASN:HD22	5:H:346:GLN:HB3	1.22	1.00
8:N:72:ARG:NH1	8:N:84:ASP:OD1	1.94	1.00
8:P:1277:ILE:HD13	8:P:1280:LEU:CB	1.82	1.00
8:P:1088:ASN:HB3	8:P:1093:ASN:HB3	1.42	0.99
9:Q:681:SER:OG	10:U:322:LEU:HD11	1.62	0.99
8:P:1050:SER:CA	8:P:1054:PHE:CD2	2.17	0.99
8:P:1277:ILE:HD12	8:P:1280:LEU:CB	1.86	0.99
8:P:69:ASN:HA	8:P:72:ARG:HD3	1.45	0.98
4:J:670:VAL:CG1	5:K:315:LYS:HB2	1.94	0.98
8:N:1277:ILE:HD11	8:N:1280:LEU:CD2	1.91	0.98
8:P:1060:LEU:HA	8:P:1065:THR:OG1	1.64	0.98
5:K:320:GLU:HB3	5:K:323:LEU:CD2	1.92	0.98
8:N:1277:ILE:HG12	8:N:1280:LEU:HD12	1.45	0.97
8:P:1277:ILE:HD12	8:P:1280:LEU:HB2	0.99	0.97
8:P:1292:GLU:HB3	8:P:1304:LYS:HG3	0.99	0.97
7:M:1037:ASN:HA	7:M:1041:PHE:HB2	1.45	0.97
8:N:376:THR:O	8:N:379:ILE:HD11	1.65	0.96
5:B:324:TYR:O	5:B:349:PRO:HG3	1.65	0.96
7:O:1027:GLN:CG	7:O:1039:ALA:CB	2.28	0.96
8:P:379:ILE:CG2	8:P:400:PHE:CE1	2.44	0.95
8:P:1060:LEU:CB	8:P:1065:THR:CG2	2.43	0.95
8:P:380:THR:OG1	8:P:400:PHE:HZ	1.33	0.95
8:N:380:THR:CG2	8:N:414:ASN:HD22	1.78	0.94
8:P:34:ALA:HB2	8:P:44:LEU:HD12	1.48	0.94
1:Y:832:VAL:HG13	1:Y:914:TYR:CD1	2.03	0.94
7:O:1027:GLN:CD	7:O:1039:ALA:HB3	1.92	0.94
8:N:12:GLN:HE22	8:N:73:SER:CB	1.69	0.93
8:P:1060:LEU:HB2	8:P:1065:THR:HG21	0.94	0.93
8:P:1292:GLU:HB3	8:P:1304:LYS:HG2	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:326:LYS:N	5:B:327:PRO:HD3	1.84	0.93
8:P:34:ALA:CB	8:P:44:LEU:CD1	2.46	0.93
8:P:380:THR:CG2	8:P:446:ALA:HA	1.99	0.93
9:T:208:LEU:O	9:T:211:LYS:HG2	1.70	0.92
5:B:324:TYR:HB3	5:B:349:PRO:HG2	1.52	0.92
5:B:324:TYR:HB3	5:B:349:PRO:CD	2.00	0.92
9:Q:595:ARG:HD2	10:U:322:LEU:CD2	2.00	0.92
1:Y:832:VAL:CG2	1:Y:914:TYR:CZ	2.52	0.91
8:P:1049:ASP:O	8:P:1054:PHE:CE2	2.23	0.90
8:P:34:ALA:HB2	8:P:44:LEU:CD1	2.00	0.90
8:P:31:ALA:HB1	8:P:40:ILE:HG12	1.55	0.89
8:P:1088:ASN:ND2	8:P:1093:ASN:HD22	1.69	0.89
6:C:370:ASP:O	6:C:374:GLN:NE2	2.06	0.89
9:Q:681:SER:OG	10:U:322:LEU:CD1	2.19	0.89
8:N:12:GLN:HE21	8:N:73:SER:HB2	1.07	0.88
4:J:670:VAL:HG12	5:K:315:LYS:CB	2.04	0.88
5:B:324:TYR:HB3	5:B:349:PRO:HD2	1.53	0.88
9:S:691:ARG:HH21	10:W:322:LEU:HD11	1.34	0.88
5:B:324:TYR:HB3	5:B:349:PRO:CG	2.04	0.87
8:P:1277:ILE:CD1	8:P:1280:LEU:HD12	2.02	0.87
9:S:594:GLY:HA3	10:W:322:LEU:HD21	0.92	0.87
8:P:69:ASN:HA	8:P:72:ARG:CD	2.04	0.87
5:B:325:THR:HA	5:B:335:TRP:CZ2	2.09	0.87
8:N:1277:ILE:CD1	8:N:1280:LEU:CG	2.07	0.87
6:I:370:ASP:O	6:I:374:GLN:NE2	2.08	0.86
5:K:320:GLU:C	5:K:322:ILE:H	1.80	0.86
9:Q:595:ARG:CD	10:U:322:LEU:HD21	2.04	0.86
5:B:324:TYR:CD2	5:B:349:PRO:O	2.28	0.86
8:P:1292:GLU:CB	8:P:1304:LYS:CG	2.47	0.86
9:Q:681:SER:HB2	10:U:322:LEU:HD11	1.56	0.86
5:B:324:TYR:CB	5:B:349:PRO:HD2	2.05	0.86
8:P:31:ALA:CB	8:P:40:ILE:HG12	2.06	0.86
5:E:318:GLU:HG3	5:E:346:GLN:HA	1.58	0.86
8:P:1304:LYS:HA	8:P:1304:LYS:CE	2.03	0.85
9:S:691:ARG:HH21	10:W:322:LEU:HD12	1.41	0.85
8:P:1277:ILE:HD11	8:P:1280:LEU:HB2	1.54	0.85
8:P:1050:SER:HB2	8:P:1054:PHE:CD2	2.12	0.85
8:P:134:ARG:O	8:P:198:MET:CE	2.25	0.84
6:C:353:LEU:HD12	6:C:369:LEU:HD23	1.59	0.84
5:B:324:TYR:O	5:B:349:PRO:HG2	1.75	0.84
8:P:1088:ASN:HB3	8:P:1093:ASN:CB	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:1277:ILE:HG12	8:N:1280:LEU:CD1	2.06	0.83
2:Z:1253:VAL:HG12	2:Z:1300:SER:CB	2.08	0.83
1:Y:1257:GLN:HA	1:Y:1261:ARG:NH1	1.92	0.83
2:Z:1254:GLY:C	2:Z:1300:SER:O	2.22	0.82
8:P:1050:SER:HA	8:P:1054:PHE:HD2	0.71	0.82
8:P:42:GLN:O	8:P:45:LYS:NZ	2.12	0.82
8:N:382:PHE:HE1	8:N:385:PHE:CE2	1.98	0.82
8:P:34:ALA:HB1	8:P:44:LEU:HD11	1.61	0.82
8:P:1060:LEU:HD12	8:P:1192:LEU:CD2	2.10	0.82
7:O:1043:SER:HB3	7:O:1047:SER:N	1.95	0.82
8:P:1060:LEU:CA	8:P:1065:THR:HG21	2.09	0.81
5:K:320:GLU:CB	5:K:323:LEU:HD21	2.11	0.81
8:N:12:GLN:HE21	8:N:73:SER:CB	1.67	0.81
8:N:1303:LEU:HG	8:N:1350:LEU:HB3	1.62	0.81
8:N:1277:ILE:CG1	8:N:1280:LEU:CG	2.52	0.81
7:O:1027:GLN:HG2	7:O:1039:ALA:HB3	0.81	0.80
5:K:320:GLU:CB	5:K:323:LEU:HG	2.08	0.80
5:B:324:TYR:HD2	5:B:348:ILE:HG22	1.48	0.79
8:P:380:THR:HG22	8:P:446:ALA:HA	1.62	0.79
8:N:382:PHE:CE1	8:N:385:PHE:CE2	2.71	0.79
8:N:382:PHE:CE1	8:N:385:PHE:HE2	2.01	0.79
7:O:979:LYS:NZ	7:O:1040:THR:HG23	1.78	0.78
7:O:1027:GLN:OE1	7:O:1039:ALA:O	2.00	0.78
8:P:34:ALA:HB1	8:P:44:LEU:CD1	2.13	0.78
1:Y:1224:ASN:O	1:Y:1225:PHE:CD1	2.37	0.78
5:E:321:ALA:C	5:E:323:LEU:H	1.90	0.78
2:1:745:ILE:HG21	2:1:815:PHE:HZ	1.41	0.77
1:Y:832:VAL:HG11	1:Y:914:TYR:CZ	2.18	0.77
1:Y:1257:GLN:HA	1:Y:1261:ARG:CZ	2.14	0.77
8:P:73:SER:CB	8:P:83:VAL:O	2.31	0.77
5:B:325:THR:CA	5:B:335:TRP:CZ2	2.68	0.76
2:Z:1254:GLY:CA	2:Z:1300:SER:HB2	2.16	0.76
2:Z:1254:GLY:N	2:Z:1300:SER:HB2	1.99	0.76
2:Z:1254:GLY:HA2	2:Z:1300:SER:HB2	1.66	0.76
8:P:380:THR:HG21	8:P:446:ALA:HA	1.68	0.76
2:1:745:ILE:HG13	2:1:823:LYS:NZ	2.01	0.76
8:P:42:GLN:HA	8:P:45:LYS:CD	2.10	0.75
7:O:1027:GLN:CD	7:O:1039:ALA:CB	2.53	0.75
5:K:320:GLU:CB	5:K:323:LEU:CD2	2.65	0.75
8:N:1277:ILE:HG13	8:N:1277:ILE:O	1.85	0.75
8:P:381:VAL:O	8:P:384:GLU:HG2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:320:GLU:HB3	5:K:323:LEU:CD1	2.17	0.74
8:N:380:THR:HG21	8:N:414:ASN:ND2	1.97	0.74
5:K:320:GLU:HB3	5:K:323:LEU:HD21	1.69	0.74
8:P:379:ILE:HG21	8:P:400:PHE:HE1	1.53	0.73
8:P:1058:GLU:OE1	8:P:1064:GLU:OE1	2.08	0.72
2:1:1109:LEU:HD13	2:1:1156:LEU:HD23	1.72	0.72
5:B:324:TYR:CD2	5:B:348:ILE:HG22	2.25	0.71
2:1:730:VAL:CG1	2:1:744:GLY:HA3	2.18	0.71
2:1:960:GLN:CG	2:1:1039:LEU:HD21	2.19	0.71
8:N:1096:ILE:HG22	8:N:1097:LEU:HD22	1.72	0.71
1:Y:1224:ASN:O	1:Y:1225:PHE:HD1	1.74	0.70
8:P:379:ILE:HG21	8:P:403:ILE:CG2	2.20	0.70
8:N:275:LEU:HD22	8:N:382:PHE:CD1	2.27	0.70
8:P:75:ILE:HD11	8:P:82:ASN:O	1.90	0.70
8:P:1292:GLU:OE2	8:P:1304:LYS:CB	2.26	0.70
2:1:1155:GLN:OE1	2:1:1155:GLN:HA	1.90	0.70
7:M:1036:PRO:O	7:M:1041:PHE:CD1	2.45	0.70
8:P:1050:SER:HA	8:P:1054:PHE:CG	2.18	0.70
5:B:326:LYS:N	5:B:327:PRO:CD	2.55	0.69
8:N:1304:LYS:HE3	8:N:1304:LYS:HA	1.74	0.69
3:5:33:UNK:CB	7:O:1038:LEU:HD21	2.23	0.69
8:N:175:SER:O	8:N:179:LEU:HG	1.92	0.69
8:P:379:ILE:HG21	8:P:403:ILE:HG22	1.75	0.69
7:M:1041:PHE:CZ	7:M:1042:ILE:HG12	2.25	0.69
8:N:1277:ILE:CD1	8:N:1280:LEU:CD1	2.71	0.69
7:O:1043:SER:HB3	7:O:1047:SER:CA	2.22	0.69
1:Y:832:VAL:HG11	1:Y:914:TYR:CD2	2.28	0.68
4:J:670:VAL:HG12	5:K:315:LYS:CG	2.24	0.68
7:M:1036:PRO:C	7:M:1041:PHE:CD1	2.72	0.68
8:N:52:ILE:O	8:N:131:ASP:OD2	2.12	0.68
5:E:318:GLU:HG3	5:E:346:GLN:CA	2.23	0.68
2:1:745:ILE:HG22	2:1:815:PHE:HE2	1.46	0.67
5:H:317:ASN:ND2	5:H:346:GLN:HB3	2.05	0.67
2:Z:1257:GLY:O	2:Z:1299:LYS:CD	2.42	0.67
8:P:1088:ASN:CB	8:P:1093:ASN:HB3	2.20	0.67
4:J:670:VAL:CG1	5:K:315:LYS:CB	2.70	0.67
9:T:208:LEU:O	9:T:211:LYS:CG	2.43	0.67
2:1:89:GLU:HG2	2:1:92:GLN:HB2	1.75	0.66
3:5:32:UNK:O	7:O:1038:LEU:HD12	1.87	0.66
8:N:380:THR:OG1	8:N:414:ASN:ND2	2.28	0.66
8:N:381:VAL:C	8:N:384:GLU:OE1	2.38	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:320:GLU:O	5:K:323:LEU:N	2.28	0.66
7:O:1224:GLU:HB3	7:O:1237:TYR:HA	1.76	0.66
7:M:1041:PHE:CE2	7:M:1042:ILE:HG13	2.29	0.66
8:P:42:GLN:H	8:P:45:LYS:HB3	1.60	0.66
8:N:1277:ILE:CG1	8:N:1280:LEU:CD1	2.73	0.66
1:Y:1258:LEU:O	1:Y:1262:ILE:HG13	1.95	0.65
2:1:745:ILE:HG22	2:1:815:PHE:CZ	1.76	0.65
8:P:1058:GLU:CD	8:P:1064:GLU:OE1	2.40	0.65
2:1:960:GLN:HG3	2:1:1039:LEU:CD2	2.24	0.64
8:N:174:VAL:HG12	8:N:178:GLN:OE1	1.96	0.64
8:P:42:GLN:C	8:P:45:LYS:HZ2	2.05	0.64
1:Y:832:VAL:CB	1:Y:914:TYR:CE1	2.80	0.64
2:1:745:ILE:CG2	2:1:815:PHE:CE1	2.52	0.63
5:K:320:GLU:C	5:K:322:ILE:N	2.48	0.63
8:P:75:ILE:O	8:P:83:VAL:HG12	1.98	0.63
8:N:1292:GLU:OE2	8:N:1303:LEU:N	2.31	0.63
8:P:1060:LEU:O	8:P:1060:LEU:HG	1.99	0.63
8:P:376:THR:HG22	8:P:379:ILE:HG13	1.80	0.63
1:Y:832:VAL:CG1	1:Y:914:TYR:CG	2.61	0.62
8:N:1303:LEU:HG	8:N:1350:LEU:HD22	1.80	0.62
5:E:318:GLU:HG3	5:E:346:GLN:H	1.64	0.62
9:S:691:ARG:NH2	10:W:322:LEU:HD12	2.14	0.62
9:T:208:LEU:HA	9:T:211:LYS:HE2	1.79	0.62
5:B:323:LEU:H	5:B:323:LEU:HD23	1.65	0.62
8:P:1057:LYS:HE3	8:P:1057:LYS:HA	1.81	0.62
2:Z:922:LYS:H	2:Z:925:ARG:HG2	1.64	0.62
2:Z:1253:VAL:HG13	2:Z:1300:SER:H	1.65	0.62
8:P:133:ASP:O	8:P:137:VAL:HG13	1.99	0.62
5:E:318:GLU:HG3	5:E:346:GLN:N	2.15	0.62
7:M:1041:PHE:CZ	7:M:1042:ILE:CG1	2.82	0.61
1:Y:832:VAL:O	1:Y:832:VAL:HG23	2.00	0.61
2:Z:1255:SER:HB2	2:Z:1301:SER:HB3	1.80	0.61
5:E:321:ALA:C	5:E:323:LEU:N	2.58	0.61
8:N:379:ILE:HG22	8:N:383:LEU:HD11	1.81	0.61
8:P:275:LEU:HD22	8:P:382:PHE:HD1	1.65	0.61
2:Z:1253:VAL:HG13	2:Z:1300:SER:N	2.14	0.61
8:N:1096:ILE:O	8:N:1096:ILE:HG23	2.01	0.61
8:N:33:ASP:HB3	8:N:1012:VAL:HG11	1.82	0.61
7:M:1035:GLY:O	7:M:1041:PHE:HE1	1.83	0.61
8:N:358:VAL:HG12	8:N:358:VAL:O	2.00	0.61
1:Y:1257:GLN:HA	1:Y:1261:ARG:NH2	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:1057:LYS:HA	8:P:1057:LYS:CE	2.30	0.60
1:Y:1257:GLN:HA	1:Y:1261:ARG:HH12	1.65	0.60
8:N:380:THR:HG23	8:N:380:THR:O	2.01	0.60
8:N:382:PHE:C	8:N:384:GLU:H	2.09	0.60
8:P:1055:GLN:OE1	8:P:1055:GLN:HA	2.00	0.60
5:K:320:GLU:O	5:K:322:ILE:N	2.35	0.60
5:K:320:GLU:O	5:K:323:LEU:HG	2.02	0.60
7:O:1026:PHE:CZ	7:O:1043:SER:O	2.55	0.60
8:P:134:ARG:HB3	8:P:198:MET:HE3	1.83	0.60
8:P:1060:LEU:CA	8:P:1065:THR:CG2	2.79	0.60
8:P:379:ILE:CG2	8:P:403:ILE:HG21	2.32	0.59
8:P:379:ILE:HD12	8:P:403:ILE:HG21	1.84	0.59
8:P:1095:GLU:OE1	8:P:1095:GLU:HA	2.02	0.59
8:P:1278:ILE:CG1	8:P:1321:LEU:HD23	2.31	0.59
1:Y:1257:GLN:CA	1:Y:1261:ARG:NH1	2.65	0.59
10:W:305:TYR:H	10:W:306:PRO:HD3	1.67	0.59
8:N:353:ALA:O	8:N:357:ASP:OD2	2.20	0.59
5:B:325:THR:C	5:B:335:TRP:CZ2	2.81	0.59
8:N:33:ASP:CB	8:N:1012:VAL:HG11	2.32	0.59
7:M:1041:PHE:CZ	7:M:1042:ILE:HD11	2.38	0.59
8:P:1088:ASN:ND2	8:P:1093:ASN:ND2	2.48	0.59
7:M:1485:LEU:HD13	7:M:1541:ASN:HD21	1.67	0.59
5:B:326:LYS:H	5:B:327:PRO:HD3	1.66	0.58
8:N:72:ARG:NH1	8:N:84:ASP:CG	2.60	0.58
5:B:319:THR:HG23	5:B:320:GLU:HG3	1.84	0.58
5:E:318:GLU:CG	5:E:346:GLN:HA	2.30	0.58
4:J:670:VAL:HG12	5:K:315:LYS:HG3	1.85	0.58
8:P:1060:LEU:HA	8:P:1065:THR:CG2	2.33	0.58
5:K:319:THR:C	5:K:321:ALA:H	2.11	0.58
7:O:1042:ILE:HG22	7:O:1042:ILE:O	2.04	0.58
7:M:1026:PHE:CZ	7:M:1043:SER:O	2.57	0.58
6:C:371:LYS:H	6:C:371:LYS:HD2	1.68	0.57
8:N:52:ILE:O	8:N:131:ASP:CG	2.48	0.57
8:P:1292:GLU:CB	8:P:1304:LYS:HG2	2.24	0.57
1:Y:1257:GLN:N	1:Y:1260:SER:HG	2.03	0.57
8:N:1095:GLU:OE2	8:N:1095:GLU:HA	2.05	0.57
5:K:315:LYS:O	5:K:315:LYS:HG2	2.04	0.57
8:P:379:ILE:CG2	8:P:403:ILE:CG2	2.82	0.56
8:P:1060:LEU:HA	8:P:1065:THR:CB	2.35	0.56
8:P:1277:ILE:CD1	8:P:1280:LEU:CG	2.66	0.56
1:O:831:LYS:HG2	1:O:923:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:1060:LEU:HD12	8:P:1192:LEU:HD23	1.85	0.56
6:C:369:LEU:HD12	6:C:370:ASP:H	1.71	0.55
2:Z:1257:GLY:O	2:Z:1299:LYS:HD2	2.05	0.55
2:1:745:ILE:HG13	2:1:823:LYS:HZ2	1.70	0.55
1:Y:717:TYR:HB2	1:Y:885:ALA:CB	2.35	0.55
5:H:309:ARG:HA	5:H:309:ARG:HH11	1.70	0.55
2:Z:1257:GLY:C	2:Z:1299:LYS:CD	2.80	0.55
2:Z:264:ILE:HG21	2:Z:347:VAL:H	1.72	0.55
2:1:89:GLU:HG2	2:1:92:GLN:CG	2.38	0.54
2:Z:1261:PHE:HB3	2:Z:1299:LYS:HE2	1.89	0.54
1:O:834:ILE:O	1:O:914:TYR:OH	2.26	0.54
8:N:1303:LEU:HD21	8:N:1385:LEU:HD11	1.89	0.54
8:N:376:THR:O	8:N:379:ILE:CD1	2.47	0.54
2:Z:1261:PHE:CB	2:Z:1299:LYS:HE2	2.37	0.54
9:S:691:ARG:NH2	10:W:322:LEU:HD11	2.13	0.54
8:P:1050:SER:HB2	8:P:1054:PHE:CE2	2.43	0.53
8:P:1088:ASN:HD22	8:P:1093:ASN:HD22	1.53	0.53
8:N:52:ILE:O	8:N:131:ASP:OD1	2.27	0.53
8:P:31:ALA:HB2	8:P:40:ILE:HG12	1.88	0.53
8:P:380:THR:HG22	8:P:446:ALA:CA	2.37	0.53
7:M:736:PHE:H	7:M:737:PRO:HD2	1.74	0.53
5:E:318:GLU:CG	5:E:346:GLN:H	2.21	0.53
8:N:1303:LEU:CG	8:N:1350:LEU:HB3	2.37	0.53
7:O:736:PHE:H	7:O:737:PRO:HD2	1.74	0.53
8:P:34:ALA:CB	8:P:44:LEU:HD11	2.25	0.53
9:S:691:ARG:NH2	10:W:322:LEU:CD1	2.54	0.52
2:1:1112:ALA:HB1	2:1:1156:LEU:HG	1.92	0.52
8:N:380:THR:OG1	8:N:415:PHE:CZ	2.60	0.52
8:N:1095:GLU:HB3	8:N:1119:ASN:OD1	2.08	0.52
8:P:1276:LYS:N	8:P:1321:LEU:HB2	2.24	0.52
4:J:670:VAL:CG1	5:K:315:LYS:HG3	2.39	0.52
8:N:378:VAL:O	8:N:378:VAL:HG22	2.09	0.52
7:O:1027:GLN:CD	7:O:1039:ALA:C	2.74	0.52
7:O:1485:LEU:HD13	7:O:1541:ASN:HD21	1.73	0.52
1:Y:832:VAL:HG11	1:Y:914:TYR:CE2	2.45	0.52
8:P:69:ASN:HA	8:P:72:ARG:HD2	1.90	0.52
8:N:69:ASN:HA	8:N:72:ARG:NH2	2.25	0.52
8:N:1303:LEU:HG	8:N:1350:LEU:CB	2.35	0.52
5:B:324:TYR:HB2	5:B:349:PRO:HD2	1.87	0.52
5:B:331:LEU:H	5:B:331:LEU:HD23	1.75	0.51
8:P:134:ARG:O	8:P:198:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:1303:LEU:O	8:P:1350:LEU:HD13	2.09	0.51
8:N:382:PHE:HA	8:N:384:GLU:OE1	2.10	0.51
9:Q:595:ARG:CD	10:U:322:LEU:CD2	2.78	0.51
6:I:369:LEU:HD12	6:I:370:ASP:H	1.76	0.51
8:N:794:ILE:HD13	8:N:794:ILE:H	1.75	0.51
2:1:730:VAL:HG13	2:1:744:GLY:CA	2.23	0.51
2:Z:1257:GLY:C	2:Z:1299:LYS:HD2	2.34	0.51
7:M:1036:PRO:C	7:M:1041:PHE:HD1	2.17	0.51
7:O:1037:ASN:O	7:O:1041:PHE:CD2	2.64	0.51
9:S:595:ARG:H	10:W:322:LEU:HD13	1.74	0.51
1:Y:831:LYS:HE2	1:Y:922:PHE:CD2	2.46	0.51
8:P:41:ARG:C	8:P:43:PHE:H	2.18	0.51
2:1:960:GLN:H	2:1:961:PRO:HD2	1.75	0.51
3:5:33:UNK:CB	7:O:1038:LEU:CD2	2.80	0.51
5:H:420:ALA:HB1	6:I:369:LEU:HD13	1.93	0.51
5:B:324:TYR:CE2	5:B:350:ILE:HA	2.46	0.51
8:N:1055:GLN:CD	8:N:1055:GLN:H	2.19	0.51
2:Z:1254:GLY:O	2:Z:1300:SER:O	2.27	0.51
2:1:89:GLU:HG2	2:1:92:GLN:CB	2.40	0.50
7:O:1043:SER:HB3	7:O:1047:SER:HA	1.92	0.50
2:Z:960:GLN:H	2:Z:961:PRO:HD2	1.75	0.50
8:N:357:ASP:N	8:N:357:ASP:OD1	2.42	0.50
8:P:52:ILE:N	8:P:133:ASP:OD2	2.44	0.50
8:P:379:ILE:HG23	8:P:403:ILE:HG21	1.93	0.50
8:P:1060:LEU:HA	8:P:1065:THR:HG1	1.74	0.50
6:C:353:LEU:CD1	6:C:369:LEU:HD23	2.38	0.50
10:U:313:TRP:HE1	10:U:358:LYS:H	1.59	0.50
7:O:1499:LEU:HD23	7:O:1499:LEU:H	1.76	0.50
2:Z:1255:SER:HB2	2:Z:1301:SER:CB	2.40	0.50
7:M:518:ASN:HA	7:M:523:ARG:HE	1.75	0.50
5:K:320:GLU:CB	5:K:323:LEU:HD11	2.41	0.50
8:N:380:THR:CB	8:N:414:ASN:HD22	2.24	0.50
8:P:379:ILE:HG13	8:P:403:ILE:HG22	1.94	0.50
8:N:382:PHE:CA	8:N:384:GLU:OE1	2.60	0.49
8:P:380:THR:HB	8:P:415:PHE:CZ	2.47	0.49
7:O:1025:GLY:HA2	7:O:1040:THR:OG1	2.12	0.49
8:P:1278:ILE:HG12	8:P:1321:LEU:HD23	1.94	0.49
9:Q:723:ILE:HG21	9:Q:739:MET:HE3	1.95	0.49
7:O:518:ASN:HA	7:O:523:ARG:HE	1.76	0.49
7:O:979:LYS:CE	7:O:1040:THR:CG2	2.88	0.49
2:1:1109:LEU:CD1	2:1:1156:LEU:HD23	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:1277:ILE:HG13	8:N:1280:LEU:H	1.78	0.49
2:1:89:GLU:CG	2:1:92:GLN:HB2	2.42	0.49
5:H:320:GLU:HG2	5:H:348:ILE:HD11	1.94	0.49
5:K:320:GLU:CB	5:K:323:LEU:CD1	2.91	0.49
7:M:1035:GLY:O	7:M:1041:PHE:CE1	2.66	0.49
7:M:1043:SER:HB3	7:M:1047:SER:N	2.28	0.49
7:M:1499:LEU:HD23	7:M:1499:LEU:H	1.77	0.49
2:Z:1253:VAL:CG1	2:Z:1300:SER:H	2.25	0.49
8:P:34:ALA:CB	8:P:44:LEU:HD12	2.20	0.48
2:Z:1257:GLY:O	2:Z:1299:LYS:HD3	2.12	0.48
2:Z:1257:GLY:C	2:Z:1299:LYS:HD3	2.37	0.48
8:N:382:PHE:CD1	8:N:385:PHE:CE2	3.02	0.48
8:N:1303:LEU:HD12	8:N:1353:SER:HB2	1.95	0.48
7:O:1037:ASN:O	7:O:1041:PHE:HD2	1.97	0.48
8:P:42:GLN:C	8:P:45:LYS:NZ	2.67	0.48
7:M:1041:PHE:CZ	7:M:1042:ILE:CD1	2.96	0.48
8:N:1304:LYS:HA	8:N:1304:LYS:CE	2.42	0.48
8:N:1344:PHE:H	8:N:1347:GLY:H	1.62	0.48
8:N:1292:GLU:CD	8:N:1303:LEU:N	2.72	0.48
1:Y:717:TYR:CB	1:Y:885:ALA:CB	2.91	0.48
1:Y:717:TYR:HB2	1:Y:885:ALA:HB2	1.95	0.48
8:N:40:ILE:HB	8:N:41:ARG:HG2	1.96	0.48
7:O:979:LYS:CE	7:O:1040:THR:HG23	2.42	0.48
1:Y:101:LEU:H	1:Y:101:LEU:HD22	1.79	0.48
8:N:74:THR:O	8:N:74:THR:HG22	2.13	0.48
2:1:745:ILE:CG2	2:1:815:PHE:CD2	2.88	0.47
5:B:324:TYR:CD2	5:B:348:ILE:CG2	2.96	0.47
5:E:324:TYR:CD1	5:E:324:TYR:N	2.82	0.47
8:N:382:PHE:CD1	8:N:385:PHE:HE2	2.31	0.47
9:Q:436:LEU:HA	9:Q:439:HIS:CE1	2.49	0.47
8:N:382:PHE:N	8:N:384:GLU:OE1	2.47	0.47
9:T:211:LYS:HE3	9:T:212:PHE:CE1	2.50	0.47
8:P:835:LEU:HD23	8:P:835:LEU:H	1.79	0.47
2:1:201:ILE:HD12	2:1:201:ILE:H	1.78	0.47
8:P:1052:LYS:HD2	8:P:1056:LYS:HA	1.97	0.47
1:O:1142:ARG:H	1:O:1142:ARG:HD3	1.80	0.47
8:P:134:ARG:C	8:P:198:MET:HE2	2.31	0.47
2:Z:1254:GLY:H	2:Z:1300:SER:N	2.12	0.47
2:1:1155:GLN:HE22	2:1:1159:ASN:HB2	1.79	0.47
8:P:51:LEU:C	8:P:133:ASP:CB	2.88	0.47
9:T:211:LYS:NZ	9:T:501:MET:HE3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:1276:LYS:HB3	8:N:1277:ILE:H	1.43	0.47
7:M:1036:PRO:O	7:M:1041:PHE:CE1	2.68	0.47
8:P:1060:LEU:HD23	8:P:1060:LEU:H	1.80	0.46
6:I:371:LYS:H	6:I:371:LYS:HD2	1.79	0.46
5:E:320:GLU:C	5:E:322:ILE:H	2.24	0.46
5:E:331:LEU:HD23	5:E:331:LEU:H	1.80	0.46
7:M:1042:ILE:HG22	7:M:1042:ILE:O	2.16	0.46
8:N:986:SER:H	8:N:991:LYS:HA	1.81	0.46
8:P:499:LEU:H	8:P:523:SER:HA	1.80	0.46
2:Z:646:TYR:CD1	2:Z:715:LEU:HD21	2.51	0.46
8:N:379:ILE:CD1	8:N:403:ILE:HG21	2.45	0.46
5:E:406:VAL:CG2	7:M:910:ARG:HH12	2.29	0.45
8:P:1303:LEU:HB3	8:P:1304:LYS:H	1.52	0.45
9:Q:681:SER:OG	10:U:322:LEU:HD12	2.10	0.45
8:P:379:ILE:HG13	8:P:403:ILE:CG2	2.47	0.45
8:N:40:ILE:C	8:N:41:ARG:HG2	2.42	0.45
1:Y:1318:HIS:CE1	1:Y:1343:LEU:HA	2.52	0.45
5:B:325:THR:O	5:B:335:TRP:CZ2	2.70	0.45
6:F:352:VAL:HG23	6:F:353:LEU:H	1.81	0.45
7:O:1437:LEU:HD23	7:O:1437:LEU:H	1.82	0.45
1:Y:832:VAL:HG22	1:Y:914:TYR:CE1	2.47	0.45
7:M:1026:PHE:HZ	7:M:1043:SER:O	1.99	0.45
8:P:1088:ASN:CB	8:P:1093:ASN:CB	2.87	0.45
8:N:72:ARG:HH12	8:N:84:ASP:CG	2.25	0.45
8:N:1593:HIS:CG	8:N:1594:ASP:H	2.34	0.45
7:O:1027:GLN:NE2	7:O:1039:ALA:HB1	2.32	0.45
9:S:595:ARG:H	10:W:322:LEU:CD1	2.28	0.45
8:N:33:ASP:HA	8:N:42:GLN:NE2	2.32	0.45
8:N:440:ILE:H	8:N:441:PRO:CD	2.29	0.45
5:B:324:TYR:HB2	5:B:348:ILE:HG23	1.99	0.45
2:1:1112:ALA:CB	2:1:1156:LEU:HG	2.47	0.44
5:E:321:ALA:O	5:E:323:LEU:N	2.50	0.44
8:N:1303:LEU:HD23	8:N:1350:LEU:HD13	1.99	0.44
8:P:1049:ASP:C	8:P:1054:PHE:CE2	2.95	0.44
8:P:1278:ILE:HG21	8:P:1333:SER:OG	2.17	0.44
8:N:794:ILE:HD13	8:N:794:ILE:N	2.31	0.44
2:1:90:PRO:O	2:1:797:ALA:HB1	2.17	0.44
8:N:382:PHE:C	8:N:384:GLU:N	2.75	0.44
1:O:1318:HIS:CE1	1:O:1343:LEU:HA	2.53	0.44
8:P:923:LEU:HD23	8:P:923:LEU:H	1.83	0.44
8:P:1277:ILE:CG1	8:P:1280:LEU:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1201:TRP:CD2	1:Y:1201:TRP:O	2.71	0.44
7:M:1515:LEU:HG	7:M:1516:THR:H	1.83	0.44
7:O:714:HIS:CE1	7:O:782:LYS:HB3	2.53	0.44
9:S:626:GLN:HA	9:S:629:ARG:HE	1.83	0.44
9:T:315:LYS:H	9:T:315:LYS:HD3	1.83	0.44
5:B:326:LYS:HD3	5:B:326:LYS:HA	1.61	0.44
8:N:43:PHE:CZ	8:N:944:GLN:HB2	2.53	0.44
8:N:1051:LYS:HB2	8:N:1053:LEU:H	1.83	0.44
8:P:41:ARG:C	8:P:43:PHE:N	2.76	0.44
2:1:960:GLN:H	2:1:961:PRO:CD	2.31	0.43
7:M:714:HIS:CE1	7:M:782:LYS:HB3	2.53	0.43
6:C:371:LYS:HA	6:C:374:GLN:HE21	1.83	0.43
7:O:1027:GLN:OE1	7:O:1038:LEU:O	2.35	0.43
7:O:1319:LEU:HD22	7:O:1319:LEU:HA	1.85	0.43
2:1:167:LEU:H	2:1:167:LEU:HD22	1.83	0.43
8:N:381:VAL:O	8:N:384:GLU:OE1	2.35	0.43
8:N:1303:LEU:CB	8:N:1350:LEU:HD22	2.48	0.43
7:O:1043:SER:O	7:O:1047:SER:OG	2.37	0.43
1:Y:832:VAL:HG13	1:Y:914:TYR:CE1	2.34	0.43
7:O:1515:LEU:HG	7:O:1516:THR:H	1.84	0.43
2:1:1155:GLN:NE2	2:1:1159:ASN:HB2	2.34	0.43
5:K:314:ASN:O	5:K:347:THR:OG1	2.31	0.43
8:N:380:THR:HG23	8:N:414:ASN:HB2	2.01	0.43
7:O:1026:PHE:HZ	7:O:1043:SER:O	1.99	0.43
1:O:1083:TYR:HB2	1:O:1092:ASP:H	1.84	0.43
2:1:745:ILE:HG13	2:1:823:LYS:CE	2.49	0.43
7:M:1408:LEU:HD12	7:M:1409:ALA:H	1.82	0.43
7:M:1437:LEU:H	7:M:1437:LEU:HD23	1.84	0.43
7:O:1408:LEU:HD12	7:O:1409:ALA:H	1.82	0.43
6:I:369:LEU:HA	6:I:373:PHE:CE2	2.53	0.43
4:J:670:VAL:CG1	5:K:315:LYS:CG	2.96	0.43
8:N:30:SER:O	8:N:32:VAL:HG12	2.19	0.43
8:P:1056:LYS:H	8:P:1056:LYS:HG3	1.54	0.43
6:C:349:THR:HB	6:C:369:LEU:N	2.34	0.42
1:Y:1257:GLN:N	1:Y:1261:ARG:NH1	2.67	0.42
2:1:89:GLU:CG	2:1:92:GLN:HG2	2.49	0.42
8:N:1303:LEU:HA	8:N:1350:LEU:HD13	2.01	0.42
8:P:1277:ILE:HD12	8:P:1277:ILE:O	2.19	0.42
1:Y:832:VAL:CB	1:Y:914:TYR:CZ	3.01	0.42
1:Y:1224:ASN:C	1:Y:1225:PHE:CD1	2.96	0.42
5:B:324:TYR:HD1	5:B:324:TYR:HA	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:380:THR:CG2	8:N:414:ASN:ND2	2.62	0.42
8:P:135:PHE:C	8:P:137:VAL:H	2.27	0.42
6:C:371:LYS:HD2	6:C:371:LYS:N	2.34	0.42
7:M:1318:LYS:H	7:M:1318:LYS:HG3	1.48	0.42
9:T:208:LEU:HD12	9:T:211:LYS:NZ	2.33	0.42
5:E:320:GLU:C	5:E:322:ILE:N	2.75	0.42
9:T:211:LYS:HE3	9:T:212:PHE:HE1	1.84	0.42
1:Y:1201:TRP:O	1:Y:1201:TRP:CE3	2.72	0.42
1:Y:1243:CYS:HA	1:Y:1259:ALA:HB2	2.01	0.42
4:G:797:LEU:HD23	9:S:46:ILE:HA	2.02	0.42
8:P:884:LEU:HD23	8:P:884:LEU:H	1.85	0.42
7:O:1027:GLN:NE2	7:O:1039:ALA:CB	2.82	0.42
5:K:318:GLU:H	5:K:346:GLN:HA	1.85	0.42
7:O:1025:GLY:HA3	7:O:1043:SER:CB	2.50	0.42
8:P:42:GLN:N	8:P:45:LYS:HB3	2.31	0.42
9:S:372:LYS:H	9:S:372:LYS:HD2	1.85	0.42
8:N:564:LEU:H	8:N:564:LEU:HD22	1.84	0.41
8:P:42:GLN:HE21	8:P:42:GLN:HB2	1.59	0.41
8:P:1418:LEU:H	8:P:1421:ILE:HG22	1.85	0.41
11:X:399:LYS:H	11:X:399:LYS:HD3	1.85	0.41
2:1:906:ALA:HB2	2:1:930:THR:HG21	2.02	0.41
8:P:377:THR:C	8:P:379:ILE:N	2.78	0.41
9:T:298:LEU:HD23	9:T:298:LEU:H	1.85	0.41
2:1:443:ILE:HD13	2:1:443:ILE:H	1.85	0.41
1:0:862:GLN:CD	1:0:862:GLN:H	2.27	0.41
7:M:736:PHE:H	7:M:737:PRO:CD	2.33	0.41
7:O:736:PHE:H	7:O:737:PRO:CD	2.33	0.41
8:N:1173:TRP:CG	8:N:1174:ASN:H	2.38	0.41
2:Z:1253:VAL:CG1	2:Z:1300:SER:HG	2.04	0.41
5:B:324:TYR:CG	5:B:349:PRO:O	2.72	0.41
2:Z:387:GLY:HA3	2:Z:448:LEU:HD23	2.03	0.41
8:N:733:ARG:HH22	8:N:795:ILE:HA	1.85	0.41
8:N:1055:GLN:CD	8:N:1055:GLN:N	2.77	0.41
1:0:654:THR:HG23	1:0:656:ASP:H	1.86	0.41
8:P:50:ASN:HD22	8:P:117:LEU:HD23	1.86	0.41
10:W:305:TYR:N	10:W:306:PRO:HD3	2.34	0.41
2:Z:238:ASN:HB2	2:Z:240:ARG:HH11	1.86	0.41
1:0:831:LYS:HD2	1:0:831:LYS:HA	1.60	0.41
5:E:321:ALA:O	5:E:324:TYR:C	2.64	0.41
8:N:1303:LEU:HD12	8:N:1353:SER:CB	2.51	0.41
1:Y:1027:HIS:CG	1:Y:1057:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:919:ASN:CG	7:O:920:ILE:H	2.29	0.40
8:P:51:LEU:CA	8:P:133:ASP:HB3	2.50	0.40
8:P:702:THR:H	8:P:705:TYR:HB3	1.86	0.40
5:K:319:THR:C	5:K:321:ALA:N	2.77	0.40
5:K:318:GLU:HG2	5:K:346:GLN:OE1	2.21	0.40
8:P:75:ILE:O	8:P:75:ILE:HG13	2.22	0.40
1:O:789:VAL:HG23	1:O:790:PHE:H	1.87	0.40
8:N:380:THR:CB	8:N:414:ASN:ND2	2.85	0.40
9:Q:322:ILE:HD12	9:Q:325:LEU:HD13	2.04	0.40
8:N:12:GLN:NE2	8:N:73:SER:HG	2.06	0.40
2:Z:121:LEU:HD12	2:Z:121:LEU:H	1.85	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	0	1072/1502 (71%)	870 (81%)	139 (13%)	63 (6%)	1	13
1	Y	1052/1502 (70%)	876 (83%)	110 (10%)	66 (6%)	1	13
2	1	1085/1391 (78%)	934 (86%)	98 (9%)	53 (5%)	1	16
2	Z	1082/1391 (78%)	934 (86%)	94 (9%)	54 (5%)	1	16
4	A	156/823 (19%)	152 (97%)	2 (1%)	2 (1%)	9	42
4	D	157/823 (19%)	152 (97%)	2 (1%)	3 (2%)	6	32
4	G	158/823 (19%)	153 (97%)	2 (1%)	3 (2%)	6	32
4	J	157/823 (19%)	149 (95%)	4 (2%)	4 (2%)	4	26
5	B	211/541 (39%)	188 (89%)	16 (8%)	7 (3%)	3	21
5	E	211/541 (39%)	188 (89%)	13 (6%)	10 (5%)	2	16
5	H	211/541 (39%)	177 (84%)	20 (10%)	14 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	211/541 (39%)	196 (93%)	10 (5%)	5 (2%)	4	27
6	C	160/472 (34%)	150 (94%)	5 (3%)	5 (3%)	3	22
6	F	161/472 (34%)	155 (96%)	3 (2%)	3 (2%)	6	32
6	I	160/472 (34%)	151 (94%)	7 (4%)	2 (1%)	9	42
6	L	161/472 (34%)	156 (97%)	4 (2%)	1 (1%)	21	59
7	M	1496/1683 (89%)	1266 (85%)	162 (11%)	68 (4%)	2	17
7	O	1497/1683 (89%)	1265 (84%)	164 (11%)	68 (4%)	2	17
8	N	1308/1655 (79%)	1018 (78%)	188 (14%)	102 (8%)	1	10
8	P	1308/1655 (79%)	1020 (78%)	186 (14%)	102 (8%)	1	10
9	Q	671/839 (80%)	593 (88%)	53 (8%)	25 (4%)	2	20
9	R	691/839 (82%)	595 (86%)	76 (11%)	20 (3%)	3	23
9	S	671/839 (80%)	589 (88%)	62 (9%)	20 (3%)	3	22
9	T	691/839 (82%)	595 (86%)	66 (10%)	30 (4%)	2	17
10	U	89/475 (19%)	77 (86%)	6 (7%)	6 (7%)	1	12
10	W	89/475 (19%)	77 (86%)	9 (10%)	3 (3%)	3	21
11	V	88/528 (17%)	71 (81%)	10 (11%)	7 (8%)	1	9
11	X	89/528 (17%)	72 (81%)	11 (12%)	6 (7%)	1	12
All	All	15093/25168 (60%)	12819 (85%)	1522 (10%)	752 (5%)	3	16

All (752) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	178	GLU
1	0	419	LYS
1	0	533	SER
1	0	693	GLU
1	0	694	LYS
1	0	710	VAL
1	0	784	ILE
1	0	885	ALA
1	0	991	ARG
1	0	1023	SER
1	0	1025	ASN
1	0	1090	GLU
1	0	1154	ASP
1	0	1198	ASN

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Mol	Chain	Res	Type
1	0	1209	LYS
1	0	1222	THR
1	0	1258	LEU
1	0	1305	SER
1	0	1312	ALA
1	0	1349	MET
1	0	1380	ASP
1	0	1381	SER
2	1	217	SER
2	1	498	ALA
2	1	679	SER
2	1	922	LYS
2	1	927	HIS
2	1	1092	LEU
2	1	1179	ASN
2	1	1210	ALA
2	1	1300	SER
2	1	1356	ASP
4	A	752	ASP
5	B	295	CYS
5	B	297	GLU
4	D	754	ASN
5	E	298	SER
5	E	299	TRP
6	F	370	ASP
4	G	726	VAL
4	G	752	ASP
5	H	299	TRP
5	H	346	GLN
4	J	639	ASP
4	J	754	ASN
7	M	36	ASN
7	M	342	TYR
7	M	620	THR
7	M	667	SER
7	M	705	ASP
7	M	736	PHE
7	M	749	ILE
7	M	794	SER
7	M	835	LYS
7	M	886	LEU
7	M	887	PHE

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Mol	Chain	Res	Type
7	M	1036	PRO
7	M	1141	SER
7	M	1143	SER
7	M	1238	ASP
7	M	1320	GLU
7	M	1516	THR
7	M	1595	VAL
7	M	1609	SER
7	M	1610	ALA
7	M	1667	VAL
8	N	23	ASN
8	N	47	ASN
8	N	54	SER
8	N	56	ASN
8	N	59	ARG
8	N	217	GLN
8	N	221	VAL
8	N	405	SER
8	N	440	ILE
8	N	457	LEU
8	N	497	ILE
8	N	552	LEU
8	N	611	SER
8	N	765	PHE
8	N	783	PHE
8	N	813	ILE
8	N	824	LEU
8	N	826	SER
8	N	928	SER
8	N	930	ALA
8	N	1032	ILE
8	N	1050	SER
8	N	1058	GLU
8	N	1239	ASP
8	N	1240	PHE
8	N	1427	SER
8	N	1512	ILE
7	O	36	ASN
7	O	342	TYR
7	O	620	THR
7	O	667	SER
7	O	705	ASP

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Mol	Chain	Res	Type
7	O	736	PHE
7	O	749	ILE
7	O	794	SER
7	O	835	LYS
7	O	886	LEU
7	O	887	PHE
7	O	1036	PRO
7	O	1141	SER
7	O	1143	SER
7	O	1238	ASP
7	O	1320	GLU
7	O	1516	THR
7	O	1595	VAL
7	O	1609	SER
7	O	1610	ALA
7	O	1667	VAL
8	P	32	VAL
8	P	49	THR
8	P	69	ASN
8	P	257	LEU
8	P	278	SER
8	P	324	SER
8	P	340	SER
8	P	410	GLN
8	P	415	PHE
8	P	416	LEU
8	P	425	LEU
8	P	442	LEU
8	P	444	ASN
8	P	457	LEU
8	P	633	SER
8	P	668	TYR
8	P	728	ILE
8	P	778	VAL
8	P	794	ILE
8	P	871	SER
8	P	892	SER
8	P	928	SER
8	P	947	ASN
8	P	964	GLN
8	P	975	GLN
8	P	1010	GLU

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Mol	Chain	Res	Type
8	P	1050	SER
8	P	1060	LEU
8	P	1254	ARG
8	P	1320	GLU
8	P	1427	SER
9	Q	67	THR
9	Q	514	LYS
9	Q	615	ASP
9	Q	754	ARG
9	R	46	ILE
9	R	60	ASN
9	R	155	VAL
9	R	295	ASN
9	R	324	ASN
9	S	44	VAL
9	S	67	THR
9	S	328	ILE
9	S	754	ARG
9	T	81	GLU
9	T	103	ILE
9	T	104	ILE
9	T	269	ASN
9	T	417	ARG
9	T	499	SER
9	T	754	ARG
9	T	768	VAL
10	U	249	ASP
10	U	348	ALA
10	W	320	SER
11	X	269	SER
11	X	299	GLN
1	Y	250	ALA
1	Y	386	SER
1	Y	407	ALA
1	Y	514	SER
1	Y	523	SER
1	Y	711	VAL
1	Y	714	LYS
1	Y	784	ILE
1	Y	858	ASP
1	Y	979	ALA
1	Y	991	ARG

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Mol	Chain	Res	Type
1	Y	1059	TYR
1	Y	1061	PRO
1	Y	1083	TYR
1	Y	1154	ASP
1	Y	1209	LYS
1	Y	1292	GLU
2	Z	141	GLN
2	Z	553	LYS
2	Z	679	SER
2	Z	745	ILE
2	Z	767	ASN
2	Z	922	LYS
2	Z	927	HIS
2	Z	932	ILE
2	Z	960	GLN
2	Z	991	ALA
2	Z	1040	LYS
2	Z	1124	ASP
2	Z	1156	LEU
1	0	165	SER
1	0	170	LYS
1	0	188	ASN
1	0	208	LYS
1	0	224	PHE
1	0	230	HIS
1	0	406	THR
1	0	454	ARG
1	0	522	ALA
1	0	625	ALA
1	0	1014	LYS
1	0	1199	ILE
1	0	1263	GLN
1	0	1440	ASP
2	1	118	SER
2	1	125	PHE
2	1	149	GLU
2	1	287	GLN
2	1	405	LYS
2	1	493	ILE
2	1	607	ASN
2	1	767	ASN
2	1	913	ALA

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Mol	Chain	Res	Type
2	1	925	ARG
2	1	945	CYS
2	1	960	GLN
2	1	988	CYS
2	1	1354	ASP
4	A	744	ALA
5	B	309	ARG
6	C	370	ASP
4	D	776	PHE
5	E	309	ARG
5	E	318	GLU
5	E	324	TYR
4	G	744	ALA
5	H	309	ARG
5	H	324	TYR
6	I	370	ASP
4	J	776	PHE
5	K	321	ALA
7	M	307	ASP
7	M	518	ASN
7	M	761	LEU
7	M	907	HIS
7	M	990	ILE
7	M	995	VAL
7	M	1034	LEU
7	M	1037	ASN
7	M	1171	SER
7	M	1273	LYS
7	M	1482	THR
7	M	1535	ALA
7	M	1558	ASP
7	M	1570	VAL
7	M	1577	LYS
7	M	1678	GLY
8	N	32	VAL
8	N	41	ARG
8	N	52	ILE
8	N	152	TYR
8	N	257	LEU
8	N	370	SER
8	N	460	ILE
8	N	474	ASP

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Mol	Chain	Res	Type
8	N	495	ASP
8	N	633	SER
8	N	650	ASP
8	N	668	TYR
8	N	683	ASP
8	N	728	ILE
8	N	794	ILE
8	N	810	MET
8	N	862	ARG
8	N	871	SER
8	N	898	VAL
8	N	964	GLN
8	N	986	SER
8	N	1056	LYS
8	N	1060	LEU
8	N	1061	THR
8	N	1092	SER
8	N	1290	SER
8	N	1344	PHE
8	N	1429	HIS
7	O	307	ASP
7	O	518	ASN
7	O	761	LEU
7	O	907	HIS
7	O	990	ILE
7	O	995	VAL
7	O	1034	LEU
7	O	1037	ASN
7	O	1171	SER
7	O	1273	LYS
7	O	1482	THR
7	O	1535	ALA
7	O	1558	ASP
7	O	1569	TYR
7	O	1570	VAL
7	O	1577	LYS
7	O	1678	GLY
8	P	200	LEU
8	P	220	PHE
8	P	277	THR
8	P	338	SER
8	P	357	ASP

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Mol	Chain	Res	Type
8	P	359	LEU
8	P	552	LEU
8	P	587	GLN
8	P	603	ASP
8	P	692	ASN
8	P	827	PRO
8	P	897	LYS
8	P	942	PRO
8	P	991	LYS
8	P	1009	PRO
8	P	1032	ILE
8	P	1092	SER
8	P	1240	PHE
8	P	1512	ILE
9	Q	79	SER
9	Q	318	LYS
9	Q	421	SER
9	Q	442	LEU
9	Q	499	SER
9	Q	697	PHE
9	Q	758	GLN
9	Q	794	TYR
9	R	321	LYS
9	R	476	ASN
9	R	499	SER
9	R	596	ASP
9	R	754	ARG
9	S	79	SER
9	S	298	LEU
9	S	357	LYS
9	S	550	PRO
9	T	113	ILE
9	T	155	VAL
9	T	316	ALA
10	U	320	SER
11	V	281	SER
11	V	300	VAL
11	V	347	TYR
11	X	300	VAL
1	Y	147	PRO
1	Y	209	HIS
1	Y	230	HIS

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Mol	Chain	Res	Type
1	Y	251	THR
1	Y	266	GLN
1	Y	292	ASN
1	Y	293	ILE
1	Y	464	SER
1	Y	522	ALA
1	Y	710	VAL
1	Y	1108	VAL
1	Y	1175	LEU
1	Y	1284	ARG
1	Y	1301	ILE
2	Z	177	ASP
2	Z	403	ALA
2	Z	405	LYS
2	Z	489	SER
2	Z	548	LEU
2	Z	625	ILE
2	Z	705	LEU
2	Z	988	CYS
2	Z	1277	ARG
1	0	187	ASP
1	0	286	GLY
1	0	290	GLY
1	0	523	SER
1	0	692	SER
1	0	913	LEU
1	0	1062	LYS
1	0	1107	LEU
1	0	1356	LYS
2	1	178	ASN
2	1	308	ASN
2	1	350	SER
2	1	352	GLY
2	1	371	ASN
2	1	376	PRO
2	1	415	CYS
2	1	818	ASP
2	1	930	THR
2	1	1040	LYS
2	1	1156	LEU
2	1	1186	ASP
2	1	1277	ARG

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Mol	Chain	Res	Type
2	1	1357	LEU
2	1	1375	ASN
5	B	393	ASP
5	B	434	GLU
6	C	342	GLU
5	E	296	LYS
5	E	422	LEU
6	F	300	ASP
5	H	291	GLN
5	H	323	LEU
5	H	332	GLN
5	H	434	GLU
5	K	295	CYS
5	K	346	GLN
7	M	137	ASN
7	M	266	ASP
7	M	298	ASP
7	M	603	GLU
7	M	726	SER
7	M	727	GLU
7	M	739	ARG
7	M	847	GLY
7	M	903	ASN
7	M	1207	CYS
7	M	1447	TYR
7	M	1474	PHE
7	M	1599	GLU
8	N	43	PHE
8	N	67	ASP
8	N	70	LYS
8	N	280	ALA
8	N	359	LEU
8	N	360	GLN
8	N	381	VAL
8	N	461	CYS
8	N	604	PRO
8	N	670	HIS
8	N	692	ASN
8	N	805	LEU
8	N	887	VAL
8	N	921	SER
8	N	942	PRO

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Mol	Chain	Res	Type
8	N	993	SER
8	N	1172	SER
8	N	1254	ARG
8	N	1307	PHE
8	N	1399	ASN
7	O	137	ASN
7	O	266	ASP
7	O	298	ASP
7	O	603	GLU
7	O	726	SER
7	O	727	GLU
7	O	739	ARG
7	O	847	GLY
7	O	903	ASN
7	O	1138	PHE
7	O	1207	CYS
7	O	1447	TYR
7	O	1474	PHE
7	O	1599	GLU
8	P	23	ASN
8	P	27	ALA
8	P	42	GLN
8	P	54	SER
8	P	89	PHE
8	P	217	GLN
8	P	371	PHE
8	P	414	ASN
8	P	473	LEU
8	P	647	GLN
8	P	650	ASP
8	P	684	LYS
8	P	862	ARG
8	P	878	PHE
8	P	929	MET
8	P	938	ASP
8	P	949	LEU
8	P	1093	ASN
8	P	1172	SER
8	P	1540	LYS
9	Q	145	ASN
9	Q	317	ASP
9	Q	678	ASP

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Mol	Chain	Res	Type
9	Q	743	ASP
9	Q	764	ASP
9	Q	766	ASN
9	R	106	SER
9	R	265	SER
9	R	698	ASP
9	S	64	LYS
9	S	82	ASP
9	S	145	ASN
9	S	321	LYS
9	S	476	ASN
9	S	764	ASP
9	T	44	VAL
9	T	49	LEU
9	T	80	PHE
9	T	105	GLU
9	T	325	LEU
9	T	423	LYS
9	T	457	TYR
9	T	678	ASP
9	T	698	ASP
10	U	250	ASP
10	U	305	TYR
11	V	354	SER
11	V	400	ILE
1	Y	135	PHE
1	Y	213	LYS
1	Y	227	ALA
1	Y	260	HIS
1	Y	261	LEU
1	Y	406	THR
1	Y	529	GLY
1	Y	617	ALA
1	Y	709	GLY
1	Y	782	ARG
1	Y	885	ALA
1	Y	1030	ASN
1	Y	1080	ALA
1	Y	1085	ALA
1	Y	1165	LEU
1	Y	1216	ILE
1	Y	1258	LEU

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Mol	Chain	Res	Type
1	Y	1463	ARG
2	Z	116	TYR
2	Z	160	LYS
2	Z	178	ASN
2	Z	190	GLU
2	Z	415	CYS
2	Z	491	THR
2	Z	494	ASN
2	Z	498	ALA
2	Z	655	GLU
2	Z	706	SER
2	Z	925	ARG
2	Z	1121	SER
2	Z	1385	ASP
1	0	186	ILE
1	0	271	ILE
1	0	289	SER
1	0	291	LEU
1	0	354	GLU
1	0	435	PHE
1	0	464	SER
1	0	1108	VAL
1	0	1358	GLU
2	1	116	TYR
2	1	136	THR
2	1	152	SER
2	1	656	HIS
2	1	994	ARG
5	B	332	GLN
4	D	755	LEU
5	E	305	LYS
5	H	290	GLU
5	H	298	SER
5	H	305	LYS
6	I	303	GLU
4	J	755	LEU
5	K	329	HIS
5	K	332	GLN
7	M	859	LYS
7	M	997	ALA
7	M	1566	ASP
7	M	1600	LEU

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Mol	Chain	Res	Type
8	N	86	ASP
8	N	197	LEU
8	N	647	GLN
8	N	748	HIS
8	N	822	ASN
8	N	892	SER
8	N	940	SER
8	N	1028	THR
8	N	1046	LYS
8	N	1171	ARG
8	N	1217	ARG
8	N	1252	LEU
7	O	859	LYS
7	O	997	ALA
8	P	409	GLU
8	P	413	GLU
8	P	796	SER
8	P	832	THR
8	P	1028	THR
8	P	1061	THR
8	P	1344	PHE
8	P	1403	ASN
9	Q	44	VAL
9	Q	84	ASP
9	Q	698	ASP
9	R	65	ASP
9	R	419	ASP
9	S	473	ARG
9	S	548	SER
9	T	63	SER
9	T	79	SER
9	T	267	ASP
9	T	295	ASN
9	T	424	ASN
9	T	473	ARG
9	T	546	ARG
9	T	586	PHE
9	T	596	ASP
11	V	269	SER
11	V	373	ASN
1	Y	140	ASN
1	Y	270	VAL

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Mol	Chain	Res	Type
1	Y	519	THR
1	Y	527	SER
1	Y	859	SER
1	Y	1045	GLU
1	Y	1113	ILE
1	Y	1296	THR
1	Y	1313	VAL
2	Z	195	ASP
2	Z	371	ASN
2	Z	580	THR
2	Z	584	GLN
2	Z	958	ASN
2	Z	1210	ALA
2	Z	1214	ASP
2	Z	1360	SER
2	Z	1375	ASN
2	Z	1387	HIS
1	0	221	PRO
1	0	411	PRO
1	0	1204	TYR
1	0	1300	LYS
2	1	115	ASP
2	1	541	SER
2	1	584	GLN
2	1	877	SER
2	1	1211	ASP
2	1	1227	GLN
2	1	1387	HIS
6	C	300	ASP
6	C	303	GLU
6	C	404	ASP
5	E	332	GLN
5	H	308	LEU
7	M	3	TRP
7	M	23	ASP
7	M	517	CYS
7	M	681	LYS
7	M	790	SER
7	M	973	ASP
7	M	1240	HIS
7	M	1483	THR
7	M	1666	MET

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Mol	Chain	Res	Type
8	N	33	ASP
8	N	413	GLU
8	N	416	LEU
8	N	432	LEU
8	N	521	PRO
8	N	523	SER
8	N	948	LEU
8	N	972	LEU
8	N	991	LYS
8	N	1277	ILE
8	N	1320	GLU
8	N	1403	ASN
7	O	3	TRP
7	O	23	ASP
7	O	517	CYS
7	O	681	LYS
7	O	790	SER
7	O	973	ASP
7	O	1240	HIS
7	O	1483	THR
7	O	1513	TYR
7	O	1600	LEU
7	O	1666	MET
8	P	74	THR
8	P	276	ASN
8	P	322	HIS
8	P	337	SER
8	P	372	ASP
8	P	420	THR
8	P	518	LEU
8	P	523	SER
8	P	700	LEU
8	P	868	LEU
8	P	870	PRO
8	P	946	TRP
8	P	952	LEU
8	P	1480	GLN
9	Q	534	PHE
9	Q	544	SER
9	Q	547	TYR
9	R	82	ASP
9	R	100	PRO

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Mol	Chain	Res	Type
9	R	154	GLU
9	R	358	ALA
9	S	766	ASN
10	U	349	ALA
10	W	305	TYR
10	W	354	ALA
11	X	354	SER
11	X	398	CYS
1	Y	1308	PHE
2	Z	115	ASP
2	Z	156	ASN
2	Z	537	LYS
2	Z	593	GLN
2	Z	879	THR
2	Z	901	ILE
1	0	1313	VAL
1	0	1314	PRO
2	1	706	SER
2	1	1250	SER
5	B	321	ALA
6	F	352	VAL
5	H	295	CYS
5	H	307	LYS
6	L	300	ASP
7	M	42	LEU
8	N	119	ASN
8	N	406	LYS
8	N	866	ARG
7	O	42	LEU
8	P	496	LEU
8	P	889	THR
8	P	898	VAL
9	Q	48	GLU
9	R	426	PRO
9	S	42	ILE
9	S	607	ARG
11	X	373	ASN
1	Y	197	ASN
1	Y	1204	TYR
2	Z	442	SER
1	0	226	PRO
1	0	1060	TYR

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Mol	Chain	Res	Type
7	M	332	VAL
7	O	332	VAL
8	P	1008	THR
8	P	1277	ILE
1	Y	832	VAL
2	Z	376	PRO
2	Z	1374	PRO
8	P	440	ILE
8	P	460	ILE
8	P	1250	ILE
9	T	428	VAL
1	Y	410	ALA
1	Y	1403	PRO
1	0	1227	ILE
5	E	322	ILE
7	M	619	VAL
7	M	1031	VAL
7	M	1042	ILE
8	P	1160	ILE
9	S	426	PRO
1	Y	1314	PRO
1	Y	1385	PHE
7	O	619	VAL
8	P	381	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	994/1353 (74%)	958 (96%)	36 (4%)	31	52
1	Y	977/1353 (72%)	951 (97%)	26 (3%)	39	61
2	1	1007/1250 (81%)	975 (97%)	32 (3%)	34	55
2	Z	1004/1250 (80%)	976 (97%)	28 (3%)	38	59
4	A	154/674 (23%)	150 (97%)	4 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	154/674 (23%)	151 (98%)	3 (2%)	50	67
4	G	155/674 (23%)	150 (97%)	5 (3%)	34	55
4	J	154/674 (23%)	148 (96%)	6 (4%)	28	49
5	B	196/439 (45%)	187 (95%)	9 (5%)	24	45
5	E	196/439 (45%)	191 (97%)	5 (3%)	40	62
5	H	196/439 (45%)	188 (96%)	8 (4%)	27	48
5	K	196/439 (45%)	187 (95%)	9 (5%)	24	45
6	C	155/377 (41%)	150 (97%)	5 (3%)	34	55
6	F	155/377 (41%)	152 (98%)	3 (2%)	50	67
6	I	155/377 (41%)	151 (97%)	4 (3%)	40	62
6	L	155/377 (41%)	152 (98%)	3 (2%)	50	67
7	M	1279/1538 (83%)	1238 (97%)	41 (3%)	34	55
7	O	1279/1538 (83%)	1238 (97%)	41 (3%)	34	55
8	N	1276/1557 (82%)	1213 (95%)	63 (5%)	22	43
8	P	1276/1557 (82%)	1218 (96%)	58 (4%)	24	46
9	Q	508/762 (67%)	496 (98%)	12 (2%)	43	64
9	R	507/762 (66%)	492 (97%)	15 (3%)	36	57
9	S	507/762 (66%)	498 (98%)	9 (2%)	51	68
9	T	507/762 (66%)	503 (99%)	4 (1%)	73	80
10	U	79/421 (19%)	77 (98%)	2 (2%)	42	63
10	W	79/421 (19%)	77 (98%)	2 (2%)	42	63
11	V	80/477 (17%)	80 (100%)	0	100	100
11	X	81/477 (17%)	79 (98%)	2 (2%)	42	63
All	All	13461/22200 (61%)	13026 (97%)	435 (3%)	35	55

All (435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	118	THR
1	0	133	TYR
1	0	185	THR
1	0	193	TRP
1	0	233	LEU
1	0	249	LYS

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Mol	Chain	Res	Type
1	0	254	LEU
1	0	273	ILE
1	0	315	THR
1	0	358	GLN
1	0	385	LYS
1	0	404	THR
1	0	452	MET
1	0	471	SER
1	0	607	GLN
1	0	630	THR
1	0	643	THR
1	0	654	THR
1	0	789	VAL
1	0	831	LYS
1	0	862	GLN
1	0	958	LYS
1	0	976	THR
1	0	977	LYS
1	0	992	CYS
1	0	1105	TYR
1	0	1143	GLN
1	0	1188	GLU
1	0	1199	ILE
1	0	1258	LEU
1	0	1278	LEU
1	0	1285	ILE
1	0	1331	ARG
1	0	1389	GLU
1	0	1446	LYS
1	0	1461	LYS
2	1	88	SER
2	1	180	LEU
2	1	275	THR
2	1	309	LEU
2	1	395	ASN
2	1	443	ILE
2	1	495	THR
2	1	502	ILE
2	1	509	THR
2	1	563	THR
2	1	605	THR
2	1	624	LEU

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Mol	Chain	Res	Type
2	1	625	ILE
2	1	653	LYS
2	1	679	SER
2	1	708	ARG
2	1	715	LEU
2	1	858	LYS
2	1	861	GLN
2	1	879	THR
2	1	922	LYS
2	1	973	LYS
2	1	1039	LEU
2	1	1043	VAL
2	1	1078	GLN
2	1	1155	GLN
2	1	1156	LEU
2	1	1169	ILE
2	1	1246	LYS
2	1	1299	LYS
2	1	1301	SER
2	1	1367	LYS
4	A	695	GLN
4	A	754	ASN
4	A	755	LEU
4	A	756	ASN
5	B	318	GLU
5	B	319	THR
5	B	322	ILE
5	B	324	TYR
5	B	326	LYS
5	B	331	LEU
5	B	361	ARG
5	B	436	MET
5	B	471	LYS
6	C	327	LYS
6	C	344	LEU
6	C	369	LEU
6	C	451	MET
6	C	462	GLN
4	D	657	GLN
4	D	690	GLN
4	D	778	LYS
5	E	324	TYR

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Mol	Chain	Res	Type
5	E	347	THR
5	E	415	LEU
5	E	435	LYS
5	E	446	ARG
6	F	370	ASP
6	F	447	PHE
6	F	449	LEU
4	G	695	GLN
4	G	727	SER
4	G	754	ASN
4	G	755	LEU
4	G	756	ASN
5	H	317	ASN
5	H	318	GLU
5	H	320	GLU
5	H	324	TYR
5	H	433	GLU
5	H	436	MET
5	H	471	LYS
5	H	525	GLU
6	I	331	LYS
6	I	369	LEU
6	I	451	MET
6	I	462	GLN
4	J	650	GLU
4	J	690	GLN
4	J	695	GLN
4	J	722	LEU
4	J	776	PHE
4	J	778	LYS
5	K	294	LYS
5	K	305	LYS
5	K	315	LYS
5	K	319	THR
5	K	320	GLU
5	K	331	LEU
5	K	435	LYS
5	K	446	ARG
5	K	508	LYS
6	L	292	HIS
6	L	340	ILE
6	L	348	GLN

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Mol	Chain	Res	Type
7	M	2	LYS
7	M	98	THR
7	M	121	VAL
7	M	136	LYS
7	M	145	LEU
7	M	180	LYS
7	M	197	LEU
7	M	228	PHE
7	M	277	LEU
7	M	288	TRP
7	M	449	LEU
7	M	553	ILE
7	M	638	VAL
7	M	681	LYS
7	M	716	LEU
7	M	837	TYR
7	M	916	ILE
7	M	964	LYS
7	M	1016	THR
7	M	1018	THR
7	M	1038	LEU
7	M	1107	GLU
7	M	1158	THR
7	M	1183	TYR
7	M	1189	MET
7	M	1273	LYS
7	M	1318	LYS
7	M	1319	LEU
7	M	1347	ILE
7	M	1396	LEU
7	M	1408	LEU
7	M	1436	LYS
7	M	1457	ILE
7	M	1479	LEU
7	M	1482	THR
7	M	1484	ARG
7	M	1487	LEU
7	M	1490	ARG
7	M	1493	LYS
7	M	1498	LEU
7	M	1516	THR
8	N	32	VAL

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Mol	Chain	Res	Type
8	N	40	ILE
8	N	41	ARG
8	N	42	GLN
8	N	43	PHE
8	N	72	ARG
8	N	131	ASP
8	N	132	ASN
8	N	155	ILE
8	N	175	SER
8	N	176	LEU
8	N	178	GLN
8	N	203	LYS
8	N	217	GLN
8	N	257	LEU
8	N	281	GLN
8	N	359	LEU
8	N	379	ILE
8	N	381	VAL
8	N	382	PHE
8	N	413	GLU
8	N	443	ILE
8	N	447	LEU
8	N	525	LYS
8	N	552	LEU
8	N	564	LEU
8	N	577	MET
8	N	656	GLN
8	N	729	HIS
8	N	753	TYR
8	N	763	GLN
8	N	766	GLU
8	N	794	ILE
8	N	833	LYS
8	N	879	ILE
8	N	903	LEU
8	N	913	ASN
8	N	923	LEU
8	N	933	LYS
8	N	980	LYS
8	N	982	ILE
8	N	1015	LYS
8	N	1021	THR

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Mol	Chain	Res	Type
8	N	1056	LYS
8	N	1060	LEU
8	N	1094	SER
8	N	1096	ILE
8	N	1192	LEU
8	N	1237	ASN
8	N	1252	LEU
8	N	1276	LYS
8	N	1277	ILE
8	N	1292	GLU
8	N	1303	LEU
8	N	1304	LYS
8	N	1317	VAL
8	N	1346	LYS
8	N	1400	PRO
8	N	1406	VAL
8	N	1431	ILE
8	N	1459	LYS
8	N	1527	LYS
8	N	1596	LYS
7	O	2	LYS
7	O	98	THR
7	O	121	VAL
7	O	136	LYS
7	O	145	LEU
7	O	180	LYS
7	O	197	LEU
7	O	228	PHE
7	O	277	LEU
7	O	288	TRP
7	O	449	LEU
7	O	553	ILE
7	O	638	VAL
7	O	681	LYS
7	O	716	LEU
7	O	837	TYR
7	O	916	ILE
7	O	964	LYS
7	O	1016	THR
7	O	1018	THR
7	O	1038	LEU
7	O	1107	GLU

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Mol	Chain	Res	Type
7	O	1138	PHE
7	O	1158	THR
7	O	1183	TYR
7	O	1191	SER
7	O	1273	LYS
7	O	1318	LYS
7	O	1319	LEU
7	O	1320	GLU
7	O	1347	ILE
7	O	1396	LEU
7	O	1408	LEU
7	O	1457	ILE
7	O	1479	LEU
7	O	1482	THR
7	O	1484	ARG
7	O	1490	ARG
7	O	1493	LYS
7	O	1498	LEU
7	O	1516	THR
8	P	22	MET
8	P	40	ILE
8	P	42	GLN
8	P	72	ARG
8	P	73	SER
8	P	133	ASP
8	P	174	VAL
8	P	178	GLN
8	P	190	GLN
8	P	193	GLN
8	P	217	GLN
8	P	218	ASN
8	P	257	LEU
8	P	281	GLN
8	P	359	LEU
8	P	381	VAL
8	P	448	ILE
8	P	552	LEU
8	P	564	LEU
8	P	647	GLN
8	P	659	GLU
8	P	766	GLU
8	P	794	ILE

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Mol	Chain	Res	Type
8	P	869	LYS
8	P	897	LYS
8	P	911	PRO
8	P	1021	THR
8	P	1031	LYS
8	P	1035	LYS
8	P	1046	LYS
8	P	1054	PHE
8	P	1055	GLN
8	P	1056	LYS
8	P	1057	LYS
8	P	1065	THR
8	P	1070	LYS
8	P	1075	ILE
8	P	1077	ARG
8	P	1095	GLU
8	P	1207	TRP
8	P	1247	PHE
8	P	1249	GLN
8	P	1276	LYS
8	P	1277	ILE
8	P	1283	LYS
8	P	1288	PHE
8	P	1303	LEU
8	P	1304	LYS
8	P	1346	LYS
8	P	1389	LEU
8	P	1406	VAL
8	P	1484	LYS
8	P	1527	LYS
8	P	1530	LYS
8	P	1559	LYS
8	P	1596	LYS
8	P	1619	THR
8	P	1647	LEU
9	Q	234	ILE
9	Q	422	ARG
9	Q	437	TRP
9	Q	501	MET
9	Q	515	LEU
9	Q	543	LYS
9	Q	592	LYS

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Mol	Chain	Res	Type
9	Q	626	GLN
9	Q	645	GLN
9	Q	672	GLN
9	Q	754	ARG
9	Q	756	LYS
9	R	222	PHE
9	R	266	LYS
9	R	283	LEU
9	R	306	LYS
9	R	321	LYS
9	R	347	LYS
9	R	411	VAL
9	R	444	LYS
9	R	514	LYS
9	R	533	ARG
9	R	592	LYS
9	R	754	ARG
9	R	766	ASN
9	R	793	LYS
9	R	812	GLN
9	S	312	LYS
9	S	314	LYS
9	S	359	ASN
9	S	543	LYS
9	S	663	ASP
9	S	672	GLN
9	S	729	ASN
9	S	754	ARG
9	S	833	ILE
9	T	276	GLN
9	T	315	LYS
9	T	413	LYS
9	T	754	ARG
10	U	249	ASP
10	U	324	LYS
10	W	249	ASP
10	W	305	TYR
11	X	302	ARG
11	X	399	LYS
1	Y	101	LEU
1	Y	124	ARG
1	Y	126	TYR

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Mol	Chain	Res	Type
1	Y	184	ILE
1	Y	207	MET
1	Y	271	ILE
1	Y	273	ILE
1	Y	274	VAL
1	Y	296	LEU
1	Y	374	LYS
1	Y	382	ILE
1	Y	454	ARG
1	Y	465	ILE
1	Y	519	THR
1	Y	577	PHE
1	Y	618	THR
1	Y	791	MET
1	Y	831	LYS
1	Y	884	VAL
1	Y	992	CYS
1	Y	1096	GLN
1	Y	1238	ARG
1	Y	1258	LEU
1	Y	1267	GLU
1	Y	1276	LEU
1	Y	1348	ARG
2	Z	110	ILE
2	Z	116	TYR
2	Z	162	ASP
2	Z	168	GLU
2	Z	234	THR
2	Z	246	ILE
2	Z	252	LYS
2	Z	452	LYS
2	Z	491	THR
2	Z	509	THR
2	Z	548	LEU
2	Z	586	TYR
2	Z	605	THR
2	Z	679	SER
2	Z	724	TRP
2	Z	745	ILE
2	Z	768	ILE
2	Z	798	LEU
2	Z	830	MET

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Mol	Chain	Res	Type
2	Z	858	LYS
2	Z	1040	LYS
2	Z	1078	GLN
2	Z	1094	ILE
2	Z	1156	LEU
2	Z	1241	LEU
2	Z	1299	LYS
2	Z	1367	LYS
2	Z	1371	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (450) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	112	GLN
1	0	117	ASN
1	0	128	ASN
1	0	134	ASN
1	0	194	ASN
1	0	197	ASN
1	0	252	ASN
1	0	449	ASN
1	0	574	HIS
1	0	607	GLN
1	0	626	ASN
1	0	862	GLN
1	0	911	ASN
1	0	1027	HIS
1	0	1082	GLN
1	0	1091	ASN
1	0	1158	HIS
1	0	1168	GLN
1	0	1272	GLN
1	0	1318	HIS
1	0	1377	ASN
1	0	1406	HIS
1	0	1453	HIS
2	1	187	ASN
2	1	192	HIS
2	1	212	ASN
2	1	220	ASN
2	1	259	ASN
2	1	271	GLN

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Mol	Chain	Res	Type
2	1	287	GLN
2	1	308	ASN
2	1	355	HIS
2	1	389	ASN
2	1	418	ASN
2	1	486	GLN
2	1	557	ASN
2	1	627	ASN
2	1	633	HIS
2	1	652	ASN
2	1	656	HIS
2	1	861	GLN
2	1	926	ASN
2	1	958	ASN
2	1	1175	ASN
2	1	1179	ASN
2	1	1239	ASN
2	1	1290	ASN
2	1	1387	HIS
2	1	1388	HIS
4	A	678	GLN
4	A	690	GLN
4	A	695	GLN
4	A	698	GLN
4	A	709	ASN
4	A	771	ASN
5	B	346	GLN
5	B	351	GLN
5	B	390	HIS
5	B	402	GLN
5	B	418	GLN
5	B	439	GLN
5	B	441	GLN
5	B	516	GLN
6	C	292	HIS
6	C	293	HIS
6	C	348	GLN
6	C	355	GLN
6	C	374	GLN
6	C	462	GLN
4	D	654	HIS
4	D	657	GLN

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Mol	Chain	Res	Type
4	D	667	GLN
4	D	675	GLN
4	D	690	GLN
4	D	695	GLN
4	D	703	GLN
4	D	756	ASN
4	D	798	ASN
5	E	287	GLN
5	E	314	ASN
5	E	351	GLN
5	E	359	ASN
5	E	365	GLN
5	E	377	ASN
5	E	385	GLN
5	E	405	ASN
5	E	418	GLN
5	E	516	GLN
6	F	279	GLN
6	F	285	GLN
6	F	289	GLN
6	F	301	HIS
6	F	374	GLN
6	F	461	HIS
4	G	667	GLN
4	G	678	GLN
4	G	695	GLN
4	G	754	ASN
4	G	771	ASN
5	H	317	ASN
5	H	332	GLN
5	H	337	GLN
5	H	351	GLN
5	H	359	ASN
5	H	363	GLN
5	H	365	GLN
5	H	390	HIS
5	H	402	GLN
5	H	405	ASN
5	H	439	GLN
5	H	441	GLN
5	H	516	GLN
6	I	275	GLN

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Mol	Chain	Res	Type
6	I	287	GLN
6	I	293	HIS
6	I	348	GLN
6	I	374	GLN
6	I	462	GLN
4	J	657	GLN
4	J	675	GLN
4	J	690	GLN
4	J	703	GLN
4	J	704	GLN
4	J	756	ASN
5	K	351	GLN
5	K	359	ASN
5	K	363	GLN
5	K	365	GLN
5	K	368	ASN
5	K	378	HIS
5	K	405	ASN
5	K	507	ASN
5	K	516	GLN
6	L	279	GLN
6	L	287	GLN
6	L	289	GLN
6	L	293	HIS
6	L	324	GLN
6	L	461	HIS
7	M	34	ASN
7	M	36	ASN
7	M	45	ASN
7	M	68	GLN
7	M	101	ASN
7	M	111	GLN
7	M	132	GLN
7	M	137	ASN
7	M	154	GLN
7	M	226	ASN
7	M	258	GLN
7	M	426	GLN
7	M	557	ASN
7	M	714	HIS
7	M	715	ASN
7	M	720	HIS

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Mol	Chain	Res	Type
7	M	724	ASN
7	M	742	GLN
7	M	763	HIS
7	M	766	GLN
7	M	798	ASN
7	M	829	ASN
7	M	873	ASN
7	M	903	ASN
7	M	935	GLN
7	M	1037	ASN
7	M	1089	ASN
7	M	1104	ASN
7	M	1123	ASN
7	M	1166	HIS
7	M	1187	ASN
7	M	1240	HIS
7	M	1288	ASN
7	M	1304	HIS
7	M	1326	ASN
7	M	1346	ASN
7	M	1410	ASN
7	M	1411	HIS
7	M	1465	GLN
7	M	1494	ASN
7	M	1541	ASN
8	N	12	GLN
8	N	42	GLN
8	N	50	ASN
8	N	68	HIS
8	N	80	GLN
8	N	111	HIS
8	N	119	ASN
8	N	151	ASN
8	N	190	GLN
8	N	215	GLN
8	N	217	GLN
8	N	281	GLN
8	N	356	HIS
8	N	388	ASN
8	N	410	GLN
8	N	414	ASN
8	N	418	ASN

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Mol	Chain	Res	Type
8	N	444	ASN
8	N	560	ASN
8	N	570	GLN
8	N	571	ASN
8	N	727	ASN
8	N	760	ASN
8	N	763	GLN
8	N	770	HIS
8	N	780	HIS
8	N	829	ASN
8	N	899	GLN
8	N	944	GLN
8	N	947	ASN
8	N	975	GLN
8	N	1041	ASN
8	N	1059	ASN
8	N	1123	HIS
8	N	1127	ASN
8	N	1180	GLN
8	N	1195	GLN
8	N	1223	ASN
8	N	1249	GLN
8	N	1335	GLN
8	N	1399	ASN
8	N	1479	GLN
8	N	1492	HIS
8	N	1497	ASN
8	N	1509	GLN
8	N	1539	ASN
7	O	34	ASN
7	O	36	ASN
7	O	45	ASN
7	O	68	GLN
7	O	101	ASN
7	O	132	GLN
7	O	137	ASN
7	O	154	GLN
7	O	226	ASN
7	O	258	GLN
7	O	426	GLN
7	O	557	ASN
7	O	714	HIS

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Mol	Chain	Res	Type
7	O	715	ASN
7	O	720	HIS
7	O	724	ASN
7	O	742	GLN
7	O	763	HIS
7	O	766	GLN
7	O	798	ASN
7	O	829	ASN
7	O	873	ASN
7	O	903	ASN
7	O	935	GLN
7	O	1037	ASN
7	O	1104	ASN
7	O	1123	ASN
7	O	1166	HIS
7	O	1187	ASN
7	O	1225	GLN
7	O	1240	HIS
7	O	1288	ASN
7	O	1304	HIS
7	O	1326	ASN
7	O	1346	ASN
7	O	1393	ASN
7	O	1410	ASN
7	O	1411	HIS
7	O	1465	GLN
7	O	1494	ASN
7	O	1541	ASN
8	P	17	HIS
8	P	42	GLN
8	P	50	ASN
8	P	60	GLN
8	P	77	ASN
8	P	111	HIS
8	P	151	ASN
8	P	178	GLN
8	P	193	GLN
8	P	196	ASN
8	P	215	GLN
8	P	217	GLN
8	P	281	GLN
8	P	299	ASN

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Mol	Chain	Res	Type
8	P	322	HIS
8	P	356	HIS
8	P	363	ASN
8	P	418	ASN
8	P	444	ASN
8	P	551	ASN
8	P	571	ASN
8	P	600	ASN
8	P	647	GLN
8	P	656	GLN
8	P	670	HIS
8	P	692	ASN
8	P	727	ASN
8	P	729	HIS
8	P	745	HIS
8	P	770	HIS
8	P	800	ASN
8	P	944	GLN
8	P	1059	ASN
8	P	1088	ASN
8	P	1093	ASN
8	P	1193	ASN
8	P	1195	GLN
8	P	1232	HIS
8	P	1249	GLN
8	P	1335	GLN
8	P	1399	ASN
8	P	1462	ASN
8	P	1492	HIS
8	P	1509	GLN
8	P	1535	ASN
8	P	1608	HIS
8	P	1624	GLN
9	Q	206	ASN
9	Q	246	ASN
9	Q	250	ASN
9	Q	252	GLN
9	Q	281	GLN
9	Q	293	ASN
9	Q	351	GLN
9	Q	356	ASN
9	Q	439	HIS

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Mol	Chain	Res	Type
9	Q	464	ASN
9	Q	612	HIS
9	Q	626	GLN
9	Q	672	GLN
9	Q	729	ASN
9	Q	762	ASN
9	Q	784	ASN
9	Q	787	HIS
9	Q	795	GLN
9	Q	812	GLN
9	R	223	ASN
9	R	227	GLN
9	R	236	ASN
9	R	301	ASN
9	R	480	GLN
9	R	505	HIS
9	R	626	GLN
9	R	658	ASN
9	R	710	ASN
9	R	733	GLN
9	R	738	GLN
9	R	784	ASN
9	R	787	HIS
9	S	224	ASN
9	S	236	ASN
9	S	276	GLN
9	S	281	GLN
9	S	301	ASN
9	S	351	GLN
9	S	505	HIS
9	S	540	ASN
9	S	563	ASN
9	S	612	HIS
9	S	621	HIS
9	S	658	ASN
9	S	672	GLN
9	S	684	ASN
9	S	719	ASN
9	S	787	HIS
9	S	795	GLN
9	T	223	ASN
9	T	246	ASN

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Mol	Chain	Res	Type
9	T	252	GLN
9	T	281	GLN
9	T	284	GLN
9	T	324	ASN
9	T	439	HIS
9	T	463	GLN
9	T	464	ASN
9	T	612	HIS
9	T	621	HIS
9	T	645	GLN
9	T	658	ASN
9	T	672	GLN
9	T	684	ASN
9	T	699	ASN
9	T	705	GLN
9	T	770	ASN
9	T	784	ASN
9	T	787	HIS
9	T	790	ASN
9	T	795	GLN
9	T	802	GLN
9	T	808	ASN
10	U	269	HIS
10	U	352	GLN
11	V	287	HIS
11	V	290	HIS
11	V	293	HIS
11	V	299	GLN
11	V	361	ASN
11	V	394	GLN
10	W	251	HIS
11	X	293	HIS
11	X	371	GLN
1	Y	134	ASN
1	Y	194	ASN
1	Y	197	ASN
1	Y	212	GLN
1	Y	222	ASN
1	Y	230	HIS
1	Y	258	ASN
1	Y	260	HIS
1	Y	266	GLN

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Mol	Chain	Res	Type
1	Y	276	HIS
1	Y	431	ASN
1	Y	432	ASN
1	Y	433	ASN
1	Y	449	ASN
1	Y	606	GLN
1	Y	631	GLN
1	Y	862	GLN
1	Y	886	ASN
1	Y	924	ASN
1	Y	1153	ASN
1	Y	1224	ASN
1	Y	1333	HIS
1	Y	1353	ASN
1	Y	1362	ASN
1	Y	1396	ASN
1	Y	1406	HIS
1	Y	1453	HIS
2	Z	113	ASN
2	Z	142	GLN
2	Z	153	GLN
2	Z	212	ASN
2	Z	220	ASN
2	Z	245	ASN
2	Z	262	ASN
2	Z	282	ASN
2	Z	344	GLN
2	Z	383	HIS
2	Z	417	ASN
2	Z	486	GLN
2	Z	494	ASN
2	Z	536	HIS
2	Z	588	ASN
2	Z	607	ASN
2	Z	627	ASN
2	Z	856	ASN
2	Z	927	HIS
2	Z	1003	ASN
2	Z	1056	HIS
2	Z	1138	ASN
2	Z	1207	ASN
2	Z	1235	GLN

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Mol	Chain	Res	Type
2	Z	1267	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	637:LEU	C	638:ASP	N	3.38

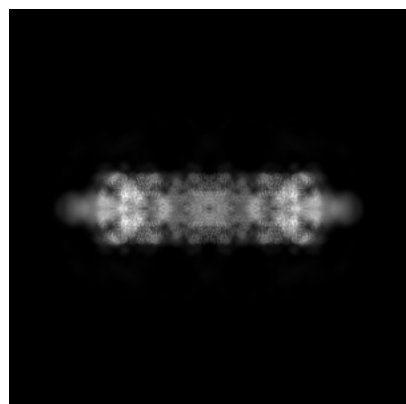
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24232. These allow visual inspection of the internal detail of the map and identification of artifacts.

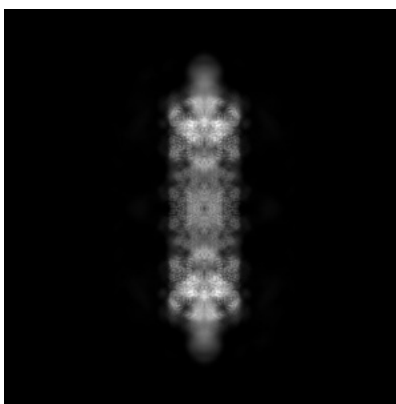
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

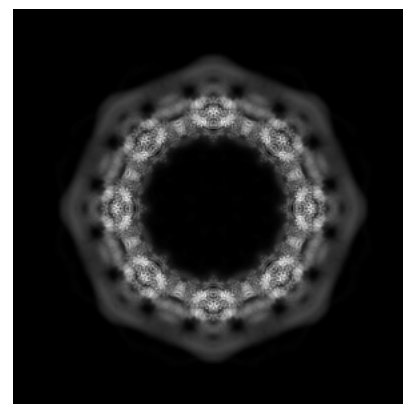
6.1.1 Primary map



X

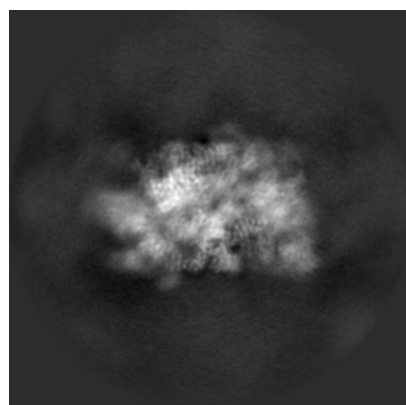


Y

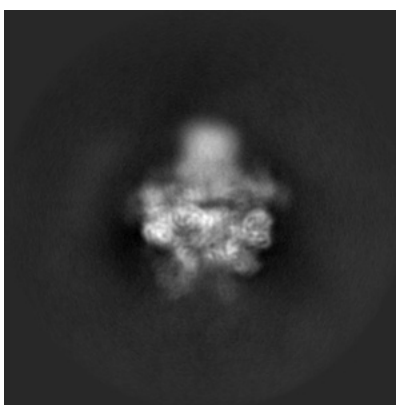


Z

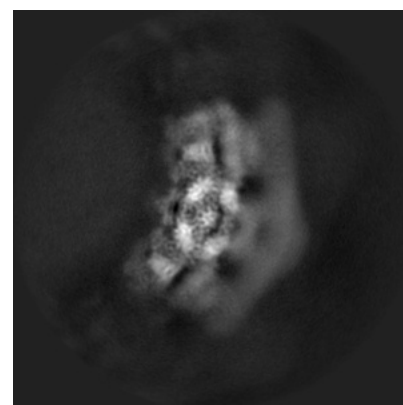
6.1.2 Raw map



X



Y

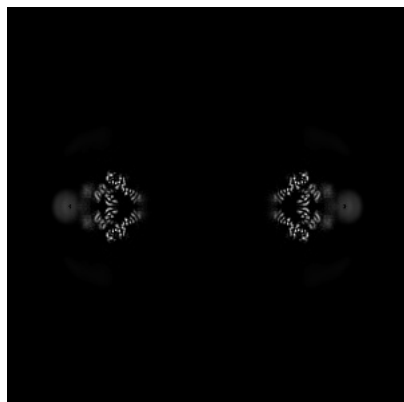


Z

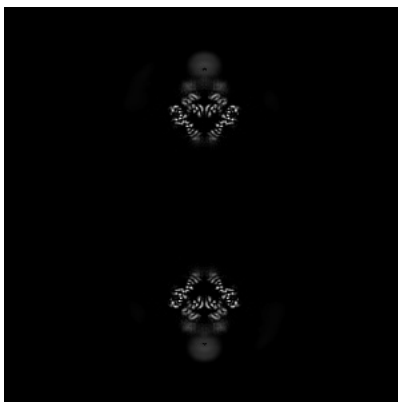
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

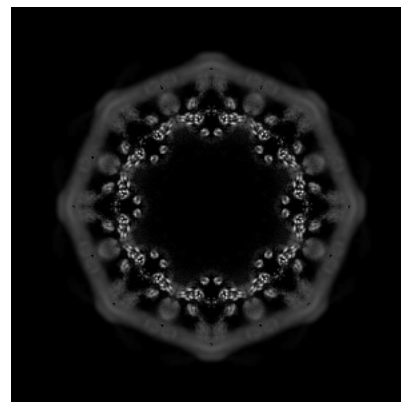
6.2.1 Primary map



X Index: 240

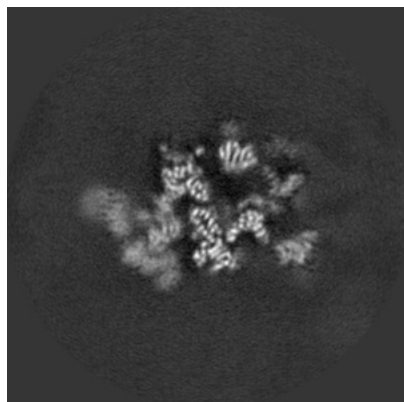


Y Index: 240

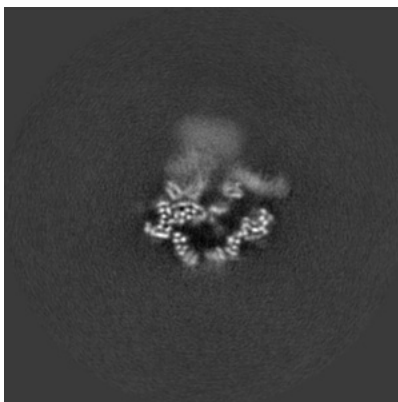


Z Index: 240

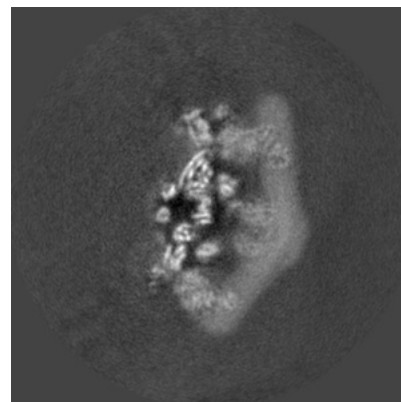
6.2.2 Raw map



X Index: 133



Y Index: 133

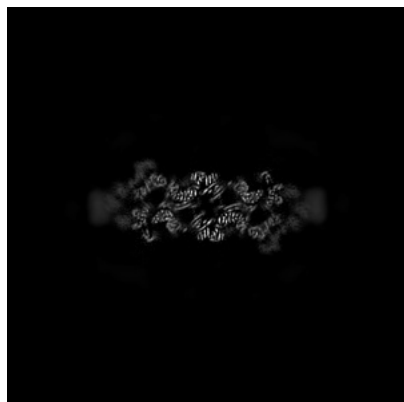


Z Index: 133

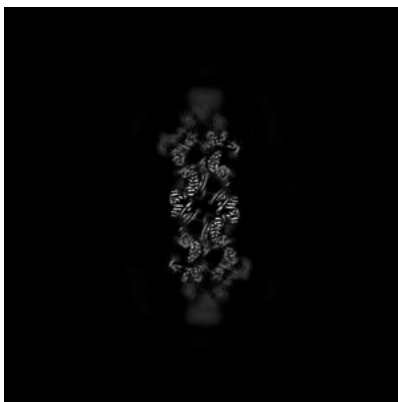
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

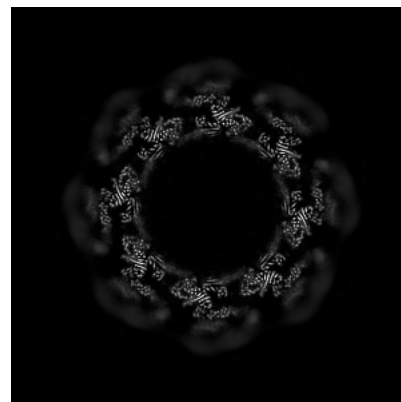
6.3.1 Primary map



X Index: 340

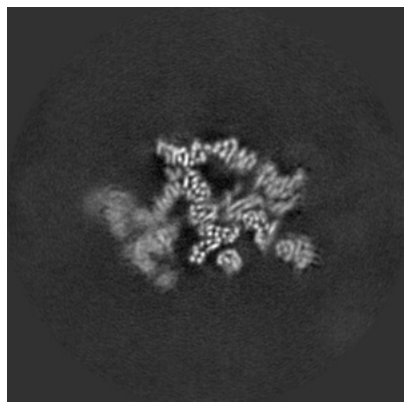


Y Index: 140

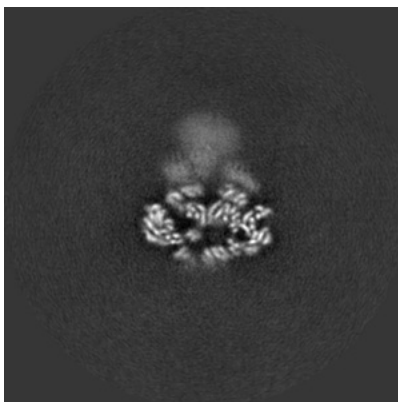


Z Index: 257

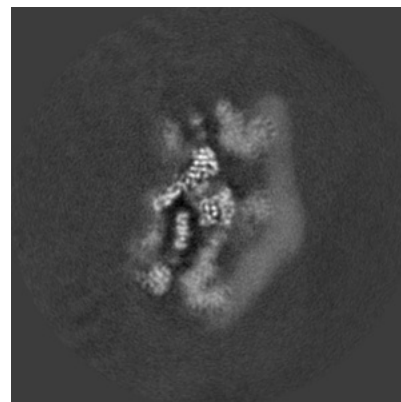
6.3.2 Raw map



X Index: 129



Y Index: 126

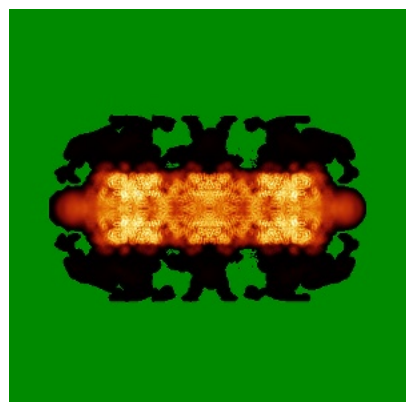


Z Index: 125

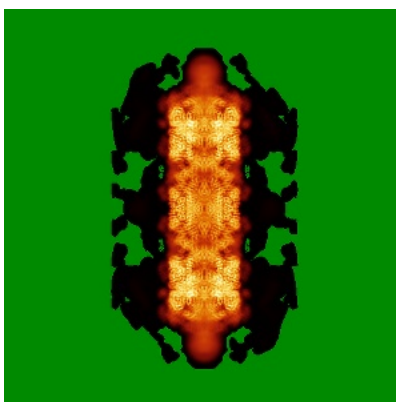
The images above show the largest variance slices of the map in three orthogonal directions.

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

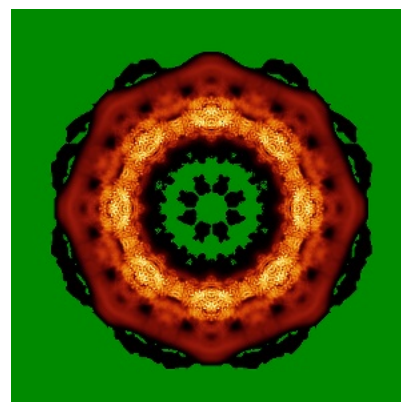
6.4.1 Primary map



X

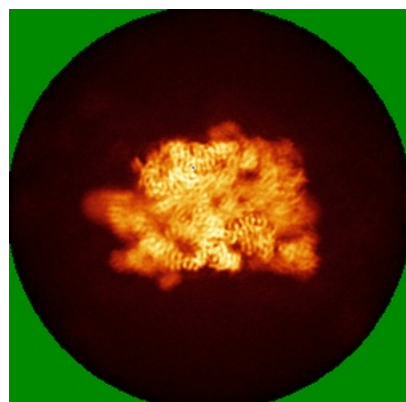


Y

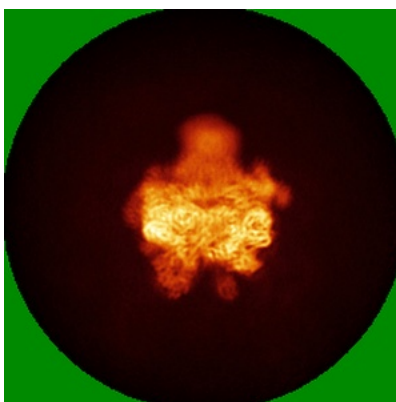


Z

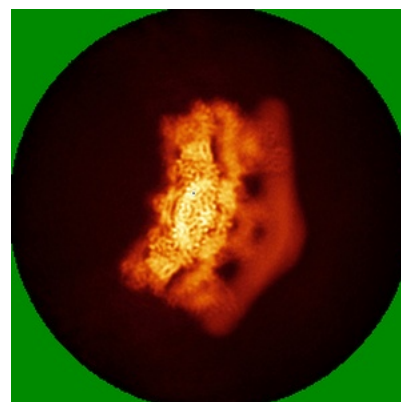
6.4.2 Raw map



X



Y

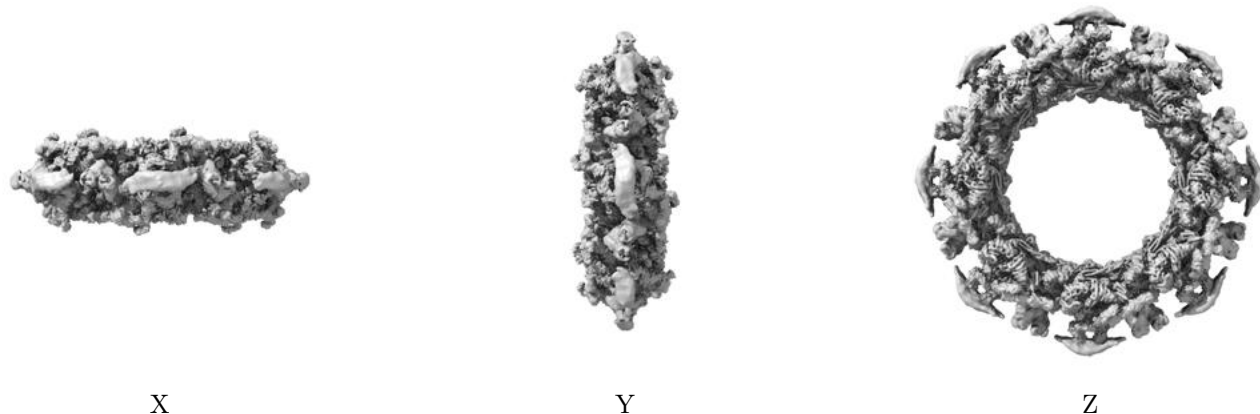


Z

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

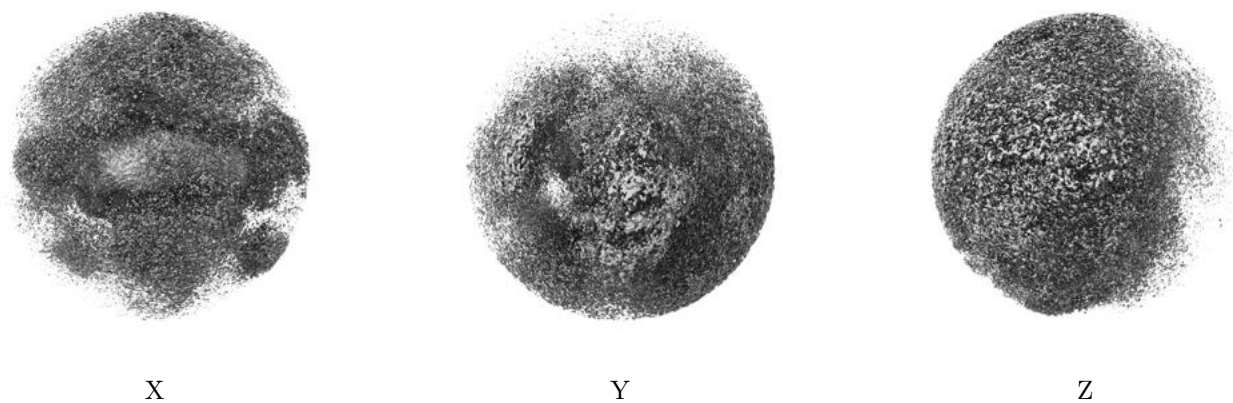
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.595. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

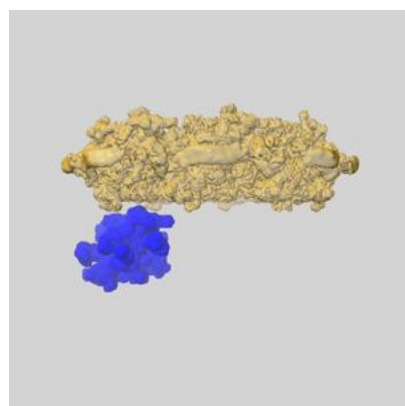
6.6 Mask visualisation [i](#)

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

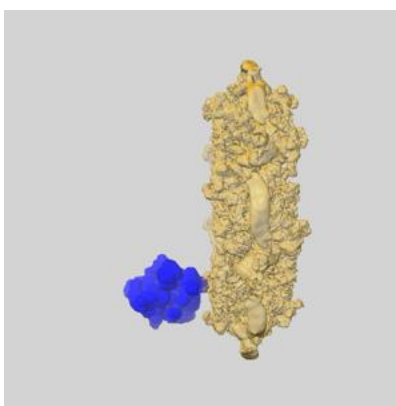
A mask typically either:

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

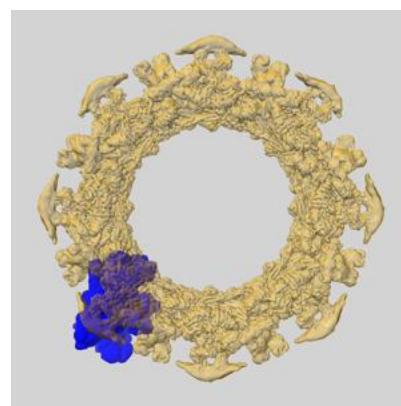
6.6.1 emd_24232_msk_1.map [i](#)



X



Y

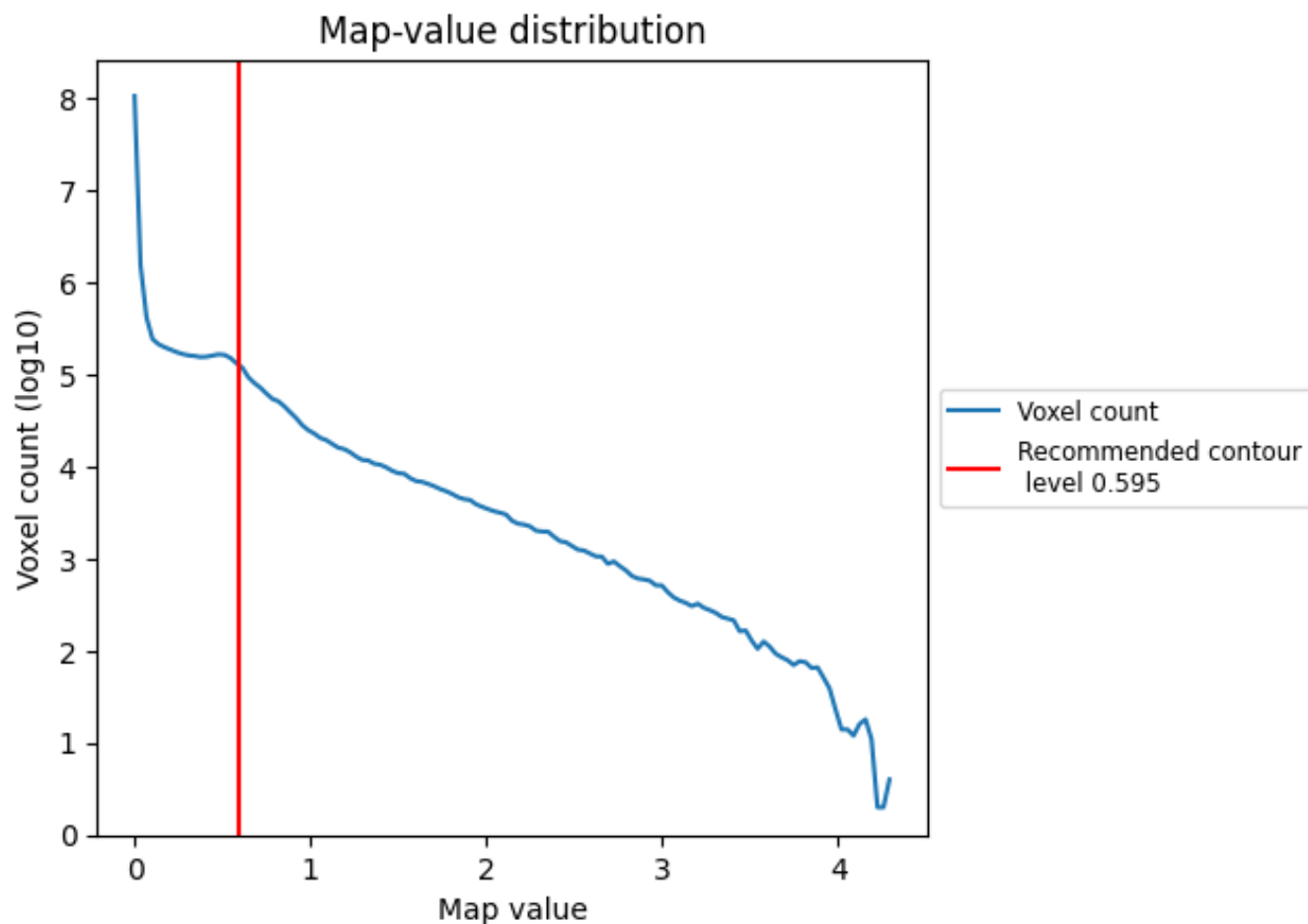


Z

7 Map analysis [i](#)

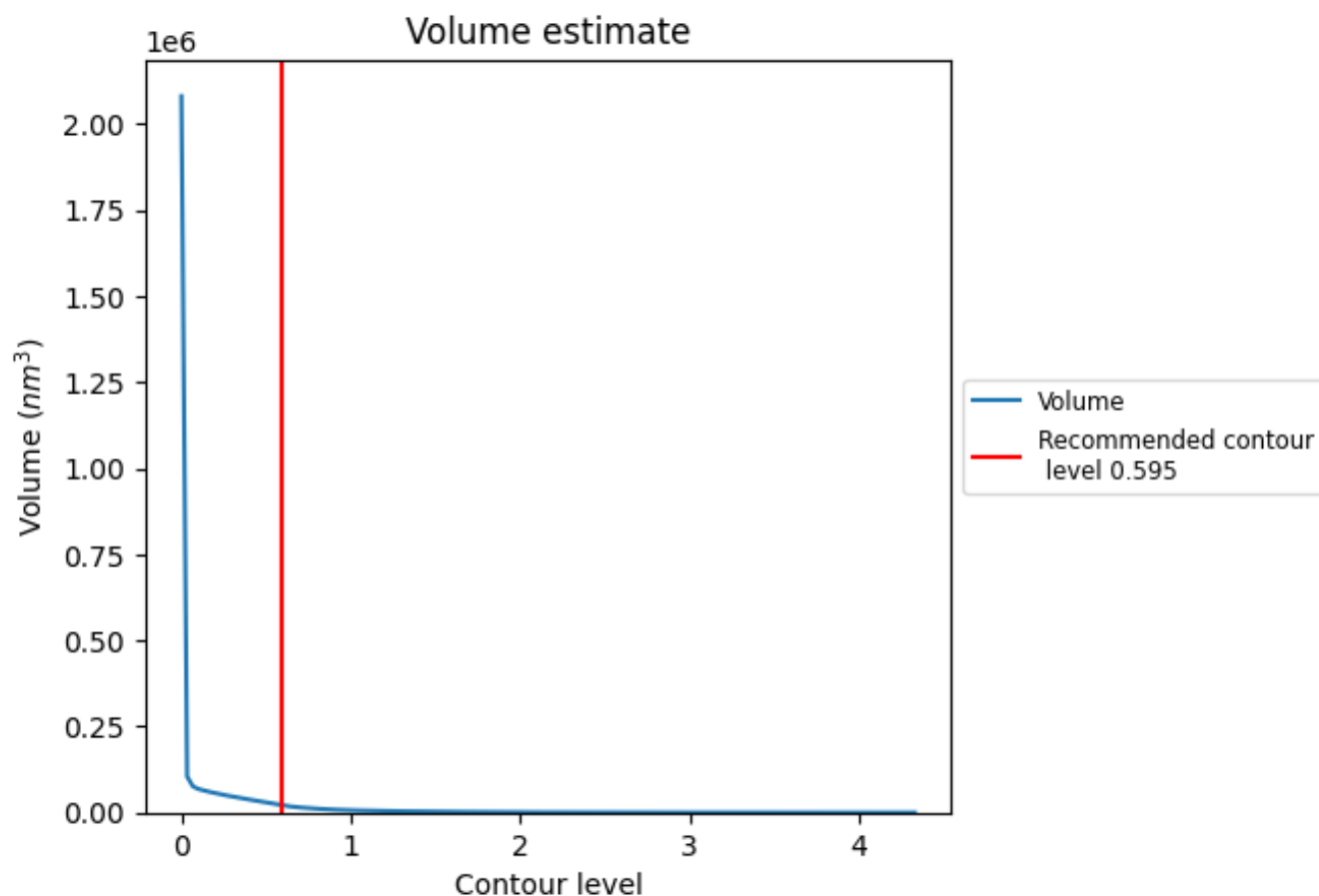
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

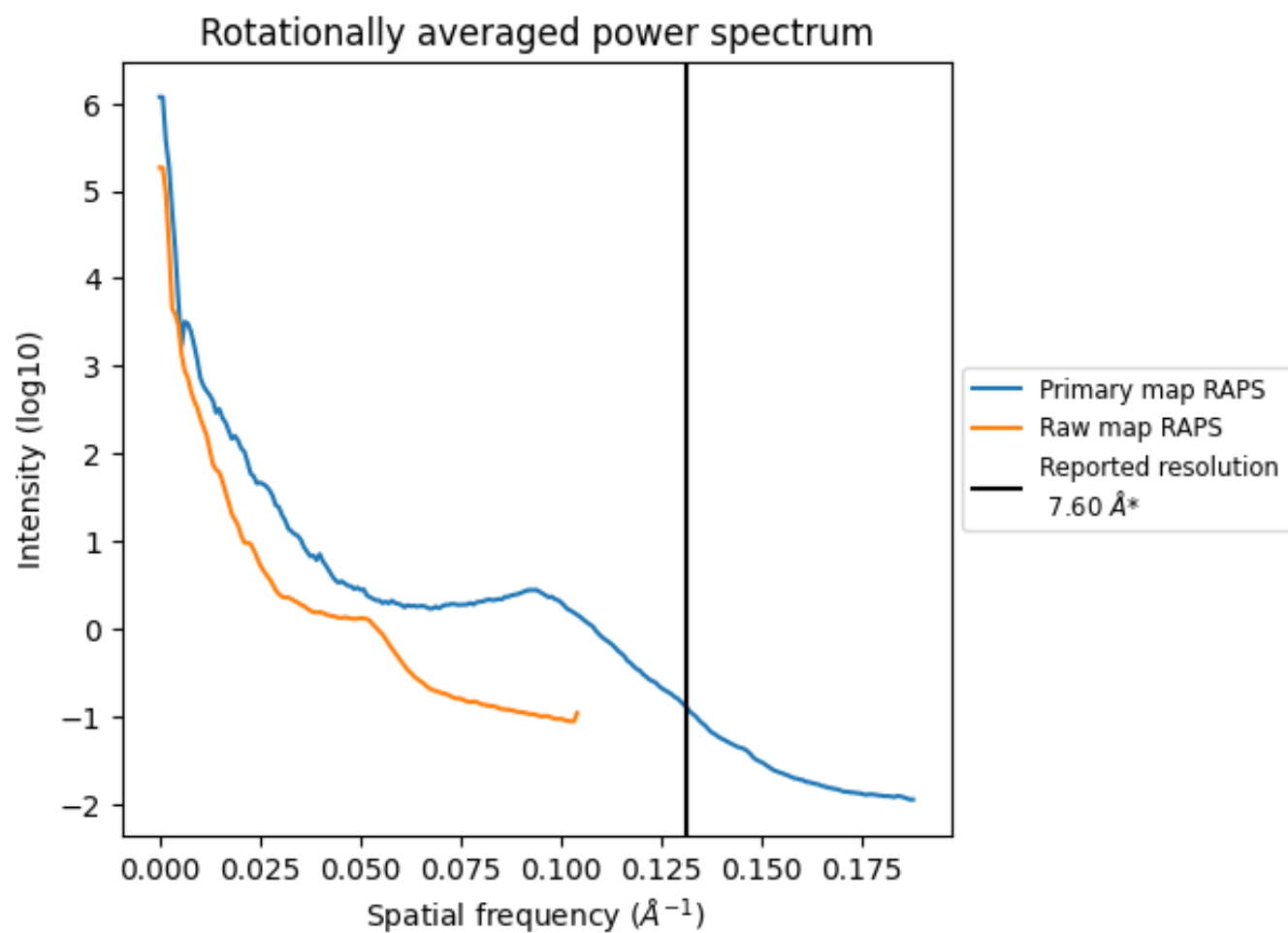
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20941 nm^3 ; this corresponds to an approximate mass of 18917 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

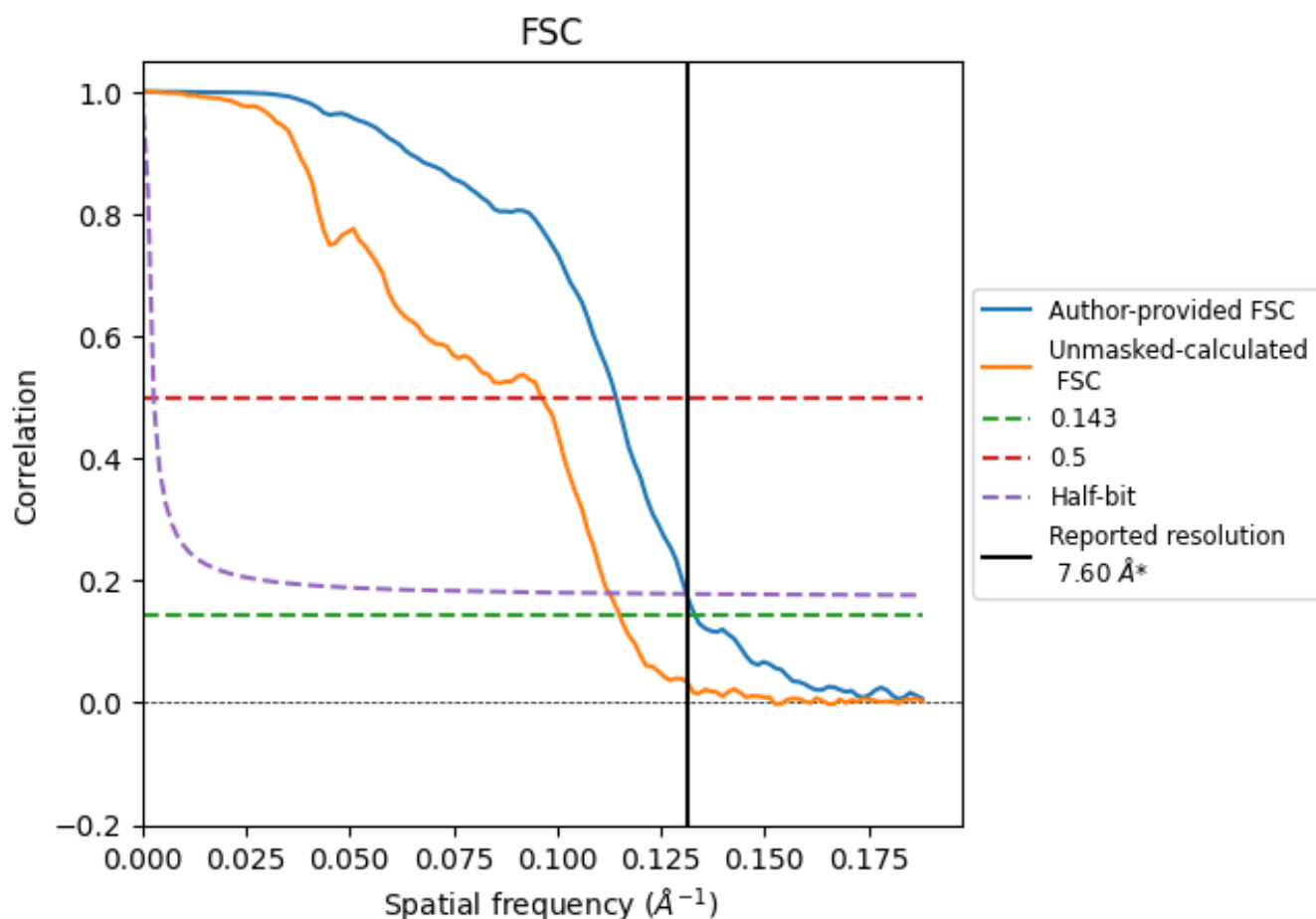


*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.132 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	7.51	8.76	7.62
Unmasked-calculated*	8.69	10.40	8.88

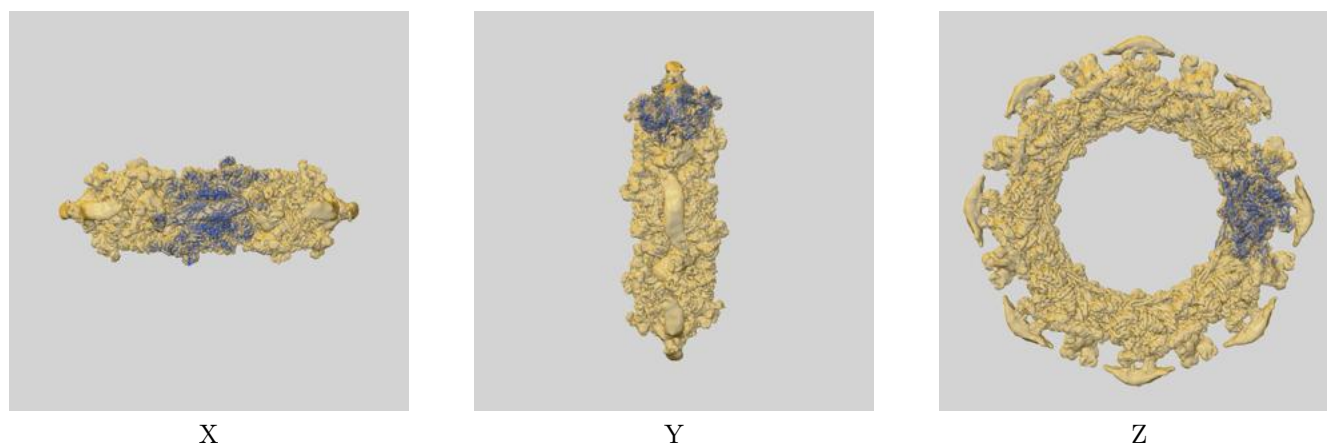
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.69 differs from the reported value 7.6 by more than 10 %

9 Map-model fit [i](#)

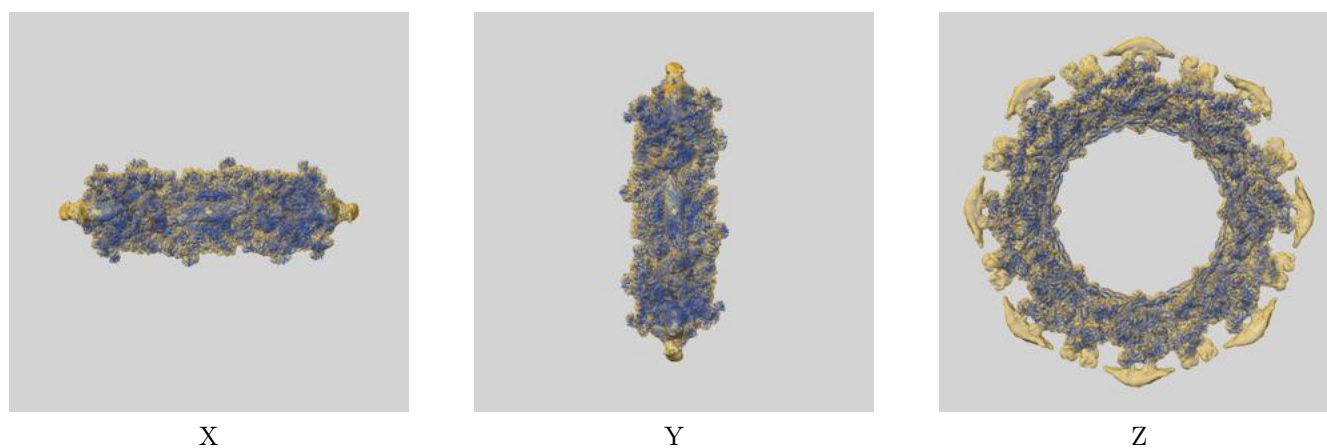
This section contains information regarding the fit between EMDB map EMD-24232 and PDB model 7N85. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

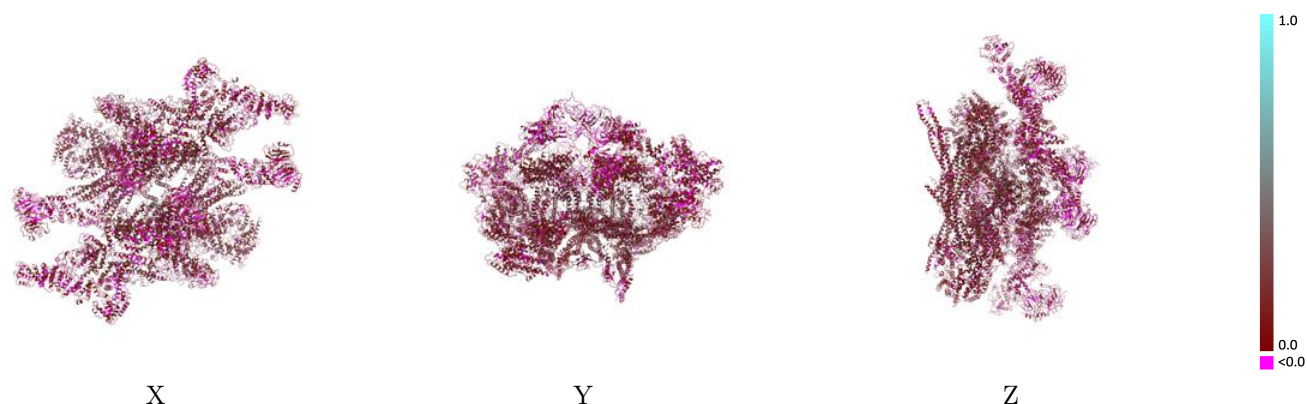


9.1.2 Map-model assembly overlay [i](#)



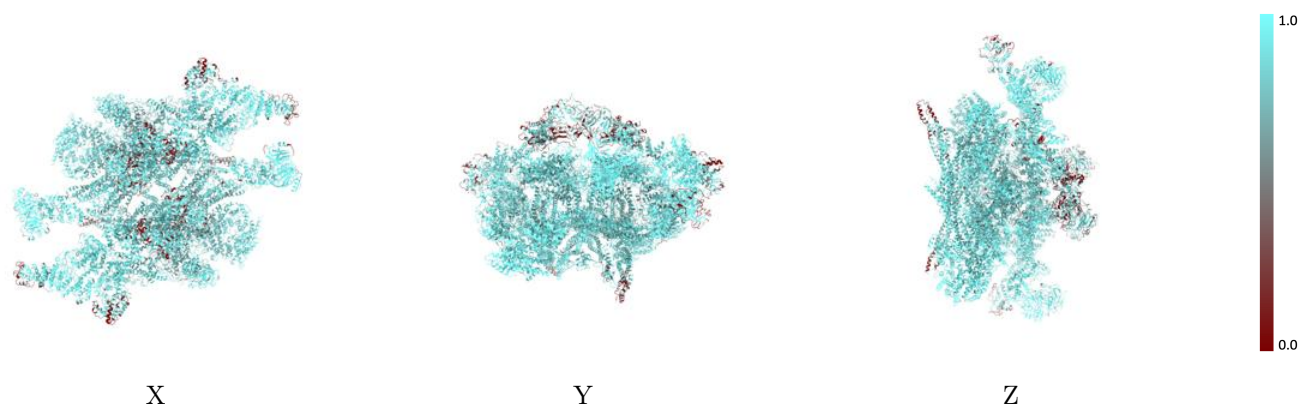
The images above show the 3D surface view of the map at the recommended contour level 0.595 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



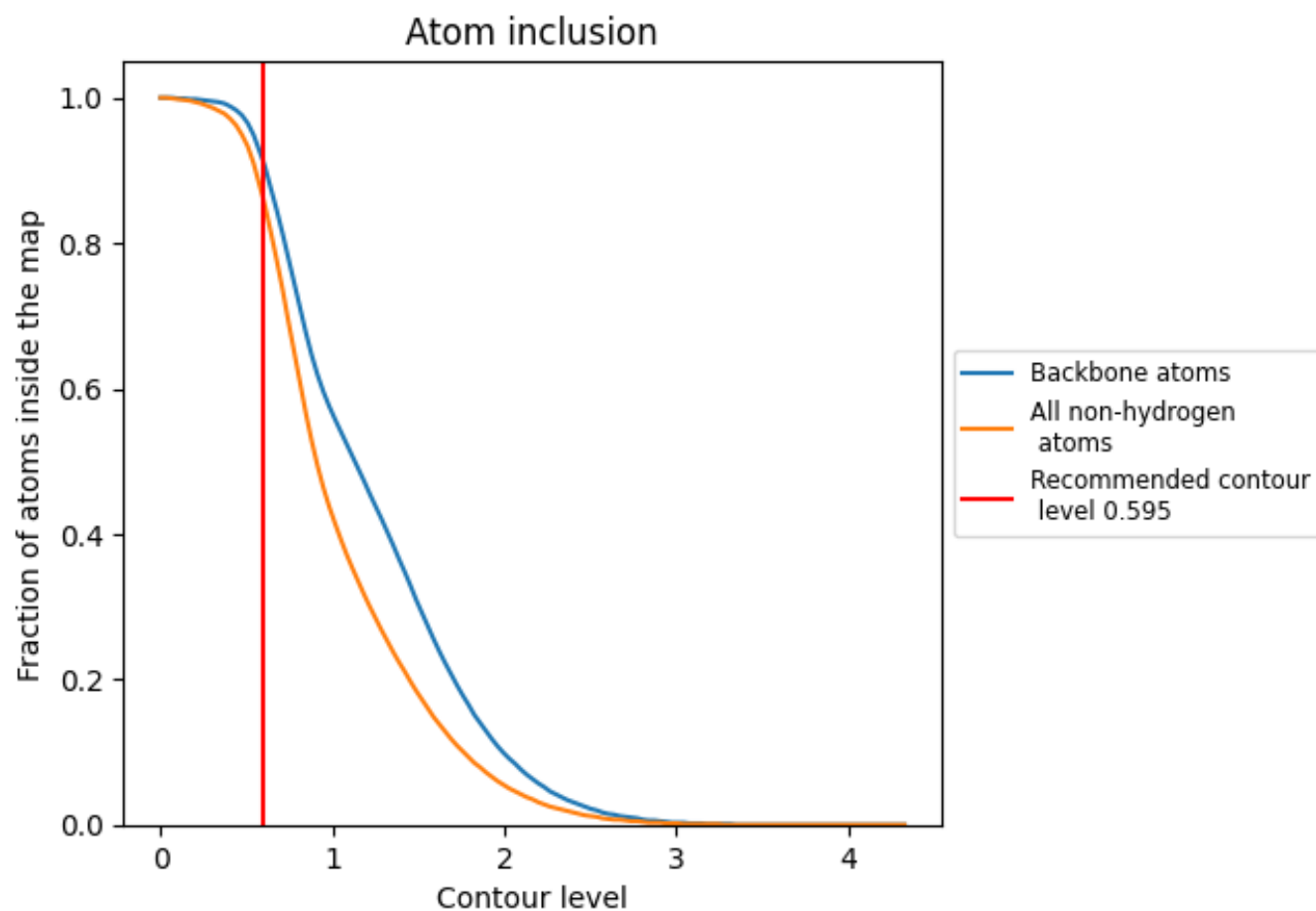
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.595).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.595) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.1130
0	 0.9440	 0.0850
1	 0.6350	 0.0560
5	 0.9560	 0.2120
6	 0.9720	 0.2110
A	 0.8240	 0.1360
B	 0.7280	 0.1140
C	 0.7580	 0.1240
D	 0.9310	 0.1530
E	 0.9240	 0.1480
F	 0.9120	 0.1380
G	 0.8330	 0.1380
H	 0.7630	 0.1140
I	 0.7570	 0.1250
J	 0.9160	 0.1540
K	 0.9040	 0.1380
L	 0.8930	 0.1440
M	 0.9400	 0.1340
N	 0.8840	 0.1320
O	 0.9250	 0.1360
P	 0.8970	 0.1310
Q	 0.8360	 0.1070
R	 0.9210	 0.1400
S	 0.8470	 0.1000
T	 0.9380	 0.1370
U	 0.9810	 0.0880
V	 0.9710	 0.0690
W	 0.9890	 0.0810
X	 0.9940	 0.0810
Y	 0.9260	 0.0850
Z	 0.6360	 0.0610

