Full wwPDB EM Validation Report

May 25, 2024 – 04:05 PM EDT

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

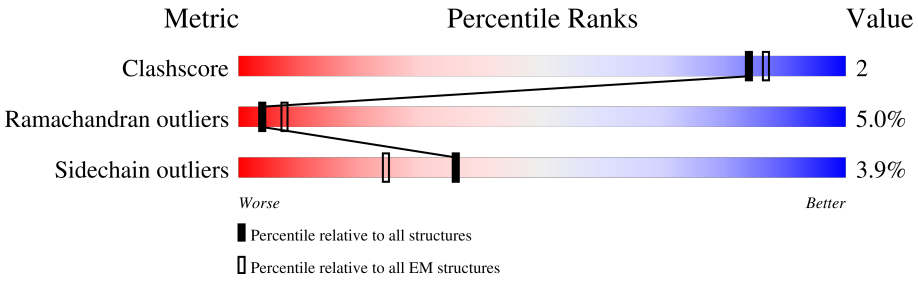
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	1502	65% 7% 27%
1	Y	1502	64% 6% 28%
2	1	1391	25% 71% 7% 20%
2	Z	1391	25% 72% 6% 20%
3	5	36	94% 6%
3	6	36	100%
4	A	823	19% 80%
4	D	823	19% 80%

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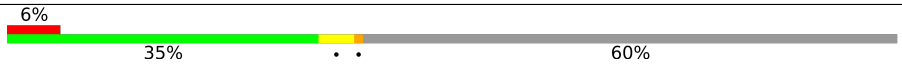
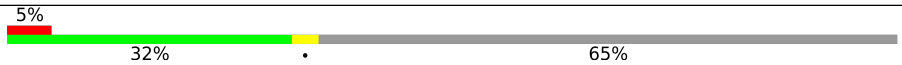
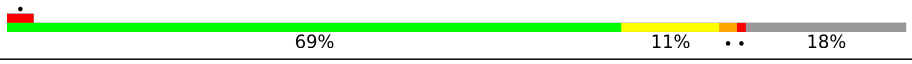
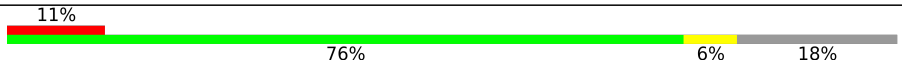
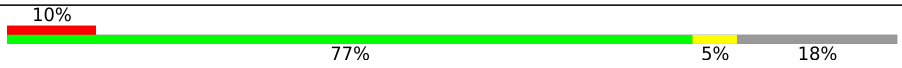
Mol	Chain	Length	Quality of chain
4	G	823	
4	J	823	
5	B	541	
5	E	541	
5	H	541	
5	K	541	
6	C	472	
6	F	472	
6	I	472	
6	L	472	
7	M	1683	
7	O	1683	
8	N	1655	
8	P	1655	
9	Q	839	
9	R	839	
9	S	839	
9	T	839	
10	U	475	
10	W	475	
11	V	528	
11	X	528	

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.

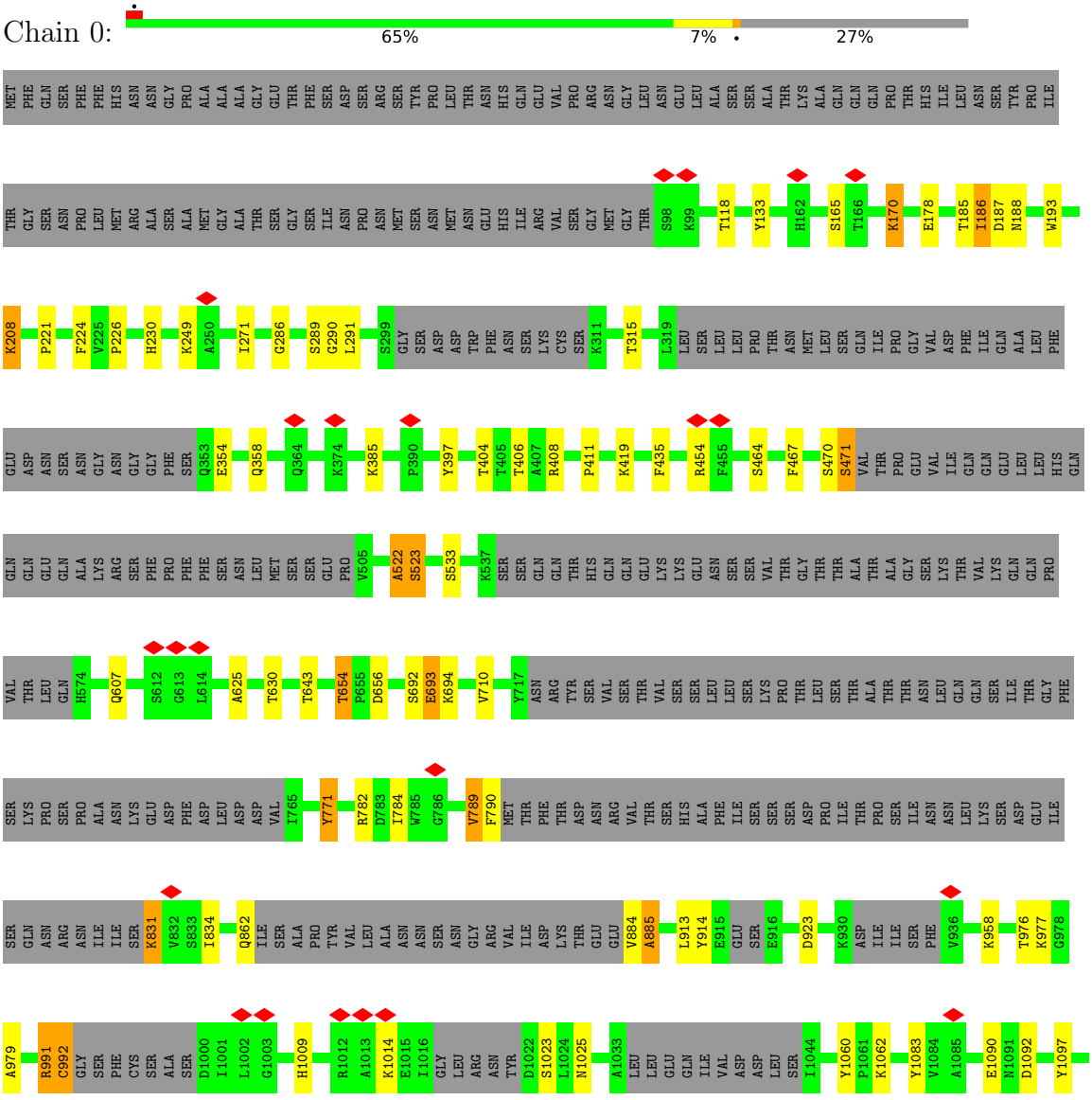
Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	92	Total	C	N	O	S	0	0
			720	465	116	136	3		
11	X	93	Total	C	N	O	S	0	0
			731	471	120	137	3		

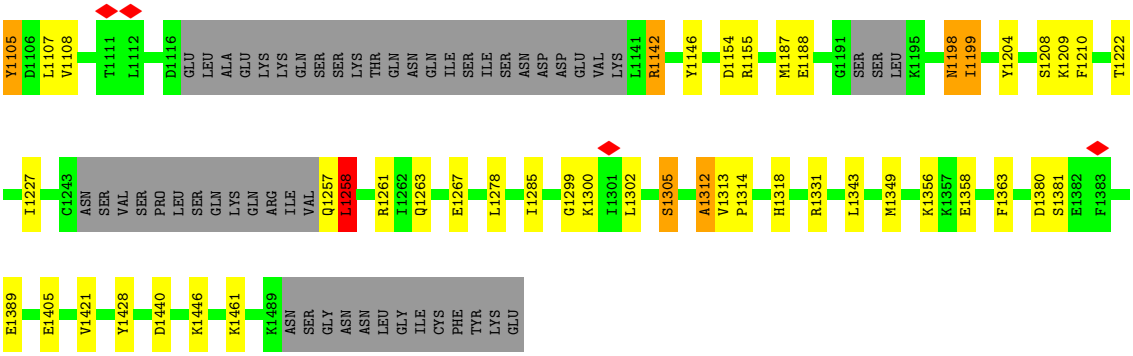
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nucleoporin NUP170

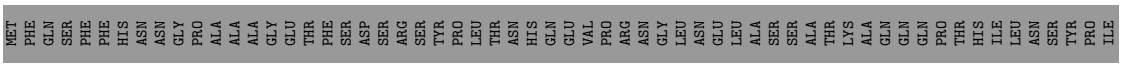
Chain 0:

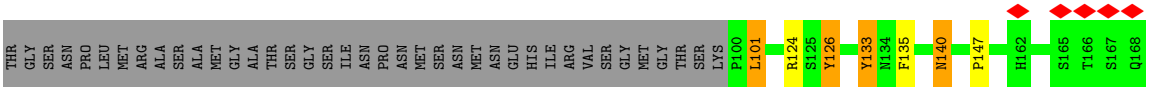


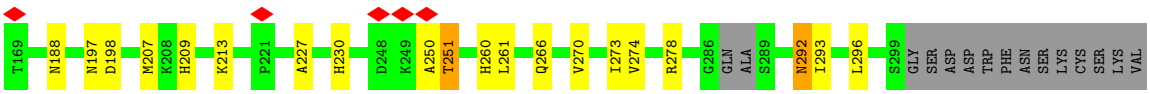


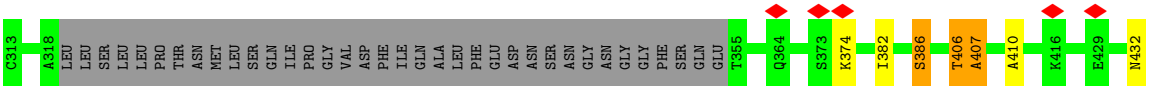
• Molecule 1: Nucleoporin NUP170

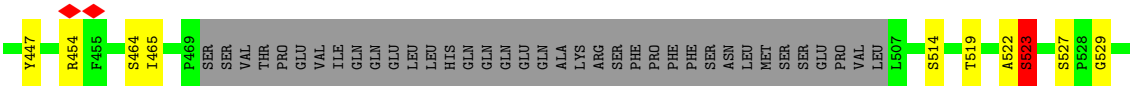
Chain Y:

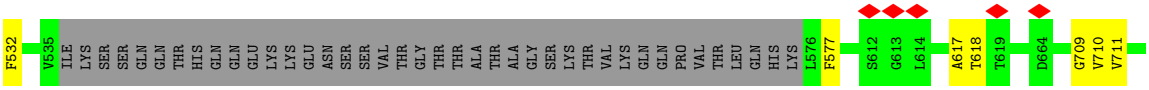


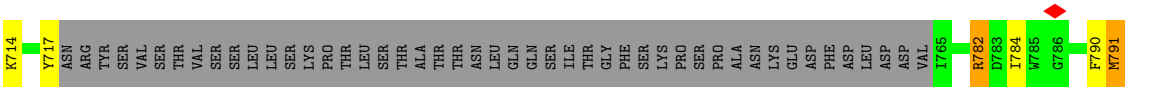


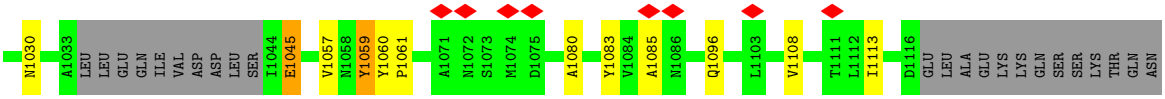


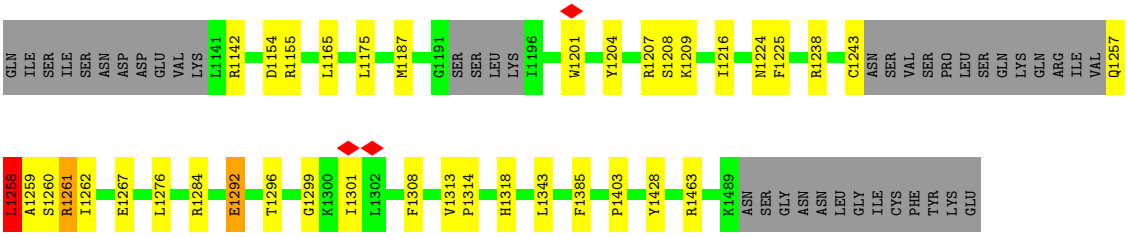






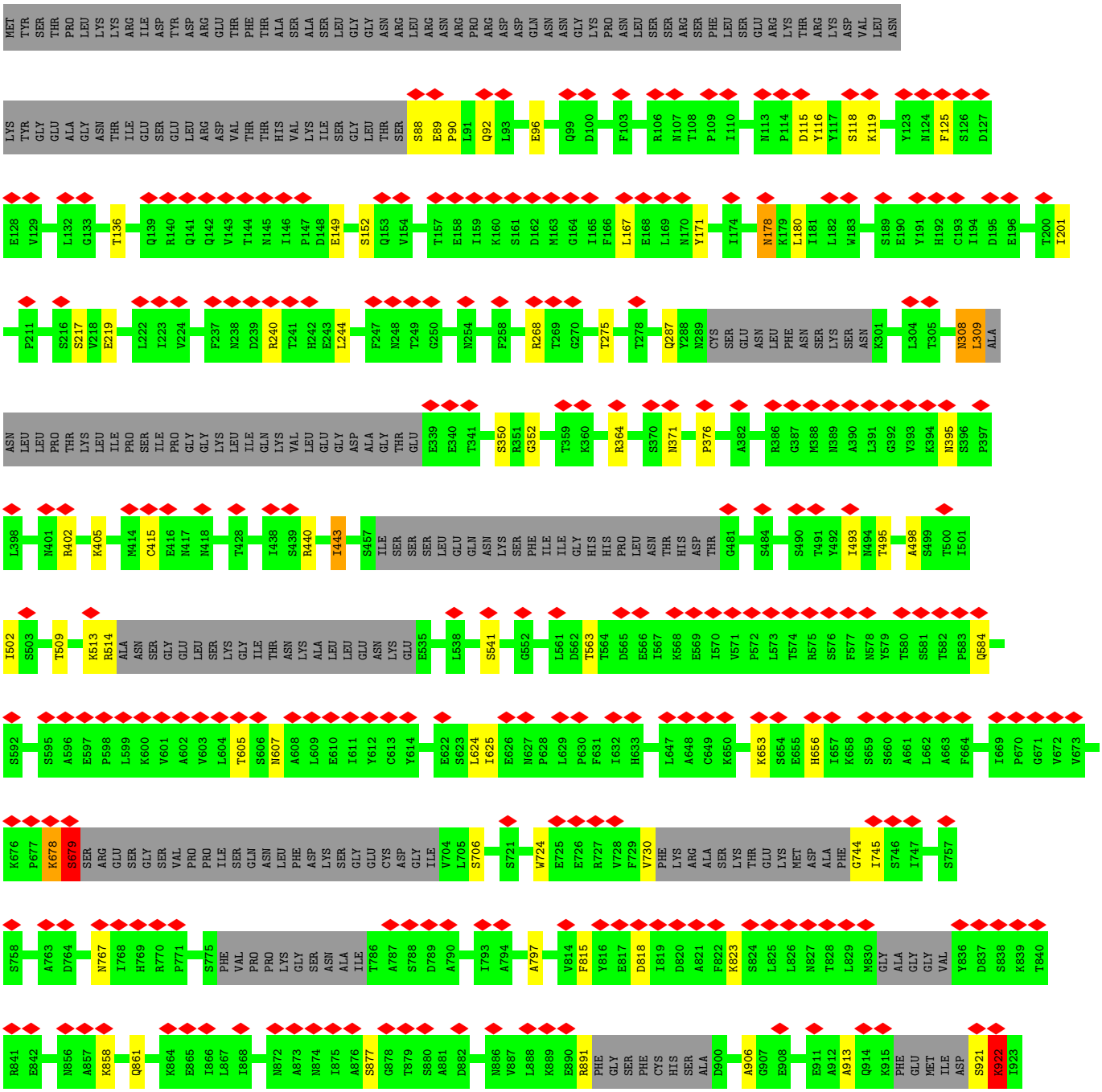


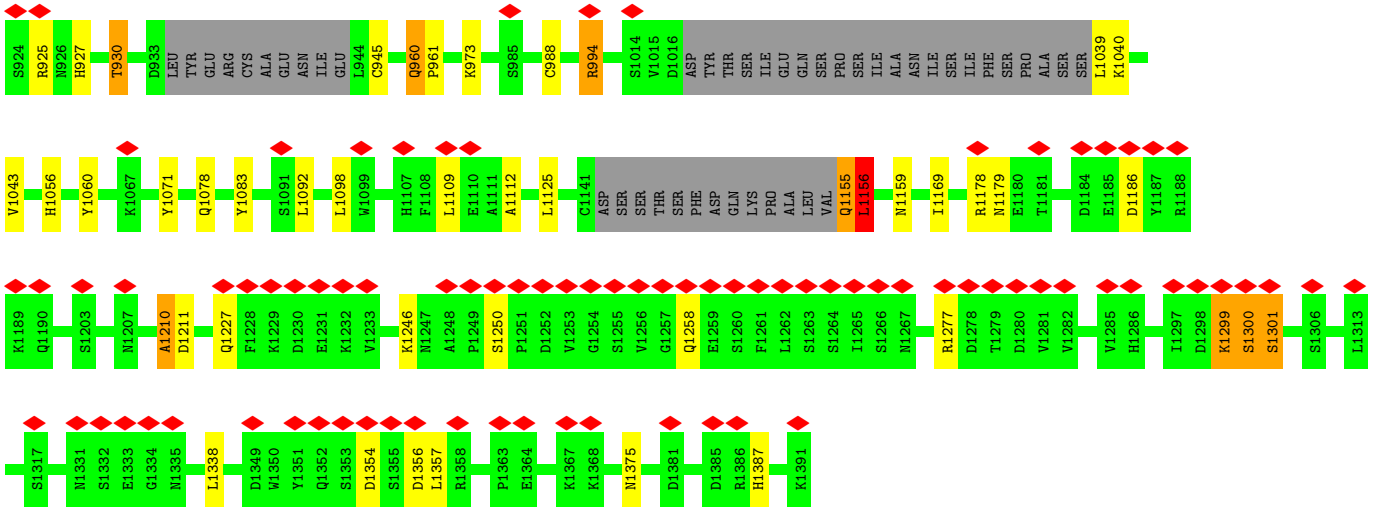




• Molecule 2: Nucleoporin NUP157

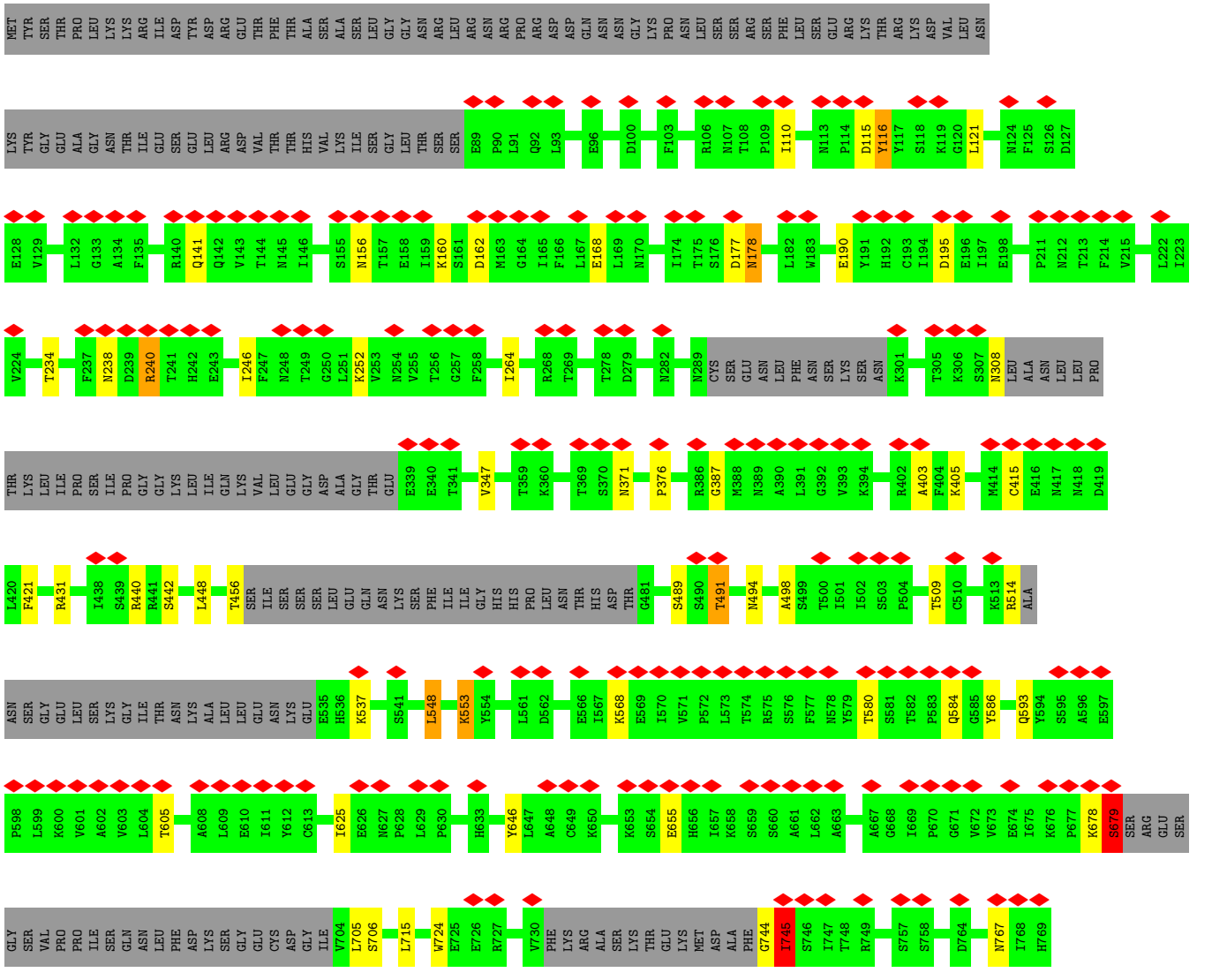
Chain 1:

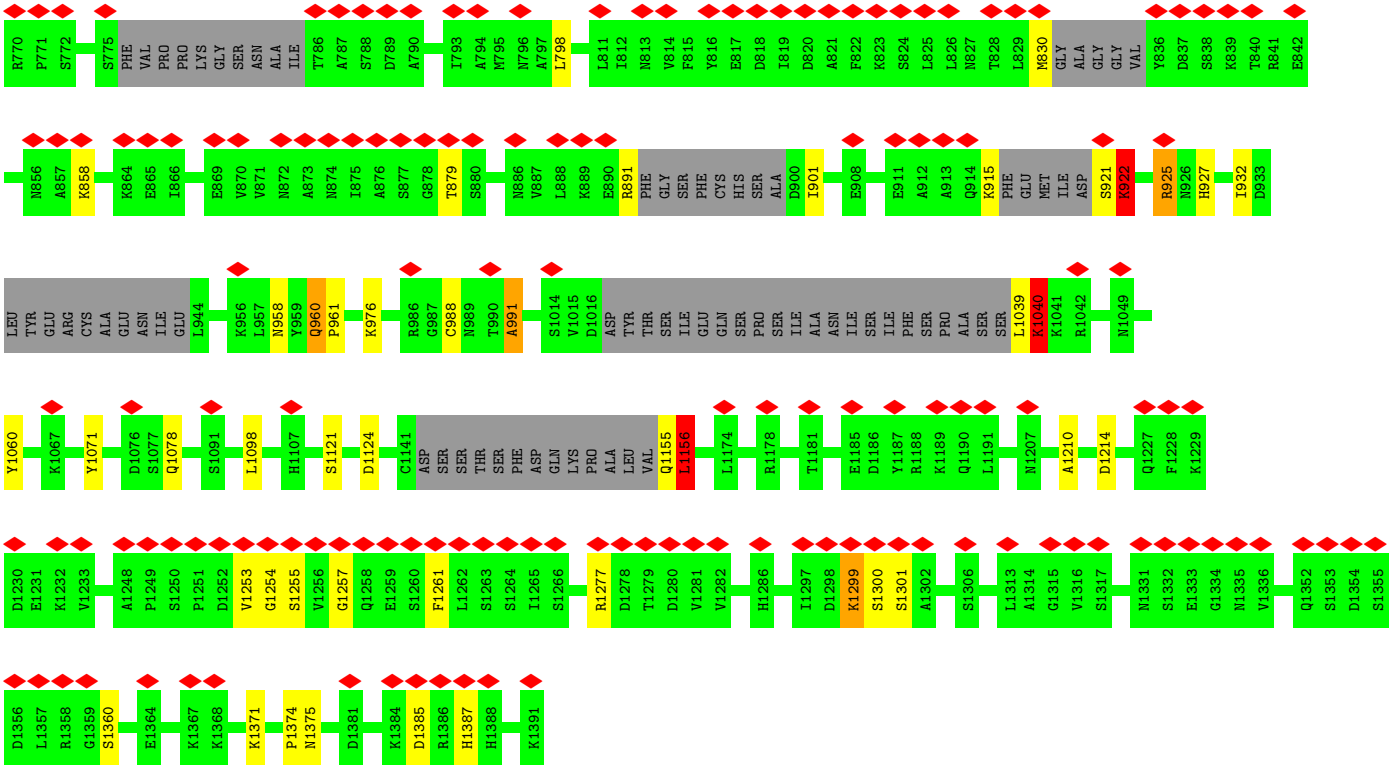




• Molecule 2: Nucleoporin NUP157

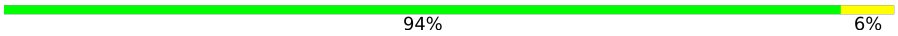
Chain Z:

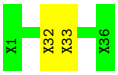




• Molecule 3: Unknown connectors

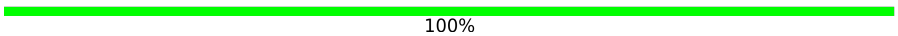
Chain 5:





• Molecule 3: Unknown connectors

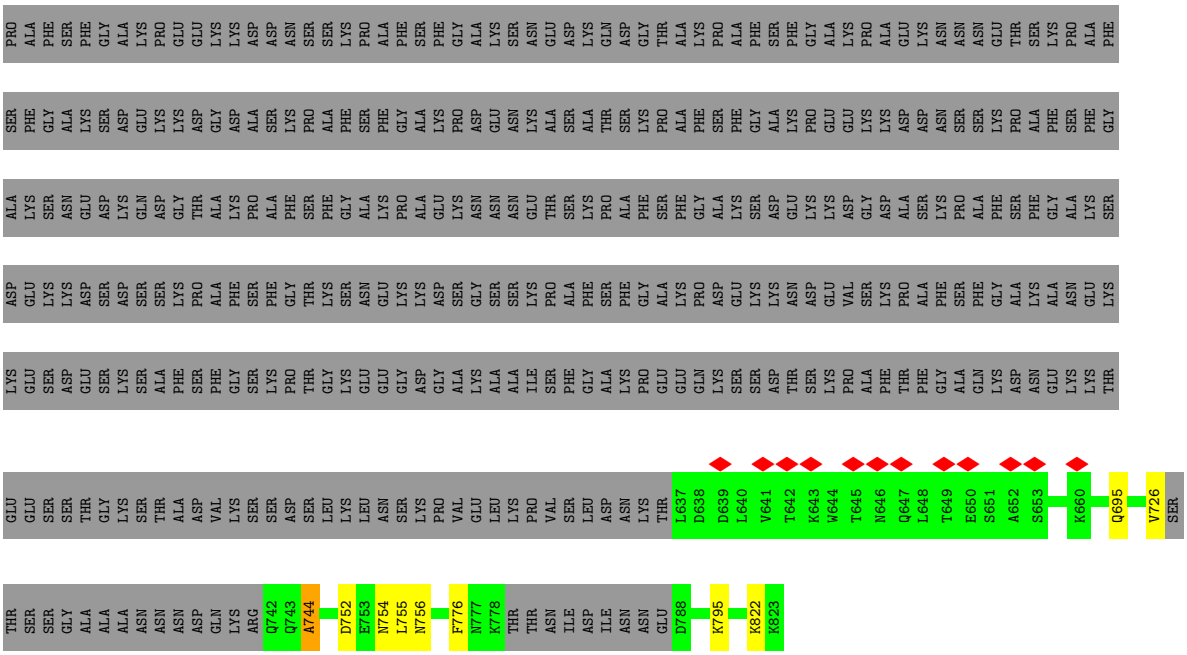
Chain 6:



There are no outlier residues recorded for this chain.

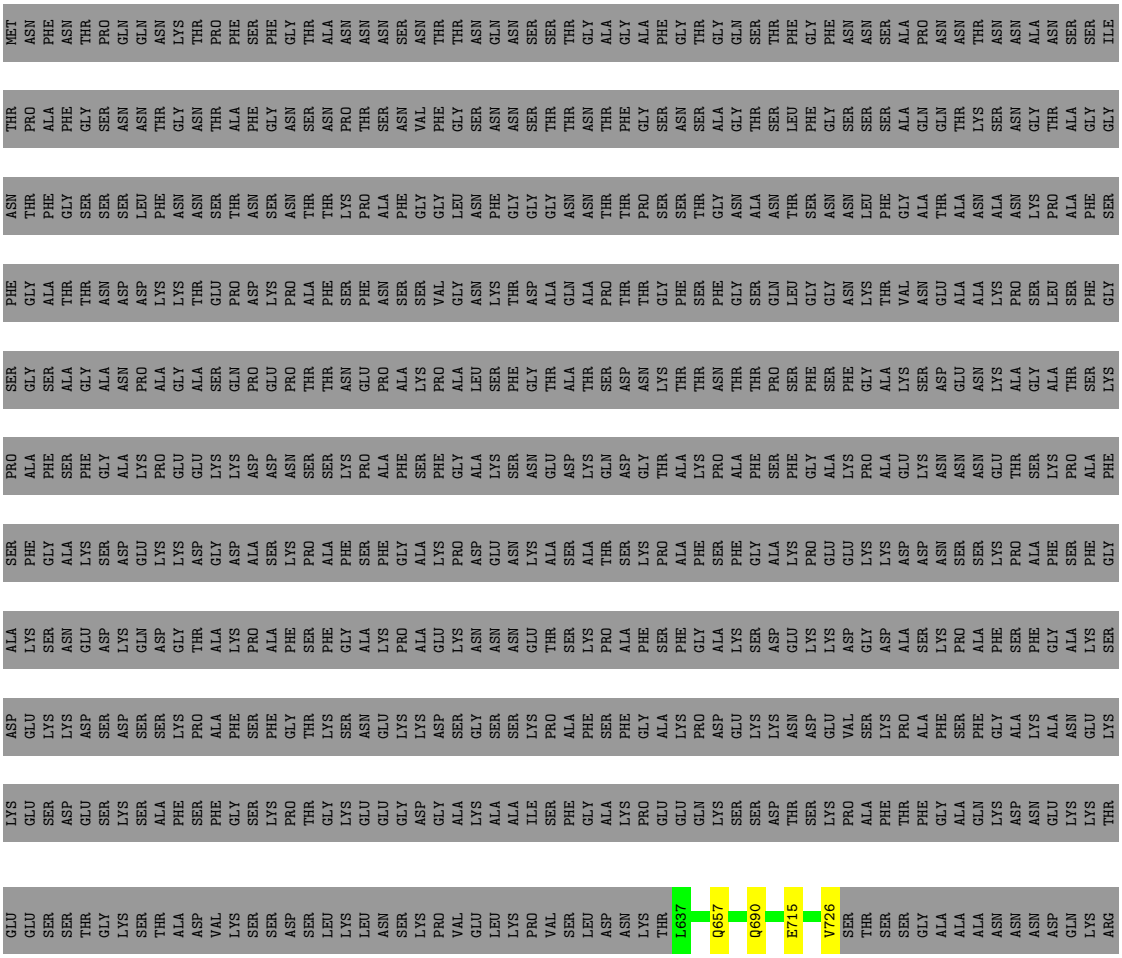
• Molecule 4: Nucleoporin NSP1

Chain A:



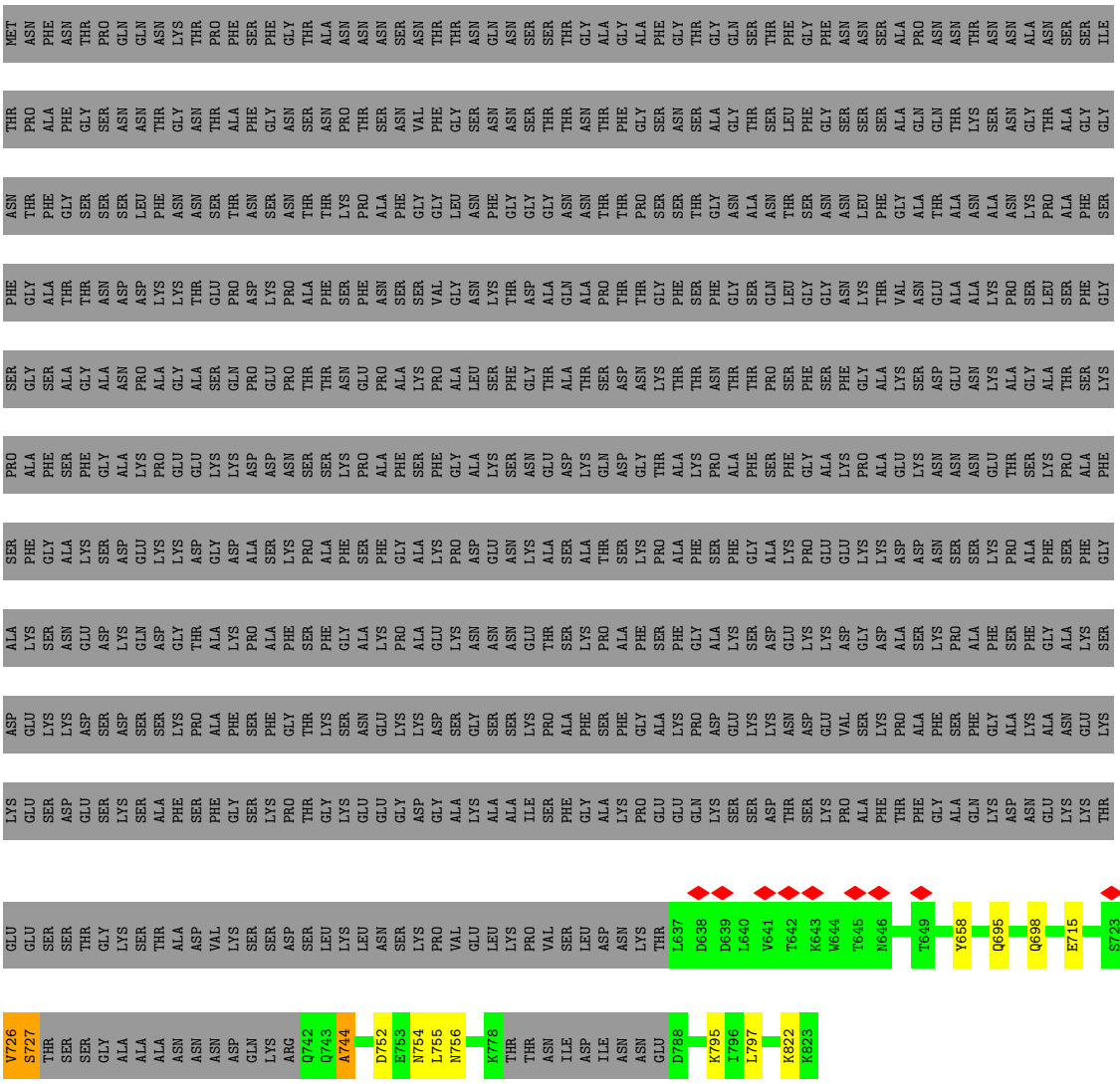
• Molecule 4: Nucleoporin NSP1

Chain D:



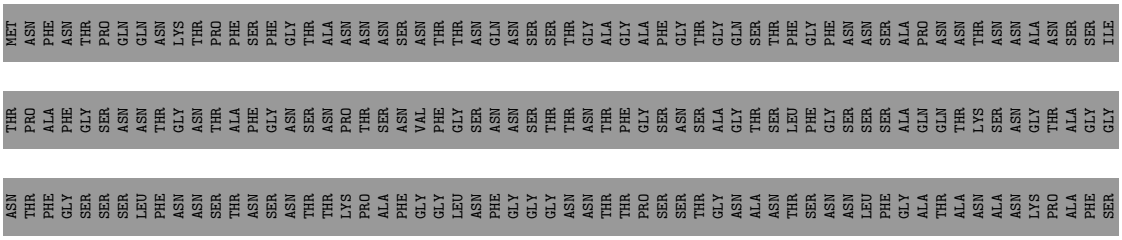
• Molecule 4: Nucleoporin NSP1

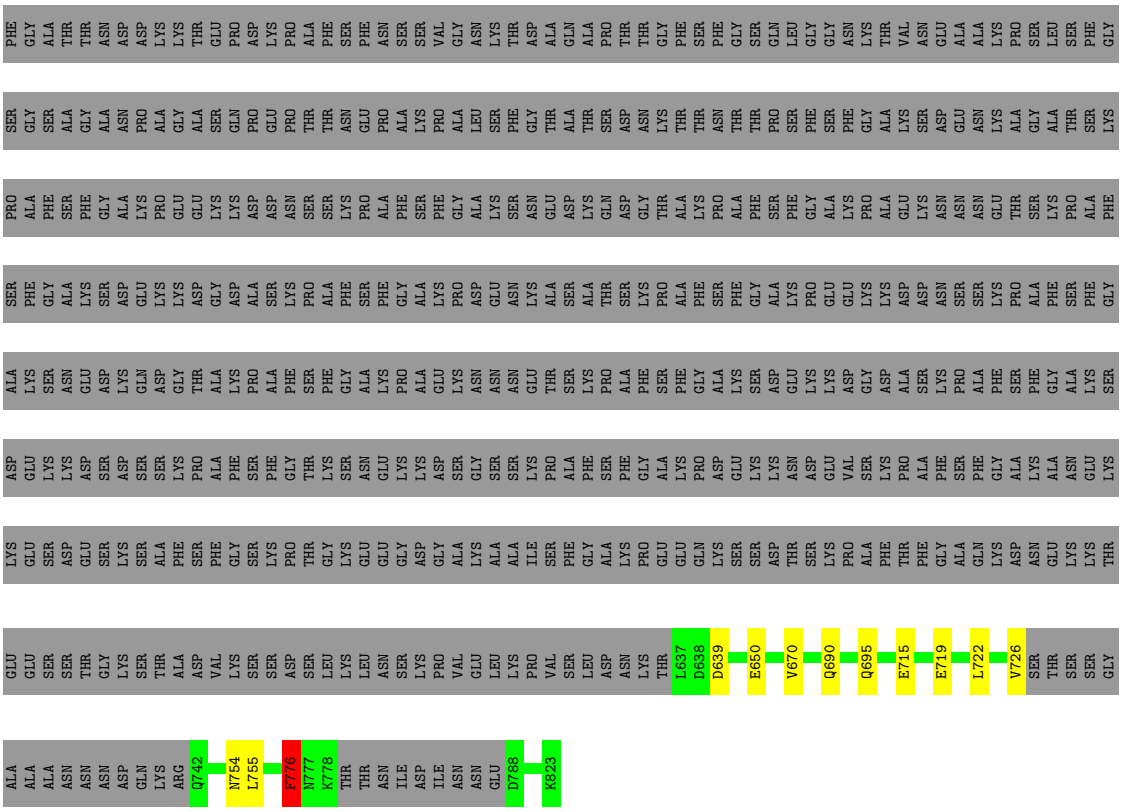
Chain G:



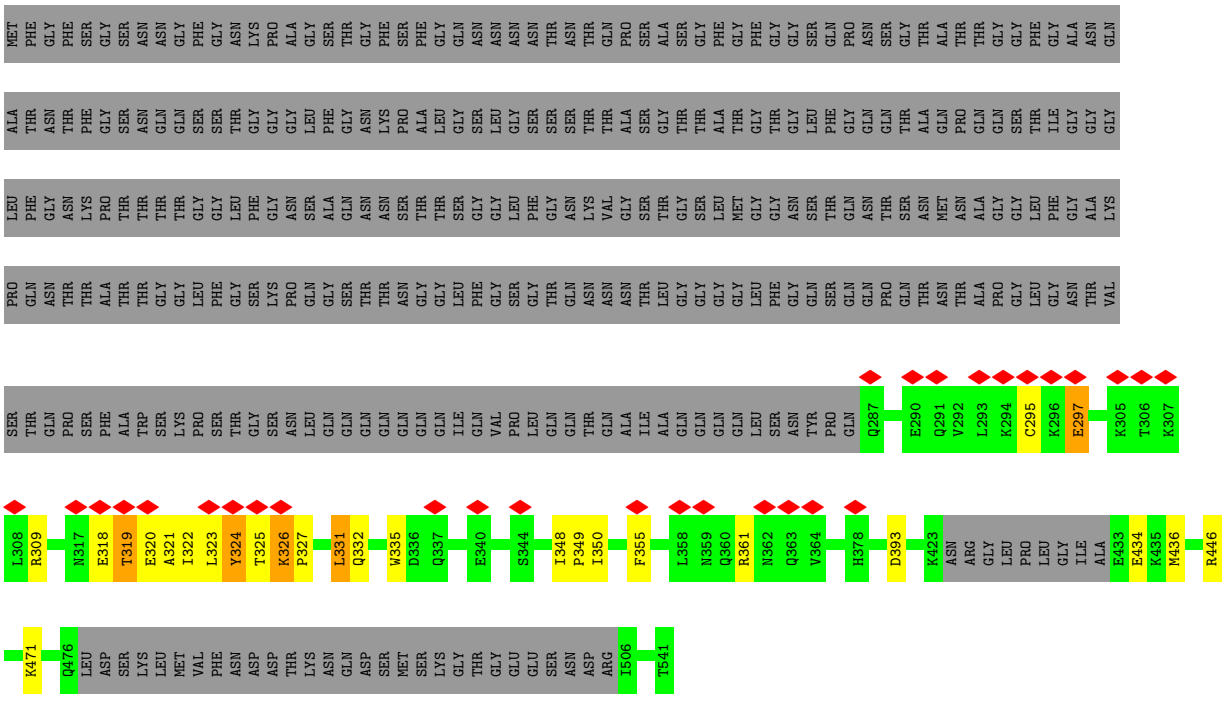
• Molecule 4: Nucleoporin NSP1

Chain J:



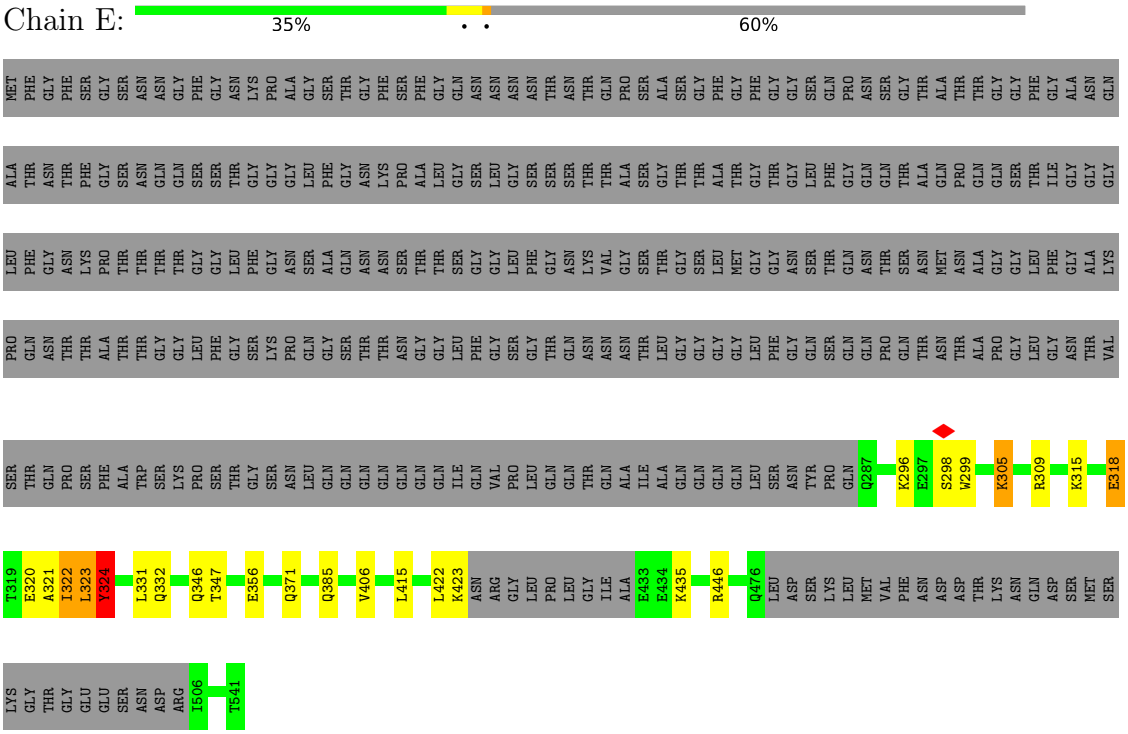


• Molecule 5: Nucleoporin NUP57



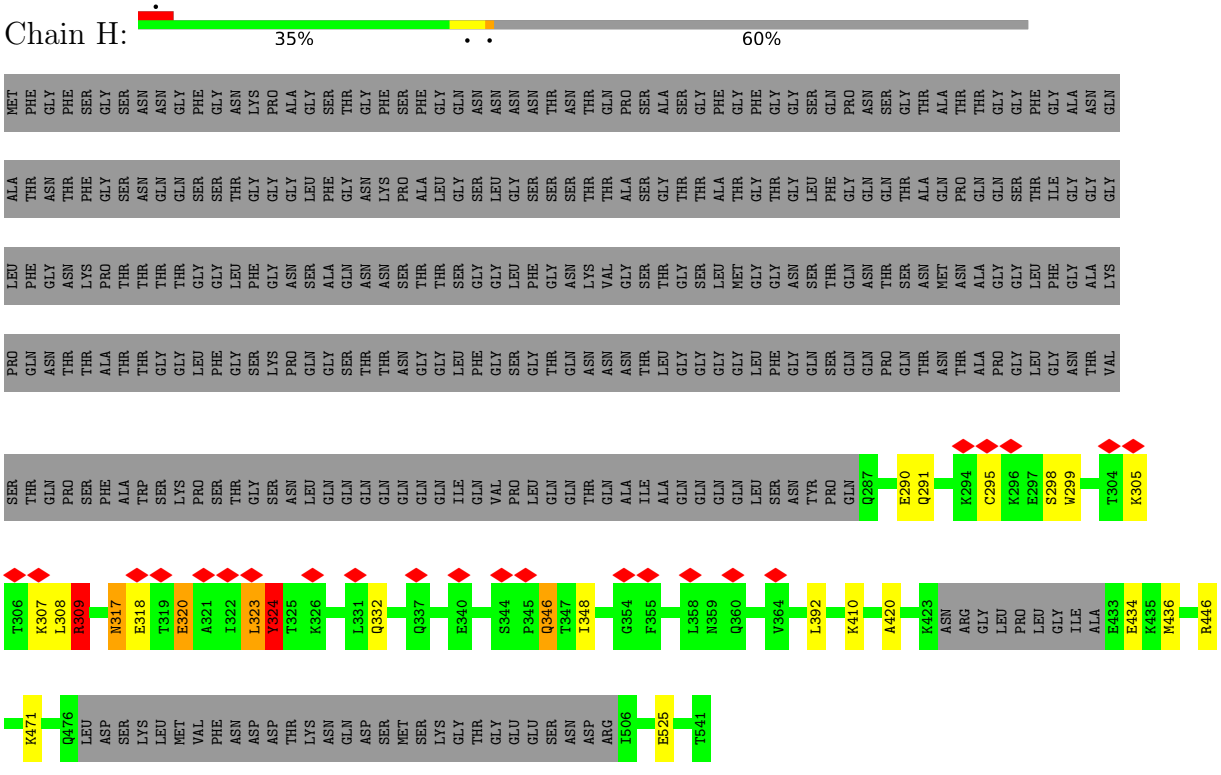
• Molecule 5: Nucleoporin NUP57

Chain E:



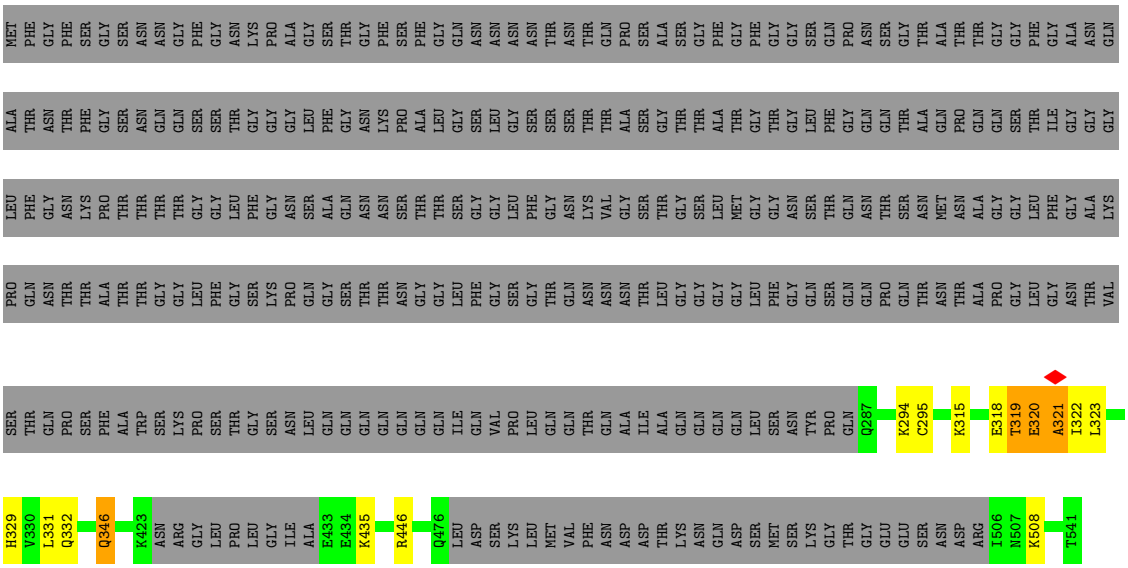
• Molecule 5: Nucleoporin NUP57

Chain H:

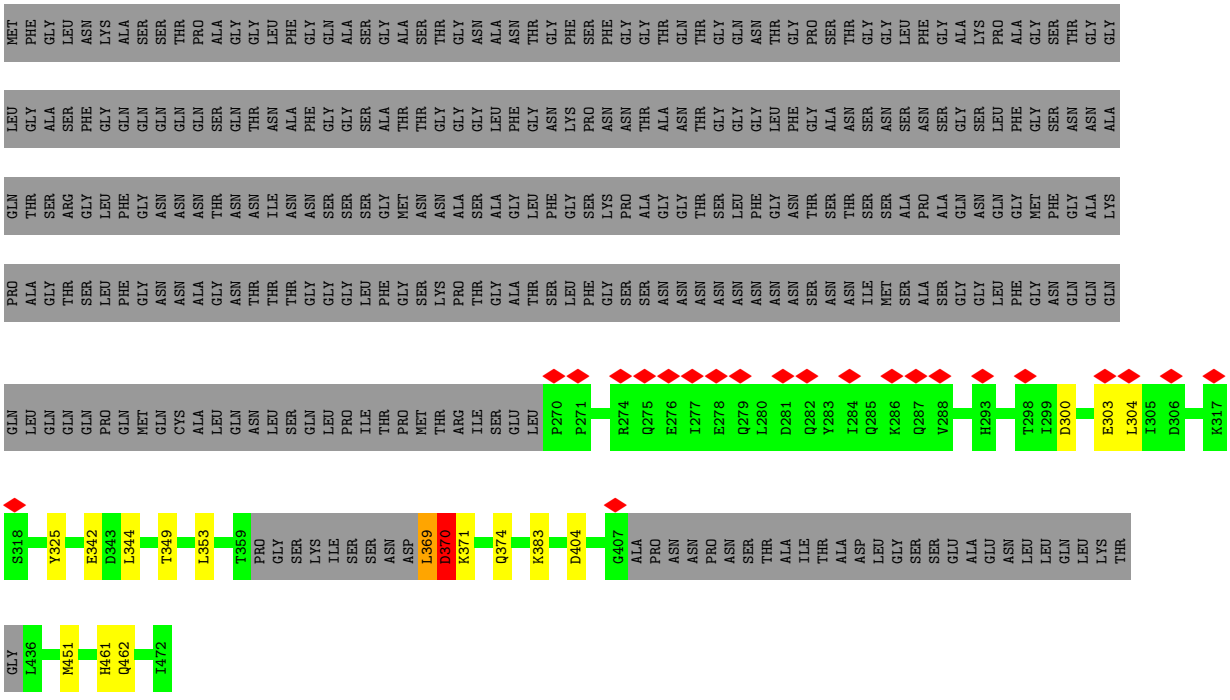


• Molecule 5: Nucleoporin NUP57

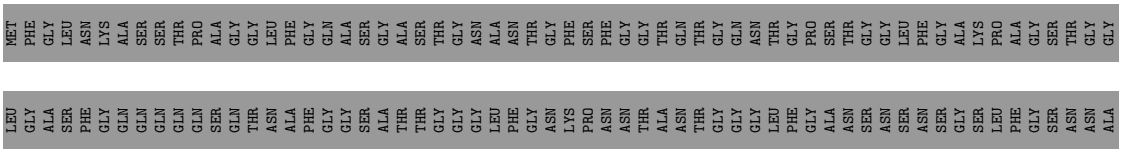
Chain K:

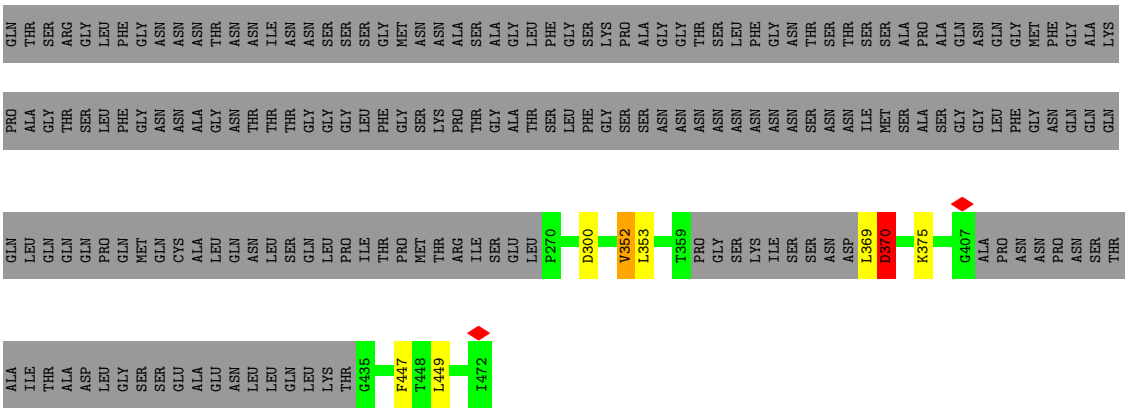


• Molecule 6: Nucleoporin NUP49/NSP49



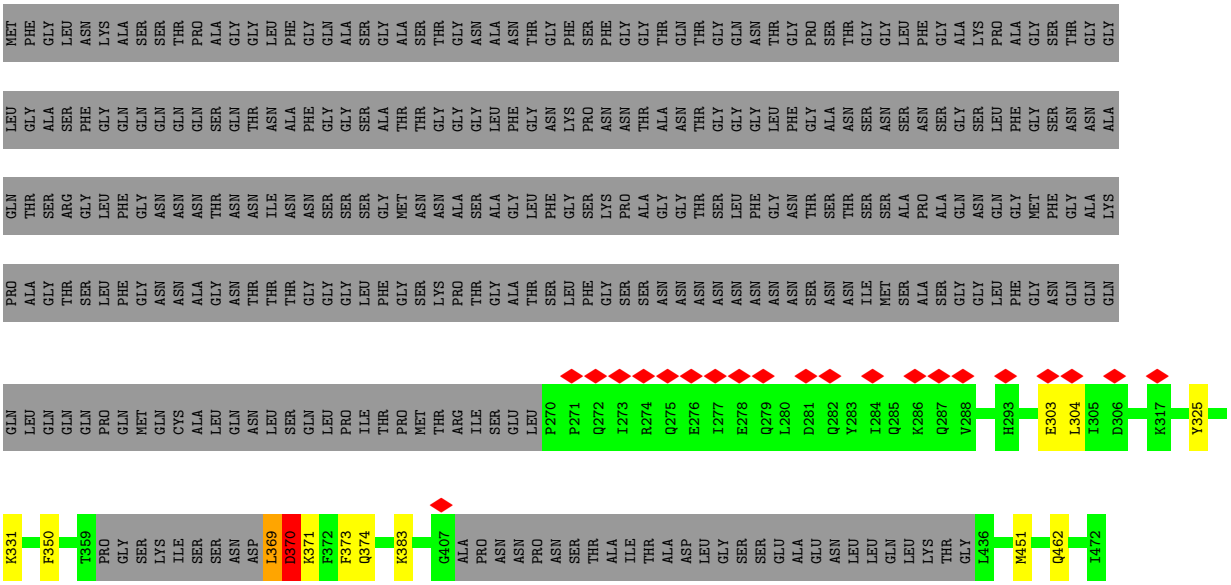
• Molecule 6: Nucleoporin NUP49/NSP49





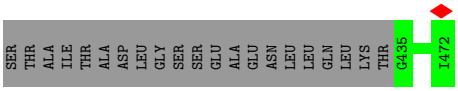
• Molecule 6: Nucleoporin NUP49/NSP49

Chain I:



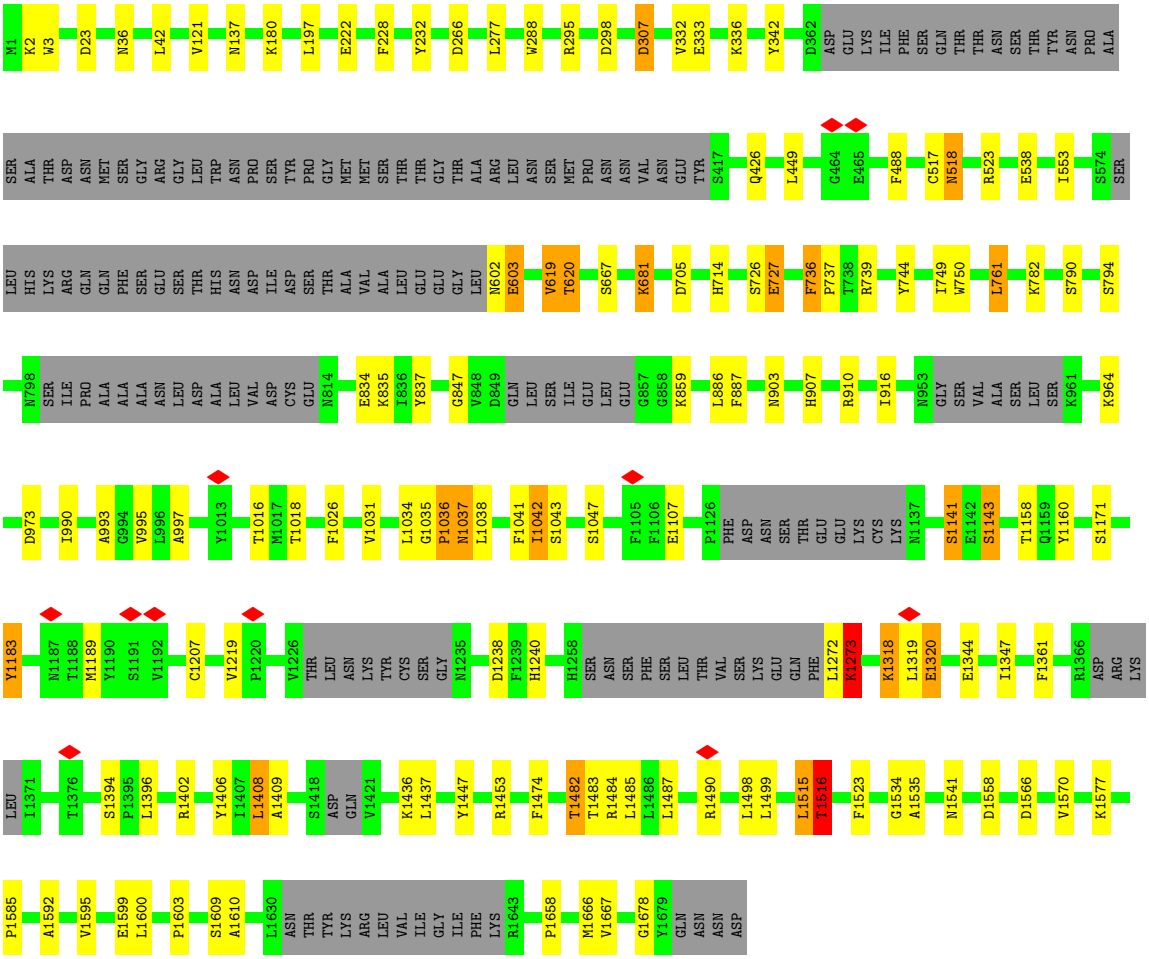
• Molecule 6: Nucleoporin NUP49/NSP49

Chain L:



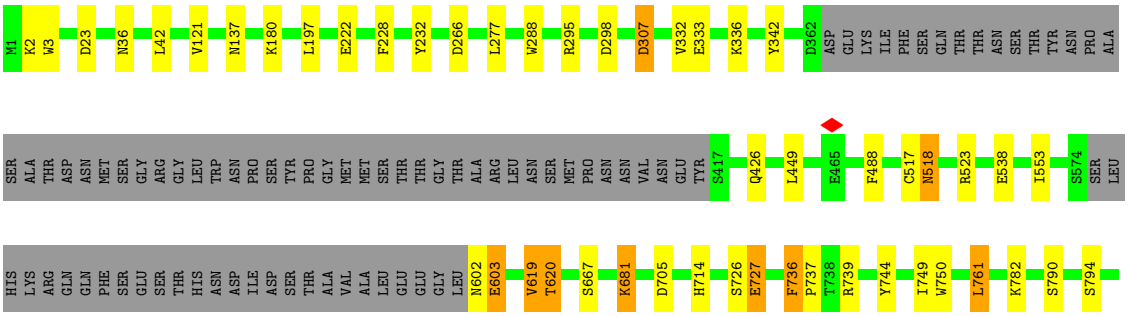
• Molecule 7: Nucleoporin NUP192

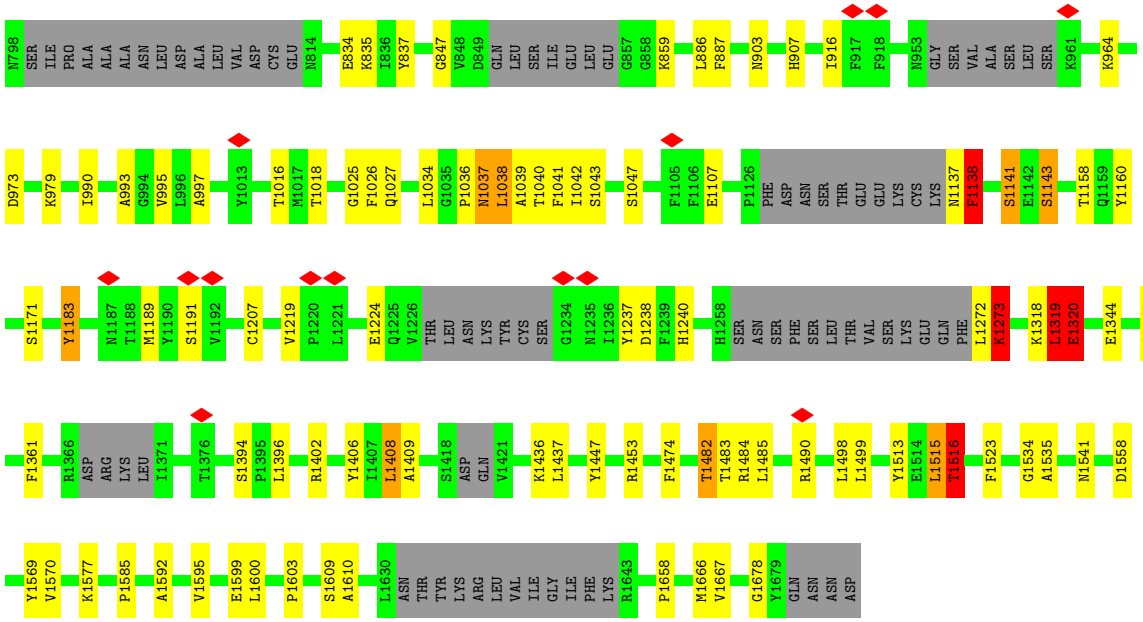
Chain M:



• Molecule 7: Nucleoporin NUP192

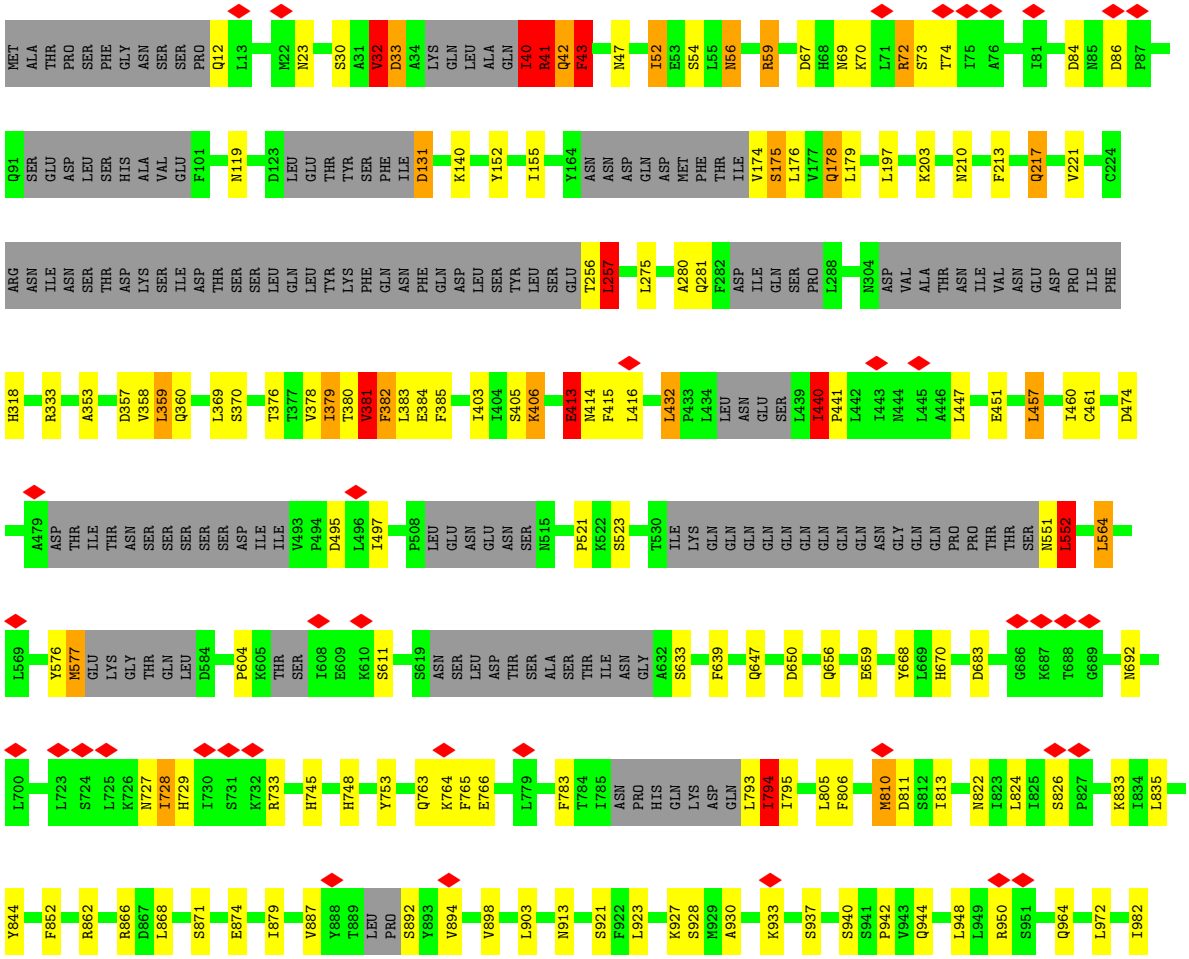
Chain O:

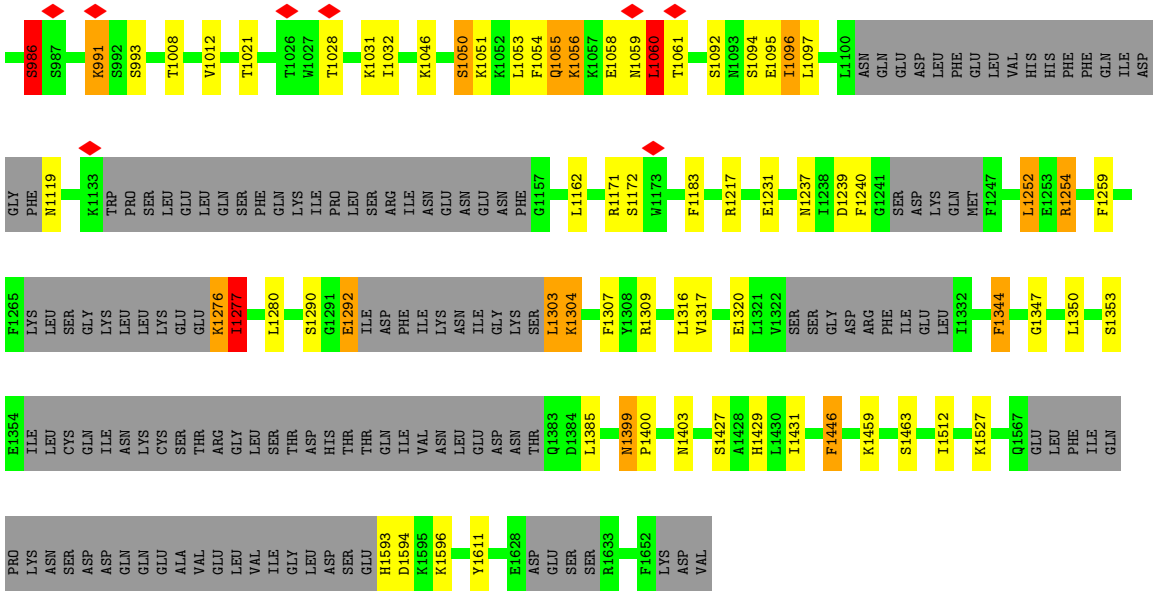




• Molecule 8: Nucleoporin NUP188

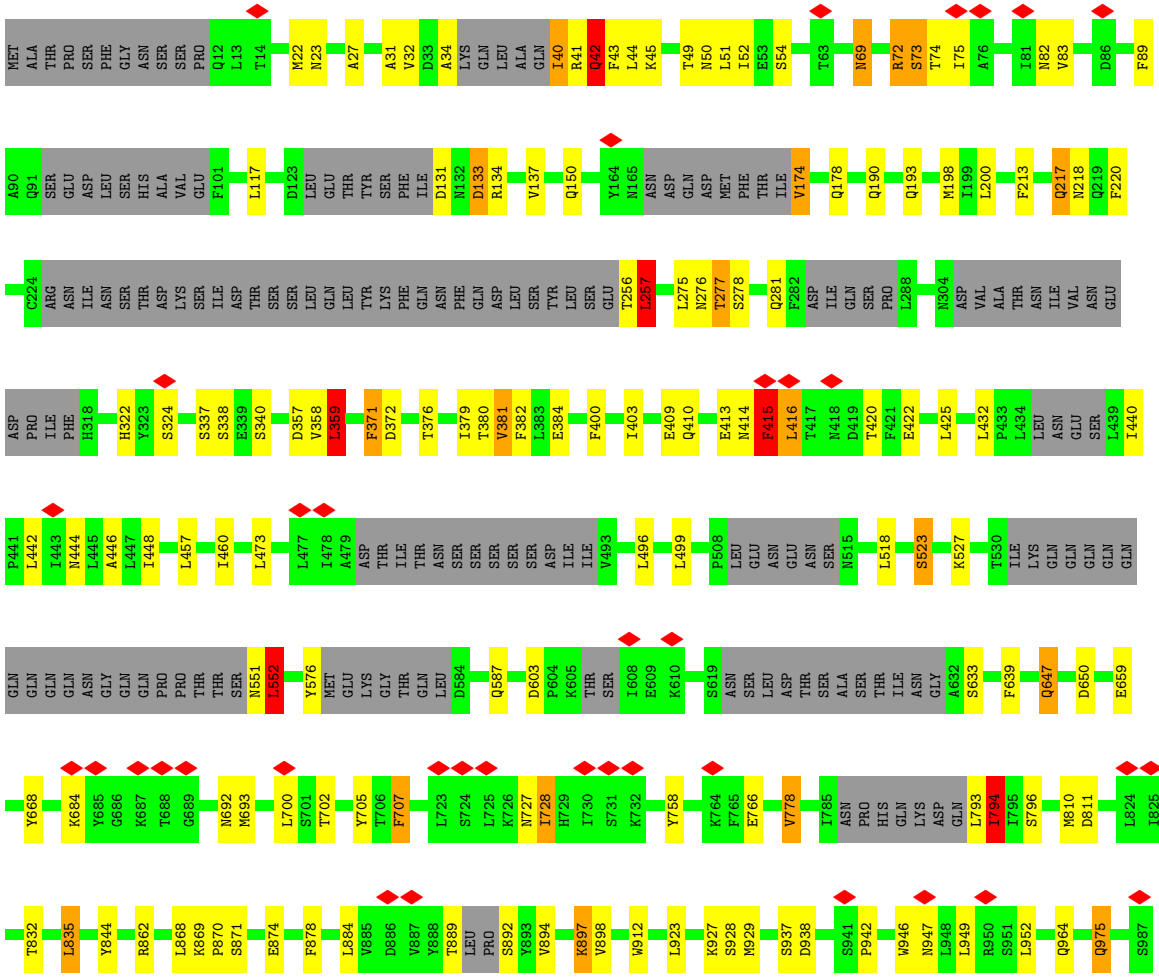
Chain N:

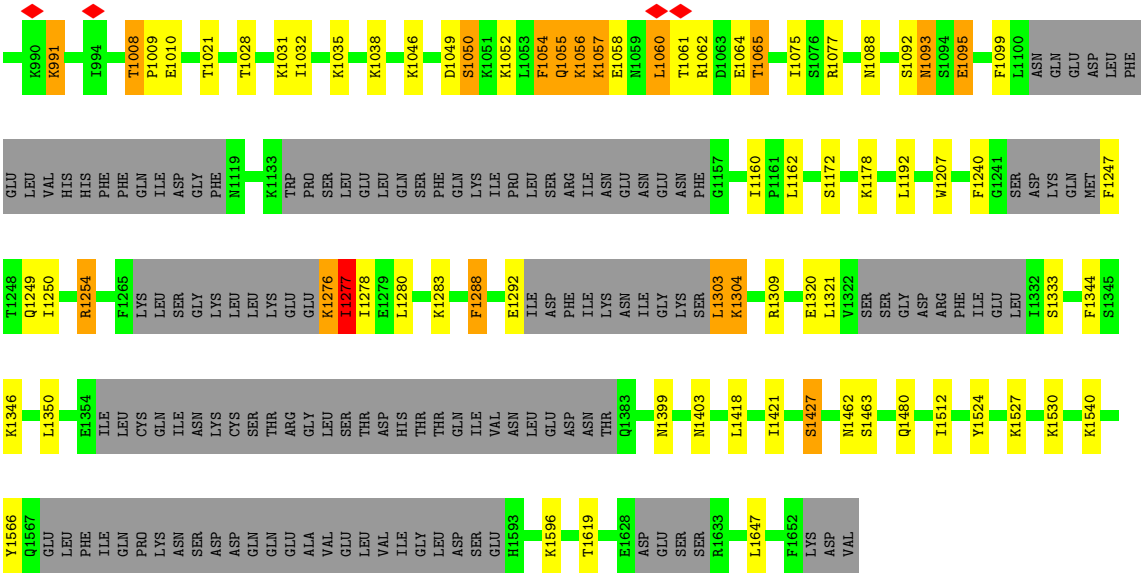




• Molecule 8: Nucleoporin NUP188

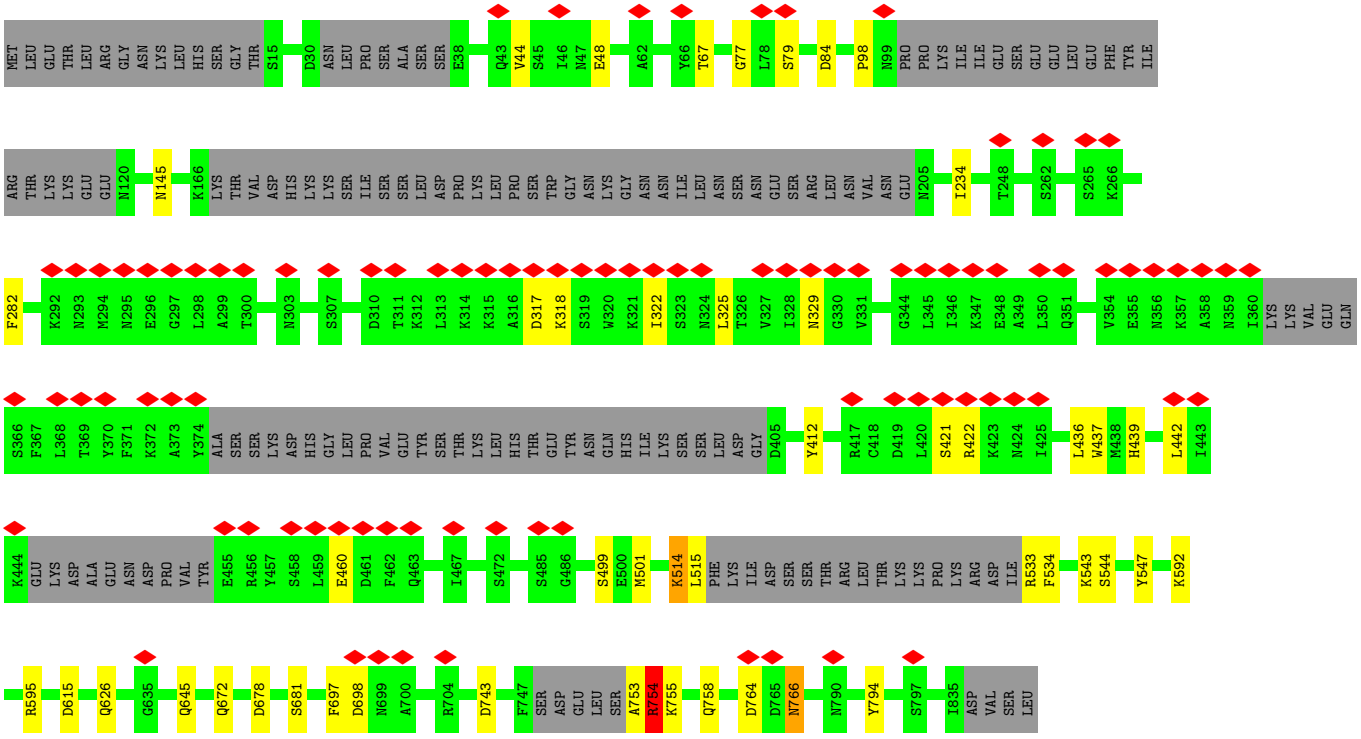
Chain P:





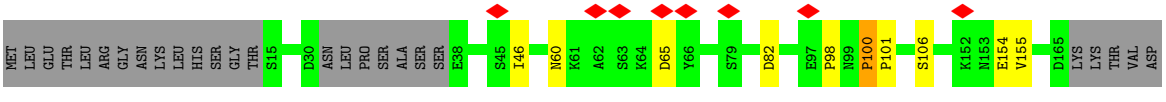
• Molecule 9: Nucleoporin NIC96

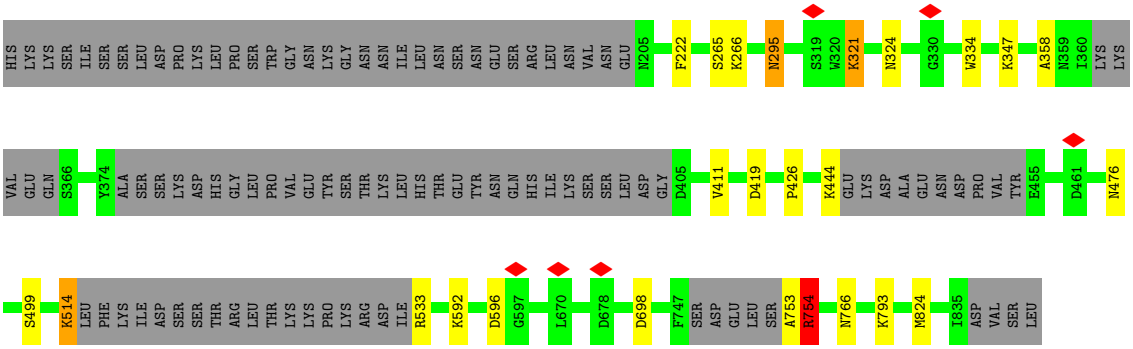
Chain Q:



• Molecule 9: Nucleoporin NIC96

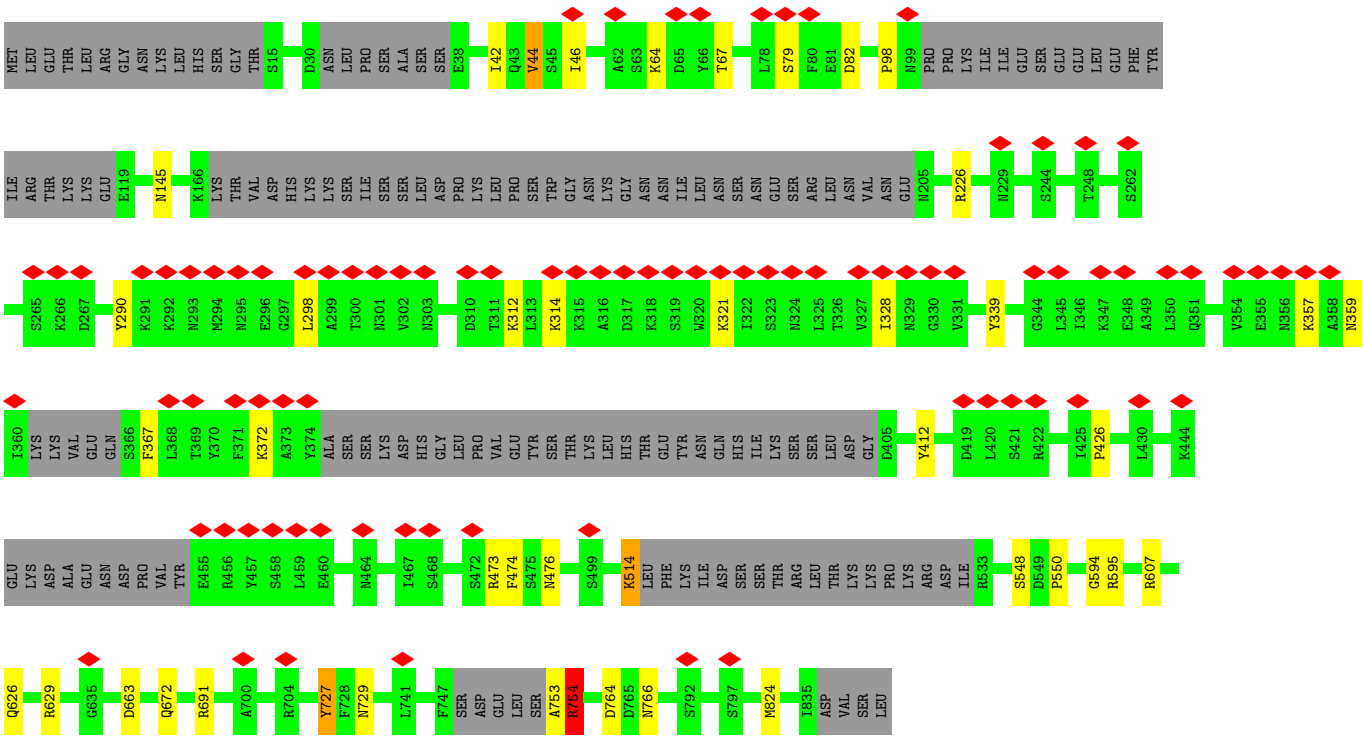
Chain R:





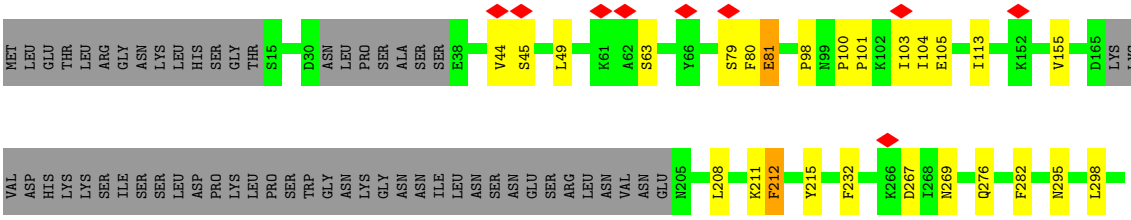
• Molecule 9: Nucleoporin NIC96

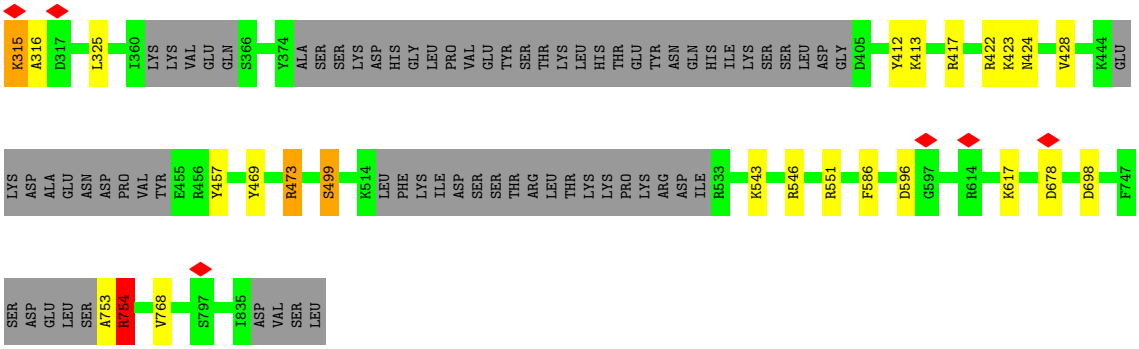
Chain S:



• Molecule 9: Nucleoporin NIC96

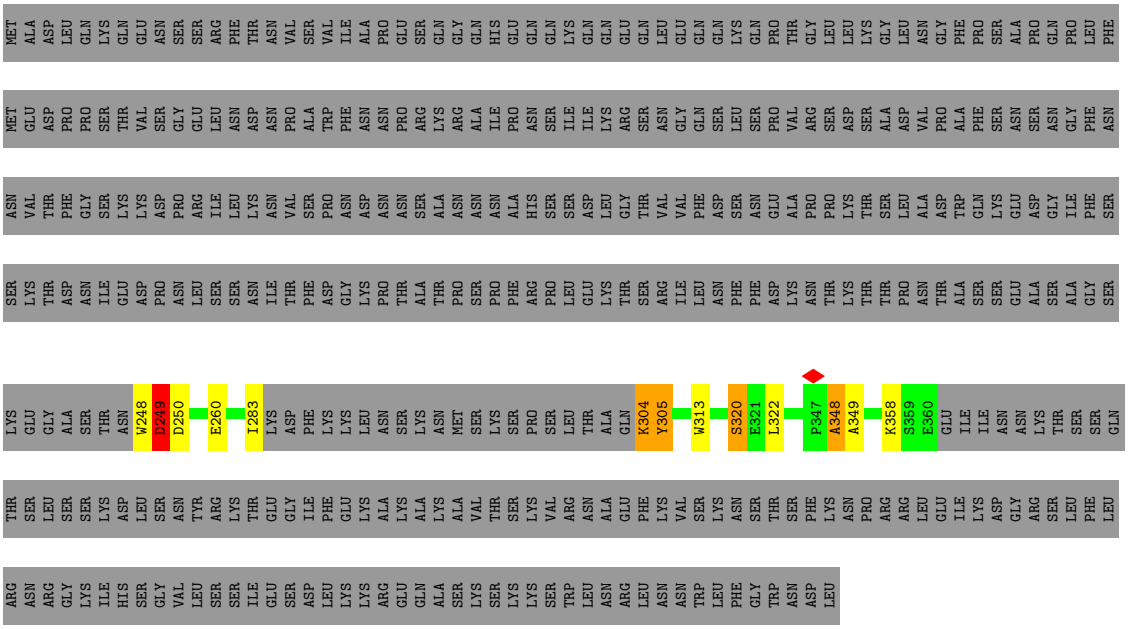
Chain T:





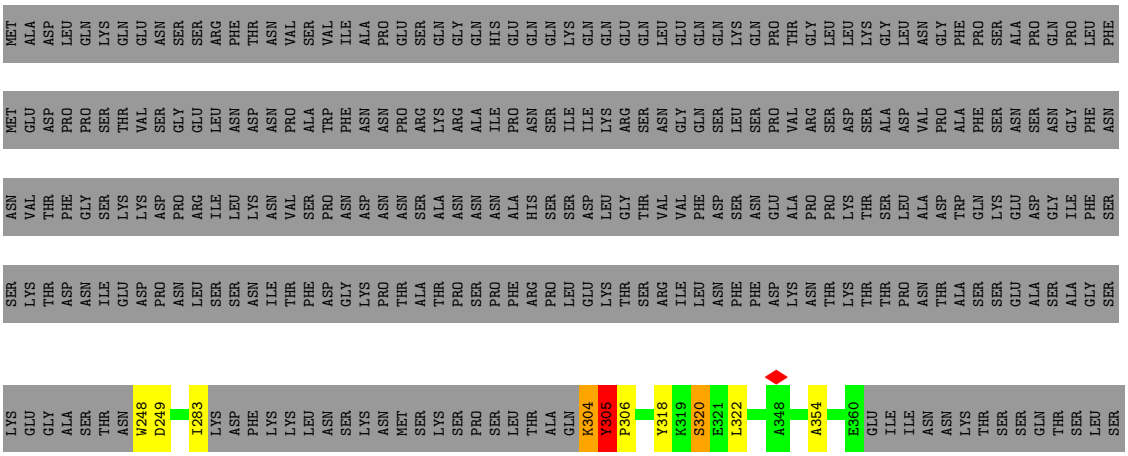
• Molecule 10: Nucleoporin NUP53

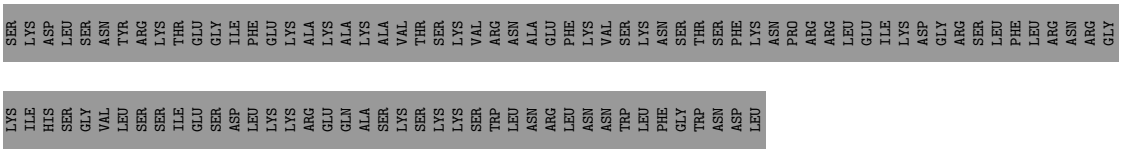
Chain U:



• Molecule 10: Nucleoporin NUP53

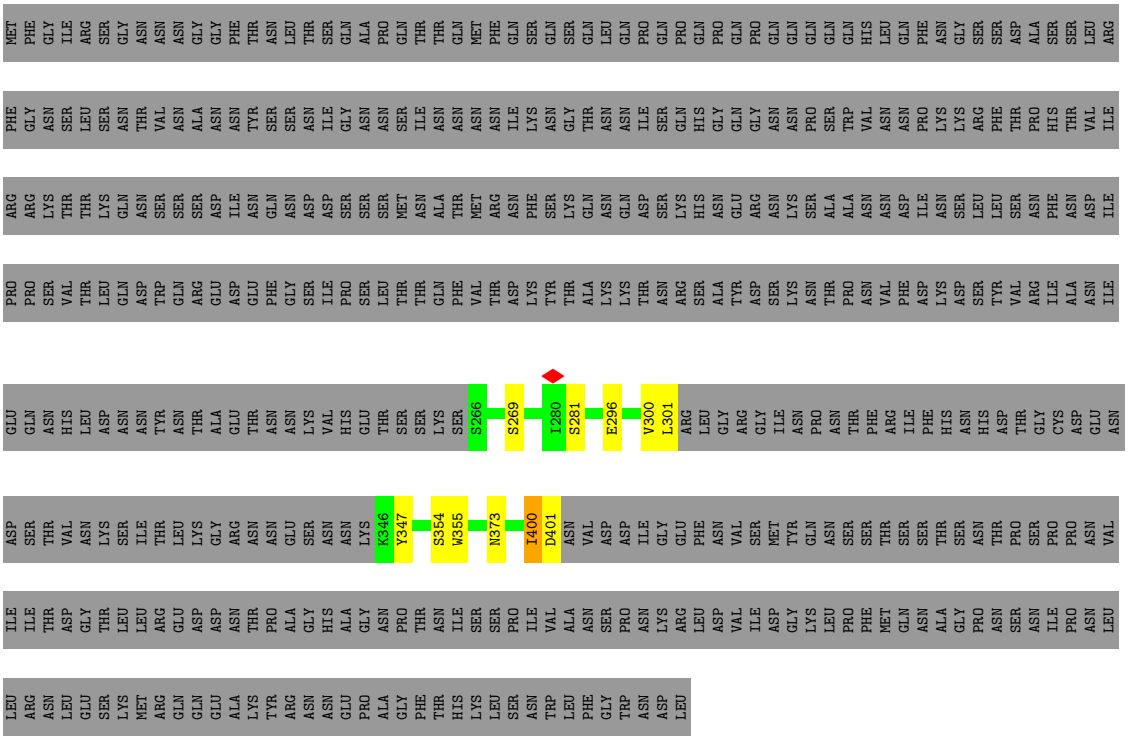
Chain W:





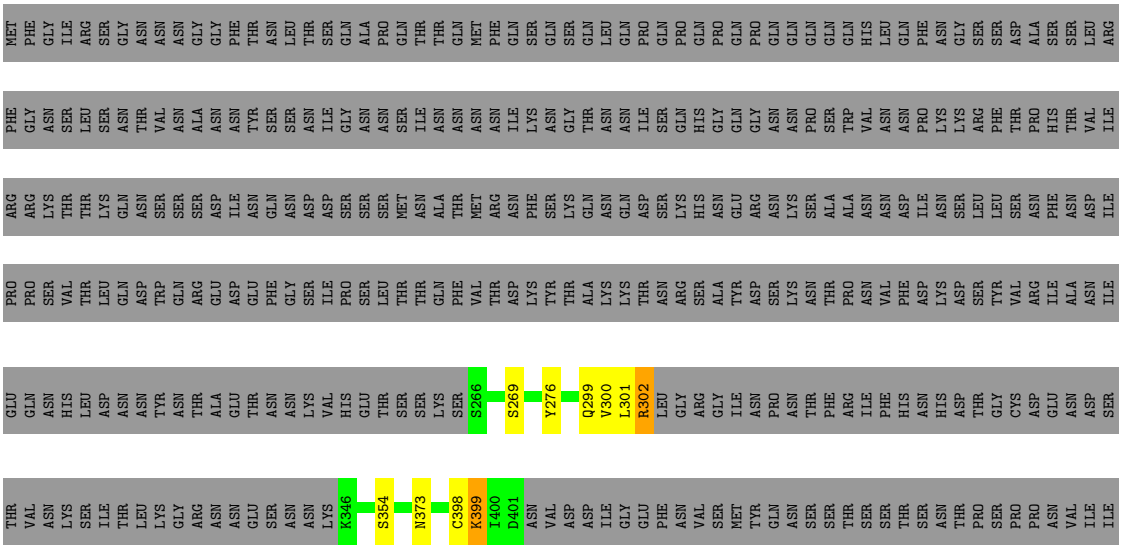
• Molecule 11: Nucleoporin ASM4

Chain V:

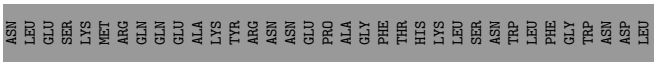


• Molecule 11: Nucleoporin ASM4

Chain X:




THR ASP GLY THR LEU LEU ARG GLU ASP ASP ASN THR PRO ALA GLY HIS ALA GLY ASN PRO THR ASN ILE SER SER PRO ILE VAL ALA ASN SER PRO ASN LYS ARG LEU ASP VAL ILE ASP GLY LYS LEU PRO PHE MET GLN ASN ALA GLY PRO ASN SER ASN ILE PRO ASN LEU LEU ARG


ASN LEU GLU SER LYS MET ARG GLN GLN GLU ALA LYS TYR ARG ASN ASN GLU PRO ALA GLY PHE THR HIS LYS LEU SER ASN TRP LEU PHE GLY TRP ASN ASP LEU

4 Experimental information (i)

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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	37651	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	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 (Å)	1276.8, 1276.8, 1276.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	1.00	11/9065 (0.1%)	1.16	45/12247 (0.4%)
1	Y	0.93	7/8920 (0.1%)	1.09	28/12052 (0.2%)
2	1	1.01	13/9072 (0.1%)	1.14	41/12276 (0.3%)
2	Z	1.09	18/9052 (0.2%)	1.24	52/12249 (0.4%)
4	A	0.91	2/1327 (0.2%)	0.92	3/1788 (0.2%)
4	D	0.91	2/1328 (0.2%)	0.89	2/1791 (0.1%)
4	G	1.15	2/1334 (0.1%)	1.21	9/1799 (0.5%)
4	J	0.92	2/1328 (0.2%)	0.92	4/1791 (0.2%)
5	B	0.86	0/1793	0.91	1/2411 (0.0%)
5	E	1.01	2/1793 (0.1%)	1.08	5/2411 (0.2%)
5	H	1.03	2/1793 (0.1%)	1.05	6/2411 (0.2%)
5	K	0.86	0/1793	0.89	0/2411
6	C	0.83	0/1364	0.90	2/1837 (0.1%)
6	F	0.99	2/1368 (0.1%)	1.14	8/1842 (0.4%)
6	I	0.84	0/1364	0.90	3/1837 (0.2%)
6	L	0.85	0/1368	0.89	0/1842
7	M	0.91	6/12128 (0.0%)	1.04	26/16436 (0.2%)
7	O	0.94	12/12132 (0.1%)	1.09	36/16441 (0.2%)
8	N	0.98	19/11142 (0.2%)	1.17	61/15068 (0.4%)
8	P	0.96	12/11142 (0.1%)	1.13	53/15069 (0.4%)
9	Q	0.98	5/5265 (0.1%)	1.08	21/7137 (0.3%)
9	R	0.94	3/5353 (0.1%)	1.02	12/7262 (0.2%)
9	S	0.94	3/5262 (0.1%)	1.04	22/7133 (0.3%)
9	T	0.93	2/5353 (0.0%)	1.05	21/7262 (0.3%)
10	U	1.44	6/752 (0.8%)	1.74	16/1016 (1.6%)
10	W	1.24	4/752 (0.5%)	1.33	9/1016 (0.9%)
11	V	1.14	2/737 (0.3%)	1.26	6/996 (0.6%)
11	X	1.22	2/748 (0.3%)	1.39	7/1010 (0.7%)
All	All	0.97	139/124828 (0.1%)	1.10	499/168841 (0.3%)

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 (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	744	GLY	N-CA	-23.98	1.10	1.46
2	Z	679	SER	CA-CB	-23.87	1.17	1.52
4	G	727	SER	CA-CB	-23.61	1.17	1.52
8	P	174	VAL	CA-CB	-19.97	1.12	1.54
2	1	679	SER	CA-CB	-19.22	1.24	1.52
1	0	470	SER	N-CA	-18.12	1.10	1.46
11	X	302	ARG	CA-CB	-17.79	1.14	1.53
5	H	324	TYR	CA-CB	-17.78	1.14	1.53
9	Q	754	ARG	CA-CB	-17.74	1.15	1.53
10	W	305	TYR	CA-CB	-17.70	1.15	1.53
8	N	1059	ASN	N-CA	-17.39	1.11	1.46
2	Z	922	LYS	CA-CB	-17.02	1.16	1.53
10	U	249	ASP	CA-CB	-16.95	1.16	1.53
9	S	754	ARG	CA-CB	-16.66	1.17	1.53
2	Z	1040	LYS	CA-CB	-16.62	1.17	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	1137	ASN	N-CA	-16.33	1.13	1.46
9	T	754	ARG	CA-CB	-16.27	1.18	1.53
2	1	309	LEU	CA-CB	-16.20	1.16	1.53
9	T	753	ALA	N-CA	-16.16	1.14	1.46
1	0	471	SER	CA-CB	-16.09	1.28	1.52
10	U	305	TYR	CA-CB	-16.03	1.18	1.53
9	Q	753	ALA	CA-CB	-16.02	1.18	1.52
5	E	324	TYR	CA-CB	-15.92	1.19	1.53
2	Z	1156	LEU	CA-CB	-15.86	1.17	1.53
2	1	922	LYS	CA-CB	-15.85	1.19	1.53
1	0	1258	LEU	CA-CB	-15.77	1.17	1.53
11	V	401	ASP	N-CA	-15.48	1.15	1.46
9	R	753	ALA	N-CA	-15.35	1.15	1.46
6	F	370	ASP	CA-CB	-15.32	1.20	1.53
1	0	885	ALA	CA-CB	-15.23	1.20	1.52
1	Y	991	ARG	CA-CB	-15.06	1.20	1.53
5	H	323	LEU	N-CA	-14.86	1.16	1.46
8	P	257	LEU	CA-CB	-14.83	1.19	1.53
4	G	726	VAL	N-CA	-14.75	1.16	1.46
1	0	991	ARG	CA-CB	-14.70	1.21	1.53
8	P	551	ASN	N-CA	-14.45	1.17	1.46
8	N	257	LEU	CA-CB	-14.40	1.20	1.53
7	O	1138	PHE	CA-CB	-14.36	1.22	1.53
1	0	1257	GLN	N-CA	-14.20	1.18	1.46
8	N	1054	PHE	CA-CB	-14.02	1.23	1.53
2	Z	745	ILE	CA-CB	-13.98	1.22	1.54
8	P	552	LEU	CA-CB	-13.96	1.21	1.53
5	E	323	LEU	CA-CB	-13.72	1.22	1.53
9	R	754	ARG	CA-CB	-13.64	1.24	1.53
8	P	358	VAL	N-CA	-13.61	1.19	1.46
2	1	678	LYS	CA-CB	-13.60	1.24	1.53
2	Z	678	LYS	N-CA	-13.58	1.19	1.46
2	Z	1039	LEU	N-CA	-13.53	1.19	1.46
2	1	308	ASN	N-CA	-13.48	1.19	1.46
10	U	248	TRP	N-CA	-13.44	1.19	1.46
9	S	514	LYS	N-CA	-13.26	1.19	1.46
8	P	794	ILE	CA-CB	-13.11	1.24	1.54
8	N	552	LEU	CA-CB	-13.11	1.23	1.53
9	Q	514	LYS	CA-CB	-12.88	1.25	1.53
10	U	304	LYS	N-CA	-12.72	1.21	1.46
10	W	304	LYS	N-CA	-12.67	1.21	1.46
8	N	1060	LEU	CA-CB	-12.62	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	301	LEU	CA-CB	-12.47	1.25	1.53
8	N	577	MET	CA-CB	-12.47	1.26	1.53
8	P	256	THR	N-CA	-12.39	1.21	1.46
7	O	1273	LYS	CA-CB	-12.38	1.26	1.53
7	M	1273	LYS	CA-CB	-12.37	1.26	1.53
2	Z	921	SER	N-CA	-12.18	1.22	1.46
8	P	576	TYR	N-CA	-12.17	1.22	1.46
2	1	514	ARG	N-CA	-12.10	1.22	1.46
8	N	1055	GLN	CA-CB	-12.08	1.27	1.53
1	Y	992	CYS	CA-CB	-12.07	1.27	1.53
8	N	41	ARG	CA-CB	-12.00	1.27	1.53
7	O	603	GLU	CA-CB	-11.96	1.27	1.53
7	M	603	GLU	CA-CB	-11.95	1.27	1.53
6	F	369	LEU	N-CA	-11.91	1.22	1.46
1	0	992	CYS	CA-CB	-11.76	1.28	1.53
8	N	576	TYR	CA-CB	-11.73	1.28	1.53
8	N	256	THR	N-CA	-11.48	1.23	1.46
2	Z	915	LYS	N-CA	-11.47	1.23	1.46
9	Q	515	LEU	CA-C	-11.45	1.23	1.52
7	O	1320	GLU	CA-CB	-11.32	1.29	1.53
8	N	551	ASN	CA-CB	-11.26	1.23	1.53
9	S	753	ALA	N-CA	-11.20	1.24	1.46
2	1	1301	SER	CA-C	-10.98	1.24	1.52
8	N	40	ILE	N-CA	-10.96	1.24	1.46
2	1	921	SER	N-CA	-10.89	1.24	1.46
9	R	514	LYS	N-CA	-10.83	1.24	1.46
10	W	283	ILE	N-CA	-10.66	1.25	1.46
2	Z	308	ASN	N-CA	-10.66	1.25	1.46
11	V	301	LEU	CA-CB	-10.66	1.29	1.53
2	Z	514	ARG	N-CA	-10.44	1.25	1.46
7	O	1319	LEU	N-CA	-10.33	1.25	1.46
2	Z	456	THR	N-CA	-10.20	1.25	1.46
8	P	359	LEU	CA-C	-9.75	1.27	1.52
2	1	1300	SER	CA-CB	-9.67	1.38	1.52
10	U	283	ILE	N-CA	-9.31	1.27	1.46
7	O	602	ASN	CA-CB	-9.18	1.29	1.53
7	M	602	ASN	CA-CB	-9.16	1.29	1.53
1	Y	791	MET	CA-C	-9.12	1.29	1.52
4	D	726	VAL	CA-CB	-9.09	1.35	1.54
4	J	726	VAL	CA-CB	-9.02	1.35	1.54
8	N	41	ARG	CA-C	-8.59	1.30	1.52
8	P	359	LEU	CA-CB	-8.56	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	794	ILE	CA-C	-8.45	1.30	1.52
1	0	884	VAL	N-CA	-8.42	1.29	1.46
2	1	1301	SER	CA-CB	-8.38	1.40	1.52
8	N	793	LEU	CA-CB	-8.22	1.34	1.53
4	A	726	VAL	N-CA	-8.19	1.29	1.46
2	1	1300	SER	N-CA	-8.16	1.30	1.46
2	1	678	LYS	N-CA	7.58	1.61	1.46
9	Q	753	ALA	N-CA	7.39	1.61	1.46
8	N	794	ILE	CA-CB	-7.38	1.37	1.54
1	0	470	SER	CA-CB	7.34	1.64	1.52
1	Y	790	PHE	CA-CB	-7.34	1.37	1.53
1	Y	790	PHE	N-CA	-7.16	1.32	1.46
2	Z	1155	GLN	N-CA	-7.11	1.32	1.46
7	O	603	GLU	CA-C	-6.93	1.34	1.52
7	M	603	GLU	CA-C	-6.92	1.34	1.52
7	O	1320	GLU	CA-C	-6.82	1.35	1.52
4	A	726	VAL	CA-CB	-6.82	1.40	1.54
7	O	1137	ASN	CA-CB	6.78	1.70	1.53
2	Z	891	ARG	CA-CB	-6.68	1.39	1.53
1	Y	991	ARG	N-CA	6.62	1.59	1.46
8	N	1055	GLN	CA-C	-6.44	1.36	1.52
1	0	991	ARG	N-CA	6.28	1.58	1.46
7	O	1272	LEU	CA-CB	6.27	1.68	1.53
7	M	1272	LEU	CA-CB	6.24	1.68	1.53
1	Y	791	MET	CA-CB	-6.24	1.40	1.53
10	U	283	ILE	CA-CB	-6.23	1.40	1.54
8	P	793	LEU	CA-CB	-6.23	1.39	1.53
2	1	891	ARG	CA-CB	6.20	1.67	1.53
1	0	884	VAL	CA-CB	-6.18	1.41	1.54
2	Z	891	ARG	N-CA	-6.17	1.34	1.46
4	J	726	VAL	N-CA	-6.09	1.34	1.46
8	N	40	ILE	CA-CB	-6.05	1.41	1.54
7	M	1272	LEU	N-CA	5.77	1.57	1.46
7	O	1272	LEU	N-CA	5.75	1.57	1.46
8	P	793	LEU	N-CA	-5.71	1.34	1.46
2	Z	1155	GLN	CA-CB	-5.66	1.41	1.53
8	N	1059	ASN	CA-CB	5.34	1.67	1.53
10	W	283	ILE	CA-CB	-5.25	1.42	1.54
4	D	726	VAL	N-CA	-5.12	1.36	1.46
2	Z	456	THR	CA-CB	-5.09	1.40	1.53

All (499) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	1040	LYS	N-CA-CB	26.00	157.41	110.60
2	Z	1156	LEU	N-CA-CB	25.77	161.94	110.40
9	Q	753	ALA	CB-CA-C	25.56	148.44	110.10
10	U	249	ASP	N-CA-CB	22.28	150.70	110.60
2	Z	679	SER	N-CA-CB	22.12	143.69	110.50
4	G	727	SER	N-CA-CB	21.58	142.88	110.50
8	N	41	ARG	CB-CA-C	21.51	153.43	110.40
8	P	359	LEU	N-CA-CB	-20.80	68.80	110.40
1	0	885	ALA	N-CA-CB	20.30	138.52	110.10
2	Z	922	LYS	N-CA-CB	20.01	146.61	110.60
2	1	678	LYS	CB-CA-C	19.70	149.79	110.40
1	0	885	ALA	CB-CA-C	19.20	138.91	110.10
11	X	302	ARG	N-CA-CB	18.95	144.70	110.60
8	P	359	LEU	CB-CA-C	18.91	146.13	110.20
7	O	1320	GLU	CB-CA-C	18.36	147.13	110.40
2	1	309	LEU	N-CA-CB	18.35	147.10	110.40
8	N	1055	GLN	CB-CA-C	18.04	146.49	110.40
2	1	1301	SER	N-CA-CB	-17.94	83.58	110.50
1	Y	991	ARG	CB-CA-C	17.92	146.24	110.40
2	1	1301	SER	CB-CA-C	17.85	144.02	110.10
7	O	1138	PHE	CB-CA-C	17.36	145.12	110.40
1	0	991	ARG	CB-CA-C	17.31	145.02	110.40
2	1	1300	SER	N-CA-CB	17.29	136.44	110.50
2	Z	308	ASN	N-CA-CB	17.23	141.61	110.60
7	O	603	GLU	CB-CA-C	17.08	144.55	110.40
7	M	603	GLU	CB-CA-C	17.03	144.46	110.40
9	T	753	ALA	CB-CA-C	-16.77	84.94	110.10
2	Z	744	GLY	N-CA-C	16.61	154.62	113.10
2	Z	745	ILE	CB-CA-C	16.53	144.65	111.60
6	F	370	ASP	N-CA-CB	16.52	140.33	110.60
1	0	471	SER	CB-CA-C	16.51	141.46	110.10
9	S	754	ARG	N-CA-CB	16.07	139.53	110.60
9	R	753	ALA	CB-CA-C	-16.01	86.08	110.10
8	N	551	ASN	CB-CA-C	15.91	142.22	110.40
2	Z	1156	LEU	N-CA-C	-15.64	68.76	111.00
8	N	552	LEU	CB-CA-C	15.49	139.62	110.20
1	Y	791	MET	CB-CA-C	15.47	141.34	110.40
8	P	174	VAL	CB-CA-C	15.44	140.73	111.40
10	U	305	TYR	N-CA-CB	15.30	138.15	110.60
1	Y	992	CYS	CB-CA-C	15.29	140.98	110.40
2	Z	1040	LYS	N-CA-C	-15.28	69.75	111.00
9	S	753	ALA	N-CA-CB	15.27	131.48	110.10
1	0	992	CYS	CB-CA-C	15.15	140.70	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	323	LEU	CB-CA-C	15.02	138.74	110.20
1	0	1258	LEU	N-CA-CB	15.01	140.41	110.40
9	R	754	ARG	CB-CA-C	14.94	140.27	110.40
1	0	470	SER	CB-CA-C	-14.92	81.75	110.10
2	Z	921	SER	N-CA-CB	14.87	132.80	110.50
7	O	1137	ASN	N-CA-C	14.83	151.04	111.00
8	P	552	LEU	CB-CA-C	14.83	138.38	110.20
2	Z	678	LYS	N-CA-CB	14.82	137.28	110.60
2	Z	456	THR	N-CA-CB	14.79	138.39	110.30
7	O	1319	LEU	N-CA-CB	14.76	139.91	110.40
9	Q	515	LEU	CB-CA-C	14.60	137.94	110.20
4	G	727	SER	CB-CA-C	14.55	137.75	110.10
9	R	514	LYS	N-CA-CB	14.52	136.74	110.60
8	P	257	LEU	N-CA-CB	14.51	139.41	110.40
8	N	577	MET	CB-CA-C	14.50	139.41	110.40
9	Q	754	ARG	N-CA-CB	14.50	136.70	110.60
8	N	576	TYR	N-CA-CB	14.37	136.47	110.60
5	E	324	TYR	CB-CA-C	14.33	139.06	110.40
7	O	1137	ASN	CB-CA-C	-14.30	81.81	110.40
1	Y	790	PHE	N-CA-CB	14.21	136.17	110.60
9	R	753	ALA	N-CA-CB	14.17	129.94	110.10
10	W	305	TYR	N-CA-CB	14.17	136.10	110.60
2	1	922	LYS	N-CA-CB	14.12	136.01	110.60
2	1	921	SER	N-CA-CB	14.07	131.60	110.50
2	1	679	SER	N-CA-CB	14.02	131.53	110.50
8	N	1059	ASN	CB-CA-C	-14.01	82.38	110.40
7	O	1320	GLU	N-CA-CB	-13.89	85.60	110.60
2	Z	891	ARG	N-CA-CB	13.84	135.51	110.60
10	U	249	ASP	N-CA-C	-13.83	73.65	111.00
2	1	308	ASN	N-CA-CB	13.79	135.43	110.60
2	1	922	LYS	CB-CA-C	13.73	137.86	110.40
2	Z	514	ARG	N-CA-CB	13.68	135.22	110.60
8	N	1060	LEU	CB-CA-C	13.65	136.14	110.20
11	X	301	LEU	CB-CA-C	13.58	136.00	110.20
9	Q	514	LYS	CB-CA-C	13.57	137.53	110.40
1	0	470	SER	N-CA-CB	13.50	130.75	110.50
9	S	514	LYS	N-CA-CB	13.46	134.82	110.60
9	T	754	ARG	CB-CA-C	13.17	136.75	110.40
8	P	576	TYR	N-CA-CB	13.13	134.23	110.60
1	Y	791	MET	N-CA-CB	-13.09	87.04	110.60
8	P	257	LEU	CB-CA-C	13.02	134.94	110.20
8	N	257	LEU	N-CA-CB	13.01	136.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	1054	PHE	CB-CA-C	12.96	136.32	110.40
8	N	1054	PHE	N-CA-CB	12.96	133.93	110.60
9	T	753	ALA	N-CA-CB	12.92	128.19	110.10
2	1	679	SER	CB-CA-C	12.82	134.47	110.10
9	T	753	ALA	N-CA-C	12.81	145.59	111.00
10	W	283	ILE	N-CA-CB	12.71	140.04	110.80
8	N	257	LEU	CB-CA-C	12.68	134.29	110.20
7	M	1272	LEU	CB-CA-C	-12.67	86.12	110.20
2	1	309	LEU	CB-CA-C	12.67	134.27	110.20
7	O	1272	LEU	CB-CA-C	-12.67	86.13	110.20
8	P	794	ILE	CB-CA-C	12.66	136.92	111.60
8	N	577	MET	N-CA-CB	12.63	133.34	110.60
5	H	324	TYR	CB-CA-C	12.63	135.66	110.40
2	Z	915	LYS	N-CA-CB	12.57	133.22	110.60
10	U	249	ASP	CB-CA-C	12.54	135.49	110.40
11	V	401	ASP	N-CA-CB	12.52	133.14	110.60
6	F	370	ASP	CB-CA-C	12.41	135.21	110.40
1	0	1258	LEU	CB-CA-C	12.38	133.72	110.20
8	N	40	ILE	N-CA-CB	12.35	139.21	110.80
10	U	248	TRP	N-CA-CB	12.33	132.80	110.60
8	P	359	LEU	N-CA-C	12.33	144.28	111.00
2	Z	679	SER	CB-CA-C	12.33	133.52	110.10
2	Z	1155	GLN	N-CA-CB	12.22	132.60	110.60
2	1	514	ARG	N-CA-CB	12.21	132.58	110.60
10	U	283	ILE	N-CA-CB	12.20	138.86	110.80
8	P	256	THR	N-CA-CB	12.11	133.31	110.30
2	1	309	LEU	N-CA-C	-12.02	78.55	111.00
9	T	754	ARG	N-CA-CB	11.99	132.19	110.60
8	N	794	ILE	CB-CA-C	11.94	135.48	111.60
9	R	753	ALA	N-CA-C	11.94	143.23	111.00
4	G	727	SER	N-CA-C	-11.79	79.17	111.00
8	N	256	THR	N-CA-CB	11.79	132.69	110.30
11	V	301	LEU	N-CA-CB	11.67	133.73	110.40
8	P	551	ASN	N-CA-CB	11.63	131.54	110.60
8	P	551	ASN	CB-CA-C	-11.60	87.21	110.40
7	O	602	ASN	N-CA-CB	11.56	131.41	110.60
7	M	1273	LYS	CB-CA-C	11.55	133.50	110.40
7	O	1273	LYS	CB-CA-C	11.53	133.47	110.40
8	P	358	VAL	N-CA-CB	11.53	136.87	111.50
7	M	602	ASN	N-CA-CB	11.49	131.29	110.60
5	E	323	LEU	N-CA-CB	11.48	133.36	110.40
9	Q	754	ARG	CB-CA-C	11.47	133.34	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	922	LYS	N-CA-C	-11.46	80.05	111.00
8	N	1059	ASN	N-CA-C	11.42	141.83	111.00
10	W	304	LYS	N-CA-CB	11.40	131.12	110.60
4	G	726	VAL	CB-CA-C	-11.35	89.84	111.40
2	Z	922	LYS	CB-CA-C	11.31	133.02	110.40
6	F	369	LEU	N-CA-CB	11.25	132.90	110.40
10	W	305	TYR	CB-CA-C	11.18	132.77	110.40
9	S	754	ARG	CB-CA-C	11.17	132.75	110.40
1	0	470	SER	N-CA-C	11.12	141.02	111.00
7	O	1272	LEU	N-CA-C	-10.97	81.39	111.00
7	M	1272	LEU	N-CA-C	-10.96	81.40	111.00
8	P	551	ASN	N-CA-C	10.94	140.54	111.00
11	X	301	LEU	N-CA-CB	10.94	132.27	110.40
10	U	305	TYR	CB-CA-C	10.90	132.19	110.40
8	P	552	LEU	N-CA-CB	10.87	132.15	110.40
2	1	678	LYS	N-CA-C	-10.80	81.84	111.00
9	Q	514	LYS	N-CA-CB	10.77	129.99	110.60
10	U	248	TRP	CB-CA-C	-10.77	88.86	110.40
8	N	793	LEU	N-CA-CB	10.77	131.93	110.40
5	H	323	LEU	N-CA-CB	10.75	131.90	110.40
10	U	304	LYS	N-CA-CB	10.71	129.88	110.60
1	0	1257	GLN	N-CA-CB	10.70	129.86	110.60
8	N	41	ARG	CA-C-O	10.66	142.48	120.10
8	N	41	ARG	CA-C-N	-10.63	93.81	117.20
11	V	401	ASP	CB-CA-C	-10.62	89.16	110.40
5	H	323	LEU	CB-CA-C	-10.61	90.04	110.20
2	Z	679	SER	N-CA-C	-10.58	82.43	111.00
2	Z	1040	LYS	CB-CA-C	10.58	131.57	110.40
9	S	514	LYS	CB-CA-C	-10.54	89.32	110.40
1	0	885	ALA	N-CA-C	-10.53	82.57	111.00
8	P	793	LEU	N-CA-CB	10.49	131.39	110.40
11	X	302	ARG	CB-CA-C	10.40	131.21	110.40
1	0	884	VAL	N-CA-CB	10.40	134.38	111.50
5	H	324	TYR	N-CA-CB	10.34	129.21	110.60
2	Z	1039	LEU	CB-CA-C	-10.34	90.56	110.20
4	J	726	VAL	N-CA-CB	10.28	134.13	111.50
1	0	1257	GLN	N-CA-C	10.25	138.68	111.00
4	G	726	VAL	N-CA-CB	10.24	134.03	111.50
4	D	726	VAL	N-CA-CB	10.23	134.02	111.50
9	Q	515	LEU	N-CA-CB	-10.17	90.06	110.40
2	Z	1039	LEU	N-CA-CB	10.13	130.67	110.40
11	X	302	ARG	N-CA-C	-10.09	83.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	248	TRP	N-CA-C	10.08	138.22	111.00
8	N	41	ARG	CA-CB-CG	10.05	135.52	113.40
2	Z	1039	LEU	N-CA-C	10.02	138.04	111.00
1	Y	991	ARG	N-CA-CB	9.99	128.59	110.60
5	H	323	LEU	N-CA-C	9.97	137.93	111.00
6	F	370	ASP	N-CA-C	-9.92	84.22	111.00
10	U	304	LYS	N-CA-C	9.89	137.71	111.00
9	Q	753	ALA	N-CA-C	-9.85	84.39	111.00
11	V	401	ASP	N-CA-C	9.83	137.54	111.00
4	A	726	VAL	N-CA-CB	9.80	133.05	111.50
7	M	602	ASN	CB-CA-C	9.75	129.90	110.40
1	Y	991	ARG	N-CA-C	-9.75	84.67	111.00
7	O	602	ASN	CB-CA-C	9.70	129.80	110.40
8	N	1055	GLN	N-CA-CB	-9.69	93.15	110.60
1	0	1257	GLN	CB-CA-C	-9.68	91.05	110.40
9	Q	753	ALA	N-CA-CB	9.64	123.60	110.10
9	T	81	GLU	N-CA-CB	9.50	127.69	110.60
8	P	257	LEU	N-CA-C	-9.45	85.47	111.00
2	Z	1156	LEU	CB-CA-C	9.43	128.12	110.20
1	0	1258	LEU	N-CA-C	-9.41	85.59	111.00
1	0	991	ARG	N-CA-CB	9.40	127.51	110.60
7	O	603	GLU	N-CA-CB	-9.37	93.73	110.60
7	O	1273	LYS	N-CA-CB	9.35	127.42	110.60
7	M	1273	LYS	N-CA-CB	9.34	127.42	110.60
7	M	603	GLU	N-CA-CB	-9.30	93.87	110.60
10	U	304	LYS	CB-CA-C	-9.29	91.82	110.40
4	G	726	VAL	N-CA-C	9.28	136.05	111.00
1	0	991	ARG	N-CA-C	-9.27	85.96	111.00
5	E	323	LEU	N-CA-C	-9.26	86.01	111.00
2	1	922	LYS	N-CA-C	-9.21	86.12	111.00
9	S	514	LYS	N-CA-C	9.06	135.46	111.00
10	W	304	LYS	N-CA-C	9.04	135.40	111.00
9	S	753	ALA	CB-CA-C	-8.96	96.66	110.10
8	P	256	THR	N-CA-C	8.95	135.16	111.00
7	O	1320	GLU	CA-C-O	-8.93	101.35	120.10
1	Y	133	TYR	CB-CG-CD2	-8.93	115.64	121.00
8	N	40	ILE	CA-CB-CG1	-8.91	94.07	111.00
8	N	577	MET	N-CA-C	-8.81	87.21	111.00
2	Z	921	SER	CB-CA-C	-8.77	93.43	110.10
9	T	98	PRO	N-CA-CB	8.74	113.79	103.30
11	V	301	LEU	CB-CA-C	8.74	126.81	110.20
2	1	308	ASN	CB-CA-C	-8.72	92.95	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	551	ASN	N-CA-CB	8.69	126.24	110.60
9	S	754	ARG	N-CA-C	-8.68	87.58	111.00
8	N	1054	PHE	N-CA-C	-8.62	87.73	111.00
10	W	304	LYS	CB-CA-C	-8.54	93.32	110.40
1	0	884	VAL	CA-CB-CG1	8.41	123.52	110.90
6	F	369	LEU	CB-CA-C	-8.41	94.22	110.20
2	Z	921	SER	N-CA-C	8.33	133.48	111.00
9	R	98	PRO	N-CA-CB	8.31	113.28	103.30
1	0	1105	TYR	CB-CG-CD1	8.29	125.97	121.00
8	P	552	LEU	CA-C-O	-8.26	102.76	120.10
8	N	256	THR	N-CA-C	8.25	133.28	111.00
10	U	305	TYR	N-CA-C	-8.15	89.00	111.00
8	N	577	MET	CA-CB-CG	8.13	127.13	113.30
8	N	257	LEU	N-CA-C	-8.12	89.06	111.00
6	F	370	ASP	CA-C-O	-8.11	103.07	120.10
8	P	358	VAL	CB-CA-C	-8.11	96.00	111.40
6	F	369	LEU	N-CA-C	8.07	132.79	111.00
2	Z	745	ILE	CA-CB-CG1	8.05	126.29	111.00
9	R	100	PRO	N-CA-CB	8.03	112.94	103.30
8	N	257	LEU	CA-C-O	-8.01	103.27	120.10
8	P	552	LEU	N-CA-C	-8.01	89.38	111.00
8	P	174	VAL	CA-CB-CG2	7.95	122.83	110.90
11	X	301	LEU	N-CA-C	-7.85	89.80	111.00
9	T	101	PRO	N-CA-CB	7.84	112.71	103.30
1	0	1105	TYR	CB-CG-CD2	-7.84	116.30	121.00
9	Q	754	ARG	N-CA-C	-7.82	89.88	111.00
1	Y	133	TYR	CB-CG-CD1	7.80	125.68	121.00
8	N	794	ILE	CA-CB-CG1	7.79	125.81	111.00
2	Z	915	LYS	CB-CA-C	-7.74	94.91	110.40
9	R	514	LYS	CB-CA-C	-7.74	94.92	110.40
8	P	257	LEU	CA-C-O	-7.73	103.87	120.10
2	1	1301	SER	N-CA-C	7.70	131.79	111.00
7	O	1183	TYR	CB-CG-CD1	7.67	125.60	121.00
7	M	1183	TYR	CB-CG-CD1	7.67	125.60	121.00
7	O	1320	GLU	CA-C-N	7.66	138.55	117.10
8	P	794	ILE	CA-CB-CG1	7.65	125.54	111.00
9	S	753	ALA	N-CA-C	7.64	131.63	111.00
9	T	754	ARG	N-CA-C	-7.64	90.37	111.00
1	0	885	ALA	CA-C-O	-7.62	104.09	120.10
6	F	370	ASP	CA-C-N	7.61	133.95	117.20
2	1	308	ASN	N-CA-C	7.60	131.51	111.00
8	P	257	LEU	CA-C-N	7.59	133.91	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	791	MET	N-CA-C	7.59	131.49	111.00
8	N	257	LEU	CA-C-N	7.57	133.86	117.20
8	N	551	ASN	N-CA-C	-7.54	90.64	111.00
7	M	1273	LYS	CA-C-O	-7.54	104.28	120.10
8	P	552	LEU	CA-C-N	7.54	133.78	117.20
9	Q	515	LEU	N-CA-C	7.53	131.32	111.00
7	O	1273	LYS	CA-C-O	-7.50	104.35	120.10
8	P	256	THR	CB-CA-C	-7.46	91.47	111.60
7	O	1183	TYR	CB-CG-CD2	-7.39	116.57	121.00
10	W	305	TYR	N-CA-C	-7.38	91.07	111.00
7	M	1183	TYR	CB-CG-CD2	-7.38	116.57	121.00
8	N	576	TYR	CB-CA-C	7.37	125.13	110.40
7	M	1273	LYS	CA-C-N	7.32	133.29	117.20
8	N	552	LEU	N-CA-CB	7.31	125.03	110.40
7	O	1273	LYS	CA-C-N	7.31	133.28	117.20
4	G	726	VAL	CA-CB-CG2	-7.29	99.96	110.90
9	Q	514	LYS	N-CA-C	-7.27	91.38	111.00
2	Z	678	LYS	CB-CA-C	-7.24	95.93	110.40
2	Z	922	LYS	CA-C-O	-7.21	104.96	120.10
9	Q	98	PRO	N-CA-CB	7.18	111.92	103.30
9	S	98	PRO	N-CA-CB	7.18	111.91	103.30
2	Z	679	SER	CA-C-O	-7.17	105.04	120.10
2	Z	456	THR	CA-CB-CG2	7.16	122.42	112.40
2	Z	745	ILE	CA-CB-CG2	-7.14	96.63	110.90
2	1	922	LYS	CA-C-O	-7.11	105.17	120.10
7	M	1658	PRO	N-CA-CB	7.08	111.80	103.30
7	M	1603	PRO	N-CA-CB	7.07	111.78	103.30
2	Z	915	LYS	N-CA-C	7.06	130.06	111.00
4	J	776	PHE	CB-CG-CD1	7.05	125.74	120.80
7	O	1658	PRO	N-CA-CB	7.03	111.73	103.30
7	O	1603	PRO	N-CA-CB	7.01	111.71	103.30
8	P	174	VAL	CA-CB-CG1	-7.01	100.39	110.90
9	S	754	ARG	CA-C-O	-6.97	105.46	120.10
4	J	726	VAL	CA-CB-CG1	6.94	121.30	110.90
8	N	794	ILE	CA-CB-CG2	-6.93	97.04	110.90
9	S	44	VAL	N-CA-CB	6.93	126.75	111.50
1	0	885	ALA	CA-C-N	6.90	132.39	117.20
4	A	726	VAL	CA-CB-CG2	6.90	121.24	110.90
7	O	1138	PHE	CA-C-O	-6.88	105.64	120.10
8	P	576	TYR	CA-CB-CG	6.87	126.45	113.40
1	Y	407	ALA	N-CA-CB	6.83	119.67	110.10
7	O	1137	ASN	N-CA-CB	6.77	122.78	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	922	LYS	CA-C-N	6.75	132.06	117.20
2	1	679	SER	N-CA-C	-6.74	92.81	111.00
2	1	921	SER	N-CA-C	6.71	129.12	111.00
2	1	678	LYS	N-CA-CB	6.70	122.67	110.60
10	W	320	SER	N-CA-CB	6.70	120.54	110.50
1	0	992	CYS	CA-CB-SG	-6.69	101.96	114.00
9	R	101	PRO	N-CA-CB	6.69	111.33	103.30
8	P	794	ILE	CA-C-O	-6.68	106.07	120.10
2	Z	308	ASN	CB-CA-C	-6.67	97.06	110.40
9	T	469	TYR	CB-CG-CD2	-6.66	117.01	121.00
1	Y	126	TYR	CB-CG-CD1	6.65	124.99	121.00
2	1	679	SER	CA-C-O	-6.65	106.13	120.10
1	0	522	ALA	N-CA-CB	6.62	119.37	110.10
8	P	794	ILE	CA-C-N	6.58	131.69	117.20
2	Z	1156	LEU	CA-C-O	-6.57	106.30	120.10
8	N	256	THR	CB-CA-C	-6.55	93.92	111.60
1	Y	523	SER	N-CA-CB	6.50	120.26	110.50
2	Z	1071	TYR	CB-CG-CD2	-6.50	117.10	121.00
9	Q	754	ARG	CA-C-O	-6.48	106.48	120.10
1	Y	992	CYS	CA-CB-SG	-6.46	102.38	114.00
2	Z	679	SER	CA-C-N	6.46	131.40	117.20
8	P	358	VAL	CA-CB-CG2	-6.44	101.24	110.90
8	P	758	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	Y	126	TYR	CB-CG-CD2	-6.40	117.16	121.00
9	S	754	ARG	CA-C-N	6.39	131.26	117.20
1	0	1146	TYR	CB-CG-CD2	-6.35	117.19	121.00
8	P	794	ILE	CA-CB-CG2	-6.31	98.29	110.90
9	S	474	PHE	CB-CG-CD1	6.29	125.20	120.80
6	C	325	TYR	CB-CG-CD2	-6.29	117.23	121.00
8	N	41	ARG	N-CA-CB	-6.28	99.30	110.60
9	T	100	PRO	N-CA-CB	6.25	110.80	103.30
8	P	758	TYR	CB-CG-CD1	6.23	124.74	121.00
2	1	679	SER	CA-C-N	6.21	130.87	117.20
8	P	794	ILE	N-CA-CB	6.21	125.08	110.80
2	1	1299	LYS	C-N-CA	6.20	137.21	121.70
10	U	348	ALA	N-CA-CB	6.16	118.72	110.10
2	1	922	LYS	CA-C-N	6.13	130.69	117.20
8	P	1288	PHE	CB-CG-CD1	6.13	125.09	120.80
2	Z	1040	LYS	CA-C-O	-6.13	107.24	120.10
9	T	469	TYR	CB-CG-CD1	6.12	124.67	121.00
7	O	1273	LYS	CA-CB-CG	6.08	126.79	113.40
7	O	1138	PHE	CA-C-N	6.08	130.59	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	986	SER	N-CA-CB	6.08	119.62	110.50
7	M	1273	LYS	CA-CB-CG	6.08	126.77	113.40
9	T	499	SER	N-CA-CB	6.07	119.60	110.50
7	M	1320	GLU	N-CA-C	6.06	127.36	111.00
9	T	81	GLU	CB-CA-C	6.05	122.50	110.40
1	0	467	PHE	CB-CG-CD1	6.04	125.03	120.80
1	0	1305	SER	N-CA-CB	6.04	119.56	110.50
1	Y	386	SER	N-CA-CB	6.03	119.54	110.50
2	1	1071	TYR	CB-CG-CD2	-6.02	117.39	121.00
4	A	744	ALA	N-CA-CB	6.00	118.50	110.10
4	G	744	ALA	N-CA-CB	6.00	118.50	110.10
7	O	1320	GLU	N-CA-C	6.00	127.19	111.00
9	T	282	PHE	CB-CG-CD1	5.99	124.99	120.80
2	Z	745	ILE	N-CA-C	-5.96	94.91	111.00
9	T	45	SER	N-CA-CB	5.95	119.43	110.50
8	N	552	LEU	N-CA-C	-5.95	94.94	111.00
8	P	639	PHE	CB-CG-CD2	-5.93	116.65	120.80
7	O	488	PHE	CB-CG-CD1	5.93	124.95	120.80
2	1	1060	TYR	CB-CG-CD2	-5.93	117.44	121.00
9	S	474	PHE	CB-CG-CD2	-5.92	116.66	120.80
4	J	776	PHE	CB-CG-CD2	-5.92	116.66	120.80
7	O	488	PHE	CB-CG-CD2	-5.91	116.67	120.80
2	Z	1071	TYR	CB-CG-CD1	5.91	124.55	121.00
7	M	488	PHE	CB-CG-CD2	-5.91	116.67	120.80
8	P	1427	SER	N-CA-CB	5.91	119.36	110.50
8	N	639	PHE	CB-CG-CD2	-5.89	116.67	120.80
5	H	324	TYR	N-CA-C	-5.89	95.11	111.00
7	M	488	PHE	CB-CG-CD1	5.85	124.90	120.80
1	Y	406	THR	N-CA-CB	5.85	121.42	110.30
9	Q	515	LEU	CA-CB-CG	-5.83	101.88	115.30
8	N	1060	LEU	CA-CB-CG	5.82	128.68	115.30
1	0	170	LYS	N-CA-CB	5.81	121.06	110.60
2	Z	1156	LEU	CA-C-N	5.80	129.97	117.20
8	N	1050	SER	N-CA-CB	5.80	119.20	110.50
2	1	921	SER	CB-CA-C	-5.78	99.13	110.10
1	0	1097	TYR	CB-CG-CD2	-5.77	117.54	121.00
2	1	1071	TYR	CB-CG-CD1	5.76	124.46	121.00
2	1	514	ARG	N-CA-C	5.74	126.51	111.00
9	S	412	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	Y	1428	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	0	397	TYR	CB-CG-CD1	5.73	124.44	121.00
9	R	514	LYS	N-CA-C	5.73	126.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	1143	SER	N-CA-CB	5.71	119.06	110.50
9	Q	754	ARG	CA-CB-CG	5.70	125.94	113.40
2	Z	678	LYS	N-CA-C	5.70	126.38	111.00
1	Y	979	ALA	N-CA-CB	5.69	118.07	110.10
1	Y	1428	TYR	CB-CG-CD1	5.69	124.42	121.00
7	O	1585	PRO	N-CA-CB	5.67	110.10	103.30
1	0	397	TYR	CB-CG-CD2	-5.66	117.61	121.00
8	P	639	PHE	CB-CG-CD1	5.66	124.76	120.80
8	N	794	ILE	N-CA-CB	-5.65	97.80	110.80
1	0	1312	ALA	N-CA-CB	5.65	118.01	110.10
7	M	1143	SER	N-CA-CB	5.65	118.98	110.50
6	C	325	TYR	CB-CG-CD1	5.64	124.38	121.00
8	N	852	PHE	CB-CG-CD1	5.64	124.75	120.80
9	Q	754	ARG	CA-C-N	5.62	129.57	117.20
8	N	1611	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	Y	1059	TYR	CB-CG-CD2	-5.60	117.64	121.00
9	T	212	PHE	CB-CG-CD1	5.58	124.71	120.80
8	N	844	TYR	CB-CG-CD2	-5.57	117.66	121.00
8	N	1446	PHE	CB-CG-CD1	5.56	124.69	120.80
8	P	975	GLN	N-CA-CB	5.55	120.59	110.60
8	P	1099	PHE	CB-CG-CD1	5.55	124.68	120.80
8	N	40	ILE	CB-CA-C	-5.54	100.53	111.60
7	O	1141	SER	N-CA-CB	5.53	118.79	110.50
4	D	726	VAL	CA-CB-CG1	5.53	119.19	110.90
8	P	1288	PHE	CB-CG-CD2	-5.52	116.94	120.80
9	S	412	TYR	CB-CG-CD1	5.51	124.31	121.00
7	M	1141	SER	N-CA-CB	5.50	118.76	110.50
8	P	358	VAL	N-CA-C	5.50	125.86	111.00
2	1	171	TYR	CB-CG-CD2	-5.49	117.71	121.00
9	Q	77	GLY	N-CA-C	-5.49	99.38	113.10
2	Z	991	ALA	N-CA-CB	5.48	117.77	110.10
7	M	1585	PRO	N-CA-CB	5.47	109.87	103.30
11	V	400	ILE	C-N-CA	5.47	135.38	121.70
1	0	979	ALA	N-CA-CB	5.46	117.75	110.10
6	I	325	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	0	1146	TYR	CB-CG-CD1	5.46	124.28	121.00
1	Y	1059	TYR	N-CA-CB	5.46	120.43	110.60
2	1	1060	TYR	CB-CG-CD1	5.46	124.27	121.00
2	1	1210	ALA	N-CA-CB	5.45	117.73	110.10
2	Z	421	PHE	CB-CG-CD2	-5.45	116.99	120.80
8	N	639	PHE	CB-CG-CD1	5.44	124.61	120.80
8	P	1524	TYR	CB-CG-CD2	-5.44	117.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1363	PHE	CB-CG-CD1	5.43	124.60	120.80
7	O	1406	TYR	CB-CG-CD2	-5.43	117.74	121.00
8	N	56	ASN	N-CA-CB	5.43	120.37	110.60
11	X	302	ARG	CA-C-O	5.43	131.49	120.10
6	I	350	PHE	CB-CG-CD1	5.41	124.59	120.80
8	N	1611	TYR	CB-CG-CD1	5.41	124.25	121.00
9	Q	412	TYR	CB-CG-CD1	5.38	124.23	121.00
2	Z	1060	TYR	CB-CG-CD2	-5.38	117.77	121.00
9	T	412	TYR	CB-CG-CD2	-5.37	117.78	121.00
7	M	1406	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	Z	1040	LYS	CA-C-N	5.35	128.96	117.20
8	N	844	TYR	CB-CG-CD1	5.34	124.21	121.00
8	N	1059	ASN	N-CA-CB	5.34	120.21	110.60
9	Q	282	PHE	CB-CG-CD1	5.33	124.53	120.80
1	0	693	GLU	N-CA-CB	5.33	120.19	110.60
1	0	1210	PHE	CB-CG-CD1	5.33	124.53	120.80
9	T	282	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	Y	140	ASN	N-CA-CB	5.31	120.15	110.60
2	1	1083	TYR	CB-CG-CD1	5.30	124.18	121.00
1	Y	251	THR	N-CA-CB	5.30	120.38	110.30
2	Z	1060	TYR	CB-CG-CD1	5.30	124.18	121.00
2	Z	421	PHE	CB-CG-CD1	5.29	124.50	120.80
10	U	320	SER	N-CA-CB	5.28	118.41	110.50
2	Z	553	LYS	N-CA-CB	5.27	120.08	110.60
1	Y	1059	TYR	CB-CG-CD1	5.25	124.15	121.00
2	1	921	SER	CA-CB-OG	5.25	125.38	111.20
1	Y	447	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	0	1198	ASN	N-CA-CB	5.24	120.03	110.60
8	N	1446	PHE	CB-CG-CD2	-5.24	117.14	120.80
9	S	754	ARG	CA-CB-CG	5.22	124.89	113.40
1	0	1428	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	Y	842	TYR	CB-CG-CD2	-5.21	117.87	121.00
2	1	514	ARG	CB-CA-C	-5.20	100.00	110.40
8	N	59	ARG	N-CA-CB	5.20	119.96	110.60
10	W	283	ILE	CA-CB-CG2	5.20	121.30	110.90
9	S	727	TYR	CB-CG-CD1	5.19	124.11	121.00
1	0	467	PHE	CB-CG-CD2	-5.19	117.17	120.80
8	P	794	ILE	N-CA-C	-5.19	97.00	111.00
8	N	852	PHE	CB-CG-CD2	-5.18	117.17	120.80
8	N	794	ILE	N-CA-C	5.18	124.98	111.00
7	M	761	LEU	N-CA-CB	5.17	120.74	110.40
5	E	324	TYR	CA-CB-CG	5.16	123.21	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	412	TYR	CB-CG-CD2	-5.16	117.91	121.00
5	B	297	GLU	N-CA-CB	5.15	119.87	110.60
2	1	1083	TYR	CB-CG-CD2	-5.15	117.91	121.00
7	O	761	LEU	N-CA-CB	5.14	120.68	110.40
10	U	283	ILE	CA-CB-CG2	5.13	121.17	110.90
8	N	576	TYR	N-CA-C	-5.13	97.15	111.00
8	N	1183	PHE	CB-CG-CD1	5.13	124.39	120.80
8	P	707	PHE	CB-CG-CD1	5.13	124.39	120.80
9	S	727	TYR	CB-CG-CD2	-5.12	117.93	121.00
8	N	1055	GLN	CA-C-N	-5.12	105.94	117.20
2	1	171	TYR	CB-CG-CD1	5.10	124.06	121.00
7	M	603	GLU	CA-C-O	-5.10	109.39	120.10
8	P	844	TYR	CB-CG-CD2	-5.09	117.95	121.00
8	P	415	PHE	CB-CG-CD1	5.09	124.36	120.80
9	R	824	MET	N-CA-C	-5.09	97.27	111.00
7	O	603	GLU	CA-C-O	-5.08	109.42	120.10
9	S	367	PHE	CB-CG-CD1	5.08	124.36	120.80
9	S	290	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	0	1097	TYR	CB-CG-CD1	5.07	124.04	121.00
9	T	412	TYR	CB-CG-CD1	5.06	124.04	121.00
9	T	215	TYR	CB-CG-CD2	-5.06	117.97	121.00
6	I	350	PHE	CB-CG-CD2	-5.05	117.26	120.80
4	G	725	VAL	C-N-CA	5.05	134.33	121.70
8	P	416	LEU	N-CA-CB	5.05	120.50	110.40
2	1	513	LYS	C-N-CA	5.05	134.32	121.70
8	P	1254	ARG	NE-CZ-NH1	5.04	122.82	120.30
7	M	307	ASP	N-CA-CB	5.04	119.67	110.60
7	O	307	ASP	N-CA-CB	5.04	119.67	110.60
1	0	771	TYR	CB-CG-CD1	5.04	124.02	121.00
8	P	359	LEU	CA-CB-CG	-5.04	103.72	115.30
1	0	1363	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	0	771	TYR	CB-CG-CD2	-5.03	117.98	121.00
9	R	295	ASN	N-CA-CB	5.02	119.64	110.60
8	P	277	THR	N-CA-CB	5.01	119.83	110.30
1	Y	447	TYR	CB-CG-CD1	5.01	124.01	121.00
7	M	1406	TYR	CB-CG-CD1	5.01	124.01	121.00

All (101) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	471	SER	CA
1	0	884	VAL	CA

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	8747	0	8800	40	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	14	0
5	H	1771	0	1832	5	0
5	K	1771	0	1831	29	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	46	0
8	N	10955	0	11304	95	0
8	P	10955	0	11301	137	0
9	Q	5192	0	4911	13	0
9	R	5279	0	4937	0	0
9	S	5189	0	4902	14	0
9	T	5279	0	4937	10	0
10	U	736	0	739	12	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	555	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 (555) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
7:O:1027:GLN:CD	7:O:1039:ALA:O	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
7:O:1027:GLN:CD	7:O:1039:ALA:HB3	1.92	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:K:320:GLU:C	5:K:322:ILE:H	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Z:1254:GLY:C	2:Z:1300:SER:O	2.22	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
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
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
5:E:321:ALA:C	5:E:323:LEU:H	1.90	0.73
8:P:379:ILE:HG21	8:P:400:PHE:HE1	1.53	0.73
8:P:134:ARG:O	8:P:198:MET:HE3	1.89	0.72
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
7:O:1027:GLN:CD	7:O:1039:ALA:CB	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:K:320:GLU:C	5:K:322:ILE:N	2.48	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
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
8:P:134:ARG:O	8:P:198:MET:HE2	1.95	0.65
2:1:745:ILE:HG22	2:1:815:PHE:CZ	1.76	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
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
8:P:75:ILE:O	8:P:83:VAL:HG12	1.98	0.63
7:M:1036:PRO:C	7:M:1041:PHE:CD1	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:N:381:VAL:C	8:N:384:GLU:OE1	2.38	0.61
2:Z:1255:SER:HB2	2:Z:1301:SER:HB3	1.80	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
8:P:134:ARG:HB3	8:P:198:MET:HE3	1.82	0.61
1:Y:1257:GLN:HA	1:Y:1261:ARG:NH2	2.14	0.60
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:P:1058:GLU:CD	8:P:1064:GLU:OE1	2.40	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:326:LYS:H	5:B:327:PRO:HD3	1.66	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
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: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
1:0:831:LYS:HG2	1:0:923:ASP:OD2	2.05	0.56
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
8:N:382:PHE:C	8:N:384:GLU:H	2.09	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: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
1:0:834:ILE:O	1:0:914:TYR:OH	2.26	0.54
5:B:325:THR:C	5:B:335:TRP:CZ2	2.81	0.54
8:N:1303:LEU:HD21	8:N:1385:LEU:HD11	1.89	0.54
5:E:321:ALA:C	5:E:323:LEU:N	2.58	0.54
8:N:376:THR:O	8:N:379:ILE:CD1	2.47	0.54
8:N:72:ARG:NH1	8:N:84:ASP:CG	2.60	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:N:357:ASP:N	8:N:357:ASP:OD1	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:K:319:THR:C	5:K:321:ALA:H	2.11	0.52
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
8:N:52:ILE:O	8:N:131:ASP:CG	2.48	0.52
4:J:670:VAL:CG1	5:K:315:LYS:HG3	2.39	0.52
9:Q:681:SER:HG	10:U:322:LEU:HD11	1.71	0.52
8:N:378:VAL:O	8:N:378:VAL:HG22	2.09	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
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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Z:1257:GLY:C	2:Z:1299:LYS:CD	2.80	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
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
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
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
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
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
9:Q:681:SER:HG	10:U:322:LEU:CD1	2.25	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
8:N:382:PHE:N	8:N:384:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:Z:1257:GLY:C	2:Z:1299:LYS:HD2	2.34	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
1:0:1142:ARG:H	1:0:1142:ARG:HD3	1.80	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: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
7:M:1036:PRO:C	7:M:1041:PHE:HD1	2.17	0.46
8:P:1060:LEU:HD23	8:P:1060:LEU:H	1.80	0.46
8:P:42:GLN:C	8:P:45:LYS:NZ	2.67	0.46
6:I:371:LYS:H	6:I:371:LYS:HD2	1.79	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:1055:GLN:CD	8:N:1055:GLN:H	2.19	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:ARG:C	8:P:43:PHE:H	2.18	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
1:0:1318:HIS:CE1	1:0:1343: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
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
7:O:1040:THR:OG1	7:O:1040:THR:O	2.36	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
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
8:N:1292:GLU:CD	8:N:1303:LEU:N	2.72	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:Z:1257:GLY:C	2:Z:1299:LYS:HD3	2.37	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
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
1:0:1083:TYR:HB2	1:0:1092: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:324:TYR:HD1	5:B:324:TYR:HA	1.68	0.42
8:N:380:THR:CG2	8:N:414:ASN:ND2	2.62	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
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:51:LEU:C	8:P:133:ASP:CB	2.88	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
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
5:E:320:GLU:C	5:E:322:ILE:H	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:N:40:ILE:C	8:N:41:ARG:HG2	2.42	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:E:320:GLU:C	5:E:322:ILE:N	2.75	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
1:0:789:VAL:HG23	1:0:790: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 17
1	Y	1052/1502 (70%)	876 (83%)	110 (10%)	66 (6%)	1 17
2	1	1085/1391 (78%)	934 (86%)	98 (9%)	53 (5%)	2 20
2	Z	1082/1391 (78%)	934 (86%)	94 (9%)	54 (5%)	2 20
4	A	156/823 (19%)	152 (97%)	2 (1%)	2 (1%)	12 48
4	D	157/823 (19%)	152 (97%)	2 (1%)	3 (2%)	8 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	G	158/823 (19%)	153 (97%)	2 (1%)	3 (2%)	8 38
4	J	157/823 (19%)	149 (95%)	4 (2%)	4 (2%)	5 32
5	B	211/541 (39%)	188 (89%)	16 (8%)	7 (3%)	4 26
5	E	211/541 (39%)	188 (89%)	13 (6%)	10 (5%)	2 21
5	H	211/541 (39%)	177 (84%)	20 (10%)	14 (7%)	1 15
5	K	211/541 (39%)	196 (93%)	10 (5%)	5 (2%)	6 33
6	C	160/472 (34%)	150 (94%)	5 (3%)	5 (3%)	4 27
6	F	161/472 (34%)	155 (96%)	3 (2%)	3 (2%)	8 38
6	I	160/472 (34%)	151 (94%)	7 (4%)	2 (1%)	12 48
6	L	161/472 (34%)	156 (97%)	4 (2%)	1 (1%)	25 66
7	M	1496/1683 (89%)	1266 (85%)	162 (11%)	68 (4%)	2 22
7	O	1497/1683 (89%)	1265 (84%)	164 (11%)	68 (4%)	2 22
8	N	1308/1655 (79%)	1018 (78%)	188 (14%)	102 (8%)	1 13
8	P	1308/1655 (79%)	1020 (78%)	186 (14%)	102 (8%)	1 13
9	Q	671/839 (80%)	593 (88%)	53 (8%)	25 (4%)	3 24
9	R	691/839 (82%)	595 (86%)	76 (11%)	20 (3%)	4 29
9	S	671/839 (80%)	589 (88%)	62 (9%)	20 (3%)	4 28
9	T	691/839 (82%)	595 (86%)	66 (10%)	30 (4%)	2 22
10	U	89/475 (19%)	77 (86%)	6 (7%)	6 (7%)	1 15
10	W	89/475 (19%)	77 (86%)	9 (10%)	3 (3%)	3 26
11	V	88/528 (17%)	71 (81%)	10 (11%)	7 (8%)	1 12
11	X	89/528 (17%)	72 (81%)	11 (12%)	6 (7%)	1 15
All	All	15093/25168 (60%)	12819 (85%)	1522 (10%)	752 (5%)	4 20

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	994/1353 (74%)	952 (96%)	42 (4%)	30	54
1	Y	977/1353 (72%)	945 (97%)	32 (3%)	38	61
2	1	1007/1250 (81%)	962 (96%)	45 (4%)	27	52
2	Z	1004/1250 (80%)	974 (97%)	30 (3%)	41	63
4	A	154/674 (23%)	147 (96%)	7 (4%)	27	52
4	D	154/674 (23%)	151 (98%)	3 (2%)	57	75
4	G	155/674 (23%)	146 (94%)	9 (6%)	20	45
4	J	154/674 (23%)	147 (96%)	7 (4%)	27	52
5	B	196/439 (45%)	185 (94%)	11 (6%)	21	46
5	E	196/439 (45%)	187 (95%)	9 (5%)	27	52
5	H	196/439 (45%)	185 (94%)	11 (6%)	21	46
5	K	196/439 (45%)	189 (96%)	7 (4%)	35	59
6	C	155/377 (41%)	147 (95%)	8 (5%)	23	48
6	F	155/377 (41%)	151 (97%)	4 (3%)	46	66
6	I	155/377 (41%)	148 (96%)	7 (4%)	27	52
6	L	155/377 (41%)	152 (98%)	3 (2%)	57	75
7	M	1279/1538 (83%)	1235 (97%)	44 (3%)	37	60
7	O	1279/1538 (83%)	1233 (96%)	46 (4%)	35	59
8	N	1276/1557 (82%)	1204 (94%)	72 (6%)	21	46
8	P	1276/1557 (82%)	1215 (95%)	61 (5%)	25	50
9	Q	508/762 (67%)	493 (97%)	15 (3%)	41	63
9	R	507/762 (66%)	494 (97%)	13 (3%)	46	66
9	S	507/762 (66%)	496 (98%)	11 (2%)	52	71
9	T	507/762 (66%)	497 (98%)	10 (2%)	55	74
10	U	79/421 (19%)	76 (96%)	3 (4%)	33	57
10	W	79/421 (19%)	75 (95%)	4 (5%)	24	48
11	V	80/477 (17%)	78 (98%)	2 (2%)	47	68
11	X	81/477 (17%)	78 (96%)	3 (4%)	34	58
All	All	13461/22200 (61%)	12942 (96%)	519 (4%)	36	56

All (519) 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	208	LYS
1	0	249	LYS
1	0	315	THR
1	0	358	GLN
1	0	385	LYS
1	0	404	THR
1	0	408	ARG
1	0	471	SER
1	0	607	GLN
1	0	630	THR
1	0	643	THR
1	0	654	THR
1	0	771	TYR
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	1009	HIS
1	0	1105	TYR
1	0	1142	ARG
1	0	1155	ARG
1	0	1187	MET
1	0	1188	GLU
1	0	1199	ILE
1	0	1258	LEU
1	0	1261	ARG
1	0	1267	GLU
1	0	1278	LEU
1	0	1285	ILE
1	0	1302	LEU
1	0	1331	ARG
1	0	1389	GLU
1	0	1405	GLU
1	0	1446	LYS
1	0	1461	LYS
2	1	88	SER

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Mol	Chain	Res	Type
2	1	96	GLU
2	1	119	LYS
2	1	178	ASN
2	1	180	LEU
2	1	219	GLU
2	1	240	ARG
2	1	244	LEU
2	1	268	ARG
2	1	275	THR
2	1	309	LEU
2	1	364	ARG
2	1	395	ASN
2	1	402	ARG
2	1	440	ARG
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
2	1	625	ILE
2	1	653	LYS
2	1	678	LYS
2	1	679	SER
2	1	724	TRP
2	1	858	LYS
2	1	861	GLN
2	1	922	LYS
2	1	973	LYS
2	1	994	ARG
2	1	1043	VAL
2	1	1056	HIS
2	1	1078	GLN
2	1	1125	LEU
2	1	1155	GLN
2	1	1156	LEU
2	1	1169	ILE
2	1	1178	ARG
2	1	1246	LYS
2	1	1258	GLN
2	1	1299	LYS

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Mol	Chain	Res	Type
2	1	1301	SER
2	1	1338	LEU
4	A	695	GLN
4	A	754	ASN
4	A	755	LEU
4	A	756	ASN
4	A	776	PHE
4	A	795	LYS
4	A	822	LYS
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	355	PHE
5	B	361	ARG
5	B	436	MET
5	B	446	ARG
5	B	471	LYS
6	C	304	LEU
6	C	344	LEU
6	C	369	LEU
6	C	370	ASP
6	C	383	LYS
6	C	451	MET
6	C	461	HIS
6	C	462	GLN
4	D	657	GLN
4	D	690	GLN
4	D	715	GLU
5	E	305	LYS
5	E	324	TYR
5	E	347	THR
5	E	356	GLU
5	E	371	GLN
5	E	415	LEU
5	E	423	LYS
5	E	435	LYS
5	E	446	ARG
6	F	370	ASP
6	F	375	LYS

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Mol	Chain	Res	Type
6	F	447	PHE
6	F	449	LEU
4	G	695	GLN
4	G	698	GLN
4	G	715	GLU
4	G	727	SER
4	G	754	ASN
4	G	755	LEU
4	G	756	ASN
4	G	795	LYS
4	G	822	LYS
5	H	309	ARG
5	H	317	ASN
5	H	318	GLU
5	H	320	GLU
5	H	324	TYR
5	H	392	LEU
5	H	410	LYS
5	H	436	MET
5	H	446	ARG
5	H	471	LYS
5	H	525	GLU
6	I	304	LEU
6	I	331	LYS
6	I	369	LEU
6	I	370	ASP
6	I	383	LYS
6	I	451	MET
6	I	462	GLN
4	J	650	GLU
4	J	690	GLN
4	J	695	GLN
4	J	715	GLU
4	J	719	GLU
4	J	722	LEU
4	J	776	PHE
5	K	294	LYS
5	K	319	THR
5	K	320	GLU
5	K	331	LEU
5	K	435	LYS
5	K	446	ARG

Continued on next page...

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Mol	Chain	Res	Type
5	K	508	LYS
6	L	292	HIS
6	L	353	LEU
6	L	375	LYS
7	M	2	LYS
7	M	121	VAL
7	M	180	LYS
7	M	197	LEU
7	M	222	GLU
7	M	228	PHE
7	M	277	LEU
7	M	288	TRP
7	M	295	ARG
7	M	333	GLU
7	M	336	LYS
7	M	426	GLN
7	M	449	LEU
7	M	538	GLU
7	M	553	ILE
7	M	681	LYS
7	M	727	GLU
7	M	750	TRP
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	1344	GLU
7	M	1347	ILE
7	M	1396	LEU
7	M	1402	ARG
7	M	1408	LEU
7	M	1436	LYS
7	M	1482	THR

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Mol	Chain	Res	Type
7	M	1484	ARG
7	M	1487	LEU
7	M	1490	ARG
7	M	1498	LEU
7	M	1516	THR
7	M	1523	PHE
8	N	32	VAL
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	140	LYS
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	318	HIS
8	N	359	LEU
8	N	379	ILE
8	N	381	VAL
8	N	382	PHE
8	N	406	LYS
8	N	413	GLU
8	N	447	LEU
8	N	451	GLU
8	N	457	LEU
8	N	552	LEU
8	N	564	LEU
8	N	577	MET
8	N	656	GLN
8	N	659	GLU
8	N	729	HIS
8	N	745	HIS
8	N	753	TYR
8	N	763	GLN
8	N	764	LYS

Continued on next page...

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Mol	Chain	Res	Type
8	N	766	GLU
8	N	794	ILE
8	N	833	LYS
8	N	868	LEU
8	N	874	GLU
8	N	903	LEU
8	N	913	ASN
8	N	923	LEU
8	N	933	LYS
8	N	950	ARG
8	N	982	ILE
8	N	1021	THR
8	N	1031	LYS
8	N	1056	LYS
8	N	1060	LEU
8	N	1094	SER
8	N	1096	ILE
8	N	1231	GLU
8	N	1237	ASN
8	N	1252	LEU
8	N	1254	ARG
8	N	1259	PHE
8	N	1276	LYS
8	N	1277	ILE
8	N	1292	GLU
8	N	1303	LEU
8	N	1304	LYS
8	N	1309	ARG
8	N	1316	LEU
8	N	1317	VAL
8	N	1400	PRO
8	N	1431	ILE
8	N	1446	PHE
8	N	1459	LYS
8	N	1527	LYS
8	N	1596	LYS
7	O	2	LYS
7	O	121	VAL
7	O	180	LYS
7	O	197	LEU
7	O	222	GLU
7	O	228	PHE

Continued on next page...

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Mol	Chain	Res	Type
7	O	277	LEU
7	O	288	TRP
7	O	295	ARG
7	O	333	GLU
7	O	336	LYS
7	O	426	GLN
7	O	449	LEU
7	O	538	GLU
7	O	553	ILE
7	O	681	LYS
7	O	727	GLU
7	O	750	TRP
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
7	O	1138	PHE
7	O	1158	THR
7	O	1183	TYR
7	O	1189	MET
7	O	1191	SER
7	O	1273	LYS
7	O	1318	LYS
7	O	1319	LEU
7	O	1320	GLU
7	O	1344	GLU
7	O	1347	ILE
7	O	1396	LEU
7	O	1402	ARG
7	O	1408	LEU
7	O	1436	LYS
7	O	1482	THR
7	O	1484	ARG
7	O	1490	ARG
7	O	1498	LEU
7	O	1516	THR
7	O	1523	PHE
8	P	22	MET
8	P	40	ILE

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Mol	Chain	Res	Type
8	P	42	GLN
8	P	72	ARG
8	P	73	SER
8	P	131	ASP
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	422	GLU
8	P	448	ILE
8	P	527	LYS
8	P	552	LEU
8	P	647	GLN
8	P	659	GLU
8	P	707	PHE
8	P	766	GLU
8	P	794	ILE
8	P	869	LYS
8	P	874	GLU
8	P	897	LYS
8	P	1021	THR
8	P	1031	LYS
8	P	1035	LYS
8	P	1038	LYS
8	P	1046	LYS
8	P	1054	PHE
8	P	1055	GLN
8	P	1056	LYS
8	P	1057	LYS
8	P	1062	ARG
8	P	1065	THR
8	P	1075	ILE
8	P	1077	ARG
8	P	1095	GLU
8	P	1178	LYS
8	P	1207	TRP

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Mol	Chain	Res	Type
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	1309	ARG
8	P	1346	LYS
8	P	1462	ASN
8	P	1527	LYS
8	P	1530	LYS
8	P	1566	TYR
8	P	1596	LYS
8	P	1619	THR
8	P	1647	LEU
9	Q	234	ILE
9	Q	329	ASN
9	Q	422	ARG
9	Q	437	TRP
9	Q	460	GLU
9	Q	501	MET
9	Q	533	ARG
9	Q	543	LYS
9	Q	592	LYS
9	Q	626	GLN
9	Q	645	GLN
9	Q	672	GLN
9	Q	754	ARG
9	Q	755	LYS
9	Q	766	ASN
9	R	222	PHE
9	R	266	LYS
9	R	321	LYS
9	R	334	TRP
9	R	347	LYS
9	R	411	VAL
9	R	444	LYS
9	R	514	LYS
9	R	533	ARG
9	R	592	LYS

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Mol	Chain	Res	Type
9	R	754	ARG
9	R	766	ASN
9	R	793	LYS
9	S	226	ARG
9	S	312	LYS
9	S	314	LYS
9	S	359	ASN
9	S	514	LYS
9	S	663	ASP
9	S	672	GLN
9	S	727	TYR
9	S	729	ASN
9	S	754	ARG
9	S	824	MET
9	T	232	PHE
9	T	276	GLN
9	T	315	LYS
9	T	413	LYS
9	T	422	ARG
9	T	473	ARG
9	T	543	LYS
9	T	551	ARG
9	T	617	LYS
9	T	754	ARG
10	U	249	ASP
10	U	260	GLU
10	U	304	LYS
11	V	296	GLU
11	V	355	TRP
10	W	248	TRP
10	W	249	ASP
10	W	304	LYS
10	W	305	TYR
11	X	276	TYR
11	X	302	ARG
11	X	399	LYS
1	Y	101	LEU
1	Y	124	ARG
1	Y	126	TYR
1	Y	188	ASN
1	Y	198	ASP
1	Y	207	MET

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Mol	Chain	Res	Type
1	Y	273	ILE
1	Y	274	VAL
1	Y	278	ARG
1	Y	296	LEU
1	Y	374	LYS
1	Y	382	ILE
1	Y	432	ASN
1	Y	454	ARG
1	Y	465	ILE
1	Y	532	PHE
1	Y	577	PHE
1	Y	618	THR
1	Y	791	MET
1	Y	831	LYS
1	Y	992	CYS
1	Y	1096	GLN
1	Y	1142	ARG
1	Y	1155	ARG
1	Y	1187	MET
1	Y	1207	ARG
1	Y	1238	ARG
1	Y	1258	LEU
1	Y	1261	ARG
1	Y	1267	GLU
1	Y	1276	LEU
1	Y	1292	GLU
2	Z	110	ILE
2	Z	116	TYR
2	Z	162	ASP
2	Z	168	GLU
2	Z	178	ASN
2	Z	234	THR
2	Z	240	ARG
2	Z	246	ILE
2	Z	252	LYS
2	Z	431	ARG
2	Z	440	ARG
2	Z	491	THR
2	Z	509	THR
2	Z	548	LEU
2	Z	568	LYS
2	Z	586	TYR

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Mol	Chain	Res	Type
2	Z	605	THR
2	Z	679	SER
2	Z	724	TRP
2	Z	745	ILE
2	Z	798	LEU
2	Z	830	MET
2	Z	858	LYS
2	Z	922	LYS
2	Z	976	LYS
2	Z	1040	LYS
2	Z	1078	GLN
2	Z	1156	LEU
2	Z	1299	LYS
2	Z	1371	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	911	ASN
1	0	1158	HIS
1	0	1318	HIS
1	0	1379	GLN
1	0	1453	HIS
2	1	184	ASN
2	1	192	HIS
2	1	355	HIS
2	1	1175	ASN
4	A	654	HIS
4	A	690	GLN
5	B	332	GLN
5	B	351	GLN
5	B	390	HIS
5	B	402	GLN
5	B	418	GLN
6	C	289	GLN
6	C	374	GLN
4	D	690	GLN
5	E	329	HIS
6	F	461	HIS
5	H	317	ASN
6	I	348	GLN
6	I	374	GLN

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Mol	Chain	Res	Type
5	K	359	ASN
6	L	293	HIS
6	L	461	HIS
7	M	9	GLN
7	M	714	HIS
7	M	720	HIS
7	M	1123	ASN
7	M	1187	ASN
7	M	1304	HIS
7	M	1326	ASN
7	M	1494	ASN
7	M	1541	ASN
8	N	12	GLN
8	N	42	GLN
8	N	414	ASN
8	N	1479	GLN
7	O	9	GLN
7	O	714	HIS
7	O	720	HIS
7	O	1037	ASN
7	O	1123	ASN
7	O	1187	ASN
7	O	1304	HIS
7	O	1326	ASN
7	O	1494	ASN
7	O	1541	ASN
8	P	42	GLN
8	P	50	ASN
8	P	178	GLN
8	P	356	HIS
8	P	745	HIS
8	P	1088	ASN
8	P	1093	ASN
8	P	1249	GLN
8	P	1509	GLN
9	Q	439	HIS
9	Q	573	HIS
9	Q	612	HIS
9	Q	821	GLN
9	R	505	HIS
9	R	612	HIS
9	R	658	ASN

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Mol	Chain	Res	Type
9	R	784	ASN
9	S	281	GLN
9	S	505	HIS
9	S	612	HIS
9	S	738	GLN
9	S	812	GLN
9	T	439	HIS
9	T	612	HIS
9	T	621	HIS
9	T	733	GLN
9	T	808	ASN
1	Y	180	ASN
1	Y	196	ASN
1	Y	230	HIS
1	Y	276	HIS
1	Y	862	GLN
1	Y	1082	GLN
1	Y	1224	ASN
1	Y	1240	ASN
1	Y	1318	HIS
1	Y	1406	HIS
2	Z	142	GLN
2	Z	271	GLN
2	Z	344	GLN
2	Z	355	HIS
2	Z	588	ASN
2	Z	1159	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

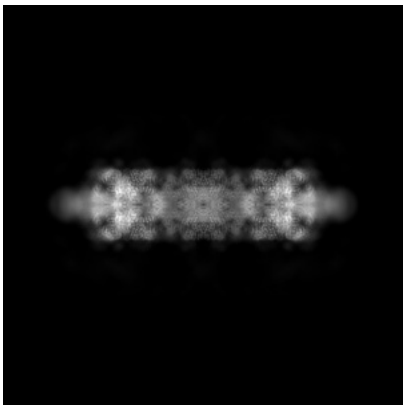
6 Map visualisation

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.

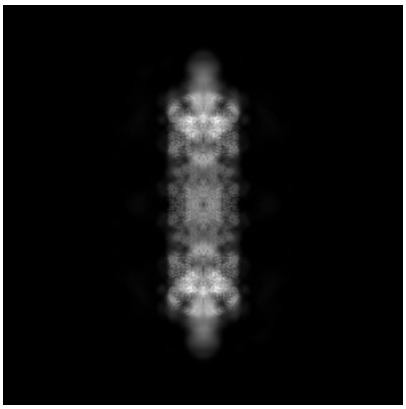
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

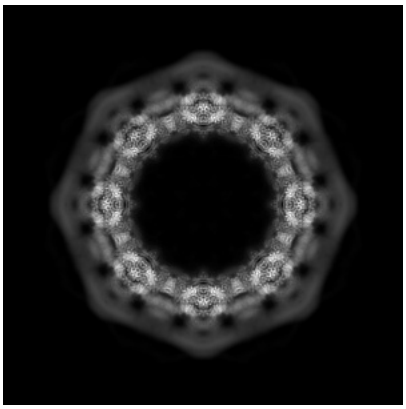
6.1.1 Primary map



X

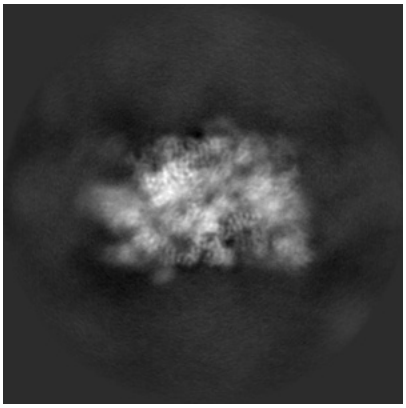


Y

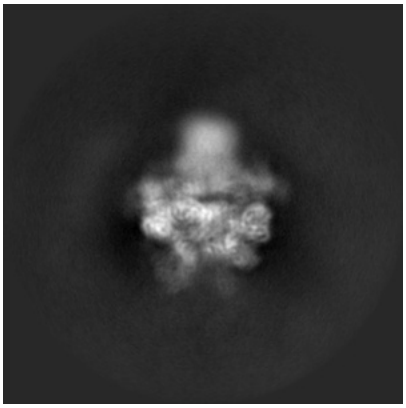


Z

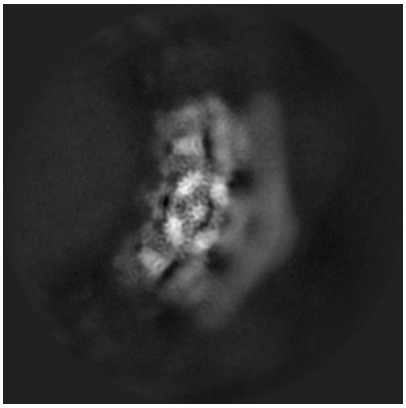
6.1.2 Raw map



X



Y

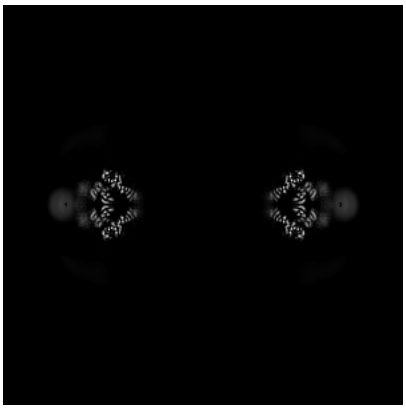


Z

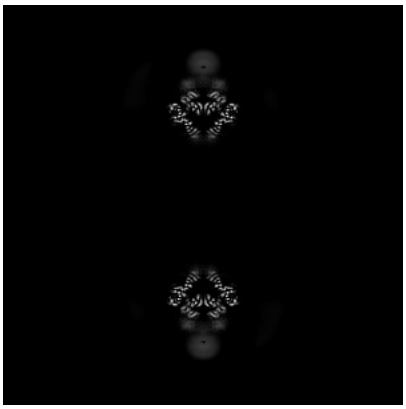
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

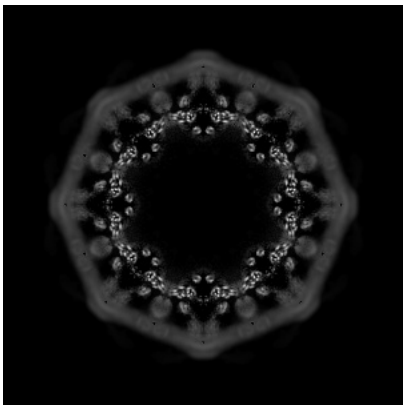
6.2.1 Primary map



X Index: 240

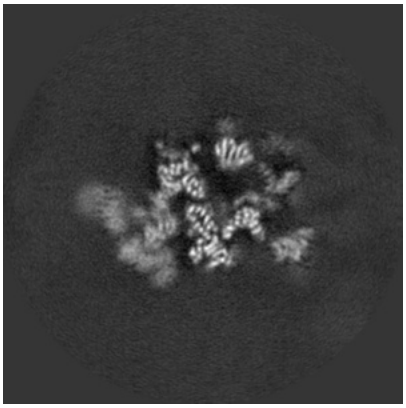


Y Index: 240

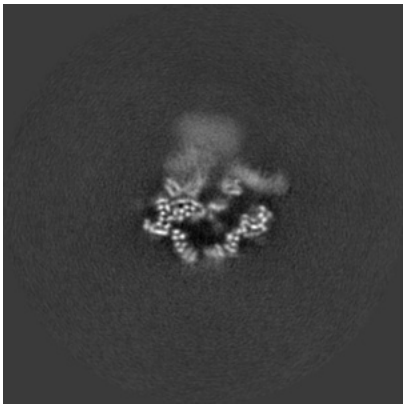


Z Index: 240

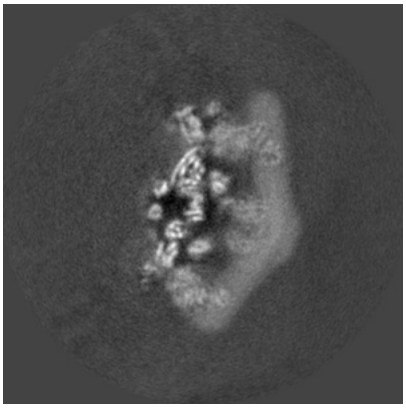
6.2.2 Raw map



X Index: 133



Y Index: 133

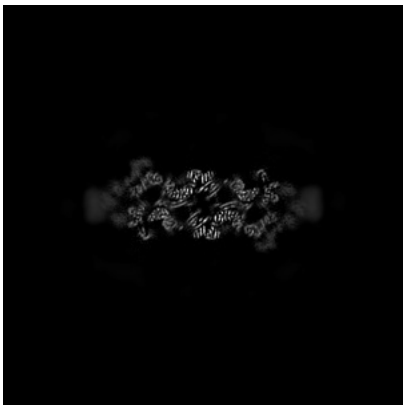


Z Index: 133

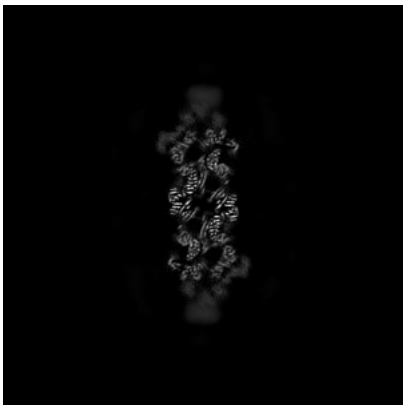
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

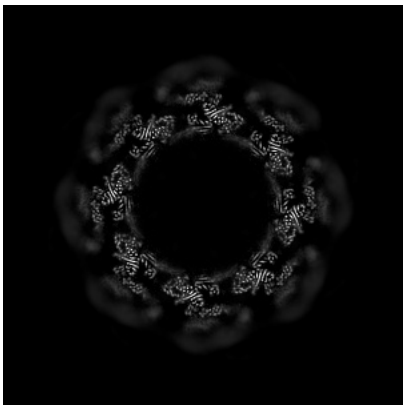
6.3.1 Primary map



X Index: 340

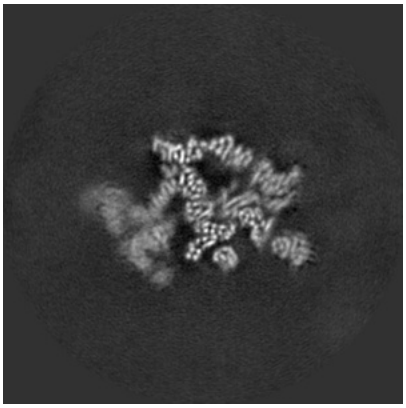


Y Index: 140

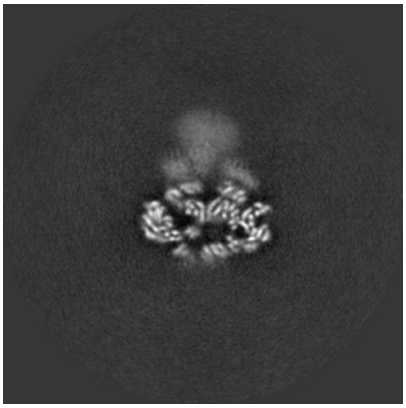


Z Index: 257

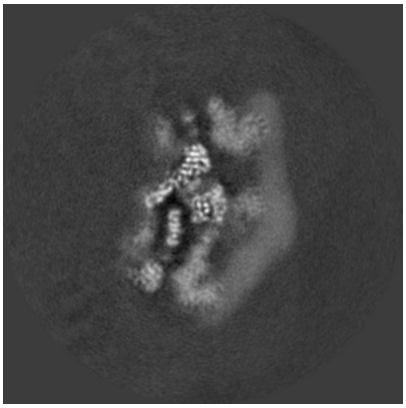
6.3.2 Raw map



X Index: 129



Y Index: 126

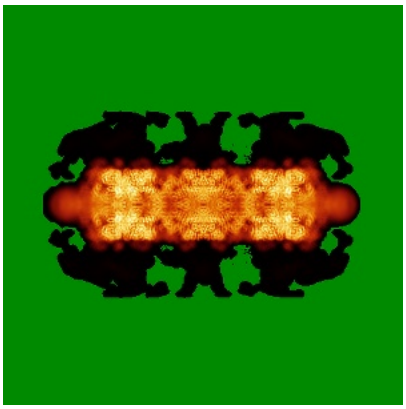


Z Index: 125

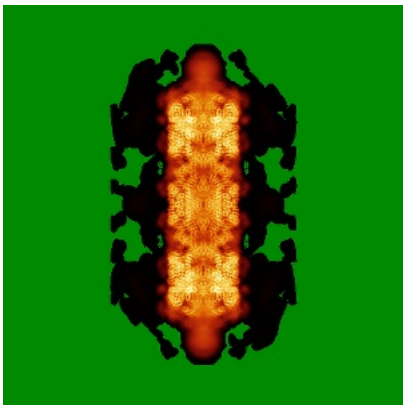
The images above show the largest variance slices of the map in three orthogonal directions.

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

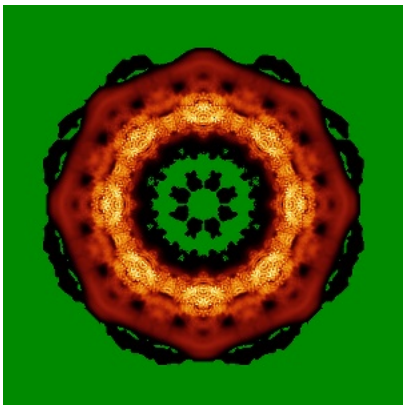
6.4.1 Primary map



X

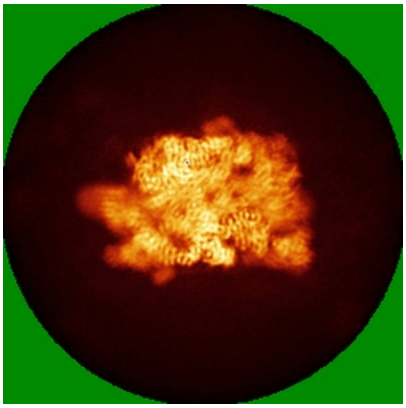


Y

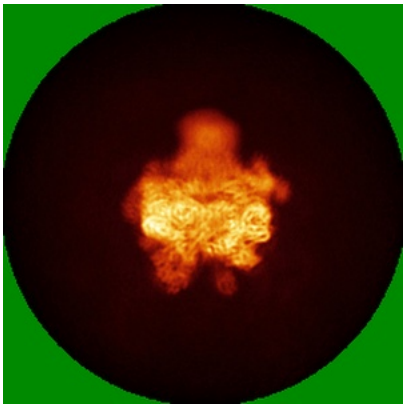


Z

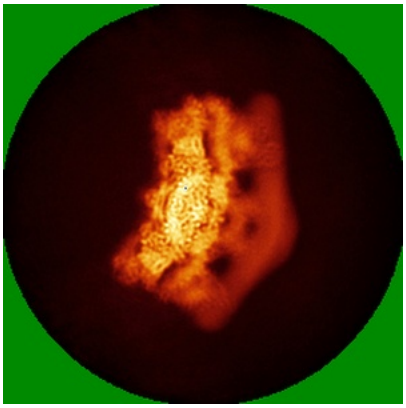
6.4.2 Raw map



X



Y

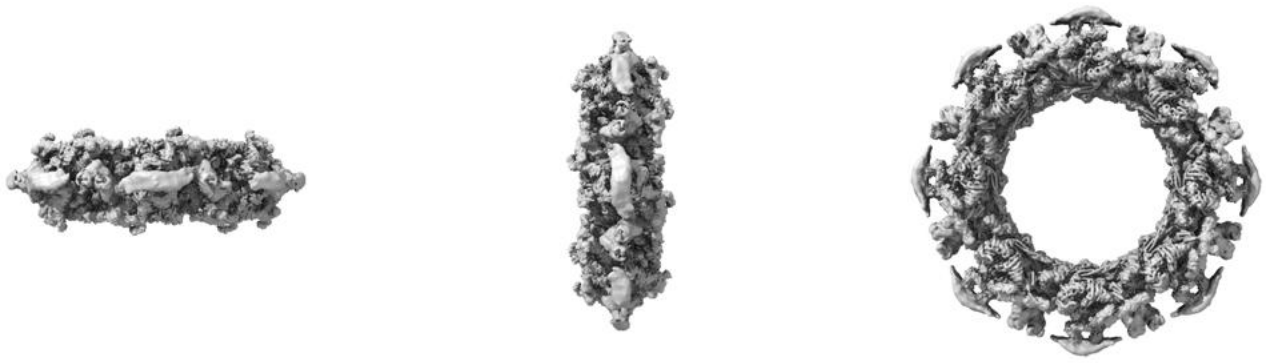


Z

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)

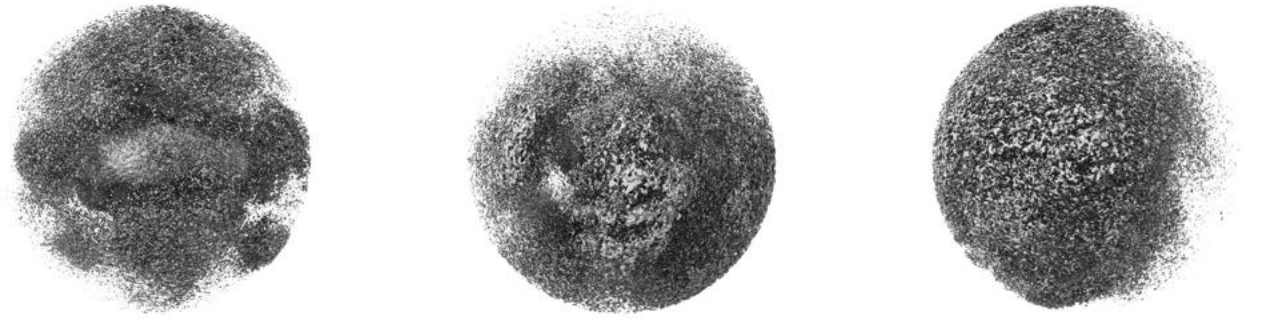
6.5.1 Primary map



X Y Z

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



X Y Z

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

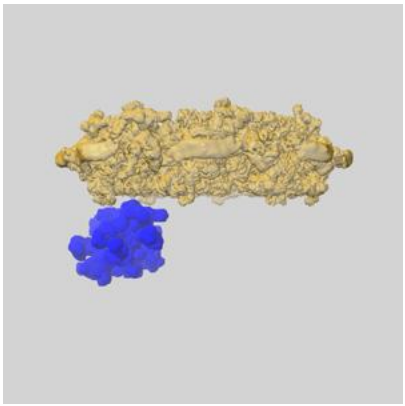
6.6 Mask visualisation (i)

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

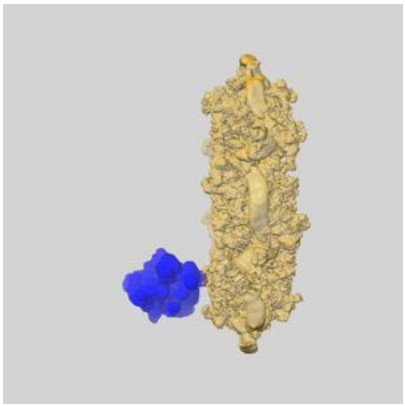
A mask typically either:

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

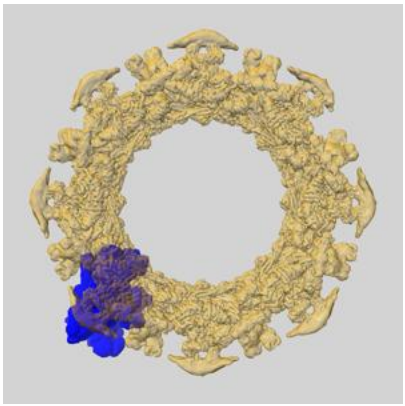
6.6.1 emd_24232_msk_1.map (i)



X



Y

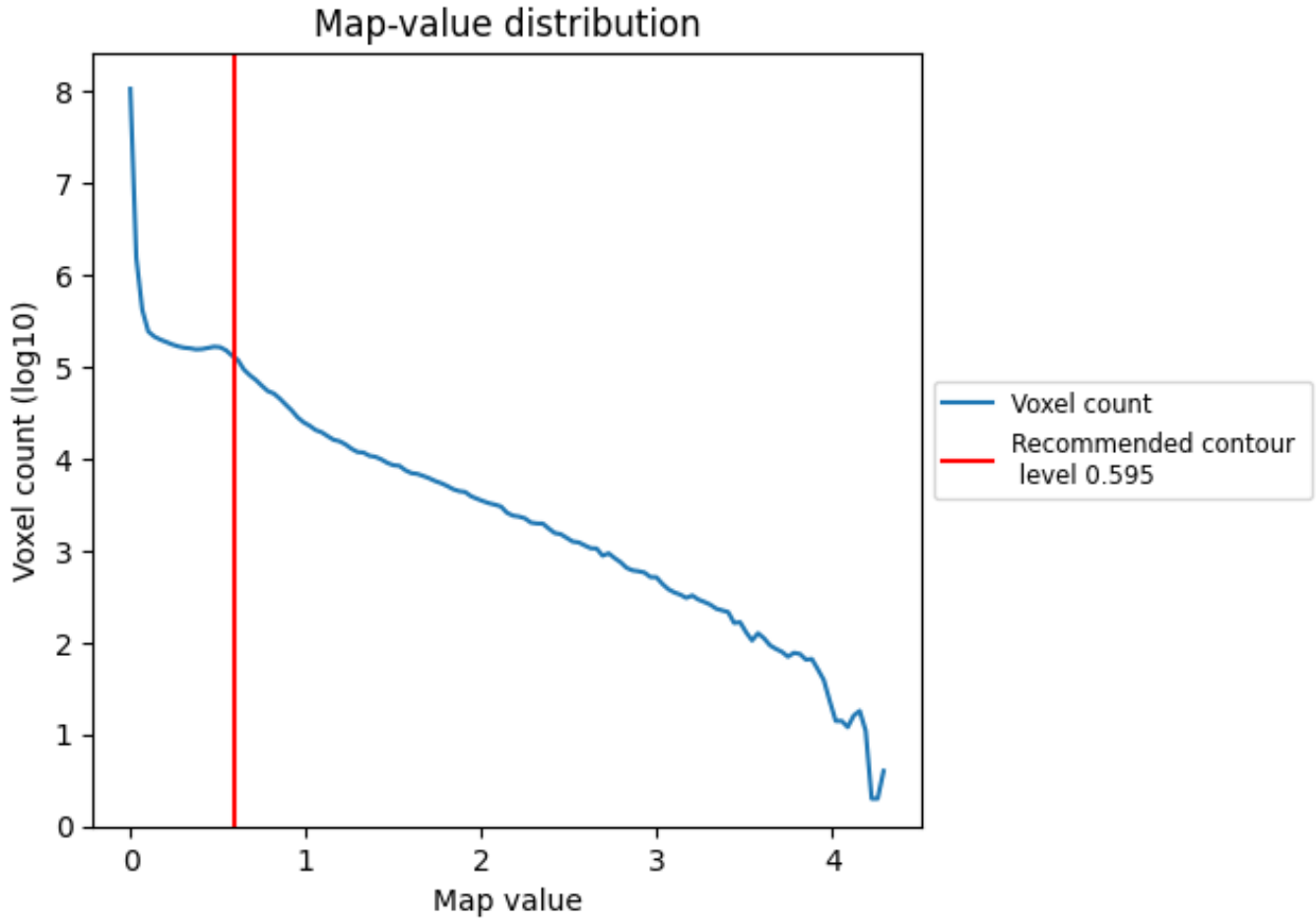


Z

7 Map analysis

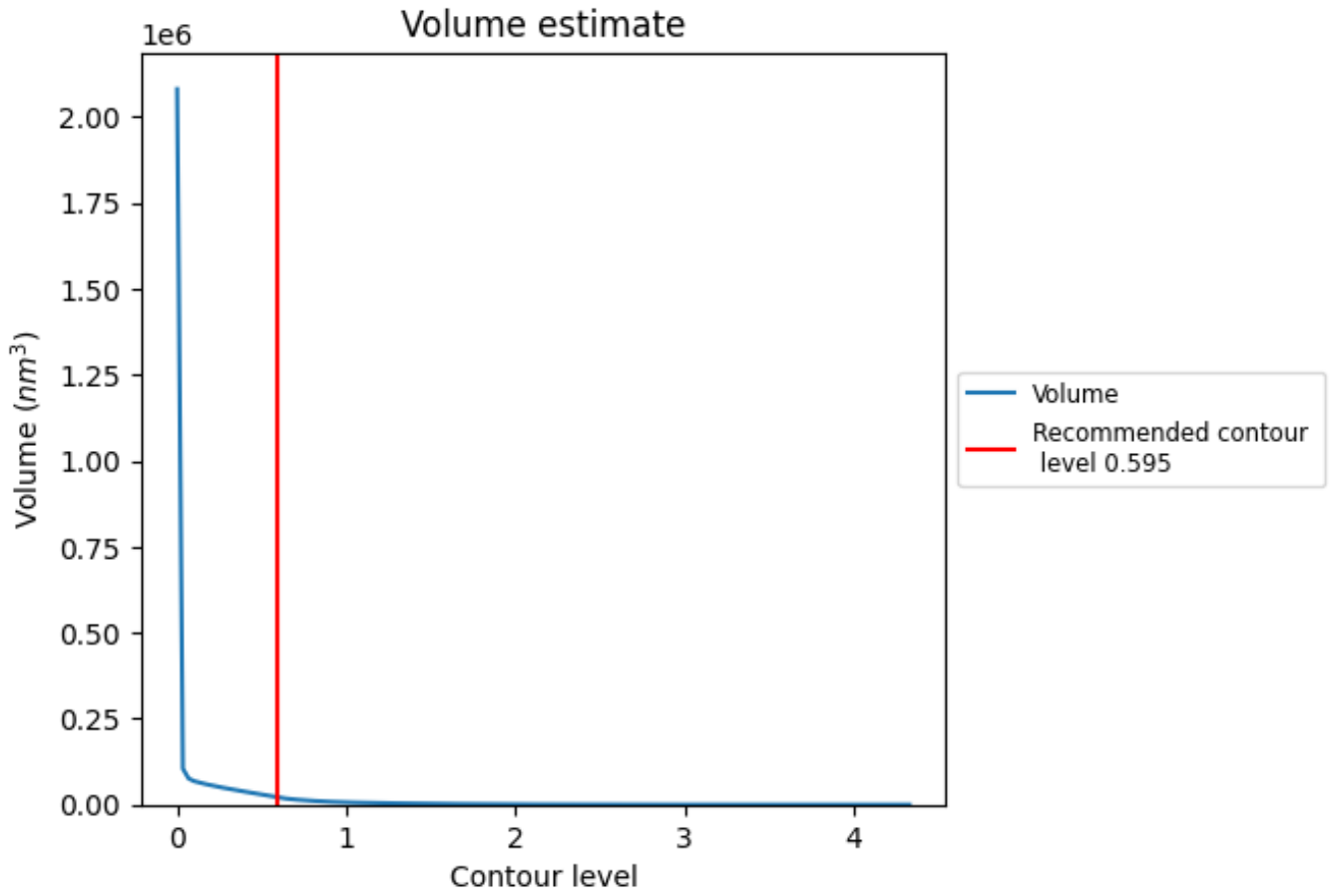
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

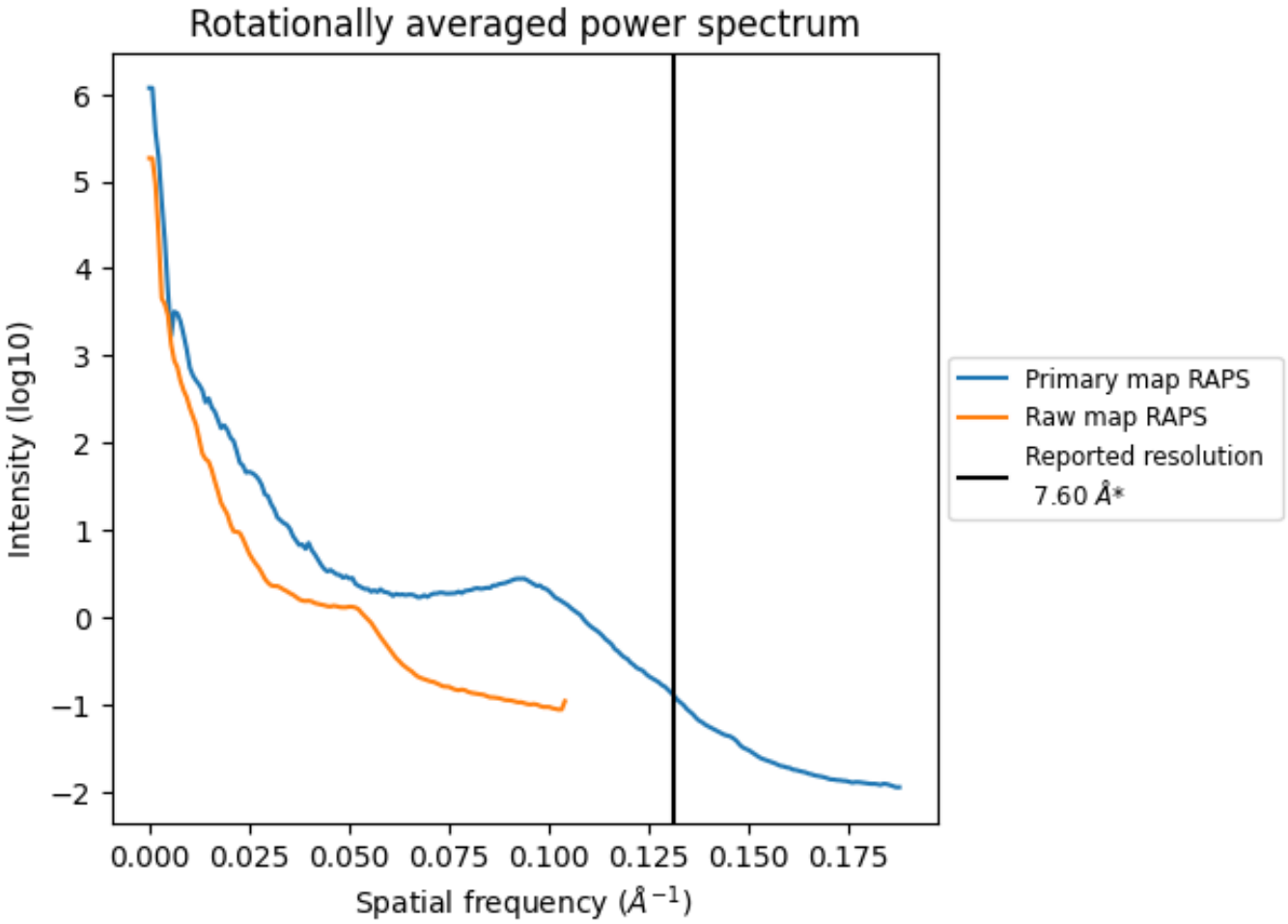
7.2 Volume estimate



The volume at the recommended contour level is 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 (i)

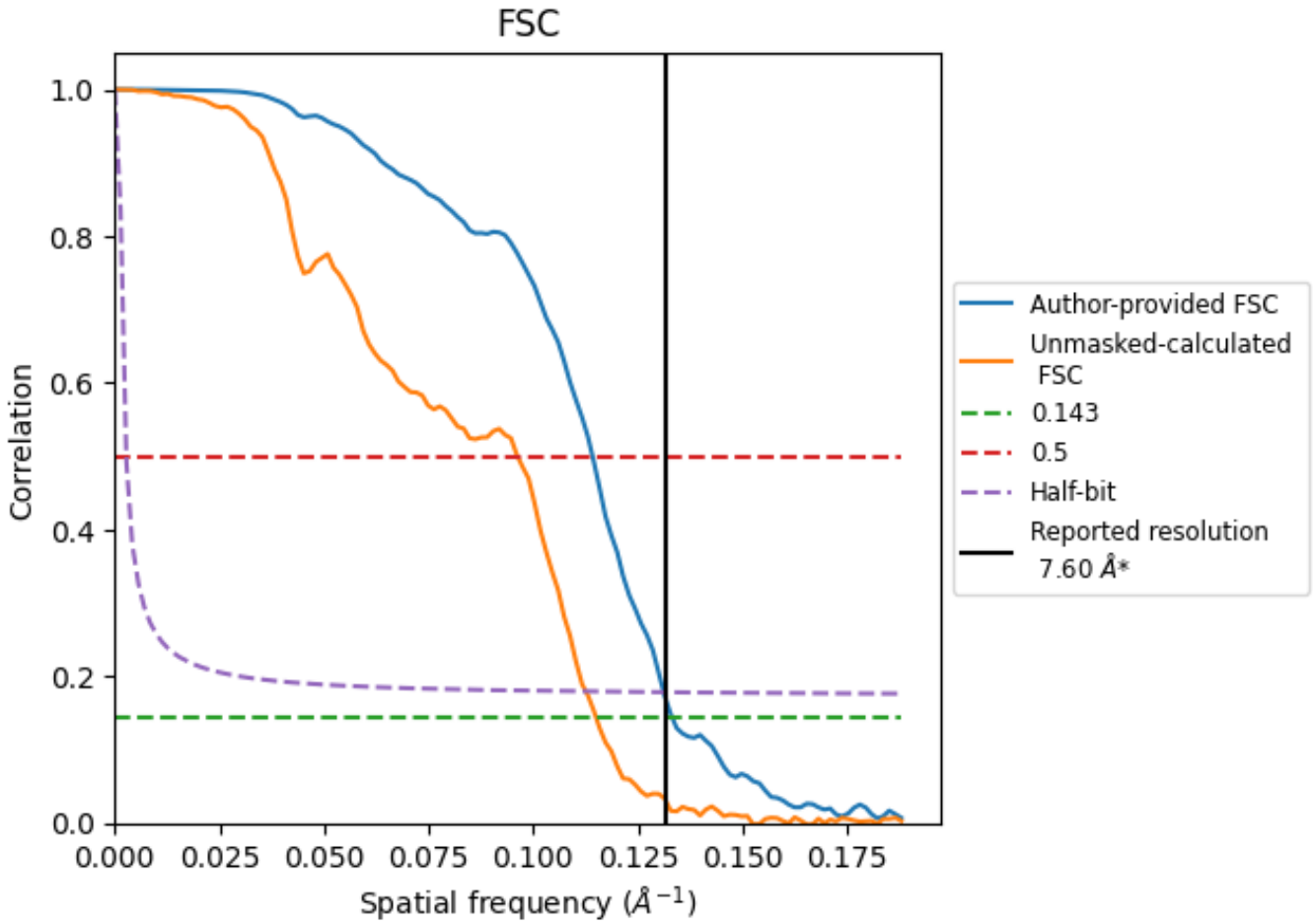


*Reported resolution corresponds to spatial frequency of 0.132 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.132 Å^{-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

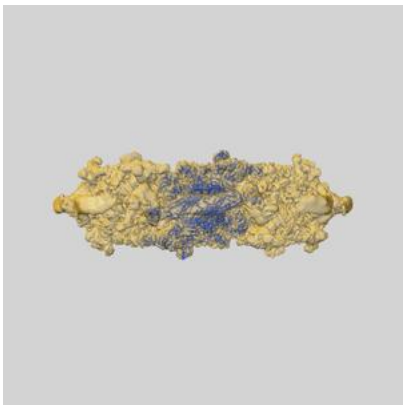
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.69 differs from the reported value 7.6 by more than 10 %

9 Map-model fit

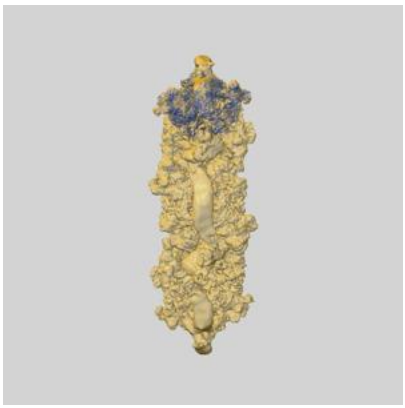
This section contains information regarding the fit between EMDB map EMD-24232 and PDB model 7N85. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

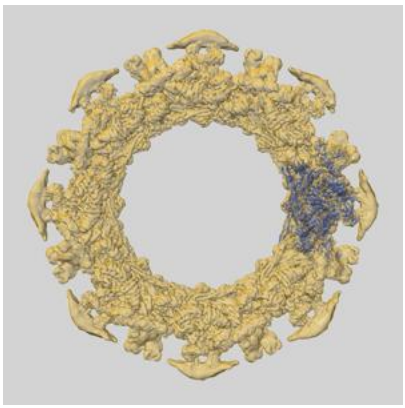
9.1.1 Map-model overlay



X

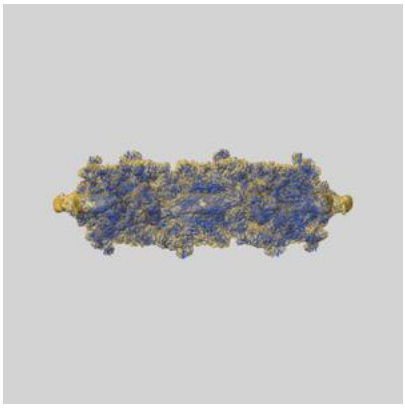


Y

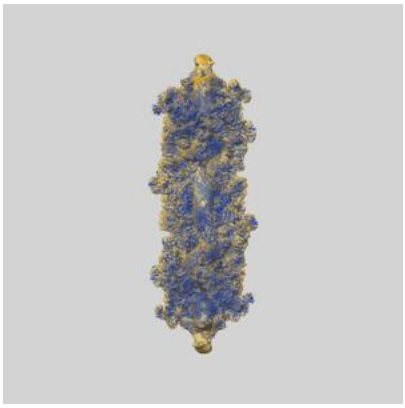


Z

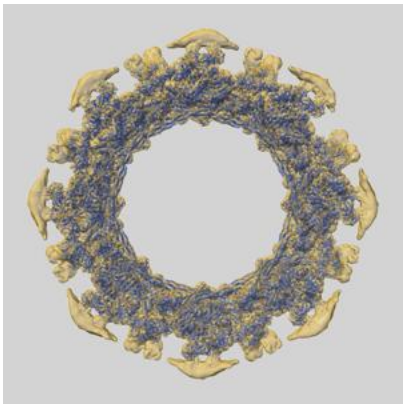
9.1.2 Map-model assembly overlay



X



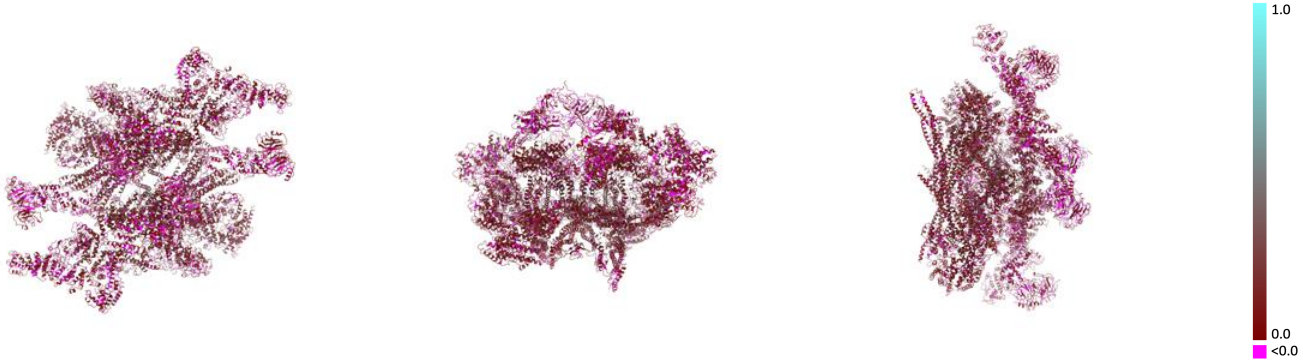
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.595 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.

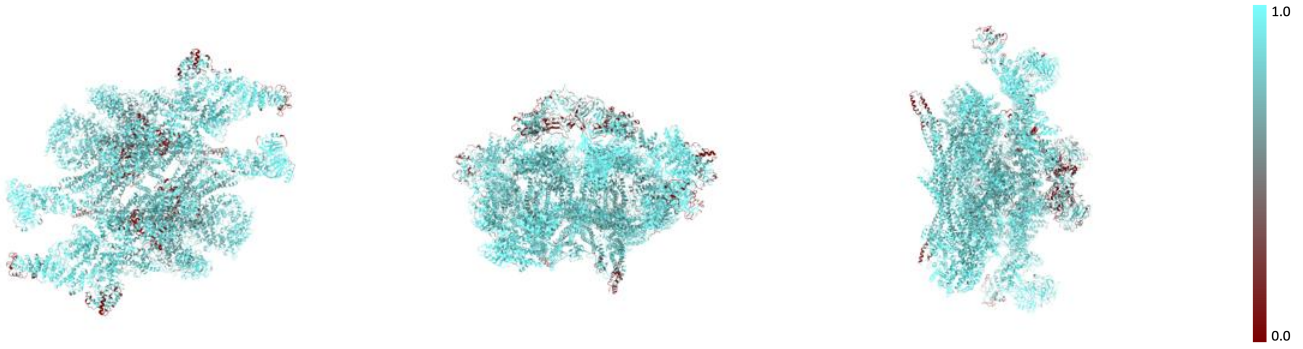
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

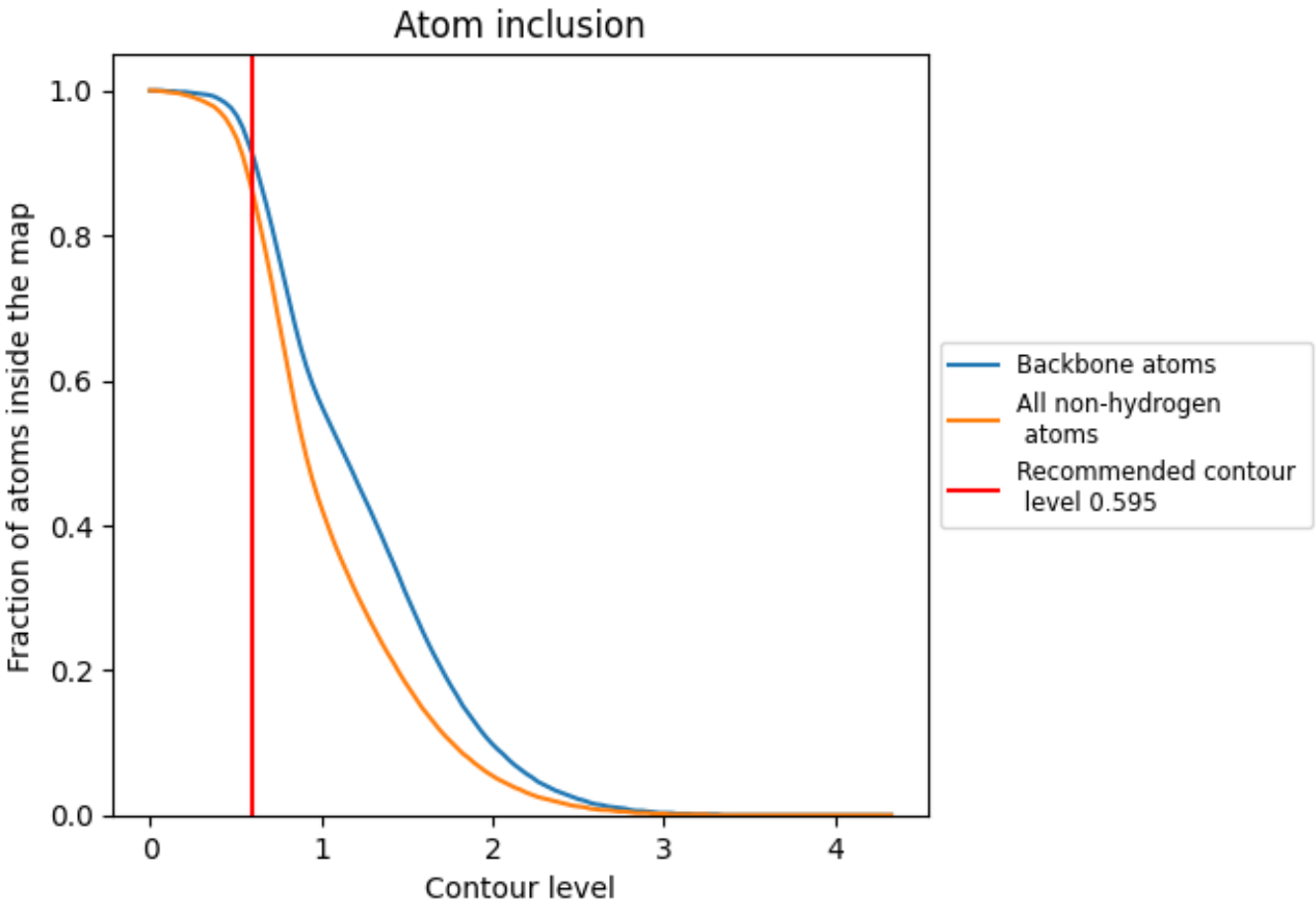
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

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