



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:29 PM BST

PDB ID : 5A9Q
EMDB ID: : EMD-3103
Title : Human nuclear pore complex
Authors : von Appen, A.; Kosinski, J.; Sparks, L.; Ori, A.; DiGuilio, A.; Vollmer, B.; Mackmull, M.; Banterle, N.; Parca, L.; Kastitis, P.; Buczak, K.; Mosalaganti, S.; Hagen, W.; Andres-Pons, A.; Lemke, E.A.; Bork, P.; Antonin, W.; Glavy, J.S.; Bui, K.H.; Beck, M.
Deposited on : 2015-07-22
Resolution : 23.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

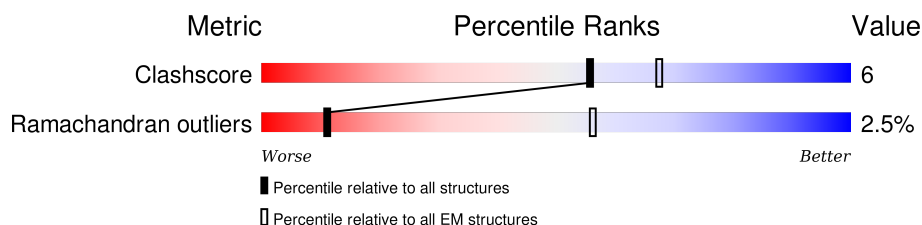
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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	114402	924
Ramachandran outliers	111179	726

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	380	 82% 17%
1	9	380	 82% 17%
1	I	380	 82% 17%
1	R	380	 82% 17%
2	1	1436	 65% 5% 30%
2	J	1436	 65% 5% 30%
2	S	1436	 65% 5% 30%
2	a	1436	 68% 30%
3	2	326	 84% 11%
3	K	326	 84% 11%
3	T	326	 84% 11%

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Mol	Chain	Length	Quality of chain
3	b	326	 90% 6% ..
4	3	1156	 40% 5% . 54%
4	C	1156	 41% . . 54%
4	L	1156	 41% . . 54%
4	U	1156	 41% . . 54%
5	4	925	 70% . 29%
5	D	925	 69% . 29%
5	M	925	 70% . 29%
5	V	925	 69% . 29%
6	5	937	 42% . 55%
6	E	937	 42% . 55%
6	N	937	 42% . 55%
6	W	937	 42% . 55%
7	6	322	 76% 12% . 11%
7	F	322	 75% 12% . 11%
7	O	322	 76% 12% . 11%
7	X	322	 76% 12% . 11%
8	7	360	 79% 8% . 11%
8	G	360	 79% 8% . 11%
8	P	360	 79% 8% . 11%
8	Y	360	 79% 8% . 11%
9	8	656	 63% . 34%
9	H	656	 63% . 34%
9	Q	656	 63% . 34%
9	Z	656	 63% . 34%

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Mol	Chain	Length	Quality of chain
10	A	1391	<div><div></div><div>74%</div><div></div><div>•</div><div>21%</div></div>
10	B	1391	<div><div></div><div>72%</div><div></div><div>6%</div><div>•</div><div>21%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 95884 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 NUP43.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	316	Total	C	N	O	0	0
			1562	930	316	316		
1	9	316	Total	C	N	O	0	0
			1562	930	316	316		
1	I	316	Total	C	N	O	0	0
			1562	930	316	316		
1	R	316	Total	C	N	O	0	0
			1562	930	316	316		

- Molecule 2 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP160.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	1009	Total	C	N	O	0	0
			4997	2979	1009	1009		
2	J	1009	Total	C	N	O	0	0
			4997	2979	1009	1009		
2	S	1009	Total	C	N	O	0	0
			4997	2979	1009	1009		
2	a	1009	Total	C	N	O	0	0
			4997	2979	1009	1009		

- Molecule 3 is a protein called NUCLEOPORIN NUP37.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	318	Total	C	N	O	0	0
			1566	930	318	318		
3	K	318	Total	C	N	O	0	0
			1566	930	318	318		
3	T	318	Total	C	N	O	0	0
			1566	930	318	318		
3	b	318	Total	C	N	O	0	0
			1566	930	318	318		

- Molecule 4 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP133.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	528	Total	C	N	O	0	0
			2629	1573	528	528		
4	C	528	Total	C	N	O	0	0
			2629	1573	528	528		
4	L	528	Total	C	N	O	0	0
			2629	1573	528	528		
4	U	528	Total	C	N	O	0	0
			2629	1573	528	528		

- Molecule 5 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP107.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	660	Total	C	N	O	0	0
			3278	1958	660	660		
5	D	660	Total	C	N	O	0	0
			3278	1958	660	660		
5	M	660	Total	C	N	O	0	0
			3278	1958	660	660		
5	V	660	Total	C	N	O	0	0
			3278	1958	660	660		

- Molecule 6 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP96.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	417	Total	C	N	O	0	0
			2073	1239	417	417		
6	E	417	Total	C	N	O	0	0
			2073	1239	417	417		
6	N	417	Total	C	N	O	0	0
			2073	1239	417	417		
6	W	417	Total	C	N	O	0	0
			2073	1239	417	417		

- Molecule 7 is a protein called PROTEIN SEC13 HOMOLOG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	6	285	Total	C	N	O	0	0
			1402	832	285	285		
7	F	285	Total	C	N	O	0	0
			1402	832	285	285		
7	O	285	Total	C	N	O	0	0
			1402	832	285	285		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	X	285	Total	C	N	O	0	0
			1402	832	285	285		

- Molecule 8 is a protein called NUCLEOPORIN SEH1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	7	322	Total	C	N	O	0	0
			1593	949	322	322		
8	G	322	Total	C	N	O	0	0
			1593	949	322	322		
8	P	322	Total	C	N	O	0	0
			1593	949	322	322		
8	Y	322	Total	C	N	O	0	0
			1593	949	322	322		

- Molecule 9 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP85.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	434	Total	C	N	O	0	0
			2153	1285	434	434		
9	H	434	Total	C	N	O	0	0
			2153	1285	434	434		
9	Q	434	Total	C	N	O	0	0
			2153	1285	434	434		
9	Z	434	Total	C	N	O	0	0
			2153	1285	434	434		


- Molecule 10 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP155.

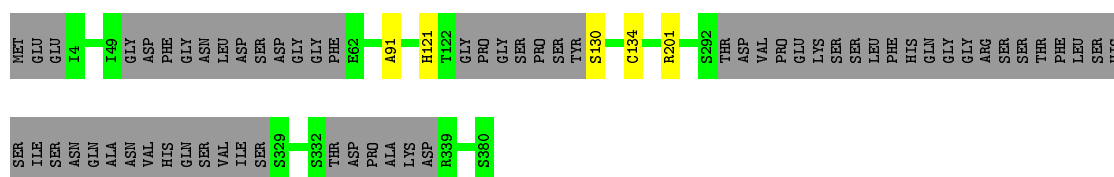
Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	1097	Total	C	N	O	0	0
			5436	3242	1097	1097		
10	B	1097	Total	C	N	O	0	0
			5436	3242	1097	1097		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

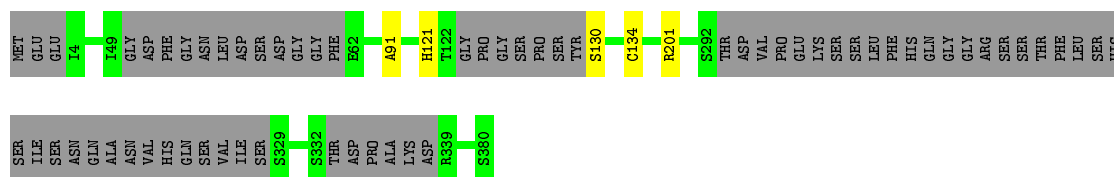
- Molecule 1: NUCLEOPORIN NUP43

Chain 0: 



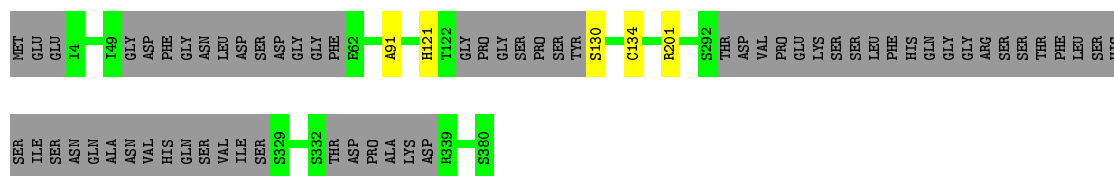
- Molecule 1: NUCLEOPORIN NUP43

Chain 9: 




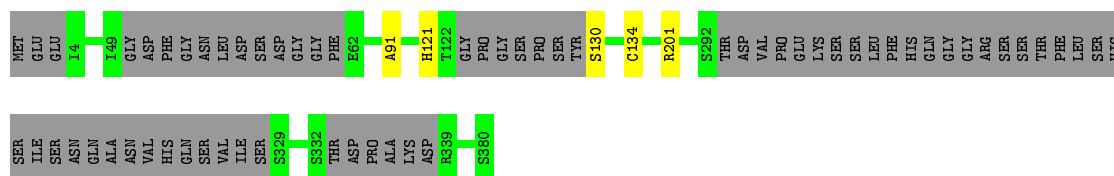
- Molecule 1: NUCLEOPORIN NUP43

Chain I: 



- Molecule 1: NUCLEOPORIN NUP43

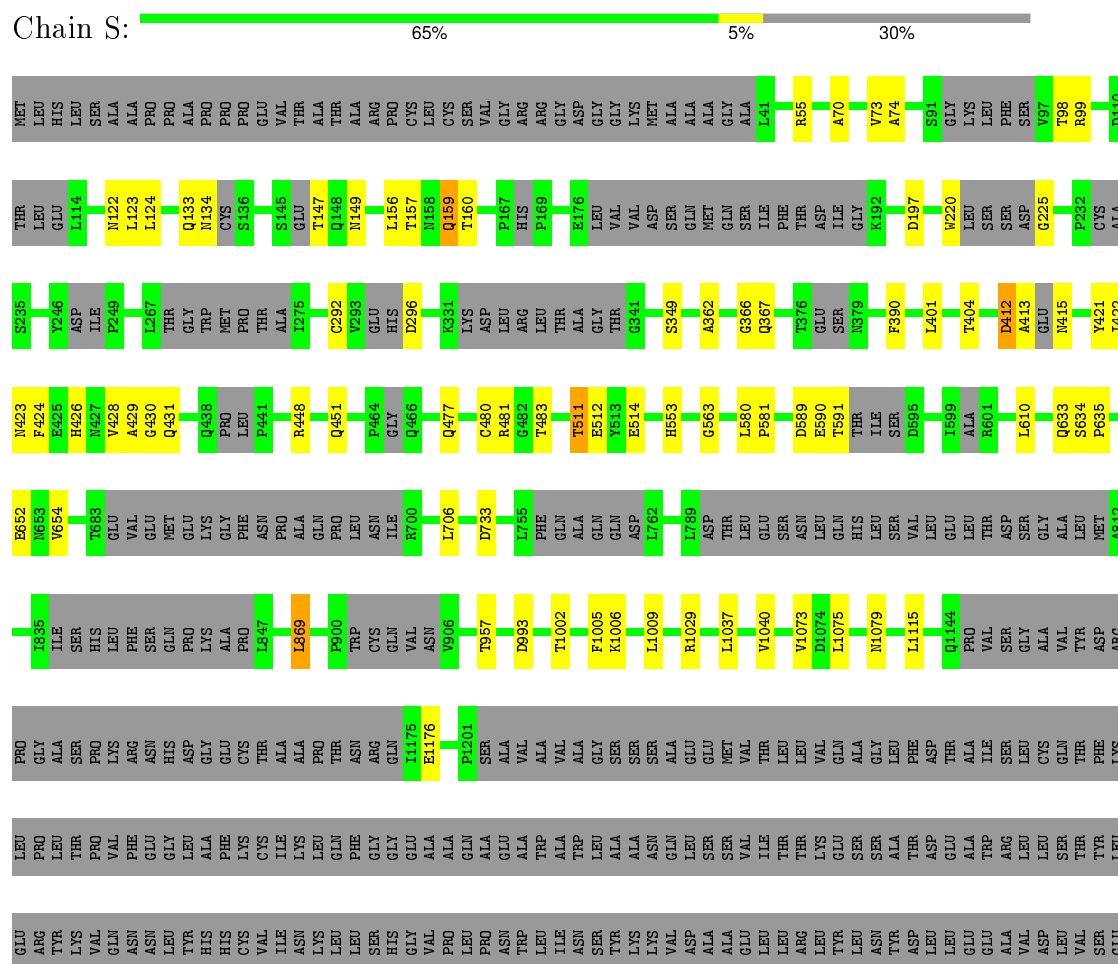
Chain R: 

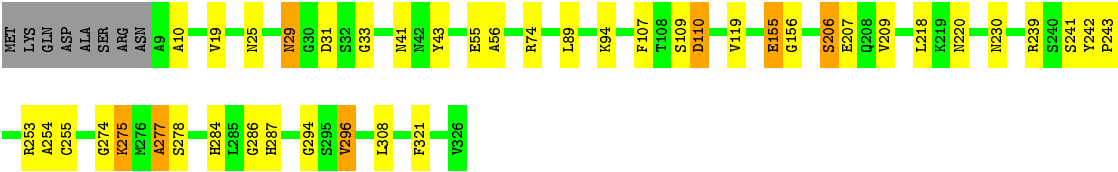


- Molecule 2: NUCLEAR PORE COMPLEX PROTEIN NUP160



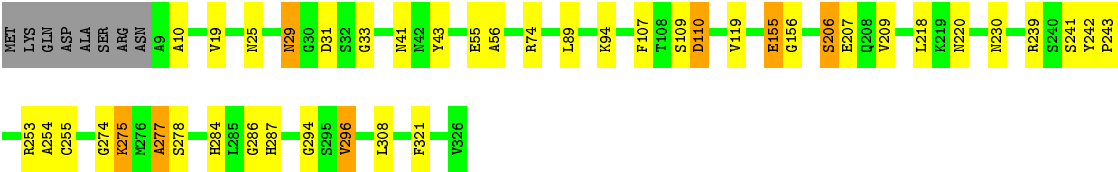
- Molecule 2: NUCLEAR PORE COMPLEX PROTEIN NUP160





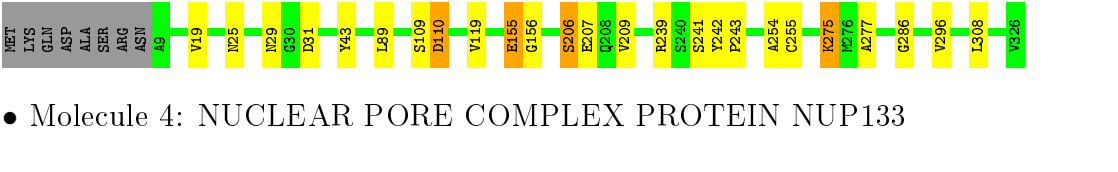
• Molecule 3: NUCLEOPORIN NUP37

Chain T: 84% 11%



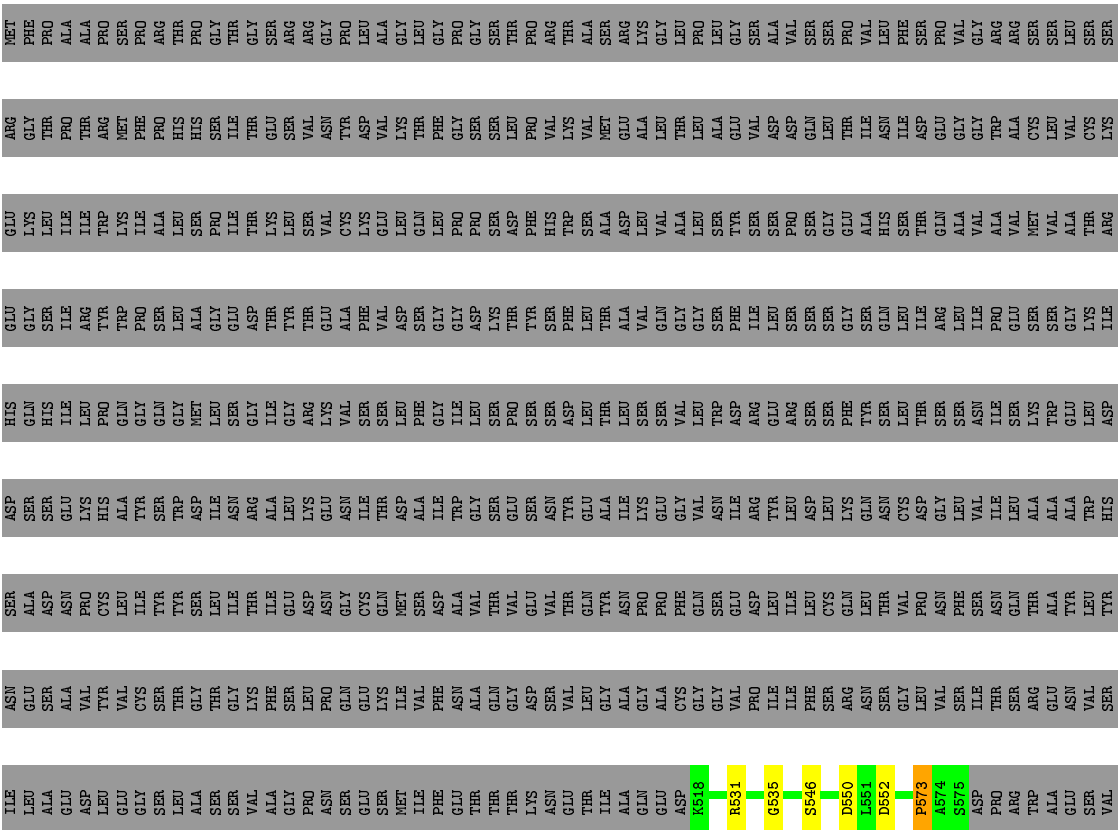
• Molecule 3: NUCLEOPORIN NUP37

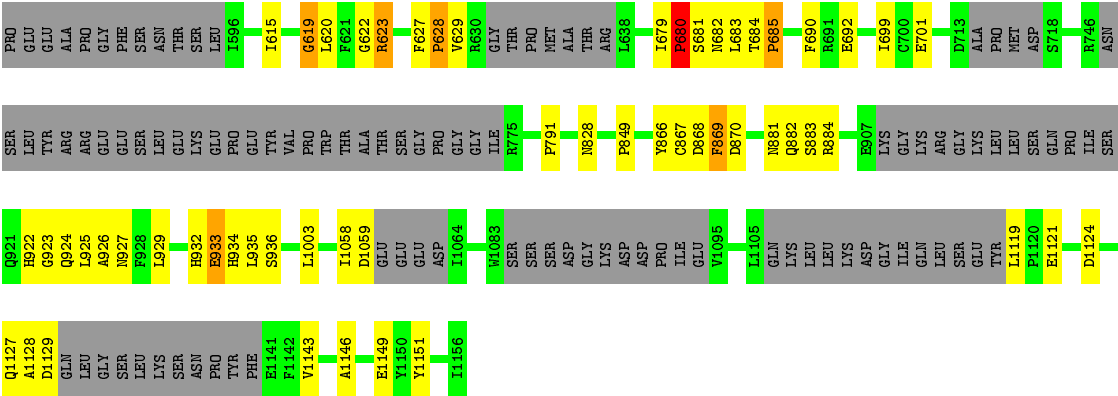
Chain b: 90% 6%



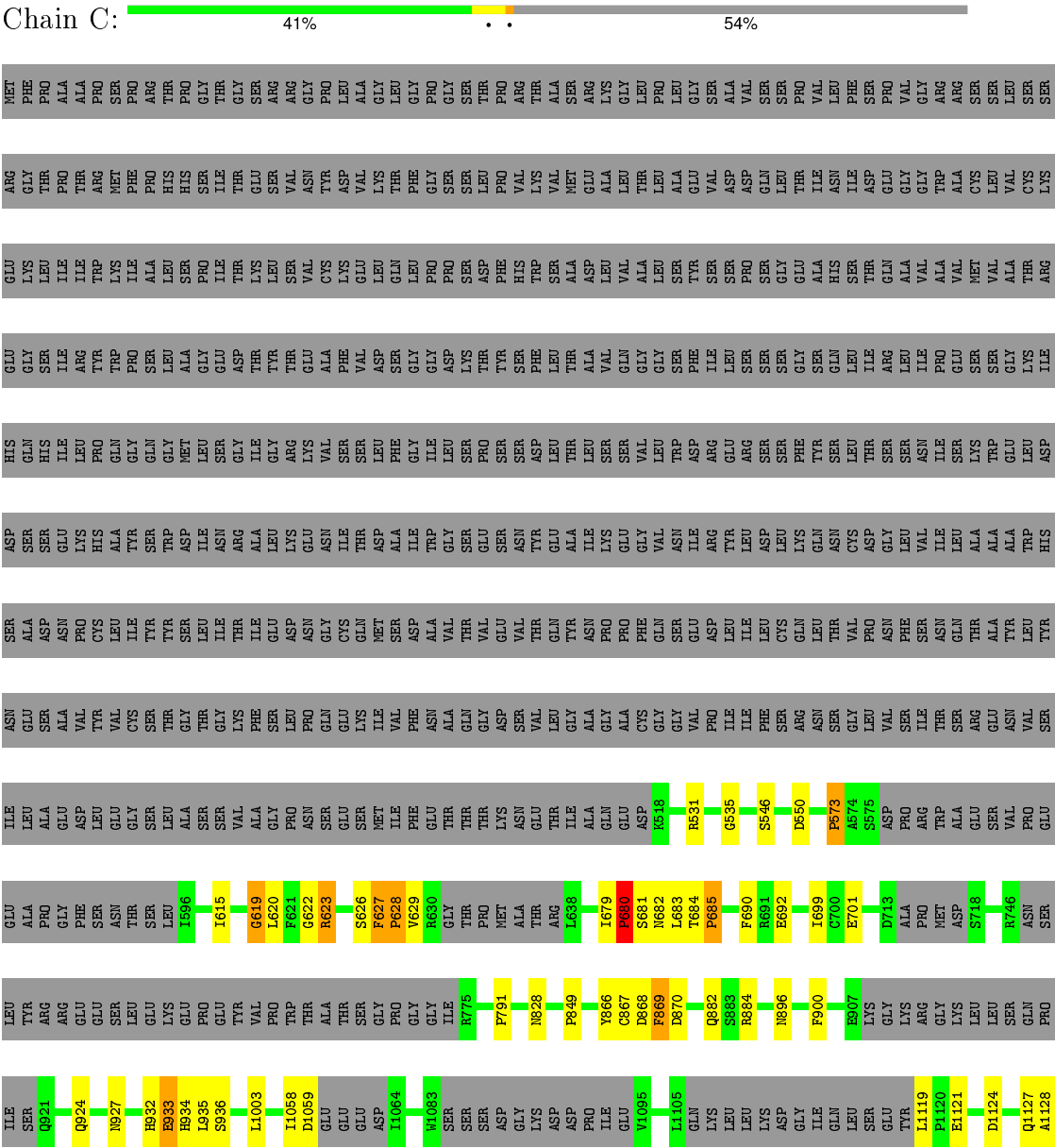
• Molecule 4: NUCLEAR PORE COMPLEX PROTEIN NUP133

Chain 3: 40% 5% 54%

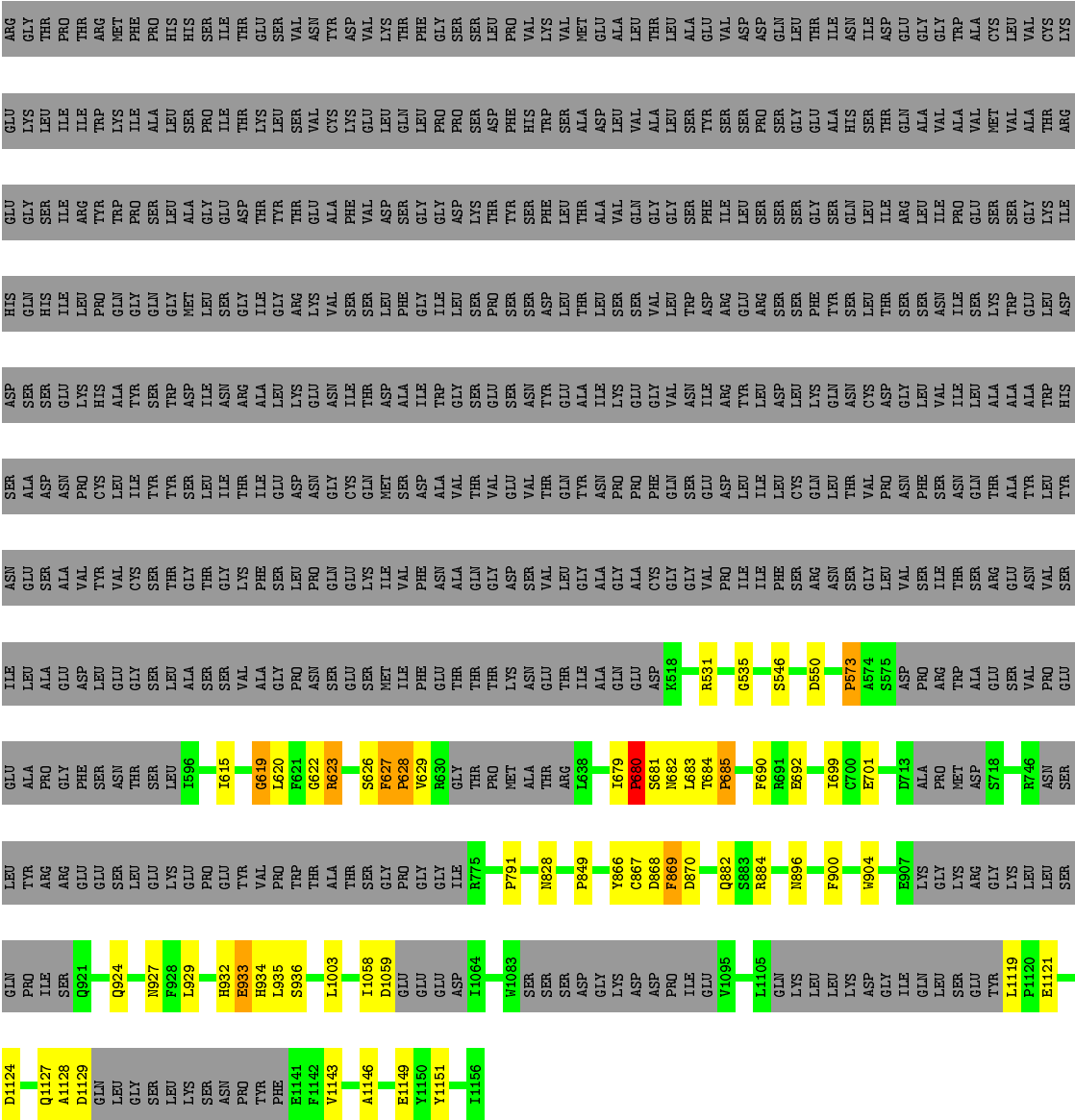




● Molecule 4: NUCLEAR PORE COMPLEX PROTEIN NUP133

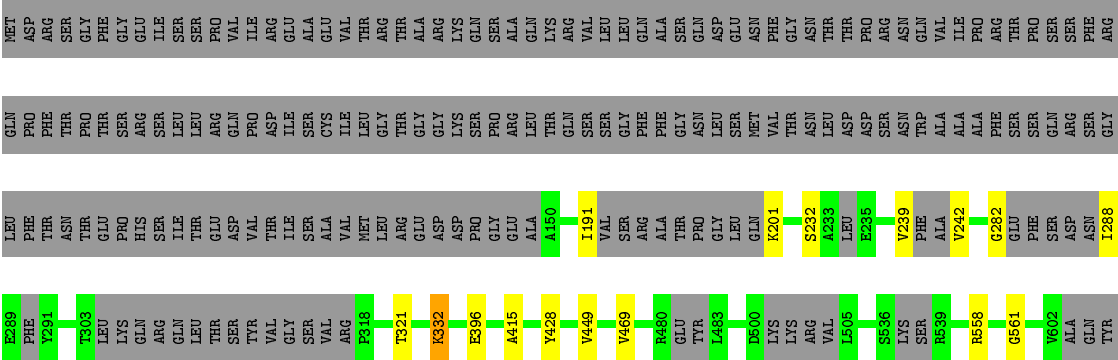


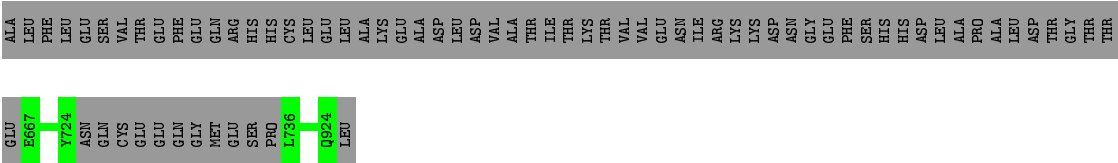




• Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107

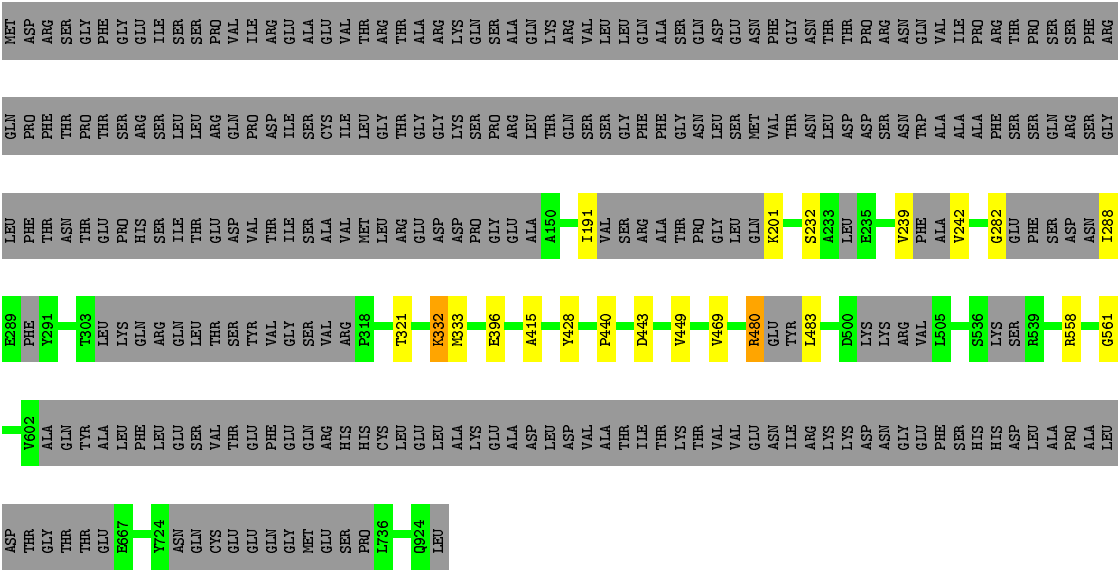
Chain 4: 70% 29%





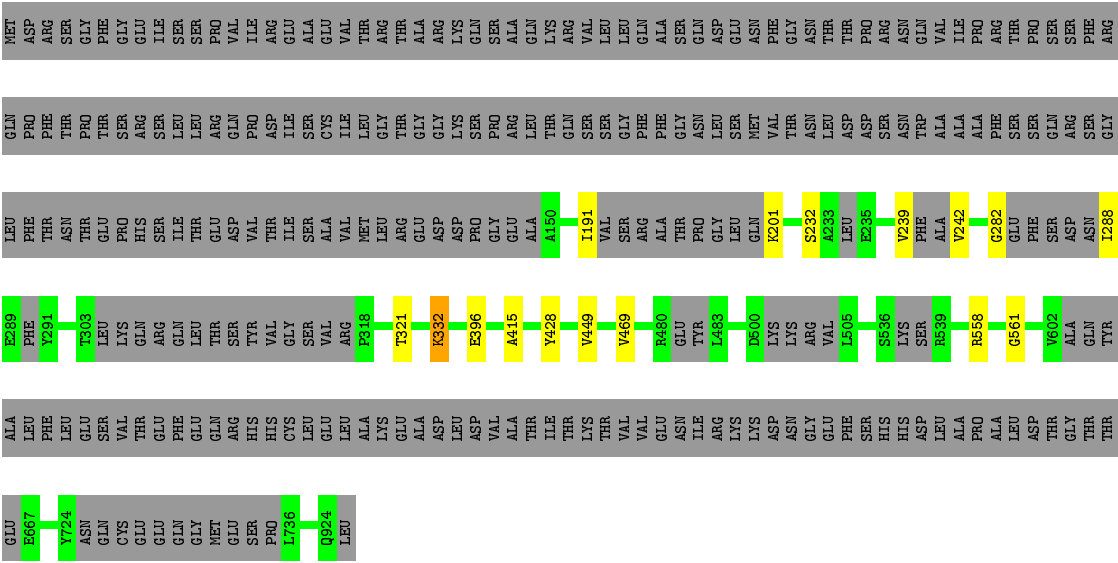
• Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107

Chain D: 69% 29%



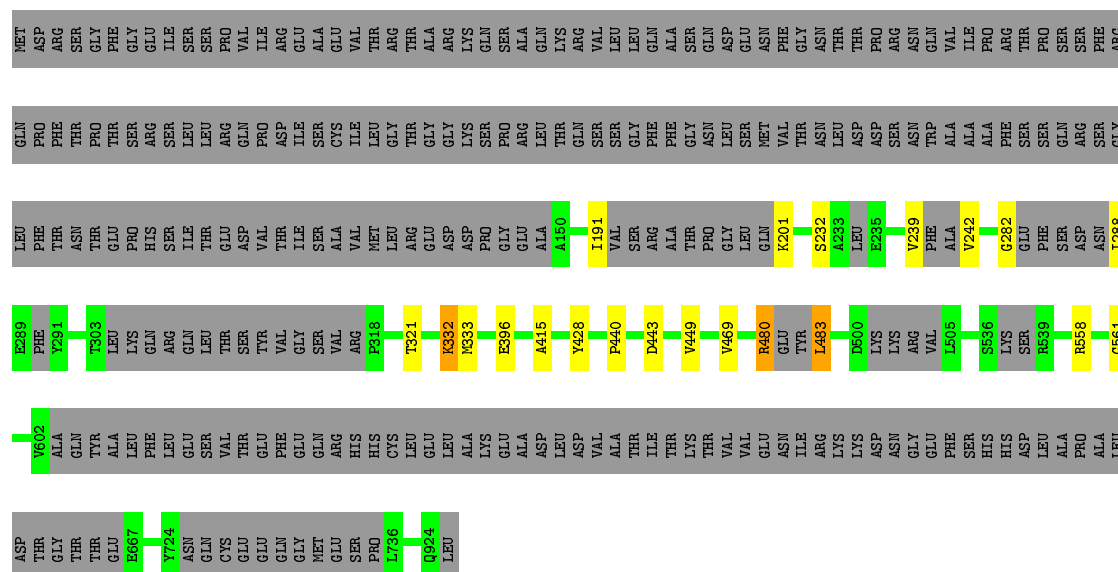
• Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107

Chain M: 70% 29%



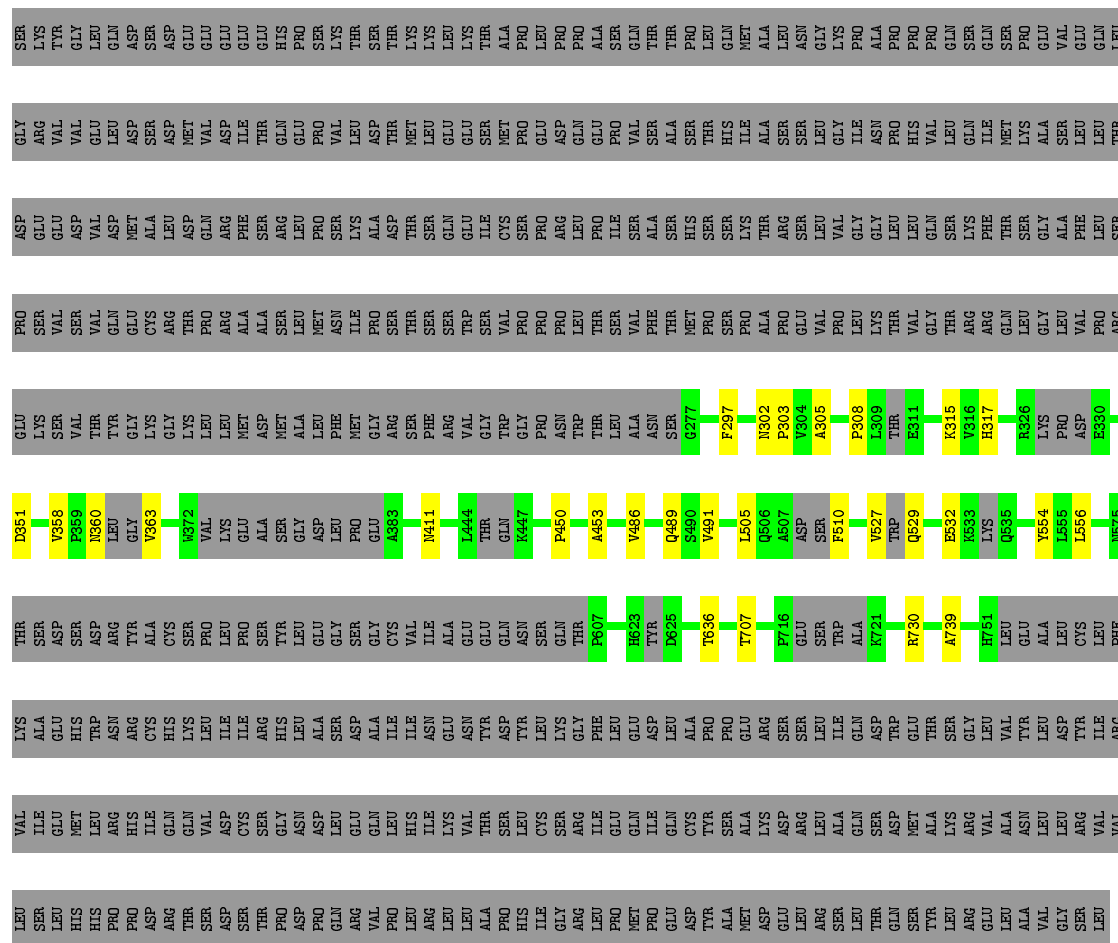
• Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107

Chain V: 69% 29%

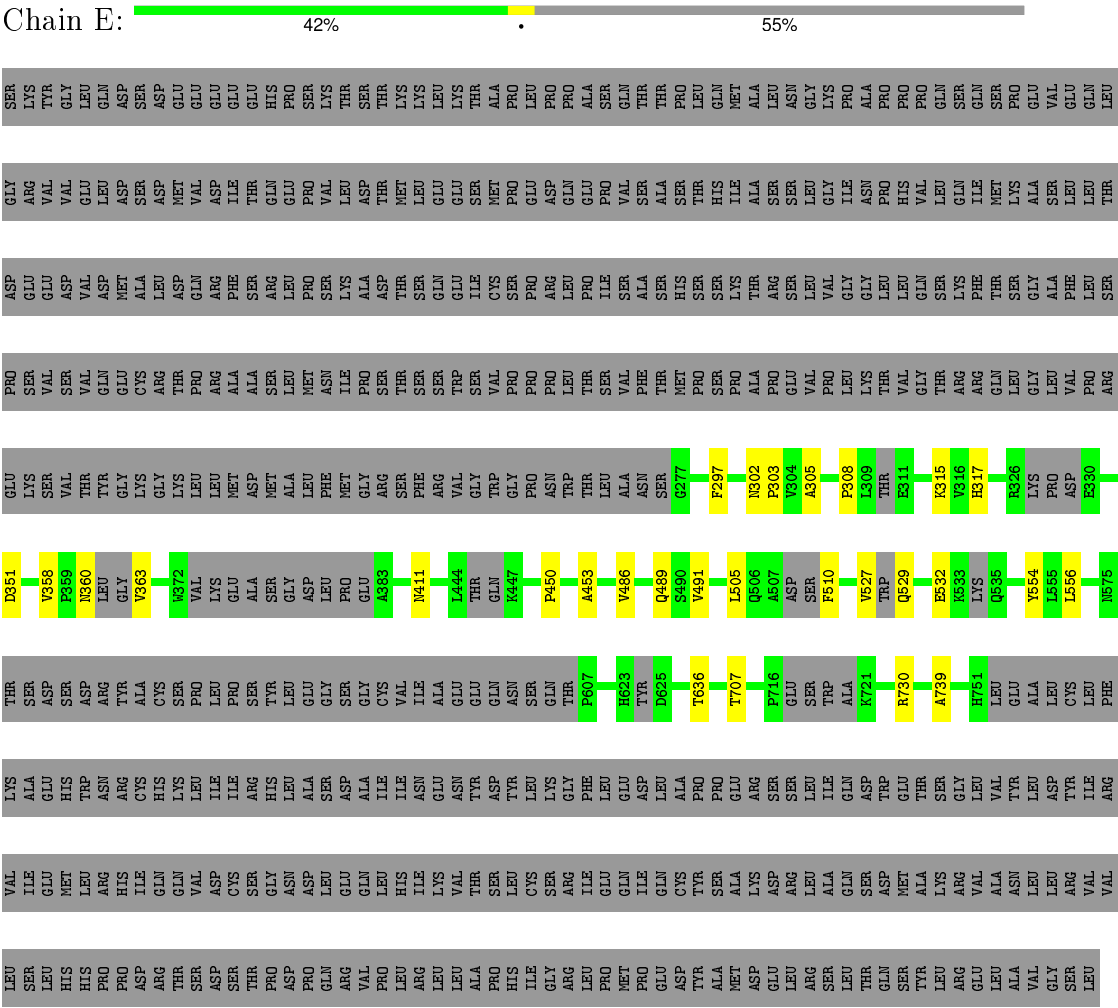


- Molecule 6: NUCLEAR PORE COMPLEX PROTEIN NUP96

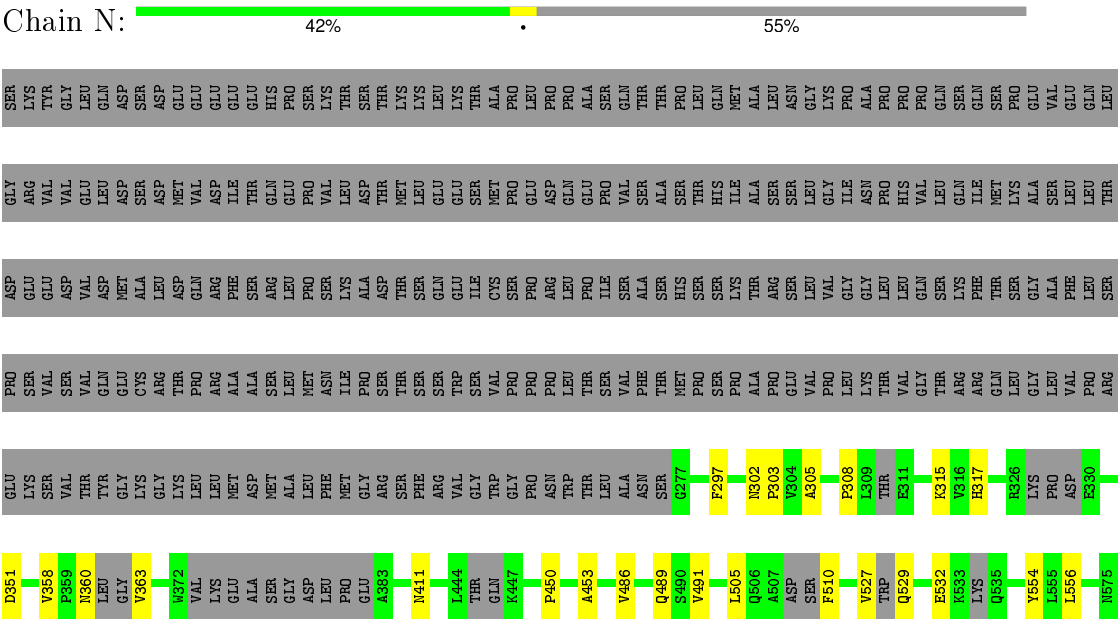
Chain 5: 42% 0% 55%

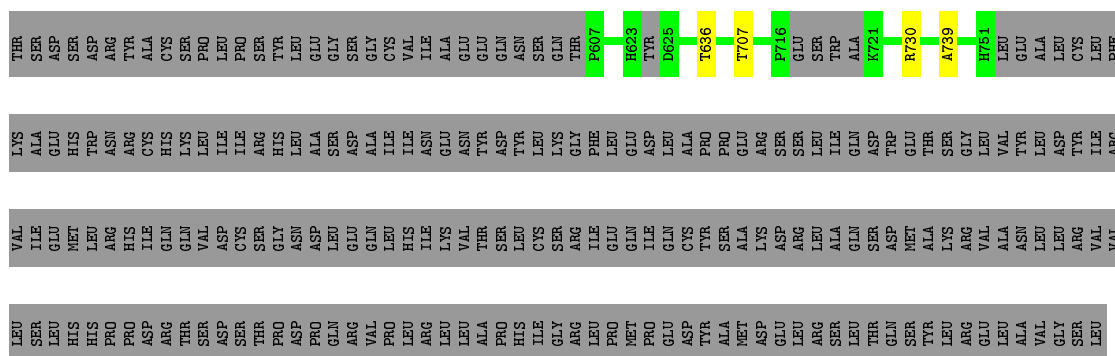


- Molecule 6: NUCLEAR PORE COMPLEX PROTEIN NUP96

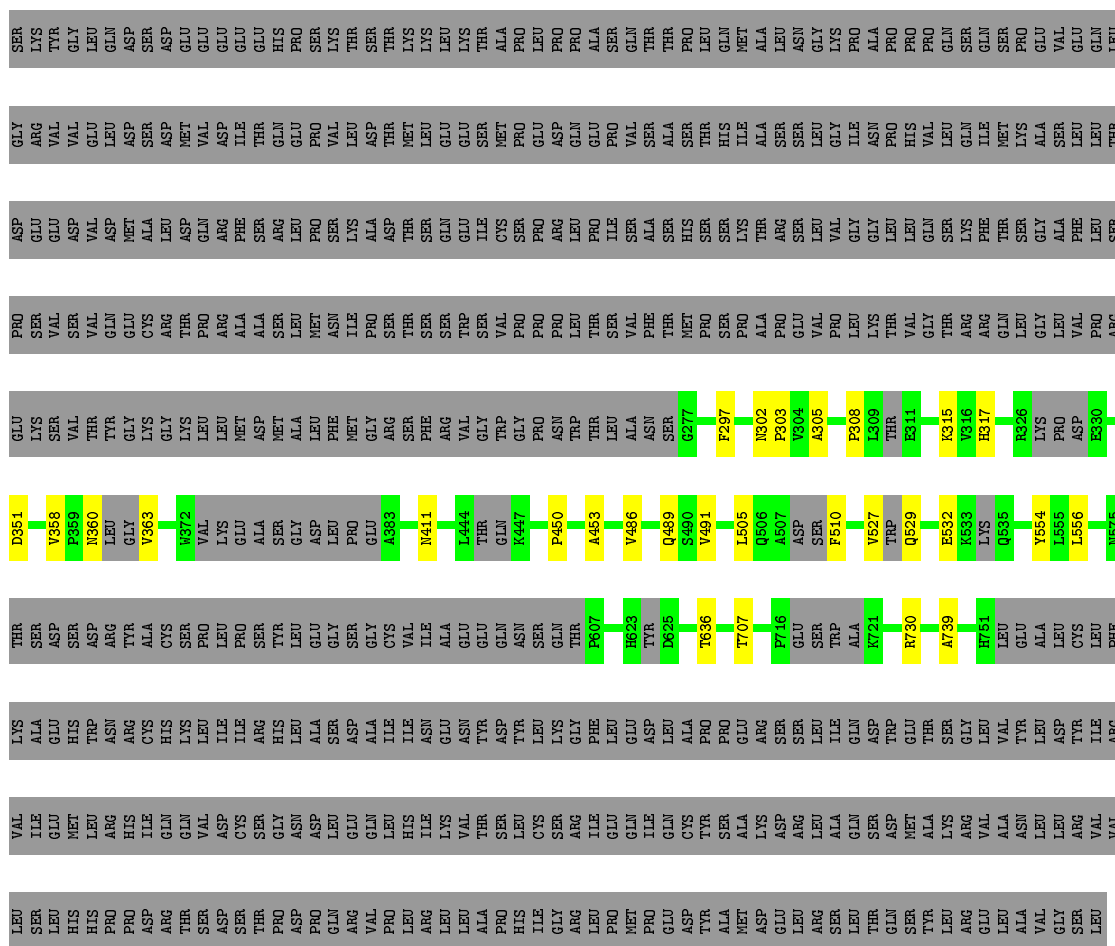


● Molecule 6: NUCLEAR PORE COMPLEX PROTEIN NUP96

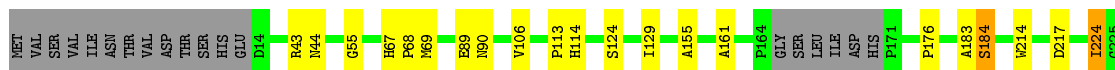
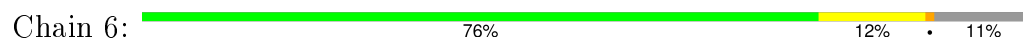


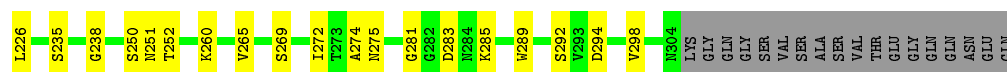


- Molecule 6: NUCLEAR PORE COMPLEX PROTEIN NUP96

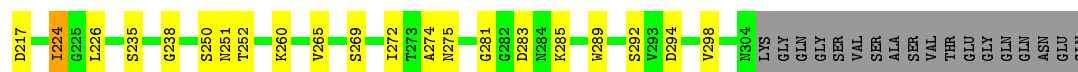
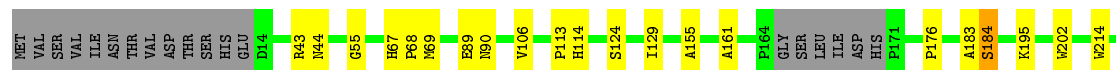
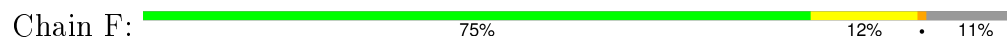


● Molecule 7: PROTEIN SEC13 HOMOLOG

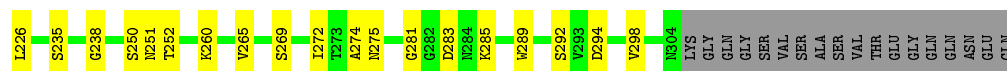
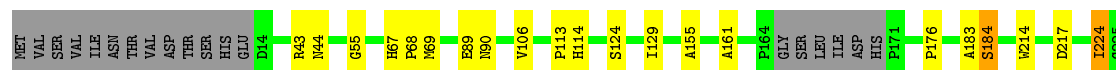
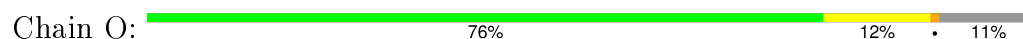




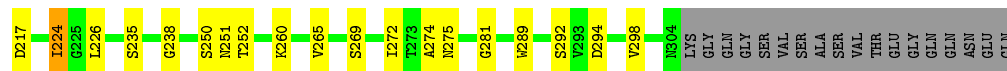
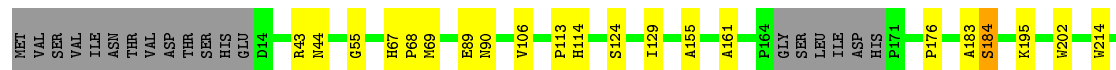
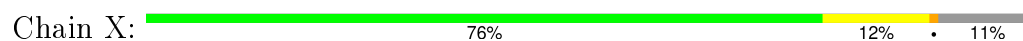
• Molecule 7: PROTEIN SEC13 HOMOLOG



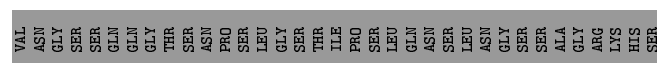
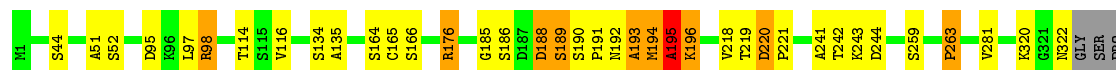
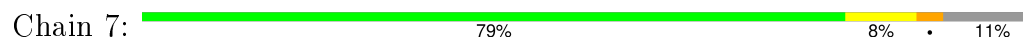
• Molecule 7: PROTEIN SEC13 HOMOLOG



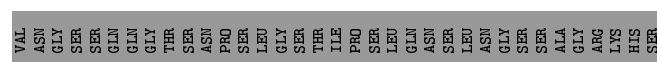
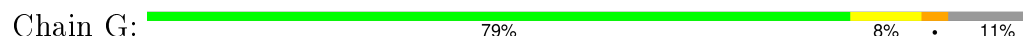
• Molecule 7: PROTEIN SEC13 HOMOLOG



• Molecule 8: NUCLEOPORIN SEH1

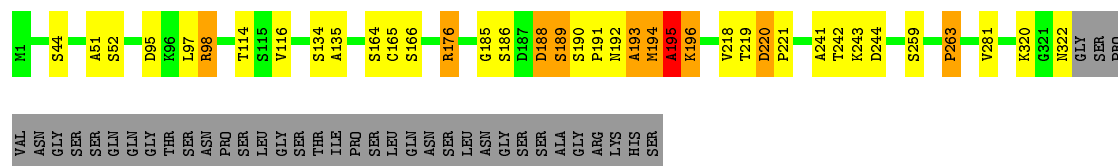


• Molecule 8: NUCLEOPORIN SEH1



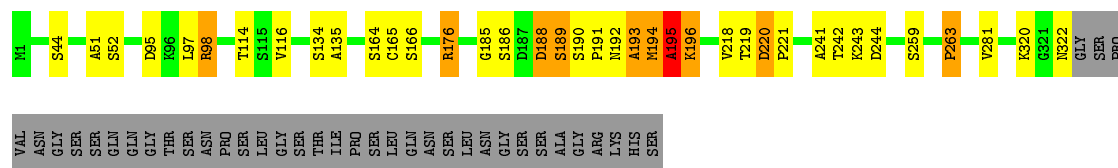
- Molecule 8: NUCLEOPORIN SEH1

Chain P: 79% 8% • 11%



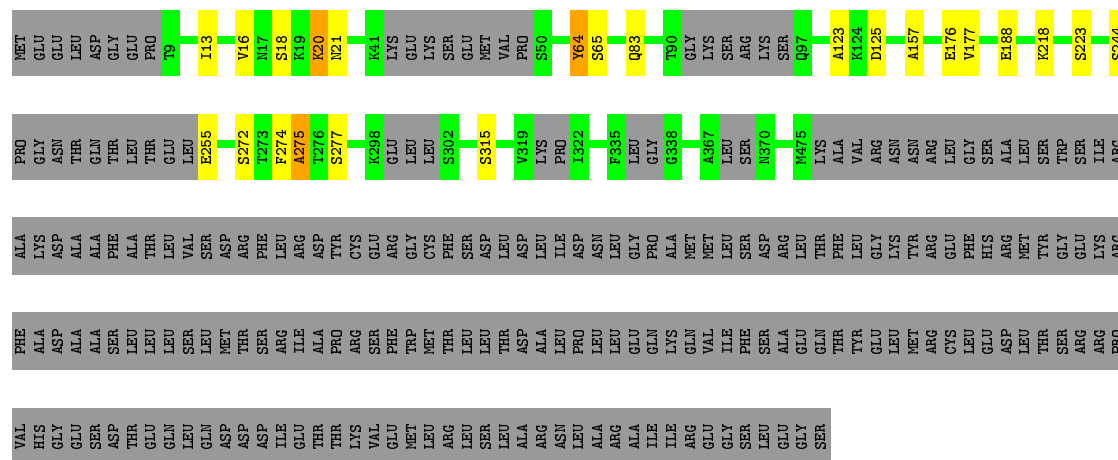
- Molecule 8: NUCLEOPORIN SEH1

Chain Y: 79% 8% • 11%



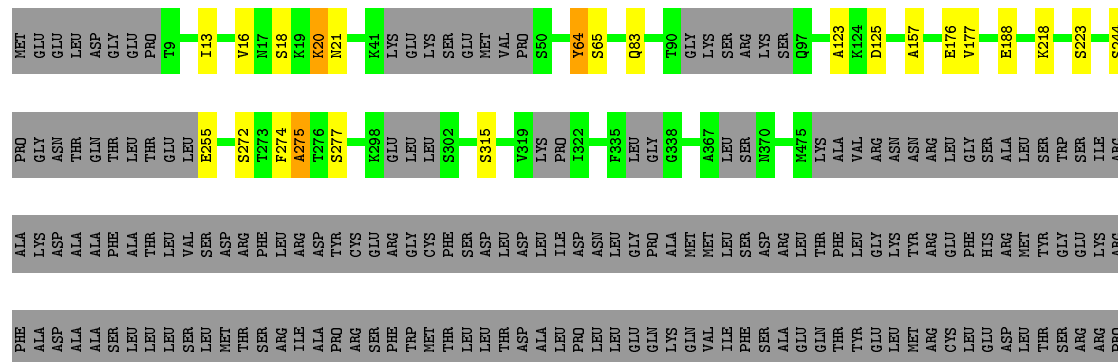
- Molecule 9: NUCLEAR PORE COMPLEX PROTEIN NUP85

Chain 8: 63% 34%



- Molecule 9: NUCLEAR PORE COMPLEX PROTEIN NUP85

Chain H:  63% 0% 34%





72% 6% 21%



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING OF TILT SERIES, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	110	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN K2 (4K X 4K)	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 > 2$	RMSZ	# $ Z > 2$
1	0	0.79	0/1557	0.76	0/2161
1	9	0.79	0/1557	0.76	0/2161
1	I	0.79	0/1557	0.76	0/2161
1	R	0.79	0/1557	0.76	0/2161
10	A	0.93	0/5409	1.18	10/7500 (0.1%)
10	B	0.93	0/5409	1.18	10/7500 (0.1%)
2	1	0.94	0/4972	1.15	8/6892 (0.1%)
2	J	0.94	0/4971	1.15	7/6889 (0.1%)
2	S	0.94	0/4971	1.15	7/6889 (0.1%)
2	a	0.94	0/4971	1.15	7/6889 (0.1%)
3	2	0.93	0/1565	1.28	7/2175 (0.3%)
3	K	0.93	0/1565	1.28	7/2175 (0.3%)
3	T	0.93	0/1565	1.28	7/2175 (0.3%)
3	b	0.93	0/1565	1.28	7/2175 (0.3%)
4	3	0.26	0/2619	0.54	6/3644 (0.2%)
4	C	0.26	0/2619	0.54	6/3644 (0.2%)
4	L	0.26	0/2619	0.54	6/3644 (0.2%)
4	U	0.26	0/2619	0.54	6/3644 (0.2%)
5	4	0.73	0/3266	0.87	2/4540 (0.0%)
5	D	0.72	1/3268 (0.0%)	0.88	4/4546 (0.1%)
5	M	0.73	0/3266	0.88	2/4540 (0.0%)
5	V	0.72	1/3268 (0.0%)	0.88	4/4546 (0.1%)
6	5	0.91	0/2061	1.09	3/2859 (0.1%)
6	E	0.91	0/2061	1.09	3/2859 (0.1%)
6	N	0.91	0/2061	1.09	3/2859 (0.1%)
6	W	0.91	0/2061	1.09	3/2859 (0.1%)
7	6	0.46	0/1400	0.79	1/1943 (0.1%)
7	F	0.46	0/1400	0.82	1/1943 (0.1%)
7	O	0.46	0/1400	0.79	1/1943 (0.1%)
7	X	0.46	0/1400	0.82	1/1943 (0.1%)
8	7	0.99	0/1592	1.28	6/2217 (0.3%)
8	G	0.99	0/1592	1.28	6/2217 (0.3%)
8	P	0.99	0/1592	1.28	6/2217 (0.3%)
8	Y	0.99	0/1592	1.28	6/2217 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
9	8	1.03	1/2145 (0.0%)	1.04	0/2980
9	H	1.03	1/2145 (0.0%)	1.04	0/2980
9	Q	1.03	1/2145 (0.0%)	1.04	0/2980
9	Z	1.03	1/2145 (0.0%)	1.04	0/2980
All	All	0.84	6/95527 (0.0%)	1.03	153/132647 (0.1%)

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
10	A	0	1
10	B	0	1
2	1	0	1
2	J	0	1
2	S	0	1
2	a	0	1
3	2	0	1
3	K	0	1
3	T	0	1
3	b	0	1
5	D	0	1
5	V	0	1
All	All	0	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	64	TYR	C-N	24.26	1.89	1.34
9	Q	64	TYR	C-N	24.23	1.89	1.34
9	Z	64	TYR	C-N	24.20	1.89	1.34
9	H	64	TYR	C-N	24.18	1.89	1.34
5	V	483	LEU	C-N	-5.78	1.22	1.33
5	D	483	LEU	C-N	-5.74	1.22	1.33

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	276	ASP	O-C-N	21.68	157.40	122.70
10	A	276	ASP	O-C-N	21.65	157.34	122.70
10	A	276	ASP	CA-C-N	-18.34	76.86	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	276	ASP	CA-C-N	-18.33	76.86	117.20
5	D	480	ARG	CA-C-N	-11.75	91.35	117.20
5	V	480	ARG	CA-C-N	-11.75	91.36	117.20
8	Y	195	ALA	N-CA-C	10.29	138.77	111.00
8	G	195	ALA	N-CA-C	10.27	138.72	111.00
8	P	195	ALA	N-CA-C	10.26	138.69	111.00
8	7	195	ALA	N-CA-C	10.25	138.68	111.00
10	B	259	SER	O-C-N	-10.04	106.63	122.70
10	A	259	SER	O-C-N	-10.02	106.66	122.70
2	S	74	ALA	N-CA-C	9.13	135.66	111.00
2	a	74	ALA	N-CA-C	9.12	135.62	111.00
2	1	74	ALA	N-CA-C	9.11	135.60	111.00
5	D	480	ARG	O-C-N	9.09	137.25	122.70
2	J	74	ALA	N-CA-C	9.09	135.54	111.00
5	V	480	ARG	O-C-N	9.04	137.17	122.70
4	C	685	PRO	N-CA-CB	8.55	113.56	103.30
4	3	685	PRO	N-CA-CB	8.53	113.54	103.30
4	U	685	PRO	N-CA-CB	8.53	113.54	103.30
4	L	685	PRO	N-CA-CB	8.51	113.51	103.30
8	Y	263	PRO	N-CA-C	8.34	133.79	112.10
8	7	263	PRO	N-CA-C	8.34	133.77	112.10
8	P	263	PRO	N-CA-C	8.33	133.75	112.10
8	G	263	PRO	N-CA-C	8.32	133.73	112.10
8	7	218	VAL	C-N-CA	-8.27	101.02	121.70
8	G	218	VAL	C-N-CA	-8.25	101.08	121.70
8	P	218	VAL	C-N-CA	-8.24	101.11	121.70
8	Y	218	VAL	C-N-CA	-8.23	101.11	121.70
10	A	259	SER	C-N-CA	7.96	141.60	121.70
10	B	259	SER	C-N-CA	7.94	141.56	121.70
3	b	109	SER	C-N-CA	7.69	140.92	121.70
3	2	109	SER	C-N-CA	7.67	140.88	121.70
3	T	109	SER	C-N-CA	7.67	140.87	121.70
3	K	109	SER	C-N-CA	7.65	140.84	121.70
4	C	680	PRO	N-CA-CB	7.06	111.77	103.30
4	L	680	PRO	N-CA-CB	7.00	111.71	103.30
4	3	680	PRO	N-CA-CB	6.99	111.69	103.30
4	U	680	PRO	N-CA-CB	6.92	111.60	103.30
4	C	573	PRO	N-CA-CB	6.79	111.44	103.30
8	7	189	SER	CB-CA-C	6.78	122.99	110.10
8	G	189	SER	CB-CA-C	6.78	122.98	110.10
8	Y	189	SER	CB-CA-C	6.78	122.98	110.10
4	3	573	PRO	N-CA-CB	6.75	111.41	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	351	ASP	C-N-CA	-6.75	104.82	121.70
4	U	573	PRO	N-CA-CB	6.75	111.40	103.30
6	N	351	ASP	C-N-CA	-6.74	104.86	121.70
8	P	189	SER	CB-CA-C	6.73	122.90	110.10
6	E	351	ASP	C-N-CA	-6.73	104.88	121.70
6	W	351	ASP	C-N-CA	-6.73	104.88	121.70
4	L	573	PRO	N-CA-CB	6.70	111.34	103.30
2	S	635	PRO	N-CA-C	6.59	129.23	112.10
2	a	635	PRO	N-CA-C	6.59	129.23	112.10
2	J	635	PRO	N-CA-C	6.57	129.19	112.10
2	1	635	PRO	N-CA-C	6.57	129.17	112.10
10	A	395	GLY	N-CA-C	-6.45	96.97	113.10
5	M	332	LYS	C-N-CA	6.45	137.84	121.70
10	B	395	GLY	N-CA-C	-6.45	96.97	113.10
5	4	332	LYS	C-N-CA	6.43	137.76	121.70
3	K	110	ASP	N-CA-C	-6.41	93.69	111.00
3	2	110	ASP	N-CA-C	-6.39	93.75	111.00
3	T	110	ASP	N-CA-C	-6.38	93.76	111.00
3	b	110	ASP	N-CA-C	-6.38	93.78	111.00
10	A	414	SER	C-N-CA	6.34	137.56	121.70
10	B	414	SER	C-N-CA	6.31	137.48	121.70
10	B	415	LYS	N-CA-CB	6.30	121.94	110.60
10	A	415	LYS	N-CA-CB	6.29	121.92	110.60
4	U	849	PRO	N-CA-CB	6.26	110.81	103.30
3	K	206	SER	C-N-CA	6.25	137.31	121.70
4	3	791	PRO	N-CA-CB	6.24	110.79	103.30
4	3	849	PRO	N-CA-CB	6.23	110.78	103.30
4	L	849	PRO	N-CA-CB	6.22	110.76	103.30
3	T	206	SER	C-N-CA	6.21	137.24	121.70
3	2	206	SER	C-N-CA	6.21	137.22	121.70
4	C	849	PRO	N-CA-CB	6.20	110.74	103.30
4	L	791	PRO	N-CA-CB	6.20	110.73	103.30
4	C	791	PRO	N-CA-CB	6.19	110.73	103.30
3	b	206	SER	C-N-CA	6.18	137.16	121.70
4	U	791	PRO	N-CA-CB	6.14	110.67	103.30
8	G	195	ALA	CB-CA-C	-5.96	101.16	110.10
8	Y	195	ALA	CB-CA-C	-5.94	101.19	110.10
8	P	195	ALA	CB-CA-C	-5.94	101.19	110.10
8	7	195	ALA	CB-CA-C	-5.93	101.20	110.10
4	L	628	PRO	N-CA-CB	5.79	110.24	103.30
4	3	628	PRO	N-CA-CB	5.76	110.21	103.30
4	U	628	PRO	N-CA-CB	5.74	110.19	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	628	PRO	N-CA-CB	5.71	110.15	103.30
10	B	395	GLY	C-N-CA	5.69	135.93	121.70
10	A	395	GLY	C-N-CA	5.66	135.86	121.70
6	5	554	TYR	CB-CA-C	-5.64	99.13	110.40
2	1	123	LEU	C-N-CA	5.63	135.79	121.70
2	S	123	LEU	C-N-CA	5.63	135.77	121.70
2	a	123	LEU	C-N-CA	5.61	135.71	121.70
2	J	123	LEU	C-N-CA	5.60	135.71	121.70
6	N	554	TYR	CB-CA-C	-5.60	99.20	110.40
5	4	449	VAL	CB-CA-C	-5.59	100.78	111.40
5	M	449	VAL	CB-CA-C	-5.57	100.81	111.40
6	W	554	TYR	CB-CA-C	-5.56	99.28	110.40
2	1	1013	HIS	O-C-N	5.56	131.60	122.70
6	E	554	TYR	CB-CA-C	-5.56	99.28	110.40
5	D	449	VAL	CB-CA-C	-5.55	100.84	111.40
5	V	449	VAL	CB-CA-C	-5.54	100.88	111.40
10	A	442	GLN	C-N-CA	5.53	135.52	121.70
10	B	442	GLN	C-N-CA	5.53	135.52	121.70
7	F	272	ILE	N-CA-C	5.49	125.81	111.00
7	X	272	ILE	N-CA-C	5.48	125.80	111.00
2	1	869	LEU	CB-CA-C	-5.46	99.82	110.20
2	a	869	LEU	CB-CA-C	-5.45	99.84	110.20
2	J	869	LEU	CB-CA-C	-5.45	99.85	110.20
2	S	869	LEU	CB-CA-C	-5.45	99.85	110.20
7	6	272	ILE	N-CA-C	5.44	125.69	111.00
7	O	272	ILE	N-CA-C	5.41	125.61	111.00
3	K	275	LYS	N-CA-C	-5.40	96.42	111.00
3	b	275	LYS	N-CA-C	-5.40	96.42	111.00
3	2	275	LYS	N-CA-C	-5.38	96.47	111.00
10	A	443	LYS	N-CA-CB	5.37	120.27	110.60
3	T	275	LYS	N-CA-C	-5.37	96.51	111.00
10	B	443	LYS	N-CA-CB	5.36	120.24	110.60
2	J	421	TYR	CB-CA-C	-5.35	99.70	110.40
2	a	421	TYR	CB-CA-C	-5.34	99.72	110.40
8	7	176	ARG	N-CA-C	-5.33	96.61	111.00
8	G	176	ARG	N-CA-C	-5.33	96.60	111.00
8	P	176	ARG	N-CA-C	-5.32	96.63	111.00
8	Y	176	ARG	N-CA-C	-5.31	96.66	111.00
2	S	421	TYR	CB-CA-C	-5.27	99.85	110.40
2	1	421	TYR	CB-CA-C	-5.26	99.87	110.40
3	T	207	GLU	N-CA-C	5.25	125.18	111.00
3	b	207	GLU	N-CA-C	5.25	125.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	207	GLU	N-CA-C	5.24	125.14	111.00
3	2	207	GLU	N-CA-C	5.23	125.11	111.00
2	1	426	HIS	C-N-CA	-5.22	108.66	121.70
2	J	426	HIS	C-N-CA	-5.22	108.66	121.70
2	a	426	HIS	C-N-CA	-5.20	108.69	121.70
6	5	453	ALA	N-CA-CB	5.20	117.38	110.10
2	S	426	HIS	C-N-CA	-5.20	108.71	121.70
3	T	156	GLY	N-CA-C	-5.19	100.11	113.10
3	2	156	GLY	N-CA-C	-5.19	100.13	113.10
3	K	156	GLY	N-CA-C	-5.17	100.17	113.10
6	N	453	ALA	N-CA-CB	5.17	117.34	110.10
3	b	156	GLY	N-CA-C	-5.17	100.18	113.10
6	E	453	ALA	N-CA-CB	5.15	117.31	110.10
6	W	453	ALA	N-CA-CB	5.14	117.30	110.10
2	a	553	HIS	CB-CA-C	-5.14	100.13	110.40
2	J	553	HIS	CB-CA-C	-5.13	100.14	110.40
2	1	553	HIS	CB-CA-C	-5.12	100.17	110.40
2	S	553	HIS	CB-CA-C	-5.11	100.18	110.40
5	V	332	LYS	N-CA-C	5.09	124.74	111.00
5	D	332	LYS	N-CA-C	5.09	124.74	111.00
3	K	155	GLU	N-CA-C	-5.08	97.28	111.00
3	b	155	GLU	N-CA-C	-5.07	97.31	111.00
3	T	155	GLU	N-CA-C	-5.06	97.33	111.00
3	2	155	GLU	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	511	THR	Peptide
3	2	286	GLY	Peptide
10	A	259	SER	Mainchain
10	B	259	SER	Mainchain
5	D	480	ARG	Mainchain
2	J	511	THR	Peptide
3	K	286	GLY	Peptide
2	S	511	THR	Peptide
3	T	286	GLY	Peptide
5	V	480	ARG	Mainchain
2	a	511	THR	Peptide
3	b	286	GLY	Peptide

5.2 Too-close contacts ⓘ

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	1562	0	681	6	0
1	9	1562	0	681	6	0
1	I	1562	0	681	6	0
1	R	1562	0	681	5	0
2	1	4997	0	2175	30	0
2	J	4997	0	2174	26	0
2	S	4997	0	2174	57	0
2	a	4997	0	2174	0	0
3	2	1566	0	702	19	0
3	K	1566	0	702	19	0
3	T	1566	0	702	18	0
3	b	1566	0	702	0	0
4	3	2629	0	1167	53	0
4	C	2629	0	1167	33	0
4	L	2629	0	1167	32	0
4	U	2629	0	1167	34	0
5	4	3278	0	1440	8	0
5	D	3278	0	1442	9	0
5	M	3278	0	1440	8	0
5	V	3278	0	1442	8	0
6	5	2073	0	907	12	0
6	E	2073	0	907	12	0
6	N	2073	0	907	12	0
6	W	2073	0	907	12	0
7	6	1402	0	648	19	0
7	F	1402	0	648	20	0
7	O	1402	0	648	20	0
7	X	1402	0	648	20	0
8	7	1593	0	731	43	0
8	G	1593	0	731	43	0
8	P	1593	0	731	42	0
8	Y	1593	0	731	43	0
9	8	2153	0	938	15	0
9	H	2153	0	938	15	0
9	Q	2153	0	938	15	0
9	Z	2153	0	938	15	0
10	A	5436	0	2392	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	5436	0	2384	117	0
All	All	95884	0	42333	825	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 6.

All (825) 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)
4:3:883:SER:CB	4:3:926:ALA:CA	1.90	1.49
10:B:844:CYS:C	10:B:885:ARG:CB	1.81	1.48
10:B:845:TYR:CB	10:B:886:GLN:HA	1.42	1.47
10:B:843:ASN:CB	10:B:919:GLN:CB	1.92	1.46
10:B:860:GLN:N	10:B:874:CYS:N	1.65	1.44
4:3:883:SER:CB	4:3:926:ALA:HA	0.96	1.42
10:B:842:ILE:HA	10:B:882:GLN:CB	1.16	1.41
10:B:860:GLN:CA	10:B:874:CYS:N	1.70	1.37
10:B:861:ASP:CB	10:B:872:ALA:HB2	1.21	1.35
10:B:861:ASP:CB	10:B:872:ALA:CB	1.80	1.35
10:B:842:ILE:CA	10:B:882:GLN:CB	2.06	1.32
10:B:852:VAL:CB	10:B:879:GLU:O	1.76	1.31
10:B:845:TYR:N	10:B:885:ARG:CB	1.92	1.30
10:B:845:TYR:CB	10:B:886:GLN:CA	2.09	1.29
10:B:858:HIS:CB	10:B:875:SER:CB	2.11	1.29
10:A:1311:ASP:CB	2:S:1009:LEU:HA	1.61	1.28
10:A:1312:PRO:HA	2:S:1005:PHE:C	1.52	1.27
10:A:1308:LYS:O	2:S:1037:LEU:CA	1.71	1.26
9:H:64:TYR:C	9:H:65:SER:N	1.89	1.26
9:Z:64:TYR:C	9:Z:65:SER:N	1.89	1.25
9:8:64:TYR:C	9:8:65:SER:N	1.89	1.25
10:A:1312:PRO:CB	2:S:1006:LYS:HA	1.66	1.25
9:Q:64:TYR:C	9:Q:65:SER:N	1.89	1.24
10:A:1312:PRO:CA	2:S:1005:PHE:O	1.84	1.23
8:Y:322:ASN:HA	9:Z:20:LYS:CB	1.71	1.21
8:P:322:ASN:HA	9:Q:20:LYS:CB	1.71	1.21
8:G:322:ASN:HA	9:H:20:LYS:CB	1.71	1.21
8:7:322:ASN:HA	9:8:20:LYS:CB	1.71	1.19
10:B:859:LEU:CB	10:B:874:CYS:C	2.12	1.19
10:B:859:LEU:CB	10:B:875:SER:N	2.06	1.18
8:P:44:SER:CB	1:R:201:ARG:CB	2.22	1.18
1:0:201:ARG:CB	8:Y:44:SER:CB	2.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:845:TYR:HA	10:B:886:GLN:N	1.60	1.17
8:7:44:SER:CB	1:9:201:ARG:CB	2.22	1.16
8:G:44:SER:CB	1:I:201:ARG:CB	2.22	1.16
8:7:188:ASP:HA	8:7:196:LYS:H	0.99	1.15
10:A:1312:PRO:CB	2:S:1005:PHE:O	1.94	1.15
8:G:188:ASP:HA	8:G:196:LYS:H	1.00	1.13
10:A:1312:PRO:CB	2:S:1006:LYS:CA	2.28	1.11
8:Y:188:ASP:HA	8:Y:196:LYS:H	0.99	1.11
10:B:858:HIS:N	10:B:875:SER:CB	2.09	1.11
10:A:1312:PRO:HA	2:S:1005:PHE:O	1.48	1.09
10:A:1312:PRO:CB	2:S:1005:PHE:C	2.21	1.09
10:A:1312:PRO:O	2:S:1005:PHE:CB	2.01	1.09
10:A:1312:PRO:CA	2:S:1005:PHE:C	2.20	1.08
10:B:856:SER:O	10:B:873:ILE:O	1.69	1.08
8:P:188:ASP:HA	8:P:196:LYS:H	1.00	1.08
10:A:1308:LYS:O	2:S:1037:LEU:HA	1.29	1.07
10:A:1319:LYS:N	2:S:1005:PHE:CB	2.18	1.06
10:B:845:TYR:CB	10:B:886:GLN:N	2.19	1.06
10:B:860:GLN:N	10:B:874:CYS:CA	2.18	1.06
10:B:859:LEU:CA	10:B:875:SER:N	2.06	1.05
10:B:859:LEU:C	10:B:874:CYS:CB	2.27	1.03
10:A:1312:PRO:HA	2:S:1005:PHE:CA	1.89	1.03
10:B:845:TYR:CA	10:B:886:GLN:N	2.20	1.02
10:A:1311:ASP:CB	2:S:1009:LEU:CA	2.40	1.00
6:W:297:PHE:HA	7:X:269:SER:CB	1.93	0.98
4:3:883:SER:CA	4:3:926:ALA:HA	1.92	0.98
6:N:297:PHE:HA	7:O:269:SER:CB	1.94	0.98
6:5:297:PHE:HA	7:6:269:SER:CB	1.94	0.98
6:E:297:PHE:HA	7:F:269:SER:CB	1.93	0.98
10:B:845:TYR:CB	10:B:885:ARG:C	2.32	0.97
4:3:881:ASN:O	4:3:926:ALA:HB2	1.63	0.96
10:B:856:SER:O	10:B:873:ILE:C	2.03	0.96
10:B:843:ASN:CA	10:B:919:GLN:CB	2.43	0.96
4:3:883:SER:H	4:3:926:ALA:HB2	1.29	0.96
10:B:853:ASP:O	10:B:876:LYS:HA	1.65	0.95
10:B:859:LEU:O	10:B:871:ASP:HA	1.65	0.95
4:3:881:ASN:CB	4:3:923:GLY:HA2	1.98	0.94
8:7:188:ASP:HA	8:7:196:LYS:N	1.82	0.94
8:P:188:ASP:HA	8:P:196:LYS:N	1.82	0.93
10:B:856:SER:O	10:B:875:SER:N	1.99	0.93
4:3:881:ASN:C	4:3:926:ALA:HB2	1.88	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:860:GLN:N	10:B:875:SER:H	1.66	0.93
8:Y:188:ASP:HA	8:Y:196:LYS:N	1.82	0.93
10:B:856:SER:O	10:B:874:CYS:C	2.08	0.91
8:G:188:ASP:HA	8:G:196:LYS:N	1.83	0.91
10:B:845:TYR:CA	10:B:885:ARG:CB	2.50	0.90
10:A:1312:PRO:N	2:S:1009:LEU:CB	2.35	0.89
8:P:322:ASN:HA	9:Q:20:LYS:CA	2.04	0.88
8:G:322:ASN:HA	9:H:20:LYS:CA	2.04	0.87
8:G:322:ASN:CA	9:H:20:LYS:CB	2.53	0.87
4:C:683:LEU:N	4:C:684:THR:HA	1.90	0.87
4:L:683:LEU:N	4:L:684:THR:HA	1.90	0.87
8:7:322:ASN:CA	9:8:20:LYS:CB	2.52	0.87
4:3:683:LEU:N	4:3:684:THR:HA	1.90	0.87
8:Y:322:ASN:CA	9:Z:20:LYS:CB	2.53	0.87
1:I:91:ALA:HB1	1:I:134:CYS:CB	2.05	0.87
1:0:91:ALA:HB1	1:0:134:CYS:CB	2.05	0.86
8:P:322:ASN:CA	9:Q:20:LYS:CB	2.53	0.86
1:R:91:ALA:HB1	1:R:134:CYS:CB	2.05	0.86
10:B:845:TYR:HA	10:B:885:ARG:C	1.95	0.86
8:7:322:ASN:HA	9:8:20:LYS:CA	2.04	0.86
8:Y:322:ASN:HA	9:Z:20:LYS:CA	2.04	0.86
10:A:1309:SER:O	2:S:1040:VAL:CB	2.22	0.86
4:U:683:LEU:N	4:U:684:THR:HA	1.90	0.86
10:B:844:CYS:O	10:B:885:ARG:CB	2.23	0.86
10:B:852:VAL:CB	10:B:879:GLU:C	2.43	0.86
1:9:91:ALA:HB1	1:9:134:CYS:CB	2.06	0.85
4:3:883:SER:H	4:3:926:ALA:CB	1.89	0.85
10:B:845:TYR:CA	10:B:885:ARG:C	2.45	0.85
10:B:859:LEU:CB	10:B:874:CYS:CB	2.53	0.85
10:B:859:LEU:O	10:B:871:ASP:CA	2.21	0.85
10:B:860:GLN:N	10:B:874:CYS:CB	2.39	0.85
10:B:861:ASP:CB	10:B:872:ALA:HB3	2.06	0.83
10:A:1312:PRO:CB	2:S:1006:LYS:N	2.40	0.83
8:Y:189:SER:HA	8:Y:220:ASP:CA	2.09	0.83
8:G:189:SER:HA	8:G:220:ASP:CA	2.09	0.82
10:B:859:LEU:CB	10:B:875:SER:CA	2.57	0.82
10:B:860:GLN:N	10:B:875:SER:N	2.27	0.82
8:7:189:SER:HA	8:7:220:ASP:CA	2.10	0.82
10:A:860:GLN:CB	10:A:882:GLN:CB	2.57	0.81
8:P:189:SER:HA	8:P:220:ASP:CA	2.09	0.81
10:B:858:HIS:CA	10:B:872:ALA:HA	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:860:GLN:HA	10:B:874:CYS:N	1.91	0.81
4:3:1143:VAL:HA	4:3:1146:ALA:HB3	1.63	0.79
6:N:707:THR:HA	6:N:739:ALA:HB1	1.65	0.79
4:3:883:SER:N	4:3:926:ALA:HB2	1.96	0.79
4:L:1143:VAL:HA	4:L:1146:ALA:HB3	1.63	0.79
10:B:845:TYR:HA	10:B:885:ARG:CB	2.11	0.79
10:B:844:CYS:CA	10:B:885:ARG:CB	2.61	0.79
10:A:1312:PRO:HA	2:S:1005:PHE:CB	2.12	0.78
4:U:1143:VAL:HA	4:U:1146:ALA:HB3	1.63	0.78
6:5:707:THR:HA	6:5:739:ALA:HB1	1.65	0.78
8:Y:51:ALA:HA	8:Y:95:ASP:O	1.84	0.78
6:W:707:THR:HA	6:W:739:ALA:HB1	1.65	0.78
8:7:51:ALA:HA	8:7:95:ASP:O	1.84	0.77
8:P:51:ALA:HA	8:P:95:ASP:O	1.84	0.77
8:P:52:SER:CB	8:P:97:LEU:HA	2.15	0.77
4:C:1143:VAL:HA	4:C:1146:ALA:HB3	1.63	0.77
8:G:51:ALA:HA	8:G:95:ASP:O	1.84	0.77
4:3:883:SER:N	4:3:926:ALA:CB	2.48	0.77
6:E:360:ASN:O	6:E:363:VAL:HA	1.85	0.77
6:E:707:THR:HA	6:E:739:ALA:HB1	1.65	0.77
8:G:52:SER:CB	8:G:97:LEU:HA	2.15	0.77
8:Y:52:SER:CB	8:Y:97:LEU:HA	2.15	0.76
6:5:360:ASN:O	6:5:363:VAL:HA	1.86	0.76
10:A:276:ASP:CB	10:A:295:SER:CB	2.63	0.76
6:W:360:ASN:O	6:W:363:VAL:HA	1.86	0.76
8:7:189:SER:HA	8:7:220:ASP:C	2.06	0.76
8:P:189:SER:HA	8:P:220:ASP:C	2.06	0.76
10:B:276:ASP:CB	10:B:295:SER:CB	2.63	0.76
8:7:52:SER:CB	8:7:97:LEU:HA	2.15	0.76
6:N:360:ASN:O	6:N:363:VAL:HA	1.85	0.75
8:G:189:SER:HA	8:G:220:ASP:C	2.06	0.75
8:Y:189:SER:HA	8:Y:220:ASP:C	2.06	0.75
4:3:881:ASN:CB	4:3:923:GLY:CA	2.64	0.74
10:B:853:ASP:O	10:B:876:LYS:CA	2.34	0.74
10:A:326:ALA:HB1	10:A:387:LEU:CB	2.17	0.74
10:B:326:ALA:HB1	10:B:387:LEU:CB	2.17	0.74
10:B:859:LEU:CB	10:B:875:SER:HA	2.18	0.74
3:T:274:GLY:HA2	3:T:277:ALA:CB	2.19	0.73
2:1:423:ASN:O	2:1:430:GLY:HA2	1.89	0.73
3:K:274:GLY:HA2	3:K:277:ALA:CB	2.19	0.73
8:G:189:SER:CB	8:G:195:ALA:H	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:189:SER:CB	8:Y:195:ALA:H	2.02	0.73
2:J:423:ASN:O	2:J:430:GLY:HA2	1.89	0.73
3:2:274:GLY:HA2	3:2:277:ALA:CB	2.19	0.72
8:P:189:SER:CB	8:P:195:ALA:H	2.02	0.72
2:S:423:ASN:O	2:S:430:GLY:HA2	1.89	0.72
10:A:22:ALA:HB1	10:A:780:ALA:HA	1.71	0.72
8:7:189:SER:CB	8:7:195:ALA:H	2.02	0.71
4:3:683:LEU:N	4:3:684:THR:CA	2.53	0.71
4:U:683:LEU:N	4:U:684:THR:CA	2.53	0.71
10:B:858:HIS:C	10:B:872:ALA:HA	2.11	0.71
5:D:321:THR:O	6:E:510:PHE:CB	2.38	0.71
5:V:321:THR:O	6:W:510:PHE:CB	2.38	0.71
4:L:683:LEU:N	4:L:684:THR:CA	2.53	0.71
10:B:22:ALA:HB1	10:B:780:ALA:HA	1.71	0.71
10:B:858:HIS:O	10:B:871:ASP:O	2.08	0.71
10:B:858:HIS:HA	10:B:872:ALA:HA	1.71	0.71
4:C:683:LEU:N	4:C:684:THR:CA	2.53	0.70
10:B:861:ASP:N	10:B:873:ILE:N	2.38	0.70
5:4:321:THR:O	6:5:510:PHE:CB	2.40	0.70
5:M:321:THR:O	6:N:510:PHE:CB	2.40	0.70
10:B:858:HIS:H	10:B:875:SER:CB	2.02	0.70
10:B:843:ASN:HA	10:B:919:GLN:CB	2.20	0.70
3:K:278:SER:O	3:K:294:GLY:HA2	1.92	0.70
4:3:682:ASN:C	4:3:684:THR:HA	2.13	0.70
4:L:682:ASN:C	4:L:684:THR:HA	2.13	0.70
3:2:278:SER:O	3:2:294:GLY:HA2	1.92	0.70
4:U:682:ASN:C	4:U:684:THR:HA	2.13	0.69
4:3:883:SER:CB	4:3:926:ALA:C	2.60	0.69
10:B:845:TYR:CB	10:B:885:ARG:O	2.39	0.69
10:B:845:TYR:HA	10:B:886:GLN:H	1.57	0.69
8:G:189:SER:HA	8:G:220:ASP:HA	1.75	0.69
4:3:866:TYR:O	4:3:868:ASP:N	2.24	0.69
10:B:843:ASN:O	10:B:885:ARG:CB	2.41	0.69
8:Y:322:ASN:HA	9:Z:20:LYS:N	2.08	0.69
3:K:274:GLY:HA2	3:K:277:ALA:HB3	1.75	0.69
8:Y:189:SER:HA	8:Y:220:ASP:HA	1.75	0.68
4:C:682:ASN:C	4:C:684:THR:HA	2.12	0.68
10:A:441:PHE:HA	10:A:444:PRO:O	1.93	0.68
4:L:866:TYR:O	4:L:868:ASP:N	2.24	0.68
6:W:360:ASN:C	6:W:363:VAL:HA	2.14	0.68
10:B:441:PHE:HA	10:B:444:PRO:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:278:SER:O	3:T:294:GLY:HA2	1.92	0.68
4:3:881:ASN:O	4:3:926:ALA:CB	2.41	0.68
8:7:188:ASP:C	8:7:195:ALA:HB3	2.14	0.68
8:G:322:ASN:HA	9:H:20:LYS:N	2.08	0.68
8:7:322:ASN:HA	9:8:20:LYS:N	2.08	0.68
6:5:360:ASN:C	6:5:363:VAL:HA	2.14	0.68
8:Y:188:ASP:C	8:Y:195:ALA:HB3	2.14	0.68
6:E:360:ASN:C	6:E:363:VAL:HA	2.14	0.68
8:7:189:SER:HA	8:7:220:ASP:HA	1.75	0.67
4:C:866:TYR:O	4:C:868:ASP:N	2.24	0.67
8:G:188:ASP:C	8:G:195:ALA:HB3	2.14	0.67
8:P:188:ASP:C	8:P:195:ALA:HB3	2.14	0.67
3:T:274:GLY:HA2	3:T:277:ALA:HB3	1.74	0.67
4:U:866:TYR:O	4:U:868:ASP:N	2.24	0.67
8:7:188:ASP:O	8:7:221:PRO:HA	1.95	0.67
8:Y:166:SER:HA	8:Y:185:GLY:O	1.95	0.67
8:G:166:SER:HA	8:G:185:GLY:O	1.95	0.67
6:N:360:ASN:C	6:N:363:VAL:HA	2.14	0.67
8:P:322:ASN:HA	9:Q:20:LYS:N	2.08	0.67
3:2:274:GLY:HA2	3:2:277:ALA:HB3	1.74	0.67
10:A:942:PRO:HA	10:A:943:GLN:CB	2.17	0.67
8:P:166:SER:HA	8:P:185:GLY:O	1.95	0.66
8:7:166:SER:HA	8:7:185:GLY:O	1.95	0.66
8:P:189:SER:HA	8:P:220:ASP:HA	1.75	0.66
10:B:863:CYS:H	10:B:871:ASP:HA	1.60	0.66
8:Y:188:ASP:O	8:Y:221:PRO:HA	1.95	0.66
4:3:881:ASN:C	4:3:926:ALA:CB	2.64	0.66
4:U:904:TRP:CB	4:U:929:LEU:CB	2.74	0.66
7:X:113:PRO:CB	7:X:161:ALA:HB2	2.27	0.65
8:P:188:ASP:O	8:P:221:PRO:HA	1.95	0.65
7:F:113:PRO:CB	7:F:161:ALA:HB2	2.27	0.65
7:6:113:PRO:CB	7:6:161:ALA:HB2	2.27	0.65
8:G:188:ASP:O	8:G:221:PRO:HA	1.95	0.65
7:O:113:PRO:CB	7:O:161:ALA:HB2	2.27	0.65
7:O:155:ALA:HB2	7:O:217:ASP:HA	1.79	0.64
7:X:155:ALA:HB2	7:X:217:ASP:HA	1.79	0.64
7:6:155:ALA:HB2	7:6:217:ASP:HA	1.79	0.63
7:F:155:ALA:HB2	7:F:217:ASP:HA	1.79	0.63
8:G:190:SER:N	8:G:220:ASP:HA	2.14	0.63
6:5:707:THR:HA	6:5:739:ALA:CB	2.29	0.63
10:B:859:LEU:C	10:B:875:SER:H	2.01	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:190:SER:N	8:P:220:ASP:HA	2.14	0.62
5:4:282:GLY:HA2	5:4:288:ILE:N	2.14	0.62
8:7:190:SER:N	8:7:220:ASP:HA	2.14	0.62
6:W:707:THR:HA	6:W:739:ALA:CB	2.28	0.62
7:O:238:GLY:O	7:O:260:LYS:HA	2.00	0.62
5:M:191:ILE:HA	5:M:201:LYS:N	2.15	0.62
7:O:224:ILE:C	7:O:226:LEU:H	2.03	0.62
5:M:282:GLY:HA2	5:M:288:ILE:N	2.14	0.62
10:B:859:LEU:C	10:B:875:SER:N	2.53	0.62
7:6:238:GLY:O	7:6:260:LYS:HA	2.00	0.62
8:Y:190:SER:N	8:Y:220:ASP:HA	2.14	0.62
5:4:191:ILE:HA	5:4:201:LYS:N	2.15	0.62
10:A:1312:PRO:CA	2:S:1005:PHE:CB	2.77	0.62
10:A:50:SER:C	10:A:58:SER:HA	2.20	0.62
3:2:29:ASN:CB	3:2:33:GLY:HA3	2.29	0.62
6:N:707:THR:HA	6:N:739:ALA:CB	2.29	0.62
5:D:191:ILE:HA	5:D:201:LYS:N	2.15	0.62
7:X:224:ILE:C	7:X:226:LEU:H	2.03	0.62
7:F:224:ILE:C	7:F:226:LEU:H	2.03	0.62
10:A:853:ASP:HA	10:A:886:GLN:CB	2.29	0.62
6:E:707:THR:HA	6:E:739:ALA:CB	2.28	0.61
5:D:282:GLY:HA2	5:D:288:ILE:N	2.14	0.61
10:B:856:SER:HA	10:B:878:ASN:H	1.64	0.61
10:B:858:HIS:C	10:B:871:ASP:O	2.36	0.61
7:F:238:GLY:O	7:F:260:LYS:HA	2.00	0.61
6:W:308:PRO:O	6:W:315:LYS:HA	2.01	0.61
6:E:308:PRO:O	6:E:315:LYS:HA	2.01	0.61
7:X:238:GLY:O	7:X:260:LYS:HA	2.00	0.61
4:C:1119:LEU:C	4:C:1121:GLU:H	2.04	0.61
3:T:29:ASN:CB	3:T:33:GLY:HA3	2.29	0.61
5:V:282:GLY:HA2	5:V:288:ILE:N	2.14	0.61
4:U:1119:LEU:C	4:U:1121:GLU:H	2.04	0.61
10:B:50:SER:C	10:B:58:SER:HA	2.20	0.61
10:B:942:PRO:HA	10:B:943:GLN:CB	2.17	0.61
3:K:29:ASN:CB	3:K:33:GLY:HA3	2.29	0.61
4:U:1124:ASP:O	4:U:1127:GLN:N	2.32	0.61
10:B:856:SER:HA	10:B:874:CYS:O	2.01	0.60
10:A:1312:PRO:C	2:S:1005:PHE:CB	2.69	0.60
8:P:165:CYS:O	8:P:186:SER:HA	2.01	0.60
5:V:191:ILE:HA	5:V:201:LYS:N	2.15	0.60
2:S:362:ALA:HB3	2:S:366:GLY:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1119:LEU:C	4:3:1121:GLU:H	2.04	0.60
2:J:362:ALA:HB3	2:J:366:GLY:H	1.67	0.60
4:L:1124:ASP:O	4:L:1127:GLN:N	2.32	0.60
10:A:312:MET:CB	10:A:313:SER:HA	2.32	0.60
4:C:868:ASP:O	4:C:870:ASP:N	2.35	0.60
6:N:297:PHE:CA	7:O:269:SER:CB	2.77	0.60
10:B:860:GLN:CA	10:B:874:CYS:CA	2.71	0.60
7:6:224:ILE:C	7:6:226:LEU:H	2.03	0.60
8:G:165:CYS:O	8:G:186:SER:HA	2.02	0.60
4:L:868:ASP:O	4:L:870:ASP:N	2.35	0.60
8:Y:165:CYS:O	8:Y:186:SER:HA	2.02	0.60
6:5:308:PRO:O	6:5:315:LYS:HA	2.01	0.60
4:3:868:ASP:O	4:3:870:ASP:N	2.35	0.60
4:U:868:ASP:O	4:U:870:ASP:N	2.35	0.60
10:B:312:MET:CB	10:B:313:SER:HA	2.32	0.60
6:5:297:PHE:CA	7:6:269:SER:CB	2.77	0.59
3:2:29:ASN:HA	3:2:33:GLY:HA3	1.83	0.59
8:7:165:CYS:O	8:7:186:SER:HA	2.01	0.59
6:N:308:PRO:O	6:N:315:LYS:HA	2.01	0.59
8:Y:114:THR:CB	8:Y:135:ALA:HB3	2.33	0.59
10:B:845:TYR:O	10:B:886:GLN:CB	2.51	0.59
4:L:1119:LEU:C	4:L:1121:GLU:H	2.04	0.59
8:7:114:THR:CB	8:7:135:ALA:HB3	2.33	0.59
3:T:29:ASN:HA	3:T:33:GLY:HA3	1.84	0.59
4:3:932:HIS:O	4:3:933:GLU:CB	2.51	0.59
4:U:932:HIS:O	4:U:933:GLU:CB	2.51	0.59
10:B:441:PHE:C	10:B:443:LYS:H	2.06	0.59
3:K:29:ASN:HA	3:K:33:GLY:HA3	1.84	0.59
10:A:441:PHE:C	10:A:443:LYS:H	2.06	0.58
8:P:114:THR:CB	8:P:135:ALA:HB3	2.33	0.58
9:Z:244:SER:HA	9:Z:255:GLU:N	2.18	0.58
9:H:244:SER:HA	9:H:255:GLU:N	2.18	0.58
2:1:362:ALA:HB3	2:1:366:GLY:H	1.66	0.58
8:G:114:THR:CB	8:G:135:ALA:HB3	2.33	0.58
4:3:883:SER:CB	4:3:925:LEU:O	2.51	0.58
2:1:220:TRP:C	2:1:225:GLY:HA2	2.24	0.58
4:C:932:HIS:O	4:C:933:GLU:CB	2.51	0.58
10:A:1312:PRO:N	2:S:1005:PHE:O	2.35	0.58
8:7:241:ALA:HB1	8:7:281:VAL:CB	2.34	0.58
9:8:244:SER:HA	9:8:255:GLU:N	2.18	0.58
10:B:845:TYR:HA	10:B:885:ARG:CA	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:858:HIS:O	10:B:871:ASP:C	2.42	0.58
8:G:241:ALA:HB1	8:G:281:VAL:CB	2.34	0.58
4:L:932:HIS:O	4:L:933:GLU:CB	2.51	0.58
8:7:189:SER:CB	8:7:194:MET:CB	2.82	0.58
7:F:250:SER:O	7:F:252:THR:N	2.35	0.58
10:B:205:LEU:C	10:B:207:SER:HA	2.25	0.58
10:B:853:ASP:O	10:B:876:LYS:CB	2.51	0.58
8:Y:241:ALA:HB1	8:Y:281:VAL:CB	2.34	0.58
10:A:205:LEU:C	10:A:207:SER:HA	2.24	0.58
10:A:1309:SER:HA	2:S:1040:VAL:CB	2.33	0.57
8:P:241:ALA:HB1	8:P:281:VAL:CB	2.34	0.57
8:Y:189:SER:CB	8:Y:194:MET:CB	2.82	0.57
3:T:29:ASN:HA	3:T:33:GLY:H	1.70	0.57
9:Q:244:SER:HA	9:Q:255:GLU:N	2.18	0.57
7:6:250:SER:O	7:6:252:THR:N	2.34	0.57
8:P:189:SER:CB	8:P:194:MET:CB	2.82	0.57
2:J:220:TRP:C	2:J:225:GLY:HA2	2.24	0.57
8:G:189:SER:CB	8:G:194:MET:CB	2.82	0.57
4:L:868:ASP:O	4:L:869:PHE:C	2.43	0.57
4:C:1124:ASP:O	4:C:1127:GLN:N	2.32	0.56
6:E:297:PHE:CA	7:F:269:SER:CB	2.76	0.56
2:S:220:TRP:C	2:S:225:GLY:HA2	2.24	0.56
4:C:868:ASP:O	4:C:869:PHE:C	2.43	0.56
3:K:29:ASN:HA	3:K:33:GLY:H	1.70	0.56
3:2:29:ASN:HA	3:2:33:GLY:H	1.70	0.56
4:3:1124:ASP:O	4:3:1127:GLN:N	2.32	0.56
4:U:868:ASP:O	4:U:869:PHE:C	2.43	0.56
10:B:845:TYR:CA	10:B:886:GLN:CA	2.76	0.56
1:0:201:ARG:CB	8:Y:44:SER:HA	2.36	0.56
10:B:205:LEU:O	10:B:207:SER:HA	2.06	0.56
10:A:205:LEU:O	10:A:207:SER:HA	2.06	0.56
7:O:250:SER:O	7:O:252:THR:N	2.35	0.56
10:B:858:HIS:O	10:B:872:ALA:HA	2.05	0.56
8:7:44:SER:HA	1:9:201:ARG:CB	2.36	0.56
10:A:376:ARG:C	10:A:380:ALA:HA	2.27	0.56
9:Q:176:GLU:HA	9:Q:177:VAL:C	2.27	0.56
2:1:590:GLU:N	2:1:591:THR:HA	2.21	0.55
9:Z:176:GLU:HA	9:Z:177:VAL:C	2.27	0.55
8:G:44:SER:HA	1:I:201:ARG:CB	2.36	0.55
10:B:376:ARG:C	10:B:380:ALA:HA	2.27	0.55
2:J:590:GLU:N	2:J:591:THR:HA	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:176:GLU:HA	9:H:177:VAL:C	2.27	0.55
10:B:863:CYS:N	10:B:871:ASP:HA	2.21	0.55
4:3:883:SER:H	4:3:926:ALA:CA	2.18	0.55
2:1:580:LEU:CB	2:1:581:PRO:HA	2.37	0.55
7:X:265:VAL:HA	7:X:281:GLY:HA3	1.89	0.55
7:F:265:VAL:HA	7:F:281:GLY:HA3	1.89	0.55
2:S:580:LEU:CB	2:S:581:PRO:HA	2.37	0.55
6:W:297:PHE:CA	7:X:269:SER:CB	2.76	0.55
4:3:868:ASP:O	4:3:869:PHE:C	2.43	0.55
8:P:44:SER:HA	1:R:201:ARG:CB	2.36	0.55
2:S:590:GLU:N	2:S:591:THR:HA	2.21	0.55
5:M:415:ALA:HB2	5:M:428:TYR:CB	2.37	0.55
8:P:322:ASN:CA	9:Q:20:LYS:N	2.70	0.55
8:G:44:SER:CA	1:I:201:ARG:CB	2.84	0.55
9:8:176:GLU:HA	9:8:177:VAL:C	2.26	0.55
7:6:265:VAL:HA	7:6:281:GLY:HA3	1.89	0.55
8:G:322:ASN:CA	9:H:20:LYS:N	2.70	0.54
8:7:322:ASN:CA	9:8:20:LYS:N	2.70	0.54
3:2:94:LYS:HA	3:2:107:PHE:O	2.08	0.54
5:4:415:ALA:HB2	5:4:428:TYR:CB	2.37	0.54
10:B:860:GLN:N	10:B:874:CYS:C	2.61	0.54
1:0:201:ARG:CB	8:Y:44:SER:CA	2.84	0.54
8:7:44:SER:CA	1:9:201:ARG:CB	2.84	0.54
2:J:580:LEU:CB	2:J:581:PRO:HA	2.37	0.54
3:2:230:ASN:O	3:2:253:ARG:HA	2.08	0.54
3:K:94:LYS:HA	3:K:107:PHE:O	2.08	0.54
8:Y:241:ALA:HB1	8:Y:281:VAL:O	2.08	0.54
3:T:230:ASN:O	3:T:253:ARG:HA	2.08	0.54
5:D:415:ALA:HB2	5:D:428:TYR:CB	2.37	0.54
8:7:241:ALA:HB1	8:7:281:VAL:O	2.08	0.54
8:G:241:ALA:HB1	8:G:281:VAL:O	2.08	0.54
4:3:881:ASN:CB	4:3:923:GLY:N	2.70	0.53
8:P:44:SER:CA	1:R:201:ARG:CB	2.84	0.53
7:F:214:TRP:O	7:F:235:SER:CB	2.56	0.53
3:K:230:ASN:O	3:K:253:ARG:HA	2.08	0.53
10:B:181:ALA:O	10:B:196:GLY:HA2	2.08	0.53
7:O:265:VAL:HA	7:O:281:GLY:HA3	1.89	0.53
8:P:241:ALA:HB1	8:P:281:VAL:O	2.08	0.53
5:D:440:PRO:HA	5:D:443:ASP:CB	2.38	0.53
5:V:415:ALA:HB2	5:V:428:TYR:CB	2.37	0.53
3:2:277:ALA:O	3:2:296:VAL:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:22:ALA:HB1	10:B:780:ALA:CA	2.38	0.53
10:A:1311:ASP:N	2:S:1009:LEU:CB	2.71	0.53
10:A:22:ALA:HB1	10:A:780:ALA:CA	2.38	0.53
3:T:94:LYS:HA	3:T:107:PHE:O	2.08	0.53
10:A:181:ALA:O	10:A:196:GLY:HA2	2.08	0.53
5:V:440:PRO:HA	5:V:443:ASP:CB	2.38	0.53
3:K:277:ALA:O	3:K:296:VAL:HA	2.08	0.53
7:6:214:TRP:O	7:6:235:SER:CB	2.56	0.53
10:A:22:ALA:HB1	10:A:780:ALA:CB	2.39	0.53
7:X:214:TRP:O	7:X:235:SER:CB	2.56	0.53
8:Y:322:ASN:CA	9:Z:20:LYS:N	2.70	0.53
7:O:214:TRP:O	7:O:235:SER:CB	2.56	0.53
3:T:277:ALA:O	3:T:296:VAL:HA	2.08	0.52
10:B:860:GLN:HA	10:B:874:CYS:CB	2.40	0.52
4:3:881:ASN:CB	4:3:922:HIS:C	2.78	0.52
10:A:1319:LYS:CB	2:S:1002:THR:O	2.57	0.52
10:B:370:PHE:HA	10:B:386:THR:O	2.10	0.52
4:3:622:GLY:O	4:3:623:ARG:O	2.27	0.52
10:B:22:ALA:HB1	10:B:780:ALA:CB	2.39	0.52
4:U:622:GLY:O	4:U:623:ARG:O	2.27	0.52
7:O:292:SER:C	7:O:294:ASP:H	2.13	0.52
2:S:422:ILE:HA	2:S:431:GLN:O	2.10	0.52
4:C:622:GLY:O	4:C:623:ARG:O	2.27	0.52
4:3:883:SER:N	4:3:926:ALA:HA	2.24	0.52
7:6:292:SER:C	7:6:294:ASP:H	2.13	0.52
4:C:1058:ILE:O	4:C:1059:ASP:CB	2.58	0.52
7:F:292:SER:C	7:F:294:ASP:H	2.13	0.52
10:A:370:PHE:HA	10:A:386:THR:O	2.10	0.52
2:J:422:ILE:HA	2:J:431:GLN:O	2.10	0.52
10:B:860:GLN:CA	10:B:874:CYS:CB	2.88	0.52
4:L:622:GLY:O	4:L:623:ARG:O	2.27	0.52
4:U:1058:ILE:O	4:U:1059:ASP:CB	2.58	0.52
7:X:67:HIS:O	7:X:69:MET:N	2.43	0.52
7:X:292:SER:C	7:X:294:ASP:H	2.13	0.52
7:6:67:HIS:O	7:6:69:MET:N	2.43	0.52
2:J:652:GLU:C	2:J:654:VAL:H	2.13	0.51
4:L:1058:ILE:O	4:L:1059:ASP:CB	2.58	0.51
2:1:422:ILE:HA	2:1:431:GLN:O	2.10	0.51
7:F:67:HIS:O	7:F:69:MET:N	2.43	0.51
2:S:652:GLU:C	2:S:654:VAL:H	2.14	0.51
2:J:1073:VAL:C	2:J:1075:LEU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:67:HIS:O	7:O:69:MET:N	2.43	0.51
6:5:527:VAL:C	6:5:529:GLN:HA	2.31	0.51
6:N:527:VAL:C	6:N:529:GLN:HA	2.31	0.51
4:3:1058:ILE:O	4:3:1059:ASP:CB	2.58	0.51
4:U:546:SER:O	4:U:550:ASP:CB	2.59	0.51
4:C:682:ASN:CA	4:C:684:THR:HA	2.41	0.51
4:L:682:ASN:CA	4:L:684:THR:HA	2.41	0.51
4:3:546:SER:O	4:3:550:ASP:CB	2.59	0.51
7:X:250:SER:O	7:X:252:THR:N	2.35	0.51
4:3:682:ASN:CA	4:3:684:THR:HA	2.41	0.50
4:L:546:SER:O	4:L:550:ASP:CB	2.59	0.50
6:E:527:VAL:C	6:E:529:GLN:HA	2.31	0.50
2:1:1073:VAL:C	2:1:1075:LEU:H	2.14	0.50
3:T:41:ASN:O	3:T:74:ARG:HA	2.11	0.50
2:S:1073:VAL:C	2:S:1075:LEU:H	2.14	0.50
3:2:41:ASN:O	3:2:74:ARG:HA	2.11	0.50
2:1:412:ASP:O	2:1:413:ALA:HB3	2.12	0.50
3:K:41:ASN:O	3:K:74:ARG:HA	2.11	0.50
4:C:546:SER:O	4:C:550:ASP:CB	2.59	0.50
4:U:682:ASN:CA	4:U:684:THR:HA	2.41	0.50
4:3:882:GLN:C	4:3:884:ARG:H	2.15	0.50
2:1:652:GLU:C	2:1:654:VAL:H	2.14	0.50
10:B:859:LEU:CB	10:B:874:CYS:CA	2.86	0.50
6:W:527:VAL:C	6:W:529:GLN:HA	2.31	0.50
9:Q:272:SER:C	9:Q:274:PHE:H	2.15	0.50
9:H:272:SER:C	9:H:274:PHE:H	2.16	0.50
10:B:376:ARG:O	10:B:380:ALA:HA	2.11	0.49
3:K:55:GLU:O	3:K:56:ALA:HB3	2.12	0.49
9:8:272:SER:C	9:8:274:PHE:H	2.15	0.49
10:B:859:LEU:O	10:B:874:CYS:CB	2.60	0.49
3:T:29:ASN:HA	3:T:33:GLY:CA	2.42	0.49
4:U:882:GLN:C	4:U:884:ARG:H	2.16	0.49
10:A:376:ARG:O	10:A:380:ALA:HA	2.11	0.49
4:L:901:LEU:CB	4:L:926:ALA:HB2	2.42	0.49
2:S:70:ALA:O	2:S:134:ASN:HA	2.12	0.49
9:Z:272:SER:C	9:Z:274:PHE:H	2.16	0.49
10:B:312:MET:CB	10:B:313:SER:CA	2.91	0.49
10:A:312:MET:CB	10:A:313:SER:CA	2.91	0.49
10:A:215:LEU:HA	10:A:230:GLY:HA2	1.94	0.49
2:J:412:ASP:O	2:J:413:ALA:HB3	2.12	0.49
2:1:424:PHE:HA	2:1:429:ALA:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:412:ASP:O	2:S:413:ALA:HB3	2.12	0.49
10:B:215:LEU:HA	10:B:230:GLY:HA2	1.94	0.49
3:T:55:GLU:O	3:T:56:ALA:HB3	2.12	0.49
3:2:55:GLU:O	3:2:56:ALA:HB3	2.12	0.48
8:P:242:THR:C	8:P:244:ASP:H	2.16	0.48
10:B:859:LEU:CB	10:B:874:CYS:O	2.59	0.48
3:2:29:ASN:HA	3:2:33:GLY:CA	2.42	0.48
8:Y:95:ASP:CB	8:Y:98:ARG:CB	2.92	0.48
4:L:882:GLN:C	4:L:884:ARG:H	2.15	0.48
2:J:70:ALA:O	2:J:134:ASN:HA	2.12	0.48
3:K:29:ASN:HA	3:K:33:GLY:CA	2.42	0.48
3:2:218:LEU:C	3:2:220:ASN:H	2.17	0.48
2:J:424:PHE:HA	2:J:429:ALA:O	2.13	0.48
2:J:589:ASP:CB	2:J:590:GLU:HA	2.44	0.48
2:S:589:ASP:CB	2:S:590:GLU:HA	2.44	0.48
2:1:70:ALA:O	2:1:134:ASN:HA	2.12	0.48
4:3:883:SER:N	4:3:926:ALA:CA	2.75	0.48
8:Y:242:THR:C	8:Y:244:ASP:H	2.16	0.48
7:O:106:VAL:HA	7:O:124:SER:HA	1.95	0.48
4:C:882:GLN:C	4:C:884:ARG:H	2.15	0.48
8:7:242:THR:C	8:7:244:ASP:H	2.16	0.48
8:7:189:SER:CA	8:7:195:ALA:H	2.27	0.48
8:P:191:PRO:C	8:P:193:ALA:H	2.14	0.48
8:P:95:ASP:CB	8:P:98:ARG:CB	2.92	0.48
8:G:95:ASP:CB	8:G:98:ARG:CB	2.92	0.48
2:1:589:ASP:CB	2:1:590:GLU:HA	2.44	0.48
4:3:934:HIS:C	4:3:936:SER:H	2.18	0.48
3:T:29:ASN:HA	3:T:33:GLY:N	2.29	0.48
2:1:413:ALA:C	2:1:415:ASN:HA	2.34	0.48
2:S:413:ALA:C	2:S:415:ASN:HA	2.34	0.48
8:G:242:THR:C	8:G:244:ASP:H	2.16	0.48
10:B:1352:LEU:C	10:B:1354:LEU:H	2.17	0.48
6:E:305:ALA:HA	6:E:317:HIS:O	2.14	0.48
7:6:274:ALA:O	7:6:275:ASN:CB	2.62	0.48
4:U:934:HIS:C	4:U:936:SER:H	2.18	0.48
4:C:934:HIS:C	4:C:936:SER:H	2.18	0.48
6:W:305:ALA:HA	6:W:317:HIS:O	2.14	0.47
7:6:106:VAL:HA	7:6:124:SER:HA	1.95	0.47
10:A:1311:ASP:CB	2:S:1009:LEU:N	2.77	0.47
8:P:189:SER:CA	8:P:195:ALA:H	2.27	0.47
3:T:218:LEU:C	3:T:220:ASN:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:274:ALA:O	7:X:275:ASN:CB	2.62	0.47
7:F:274:ALA:O	7:F:275:ASN:CB	2.62	0.47
2:S:424:PHE:HA	2:S:429:ALA:O	2.13	0.47
8:G:191:PRO:C	8:G:193:ALA:H	2.14	0.47
5:M:239:VAL:C	5:M:242:VAL:HA	2.35	0.47
8:G:189:SER:CA	8:G:195:ALA:H	2.27	0.47
8:7:95:ASP:CB	8:7:98:ARG:CB	2.92	0.47
2:S:610:LEU:CB	2:S:733:ASP:CB	2.93	0.47
7:X:106:VAL:HA	7:X:124:SER:HA	1.95	0.47
6:5:305:ALA:HA	6:5:317:HIS:O	2.15	0.47
7:O:274:ALA:O	7:O:275:ASN:CB	2.62	0.47
4:U:924:GLN:HA	4:U:927:ASN:CB	2.45	0.47
10:A:856:SER:O	10:A:882:GLN:CB	2.63	0.47
3:2:274:GLY:HA2	3:2:277:ALA:HB2	1.96	0.47
4:L:924:GLN:HA	4:L:927:ASN:CB	2.45	0.47
2:S:98:THR:HA	2:S:99:ARG:HA	1.51	0.47
2:J:413:ALA:C	2:J:415:ASN:HA	2.34	0.47
10:B:340:LYS:C	10:B:342:ILE:HA	2.35	0.47
5:V:239:VAL:C	5:V:242:VAL:HA	2.34	0.47
5:4:239:VAL:C	5:4:242:VAL:HA	2.34	0.47
10:A:340:LYS:C	10:A:342:ILE:HA	2.35	0.47
10:A:38:ARG:HA	10:A:484:THR:CB	2.45	0.47
5:D:239:VAL:C	5:D:242:VAL:HA	2.34	0.47
10:A:1352:LEU:C	10:A:1354:LEU:H	2.17	0.47
8:Y:190:SER:HA	8:Y:219:THR:CB	2.45	0.47
4:L:934:HIS:C	4:L:936:SER:H	2.18	0.47
2:1:157:THR:C	2:1:159:GLN:H	2.19	0.47
8:P:190:SER:HA	8:P:219:THR:CB	2.45	0.47
2:S:157:THR:C	2:S:159:GLN:H	2.19	0.47
10:B:38:ARG:HA	10:B:484:THR:CB	2.45	0.47
2:J:610:LEU:CB	2:J:733:ASP:CB	2.93	0.47
2:1:292:CYS:HA	2:1:296:ASP:N	2.30	0.47
8:G:190:SER:HA	8:G:219:THR:CB	2.45	0.46
7:O:292:SER:C	7:O:294:ASP:N	2.69	0.46
8:7:322:ASN:CB	9:8:20:LYS:CB	2.94	0.46
3:K:29:ASN:HA	3:K:33:GLY:N	2.29	0.46
4:3:924:GLN:HA	4:3:927:ASN:CB	2.45	0.46
3:K:218:LEU:C	3:K:220:ASN:H	2.17	0.46
2:1:610:LEU:CB	2:1:733:ASP:CB	2.93	0.46
7:F:106:VAL:HA	7:F:124:SER:HA	1.95	0.46
6:N:305:ALA:HA	6:N:317:HIS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:322:ASN:CB	9:Z:20:LYS:CB	2.94	0.46
8:Y:189:SER:CA	8:Y:195:ALA:H	2.27	0.46
8:G:322:ASN:CB	9:H:20:LYS:CB	2.94	0.46
10:A:856:SER:CB	10:A:882:GLN:O	2.63	0.46
2:J:292:CYS:HA	2:J:296:ASP:N	2.30	0.46
3:K:274:GLY:HA2	3:K:277:ALA:HB2	1.96	0.46
2:J:157:THR:C	2:J:159:GLN:H	2.19	0.46
7:6:292:SER:C	7:6:294:ASP:N	2.69	0.46
2:S:292:CYS:HA	2:S:296:ASP:N	2.30	0.46
4:C:924:GLN:HA	4:C:927:ASN:CB	2.45	0.46
4:L:882:GLN:C	4:L:884:ARG:N	2.69	0.46
8:P:189:SER:CA	8:P:195:ALA:N	2.79	0.46
4:U:882:GLN:C	4:U:884:ARG:N	2.69	0.46
8:P:322:ASN:CB	9:Q:20:LYS:CB	2.94	0.46
4:3:882:GLN:C	4:3:884:ARG:N	2.69	0.46
2:S:70:ALA:HB1	2:S:133:GLN:O	2.16	0.46
10:B:856:SER:HA	10:B:878:ASN:N	2.31	0.45
8:7:190:SER:HA	8:7:219:THR:CB	2.45	0.45
4:C:882:GLN:C	4:C:884:ARG:N	2.69	0.45
8:G:189:SER:CA	8:G:195:ALA:N	2.79	0.45
10:A:942:PRO:HA	10:A:943:GLN:HA	1.48	0.45
3:2:29:ASN:HA	3:2:33:GLY:N	2.29	0.45
8:Y:189:SER:CA	8:Y:195:ALA:N	2.79	0.45
3:2:284:HIS:CB	3:2:287:HIS:CB	2.94	0.45
3:K:284:HIS:CB	3:K:287:HIS:CB	2.94	0.45
10:B:862:ILE:N	10:B:871:ASP:C	2.63	0.45
10:B:852:VAL:CB	10:B:879:GLU:CA	2.95	0.45
8:7:189:SER:CA	8:7:195:ALA:N	2.79	0.45
4:3:682:ASN:HA	4:3:684:THR:HA	1.98	0.45
7:X:292:SER:C	7:X:294:ASP:N	2.69	0.45
2:J:70:ALA:HB1	2:J:133:GLN:O	2.16	0.45
4:C:1143:VAL:HA	4:C:1146:ALA:CB	2.41	0.45
7:F:292:SER:C	7:F:294:ASP:N	2.69	0.45
3:T:29:ASN:CA	3:T:33:GLY:HA3	2.47	0.45
2:S:590:GLU:N	2:S:591:THR:CA	2.79	0.45
2:S:477:GLN:HA	2:S:481:ARG:O	2.17	0.45
6:E:527:VAL:O	6:E:529:GLN:HA	2.17	0.45
2:1:70:ALA:HB1	2:1:133:GLN:O	2.16	0.45
2:1:367:GLN:HA	2:1:390:PHE:O	2.17	0.45
2:J:367:GLN:HA	2:J:390:PHE:O	2.17	0.45
8:G:116:VAL:HA	8:G:134:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:322:ASN:H	9:Q:18:SER:CB	2.30	0.45
4:U:1143:VAL:HA	4:U:1146:ALA:CB	2.41	0.45
3:K:29:ASN:CA	3:K:33:GLY:HA3	2.47	0.45
2:1:590:GLU:N	2:1:591:THR:CA	2.79	0.45
2:J:590:GLU:N	2:J:591:THR:CA	2.79	0.45
3:T:284:HIS:CB	3:T:287:HIS:CB	2.94	0.45
8:Y:116:VAL:HA	8:Y:134:SER:HA	1.99	0.45
2:S:367:GLN:HA	2:S:390:PHE:O	2.17	0.45
8:G:322:ASN:H	9:H:18:SER:CB	2.30	0.45
4:3:1143:VAL:HA	4:3:1146:ALA:CB	2.41	0.45
8:7:116:VAL:HA	8:7:134:SER:HA	1.99	0.45
4:3:619:GLY:HA2	4:3:620:LEU:CB	2.47	0.45
8:Y:322:ASN:H	9:Z:18:SER:CB	2.30	0.44
6:W:527:VAL:O	6:W:529:GLN:HA	2.17	0.44
4:U:619:GLY:HA2	4:U:620:LEU:CB	2.47	0.44
10:A:395:GLY:N	10:A:400:SER:CB	2.80	0.44
4:C:1119:LEU:C	4:C:1121:GLU:N	2.71	0.44
4:U:1119:LEU:C	4:U:1121:GLU:N	2.71	0.44
9:Q:244:SER:CA	9:Q:255:GLU:N	2.81	0.44
4:C:619:GLY:HA2	4:C:620:LEU:CB	2.47	0.44
4:3:883:SER:CB	4:3:929:LEU:CB	2.95	0.44
4:L:682:ASN:HA	4:L:684:THR:HA	1.98	0.44
4:U:682:ASN:HA	4:U:684:THR:HA	1.98	0.44
10:A:1355:ASP:CB	10:A:1358:CYS:CB	2.96	0.44
10:B:395:GLY:N	10:B:400:SER:CB	2.80	0.44
4:C:682:ASN:HA	4:C:684:THR:HA	1.98	0.44
2:J:477:GLN:HA	2:J:481:ARG:O	2.17	0.44
6:W:489:GLN:C	6:W:491:VAL:H	2.20	0.44
4:L:1119:LEU:C	4:L:1121:GLU:N	2.71	0.44
4:C:690:PHE:C	4:C:692:GLU:N	2.70	0.44
8:7:322:ASN:H	9:8:18:SER:CB	2.30	0.44
2:J:98:THR:HA	2:J:99:ARG:HA	1.51	0.44
7:O:43:ARG:O	7:O:44:ASN:CB	2.66	0.44
7:6:43:ARG:O	7:6:44:ASN:CB	2.66	0.44
9:H:244:SER:CA	9:H:255:GLU:N	2.81	0.44
6:5:527:VAL:O	6:5:529:GLN:HA	2.17	0.44
4:U:615:ILE:O	4:U:620:LEU:CB	2.66	0.44
4:C:615:ILE:O	4:C:620:LEU:CB	2.66	0.44
6:5:489:GLN:C	6:5:491:VAL:H	2.20	0.44
2:1:477:GLN:HA	2:1:481:ARG:O	2.17	0.44
10:B:856:SER:O	10:B:874:CYS:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:29:ASN:CA	3:2:33:GLY:HA3	2.47	0.44
4:L:680:PRO:O	4:L:681:SER:C	2.56	0.44
7:F:43:ARG:O	7:F:44:ASN:CB	2.66	0.44
9:8:244:SER:CA	9:8:255:GLU:N	2.81	0.43
4:3:615:ILE:O	4:3:620:LEU:CB	2.66	0.43
7:X:43:ARG:O	7:X:44:ASN:CB	2.66	0.43
9:Q:123:ALA:C	9:Q:125:ASP:N	2.72	0.43
10:B:857:LEU:HA	10:B:873:ILE:HA	1.99	0.43
4:L:619:GLY:HA2	4:L:620:LEU:CB	2.47	0.43
4:L:690:PHE:C	4:L:692:GLU:N	2.70	0.43
5:V:558:ARG:HA	5:V:561:GLY:O	2.18	0.43
5:D:558:ARG:HA	5:D:561:GLY:O	2.18	0.43
8:7:193:ALA:O	8:7:194:MET:CB	2.66	0.43
10:B:859:LEU:CA	10:B:874:CYS:CB	2.96	0.43
6:N:527:VAL:O	6:N:529:GLN:HA	2.17	0.43
4:L:615:ILE:O	4:L:620:LEU:CB	2.66	0.43
6:N:489:GLN:C	6:N:491:VAL:H	2.20	0.43
10:B:863:CYS:H	10:B:871:ASP:CA	2.29	0.43
8:Y:189:SER:N	8:Y:195:ALA:HB3	2.33	0.43
9:Z:274:PHE:O	9:Z:275:ALA:HB2	2.18	0.43
5:4:558:ARG:HA	5:4:561:GLY:O	2.18	0.43
9:Z:123:ALA:C	9:Z:125:ASP:N	2.72	0.43
8:G:193:ALA:O	8:G:194:MET:CB	2.67	0.43
8:P:193:ALA:O	8:P:194:MET:CB	2.67	0.43
7:X:289:TRP:HA	7:X:298:VAL:O	2.19	0.43
6:E:489:GLN:C	6:E:491:VAL:H	2.20	0.43
7:X:89:GLU:O	7:X:90:ASN:CB	2.66	0.43
7:O:224:ILE:C	7:O:226:LEU:N	2.72	0.43
9:Z:244:SER:CA	9:Z:255:GLU:N	2.81	0.43
9:Q:274:PHE:O	9:Q:275:ALA:HB2	2.18	0.43
4:L:901:LEU:CB	4:L:926:ALA:CB	2.97	0.43
5:M:558:ARG:HA	5:M:561:GLY:O	2.18	0.43
7:O:289:TRP:HA	7:O:298:VAL:O	2.19	0.43
8:P:220:ASP:CB	8:P:243:LYS:CB	2.97	0.43
2:S:413:ALA:O	2:S:415:ASN:HA	2.19	0.43
4:C:680:PRO:O	4:C:681:SER:C	2.56	0.43
7:F:289:TRP:HA	7:F:298:VAL:O	2.19	0.43
8:7:191:PRO:C	8:7:193:ALA:H	2.14	0.43
8:G:220:ASP:CB	8:G:243:LYS:CB	2.97	0.43
8:P:189:SER:N	8:P:195:ALA:HB3	2.33	0.43
4:U:933:GLU:O	4:U:935:LEU:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:413:ALA:O	2:J:415:ASN:HA	2.19	0.43
8:Y:191:PRO:C	8:Y:193:ALA:H	2.14	0.42
8:Y:220:ASP:CB	8:Y:243:LYS:CB	2.97	0.42
7:X:183:ALA:O	7:X:184:SER:CB	2.67	0.42
2:1:122:ASN:C	2:1:124:LEU:H	2.23	0.42
10:B:1355:ASP:CB	10:B:1358:CYS:CB	2.96	0.42
7:6:289:TRP:HA	7:6:298:VAL:O	2.19	0.42
9:H:123:ALA:C	9:H:125:ASP:N	2.72	0.42
8:Y:190:SER:N	8:Y:220:ASP:CA	2.82	0.42
7:F:89:GLU:O	7:F:90:ASN:CB	2.67	0.42
2:S:122:ASN:C	2:S:124:LEU:H	2.22	0.42
8:Y:193:ALA:O	8:Y:194:MET:CB	2.67	0.42
2:1:413:ALA:O	2:1:415:ASN:HA	2.19	0.42
4:U:680:PRO:O	4:U:681:SER:C	2.56	0.42
8:P:116:VAL:HA	8:P:134:SER:HA	1.99	0.42
9:8:123:ALA:C	9:8:125:ASP:N	2.72	0.42
5:M:191:ILE:CA	5:M:201:LYS:N	2.82	0.42
4:U:1119:LEU:O	4:U:1121:GLU:N	2.52	0.42
4:L:1119:LEU:O	4:L:1121:GLU:N	2.52	0.42
7:6:89:GLU:O	7:6:90:ASN:CB	2.66	0.42
2:J:122:ASN:C	2:J:124:LEU:H	2.22	0.42
8:G:189:SER:N	8:G:195:ALA:HB3	2.33	0.42
10:B:942:PRO:HA	10:B:943:GLN:HA	1.48	0.42
9:H:274:PHE:O	9:H:275:ALA:HB2	2.18	0.42
8:Y:190:SER:N	8:Y:194:MET:CB	2.83	0.42
8:P:190:SER:N	8:P:194:MET:CB	2.83	0.42
2:1:292:CYS:CA	2:1:296:ASP:N	2.83	0.42
1:0:121:HIS:N	1:0:130:SER:O	2.51	0.42
7:O:89:GLU:O	7:O:90:ASN:CB	2.66	0.42
7:F:195:LYS:O	7:F:202:TRP:HA	2.20	0.42
7:X:195:LYS:O	7:X:202:TRP:HA	2.20	0.42
4:3:680:PRO:O	4:3:681:SER:C	2.56	0.42
3:K:274:GLY:CA	3:K:277:ALA:HB3	2.46	0.42
3:2:274:GLY:CA	3:2:277:ALA:HB3	2.46	0.42
10:B:847:ARG:O	10:B:883:ARG:HA	2.19	0.42
2:J:156:LEU:HA	2:J:160:THR:O	2.20	0.42
4:3:690:PHE:C	4:3:692:GLU:N	2.70	0.42
8:7:220:ASP:CB	8:7:243:LYS:CB	2.97	0.42
4:C:1119:LEU:O	4:C:1121:GLU:N	2.52	0.42
7:F:183:ALA:O	7:F:184:SER:CB	2.67	0.42
8:7:189:SER:N	8:7:195:ALA:HB3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:190:SER:N	8:G:194:MET:CB	2.83	0.42
5:4:191:ILE:CA	5:4:201:LYS:N	2.82	0.42
4:C:933:GLU:O	4:C:935:LEU:N	2.44	0.42
2:S:292:CYS:CA	2:S:296:ASP:N	2.83	0.42
2:S:156:LEU:HA	2:S:160:THR:O	2.20	0.42
7:6:183:ALA:O	7:6:184:SER:CB	2.67	0.42
10:B:856:SER:O	10:B:872:ALA:O	2.38	0.42
8:7:190:SER:N	8:7:220:ASP:CA	2.82	0.42
4:L:531:ARG:O	4:L:535:GLY:O	2.38	0.42
8:G:188:ASP:CA	8:G:195:ALA:HB3	2.50	0.41
4:3:1119:LEU:O	4:3:1121:GLU:N	2.52	0.41
1:0:121:HIS:CB	1:0:130:SER:CB	2.98	0.41
8:G:190:SER:N	8:G:220:ASP:CA	2.82	0.41
8:P:188:ASP:CA	8:P:195:ALA:HB3	2.50	0.41
4:L:1143:VAL:HA	4:L:1146:ALA:CB	2.41	0.41
3:T:274:GLY:HA2	3:T:277:ALA:HB2	1.96	0.41
4:C:1127:GLN:C	4:C:1129:ASP:N	2.74	0.41
2:J:292:CYS:CA	2:J:296:ASP:N	2.83	0.41
4:U:690:PHE:C	4:U:692:GLU:N	2.70	0.41
4:U:531:ARG:O	4:U:535:GLY:O	2.38	0.41
1:R:121:HIS:CB	1:R:130:SER:CB	2.98	0.41
4:3:881:ASN:CB	4:3:922:HIS:O	2.68	0.41
10:A:1309:SER:CA	2:S:1040:VAL:CB	2.98	0.41
5:M:282:GLY:CA	5:M:288:ILE:N	2.83	0.41
4:3:1127:GLN:C	4:3:1129:ASP:N	2.74	0.41
1:I:121:HIS:CB	1:I:130:SER:CB	2.98	0.41
4:3:699:ILE:C	4:3:701:GLU:H	2.24	0.41
7:O:183:ALA:O	7:O:184:SER:CB	2.67	0.41
10:B:842:ILE:CB	10:B:882:GLN:CB	2.92	0.41
8:7:190:SER:N	8:7:194:MET:CB	2.83	0.41
8:G:191:PRO:O	8:G:192:ASN:CB	2.69	0.41
8:P:191:PRO:O	8:P:192:ASN:CB	2.69	0.41
4:L:1127:GLN:C	4:L:1129:ASP:N	2.74	0.41
2:S:349:SER:HA	2:S:401:LEU:O	2.20	0.41
8:P:320:LYS:O	9:Q:13:ILE:CB	2.69	0.41
5:V:191:ILE:CA	5:V:201:LYS:N	2.82	0.41
9:8:274:PHE:O	9:8:275:ALA:HB2	2.18	0.41
4:C:531:ARG:O	4:C:535:GLY:O	2.38	0.41
2:J:349:SER:HA	2:J:401:LEU:O	2.20	0.41
4:3:933:GLU:O	4:3:935:LEU:N	2.44	0.41
1:I:121:HIS:N	1:I:130:SER:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:531:ARG:O	4:3:535:GLY:O	2.38	0.41
2:S:511:THR:HA	2:S:512:GLU:HA	1.86	0.41
10:B:858:HIS:C	10:B:872:ALA:CA	2.86	0.41
8:P:189:SER:C	8:P:220:ASP:N	2.74	0.41
5:D:282:GLY:CA	5:D:288:ILE:N	2.82	0.41
8:Y:320:LYS:O	9:Z:13:ILE:CB	2.68	0.41
1:9:121:HIS:CB	1:9:130:SER:CB	2.98	0.41
1:9:121:HIS:N	1:9:130:SER:O	2.51	0.41
2:1:156:LEU:HA	2:1:160:THR:O	2.20	0.41
8:Y:188:ASP:CA	8:Y:195:ALA:HB3	2.50	0.41
5:4:282:GLY:CA	5:4:288:ILE:N	2.82	0.41
7:F:283:ASP:C	7:F:285:LYS:H	2.24	0.41
2:1:394:GLU:CB	2:1:410:TRP:CB	2.99	0.41
2:1:511:THR:HA	2:1:512:GLU:HA	1.86	0.41
8:G:320:LYS:O	9:H:13:ILE:CB	2.69	0.41
10:B:856:SER:C	10:B:873:ILE:O	2.52	0.41
10:A:1311:ASP:H	2:S:1009:LEU:CB	2.33	0.41
8:7:189:SER:C	8:7:220:ASP:N	2.74	0.41
8:G:189:SER:C	8:G:220:ASP:N	2.74	0.41
10:B:326:ALA:CB	10:B:387:LEU:CB	2.95	0.41
5:D:191:ILE:CA	5:D:201:LYS:N	2.82	0.41
4:U:1127:GLN:C	4:U:1129:ASP:N	2.74	0.41
4:3:1119:LEU:C	4:3:1121:GLU:N	2.71	0.41
10:A:1352:LEU:CB	2:S:1029:ARG:O	2.69	0.41
4:U:699:ILE:C	4:U:701:GLU:H	2.24	0.41
4:U:896:ASN:O	4:U:900:PHE:N	2.52	0.41
4:L:699:ILE:C	4:L:701:GLU:H	2.24	0.41
4:3:1149:GLU:C	4:3:1151:TYR:H	2.24	0.41
4:C:896:ASN:O	4:C:900:PHE:N	2.52	0.41
7:O:283:ASP:C	7:O:285:LYS:H	2.23	0.41
7:X:224:ILE:C	7:X:226:LEU:N	2.72	0.41
4:U:1149:GLU:C	4:U:1151:TYR:H	2.24	0.41
10:B:350:ASN:HA	10:B:353:SER:O	2.21	0.41
8:Y:189:SER:C	8:Y:220:ASP:N	2.74	0.40
3:T:10:ALA:HB1	3:T:321:PHE:O	2.21	0.40
2:1:349:SER:HA	2:1:401:LEU:O	2.20	0.40
8:7:320:LYS:O	9:8:13:ILE:CB	2.69	0.40
7:6:283:ASP:C	7:6:285:LYS:H	2.23	0.40
8:7:191:PRO:O	8:7:192:ASN:CB	2.69	0.40
8:Y:191:PRO:O	8:Y:192:ASN:CB	2.69	0.40
2:1:147:THR:C	2:1:149:ASN:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:10:ALA:HB1	3:2:321:PHE:O	2.21	0.40
4:C:626:SER:O	4:C:627:PHE:C	2.60	0.40
4:U:626:SER:O	4:U:627:PHE:C	2.60	0.40
8:7:188:ASP:CA	8:7:195:ALA:HB3	2.51	0.40
4:C:699:ILE:C	4:C:701:GLU:H	2.24	0.40
4:C:1149:GLU:C	4:C:1151:TYR:H	2.25	0.40
10:B:860:GLN:N	10:B:872:ALA:C	2.74	0.40
10:A:326:ALA:CB	10:A:387:LEU:CB	2.95	0.40
2:1:849:GLN:C	2:1:851:GLY:H	2.25	0.40
4:L:1002:LEU:O	4:L:1004:HIS:N	2.55	0.40
10:B:542:HIS:O	10:B:543:GLN:CB	2.69	0.40
2:1:331:LYS:O	2:1:341:GLY:HA2	2.22	0.40
3:K:10:ALA:HB1	3:K:321:PHE:O	2.21	0.40
2:S:147:THR:C	2:S:149:ASN:H	2.25	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	306/380 (80%)	296 (97%)	10 (3%)	0	100	100
1	9	306/380 (80%)	296 (97%)	10 (3%)	0	100	100
1	I	306/380 (80%)	296 (97%)	10 (3%)	0	100	100
1	R	306/380 (80%)	296 (97%)	10 (3%)	0	100	100
2	1	959/1436 (67%)	873 (91%)	63 (7%)	23 (2%)	7	47
2	J	957/1436 (67%)	873 (91%)	62 (6%)	22 (2%)	8	48
2	S	957/1436 (67%)	873 (91%)	62 (6%)	22 (2%)	8	48
2	a	957/1436 (67%)	873 (91%)	62 (6%)	22 (2%)	8	48
3	2	316/326 (97%)	280 (89%)	15 (5%)	21 (7%)	1	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	316/326 (97%)	279 (88%)	16 (5%)	21 (7%)	1	24
3	T	316/326 (97%)	280 (89%)	15 (5%)	21 (7%)	1	24
3	b	316/326 (97%)	279 (88%)	16 (5%)	21 (7%)	1	24
4	3	508/1156 (44%)	437 (86%)	55 (11%)	16 (3%)	5	42
4	C	508/1156 (44%)	437 (86%)	56 (11%)	15 (3%)	5	42
4	L	508/1156 (44%)	437 (86%)	56 (11%)	15 (3%)	5	42
4	U	508/1156 (44%)	437 (86%)	56 (11%)	15 (3%)	5	42
5	4	636/925 (69%)	607 (95%)	25 (4%)	4 (1%)	30	74
5	D	640/925 (69%)	607 (95%)	28 (4%)	5 (1%)	24	69
5	M	636/925 (69%)	608 (96%)	24 (4%)	4 (1%)	30	74
5	V	640/925 (69%)	607 (95%)	27 (4%)	6 (1%)	21	67
6	5	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	6	44
6	E	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	6	44
6	N	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	6	44
6	W	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	6	44
7	6	281/322 (87%)	235 (84%)	38 (14%)	8 (3%)	6	44
7	F	281/322 (87%)	231 (82%)	42 (15%)	8 (3%)	6	44
7	O	281/322 (87%)	235 (84%)	38 (14%)	8 (3%)	6	44
7	X	281/322 (87%)	230 (82%)	43 (15%)	8 (3%)	6	44
8	7	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	5	40
8	G	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	5	40
8	P	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	5	40
8	Y	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	5	40
9	8	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	7	45
9	H	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	7	45
9	Q	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	7	45
9	Z	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	7	45
10	A	1043/1391 (75%)	961 (92%)	58 (6%)	24 (2%)	8	48
10	B	1043/1391 (75%)	961 (92%)	58 (6%)	24 (2%)	8	48
All	All	18636/28774 (65%)	16944 (91%)	1227 (7%)	465 (2%)	11	46

All (465) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	55	ARG
2	1	73	VAL
2	1	159	GLN
2	1	404	THR
2	1	428	VAL
2	1	448	ARG
2	1	480	CYS
2	1	514	GLU
2	1	634	SER
2	1	706	LEU
2	1	957	THR
2	1	1013	HIS
2	1	1115	LEU
2	1	1176	GLU
3	2	19	VAL
3	2	29	ASN
3	2	89	LEU
3	2	110	ASP
3	2	119	VAL
3	2	155	GLU
3	2	239	ARG
3	2	242	TYR
3	2	254	ALA
3	2	308	LEU
4	3	619	GLY
4	3	623	ARG
4	3	627	PHE
4	3	679	ILE
4	3	680	PRO
4	3	685	PRO
4	3	867	CYS
4	3	869	PHE
4	3	933	GLU
5	4	332	LYS
6	5	303	PRO
6	5	358	VAL
6	5	411	ASN
6	5	532	GLU
7	6	251	ASN
8	7	164	SER
8	7	188	ASP
8	7	193	ALA
8	7	194	MET

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Mol	Chain	Res	Type
8	7	195	ALA
8	7	220	ASP
9	8	157	ALA
9	8	188	GLU
10	A	332	ARG
10	A	443	LYS
10	A	543	GLN
10	A	802	GLN
10	A	1320	PRO
10	A	1343	ASN
10	A	1351	ASN
10	A	1369	SER
10	B	332	ARG
10	B	443	LYS
10	B	543	GLN
10	B	802	GLN
10	B	1320	PRO
10	B	1343	ASN
10	B	1351	ASN
10	B	1369	SER
4	C	619	GLY
4	C	623	ARG
4	C	627	PHE
4	C	679	ILE
4	C	680	PRO
4	C	685	PRO
4	C	867	CYS
4	C	869	PHE
4	C	933	GLU
5	D	332	LYS
6	E	303	PRO
6	E	358	VAL
6	E	411	ASN
6	E	532	GLU
7	F	251	ASN
8	G	164	SER
8	G	188	ASP
8	G	193	ALA
8	G	194	MET
8	G	195	ALA
8	G	220	ASP
9	H	157	ALA

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Mol	Chain	Res	Type
9	H	188	GLU
2	J	55	ARG
2	J	73	VAL
2	J	159	GLN
2	J	404	THR
2	J	428	VAL
2	J	448	ARG
2	J	480	CYS
2	J	514	GLU
2	J	634	SER
2	J	706	LEU
2	J	957	THR
2	J	1115	LEU
2	J	1176	GLU
3	K	19	VAL
3	K	29	ASN
3	K	89	LEU
3	K	110	ASP
3	K	119	VAL
3	K	155	GLU
3	K	239	ARG
3	K	242	TYR
3	K	254	ALA
3	K	308	LEU
4	L	619	GLY
4	L	623	ARG
4	L	627	PHE
4	L	679	ILE
4	L	680	PRO
4	L	685	PRO
4	L	867	CYS
4	L	869	PHE
4	L	933	GLU
5	M	332	LYS
6	N	303	PRO
6	N	358	VAL
6	N	411	ASN
6	N	532	GLU
7	O	251	ASN
8	P	164	SER
8	P	188	ASP
8	P	193	ALA

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Mol	Chain	Res	Type
8	P	194	MET
8	P	195	ALA
8	P	220	ASP
9	Q	157	ALA
9	Q	188	GLU
2	S	55	ARG
2	S	73	VAL
2	S	159	GLN
2	S	404	THR
2	S	428	VAL
2	S	448	ARG
2	S	480	CYS
2	S	514	GLU
2	S	634	SER
2	S	706	LEU
2	S	957	THR
2	S	1115	LEU
2	S	1176	GLU
3	T	19	VAL
3	T	29	ASN
3	T	89	LEU
3	T	110	ASP
3	T	119	VAL
3	T	155	GLU
3	T	239	ARG
3	T	242	TYR
3	T	254	ALA
3	T	308	LEU
4	U	619	GLY
4	U	623	ARG
4	U	627	PHE
4	U	680	PRO
4	U	685	PRO
4	U	867	CYS
4	U	869	PHE
4	U	933	GLU
5	V	332	LYS
6	W	303	PRO
6	W	358	VAL
6	W	411	ASN
6	W	532	GLU
7	X	251	ASN

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Mol	Chain	Res	Type
8	Y	164	SER
8	Y	188	ASP
8	Y	193	ALA
8	Y	194	MET
8	Y	195	ALA
8	Y	220	ASP
9	Z	157	ALA
9	Z	188	GLU
2	a	55	ARG
2	a	73	VAL
2	a	159	GLN
2	a	404	THR
2	a	428	VAL
2	a	448	ARG
2	a	480	CYS
2	a	514	GLU
2	a	634	SER
2	a	706	LEU
2	a	957	THR
2	a	1115	LEU
2	a	1176	GLU
3	b	19	VAL
3	b	29	ASN
3	b	89	LEU
3	b	110	ASP
3	b	119	VAL
3	b	155	GLU
3	b	239	ARG
3	b	242	TYR
3	b	254	ALA
3	b	308	LEU
2	1	451	GLN
2	1	483	THR
2	1	633	GLN
3	2	43	TYR
3	2	241	SER
4	3	629	VAL
4	3	1003	LEU
6	5	486	VAL
6	5	505	LEU
6	5	730	ARG
7	6	114	HIS

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Mol	Chain	Res	Type
7	6	176	PRO
8	7	98	ARG
8	7	176	ARG
8	7	259	SER
9	8	16	VAL
9	8	20	LYS
9	8	315	SER
10	A	260	SER
10	A	312	MET
10	A	415	LYS
10	A	961	GLY
10	A	1235	LEU
10	A	1346	ARG
10	B	260	SER
10	B	312	MET
10	B	415	LYS
10	B	961	GLY
10	B	1235	LEU
10	B	1346	ARG
4	C	629	VAL
4	C	1003	LEU
6	E	486	VAL
6	E	505	LEU
6	E	730	ARG
7	F	114	HIS
8	G	98	ARG
8	G	176	ARG
8	G	259	SER
9	H	16	VAL
9	H	20	LYS
9	H	315	SER
2	J	483	THR
2	J	633	GLN
3	K	43	TYR
3	K	241	SER
4	L	629	VAL
4	L	1003	LEU
6	N	486	VAL
6	N	505	LEU
6	N	730	ARG
7	O	114	HIS
7	O	176	PRO

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Mol	Chain	Res	Type
8	P	98	ARG
8	P	176	ARG
8	P	259	SER
9	Q	16	VAL
9	Q	20	LYS
9	Q	315	SER
2	S	451	GLN
2	S	483	THR
2	S	633	GLN
3	T	43	TYR
3	T	241	SER
4	U	629	VAL
4	U	679	ILE
4	U	1003	LEU
6	W	486	VAL
6	W	505	LEU
6	W	730	ARG
7	X	114	HIS
8	Y	98	ARG
8	Y	176	ARG
8	Y	259	SER
9	Z	16	VAL
9	Z	20	LYS
9	Z	315	SER
2	a	483	THR
2	a	633	GLN
3	b	43	TYR
3	b	241	SER
2	1	412	ASP
2	1	563	GLY
2	1	993	ASP
3	2	206	SER
3	2	255	CYS
4	3	628	PRO
4	3	828	ASN
7	6	184	SER
8	7	196	LYS
9	8	21	ASN
9	8	223	SER
10	A	204	PRO
10	A	1365	GLN
10	B	204	PRO

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Mol	Chain	Res	Type
10	B	1365	GLN
4	C	628	PRO
4	C	828	ASN
7	F	184	SER
8	G	196	LYS
9	H	21	ASN
9	H	223	SER
2	J	412	ASP
2	J	451	GLN
2	J	563	GLY
2	J	993	ASP
3	K	206	SER
3	K	255	CYS
4	L	628	PRO
4	L	828	ASN
7	O	184	SER
8	P	196	LYS
9	Q	21	ASN
9	Q	223	SER
2	S	412	ASP
2	S	563	GLY
2	S	993	ASP
3	T	206	SER
3	T	255	CYS
4	U	628	PRO
4	U	828	ASN
7	X	184	SER
8	Y	196	LYS
9	Z	21	ASN
9	Z	223	SER
2	a	412	ASP
2	a	451	GLN
2	a	563	GLY
2	a	993	ASP
3	b	206	SER
3	b	255	CYS
3	2	31	ASP
3	2	243	PRO
3	2	277	ALA
7	6	55	GLY
9	8	83	GLN
9	8	218	LYS

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Mol	Chain	Res	Type
9	8	275	ALA
9	8	277	SER
10	A	40	TYR
10	A	275	GLU
10	B	40	TYR
10	B	275	GLU
5	D	232	SER
5	D	333	MET
7	F	55	GLY
8	G	263	PRO
9	H	83	GLN
9	H	218	LYS
9	H	275	ALA
9	H	277	SER
3	K	31	ASP
3	K	243	PRO
3	K	277	ALA
7	O	55	GLY
8	P	263	PRO
9	Q	83	GLN
9	Q	218	LYS
9	Q	275	ALA
9	Q	277	SER
3	T	31	ASP
3	T	243	PRO
3	T	277	ALA
5	V	232	SER
5	V	333	MET
7	X	55	GLY
8	Y	263	PRO
9	Z	83	GLN
9	Z	218	LYS
9	Z	275	ALA
9	Z	277	SER
3	b	31	ASP
3	b	243	PRO
3	b	277	ALA
2	1	869	LEU
2	1	1079	ASN
3	2	25	ASN
3	2	275	LYS
4	3	1128	ALA

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Mol	Chain	Res	Type
5	4	232	SER
6	5	302	ASN
7	6	68	PRO
8	7	263	PRO
10	A	274	SER
10	A	278	PRO
10	A	910	GLN
10	B	274	SER
10	B	278	PRO
10	B	910	GLN
4	C	1128	ALA
6	E	302	ASN
7	F	68	PRO
2	J	869	LEU
2	J	1079	ASN
3	K	25	ASN
3	K	275	LYS
4	L	1128	ALA
5	M	232	SER
6	N	302	ASN
7	O	68	PRO
2	S	869	LEU
2	S	1079	ASN
3	T	25	ASN
3	T	275	LYS
4	U	1128	ALA
6	W	302	ASN
7	X	68	PRO
2	a	869	LEU
2	a	1079	ASN
3	b	25	ASN
3	b	275	LYS
3	2	296	VAL
4	3	552	ASP
6	5	556	LEU
6	5	636	THR
10	A	158	GLN
10	B	158	GLN
6	E	556	LEU
6	E	636	THR
3	K	296	VAL
6	N	556	LEU

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Mol	Chain	Res	Type
6	N	636	THR
3	T	296	VAL
5	V	483	LEU
6	W	556	LEU
6	W	636	THR
3	b	296	VAL
3	2	209	VAL
5	4	469	VAL
5	D	469	VAL
6	E	450	PRO
3	K	209	VAL
5	M	469	VAL
3	T	209	VAL
5	V	469	VAL
6	W	450	PRO
3	b	209	VAL
2	1	197	ASP
5	4	396	GLU
6	5	450	PRO
7	6	129	ILE
5	D	396	GLU
7	F	129	ILE
7	F	176	PRO
2	J	197	ASP
5	M	396	GLU
6	N	450	PRO
7	O	129	ILE
2	S	197	ASP
5	V	396	GLU
7	X	129	ILE
7	X	176	PRO
2	a	197	ASP
10	A	942	PRO
10	B	942	PRO
4	3	573	PRO
7	6	224	ILE
10	A	76	PRO
10	B	76	PRO
7	F	224	ILE
7	O	224	ILE
7	X	224	ILE
4	C	573	PRO

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Mol	Chain	Res	Type
4	L	573	PRO
4	U	573	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.