



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:26 PM UTC

PDB ID : 5A9Q / pdb_00005a9q
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.; Kastritis, 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

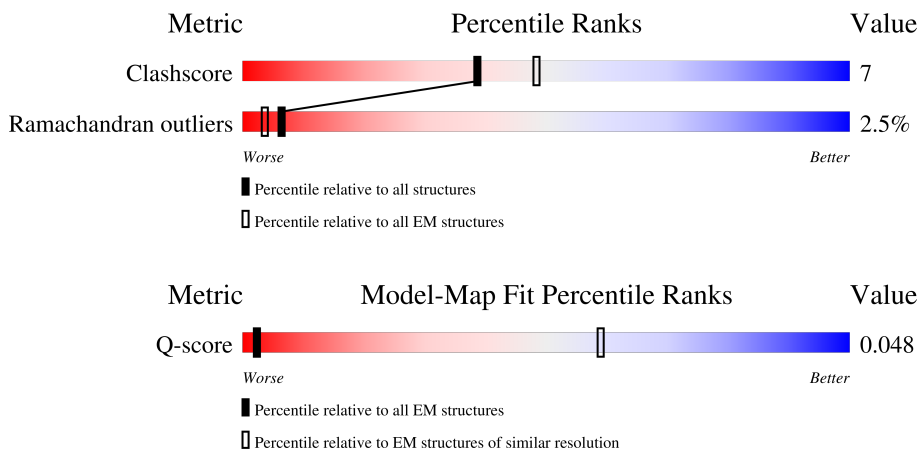
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



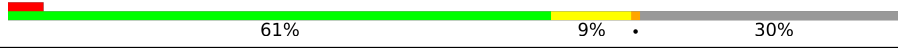
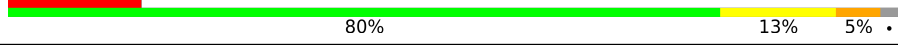
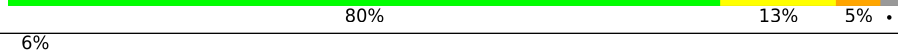
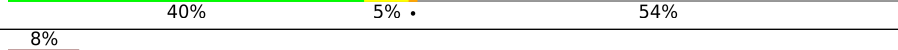
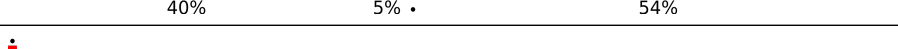
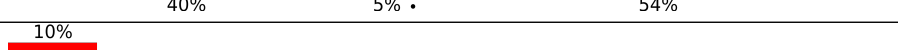
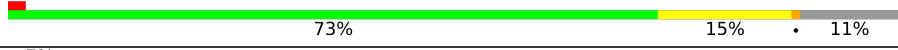
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	17 (22.90 - 23.50)

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

Mol	Chain	Length	Quality of chain
1	0	380	 8% 80% 17%
1	9	380	 8% 80% 17%
1	I	380	 8% 80% 17%
1	R	380	 8% 80% 17%
2	1	1436	 14% 61% 8% 30%

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Mol	Chain	Length	Quality of chain
2	J	1436	
2	S	1436	
2	a	1436	
3	2	326	
3	K	326	
3	T	326	
3	b	326	
4	3	1156	
4	C	1156	
4	L	1156	
4	U	1156	
5	4	925	
5	D	925	
5	M	925	
5	V	925	
6	5	937	
6	E	937	
6	N	937	
6	W	937	
7	6	322	
7	F	322	
7	O	322	
7	X	322	
8	7	360	
8	G	360	

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Mol	Chain	Length	Quality of chain
8	P	360	75%9%11%
8	Y	360	75%9%11%
9	8	656	58%8%34%
9	H	656	58%8%34%
9	Q	656	58%8%34%
9	Z	656	58%8%34%
10	A	1391	16%69%8%21%
10	B	1391	10%68%10%21%

2 Entry composition [i](#)

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.

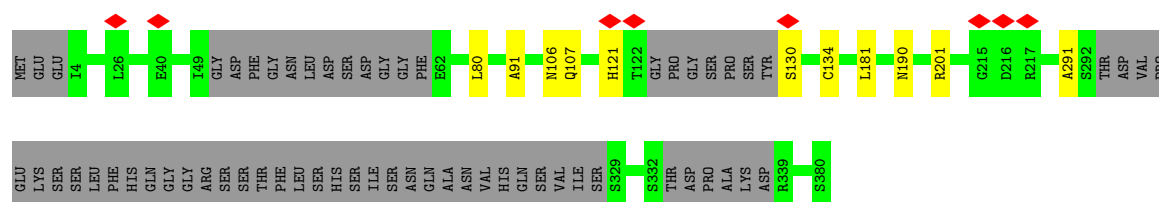
Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	1097	Total	C	N	O	0	0
			5436	3242	1097	1097		
10	B	1097	Total	C	N	O	0	0
			5436	3242	1097	1097		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

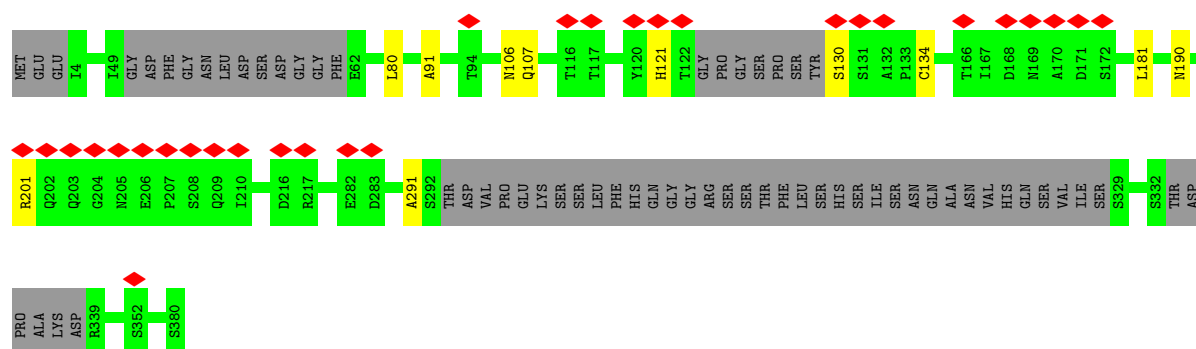
• Molecule 1: NUCLEOPORIN NUP43

Chain 0: 



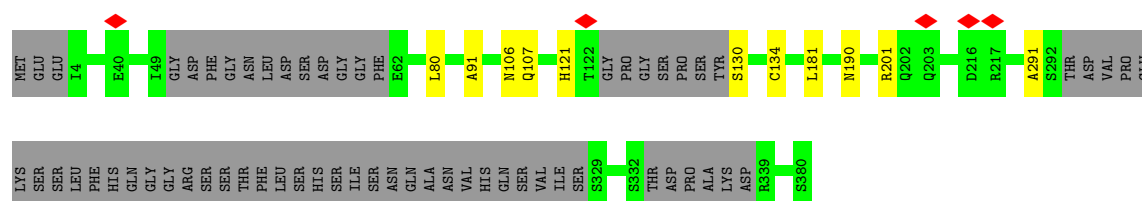
• Molecule 1: NUCLEOPORIN NUP43

Chain 9: 



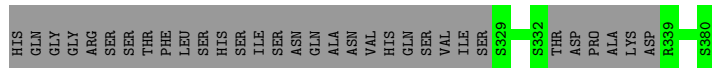
• Molecule 1: NUCLEOPORIN NUP43

Chain I: 



• Molecule 1: NUCLEOPORIN NUP43

Response	Percentage
Yes	80%
No	17%



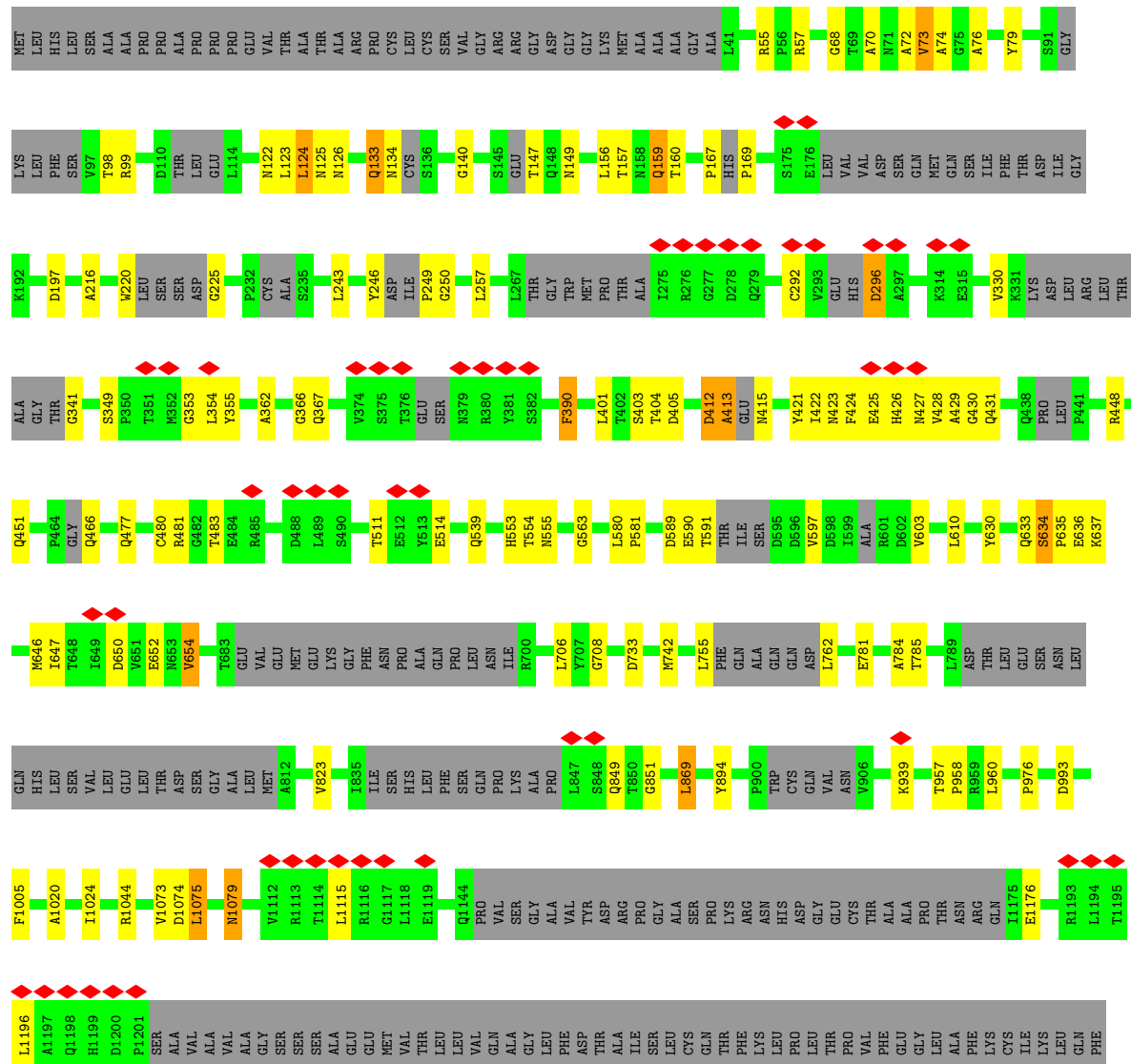
Chain 1:





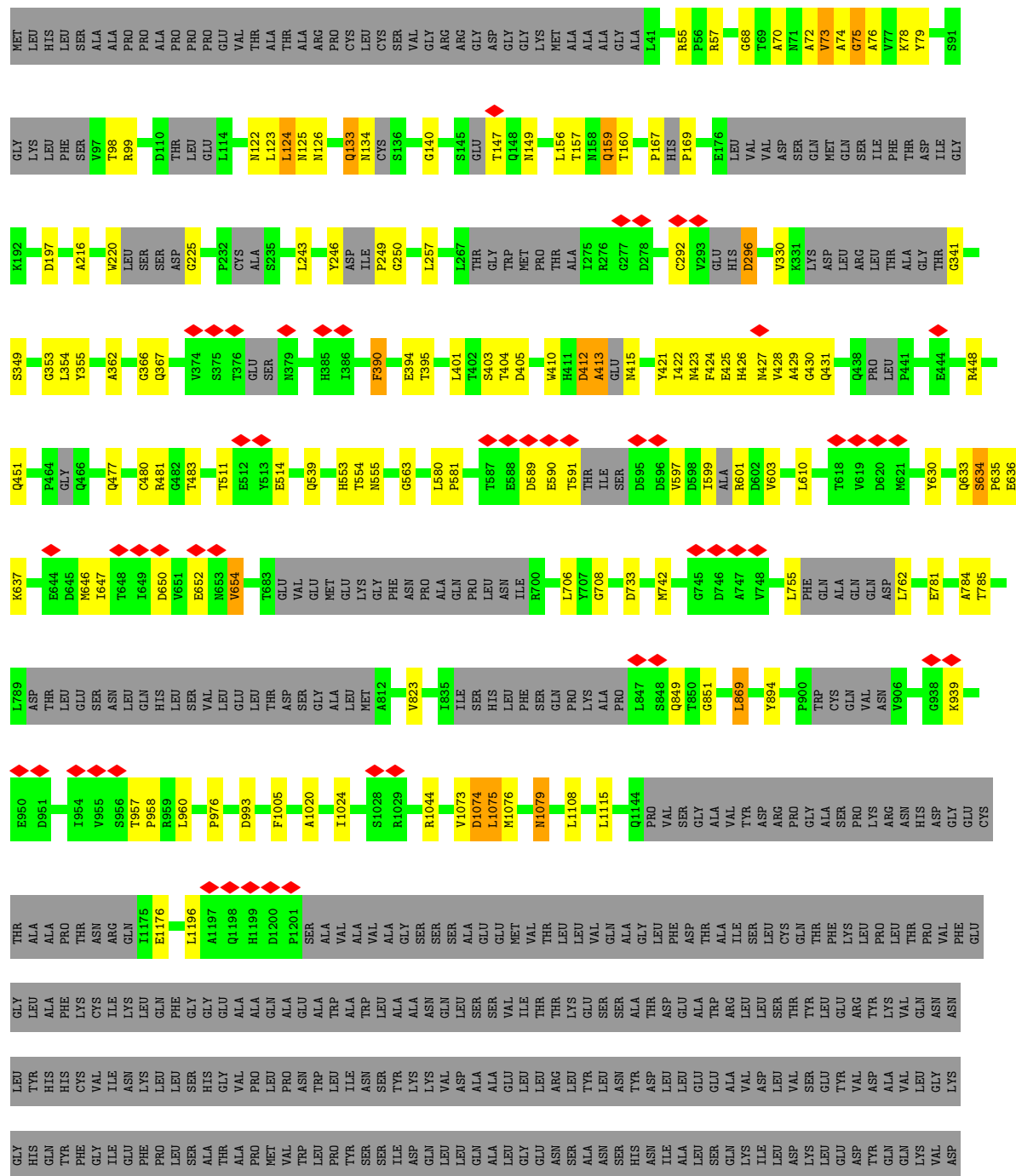
• Molecule 2: NUCLEAR PORE COMPLEX PROTEIN NUP160

Chain J: 61% 8% 30%





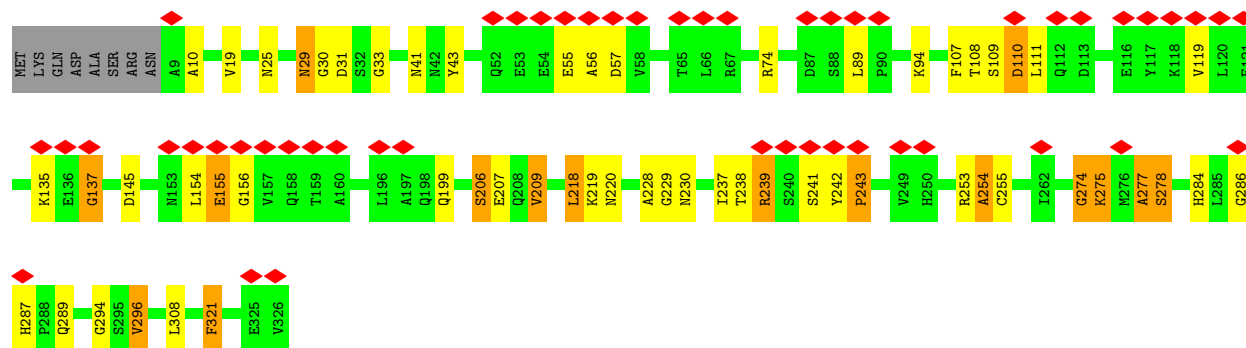
- Molecule 2: NUCLEAR PORE COMPLEX PROTEIN NUP160



LYS
ALA
THR
GLN
ASP
ARG
LEU
LEU
TYR
ARG
THR
LEU

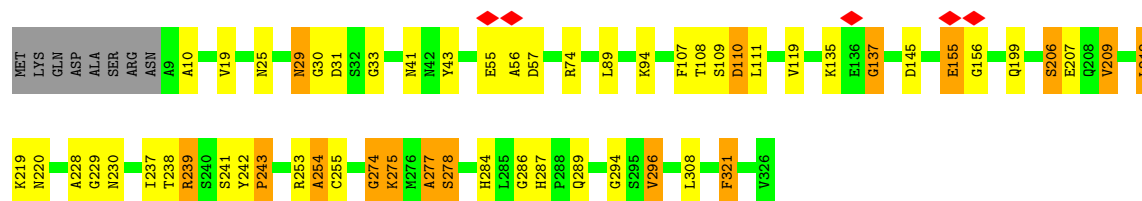
• Molecule 3: NUCLEOPORIN NUP37

Chain 2:  15% 80% 13% 5% .



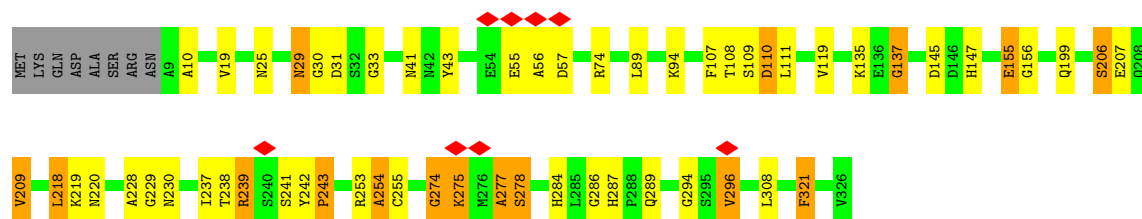
• Molecule 3: NUCLEOPORIN NUP37

Chain K:  80% 13% 5% .



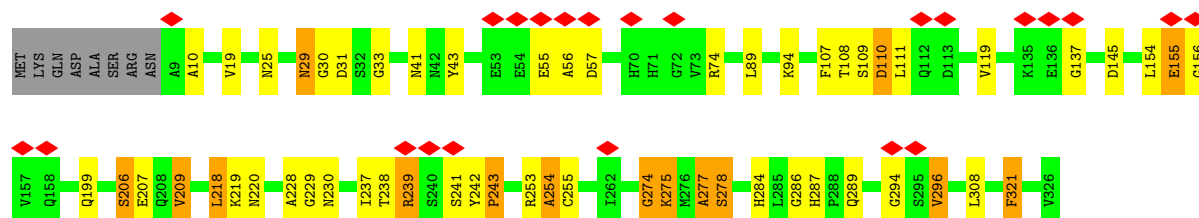
• Molecule 3: NUCLEOPORIN NUP37

Chain T:  80% 13% 5% .

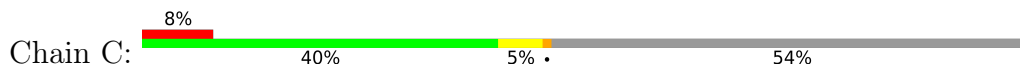


• Molecule 3: NUCLEOPORIN NUP37

Chain b:  7% 80% 13% 5% .

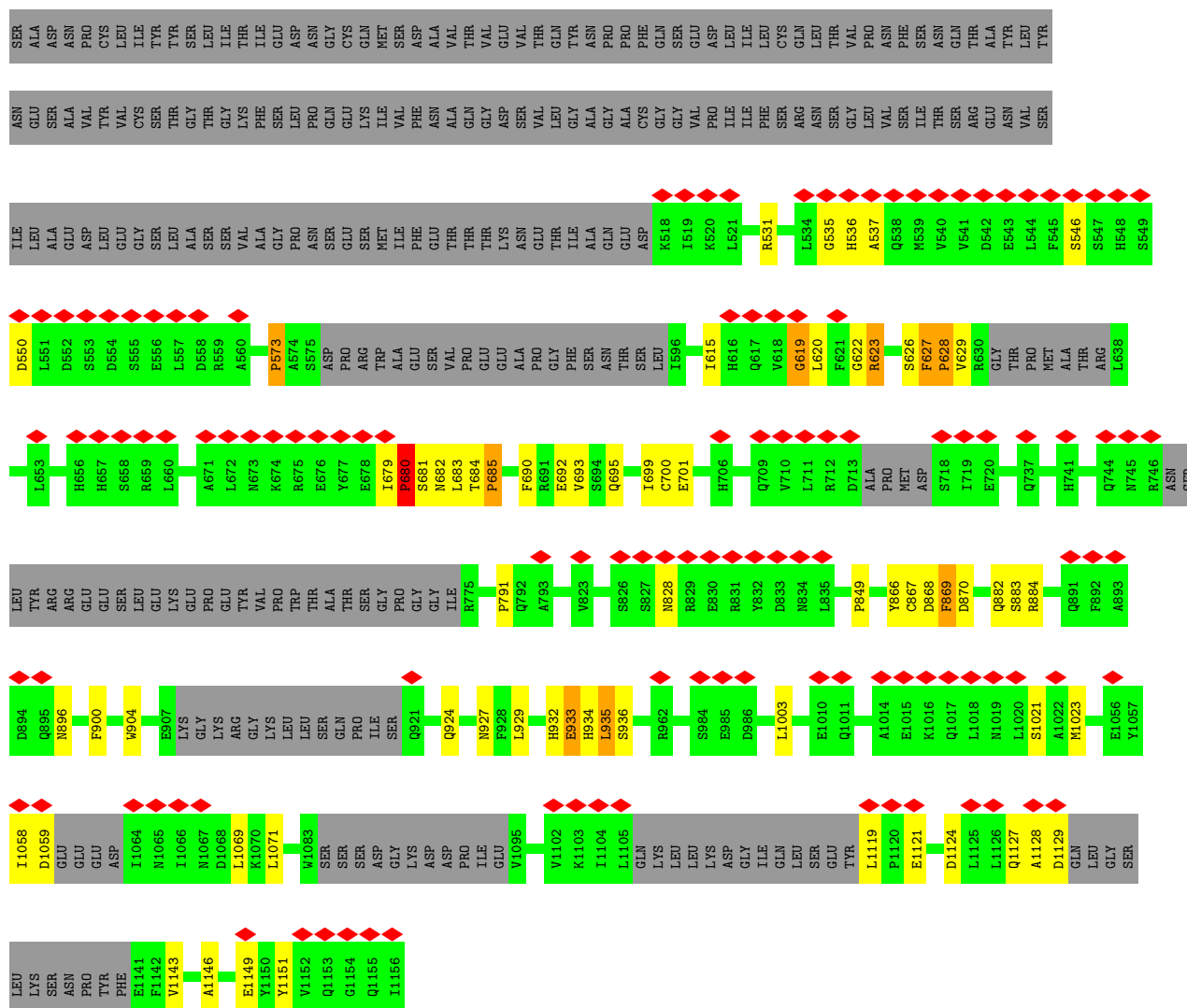


Chain 3: 6% 40% 5% 49%



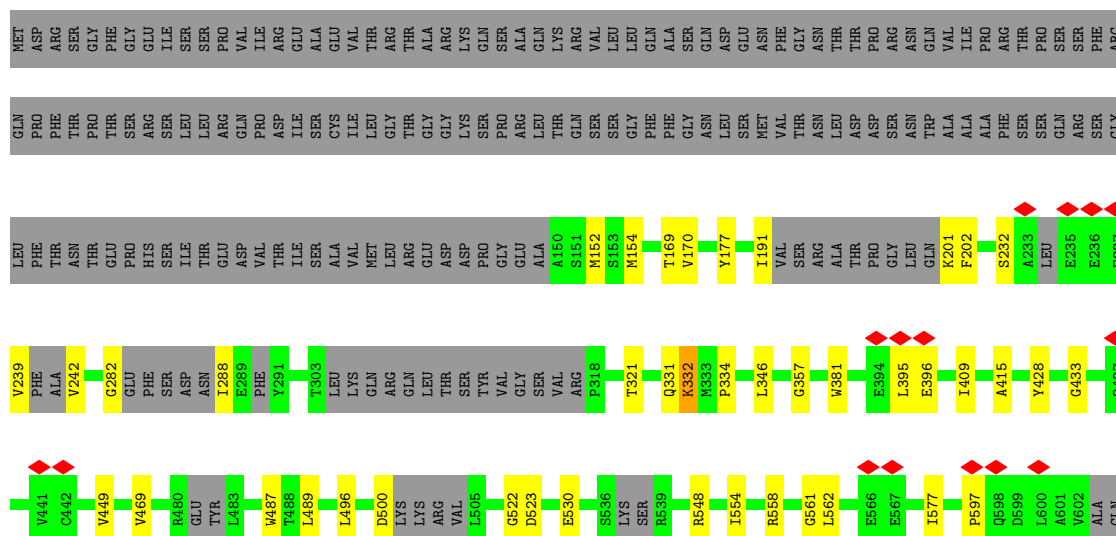
- Molecule 4: NUCLEAR PORE COMPLEX PROTEIN NUP133

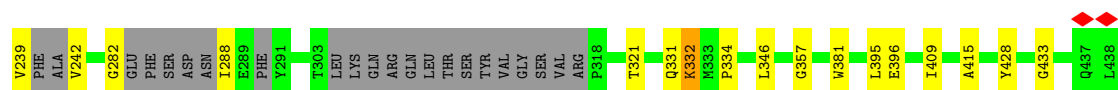
[illegible]

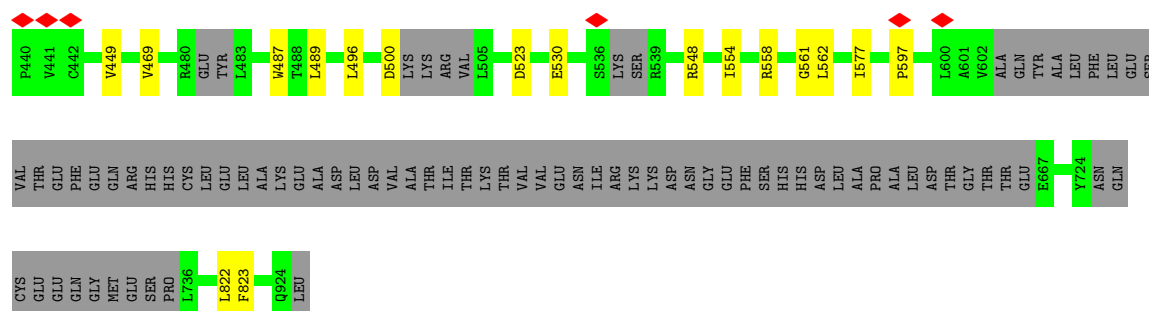


● Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107

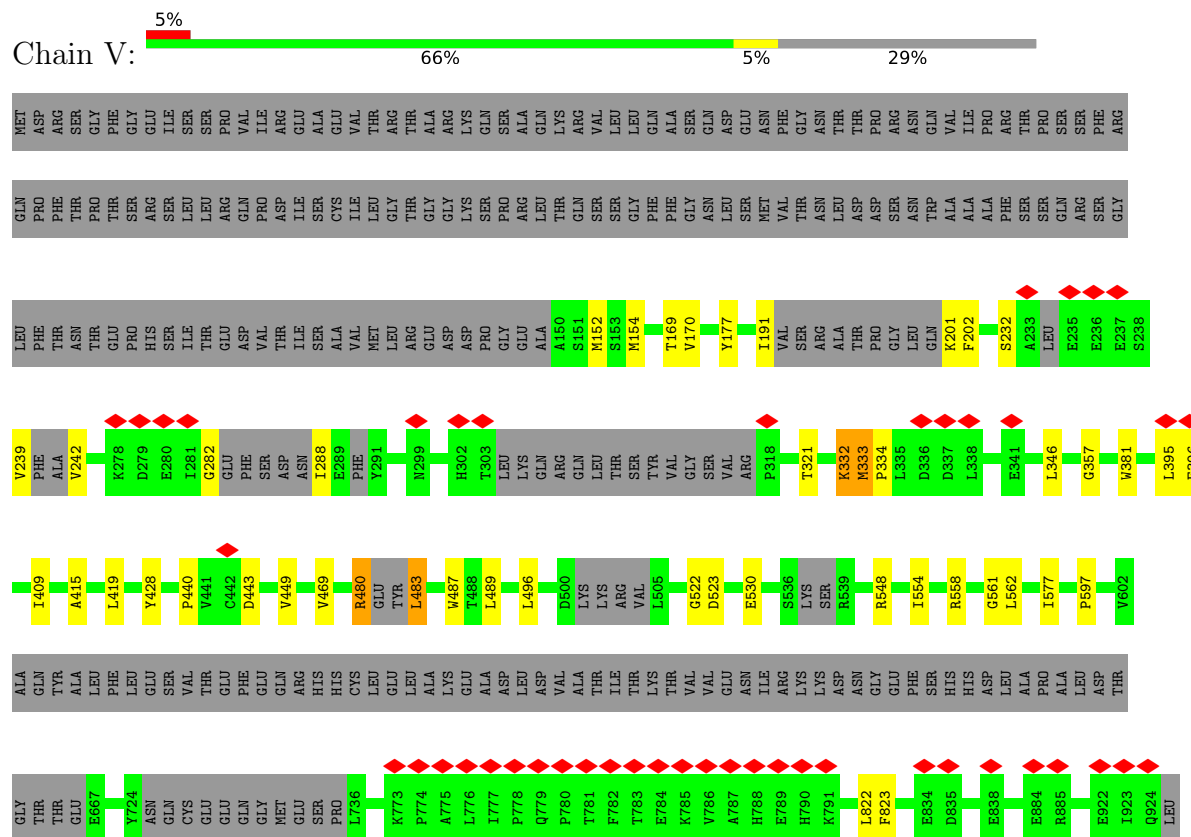
Chain 4: 67% 5% 29%



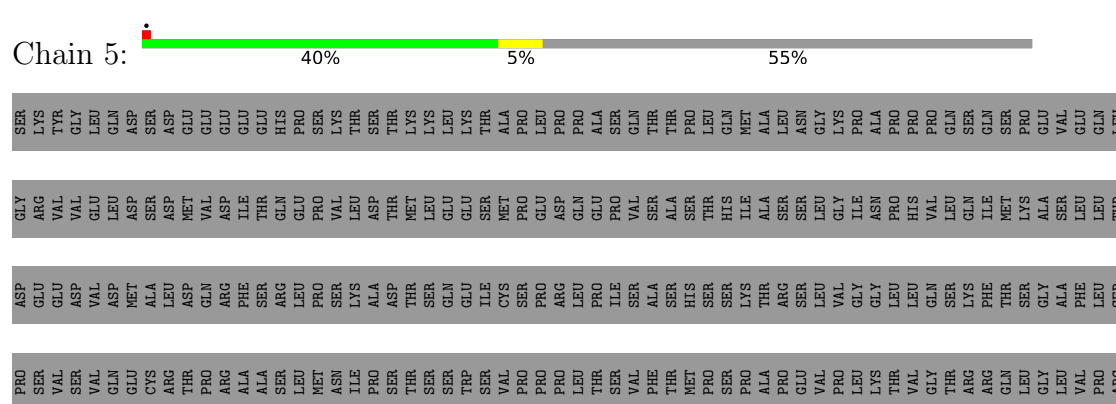


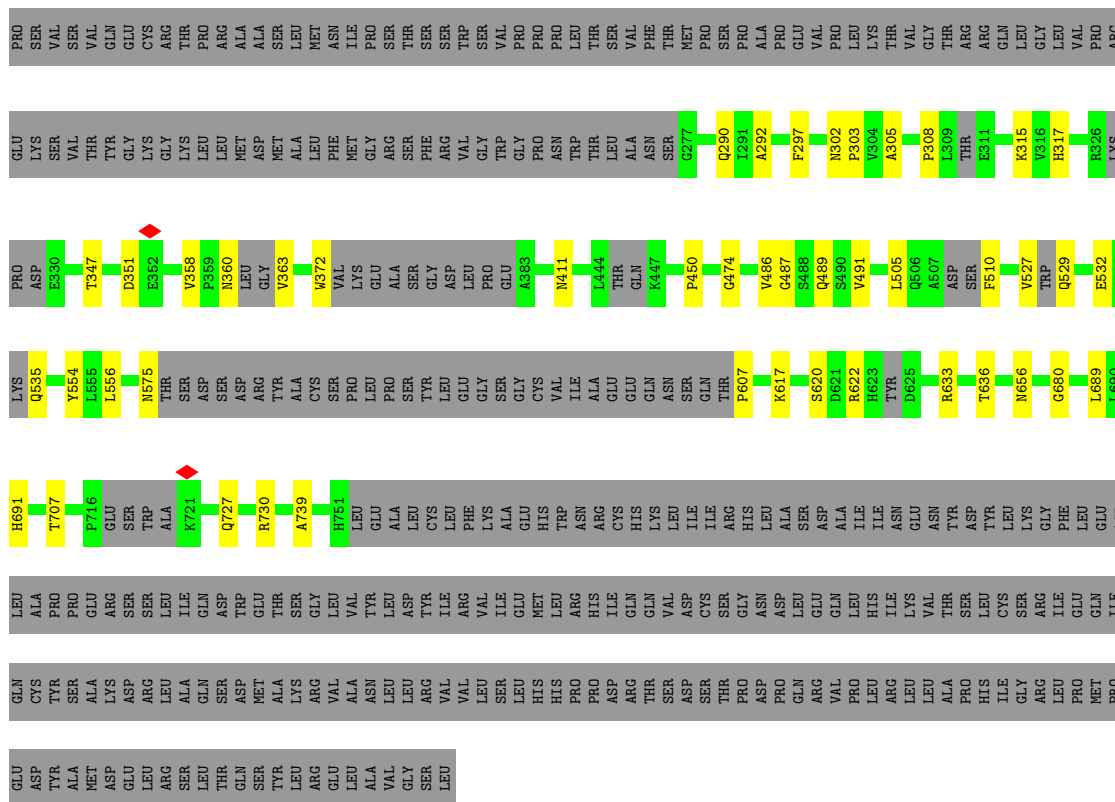


• Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107

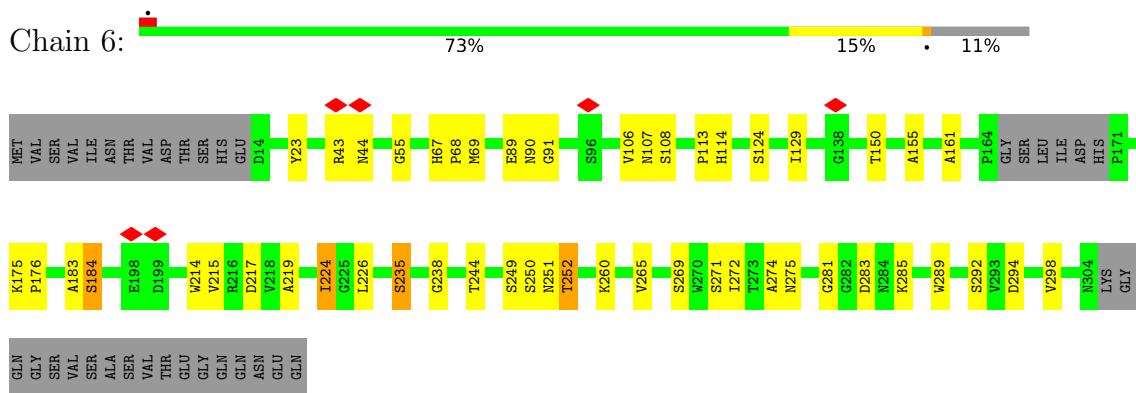


• Molecule 6: NUCLEAR PORE COMPLEX PROTEIN NUP96

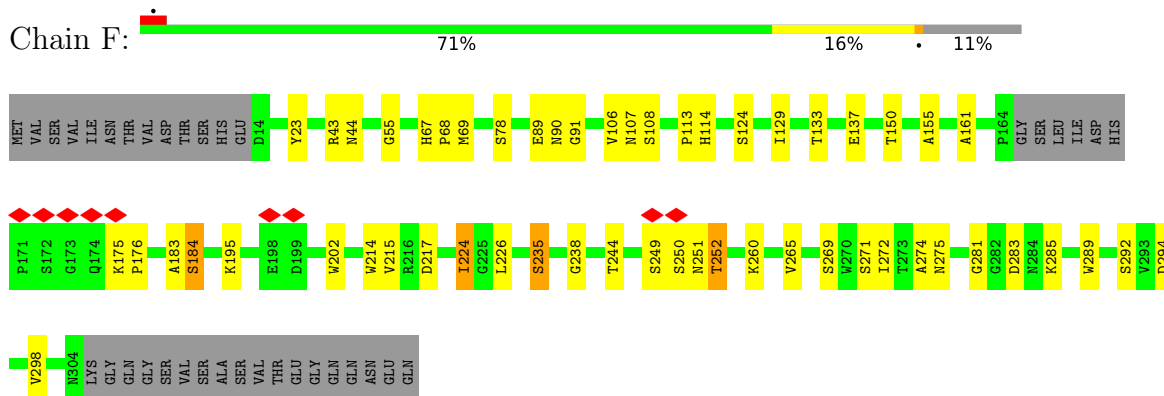




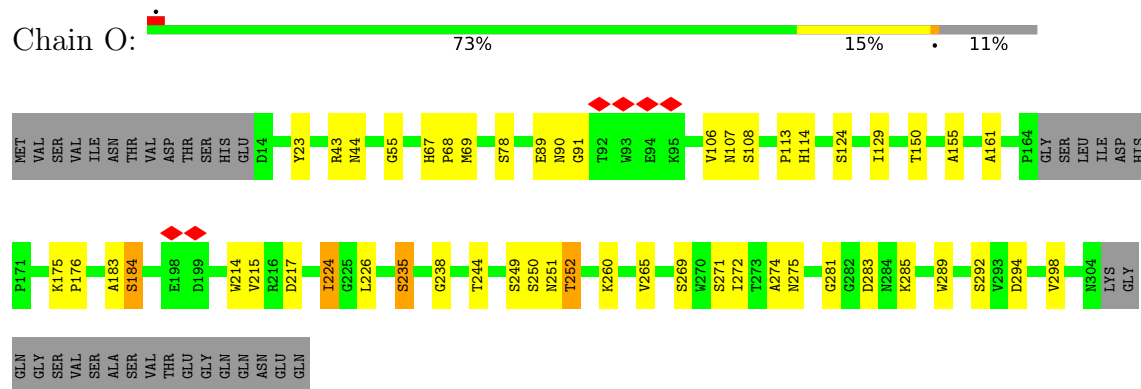
● Molecule 7: PROTEIN SEC13 HOMOLOG



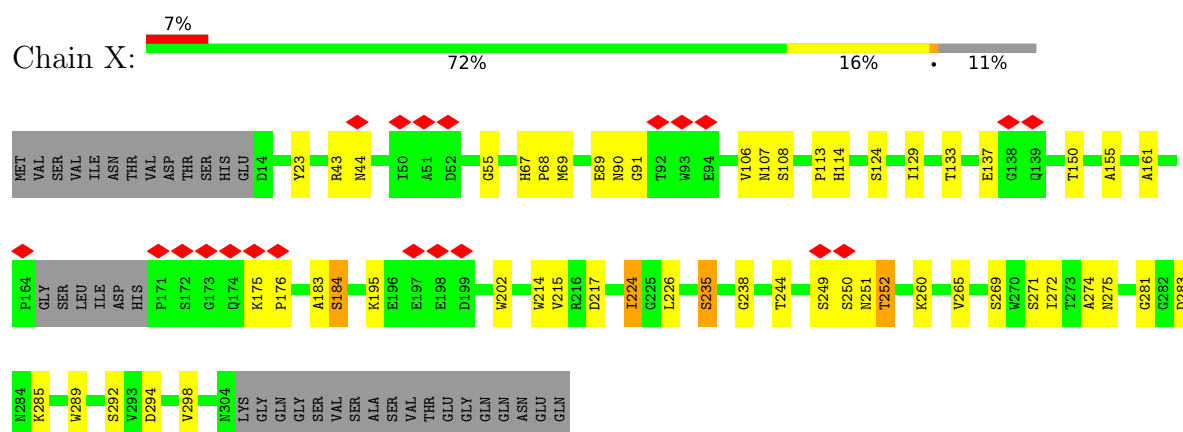
● Molecule 7: PROTEIN SEC13 HOMOLOG



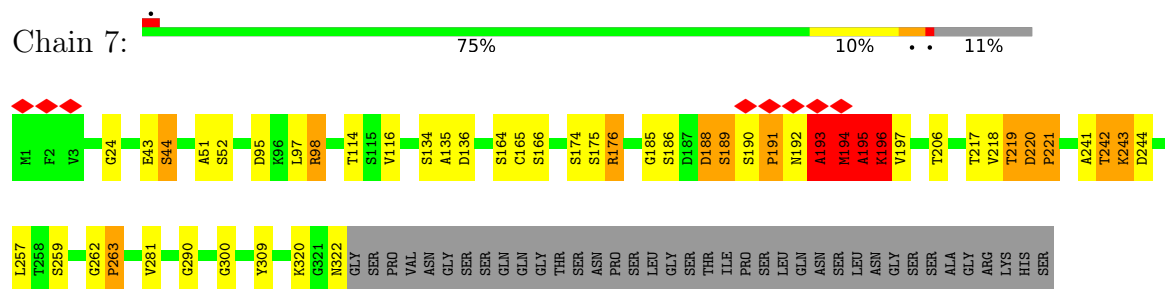
- Molecule 7: PROTEIN SEC13 HOMOLOG



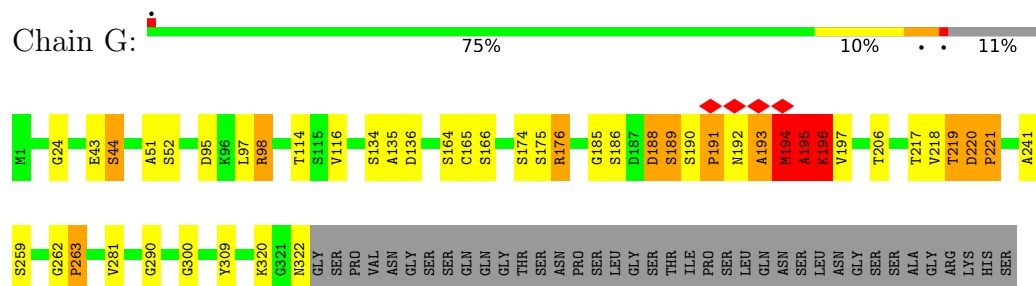
- Molecule 7: PROTEIN SEC13 HOMOLOG



- Molecule 8: NUCLEOPORIN SEH1

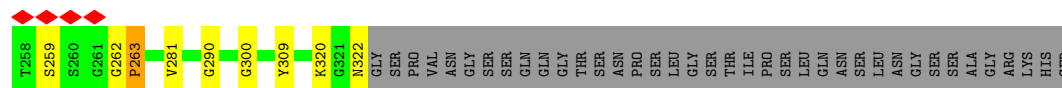


- Molecule 8: NUCLEOPORIN SEH1



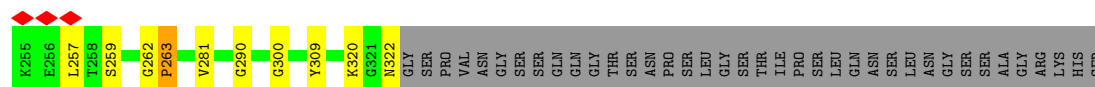
- Molecule 8: NUCLEOPORIN SEH1

Frequency	Percentage
Daily	75%
Weekly	9%
Monthly	11%
Other	5%



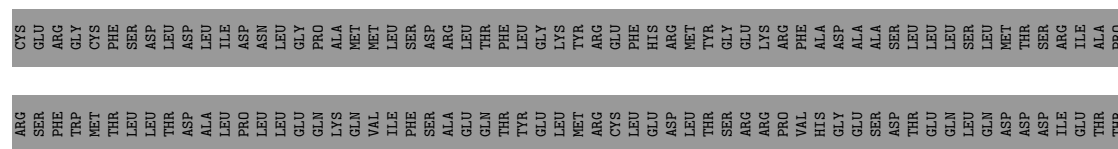
- Molecule 8: NUCLEOPORIN SEH1

Frequency	Percentage
Daily	75%
Weekly	9%
Monthly	11%
Other	5%



- Molecule 9: NUCLEAR PORE COMPLEX PROTEIN NUP85

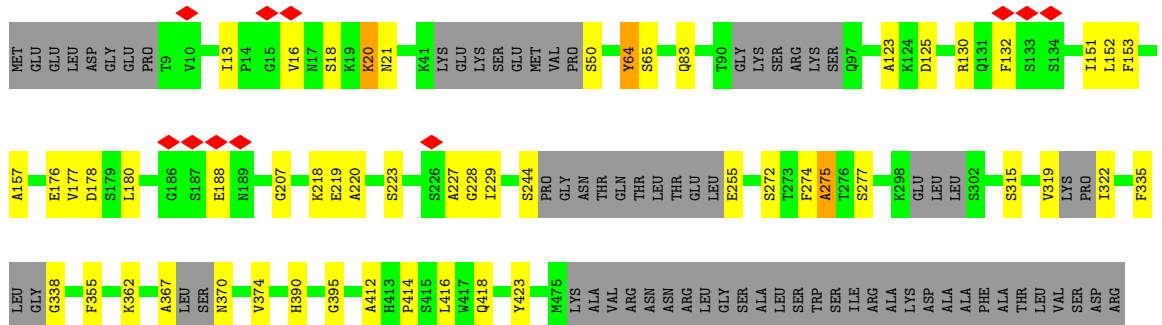
Frequency	Percentage
Daily	58%
Weekly	8%
Monthly	34%



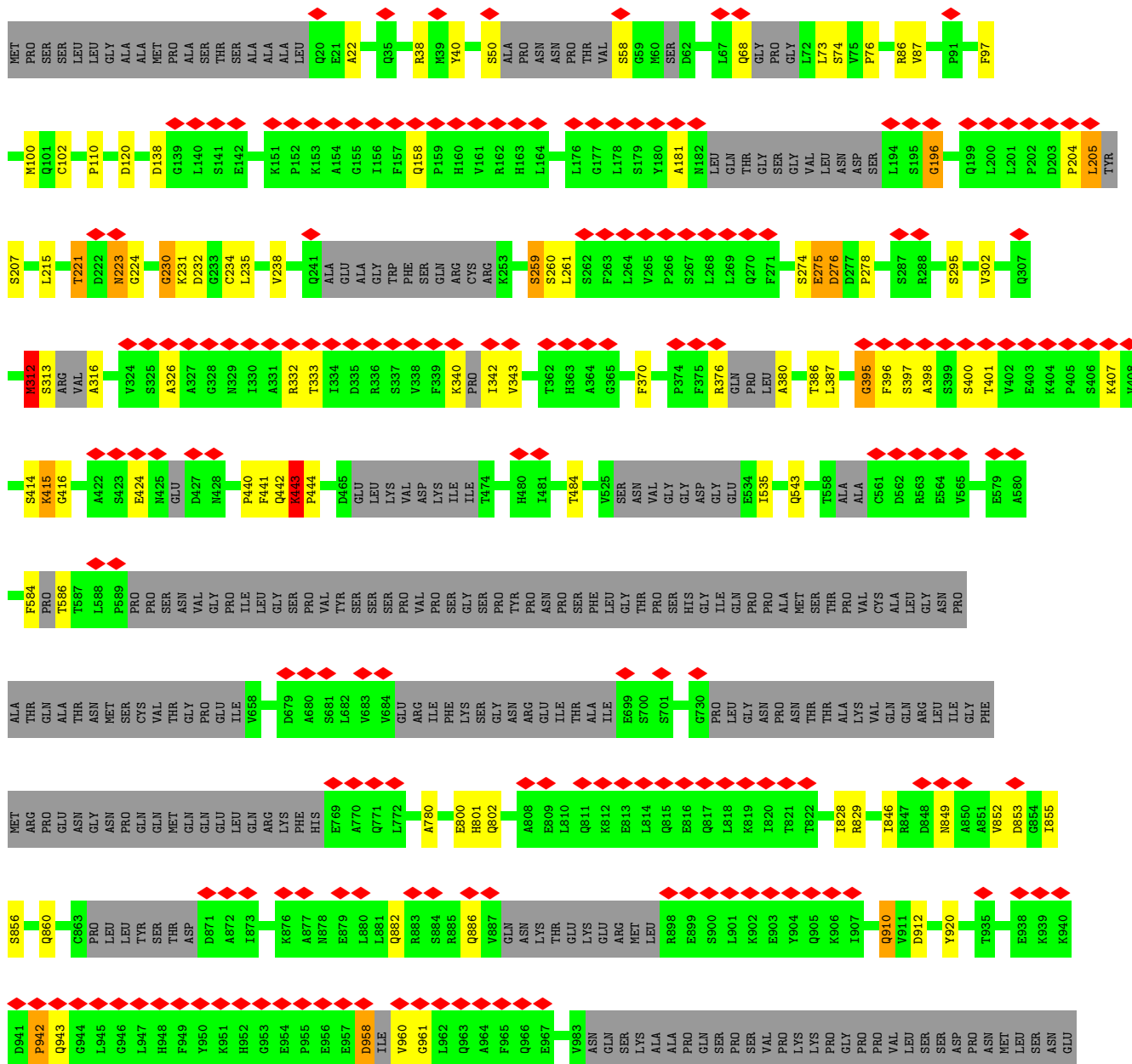
- Molecule 9: NUCLEAR PORE COMPLEX PROTEIN NUP85

Frequency	Percentage
Daily	58%
Weekly	8%
Monthly	34%

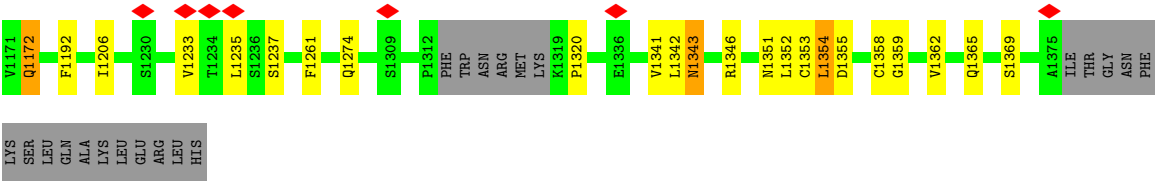




- Molecule 10: NUCLEAR PORE COMPLEX PROTEIN NUP155







4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING OF TILT SERIES	Depositor
Microscope	FEI TITAN KRIOS	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
Maximum voxel value	15.038	Depositor
Minimum voxel value	-7.184	Depositor
Average voxel value	-0.000	Depositor
Voxel value standard deviation	1.629	Depositor
Recommended contour level	3.5	Depositor
Tomogram size ($\text{\AA}$)	1422.72, 1422.72, 1422.72	wwPDB
Tomogram dimensions	208, 208, 208	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing ($\text{\AA}$)	6.8399997, 6.8399997, 6.8399997	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	1.22	2/1557 (0.1%)	1.02	2/2161 (0.1%)
1	9	1.22	2/1557 (0.1%)	1.02	2/2161 (0.1%)
1	I	1.22	2/1557 (0.1%)	1.02	2/2161 (0.1%)
1	R	1.22	2/1557 (0.1%)	1.02	2/2161 (0.1%)
2	1	1.59	7/4972 (0.1%)	1.81	108/6892 (1.6%)
2	J	1.60	6/4971 (0.1%)	1.83	107/6889 (1.6%)
2	S	1.58	6/4971 (0.1%)	1.81	106/6889 (1.5%)
2	a	1.59	6/4971 (0.1%)	1.81	104/6889 (1.5%)
3	2	1.53	0/1565	1.91	43/2175 (2.0%)
3	K	1.53	0/1565	1.91	41/2175 (1.9%)
3	T	1.53	0/1565	1.91	42/2175 (1.9%)
3	b	1.53	0/1565	1.91	43/2175 (2.0%)
4	3	0.41	0/2619	1.07	9/3644 (0.2%)
4	C	0.41	0/2619	1.07	8/3644 (0.2%)
4	L	0.41	0/2619	1.07	9/3644 (0.2%)
4	U	0.40	0/2619	1.07	9/3644 (0.2%)
5	4	1.25	0/3266	1.49	32/4540 (0.7%)
5	D	1.23	3/3268 (0.1%)	1.45	30/4546 (0.7%)
5	M	1.25	0/3266	1.49	31/4540 (0.7%)
5	V	1.22	3/3268 (0.1%)	1.45	32/4546 (0.7%)
6	5	1.55	0/2061	1.76	23/2859 (0.8%)
6	E	1.55	0/2061	1.75	23/2859 (0.8%)
6	N	1.55	0/2061	1.76	23/2859 (0.8%)
6	W	1.55	0/2061	1.75	23/2859 (0.8%)
7	6	0.71	0/1400	1.38	18/1943 (0.9%)
7	F	0.72	0/1400	1.42	18/1943 (0.9%)
7	O	0.71	0/1400	1.38	18/1943 (0.9%)
7	X	0.72	0/1400	1.42	17/1943 (0.9%)
8	7	1.64	12/1592 (0.8%)	1.92	41/2217 (1.8%)
8	G	1.64	11/1592 (0.7%)	1.92	41/2217 (1.8%)
8	P	1.65	11/1592 (0.7%)	1.92	41/2217 (1.8%)
8	Y	1.65	13/1592 (0.8%)	1.93	44/2217 (2.0%)
9	8	1.75	1/2145 (0.0%)	1.72	31/2980 (1.0%)
9	H	1.74	1/2145 (0.0%)	1.72	31/2980 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	Q	1.75	1/2145 (0.0%)	1.73	33/2980 (1.1%)
9	Z	1.74	1/2145 (0.0%)	1.72	31/2980 (1.0%)
10	A	1.56	1/5409 (0.0%)	1.83	94/7500 (1.3%)
10	B	1.56	1/5409 (0.0%)	1.83	93/7500 (1.2%)
All	All	1.40	92/95527 (0.1%)	1.64	1405/132647 (1.1%)

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
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
10	A	0	1
10	B	0	1
All	All	0	12

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	64	TYR	C-N	40.99	1.89	1.33
9	Q	64	TYR	C-N	40.95	1.89	1.33
9	Z	64	TYR	C-N	40.89	1.89	1.33
9	H	64	TYR	C-N	40.86	1.89	1.33
2	J	124	LEU	CA-C	10.39	1.59	1.53
2	J	123	LEU	C-N	9.87	1.41	1.33
8	P	194	MET	CA-C	8.22	1.63	1.52
8	7	194	MET	CA-C	8.20	1.63	1.52
8	Y	194	MET	CA-C	8.17	1.63	1.52
8	G	194	MET	CA-C	8.12	1.63	1.52
2	J	124	LEU	N-CA	7.72	1.51	1.46
5	V	483	LEU	C-N	-7.44	1.22	1.33
5	D	483	LEU	C-N	-7.38	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	194	MET	C-N	7.16	1.43	1.33
8	P	194	MET	C-N	7.09	1.43	1.33
8	Y	194	MET	C-N	7.06	1.43	1.33
8	7	194	MET	C-N	6.95	1.43	1.33
2	S	1024	ILE	CA-CB	-6.71	1.50	1.54
8	P	195	ALA	CA-C	6.63	1.61	1.52
8	G	195	ALA	CA-C	6.63	1.61	1.52
8	7	195	ALA	CA-C	6.56	1.61	1.52
2	J	1024	ILE	CA-CB	-6.55	1.50	1.54
2	a	1024	ILE	CA-CB	-6.51	1.50	1.54
2	1	1024	ILE	CA-CB	-6.46	1.50	1.54
8	Y	195	ALA	CA-C	6.44	1.61	1.52
8	G	196	LYS	C-N	6.35	1.42	1.33
8	P	196	LYS	C-N	6.33	1.42	1.33
8	Y	196	LYS	C-N	6.32	1.42	1.33
2	a	124	LEU	C-N	6.31	1.42	1.33
2	S	124	LEU	C-N	6.27	1.42	1.33
8	P	218	VAL	CA-C	-6.25	1.45	1.52
8	7	196	LYS	C-N	6.24	1.42	1.33
8	G	218	VAL	CA-C	-6.23	1.45	1.52
2	J	124	LEU	C-N	6.22	1.42	1.33
2	1	124	LEU	C-N	6.20	1.42	1.33
8	Y	218	VAL	CA-C	-6.19	1.45	1.52
8	7	218	VAL	CA-C	-6.16	1.45	1.52
8	7	195	ALA	N-CA	5.97	1.53	1.46
8	Y	191	PRO	CA-C	-5.95	1.47	1.53
8	Y	195	ALA	N-CA	5.94	1.53	1.46
8	P	195	ALA	N-CA	5.89	1.53	1.46
1	I	80	LEU	N-CA	-5.82	1.39	1.46
8	G	195	ALA	N-CA	5.80	1.53	1.46
1	R	80	LEU	N-CA	-5.80	1.39	1.46
5	V	483	LEU	CA-C	-5.74	1.45	1.52
1	9	80	LEU	N-CA	-5.73	1.39	1.46
1	0	80	LEU	N-CA	-5.73	1.39	1.46
5	D	483	LEU	CA-C	-5.72	1.45	1.52
8	Y	242	THR	CA-C	-5.59	1.46	1.53
1	R	291	ALA	N-CA	5.58	1.53	1.46
8	Y	195	ALA	C-N	5.58	1.41	1.33
1	0	291	ALA	N-CA	5.56	1.53	1.46
8	G	242	THR	CA-C	-5.50	1.46	1.53
8	P	242	THR	CA-C	-5.49	1.46	1.53
1	9	291	ALA	N-CA	5.46	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	195	ALA	C-N	5.46	1.41	1.33
8	7	195	ALA	C-N	5.45	1.41	1.33
2	a	123	LEU	C-N	5.45	1.41	1.33
8	P	219	THR	N-CA	-5.43	1.39	1.46
2	1	123	LEU	C-N	5.42	1.41	1.33
8	7	242	THR	CA-C	-5.41	1.46	1.53
8	Y	219	THR	N-CA	-5.41	1.39	1.46
1	I	291	ALA	N-CA	5.40	1.53	1.46
8	P	195	ALA	C-N	5.39	1.41	1.33
2	S	123	LEU	C-N	5.39	1.41	1.33
2	a	72	ALA	C-N	5.38	1.41	1.33
8	G	219	THR	N-CA	-5.37	1.39	1.46
8	7	219	THR	N-CA	-5.35	1.39	1.46
8	Y	197	VAL	CA-C	5.33	1.58	1.52
2	J	72	ALA	C-N	5.29	1.40	1.33
2	S	72	ALA	C-N	5.28	1.40	1.33
2	1	72	ALA	C-N	5.27	1.40	1.33
8	P	196	LYS	CA-C	5.24	1.59	1.52
2	1	1013	HIS	C-N	-5.23	1.26	1.33
8	G	196	LYS	CA-C	5.19	1.59	1.52
10	A	87	VAL	CA-CB	-5.14	1.50	1.54
5	V	480	ARG	C-N	5.14	1.40	1.33
8	Y	196	LYS	CA-C	5.14	1.59	1.52
5	D	480	ARG	C-N	5.14	1.40	1.33
8	7	196	LYS	CA-C	5.12	1.59	1.52
2	S	124	LEU	CA-C	5.12	1.59	1.52
8	7	193	ALA	C-N	5.08	1.40	1.33
8	G	197	VAL	CA-C	5.08	1.58	1.52
8	P	197	VAL	CA-C	5.05	1.58	1.52
8	7	197	VAL	CA-C	5.05	1.58	1.52
10	B	87	VAL	CA-CB	-5.04	1.50	1.54
2	1	124	LEU	CA-C	5.02	1.59	1.52
2	S	125	ASN	C-N	5.01	1.39	1.33
2	1	73	VAL	C-N	5.01	1.40	1.33
2	a	73	VAL	C-N	5.01	1.40	1.33
8	Y	193	ALA	C-N	5.00	1.40	1.33
2	a	75	GLY	N-CA	5.00	1.52	1.45

All (1405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	276	ASP	O-C-N	28.48	157.40	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	276	ASP	O-C-N	28.43	157.34	122.65
5	M	332	LYS	CA-C-N	14.94	137.84	120.06
5	M	332	LYS	C-N-CA	14.94	137.84	120.06
7	F	272	ILE	N-CA-C	14.90	125.81	110.62
5	4	332	LYS	CA-C-N	14.88	137.76	120.06
5	4	332	LYS	C-N-CA	14.88	137.76	120.06
7	X	272	ILE	N-CA-C	14.88	125.80	110.62
7	6	272	ILE	N-CA-C	14.78	125.69	110.62
7	O	272	ILE	N-CA-C	14.70	125.61	110.62
8	7	218	VAL	CA-C-N	-14.44	101.02	122.39
8	7	218	VAL	C-N-CA	-14.44	101.02	122.39
2	J	124	LEU	N-CA-C	14.41	120.60	108.78
8	G	218	VAL	CA-C-N	-14.40	101.08	122.39
8	G	218	VAL	C-N-CA	-14.40	101.08	122.39
8	P	218	VAL	CA-C-N	-14.38	101.11	122.39
8	P	218	VAL	C-N-CA	-14.38	101.11	122.39
8	Y	218	VAL	CA-C-N	-14.38	101.11	122.39
8	Y	218	VAL	C-N-CA	-14.38	101.11	122.39
8	Y	195	ALA	N-CA-C	13.13	138.77	110.80
8	G	195	ALA	N-CA-C	13.11	138.72	110.80
8	P	195	ALA	N-CA-C	13.09	138.69	110.80
8	7	195	ALA	N-CA-C	13.09	138.68	110.80
10	A	395	GLY	N-CA-C	-12.35	96.97	112.77
10	B	395	GLY	N-CA-C	-12.34	96.97	112.77
8	P	262	GLY	CA-C-N	12.23	135.12	119.84
8	P	262	GLY	C-N-CA	12.23	135.12	119.84
8	G	262	GLY	CA-C-N	12.21	135.11	119.84
8	G	262	GLY	C-N-CA	12.21	135.11	119.84
8	Y	262	GLY	CA-C-N	12.18	135.06	119.84
8	Y	262	GLY	C-N-CA	12.18	135.06	119.84
8	7	262	GLY	CA-C-N	12.15	135.02	119.84
8	7	262	GLY	C-N-CA	12.15	135.02	119.84
10	B	259	SER	O-C-N	-12.00	106.63	122.59
10	A	259	SER	O-C-N	-11.98	106.66	122.59
2	J	123	LEU	CA-C-N	11.73	135.71	123.04
2	J	123	LEU	C-N-CA	11.73	135.71	123.04
2	S	74	ALA	N-CA-C	11.67	135.66	110.80
2	a	74	ALA	N-CA-C	11.65	135.62	110.80
2	1	74	ALA	N-CA-C	11.64	135.60	110.80
6	5	351	ASP	CA-C-N	-11.63	104.82	120.63
6	5	351	ASP	C-N-CA	-11.63	104.82	120.63
2	J	74	ALA	N-CA-C	11.61	135.54	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	351	ASP	CA-C-N	-11.60	104.86	120.63
6	N	351	ASP	C-N-CA	-11.60	104.86	120.63
6	E	351	ASP	CA-C-N	-11.58	104.88	120.63
6	E	351	ASP	C-N-CA	-11.58	104.88	120.63
6	W	351	ASP	CA-C-N	-11.58	104.88	120.63
6	W	351	ASP	C-N-CA	-11.58	104.88	120.63
2	1	427	ASN	N-CA-C	-11.26	99.08	111.36
2	S	427	ASN	N-CA-C	-11.25	99.10	111.36
2	J	427	ASN	N-CA-C	-11.24	99.11	111.36
5	D	480	ARG	O-C-N	11.22	137.25	123.44
2	a	427	ASN	N-CA-C	-11.20	99.15	111.36
5	V	480	ARG	O-C-N	11.16	137.17	123.44
10	A	259	SER	CA-C-N	10.51	141.60	121.54
10	A	259	SER	C-N-CA	10.51	141.60	121.54
10	B	259	SER	CA-C-N	10.48	141.56	121.54
10	B	259	SER	C-N-CA	10.48	141.56	121.54
8	Y	263	PRO	N-CA-C	10.35	133.79	112.47
8	7	263	PRO	N-CA-C	10.34	133.77	112.47
8	P	263	PRO	N-CA-C	10.33	133.75	112.47
8	G	263	PRO	N-CA-C	10.32	133.73	112.47
3	b	109	SER	CA-C-N	10.15	140.92	121.54
3	b	109	SER	C-N-CA	10.15	140.92	121.54
3	2	109	SER	CA-C-N	10.12	140.88	121.54
3	2	109	SER	C-N-CA	10.12	140.88	121.54
3	T	109	SER	CA-C-N	10.12	140.87	121.54
3	T	109	SER	C-N-CA	10.12	140.87	121.54
3	K	109	SER	CA-C-N	10.10	140.84	121.54
3	K	109	SER	C-N-CA	10.10	140.84	121.54
3	K	30	GLY	N-CA-C	-9.83	101.64	115.30
3	b	30	GLY	N-CA-C	-9.82	101.65	115.30
4	C	685	PRO	N-CA-CB	9.81	113.56	103.25
4	3	685	PRO	N-CA-CB	9.80	113.54	103.25
4	U	685	PRO	N-CA-CB	9.80	113.54	103.25
4	L	685	PRO	N-CA-CB	9.77	113.51	103.25
3	T	30	GLY	N-CA-C	-9.77	101.72	115.30
3	2	30	GLY	N-CA-C	-9.75	101.75	115.30
5	M	169	THR	CA-C-N	9.69	132.54	120.72
5	M	169	THR	C-N-CA	9.69	132.54	120.72
2	S	869	LEU	CA-C-N	9.67	132.18	120.09
2	S	869	LEU	C-N-CA	9.67	132.18	120.09
5	4	169	THR	CA-C-N	9.65	132.49	120.72
5	4	169	THR	C-N-CA	9.65	132.49	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	869	LEU	CA-C-N	9.64	132.14	120.09
2	1	869	LEU	C-N-CA	9.64	132.14	120.09
5	D	169	THR	CA-C-N	9.62	132.45	120.72
5	D	169	THR	C-N-CA	9.62	132.45	120.72
5	M	170	VAL	N-CA-C	9.61	119.45	110.42
2	J	869	LEU	CA-C-N	9.59	132.08	120.09
2	J	869	LEU	C-N-CA	9.59	132.08	120.09
5	4	170	VAL	N-CA-C	9.58	119.43	110.42
5	V	170	VAL	N-CA-C	9.57	119.41	110.42
2	a	869	LEU	CA-C-N	9.56	132.04	120.09
2	a	869	LEU	C-N-CA	9.56	132.04	120.09
5	V	169	THR	CA-C-N	9.56	132.38	120.72
5	V	169	THR	C-N-CA	9.56	132.38	120.72
5	D	170	VAL	N-CA-C	9.50	119.35	110.42
3	T	156	GLY	N-CA-C	-9.32	100.11	112.14
3	2	156	GLY	N-CA-C	-9.31	100.13	112.14
3	K	156	GLY	N-CA-C	-9.28	100.17	112.14
3	b	156	GLY	N-CA-C	-9.27	100.18	112.14
2	1	76	ALA	N-CA-C	-9.12	101.22	111.71
2	a	76	ALA	N-CA-C	-9.08	101.27	111.71
9	H	227	ALA	CA-C-N	9.08	131.75	120.22
9	H	227	ALA	C-N-CA	9.08	131.75	120.22
9	8	227	ALA	CA-C-N	9.07	131.75	120.22
9	8	227	ALA	C-N-CA	9.07	131.75	120.22
2	J	76	ALA	N-CA-C	-9.07	101.28	111.71
9	Z	227	ALA	CA-C-N	9.07	131.74	120.22
9	Z	227	ALA	C-N-CA	9.07	131.74	120.22
9	Q	227	ALA	CA-C-N	9.04	131.70	120.22
9	Q	227	ALA	C-N-CA	9.04	131.70	120.22
2	S	76	ALA	N-CA-C	-9.04	101.31	111.71
10	B	1343	ASN	CA-C-N	8.86	131.95	120.44
10	B	1343	ASN	C-N-CA	8.86	131.95	120.44
8	Y	206	THR	N-CA-C	-8.84	101.57	111.82
8	G	206	THR	N-CA-C	-8.82	101.59	111.82
8	7	206	THR	N-CA-C	-8.82	101.59	111.82
10	A	1343	ASN	CA-C-N	8.81	131.90	120.44
10	A	1343	ASN	C-N-CA	8.81	131.90	120.44
8	P	206	THR	N-CA-C	-8.81	101.60	111.82
5	4	449	VAL	CB-CA-C	-8.42	100.78	112.14
5	M	449	VAL	CB-CA-C	-8.39	100.81	112.14
10	B	223	ASN	N-CA-C	-8.39	102.09	111.82
10	A	414	SER	CA-C-N	8.39	137.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	414	SER	C-N-CA	8.39	137.56	121.54
2	J	597	VAL	N-CA-C	-8.38	100.91	110.05
2	a	597	VAL	N-CA-C	-8.38	100.92	110.05
5	D	449	VAL	CB-CA-C	-8.37	100.84	112.14
2	1	597	VAL	N-CA-C	-8.35	100.95	110.05
2	S	597	VAL	N-CA-C	-8.35	100.95	110.05
10	B	414	SER	CA-C-N	8.35	137.48	121.54
10	B	414	SER	C-N-CA	8.35	137.48	121.54
5	V	449	VAL	CB-CA-C	-8.34	100.88	112.14
10	A	223	ASN	N-CA-C	-8.33	102.16	111.82
3	K	206	SER	CA-C-N	8.26	137.31	121.54
3	K	206	SER	C-N-CA	8.26	137.31	121.54
3	T	206	SER	CA-C-N	8.22	137.24	121.54
3	T	206	SER	C-N-CA	8.22	137.24	121.54
3	2	206	SER	CA-C-N	8.21	137.22	121.54
3	2	206	SER	C-N-CA	8.21	137.22	121.54
2	1	426	HIS	CA-C-N	-8.19	108.66	120.29
2	1	426	HIS	C-N-CA	-8.19	108.66	120.29
2	J	426	HIS	CA-C-N	-8.19	108.66	120.29
2	J	426	HIS	C-N-CA	-8.19	108.66	120.29
3	b	206	SER	CA-C-N	8.18	137.16	121.54
3	b	206	SER	C-N-CA	8.18	137.16	121.54
7	6	23	TYR	N-CA-C	-8.17	100.36	110.41
2	a	426	HIS	CA-C-N	-8.17	108.69	120.29
2	a	426	HIS	C-N-CA	-8.17	108.69	120.29
2	S	784	ALA	N-CA-C	8.16	120.26	111.36
2	S	426	HIS	CA-C-N	-8.15	108.71	120.29
2	S	426	HIS	C-N-CA	-8.15	108.71	120.29
7	O	23	TYR	N-CA-C	-8.15	100.38	110.41
2	S	635	PRO	N-CA-C	8.14	129.23	112.47
2	a	635	PRO	N-CA-C	8.14	129.23	112.47
2	J	635	PRO	N-CA-C	8.12	129.19	112.47
4	C	680	PRO	N-CA-CB	8.11	111.77	103.25
2	1	635	PRO	N-CA-C	8.11	129.17	112.47
2	1	784	ALA	N-CA-C	8.11	120.20	111.36
2	a	784	ALA	N-CA-C	8.07	120.16	111.36
7	F	23	TYR	N-CA-C	-8.06	100.49	110.41
4	L	680	PRO	N-CA-CB	8.05	111.71	103.25
2	J	784	ALA	N-CA-C	8.05	120.14	111.36
4	3	680	PRO	N-CA-CB	8.04	111.69	103.25
3	K	110	ASP	N-CA-C	-8.03	93.69	110.80
3	2	110	ASP	N-CA-C	-8.01	93.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	110	ASP	N-CA-C	-8.00	93.76	110.80
3	b	110	ASP	N-CA-C	-7.99	93.78	110.80
4	U	680	PRO	N-CA-CB	7.95	111.60	103.25
3	2	289	GLN	CB-CA-C	-7.88	103.34	110.44
3	K	289	GLN	CB-CA-C	-7.88	103.35	110.44
3	T	289	GLN	CB-CA-C	-7.85	103.38	110.44
3	b	289	GLN	CB-CA-C	-7.82	103.40	110.44
7	O	249	SER	N-CA-C	7.81	122.52	113.38
4	C	573	PRO	N-CA-CB	7.80	111.44	103.25
7	X	249	SER	N-CA-C	7.79	122.50	113.38
7	F	249	SER	N-CA-C	7.78	122.48	113.38
7	6	249	SER	N-CA-C	7.77	122.47	113.38
4	3	573	PRO	N-CA-CB	7.77	111.41	103.25
4	U	573	PRO	N-CA-CB	7.76	111.40	103.25
4	L	573	PRO	N-CA-CB	7.71	111.34	103.25
2	J	76	ALA	CA-C-N	7.70	131.01	120.46
2	J	76	ALA	C-N-CA	7.70	131.01	120.46
2	a	76	ALA	CA-C-N	7.70	131.01	120.46
2	a	76	ALA	C-N-CA	7.70	131.01	120.46
2	S	76	ALA	CA-C-N	7.67	130.97	120.46
2	S	76	ALA	C-N-CA	7.67	130.97	120.46
2	1	76	ALA	CA-C-N	7.66	130.96	120.46
2	1	76	ALA	C-N-CA	7.66	130.96	120.46
7	X	23	TYR	N-CA-C	-7.59	100.54	110.33
3	2	209	VAL	CA-C-N	-7.56	112.42	120.66
3	2	209	VAL	C-N-CA	-7.56	112.42	120.66
3	T	209	VAL	CA-C-N	-7.55	112.43	120.66
3	T	209	VAL	C-N-CA	-7.55	112.43	120.66
3	K	209	VAL	CA-C-N	-7.54	112.44	120.66
3	K	209	VAL	C-N-CA	-7.54	112.44	120.66
10	B	395	GLY	CA-C-N	7.53	135.93	121.54
10	B	395	GLY	C-N-CA	7.53	135.93	121.54
3	b	209	VAL	CA-C-N	-7.52	112.46	120.66
3	b	209	VAL	C-N-CA	-7.52	112.46	120.66
10	A	395	GLY	CA-C-N	7.50	135.86	121.54
10	A	395	GLY	C-N-CA	7.50	135.86	121.54
10	B	235	LEU	N-CA-C	7.48	120.74	108.99
8	7	189	SER	CB-CA-C	7.47	122.99	110.43
8	G	189	SER	CB-CA-C	7.47	122.98	110.43
8	Y	189	SER	CB-CA-C	7.47	122.98	110.43
8	Y	192	ASN	N-CA-C	-7.46	98.37	113.29
2	1	123	LEU	CA-C-N	7.46	135.79	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	123	LEU	C-N-CA	7.46	135.79	121.54
8	G	192	ASN	N-CA-C	-7.46	98.38	113.29
10	A	235	LEU	N-CA-C	7.45	120.69	108.99
10	A	398	ALA	N-CA-C	7.45	119.04	111.07
2	S	123	LEU	CA-C-N	7.45	135.77	121.54
2	S	123	LEU	C-N-CA	7.45	135.77	121.54
10	B	398	ALA	N-CA-C	7.44	119.03	111.07
8	7	192	ASN	N-CA-C	-7.43	98.43	113.29
2	a	123	LEU	CA-C-N	7.42	135.71	121.54
2	a	123	LEU	C-N-CA	7.42	135.71	121.54
8	P	189	SER	CB-CA-C	7.42	122.90	110.43
8	P	192	ASN	N-CA-C	-7.42	98.46	113.29
10	B	1233	VAL	CA-C-N	-7.41	112.68	123.05
10	B	1233	VAL	C-N-CA	-7.41	112.68	123.05
10	A	1233	VAL	CA-C-N	-7.40	112.69	123.05
10	A	1233	VAL	C-N-CA	-7.40	112.69	123.05
7	X	175	LYS	N-CA-C	-7.38	98.98	109.24
7	F	175	LYS	N-CA-C	-7.37	99.00	109.24
10	B	120	ASP	CB-CA-C	-7.30	108.16	116.63
10	A	120	ASP	CB-CA-C	-7.30	108.16	116.63
10	A	828	ILE	CA-C-N	7.29	131.54	120.82
10	A	828	ILE	C-N-CA	7.29	131.54	120.82
10	B	828	ILE	CA-C-N	7.27	131.51	120.82
10	B	828	ILE	C-N-CA	7.27	131.51	120.82
3	2	108	THR	CA-C-N	-7.22	112.81	122.99
3	2	108	THR	C-N-CA	-7.22	112.81	122.99
3	K	108	THR	CA-C-N	-7.19	112.85	122.99
3	K	108	THR	C-N-CA	-7.19	112.85	122.99
4	3	791	PRO	N-CA-CB	7.18	110.79	103.25
3	T	108	THR	CA-C-N	-7.18	112.87	122.99
3	T	108	THR	C-N-CA	-7.18	112.87	122.99
3	b	108	THR	CA-C-N	-7.17	112.88	122.99
3	b	108	THR	C-N-CA	-7.17	112.88	122.99
3	K	155	GLU	CA-C-N	-7.16	113.54	120.34
3	K	155	GLU	C-N-CA	-7.16	113.54	120.34
3	b	155	GLU	CA-C-N	-7.16	113.54	120.34
3	b	155	GLU	C-N-CA	-7.16	113.54	120.34
10	B	1353	CYS	N-CA-C	-7.15	105.39	112.97
2	1	216	ALA	CA-C-N	-7.15	112.85	122.72
2	1	216	ALA	C-N-CA	-7.15	112.85	122.72
2	1	354	LEU	N-CA-C	7.15	119.15	111.36
2	J	354	LEU	N-CA-C	7.13	119.13	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	791	PRO	N-CA-CB	7.13	110.73	103.25
4	C	791	PRO	N-CA-CB	7.12	110.73	103.25
2	J	216	ALA	CA-C-N	-7.11	112.90	122.72
2	J	216	ALA	C-N-CA	-7.11	112.90	122.72
10	A	1353	CYS	N-CA-C	-7.11	105.44	112.97
2	1	1079	ASN	CA-C-N	7.10	131.10	120.31
2	1	1079	ASN	C-N-CA	7.10	131.10	120.31
2	S	216	ALA	CA-C-N	-7.09	112.93	122.72
2	S	216	ALA	C-N-CA	-7.09	112.93	122.72
3	T	155	GLU	CA-C-N	-7.09	113.61	120.34
3	T	155	GLU	C-N-CA	-7.09	113.61	120.34
4	U	791	PRO	N-CA-CB	7.07	110.67	103.25
2	a	354	LEU	N-CA-C	7.07	119.06	111.36
2	a	1079	ASN	CA-C-N	7.07	131.05	120.31
2	a	1079	ASN	C-N-CA	7.07	131.05	120.31
2	S	354	LEU	N-CA-C	7.06	119.06	111.36
2	J	1079	ASN	CA-C-N	7.05	131.02	120.31
2	J	1079	ASN	C-N-CA	7.05	131.02	120.31
2	S	1079	ASN	CA-C-N	7.05	131.02	120.31
2	S	1079	ASN	C-N-CA	7.05	131.02	120.31
2	a	216	ALA	CA-C-N	-7.05	113.00	122.72
2	a	216	ALA	C-N-CA	-7.05	113.00	122.72
2	a	553	HIS	CB-CA-C	-7.03	100.13	110.96
4	U	849	PRO	N-CA-CB	7.03	110.81	103.15
3	2	155	GLU	CA-C-N	-7.03	113.67	120.34
3	2	155	GLU	C-N-CA	-7.03	113.67	120.34
2	J	553	HIS	CB-CA-C	-7.03	100.14	110.96
8	7	242	THR	CA-C-N	-7.01	109.30	122.27
8	7	242	THR	C-N-CA	-7.01	109.30	122.27
2	1	553	HIS	CB-CA-C	-7.01	100.17	110.96
4	3	849	PRO	N-CA-CB	7.00	110.78	103.15
2	S	553	HIS	CB-CA-C	-7.00	100.18	110.96
2	a	1024	ILE	N-CA-CB	7.00	115.91	110.45
4	L	849	PRO	N-CA-CB	6.98	110.76	103.15
2	J	1024	ILE	N-CA-CB	6.98	115.90	110.45
8	Y	242	THR	CA-C-N	-6.98	109.36	122.27
8	Y	242	THR	C-N-CA	-6.98	109.36	122.27
5	D	334	PRO	N-CA-C	6.97	123.06	113.65
8	Y	221	PRO	CA-C-N	-6.97	113.65	122.43
8	Y	221	PRO	C-N-CA	-6.97	113.65	122.43
4	C	849	PRO	N-CA-CB	6.96	110.74	103.15
9	H	220	ALA	N-CA-C	6.96	118.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	242	THR	CA-C-N	-6.96	109.38	122.27
8	P	242	THR	C-N-CA	-6.96	109.38	122.27
2	1	1024	ILE	N-CA-CB	6.96	115.88	110.45
8	G	242	THR	CA-C-N	-6.96	109.40	122.27
8	G	242	THR	C-N-CA	-6.96	109.40	122.27
8	G	221	PRO	CA-C-N	-6.95	113.67	122.43
8	G	221	PRO	C-N-CA	-6.95	113.67	122.43
2	S	1024	ILE	N-CA-CB	6.95	115.87	110.45
5	V	334	PRO	N-CA-C	6.94	123.02	113.65
9	Z	220	ALA	N-CA-C	6.93	118.92	111.36
8	Y	196	LYS	CA-C-N	6.93	132.45	123.03
8	Y	196	LYS	C-N-CA	6.93	132.45	123.03
9	8	220	ALA	N-CA-C	6.92	118.90	111.36
8	P	221	PRO	CA-C-N	-6.92	113.71	122.43
8	P	221	PRO	C-N-CA	-6.92	113.71	122.43
8	7	196	LYS	CA-C-N	6.91	132.50	122.69
8	7	196	LYS	C-N-CA	6.91	132.50	122.69
9	Q	220	ALA	N-CA-C	6.91	118.89	111.36
8	G	196	LYS	CA-C-N	6.88	132.46	122.69
8	G	196	LYS	C-N-CA	6.88	132.46	122.69
8	P	44	SER	N-CA-C	-6.88	100.26	110.23
8	7	221	PRO	CA-C-N	-6.88	113.77	122.43
8	7	221	PRO	C-N-CA	-6.88	113.77	122.43
8	G	44	SER	N-CA-C	-6.87	100.27	110.23
8	Y	44	SER	N-CA-C	-6.85	100.30	110.23
10	B	234	CYS	N-CA-C	6.84	118.62	111.03
2	J	250	GLY	N-CA-C	-6.83	104.56	115.08
8	P	196	LYS	CA-C-N	6.83	132.38	122.69
8	P	196	LYS	C-N-CA	6.83	132.38	122.69
10	B	910	GLN	CA-C-N	6.82	129.81	120.46
10	B	910	GLN	C-N-CA	6.82	129.81	120.46
8	7	44	SER	N-CA-C	-6.82	100.34	110.23
10	A	910	GLN	CA-C-N	6.81	129.79	120.46
10	A	910	GLN	C-N-CA	6.81	129.79	120.46
2	a	250	GLY	N-CA-C	-6.81	104.60	115.08
2	1	250	GLY	N-CA-C	-6.78	104.64	115.08
10	A	234	CYS	N-CA-C	6.78	118.55	111.03
10	B	415	LYS	N-CA-CB	6.78	121.94	110.49
2	1	1013	HIS	O-C-N	6.77	131.60	122.59
2	a	140	GLY	N-CA-C	-6.77	106.36	115.36
10	A	415	LYS	N-CA-CB	6.76	121.92	110.49
2	J	140	GLY	N-CA-C	-6.76	106.37	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	250	GLY	N-CA-C	-6.76	104.67	115.08
2	S	140	GLY	N-CA-C	-6.76	106.37	115.36
3	T	207	GLU	N-CA-C	6.75	125.18	110.80
3	K	275	LYS	N-CA-C	-6.75	96.42	110.80
3	b	275	LYS	N-CA-C	-6.75	96.42	110.80
3	b	207	GLU	N-CA-C	6.75	125.17	110.80
2	1	140	GLY	N-CA-C	-6.74	106.39	115.36
9	Z	151	ILE	CB-CA-C	-6.74	103.34	111.97
2	S	296	ASP	N-CA-C	-6.74	99.32	110.17
3	K	207	GLU	N-CA-C	6.73	125.14	110.80
3	2	275	LYS	N-CA-C	-6.73	96.47	110.80
9	H	151	ILE	CB-CA-C	-6.73	103.36	111.97
2	1	555	ASN	N-CA-C	-6.72	102.18	110.65
3	2	207	GLU	N-CA-C	6.72	125.11	110.80
6	5	292	ALA	CA-C-N	-6.72	110.82	122.37
6	5	292	ALA	C-N-CA	-6.72	110.82	122.37
9	8	151	ILE	CB-CA-C	-6.72	103.37	111.97
3	T	275	LYS	N-CA-C	-6.71	96.51	110.80
2	1	296	ASP	N-CA-C	-6.71	99.37	110.17
6	N	292	ALA	CA-C-N	-6.71	110.84	122.37
6	N	292	ALA	C-N-CA	-6.71	110.84	122.37
9	Z	423	TYR	N-CA-C	-6.71	103.97	111.28
2	a	296	ASP	N-CA-C	-6.70	99.38	110.17
9	Q	151	ILE	CB-CA-C	-6.70	103.39	111.97
10	A	958	ASP	CB-CA-C	-6.69	107.83	115.79
10	B	958	ASP	CB-CA-C	-6.69	107.83	115.79
6	W	292	ALA	CA-C-N	-6.69	110.86	122.37
6	W	292	ALA	C-N-CA	-6.69	110.86	122.37
2	J	296	ASP	N-CA-C	-6.68	99.41	110.17
9	Q	423	TYR	N-CA-C	-6.68	104.00	111.28
7	6	150	THR	N-CA-C	6.67	118.35	111.14
9	H	423	TYR	N-CA-C	-6.67	104.00	111.28
2	J	403	SER	N-CA-C	-6.67	101.27	110.35
6	E	292	ALA	CA-C-N	-6.67	110.90	122.37
6	E	292	ALA	C-N-CA	-6.67	110.90	122.37
8	G	176	ARG	N-CA-C	-6.67	96.60	110.80
8	7	176	ARG	N-CA-C	-6.66	96.61	110.80
4	L	628	PRO	N-CA-CB	6.66	110.24	103.25
7	O	150	THR	N-CA-C	6.66	118.33	111.14
8	P	176	ARG	N-CA-C	-6.65	96.63	110.80
2	S	403	SER	N-CA-C	-6.65	101.31	110.35
2	S	555	ASN	N-CA-C	-6.64	102.28	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	555	ASN	N-CA-C	-6.64	102.28	110.65
8	Y	176	ARG	N-CA-C	-6.64	96.66	110.80
7	F	150	THR	N-CA-C	6.64	118.31	111.14
7	X	150	THR	N-CA-C	6.64	118.31	111.14
2	a	555	ASN	N-CA-C	-6.64	102.29	110.65
9	8	423	TYR	N-CA-C	-6.63	104.05	111.28
4	3	628	PRO	N-CA-CB	6.63	110.21	103.25
2	J	1074	ASP	CA-C-N	6.61	131.76	120.72
2	J	1074	ASP	C-N-CA	6.61	131.76	120.72
2	a	1074	ASP	CA-C-N	6.61	131.76	120.72
2	a	1074	ASP	C-N-CA	6.61	131.76	120.72
9	8	130	ARG	CA-C-N	-6.61	110.50	121.80
9	8	130	ARG	C-N-CA	-6.61	110.50	121.80
4	U	628	PRO	N-CA-CB	6.61	110.19	103.25
2	a	403	SER	N-CA-C	-6.60	101.37	110.35
2	S	1074	ASP	CA-C-N	6.60	131.74	120.72
2	S	1074	ASP	C-N-CA	6.60	131.74	120.72
9	Z	130	ARG	CA-C-N	-6.60	110.52	121.80
9	Z	130	ARG	C-N-CA	-6.60	110.52	121.80
2	1	1074	ASP	CA-C-N	6.58	131.72	120.72
2	1	1074	ASP	C-N-CA	6.58	131.72	120.72
9	H	130	ARG	CA-C-N	-6.58	110.55	121.80
9	H	130	ARG	C-N-CA	-6.58	110.55	121.80
4	C	628	PRO	N-CA-CB	6.57	110.15	103.25
8	7	194	MET	CA-C-N	6.57	134.09	121.54
8	7	194	MET	C-N-CA	6.57	134.09	121.54
2	J	427	ASN	CA-C-N	6.56	133.78	121.97
2	J	427	ASN	C-N-CA	6.56	133.78	121.97
8	G	194	MET	CA-C-N	6.56	134.07	121.54
8	G	194	MET	C-N-CA	6.56	134.07	121.54
9	Q	130	ARG	CA-C-N	-6.55	110.60	121.80
9	Q	130	ARG	C-N-CA	-6.55	110.60	121.80
2	a	427	ASN	CA-C-N	6.55	133.76	121.97
2	a	427	ASN	C-N-CA	6.55	133.76	121.97
5	V	332	LYS	N-CA-C	6.55	124.74	110.80
5	D	332	LYS	N-CA-C	6.54	124.74	110.80
2	1	427	ASN	CA-C-N	6.54	133.74	121.97
2	1	427	ASN	C-N-CA	6.54	133.74	121.97
8	P	194	MET	CA-C-N	6.54	134.03	121.54
8	P	194	MET	C-N-CA	6.54	134.03	121.54
2	S	427	ASN	CA-C-N	6.53	133.73	121.97
2	S	427	ASN	C-N-CA	6.53	133.73	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	261	LEU	N-CA-C	-6.53	104.08	111.07
10	A	261	LEU	N-CA-C	-6.53	104.09	111.07
8	Y	194	MET	CA-C-N	6.52	134.00	121.54
8	Y	194	MET	C-N-CA	6.52	134.00	121.54
5	D	530	GLU	CA-C-N	6.50	128.99	120.28
5	D	530	GLU	C-N-CA	6.50	128.99	120.28
5	V	530	GLU	CA-C-N	6.50	128.99	120.28
5	V	530	GLU	C-N-CA	6.50	128.99	120.28
7	O	107	ASN	N-CA-C	6.48	120.05	111.75
5	M	530	GLU	CA-C-N	6.48	128.96	120.28
5	M	530	GLU	C-N-CA	6.48	128.96	120.28
2	S	1044	ARG	N-CA-C	-6.47	104.27	111.71
3	T	238	THR	CA-C-N	6.47	133.89	121.54
3	T	238	THR	C-N-CA	6.47	133.89	121.54
3	2	238	THR	CA-C-N	6.45	133.87	121.54
3	2	238	THR	C-N-CA	6.45	133.87	121.54
3	b	238	THR	CA-C-N	6.45	133.87	121.54
3	b	238	THR	C-N-CA	6.45	133.87	121.54
5	4	530	GLU	CA-C-N	6.45	128.92	120.28
5	4	530	GLU	C-N-CA	6.45	128.92	120.28
7	6	107	ASN	N-CA-C	6.45	120.01	111.75
2	J	1044	ARG	N-CA-C	-6.45	104.29	111.71
8	G	217	THR	CA-C-N	-6.44	113.71	122.91
8	G	217	THR	C-N-CA	-6.44	113.71	122.91
2	1	1044	ARG	N-CA-C	-6.43	104.31	111.71
8	Y	192	ASN	CA-C-N	6.43	133.83	121.54
8	Y	192	ASN	C-N-CA	6.43	133.83	121.54
8	G	192	ASN	CA-C-N	6.43	133.82	121.54
8	G	192	ASN	C-N-CA	6.43	133.82	121.54
8	Y	217	THR	CA-C-N	-6.43	113.71	122.91
8	Y	217	THR	C-N-CA	-6.43	113.71	122.91
8	P	217	THR	CA-C-N	-6.42	113.73	122.91
8	P	217	THR	C-N-CA	-6.42	113.73	122.91
2	a	1044	ARG	N-CA-C	-6.42	104.33	111.71
2	1	79	TYR	CA-C-N	-6.41	113.96	123.00
2	1	79	TYR	C-N-CA	-6.41	113.96	123.00
3	K	238	THR	CA-C-N	6.41	133.79	121.54
3	K	238	THR	C-N-CA	6.41	133.79	121.54
8	7	192	ASN	CA-C-N	6.41	133.79	121.54
8	7	192	ASN	C-N-CA	6.41	133.79	121.54
7	X	107	ASN	N-CA-C	6.41	119.96	111.75
2	a	79	TYR	CA-C-N	-6.41	113.97	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	79	TYR	C-N-CA	-6.41	113.97	123.00
7	F	107	ASN	N-CA-C	6.40	119.95	111.75
8	P	192	ASN	CA-C-N	6.40	133.77	121.54
8	P	192	ASN	C-N-CA	6.40	133.77	121.54
2	J	79	TYR	CA-C-N	-6.39	113.99	123.00
2	J	79	TYR	C-N-CA	-6.39	113.99	123.00
10	A	829	ARG	N-CA-C	6.39	118.55	110.24
2	S	79	TYR	CA-C-N	-6.39	113.99	123.00
2	S	79	TYR	C-N-CA	-6.39	113.99	123.00
8	7	217	THR	CA-C-N	-6.39	113.78	122.91
8	7	217	THR	C-N-CA	-6.39	113.78	122.91
10	B	829	ARG	N-CA-C	6.38	118.53	110.24
2	J	126	ASN	N-CA-C	6.38	118.10	110.19
8	P	43	GLU	N-CA-C	-6.35	104.35	111.28
3	K	155	GLU	N-CA-C	-6.35	97.28	110.80
8	G	290	GLY	N-CA-C	-6.34	106.32	115.27
2	a	126	ASN	N-CA-C	6.34	118.06	110.19
2	S	341	GLY	N-CA-C	-6.34	102.90	112.60
3	b	155	GLU	N-CA-C	-6.33	97.31	110.80
8	Y	290	GLY	N-CA-C	-6.33	106.34	115.27
2	J	341	GLY	N-CA-C	-6.33	102.92	112.60
3	T	155	GLU	N-CA-C	-6.32	97.33	110.80
10	A	849	ASN	CB-CA-C	-6.32	108.64	117.23
3	2	155	GLU	N-CA-C	-6.31	97.36	110.80
2	J	124	LEU	CB-CA-C	-6.31	107.98	117.07
10	B	196	GLY	N-CA-C	-6.31	105.98	115.32
10	B	849	ASN	CB-CA-C	-6.31	108.65	117.23
8	P	290	GLY	N-CA-C	-6.31	106.37	115.27
6	W	347	THR	CA-C-N	-6.31	114.83	122.90
6	W	347	THR	C-N-CA	-6.31	114.83	122.90
10	B	1342	LEU	CB-CA-C	-6.31	100.94	109.71
6	N	347	THR	CA-C-N	-6.31	114.83	122.90
6	N	347	THR	C-N-CA	-6.31	114.83	122.90
6	5	347	THR	CA-C-N	-6.30	114.83	122.90
6	5	347	THR	C-N-CA	-6.30	114.83	122.90
2	S	126	ASN	N-CA-C	6.29	117.99	110.19
10	A	196	GLY	N-CA-C	-6.29	106.01	115.32
2	1	126	ASN	N-CA-C	6.29	117.98	110.19
9	Z	229	ILE	N-CA-CB	6.27	117.89	110.55
8	7	290	GLY	N-CA-C	-6.27	106.43	115.27
2	a	341	GLY	N-CA-C	-6.26	103.02	112.60
10	A	1342	LEU	CB-CA-C	-6.26	101.01	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	229	ILE	N-CA-CB	6.26	117.87	110.55
7	O	91	GLY	N-CA-C	-6.26	106.79	114.92
5	V	480	ARG	CA-C-N	6.25	133.49	121.54
5	V	480	ARG	C-N-CA	6.25	133.49	121.54
2	1	341	GLY	N-CA-C	-6.25	103.03	112.60
8	Y	43	GLU	N-CA-C	-6.25	104.47	111.28
6	E	292	ALA	N-CA-C	-6.24	99.55	109.23
2	J	57	ARG	CA-C-N	-6.24	110.59	122.08
2	J	57	ARG	C-N-CA	-6.24	110.59	122.08
9	Q	229	ILE	N-CA-CB	6.24	117.85	110.55
8	P	257	LEU	N-CA-C	-6.24	100.03	109.95
5	D	480	ARG	CA-C-N	6.23	133.44	121.54
5	D	480	ARG	C-N-CA	6.23	133.44	121.54
8	G	43	GLU	N-CA-C	-6.23	104.49	111.28
6	E	347	THR	CA-C-N	-6.23	114.93	122.90
6	E	347	THR	C-N-CA	-6.23	114.93	122.90
3	2	219	LYS	N-CA-C	-6.22	104.75	113.20
7	X	133	THR	N-CA-C	-6.21	100.79	110.42
2	S	57	ARG	CA-C-N	-6.21	110.65	122.08
2	S	57	ARG	C-N-CA	-6.21	110.65	122.08
10	B	1354	LEU	N-CA-C	-6.21	102.83	110.65
8	Y	257	LEU	N-CA-C	-6.21	100.08	109.95
6	5	292	ALA	N-CA-C	-6.21	99.61	109.23
8	7	43	GLU	N-CA-C	-6.21	104.51	111.28
6	W	292	ALA	N-CA-C	-6.21	99.61	109.23
10	A	1354	LEU	N-CA-C	-6.20	102.83	110.65
2	a	57	ARG	CA-C-N	-6.20	110.67	122.08
2	a	57	ARG	C-N-CA	-6.20	110.67	122.08
8	7	257	LEU	N-CA-C	-6.20	100.09	109.95
6	N	292	ALA	N-CA-C	-6.20	99.62	109.23
8	G	257	LEU	N-CA-C	-6.20	100.10	109.95
3	K	219	LYS	N-CA-C	-6.19	104.78	113.20
2	1	57	ARG	CA-C-N	-6.19	110.69	122.08
2	1	57	ARG	C-N-CA	-6.19	110.69	122.08
10	B	801	HIS	CA-C-N	6.19	133.37	121.54
10	B	801	HIS	C-N-CA	6.19	133.37	121.54
3	K	228	ALA	CA-C-N	6.18	131.37	120.74
3	K	228	ALA	C-N-CA	6.18	131.37	120.74
10	A	102	CYS	N-CA-C	6.18	119.21	111.24
3	b	219	LYS	N-CA-C	-6.18	104.80	113.20
10	B	102	CYS	N-CA-C	6.18	119.21	111.24
10	A	801	HIS	CA-C-N	6.18	133.34	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	801	HIS	C-N-CA	6.18	133.34	121.54
7	F	91	GLY	N-CA-C	-6.18	106.89	114.92
9	8	229	ILE	N-CA-CB	6.17	117.77	110.55
3	T	219	LYS	N-CA-C	-6.17	104.80	113.20
2	a	976	PRO	CA-C-N	-6.17	111.52	120.29
2	a	976	PRO	C-N-CA	-6.17	111.52	120.29
7	F	133	THR	N-CA-C	-6.17	100.86	110.42
10	A	238	VAL	CB-CA-C	-6.16	102.29	110.98
9	H	132	PHE	N-CA-C	-6.16	98.85	108.90
3	T	243	PRO	N-CA-C	-6.16	99.78	112.47
10	B	855	ILE	N-CA-CB	6.16	118.91	110.54
3	b	243	PRO	N-CA-C	-6.15	99.81	112.47
3	2	243	PRO	N-CA-C	-6.15	99.81	112.47
3	T	228	ALA	CA-C-N	6.14	131.30	120.74
3	T	228	ALA	C-N-CA	6.14	131.30	120.74
2	1	976	PRO	CA-C-N	-6.14	111.57	120.29
2	1	976	PRO	C-N-CA	-6.14	111.57	120.29
2	J	976	PRO	CA-C-N	-6.14	111.58	120.29
2	J	976	PRO	C-N-CA	-6.14	111.58	120.29
9	Q	132	PHE	N-CA-C	-6.13	98.90	108.90
2	1	403	SER	N-CA-C	-6.13	101.34	110.23
9	Z	132	PHE	N-CA-C	-6.13	98.92	108.90
3	K	243	PRO	N-CA-C	-6.12	99.87	112.47
3	b	228	ALA	CA-C-N	6.12	131.26	120.74
3	b	228	ALA	C-N-CA	6.12	131.26	120.74
10	A	397	SER	CA-C-N	6.12	128.39	120.44
10	A	397	SER	C-N-CA	6.12	128.39	120.44
9	8	132	PHE	N-CA-C	-6.11	98.94	108.90
10	A	1261	PHE	N-CA-CB	6.11	119.21	110.16
9	Q	430	LEU	CA-C-N	6.11	126.72	120.00
9	Q	430	LEU	C-N-CA	6.11	126.72	120.00
10	A	855	ILE	N-CA-CB	6.10	118.84	110.54
6	5	554	TYR	CB-CA-C	-6.10	99.13	109.38
2	a	1020	ALA	N-CA-C	-6.10	104.63	111.28
3	2	228	ALA	CA-C-N	6.09	131.22	120.74
3	2	228	ALA	C-N-CA	6.09	131.22	120.74
2	J	1020	ALA	N-CA-C	-6.09	104.64	111.28
10	B	1261	PHE	N-CA-CB	6.09	119.17	110.16
2	J	425	GLU	CA-C-N	-6.09	112.98	122.67
2	J	425	GLU	C-N-CA	-6.09	112.98	122.67
6	N	351	ASP	N-CA-C	-6.09	97.83	110.80
2	1	425	GLU	CA-C-N	-6.09	112.99	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	425	GLU	C-N-CA	-6.09	112.99	122.67
6	5	351	ASP	N-CA-C	-6.09	97.83	110.80
10	B	397	SER	CA-C-N	6.09	128.35	120.44
10	B	397	SER	C-N-CA	6.09	128.35	120.44
2	1	1020	ALA	N-CA-C	-6.08	104.65	111.28
2	S	976	PRO	CA-C-N	-6.08	111.66	120.29
2	S	976	PRO	C-N-CA	-6.08	111.66	120.29
6	W	351	ASP	N-CA-C	-6.08	97.85	110.80
10	B	416	GLY	CA-C-N	-6.08	115.12	122.90
10	B	416	GLY	C-N-CA	-6.08	115.12	122.90
2	S	425	GLU	CA-C-N	-6.08	113.01	122.67
2	S	425	GLU	C-N-CA	-6.08	113.01	122.67
6	E	351	ASP	N-CA-C	-6.07	97.86	110.80
6	N	554	TYR	CB-CA-C	-6.06	99.20	109.38
2	a	425	GLU	CA-C-N	-6.06	113.04	122.67
2	a	425	GLU	C-N-CA	-6.06	113.04	122.67
3	K	137	GLY	N-CA-C	-6.05	102.33	110.56
10	A	416	GLY	CA-C-N	-6.04	115.17	122.90
10	A	416	GLY	C-N-CA	-6.04	115.17	122.90
2	S	1020	ALA	N-CA-C	-6.04	104.69	111.28
9	Z	50	SER	CA-C-N	-6.04	115.55	123.34
9	Z	50	SER	C-N-CA	-6.04	115.55	123.34
2	a	958	PRO	CA-C-N	6.03	128.97	120.28
2	a	958	PRO	C-N-CA	6.03	128.97	120.28
3	T	137	GLY	N-CA-C	-6.03	102.36	110.56
7	X	108	SER	N-CA-C	6.03	118.01	108.79
3	b	137	GLY	N-CA-C	-6.02	102.37	110.56
3	2	137	GLY	N-CA-C	-6.02	102.37	110.56
9	H	50	SER	CA-C-N	-6.02	115.57	123.34
9	H	50	SER	C-N-CA	-6.02	115.57	123.34
7	F	108	SER	N-CA-C	6.02	118.00	108.79
6	N	689	LEU	CA-C-N	6.02	128.35	120.28
6	N	689	LEU	C-N-CA	6.02	128.35	120.28
6	E	689	LEU	CA-C-N	6.02	128.34	120.28
6	E	689	LEU	C-N-CA	6.02	128.34	120.28
7	O	108	SER	N-CA-C	6.02	118.00	108.79
6	W	554	TYR	CB-CA-C	-6.01	99.28	109.38
10	B	86	ARG	CA-C-N	-6.01	118.10	123.33
10	B	86	ARG	C-N-CA	-6.01	118.10	123.33
9	8	50	SER	CA-C-N	-6.01	115.59	123.34
9	8	50	SER	C-N-CA	-6.01	115.59	123.34
10	B	231	LYS	N-CA-C	-6.01	102.32	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	309	TYR	N-CA-C	-6.01	104.73	111.28
6	E	554	TYR	CB-CA-C	-6.01	99.28	109.38
6	E	680	GLY	N-CA-C	-6.01	106.80	115.27
9	Q	50	SER	CA-C-N	-6.01	115.59	123.34
9	Q	50	SER	C-N-CA	-6.01	115.59	123.34
8	G	309	TYR	N-CA-C	-6.00	104.74	111.28
6	W	689	LEU	CA-C-N	6.00	128.32	120.28
6	W	689	LEU	C-N-CA	6.00	128.32	120.28
6	5	689	LEU	CA-C-N	6.00	128.31	120.28
6	5	689	LEU	C-N-CA	6.00	128.31	120.28
7	6	108	SER	N-CA-C	6.00	117.96	108.79
2	S	958	PRO	CA-C-N	6.00	128.91	120.28
2	S	958	PRO	C-N-CA	6.00	128.91	120.28
10	A	231	LYS	N-CA-C	-5.99	102.35	110.68
6	W	680	GLY	N-CA-C	-5.99	106.82	115.27
2	1	958	PRO	CA-C-N	5.99	128.91	120.28
2	1	958	PRO	C-N-CA	5.99	128.91	120.28
6	N	680	GLY	N-CA-C	-5.99	106.82	115.27
10	A	846	ILE	CB-CA-C	-5.99	104.22	111.88
5	D	357	GLY	N-CA-C	-5.98	106.91	115.64
3	2	57	ASP	N-CA-C	-5.98	100.75	110.20
8	P	309	TYR	N-CA-C	-5.98	104.77	111.28
10	B	846	ILE	CB-CA-C	-5.97	104.23	111.88
3	T	57	ASP	N-CA-C	-5.97	100.76	110.20
5	V	357	GLY	N-CA-C	-5.97	106.92	115.64
2	J	958	PRO	CA-C-N	5.97	128.88	120.28
2	J	958	PRO	C-N-CA	5.97	128.88	120.28
8	Y	309	TYR	N-CA-C	-5.97	104.77	111.28
3	K	57	ASP	N-CA-C	-5.97	100.77	110.20
6	5	680	GLY	N-CA-C	-5.96	106.86	115.27
5	4	357	GLY	N-CA-C	-5.96	106.94	115.64
10	A	86	ARG	CA-C-N	-5.96	118.14	123.33
10	A	86	ARG	C-N-CA	-5.96	118.14	123.33
2	S	708	GLY	N-CA-C	-5.96	103.54	113.02
2	1	355	TYR	CB-CA-C	-5.96	101.08	110.79
10	B	205	LEU	CB-CA-C	-5.94	104.06	111.43
9	8	228	GLY	N-CA-C	5.94	121.33	113.37
8	P	175	SER	CA-C-N	5.94	132.88	121.54
8	P	175	SER	C-N-CA	5.94	132.88	121.54
5	M	357	GLY	N-CA-C	-5.93	106.98	115.64
2	J	708	GLY	N-CA-C	-5.93	103.59	113.02
2	a	939	LYS	CA-C-N	-5.93	114.69	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	939	LYS	C-N-CA	-5.93	114.69	123.11
8	G	175	SER	CA-C-N	5.92	132.86	121.54
8	G	175	SER	C-N-CA	5.92	132.86	121.54
2	a	708	GLY	N-CA-C	-5.92	103.61	113.02
8	7	175	SER	CA-C-N	5.92	132.84	121.54
8	7	175	SER	C-N-CA	5.92	132.84	121.54
9	Q	228	GLY	N-CA-C	5.92	121.30	113.37
2	J	636	GLU	CB-CA-C	-5.91	100.81	114.41
8	Y	175	SER	CA-C-N	5.91	132.83	121.54
8	Y	175	SER	C-N-CA	5.91	132.83	121.54
3	b	57	ASP	N-CA-C	-5.91	100.86	110.20
2	S	636	GLU	CB-CA-C	-5.91	100.82	114.41
2	J	630	TYR	N-CA-CB	5.91	118.90	110.16
2	1	708	GLY	N-CA-C	-5.90	103.64	113.02
7	F	215	VAL	N-CA-C	-5.90	101.10	108.89
7	X	215	VAL	N-CA-C	-5.90	101.10	108.89
2	a	636	GLU	CB-CA-C	-5.90	100.84	114.41
5	D	419	LEU	N-CA-C	-5.89	105.37	113.56
10	A	205	LEU	CB-CA-C	-5.89	104.12	111.43
2	J	355	TYR	CB-CA-C	-5.89	101.19	110.79
2	1	636	GLU	CB-CA-C	-5.89	100.87	114.41
5	M	496	LEU	N-CA-C	-5.89	104.86	111.28
9	Q	416	LEU	N-CA-C	-5.88	105.36	112.54
2	a	630	TYR	N-CA-CB	5.88	118.87	110.16
9	H	228	GLY	N-CA-C	5.88	121.25	113.37
2	S	939	LYS	CA-C-N	-5.87	114.77	123.11
2	S	939	LYS	C-N-CA	-5.87	114.77	123.11
2	S	355	TYR	CB-CA-C	-5.87	101.22	110.79
5	V	419	LEU	N-CA-C	-5.87	105.40	113.56
5	4	496	LEU	N-CA-C	-5.87	104.88	111.28
2	1	630	TYR	N-CA-CB	5.87	118.85	110.16
9	8	416	LEU	N-CA-C	-5.86	105.39	112.54
7	6	215	VAL	N-CA-C	-5.86	101.16	108.89
10	B	97	PHE	N-CA-C	-5.86	105.01	114.09
2	1	939	LYS	CA-C-N	-5.86	114.79	123.11
2	1	939	LYS	C-N-CA	-5.86	114.79	123.11
10	A	97	PHE	N-CA-C	-5.86	105.01	114.09
10	B	100	MET	CB-CA-C	-5.85	103.75	111.42
6	N	691	HIS	CB-CA-C	-5.85	103.96	111.22
9	H	416	LEU	N-CA-C	-5.85	105.40	112.54
7	O	215	VAL	N-CA-C	-5.85	101.17	108.89
9	Z	228	GLY	N-CA-C	5.85	121.20	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	355	TYR	CB-CA-C	-5.85	101.26	110.79
6	E	691	HIS	CB-CA-C	-5.84	103.98	111.22
9	Z	416	LEU	N-CA-C	-5.83	105.42	112.54
5	D	346	LEU	CB-CA-C	-5.83	101.98	110.96
2	S	630	TYR	N-CA-CB	5.83	118.79	110.16
2	1	647	ILE	N-CA-C	5.83	116.47	110.82
2	J	939	LYS	CA-C-N	-5.83	114.84	123.11
2	J	939	LYS	C-N-CA	-5.83	114.84	123.11
10	B	224	GLY	N-CA-C	-5.83	106.61	115.00
6	W	691	HIS	CB-CA-C	-5.82	104.00	111.22
10	A	224	GLY	N-CA-C	-5.82	106.62	115.00
2	J	73	VAL	CA-C-N	5.82	132.65	121.54
2	J	73	VAL	C-N-CA	5.82	132.65	121.54
5	V	496	LEU	N-CA-C	-5.81	104.94	111.28
2	a	73	VAL	CA-C-N	5.81	132.64	121.54
2	a	73	VAL	C-N-CA	5.81	132.64	121.54
2	S	647	ILE	N-CA-C	5.81	116.45	110.82
5	V	346	LEU	CB-CA-C	-5.81	102.02	110.96
5	V	597	PRO	N-CA-C	-5.81	106.89	114.03
2	J	647	ILE	N-CA-C	5.80	116.45	110.82
5	D	496	LEU	N-CA-C	-5.80	104.96	111.28
6	5	691	HIS	CB-CA-C	-5.78	104.05	111.22
10	A	333	THR	N-CA-C	-5.78	105.06	111.71
10	B	1206	ILE	CB-CA-C	5.78	121.12	112.16
3	b	239	ARG	N-CA-C	-5.78	98.50	110.80
5	D	597	PRO	N-CA-C	-5.78	106.93	114.03
6	5	727	GLN	N-CA-C	-5.77	105.07	111.71
2	1	73	VAL	CA-C-N	5.77	132.57	121.54
2	1	73	VAL	C-N-CA	5.77	132.57	121.54
9	8	207	GLY	N-CA-C	-5.77	107.14	115.27
5	M	554	ILE	CB-CA-C	-5.77	104.35	112.14
2	S	73	VAL	CA-C-N	5.77	132.55	121.54
2	S	73	VAL	C-N-CA	5.77	132.55	121.54
5	M	433	GLY	N-CA-C	-5.76	106.80	115.32
2	a	647	ILE	N-CA-C	5.76	116.41	110.82
5	4	433	GLY	N-CA-C	-5.76	106.80	115.32
3	2	239	ARG	N-CA-C	-5.75	98.55	110.80
9	Z	207	GLY	N-CA-C	-5.75	107.16	115.27
2	a	654	VAL	N-CA-C	-5.75	103.99	112.04
3	T	239	ARG	N-CA-C	-5.75	98.55	110.80
6	E	727	GLN	N-CA-C	-5.75	105.10	111.71
6	N	727	GLN	N-CA-C	-5.75	105.10	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	207	GLY	N-CA-C	-5.75	107.17	115.27
10	A	1206	ILE	CB-CA-C	5.74	121.06	112.16
9	H	395	GLY	CA-C-N	-5.74	110.70	121.95
9	H	395	GLY	C-N-CA	-5.74	110.70	121.95
6	W	727	GLN	N-CA-C	-5.74	105.11	111.71
10	A	800	GLU	CA-C-N	-5.74	112.24	122.45
10	A	800	GLU	C-N-CA	-5.74	112.24	122.45
3	K	239	ARG	N-CA-C	-5.74	98.58	110.80
10	B	800	GLU	CA-C-N	-5.73	112.25	122.45
10	B	800	GLU	C-N-CA	-5.73	112.25	122.45
2	1	654	VAL	N-CA-C	-5.73	104.02	112.04
10	A	535	ILE	CB-CA-C	-5.73	105.60	112.19
10	B	535	ILE	CB-CA-C	-5.73	105.61	112.19
10	B	333	THR	N-CA-C	-5.72	105.13	111.71
9	H	207	GLY	N-CA-C	-5.72	107.20	115.27
5	M	500	ASP	CB-CA-C	-5.72	103.65	111.95
5	4	597	PRO	N-CA-C	-5.72	107.00	114.03
2	S	654	VAL	N-CA-C	-5.72	104.03	112.04
8	7	243	LYS	CA-C-N	5.72	132.46	121.54
8	7	243	LYS	C-N-CA	5.72	132.46	121.54
5	4	554	ILE	CB-CA-C	-5.71	104.43	112.14
5	4	500	ASP	CB-CA-C	-5.71	103.67	111.95
9	Z	395	GLY	CA-C-N	-5.71	110.77	121.95
9	Z	395	GLY	C-N-CA	-5.71	110.77	121.95
2	a	405	ASP	CA-C-N	-5.71	116.12	123.19
2	a	405	ASP	C-N-CA	-5.71	116.12	123.19
9	8	395	GLY	CA-C-N	-5.70	110.78	121.95
9	8	395	GLY	C-N-CA	-5.70	110.78	121.95
9	Q	395	GLY	CA-C-N	-5.70	110.78	121.95
9	Q	395	GLY	C-N-CA	-5.70	110.78	121.95
5	M	170	VAL	CB-CA-C	-5.70	104.52	111.87
5	M	597	PRO	N-CA-C	-5.68	107.05	114.03
8	P	243	LYS	CA-C-N	5.68	132.38	121.54
8	P	243	LYS	C-N-CA	5.68	132.38	121.54
10	A	312	MET	CA-C-N	5.68	131.92	121.70
10	A	312	MET	C-N-CA	5.68	131.92	121.70
2	J	405	ASP	CA-C-N	-5.68	116.15	123.19
2	J	405	ASP	C-N-CA	-5.68	116.15	123.19
2	J	654	VAL	N-CA-C	-5.68	104.09	112.04
7	6	175	LYS	CA-C-N	5.67	126.93	119.84
7	6	175	LYS	C-N-CA	5.67	126.93	119.84
8	G	243	LYS	CA-C-N	5.67	132.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	243	LYS	C-N-CA	5.67	132.37	121.54
7	O	175	LYS	CA-C-N	5.67	126.92	119.84
7	O	175	LYS	C-N-CA	5.67	126.92	119.84
2	S	243	LEU	CB-CA-C	-5.67	102.53	110.13
5	4	548	ARG	CA-C-N	5.67	127.81	120.44
5	4	548	ARG	C-N-CA	5.67	127.81	120.44
8	G	300	GLY	N-CA-C	-5.67	106.93	115.32
8	Y	300	GLY	N-CA-C	-5.67	106.93	115.32
10	B	312	MET	CA-C-N	5.66	131.90	121.70
10	B	312	MET	C-N-CA	5.66	131.90	121.70
8	Y	243	LYS	CA-C-N	5.66	132.36	121.54
8	Y	243	LYS	C-N-CA	5.66	132.36	121.54
10	B	1237	SER	N-CA-C	-5.66	105.01	111.07
2	1	405	ASP	CA-C-N	-5.66	116.17	123.19
2	1	405	ASP	C-N-CA	-5.66	116.17	123.19
8	7	300	GLY	N-CA-C	-5.66	106.94	115.32
2	J	243	LEU	CB-CA-C	-5.66	102.55	110.13
5	4	170	VAL	CB-CA-C	-5.65	104.58	111.87
2	a	243	LEU	CB-CA-C	-5.65	102.56	110.13
5	M	548	ARG	CA-C-N	5.64	127.77	120.44
5	M	548	ARG	C-N-CA	5.64	127.77	120.44
8	P	300	GLY	N-CA-C	-5.64	106.97	115.32
5	D	170	VAL	CB-CA-C	-5.64	104.60	111.87
2	1	243	LEU	CB-CA-C	-5.63	102.58	110.13
10	A	442	GLN	CA-C-N	5.62	135.52	121.80
10	A	442	GLN	C-N-CA	5.62	135.52	121.80
10	B	442	GLN	CA-C-N	5.62	135.52	121.80
10	B	442	GLN	C-N-CA	5.62	135.52	121.80
3	K	278	SER	CB-CA-C	-5.62	103.91	112.11
10	A	1237	SER	N-CA-C	-5.62	105.06	111.07
10	B	275	GLU	CA-C-N	-5.62	110.50	121.06
10	B	275	GLU	C-N-CA	-5.62	110.50	121.06
2	J	637	LYS	N-CA-C	-5.62	100.46	109.39
7	6	91	GLY	N-CA-C	-5.61	106.78	114.64
2	J	133	GLN	N-CA-C	-5.61	105.17	111.28
5	V	170	VAL	CB-CA-C	-5.61	104.64	111.87
2	1	637	LYS	N-CA-C	-5.61	100.48	109.39
2	S	405	ASP	CA-C-N	-5.61	116.24	123.19
2	S	405	ASP	C-N-CA	-5.61	116.24	123.19
2	a	637	LYS	N-CA-C	-5.61	100.48	109.39
10	B	230	GLY	N-CA-C	-5.60	104.89	112.57
5	D	554	ILE	CB-CA-C	-5.60	104.58	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	125	ASN	CA-C-N	5.60	131.03	121.29
2	1	125	ASN	C-N-CA	5.60	131.03	121.29
5	V	548	ARG	CA-C-N	5.60	127.72	120.44
5	V	548	ARG	C-N-CA	5.60	127.72	120.44
10	A	275	GLU	CA-C-N	-5.59	110.54	121.06
10	A	275	GLU	C-N-CA	-5.59	110.54	121.06
5	V	554	ILE	CB-CA-C	-5.59	104.59	112.14
10	B	238	VAL	CB-CA-C	-5.59	102.31	110.81
2	S	637	LYS	N-CA-C	-5.59	100.51	109.39
2	S	125	ASN	CA-C-N	5.58	131.01	121.29
2	S	125	ASN	C-N-CA	5.58	131.01	121.29
3	T	278	SER	CB-CA-C	-5.58	103.96	112.11
10	A	407	LYS	CA-C-N	5.58	129.28	120.47
10	A	407	LYS	C-N-CA	5.58	129.28	120.47
10	B	440	PRO	N-CA-C	-5.58	106.89	113.86
2	S	133	GLN	N-CA-C	-5.58	105.20	111.28
3	b	278	SER	CB-CA-C	-5.58	103.97	112.11
7	X	91	GLY	N-CA-C	-5.57	106.84	114.64
10	A	230	GLY	N-CA-C	-5.57	104.94	112.57
10	A	443	LYS	N-CA-CB	5.56	120.27	110.37
5	D	548	ARG	CA-C-N	5.56	127.67	120.44
5	D	548	ARG	C-N-CA	5.56	127.67	120.44
3	2	278	SER	CB-CA-C	-5.55	104.00	112.11
2	a	133	GLN	N-CA-C	-5.55	105.23	111.28
10	B	920	TYR	N-CA-CB	5.55	118.28	110.12
8	Y	190	SER	N-CA-C	5.55	117.90	109.41
2	a	125	ASN	CA-C-N	5.55	130.95	121.29
2	a	125	ASN	C-N-CA	5.55	130.95	121.29
10	B	443	LYS	N-CA-CB	5.55	120.24	110.37
2	J	635	PRO	CA-C-N	-5.55	114.02	122.23
2	J	635	PRO	C-N-CA	-5.55	114.02	122.23
5	4	346	LEU	CB-CA-C	-5.54	102.18	110.88
10	B	407	LYS	CA-C-N	5.54	129.22	120.47
10	B	407	LYS	C-N-CA	5.54	129.22	120.47
2	J	125	ASN	CA-C-N	5.54	130.93	121.29
2	J	125	ASN	C-N-CA	5.54	130.93	121.29
5	M	346	LEU	CB-CA-C	-5.54	102.19	110.88
10	A	920	TYR	N-CA-CB	5.53	118.25	110.12
2	a	960	LEU	N-CA-C	-5.53	105.25	111.28
2	S	68	GLY	CA-C-N	-5.52	114.18	122.47
2	S	68	GLY	C-N-CA	-5.52	114.18	122.47
2	1	960	LEU	N-CA-C	-5.52	105.26	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	635	PRO	CA-C-N	-5.52	114.06	122.23
2	S	635	PRO	C-N-CA	-5.52	114.06	122.23
10	A	1233	VAL	N-CA-C	-5.52	100.74	108.80
4	U	700	CYS	N-CA-C	-5.52	106.86	113.21
10	A	1055	VAL	CA-C-N	5.52	128.12	120.29
10	A	1055	VAL	C-N-CA	5.52	128.12	120.29
6	5	656	ASN	N-CA-C	-5.51	105.90	113.56
2	1	133	GLN	N-CA-C	-5.50	105.29	111.28
10	A	440	PRO	N-CA-C	-5.50	106.99	113.86
2	a	785	THR	N-CA-C	5.50	118.04	109.52
10	B	1233	VAL	N-CA-C	-5.49	100.78	108.80
2	1	785	THR	N-CA-C	5.49	118.03	109.52
5	4	331	GLN	CA-C-N	5.49	132.02	121.54
5	4	331	GLN	C-N-CA	5.49	132.02	121.54
2	a	635	PRO	CA-C-N	-5.49	114.11	122.23
2	a	635	PRO	C-N-CA	-5.49	114.11	122.23
2	1	635	PRO	CA-C-N	-5.48	114.11	122.23
2	1	635	PRO	C-N-CA	-5.48	114.11	122.23
6	E	656	ASN	N-CA-C	-5.48	105.94	113.56
6	N	656	ASN	N-CA-C	-5.48	105.94	113.56
5	D	381	TRP	CB-CA-C	-5.48	102.04	110.81
2	S	785	THR	N-CA-C	5.48	118.01	109.52
10	B	316	ALA	N-CA-C	-5.48	102.78	110.50
2	1	68	GLY	CA-C-N	-5.48	114.26	122.47
2	1	68	GLY	C-N-CA	-5.48	114.26	122.47
9	H	414	PRO	N-CA-C	5.48	123.75	112.47
2	1	539	GLN	CB-CA-C	-5.47	101.71	110.79
2	J	539	GLN	CB-CA-C	-5.47	101.71	110.79
6	W	656	ASN	N-CA-C	-5.47	105.96	113.56
4	C	700	CYS	N-CA-C	-5.47	106.92	113.21
5	V	381	TRP	CB-CA-C	-5.47	102.06	110.81
9	8	414	PRO	N-CA-C	5.46	123.72	112.47
10	B	1055	VAL	CA-C-N	5.46	128.04	120.29
10	B	1055	VAL	C-N-CA	5.46	128.04	120.29
5	M	331	GLN	CA-C-N	5.46	131.97	121.54
5	M	331	GLN	C-N-CA	5.46	131.97	121.54
2	S	539	GLN	CB-CA-C	-5.46	101.73	110.79
10	A	316	ALA	N-CA-C	-5.46	102.81	110.50
5	D	409	ILE	CB-CA-C	-5.45	104.78	112.14
9	H	374	VAL	CB-CA-C	-5.45	104.78	112.14
3	K	229	GLY	N-CA-C	-5.45	107.01	113.99
5	V	409	ILE	CB-CA-C	-5.45	104.78	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	539	GLN	CB-CA-C	-5.45	101.74	110.79
3	b	199	GLN	CA-C-N	-5.45	114.70	122.77
3	b	199	GLN	C-N-CA	-5.45	114.70	122.77
4	L	700	CYS	N-CA-C	-5.45	106.94	113.21
5	M	409	ILE	CB-CA-C	-5.45	104.78	112.14
2	a	68	GLY	CA-C-N	-5.45	114.30	122.47
2	a	68	GLY	C-N-CA	-5.45	114.30	122.47
5	4	381	TRP	CB-CA-C	-5.45	102.09	110.81
9	Z	414	PRO	N-CA-C	5.45	123.69	112.47
2	J	68	GLY	CA-C-N	-5.45	114.30	122.47
2	J	68	GLY	C-N-CA	-5.45	114.30	122.47
7	6	272	ILE	CB-CA-C	-5.45	104.79	112.14
7	F	272	ILE	CB-CA-C	-5.45	104.79	112.14
2	J	785	THR	N-CA-C	5.45	117.96	109.52
5	M	381	TRP	CB-CA-C	-5.44	102.10	110.81
2	S	1005	PHE	CB-CA-C	-5.44	102.34	110.88
7	X	272	ILE	CB-CA-C	-5.44	104.79	112.14
3	2	237	ILE	CA-C-N	-5.44	113.29	123.03
3	2	237	ILE	C-N-CA	-5.44	113.29	123.03
9	Q	414	PRO	N-CA-C	5.44	123.68	112.47
2	J	960	LEU	N-CA-C	-5.44	105.35	111.28
3	K	237	ILE	CA-C-N	-5.44	113.29	123.03
3	K	237	ILE	C-N-CA	-5.44	113.29	123.03
4	3	700	CYS	N-CA-C	-5.43	106.96	113.21
8	7	242	THR	N-CA-C	-5.43	101.53	109.63
7	O	272	ILE	CB-CA-C	-5.43	104.81	112.14
3	T	237	ILE	CA-C-N	-5.43	113.31	123.03
3	T	237	ILE	C-N-CA	-5.43	113.31	123.03
2	J	1005	PHE	CB-CA-C	-5.43	102.36	110.88
3	T	199	GLN	CA-C-N	-5.42	114.75	122.77
3	T	199	GLN	C-N-CA	-5.42	114.75	122.77
8	G	242	THR	N-CA-C	-5.42	101.55	109.63
3	b	111	LEU	N-CA-C	-5.42	103.91	111.39
3	b	229	GLY	N-CA-C	-5.42	107.05	113.99
2	1	1005	PHE	CB-CA-C	-5.42	102.38	110.88
3	2	111	LEU	N-CA-C	-5.41	103.92	111.39
3	b	237	ILE	CA-C-N	-5.41	113.35	123.03
3	b	237	ILE	C-N-CA	-5.41	113.35	123.03
2	S	330	VAL	CA-C-N	5.41	131.86	121.54
2	S	330	VAL	C-N-CA	5.41	131.86	121.54
2	a	1005	PHE	CB-CA-C	-5.41	102.39	110.88
10	A	302	VAL	N-CA-C	5.40	114.52	106.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	374	VAL	CB-CA-C	-5.40	104.85	112.14
9	Z	374	VAL	CB-CA-C	-5.40	104.85	112.14
5	4	409	ILE	CB-CA-C	-5.40	104.85	112.14
3	K	111	LEU	N-CA-C	-5.40	103.94	111.39
8	Y	242	THR	N-CA-C	-5.40	101.59	109.63
4	L	883	SER	N-CA-C	-5.39	106.77	113.19
2	S	960	LEU	N-CA-C	-5.39	105.40	111.28
6	5	474	GLY	N-CA-C	-5.39	107.67	115.27
4	C	883	SER	N-CA-C	-5.39	106.77	113.19
1	0	181	LEU	N-CA-C	-5.39	99.32	110.80
1	I	181	LEU	N-CA-C	-5.39	99.32	110.80
8	P	242	THR	N-CA-C	-5.39	101.61	109.63
2	J	330	VAL	CA-C-N	5.38	131.82	121.54
2	J	330	VAL	C-N-CA	5.38	131.82	121.54
3	T	111	LEU	N-CA-C	-5.38	103.96	111.39
3	T	229	GLY	N-CA-C	-5.38	107.10	113.99
8	7	194	MET	N-CA-C	5.38	122.25	110.80
1	9	181	LEU	N-CA-C	-5.38	99.35	110.80
8	G	24	GLY	N-CA-C	-5.38	107.93	114.92
10	B	852	VAL	CB-CA-C	-5.37	105.00	112.04
8	P	24	GLY	N-CA-C	-5.37	107.94	114.92
9	Q	374	VAL	CB-CA-C	-5.37	104.89	112.14
6	N	474	GLY	N-CA-C	-5.37	107.70	115.27
1	R	181	LEU	N-CA-C	-5.37	99.36	110.80
10	A	852	VAL	CB-CA-C	-5.37	105.01	112.04
9	H	355	PHE	CA-C-N	-5.37	114.84	122.41
9	H	355	PHE	C-N-CA	-5.37	114.84	122.41
2	1	330	VAL	CA-C-N	5.36	131.78	121.54
2	1	330	VAL	C-N-CA	5.36	131.78	121.54
3	2	218	LEU	CB-CA-C	-5.36	108.81	115.89
4	U	883	SER	N-CA-C	-5.36	106.81	113.19
8	7	257	LEU	CA-C-N	-5.36	115.65	122.77
8	7	257	LEU	C-N-CA	-5.36	115.65	122.77
10	B	302	VAL	N-CA-C	5.36	114.45	106.85
8	Y	194	MET	N-CA-C	5.36	122.21	110.80
3	2	110	ASP	CA-C-N	5.35	129.96	122.36
3	2	110	ASP	C-N-CA	5.35	129.96	122.36
8	G	194	MET	N-CA-C	5.35	122.20	110.80
9	Q	219	GLU	CA-C-N	5.35	127.89	120.29
9	Q	219	GLU	C-N-CA	5.35	127.89	120.29
2	a	330	VAL	CA-C-N	5.35	131.76	121.54
2	a	330	VAL	C-N-CA	5.35	131.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	883	SER	N-CA-C	-5.35	106.82	113.19
3	K	110	ASP	CA-C-N	5.35	129.96	122.36
3	K	110	ASP	C-N-CA	5.35	129.96	122.36
10	B	110	PRO	N-CA-C	5.35	117.22	110.70
2	J	654	VAL	CA-C-N	5.35	127.70	120.38
2	J	654	VAL	C-N-CA	5.35	127.70	120.38
5	V	333	MET	N-CA-C	5.35	121.62	109.81
3	b	110	ASP	CA-C-N	5.35	129.95	122.36
3	b	110	ASP	C-N-CA	5.35	129.95	122.36
2	1	654	VAL	CA-C-N	5.34	127.70	120.38
2	1	654	VAL	C-N-CA	5.34	127.70	120.38
3	K	199	GLN	CA-C-N	-5.34	114.87	122.77
3	K	199	GLN	C-N-CA	-5.34	114.87	122.77
9	Q	355	PHE	CA-C-N	-5.34	114.88	122.41
9	Q	355	PHE	C-N-CA	-5.34	114.88	122.41
8	Y	24	GLY	N-CA-C	-5.34	107.98	114.92
9	Z	355	PHE	CA-C-N	-5.34	114.88	122.41
9	Z	355	PHE	C-N-CA	-5.34	114.88	122.41
9	8	355	PHE	CA-C-N	-5.34	114.88	122.41
9	8	355	PHE	C-N-CA	-5.34	114.88	122.41
5	D	333	MET	N-CA-C	5.34	121.61	109.81
2	J	353	GLY	CA-C-N	5.34	127.87	120.29
2	J	353	GLY	C-N-CA	5.34	127.87	120.29
3	K	218	LEU	CB-CA-C	-5.33	108.85	115.89
8	P	194	MET	N-CA-C	5.33	122.17	110.80
6	E	474	GLY	N-CA-C	-5.33	107.75	115.27
8	Y	257	LEU	CA-C-N	-5.33	115.68	122.77
8	Y	257	LEU	C-N-CA	-5.33	115.68	122.77
8	G	257	LEU	CA-C-N	-5.33	115.68	122.77
8	G	257	LEU	C-N-CA	-5.33	115.68	122.77
3	T	110	ASP	CA-C-N	5.33	129.93	122.36
3	T	110	ASP	C-N-CA	5.33	129.93	122.36
3	2	229	GLY	N-CA-C	-5.33	107.17	113.99
2	1	869	LEU	CB-CA-C	-5.33	99.82	110.42
3	2	199	GLN	CA-C-N	-5.33	114.89	122.77
3	2	199	GLN	C-N-CA	-5.33	114.89	122.77
3	T	218	LEU	CB-CA-C	-5.32	108.86	115.89
2	a	654	VAL	CA-C-N	5.32	127.67	120.38
2	a	654	VAL	C-N-CA	5.32	127.67	120.38
8	P	257	LEU	CA-C-N	-5.32	115.69	122.77
8	P	257	LEU	C-N-CA	-5.32	115.69	122.77
9	Z	219	GLU	CA-C-N	5.32	127.84	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Z	219	GLU	C-N-CA	5.32	127.84	120.29
10	B	396	PHE	N-CA-C	-5.32	99.47	110.80
2	S	654	VAL	CA-C-N	5.32	127.67	120.38
2	S	654	VAL	C-N-CA	5.32	127.67	120.38
2	S	784	ALA	CA-C-N	-5.32	114.24	122.59
2	S	784	ALA	C-N-CA	-5.32	114.24	122.59
5	V	577	ILE	CB-CA-C	-5.32	104.96	112.14
2	a	869	LEU	CB-CA-C	-5.32	99.84	110.42
2	a	603	VAL	CB-CA-C	-5.31	104.97	112.14
6	W	474	GLY	N-CA-C	-5.31	107.78	115.27
5	D	577	ILE	CB-CA-C	-5.31	104.97	112.14
2	J	869	LEU	CB-CA-C	-5.31	99.85	110.42
2	S	869	LEU	CB-CA-C	-5.31	99.85	110.42
8	7	24	GLY	N-CA-C	-5.31	108.02	114.92
2	S	603	VAL	CB-CA-C	-5.31	104.97	112.14
3	b	218	LEU	CB-CA-C	-5.31	108.88	115.89
5	D	562	LEU	N-CA-C	-5.31	102.05	109.96
10	A	396	PHE	N-CA-C	-5.30	99.50	110.80
2	J	603	VAL	CB-CA-C	-5.30	104.98	112.14
2	J	784	ALA	CA-C-N	-5.30	114.26	122.59
2	J	784	ALA	C-N-CA	-5.30	114.26	122.59
2	S	894	TYR	CB-CA-C	-5.30	102.21	111.23
2	a	353	GLY	CA-C-N	5.30	127.82	120.29
2	a	353	GLY	C-N-CA	5.30	127.82	120.29
7	O	235	SER	N-CA-C	5.30	117.04	109.14
10	A	110	PRO	N-CA-C	5.30	117.16	110.70
5	4	562	LEU	N-CA-C	-5.29	102.07	109.96
9	8	219	GLU	CA-C-N	5.29	127.80	120.29
9	8	219	GLU	C-N-CA	5.29	127.80	120.29
7	O	271	SER	N-CA-C	-5.29	101.84	110.20
8	G	191	PRO	N-CA-CB	5.29	108.81	103.25
2	J	257	LEU	CA-C-N	5.29	128.35	120.31
2	J	257	LEU	C-N-CA	5.29	128.35	120.31
9	H	219	GLU	CA-C-N	5.29	127.80	120.29
9	H	219	GLU	C-N-CA	5.29	127.80	120.29
5	V	562	LEU	N-CA-C	-5.29	102.09	109.96
2	1	603	VAL	CB-CA-C	-5.28	105.01	112.14
2	S	353	GLY	CA-C-N	5.28	127.79	120.29
2	S	353	GLY	C-N-CA	5.28	127.79	120.29
5	4	487	TRP	N-CA-CB	5.28	117.99	110.44
7	6	235	SER	N-CA-C	5.28	117.01	109.14
2	1	257	LEU	CA-C-N	5.28	128.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	257	LEU	C-N-CA	5.28	128.33	120.31
5	M	562	LEU	N-CA-C	-5.28	102.09	109.96
10	A	221	THR	N-CA-C	-5.28	101.56	109.95
10	B	1342	LEU	N-CA-C	5.28	118.12	110.42
8	P	191	PRO	N-CA-CB	5.28	108.79	103.25
7	6	252	THR	CA-C-N	-5.27	115.34	123.14
7	6	252	THR	C-N-CA	-5.27	115.34	123.14
7	6	271	SER	N-CA-C	-5.27	101.87	110.20
8	7	191	PRO	N-CA-CB	5.27	108.78	103.25
2	S	257	LEU	CA-C-N	5.27	128.32	120.31
2	S	257	LEU	C-N-CA	5.27	128.32	120.31
7	O	252	THR	CA-C-N	-5.27	115.34	123.14
7	O	252	THR	C-N-CA	-5.27	115.34	123.14
5	D	177	TYR	N-CA-CB	5.27	117.86	110.12
9	Q	418	GLN	N-CA-CB	5.27	117.86	110.12
9	8	418	GLN	N-CA-CB	5.26	117.86	110.12
10	B	221	THR	N-CA-C	-5.26	101.58	109.95
6	W	617	LYS	CB-CA-C	-5.26	102.62	110.88
6	E	290	GLN	N-CA-C	-5.26	104.64	111.74
7	X	252	THR	CA-C-N	-5.26	115.36	123.14
7	X	252	THR	C-N-CA	-5.26	115.36	123.14
2	1	784	ALA	CA-C-N	-5.26	114.34	122.59
2	1	784	ALA	C-N-CA	-5.26	114.34	122.59
10	A	100	MET	CB-CA-C	-5.25	103.77	111.23
10	B	1341	VAL	CA-C-N	5.25	129.76	121.56
10	B	1341	VAL	C-N-CA	5.25	129.76	121.56
5	D	487	TRP	N-CA-CB	5.25	117.95	110.44
2	J	894	TYR	CB-CA-C	-5.25	102.30	111.23
2	a	784	ALA	CA-C-N	-5.25	114.34	122.59
2	a	784	ALA	C-N-CA	-5.25	114.34	122.59
10	A	1341	VAL	CA-C-N	5.25	129.75	121.56
10	A	1341	VAL	C-N-CA	5.25	129.75	121.56
10	A	1342	LEU	N-CA-C	5.25	118.09	110.42
7	F	252	THR	CA-C-N	-5.25	115.37	123.14
7	F	252	THR	C-N-CA	-5.25	115.37	123.14
6	W	290	GLN	N-CA-C	-5.25	104.65	111.74
6	E	617	LYS	CB-CA-C	-5.25	102.64	110.88
2	1	894	TYR	CB-CA-C	-5.25	102.31	111.23
3	b	145	ASP	N-CA-C	-5.25	106.14	112.54
10	A	1140	PHE	N-CA-C	-5.25	105.56	111.28
6	5	633	ARG	N-CA-C	-5.25	105.56	111.28
5	M	487	TRP	N-CA-CB	5.25	117.94	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	424	GLU	N-CA-C	-5.24	103.96	110.41
6	N	617	LYS	CB-CA-C	-5.24	102.65	110.88
2	1	353	GLY	CA-C-N	5.24	127.73	120.29
2	1	353	GLY	C-N-CA	5.24	127.73	120.29
2	S	650	ASP	CA-C-N	-5.24	115.83	123.06
2	S	650	ASP	C-N-CA	-5.24	115.83	123.06
7	X	235	SER	N-CA-C	5.24	116.95	109.14
2	1	296	ASP	CA-C-N	-5.24	113.10	122.32
2	1	296	ASP	C-N-CA	-5.24	113.10	122.32
9	H	418	GLN	N-CA-CB	5.24	117.82	110.12
6	W	633	ARG	N-CA-C	-5.24	105.57	111.28
9	Z	418	GLN	N-CA-CB	5.24	117.82	110.12
2	a	894	TYR	CB-CA-C	-5.24	102.33	111.23
2	1	823	VAL	CB-CA-C	-5.24	105.07	112.14
2	J	1075	LEU	N-CA-C	-5.24	106.15	112.54
2	J	823	VAL	CB-CA-C	-5.23	105.08	112.14
6	5	290	GLN	N-CA-C	-5.23	104.68	111.74
10	A	1274	GLN	CB-CA-C	-5.23	102.67	110.88
2	J	742	MET	CA-C-N	-5.23	114.61	122.24
2	J	742	MET	C-N-CA	-5.23	114.61	122.24
8	Y	191	PRO	N-CA-CB	5.23	108.78	102.72
2	S	823	VAL	CB-CA-C	-5.23	105.08	112.14
2	a	72	ALA	CA-C-N	5.23	131.38	121.97
2	a	72	ALA	C-N-CA	5.23	131.38	121.97
10	B	1140	PHE	N-CA-C	-5.22	105.58	111.28
7	F	271	SER	N-CA-C	-5.22	101.95	110.20
5	M	577	ILE	CB-CA-C	-5.22	105.09	112.14
5	V	487	TRP	N-CA-CB	5.22	117.91	110.44
2	a	823	VAL	CB-CA-C	-5.22	105.09	112.14
5	M	177	TYR	N-CA-CB	5.22	117.79	110.12
5	V	177	TYR	N-CA-CB	5.22	117.80	110.12
7	F	235	SER	N-CA-C	5.22	116.92	109.14
6	5	535	GLN	N-CA-C	-5.22	104.40	111.55
10	B	1274	GLN	CB-CA-C	-5.22	102.69	110.88
6	N	633	ARG	N-CA-C	-5.22	105.59	111.28
2	a	296	ASP	CA-C-N	-5.22	113.14	122.32
2	a	296	ASP	C-N-CA	-5.22	113.14	122.32
5	4	395	LEU	CB-CA-C	-5.21	104.97	113.37
2	J	355	TYR	N-CA-C	5.21	117.22	107.99
9	8	412	ALA	N-CA-C	5.21	116.96	111.28
2	1	646	MET	N-CA-C	5.21	116.82	111.03
6	N	290	GLN	N-CA-C	-5.21	104.70	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	177	TYR	N-CA-CB	5.21	117.78	110.12
5	M	395	LEU	CB-CA-C	-5.21	104.98	113.37
2	a	646	MET	N-CA-C	5.21	116.81	111.03
5	4	577	ILE	CB-CA-C	-5.21	105.11	112.14
2	a	355	TYR	N-CA-C	5.21	117.21	107.99
5	V	395	LEU	CB-CA-C	-5.21	104.99	113.37
2	a	257	LEU	CA-C-N	5.21	128.22	120.31
2	a	257	LEU	C-N-CA	5.21	128.22	120.31
2	J	296	ASP	CA-C-N	-5.20	113.16	122.32
2	J	296	ASP	C-N-CA	-5.20	113.16	122.32
10	B	343	VAL	CB-CA-C	-5.20	105.31	111.97
10	B	424	GLU	N-CA-C	-5.20	104.01	110.41
10	B	1089	ARG	N-CA-C	-5.20	105.69	111.36
8	Y	197	VAL	N-CA-C	5.20	116.19	108.65
10	A	343	VAL	CB-CA-C	-5.20	105.32	111.97
9	H	362	LYS	CB-CA-C	-5.20	102.72	110.88
9	H	390	HIS	CA-C-N	5.20	128.46	120.82
9	H	390	HIS	C-N-CA	5.20	128.46	120.82
6	N	535	GLN	N-CA-C	-5.20	104.43	111.55
9	Z	412	ALA	N-CA-C	5.20	116.95	111.28
6	5	617	LYS	CB-CA-C	-5.20	102.72	110.88
2	J	646	MET	N-CA-C	5.20	116.80	111.03
2	S	646	MET	N-CA-C	5.20	116.80	111.03
8	7	174	SER	CA-C-N	-5.20	115.40	122.93
8	7	174	SER	C-N-CA	-5.20	115.40	122.93
10	A	1089	ARG	N-CA-C	-5.20	105.70	111.36
9	Z	362	LYS	CB-CA-C	-5.20	102.72	110.88
10	B	912	ASP	N-CA-C	-5.19	106.05	112.38
2	S	742	MET	CA-C-N	-5.19	114.66	122.24
2	S	742	MET	C-N-CA	-5.19	114.66	122.24
2	J	650	ASP	CA-C-N	-5.19	115.90	123.06
2	J	650	ASP	C-N-CA	-5.19	115.90	123.06
2	a	1075	LEU	N-CA-C	-5.19	106.21	112.54
9	H	412	ALA	N-CA-C	5.19	116.94	111.28
5	4	334	PRO	N-CA-C	5.19	123.16	112.47
9	8	362	LYS	CB-CA-C	-5.19	102.73	110.88
5	D	395	LEU	CB-CA-C	-5.19	105.02	113.37
2	J	72	ALA	CA-C-N	5.19	131.31	121.97
2	J	72	ALA	C-N-CA	5.19	131.31	121.97
5	M	334	PRO	N-CA-C	5.19	123.16	112.47
9	Q	412	ALA	N-CA-C	5.19	116.94	111.28
7	X	271	SER	N-CA-C	-5.19	102.00	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	296	ASP	CA-C-N	-5.19	113.19	122.32
2	S	296	ASP	C-N-CA	-5.19	113.19	122.32
2	1	742	MET	CA-C-N	-5.18	114.67	122.24
2	1	742	MET	C-N-CA	-5.18	114.67	122.24
10	A	912	ASP	N-CA-C	-5.18	106.06	112.38
6	E	535	GLN	N-CA-C	-5.18	104.45	111.55
2	J	554	THR	N-CA-C	-5.18	103.84	110.53
2	1	355	TYR	N-CA-C	5.18	117.16	107.99
2	1	650	ASP	CA-C-N	-5.18	115.91	123.06
2	1	650	ASP	C-N-CA	-5.18	115.91	123.06
2	1	1075	LEU	N-CA-C	-5.18	106.22	112.54
3	K	321	PHE	N-CA-CB	5.18	119.07	110.52
5	M	523	ASP	CA-C-O	-5.18	116.14	122.41
6	E	633	ARG	N-CA-C	-5.18	105.64	111.28
3	b	321	PHE	N-CA-CB	5.18	119.06	110.52
2	1	72	ALA	CA-C-N	5.18	131.29	121.97
2	1	72	ALA	C-N-CA	5.18	131.29	121.97
3	K	145	ASP	N-CA-C	-5.18	106.22	112.54
2	a	650	ASP	CA-C-N	-5.18	115.92	123.06
2	a	650	ASP	C-N-CA	-5.18	115.92	123.06
6	W	535	GLN	N-CA-C	-5.17	104.46	111.55
10	B	138	ASP	N-CA-C	-5.17	107.00	113.72
9	Q	153	PHE	CA-C-N	-5.17	112.67	121.97
9	Q	153	PHE	C-N-CA	-5.17	112.67	121.97
8	P	174	SER	CA-C-N	-5.17	115.44	122.93
8	P	174	SER	C-N-CA	-5.17	115.44	122.93
9	Q	362	LYS	CB-CA-C	-5.17	102.77	110.88
8	Y	174	SER	CA-C-N	-5.17	115.44	122.93
8	Y	174	SER	C-N-CA	-5.17	115.44	122.93
10	A	1082	TRP	N-CA-C	-5.16	105.77	111.71
10	B	1172	GLN	N-CA-C	-5.16	106.24	112.54
2	S	72	ALA	CA-C-N	5.16	131.27	121.97
2	S	72	ALA	C-N-CA	5.16	131.27	121.97
3	2	145	ASP	N-CA-C	-5.16	106.24	112.54
2	S	355	TYR	N-CA-C	5.16	117.12	107.99
2	a	742	MET	CA-C-N	-5.16	114.71	122.24
2	a	742	MET	C-N-CA	-5.16	114.71	122.24
3	2	321	PHE	N-CA-CB	5.16	119.03	110.52
10	A	316	ALA	CA-C-N	-5.16	112.72	121.85
10	A	316	ALA	C-N-CA	-5.16	112.72	121.85
6	E	372	TRP	CB-CA-C	-5.16	104.44	112.07
3	T	145	ASP	N-CA-C	-5.16	106.25	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	108	THR	N-CA-C	-5.15	101.29	109.59
6	5	372	TRP	CB-CA-C	-5.15	104.44	112.07
6	N	691	HIS	CA-C-N	-5.15	116.81	123.19
6	N	691	HIS	C-N-CA	-5.15	116.81	123.19
2	S	554	THR	N-CA-C	-5.15	103.89	110.53
8	7	136	ASP	N-CA-C	-5.14	105.80	111.71
10	A	138	ASP	N-CA-C	-5.14	107.04	113.72
6	W	691	HIS	CA-C-N	-5.14	116.81	123.19
6	W	691	HIS	C-N-CA	-5.14	116.81	123.19
8	Y	197	VAL	CB-CA-C	-5.14	102.44	110.52
2	J	634	SER	CA-C-N	5.14	126.27	119.84
2	J	634	SER	C-N-CA	5.14	126.27	119.84
3	T	108	THR	N-CA-C	-5.14	101.31	109.59
10	A	1172	GLN	N-CA-C	-5.14	106.27	112.54
7	F	137	GLU	N-CA-C	5.14	116.54	109.29
3	T	321	PHE	N-CA-CB	5.14	119.00	110.52
8	Y	136	ASP	N-CA-C	-5.14	105.80	111.71
6	N	372	TRP	CB-CA-C	-5.14	104.47	112.07
2	S	1075	LEU	N-CA-C	-5.14	106.27	112.54
6	W	372	TRP	CB-CA-C	-5.14	104.47	112.07
9	8	390	HIS	CA-C-N	5.13	128.37	120.82
9	8	390	HIS	C-N-CA	5.13	128.37	120.82
8	G	136	ASP	N-CA-C	-5.13	105.81	111.71
9	Z	153	PHE	CA-C-N	-5.13	112.73	121.97
9	Z	153	PHE	C-N-CA	-5.13	112.73	121.97
9	Z	390	HIS	CA-C-N	5.13	128.36	120.82
9	Z	390	HIS	C-N-CA	5.13	128.36	120.82
9	8	153	PHE	CA-C-N	-5.13	112.74	121.97
9	8	153	PHE	C-N-CA	-5.13	112.74	121.97
8	G	174	SER	CA-C-N	-5.13	115.49	122.93
8	G	174	SER	C-N-CA	-5.13	115.49	122.93
7	O	244	THR	N-CA-C	5.13	117.60	109.50
2	1	554	THR	N-CA-C	-5.13	103.92	110.53
2	J	1196	LEU	N-CA-C	-5.13	105.69	111.28
2	a	554	THR	N-CA-C	-5.13	103.92	110.53
2	a	1196	LEU	N-CA-C	-5.13	105.69	111.28
10	B	1082	TRP	N-CA-C	-5.12	105.82	111.71
3	2	274	GLY	CA-C-N	5.12	131.32	121.54
3	2	274	GLY	C-N-CA	5.12	131.32	121.54
5	4	523	ASP	CA-C-O	-5.12	116.21	122.41
10	A	401	THR	N-CA-C	-5.12	105.75	112.41
3	2	108	THR	N-CA-C	-5.12	101.35	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	136	ASP	N-CA-C	-5.12	105.82	111.71
9	8	152	LEU	CA-C-N	-5.12	113.60	122.14
9	8	152	LEU	C-N-CA	-5.12	113.60	122.14
10	B	316	ALA	CA-C-N	-5.11	112.80	121.85
10	B	316	ALA	C-N-CA	-5.11	112.80	121.85
9	H	153	PHE	CA-C-N	-5.11	112.77	121.97
9	H	153	PHE	C-N-CA	-5.11	112.77	121.97
3	K	108	THR	N-CA-C	-5.11	101.36	109.59
6	E	691	HIS	CA-C-N	-5.11	116.85	123.19
6	E	691	HIS	C-N-CA	-5.11	116.85	123.19
10	B	73	LEU	N-CA-C	-5.11	107.00	113.23
2	S	634	SER	CA-C-N	5.11	126.23	119.84
2	S	634	SER	C-N-CA	5.11	126.23	119.84
2	S	1196	LEU	N-CA-C	-5.11	105.71	111.28
2	a	426	HIS	N-CA-C	5.11	118.82	112.59
7	F	78	SER	N-CA-C	5.11	115.08	107.88
1	R	190	ASN	N-CA-C	5.11	116.43	109.18
6	5	691	HIS	CA-C-N	-5.10	116.86	123.19
6	5	691	HIS	C-N-CA	-5.10	116.86	123.19
10	B	401	THR	N-CA-C	-5.10	105.78	112.41
9	Q	390	HIS	CA-C-N	5.10	128.31	120.82
9	Q	390	HIS	C-N-CA	5.10	128.31	120.82
2	a	634	SER	CA-C-N	5.10	126.21	119.84
2	a	634	SER	C-N-CA	5.10	126.21	119.84
3	b	274	GLY	CA-C-N	5.10	131.28	121.54
3	b	274	GLY	C-N-CA	5.10	131.28	121.54
5	D	202	PHE	N-CA-C	-5.09	103.32	110.50
2	J	426	HIS	N-CA-C	5.09	118.81	112.59
2	1	634	SER	CA-C-N	5.09	126.21	119.84
2	1	634	SER	C-N-CA	5.09	126.21	119.84
1	9	190	ASN	N-CA-C	5.09	116.41	109.18
3	T	274	GLY	CA-C-N	5.09	131.27	121.54
3	T	274	GLY	C-N-CA	5.09	131.27	121.54
9	H	152	LEU	CA-C-N	-5.09	113.64	122.14
9	H	152	LEU	C-N-CA	-5.09	113.64	122.14
2	1	390	PHE	N-CA-C	-5.09	100.41	109.06
2	1	426	HIS	N-CA-C	5.09	118.80	112.59
7	6	244	THR	N-CA-C	5.08	117.53	109.50
2	S	781	GLU	CA-C-N	5.08	128.73	120.60
2	S	781	GLU	C-N-CA	5.08	128.73	120.60
9	Z	152	LEU	CA-C-N	-5.08	113.65	122.14
9	Z	152	LEU	C-N-CA	-5.08	113.65	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	137	GLU	N-CA-C	5.08	116.45	109.29
2	1	781	GLU	CA-C-N	5.07	128.72	120.60
2	1	781	GLU	C-N-CA	5.07	128.72	120.60
2	1	413	ALA	CB-CA-C	-5.07	109.24	116.34
5	M	202	PHE	N-CA-C	-5.07	103.35	110.50
5	V	522	GLY	N-CA-C	-5.07	107.86	113.79
5	4	202	PHE	N-CA-C	-5.07	103.35	110.50
10	A	73	LEU	N-CA-C	-5.07	107.05	113.23
1	I	190	ASN	N-CA-C	5.07	116.38	109.18
2	J	781	GLU	CA-C-N	5.07	128.71	120.60
2	J	781	GLU	C-N-CA	5.07	128.71	120.60
1	0	190	ASN	N-CA-C	5.06	116.37	109.18
2	1	466	GLN	N-CA-C	-5.06	105.96	113.40
2	J	421	TYR	CB-CA-C	-5.06	99.70	109.37
2	S	413	ALA	CB-CA-C	-5.06	109.25	116.34
2	a	781	GLU	CA-C-N	5.06	128.69	120.60
2	a	781	GLU	C-N-CA	5.06	128.69	120.60
2	S	390	PHE	N-CA-C	-5.05	100.47	109.06
5	V	202	PHE	N-CA-C	-5.05	103.37	110.50
2	a	413	ALA	CB-CA-C	-5.05	109.27	116.34
3	2	154	LEU	CA-C-N	5.05	131.19	121.54
3	2	154	LEU	C-N-CA	5.05	131.19	121.54
5	M	489	LEU	N-CA-C	-5.05	105.78	111.28
2	a	421	TYR	CB-CA-C	-5.05	99.72	109.37
2	S	426	HIS	N-CA-C	5.05	118.75	112.59
5	D	522	GLY	N-CA-C	-5.05	107.89	113.79
4	L	935	LEU	N-CA-C	-5.05	106.40	113.37
3	b	154	LEU	CA-C-N	5.05	131.18	121.54
3	b	154	LEU	C-N-CA	5.05	131.18	121.54
5	4	489	LEU	N-CA-C	-5.04	105.78	111.28
10	A	395	GLY	O-C-N	5.04	127.08	122.19
2	J	390	PHE	N-CA-C	-5.04	100.48	109.06
4	U	935	LEU	N-CA-C	-5.04	106.41	113.37
7	F	244	THR	N-CA-C	5.04	117.47	109.50
2	1	1196	LEU	N-CA-C	-5.04	105.79	111.28
7	X	244	THR	N-CA-C	5.04	117.46	109.50
3	K	274	GLY	CA-C-N	5.04	131.16	121.54
3	K	274	GLY	C-N-CA	5.04	131.16	121.54
2	J	413	ALA	CB-CA-C	-5.04	109.29	116.34
9	Q	152	LEU	CA-C-N	-5.04	113.73	122.14
9	Q	152	LEU	C-N-CA	-5.04	113.73	122.14
2	a	390	PHE	N-CA-C	-5.04	100.50	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	489	LEU	N-CA-C	-5.03	105.80	111.28
7	6	219	ALA	N-CA-C	5.03	116.61	108.41
7	O	78	SER	N-CA-C	5.02	114.96	107.88
4	3	935	LEU	N-CA-C	-5.02	106.44	113.37
10	B	1192	PHE	N-CA-C	5.02	117.71	111.24
2	J	466	GLN	N-CA-C	-5.02	106.02	113.40
7	O	271	SER	CB-CA-C	5.02	118.01	109.53
2	S	466	GLN	N-CA-C	-5.02	106.03	113.40
3	T	147	HIS	N-CA-CB	-5.01	104.85	112.47
5	4	522	GLY	N-CA-C	-5.01	107.92	113.79
2	1	137	VAL	N-CA-C	-5.01	103.12	109.58
10	A	1192	PHE	N-CA-C	5.01	117.70	111.24
7	6	271	SER	CB-CA-C	5.01	117.99	109.53
5	V	523	ASP	CA-C-O	-5.00	116.36	122.41
2	1	581	PRO	CA-C-N	5.00	126.94	120.44
2	1	581	PRO	C-N-CA	5.00	126.94	120.44
2	S	581	PRO	CA-C-N	5.00	126.94	120.44
2	S	581	PRO	C-N-CA	5.00	126.94	120.44

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	7	0
1	9	1562	0	681	7	0
1	I	1562	0	681	7	0
1	R	1562	0	681	6	0
2	1	4997	0	2175	37	0
2	J	4997	0	2174	34	0
2	S	4997	0	2174	64	0
2	a	4997	0	2174	45	0
3	2	1566	0	702	21	0
3	K	1566	0	702	21	0
3	T	1566	0	702	20	0
3	b	1566	0	702	19	0
4	3	2629	0	1167	59	0
4	C	2629	0	1167	37	0
4	L	2629	0	1167	39	0
4	U	2629	0	1167	39	0
5	4	3278	0	1440	10	0
5	D	3278	0	1442	11	0
5	M	3278	0	1440	10	0
5	V	3278	0	1442	10	0
6	5	2073	0	907	15	0
6	E	2073	0	907	15	0
6	N	2073	0	907	16	0
6	W	2073	0	907	16	0
7	6	1402	0	648	20	0
7	F	1402	0	648	22	0
7	O	1402	0	648	20	0
7	X	1402	0	648	22	0
8	7	1593	0	731	44	0
8	G	1593	0	731	43	0
8	P	1593	0	731	44	0
8	Y	1593	0	731	43	0
9	8	2153	0	938	20	0
9	H	2153	0	938	20	0
9	Q	2153	0	938	20	0
9	Z	2153	0	938	20	0
10	A	5436	0	2392	68	0
10	B	5436	0	2384	134	0
All	All	95884	0	42333	1013	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 7.

All (1013) 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)
10:B:844:CYS:C	10:B:885:ARG:CB	1.81	1.52
4:3:883:SER:CB	4:3:926:ALA:CA	1.90	1.49
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:A:1312:PRO:HA	2:S:1005:PHE:C	1.52	1.32
10:B:852:VAL:CB	10:B:879:GLU:O	1.76	1.31
9:Z:64:TYR:C	9:Z:65:SER:N	1.89	1.30
9:8:64:TYR:C	9:8:65:SER:N	1.89	1.30
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
9:H:64:TYR:C	9:H:65:SER:N	1.89	1.28
10:A:1311:ASP:CB	2:S:1009:LEU:HA	1.61	1.28
9:Q:64:TYR:C	9:Q:65:SER:N	1.89	1.28
10:A:1308:LYS:O	2:S:1037:LEU:CA	1.71	1.26
10:B:1362:VAL:HA	2:a:1076:MET:CB	1.66	1.25
10:A:1312:PRO:CB	2:S:1006:LYS:HA	1.66	1.25
10:B:859:LEU:CB	10:B:874:CYS:C	2.12	1.23
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:G:322:ASN:HA	9:H:20:LYS:CB	1.71	1.21
8:P:322:ASN:HA	9:Q: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:875:SER:N	2.06	1.18
8:P:44:SER:CB	1:R:201:ARG:CB	2.22	1.18
1:O:201:ARG:CB	8:Y:44:SER:CB	2.22	1.17
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
10:A:1312:PRO:CB	2:S:1005:PHE:C	2.21	1.13
10:A:1312:PRO:CA	2:S:1005:PHE:C	2.20	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:188:ASP:HA	8:G:196:LYS:H	1.00	1.13
10:B:1362:VAL:CA	2:a:1076:MET:CB	2.27	1.12
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:O	2:S:1005:PHE:CB	2.01	1.09
10:B:856:SER:O	10:B:873:ILE:O	1.69	1.08
10:B:859:LEU:C	10:B:874:CYS:CB	2.27	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: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:B:845:TYR:CB	10:B:885:ARG:C	2.32	1.02
10:B:856:SER:O	10:B:873:ILE:C	2.03	1.01
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
4:3:881:ASN:C	4:3:926:ALA:HB2	1.88	0.97
4:3:881:ASN:O	4:3:926:ALA:HB2	1.63	0.96
10:B:856:SER:O	10:B:874:CYS:C	2.08	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
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
10:B:859:LEU:O	10:B:871:ASP:HA	1.65	0.93
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
8:G:188:ASP:HA	8:G:196:LYS:N	1.83	0.91
10:B:845:TYR:HA	10:B:885:ARG:C	1.95	0.91
10:B:852:VAL:CB	10:B:879:GLU:C	2.43	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:845:TYR:CA	10:B:885:ARG:C	2.45	0.90
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
4:3:683:LEU:N	4:3:684:THR:HA	1.90	0.87
8:7:322:ASN:CA	9:8:20:LYS:CB	2.52	0.87
1:I:91:ALA:HB1	1:I:134:CYS:CB	2.05	0.87
8:Y:322:ASN:CA	9:Z:20:LYS:CB	2.53	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
8:7:322:ASN:HA	9:8:20:LYS:CA	2.04	0.86
10:A:1309:SER:O	2:S:1040:VAL:CB	2.22	0.86
8:Y:322:ASN:HA	9:Z:20:LYS:CA	2.04	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
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:859:LEU:CB	10:B:874:CYS:CB	2.53	0.85
10:B:1359:GLY:HA2	2:a:1074:ASP:O	1.76	0.85
10:B:1362:VAL:CB	2:a:1076:MET:CB	2.56	0.83
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
10:B:860:GLN:N	10:B:874:CYS:CB	2.39	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:B:859:LEU:O	10:B:871:ASP:CA	2.21	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
10:B:860:GLN:HA	10:B:874:CYS:N	1.91	0.81
8:7:189:SER:HA	8:7:220:ASP:C	2.06	0.81
8:P:189:SER:HA	8:P:220:ASP:C	2.06	0.81
8:G:189:SER:HA	8:G:220:ASP:C	2.06	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1143:VAL:HA	4:3:1146:ALA:HB3	1.63	0.79
8:Y:189:SER:HA	8:Y:220:ASP:C	2.06	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:844:CYS:CA	10:B:885:ARG:CB	2.61	0.79
10:B:845:TYR:HA	10:B:885:ARG:CB	2.11	0.79
10:A:1312:PRO:HA	2:S:1005:PHE:CB	2.12	0.78
6:5:707:THR:HA	6:5:739:ALA:HB1	1.65	0.78
4:U:1143:VAL:HA	4:U:1146:ALA:HB3	1.63	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
4:C:1143:VAL:HA	4:C:1146:ALA:HB3	1.63	0.77
8:P:52:SER:CB	8:P:97:LEU:HA	2.15	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
10:B:858:HIS:C	10:B:872:ALA:HA	2.11	0.76
6:W:360:ASN:O	6:W:363:VAL:HA	1.86	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
4:3:682:ASN:C	4:3:684:THR:HA	2.13	0.74
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
4:L:682:ASN:C	4:L:684:THR:HA	2.13	0.74
10:B:859:LEU:CB	10:B:875:SER:HA	2.18	0.74
4:U:682:ASN:C	4:U:684:THR:HA	2.13	0.74
4:3:883:SER:CB	4:3:926:ALA:C	2.60	0.74
2:1:423:ASN:O	2:1:430:GLY:HA2	1.89	0.73
4:C:682:ASN:C	4:C:684:THR:HA	2.12	0.73
3:T:274:GLY:HA2	3:T:277:ALA:CB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:360:ASN:C	6:W:363:VAL:HA	2.14	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
2:J:423:ASN:O	2:J:430:GLY:HA2	1.89	0.73
8:Y:189:SER:CB	8:Y:195:ALA:H	2.02	0.73
3:b:274:GLY:HA2	3:b:277:ALA:CB	2.19	0.73
3:2:274:GLY:HA2	3:2:277:ALA:CB	2.19	0.72
6:5:360:ASN:C	6:5:363:VAL:HA	2.14	0.72
8:7:188:ASP:C	8:7:195:ALA:HB3	2.14	0.72
8:P:189:SER:CB	8:P:195:ALA:H	2.02	0.72
8:Y:188:ASP:C	8:Y:195:ALA:HB3	2.14	0.72
2:a:423:ASN:O	2:a:430:GLY:HA2	1.89	0.72
6:E:360:ASN:C	6:E:363:VAL:HA	2.14	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:G:188:ASP:C	8:G:195:ALA:HB3	2.14	0.72
8:P:188:ASP:C	8:P:195:ALA:HB3	2.14	0.72
8:7:189:SER:CB	8:7:195:ALA:H	2.02	0.71
6:N:360:ASN:C	6:N:363:VAL:HA	2.14	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
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
10:B:22:ALA:HB1	10:B:780:ALA:HA	1.71	0.71
4:L:683:LEU:N	4:L:684:THR:CA	2.53	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
4:3:881:ASN:C	4:3:926:ALA:CB	2.64	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
3:2:278:SER:O	3:2:294:GLY:HA2	1.92	0.70
10:B:845:TYR:HA	10:B:886:GLN:H	1.57	0.69
4:3:866:TYR:O	4:3:868:ASP:N	2.24	0.69
10:B:845:TYR:CB	10:B:885:ARG:O	2.39	0.69
8:G:189:SER:HA	8:G:220:ASP:HA	1.75	0.69
10:B:843:ASN:O	10:B:885:ARG:CB	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:B:441:PHE:HA	10:B:444:PRO:O	1.93	0.68
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
3:b:278:SER:O	3:b:294:GLY:HA2	1.92	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
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
10:B:859:LEU:C	10:B:875:SER:H	2.01	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:G:166:SER:HA	8:G:185:GLY:O	1.95	0.67
8:Y:166:SER:HA	8:Y:185:GLY:O	1.95	0.67
7:O:224:ILE:C	7:O:226:LEU:H	2.03	0.67
3:2:274:GLY:HA2	3:2:277:ALA:HB3	1.74	0.67
10:B:859:LEU:C	10:B:875:SER:N	2.53	0.67
8:P:322:ASN:HA	9:Q:20:LYS:N	2.08	0.67
10:A:942:PRO:HA	10:A:943:GLN:CB	2.17	0.67
10:A:50:SER:C	10:A:58:SER:HA	2.20	0.67
8:P:166:SER:HA	8:P:185:GLY:O	1.95	0.66
3:b:274:GLY:HA2	3:b:277:ALA:HB3	1.75	0.66
7:F:224:ILE:C	7:F:226:LEU:H	2.03	0.66
7:X:224:ILE:C	7:X:226:LEU:H	2.03	0.66
8:7:166:SER:HA	8:7:185:GLY:O	1.95	0.66
10:B:858:HIS:C	10:B:871:ASP:O	2.36	0.66
8:P:189:SER:HA	8:P:220:ASP:HA	1.75	0.66
4:U:1119:LEU:C	4:U:1121:GLU:H	2.04	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
10:B:50:SER:C	10:B:58:SER:HA	2.20	0.66
4:U:904:TRP:CB	4:U:929:LEU:CB	2.74	0.66
4:C:1119:LEU:C	4:C:1121:GLU:H	2.04	0.66
4:L:1119:LEU:C	4:L:1121:GLU:H	2.04	0.65
7:X:113:PRO:CB	7:X:161:ALA:HB2	2.27	0.65
10:A:1312:PRO:C	2:S:1005:PHE:CB	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:113:PRO:CB	7:F:161:ALA:HB2	2.27	0.65
8:P:188:ASP:O	8:P:221:PRO:HA	1.95	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
4:3:1119:LEU:C	4:3:1121:GLU:H	2.04	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
7:6:224:ILE:C	7:6:226:LEU:H	2.03	0.64
7:X:155:ALA:HB2	7:X:217:ASP:HA	1.79	0.64
10:A:441:PHE:C	10:A:443:LYS:H	2.06	0.64
10:B:441:PHE:C	10:B:443:LYS:H	2.06	0.63
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
2:1:220:TRP:C	2:1:225:GLY:HA2	2.24	0.63
6:5:707:THR:HA	6:5:739:ALA:CB	2.29	0.63
5:4:282:GLY:HA2	5:4:288:ILE:N	2.14	0.62
10:B:858:HIS:O	10:B:871:ASP:C	2.42	0.62
8:P:190:SER:N	8:P:220:ASP:HA	2.14	0.62
8:7:190:SER:N	8:7:220:ASP:HA	2.14	0.62
10:B:205:LEU:C	10:B:207:SER:HA	2.25	0.62
10:A:205:LEU:C	10:A:207:SER:HA	2.24	0.62
7:O:238:GLY:O	7:O:260:LYS:HA	2.00	0.62
6:W:707:THR:HA	6:W:739:ALA:CB	2.28	0.62
5:M:191:ILE:HA	5:M:201:LYS:N	2.15	0.62
2:a:220:TRP:C	2:a:225:GLY:HA2	2.24	0.62
5:M:282:GLY:HA2	5:M:288:ILE:N	2.14	0.62
7:6:238:GLY:O	7:6:260:LYS:HA	2.00	0.62
5:4:191:ILE:HA	5:4:201:LYS:N	2.15	0.62
8:Y:190:SER:N	8:Y:220:ASP:HA	2.14	0.62
3:b:29:ASN:CB	3:b:33:GLY:HA3	2.29	0.62
3:2:29:ASN:CB	3:2:33:GLY:HA3	2.29	0.62
10:A:1312:PRO:CA	2:S:1005:PHE:CB	2.77	0.62
5:D:191:ILE:HA	5:D:201:LYS:N	2.15	0.62
6:N:707:THR:HA	6:N:739:ALA:CB	2.29	0.62
10:A:853:ASP:HA	10:A:886:GLN:CB	2.29	0.62
2:J:220:TRP:C	2:J:225:GLY:HA2	2.24	0.61
5:D:282:GLY:HA2	5:D:288:ILE:N	2.14	0.61
6:E:707:THR:HA	6:E:739:ALA:CB	2.28	0.61
10:B:856:SER:HA	10:B:878:ASN:H	1.64	0.61
6:E:308:PRO:O	6:E:315:LYS:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:238:GLY:O	7:F:260:LYS:HA	2.00	0.61
4:L:868:ASP:O	4:L:869:PHE:C	2.43	0.61
6:W:308:PRO:O	6:W:315:LYS:HA	2.01	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
7:X:238:GLY:O	7:X:260:LYS:HA	2.00	0.61
4:C:868:ASP:O	4:C:869:PHE:C	2.43	0.61
2:S:220:TRP:C	2:S:225:GLY:HA2	2.24	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
4:U:868:ASP:O	4:U:869:PHE:C	2.43	0.61
10:B:856:SER:HA	10:B:874:CYS:O	2.01	0.60
8:P:165:CYS:O	8:P:186:SER:HA	2.01	0.60
2:S:362:ALA:HB3	2:S:366:GLY:H	1.67	0.60
5:V:191:ILE:HA	5:V:201:LYS:N	2.15	0.60
10:A:376:ARG:C	10:A:380:ALA:HA	2.27	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
10:B:376:ARG:C	10:B:380:ALA:HA	2.27	0.60
4:C:868:ASP:O	4:C:870:ASP:N	2.35	0.60
9:Q:176:GLU:HA	9:Q:177:VAL:C	2.27	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
8:G:165:CYS:O	8:G:186:SER:HA	2.02	0.60
6:5:308:PRO:O	6:5:315:LYS:HA	2.01	0.60
9:H:176:GLU:HA	9:H:177:VAL:C	2.27	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
4:3:868:ASP:O	4:3:870:ASP:N	2.35	0.60
10:B:312:MET:CB	10:B:313:SER:HA	2.32	0.60
4:U:868:ASP:O	4:U:870:ASP:N	2.35	0.60
4:3:868:ASP:O	4:3:869:PHE:C	2.43	0.59
2:a:362:ALA:HB3	2:a:366:GLY:H	1.66	0.59
3:2:29:ASN:HA	3:2:33:GLY:HA3	1.83	0.59
6:5:297:PHE:CA	7:6:269:SER:CB	2.77	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
9:Z:176:GLU:HA	9:Z:177:VAL:C	2.27	0.59
8:Y:114:THR:CB	8:Y:135:ALA:HB3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:845:TYR:O	10:B:886:GLN:CB	2.51	0.59
8:7:114:THR:CB	8:7:135:ALA:HB3	2.33	0.59
9:8:176:GLU:HA	9:8:177:VAL:C	2.26	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:860:GLN:N	10:B:874:CYS:C	2.61	0.59
3:K:29:ASN:HA	3:K:33:GLY:HA3	1.84	0.59
8:P:114:THR:CB	8:P:135:ALA:HB3	2.33	0.58
3:b:29:ASN:HA	3:b:33:GLY:HA3	1.84	0.58
2:1:362:ALA:HB3	2:1:366:GLY:H	1.66	0.58
9:H:244:SER:HA	9:H:255:GLU:N	2.18	0.58
9:Z:244:SER:HA	9:Z:255:GLU:N	2.18	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
4:C:932:HIS:O	4:C:933:GLU:CB	2.51	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:A:1312:PRO:N	2:S:1005:PHE:O	2.35	0.58
10:B:845:TYR:HA	10:B:885:ARG:CA	2.32	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: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: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
4:3:881:ASN:CB	4:3:922:HIS:C	2.78	0.57
7:6:292:SER:C	7:6:294:ASP:H	2.13	0.57
3:T:29:ASN:HA	3:T:33:GLY:H	1.70	0.57
8:Y:189:SER:CB	8:Y:194:MET:CB	2.82	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
3:b:29:ASN:HA	3:b:33:GLY:H	1.70	0.57
7:O:292:SER:C	7:O:294:ASP:H	2.13	0.57
8:P:189:SER:CB	8:P:194:MET:CB	2.82	0.57
8:G:189:SER:CB	8:G:194:MET:CB	2.82	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
7:F:292:SER:C	7:F:294:ASP:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:652:GLU:C	2:J:654:VAL:H	2.13	0.56
3:K:29:ASN:HA	3:K:33:GLY:H	1.70	0.56
2:1:1073:VAL:C	2:1:1075:LEU:H	2.14	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
2:a:590:GLU:N	2:a:591:THR:HA	2.21	0.56
2:a:652:GLU:C	2:a:654:VAL:H	2.13	0.56
2:a:1073:VAL:C	2:a:1075:LEU:H	2.14	0.56
1:0:201:ARG:CB	8:Y:44:SER:HA	2.36	0.56
10:B:845:TYR:CA	10:B:886:GLN:CA	2.76	0.56
2:S:652:GLU:C	2:S:654:VAL:H	2.14	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
2:J:1073:VAL:C	2:J:1075:LEU:H	2.14	0.56
7:O:250:SER:O	7:O:252:THR:N	2.35	0.56
8:7:44:SER:HA	1:9:201:ARG:CB	2.36	0.56
2:1:590:GLU:N	2:1:591:THR:HA	2.21	0.55
6:5:527:VAL:C	6:5:529:GLN:HA	2.31	0.55
6:N:527:VAL:C	6:N:529:GLN:HA	2.31	0.55
8:G:44:SER:HA	1:I:201:ARG:CB	2.36	0.55
6:E:527:VAL:C	6:E:529:GLN:HA	2.31	0.55
2:J:590:GLU:N	2:J:591:THR:HA	2.21	0.55
2:S:1073:VAL:C	2:S:1075:LEU:H	2.14	0.55
10:B:863:CYS:N	10:B:871:ASP:HA	2.21	0.55
7:X:292:SER:C	7:X:294:ASP:H	2.13	0.55
2:1:580:LEU:CB	2:1:581:PRO:HA	2.37	0.55
4:3:883:SER:H	4:3:926:ALA:CA	2.18	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:527:VAL:C	6:W:529:GLN:HA	2.31	0.55
6:W:297:PHE:CA	7:X:269:SER:CB	2.76	0.55
2:1:652:GLU:C	2:1:654:VAL:H	2.14	0.55
5:M:415:ALA:HB2	5:M:428:TYR:CB	2.37	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
7:6:265:VAL:HA	7:6:281:GLY:HA3	1.89	0.55
10:B:858:HIS:O	10:B:872:ALA:HA	2.05	0.55
8:G:44:SER:CA	1:I:201:ARG:CB	2.84	0.55
8:P:322:ASN:CA	9:Q:20:LYS:N	2.70	0.55
9:Q:272:SER:C	9:Q:274:PHE:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:322:ASN:CA	9:H:20:LYS:N	2.70	0.54
8:7:191:PRO:C	8:7:193:ALA:H	2.14	0.54
8:7:322:ASN:CA	9:8:20:LYS:N	2.70	0.54
9:H:272:SER:C	9:H:274:PHE:H	2.16	0.54
3:2:94:LYS:HA	3:2:107:PHE:O	2.08	0.54
9:8:272:SER:C	9:8:274:PHE:H	2.15	0.54
10:B:1362:VAL:N	2:a:1076:MET:CB	2.70	0.54
5:4:415:ALA:HB2	5:4:428:TYR:CB	2.37	0.54
4:3:882:GLN:C	4:3:884:ARG:H	2.15	0.54
4:U:882:GLN:C	4:U:884:ARG:H	2.16	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
9:Z:272:SER:C	9:Z:274:PHE:H	2.16	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
2:a:580:LEU:CB	2:a:581:PRO:HA	2.37	0.54
5:D:415:ALA:HB2	5:D:428:TYR:CB	2.37	0.54
3:T:230:ASN:O	3:T:253:ARG:HA	2.08	0.54
8:Y:241:ALA:HB1	8:Y:281:VAL:O	2.08	0.54
3:b:94:LYS:HA	3:b:107:PHE:O	2.07	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
3:b:230:ASN:O	3:b:253:ARG:HA	2.07	0.54
4:3:881:ASN:CB	4:3:923:GLY:N	2.70	0.53
10:B:181:ALA:O	10:B:196:GLY:HA2	2.08	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
4:L:882:GLN:C	4:L:884:ARG:H	2.15	0.53
7:O:265:VAL:HA	7:O:281:GLY:HA3	1.89	0.53
8:P:44:SER:CA	1:R:201:ARG:CB	2.84	0.53
8:P:242:THR:C	8:P:244:ASP:H	2.16	0.53
5:D:440:PRO:HA	5:D:443:ASP:CB	2.38	0.53
8:P:241:ALA:HB1	8:P:281:VAL:O	2.08	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
10:B:22:ALA:HB1	10:B:780:ALA:CA	2.38	0.53
10:A:22:ALA:HB1	10:A:780:ALA:CA	2.38	0.53
10:A:1311:ASP:N	2:S:1009:LEU:CB	2.71	0.53
3:T:94:LYS:HA	3:T:107:PHE:O	2.08	0.53
8:Y:191:PRO:C	8:Y:193:ALA:H	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:242:THR:C	8:Y:244:ASP:H	2.16	0.53
3:2:218:LEU:C	3:2:220:ASN:H	2.17	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
7:6:214:TRP:O	7:6:235:SER:CB	2.56	0.53
8:7:242:THR:C	8:7:244:ASP:H	2.16	0.53
3:K:277:ALA:O	3:K:296:VAL:HA	2.08	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
4:C:882:GLN:C	4:C:884:ARG:H	2.15	0.53
7:O:214:TRP:O	7:O:235:SER:CB	2.56	0.53
8:Y:322:ASN:CA	9:Z:20:LYS:N	2.70	0.53
4:3:934:HIS:C	4:3:936:SER:H	2.18	0.52
4:C:934:HIS:C	4:C:936:SER:H	2.18	0.52
8:G:242:THR:C	8:G:244:ASP:H	2.16	0.52
3:T:277:ALA:O	3:T:296:VAL:HA	2.08	0.52
2:1:413:ALA:C	2:1:415:ASN:HA	2.34	0.52
10:B:860:GLN:HA	10:B:874:CYS:CB	2.40	0.52
10:B:1352:LEU:C	10:B:1354:LEU:H	2.17	0.52
2:S:413:ALA:C	2:S:415:ASN:HA	2.34	0.52
4:3:622:GLY:O	4:3:623:ARG:O	2.27	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
10:B:22:ALA:HB1	10:B:780:ALA:CB	2.39	0.52
8:P:191:PRO:C	8:P:193:ALA:H	2.14	0.52
3:T:218:LEU:C	3:T:220:ASN:H	2.17	0.52
4:U:622:GLY:O	4:U:623:ARG:O	2.27	0.52
2:a:413:ALA:C	2:a:415:ASN:HA	2.34	0.52
5:D:239:VAL:C	5:D:242:VAL:HA	2.34	0.52
3:b:277:ALA:O	3:b:296:VAL:HA	2.08	0.52
4:C:622:GLY:O	4:C:623:ARG:O	2.27	0.52
2:S:422:ILE:HA	2:S:431:GLN:O	2.10	0.52
4:3:883:SER:N	4:3:926:ALA:HA	2.24	0.52
4:C:1058:ILE:O	4:C:1059:ASP:CB	2.58	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
7:6:67:HIS:O	7:6:69:MET:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:340:LYS:C	10:A:342:ILE:HA	2.35	0.52
10:B:340:LYS:C	10:B:342:ILE:HA	2.35	0.52
2:J:413:ALA:C	2:J:415:ASN:HA	2.34	0.52
5:V:239:VAL:C	5:V:242:VAL:HA	2.34	0.52
3:b:218:LEU:C	3:b:220:ASN:H	2.17	0.52
2:1:422:ILE:HA	2:1:431:GLN:O	2.10	0.51
4:L:1058:ILE:O	4:L:1059:ASP:CB	2.58	0.51
2:a:157:THR:C	2:a:159:GLN:H	2.18	0.51
2:a:422:ILE:HA	2:a:431:GLN:O	2.10	0.51
2:1:157:THR:C	2:1:159:GLN:H	2.19	0.51
5:4:239:VAL:C	5:4:242:VAL:HA	2.34	0.51
10:A:1352:LEU:C	10:A:1354:LEU:H	2.17	0.51
4:L:934:HIS:C	4:L:936:SER:H	2.18	0.51
2:S:157:THR:C	2:S:159:GLN:H	2.19	0.51
7:F:67:HIS:O	7:F:69:MET:N	2.43	0.51
5:M:239:VAL:C	5:M:242:VAL:HA	2.35	0.51
7:O:67:HIS:O	7:O:69:MET:N	2.43	0.51
3:K:218:LEU:C	3:K:220:ASN:H	2.17	0.51
4:U:934:HIS:C	4:U:936:SER:H	2.18	0.51
4:3:1058:ILE:O	4:3:1059:ASP:CB	2.58	0.51
2:J:157:THR:C	2:J:159:GLN:H	2.19	0.51
4:U:546:SER:O	4:U:550:ASP:CB	2.59	0.51
4:3:546:SER:O	4:3:550:ASP:CB	2.59	0.51
7:F:292:SER:C	7:F:294:ASP:N	2.69	0.51
4:L:682:ASN:CA	4:L:684:THR:HA	2.41	0.51
7:X:250:SER:O	7:X:252:THR:N	2.35	0.51
4:L:882:GLN:C	4:L:884:ARG:N	2.69	0.50
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
3:T:41:ASN:O	3:T:74:ARG:HA	2.11	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
4:C:546:SER:O	4:C:550:ASP:CB	2.59	0.50
3:K:41:ASN:O	3:K:74:ARG:HA	2.11	0.50
4:U:682:ASN:CA	4:U:684:THR:HA	2.41	0.50
10:B:859:LEU:CB	10:B:874:CYS:CA	2.86	0.50
7:X:292:SER:C	7:X:294:ASP:N	2.69	0.50
2:a:412:ASP:O	2:a:413:ALA:HB3	2.12	0.50
3:b:55:GLU:O	3:b:56:ALA:HB3	2.12	0.50
10:B:376:ARG:O	10:B:380:ALA:HA	2.11	0.49
4:C:682:ASN:CA	4:C:684:THR:HA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:55:GLU:O	3:K:56:ALA:HB3	2.12	0.49
6:W:489:GLN:C	6:W:491:VAL:H	2.20	0.49
10:B:859:LEU:O	10:B:874:CYS:CB	2.60	0.49
10:B:862:ILE:N	10:B:871:ASP:C	2.63	0.49
7:O:292:SER:C	7:O:294:ASP:N	2.69	0.49
3:T:29:ASN:HA	3:T:33:GLY:CA	2.42	0.49
3:b:41:ASN:O	3:b:74:ARG:HA	2.11	0.49
7:6:292:SER:C	7:6:294:ASP:N	2.69	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
3:b:29:ASN:HA	3:b:33:GLY:CA	2.43	0.49
4:3:1119:LEU:C	4:3:1121:GLU:N	2.71	0.49
8:G:191:PRO:C	8:G:193:ALA:H	2.14	0.49
10:B:312:MET:CB	10:B:313:SER:CA	2.91	0.49
2:1:424:PHE:HA	2:1:429:ALA:O	2.13	0.49
10:A:215:LEU:HA	10:A:230:GLY:HA2	1.94	0.49
10:A:312:MET:CB	10:A:313:SER:CA	2.91	0.49
10:B:1362:VAL:CB	2:a:1076:MET:CA	2.91	0.49
2:J:412:ASP:O	2:J:413:ALA:HB3	2.12	0.49
2:S:412:ASP:O	2:S:413:ALA:HB3	2.12	0.49
6:N:489:GLN:C	6:N:491:VAL:H	2.20	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
6:E:489:GLN:C	6:E:491:VAL:H	2.20	0.48
2:a:70:ALA:O	2:a:134:ASN:HA	2.13	0.48
3:2:29:ASN:HA	3:2:33:GLY:CA	2.42	0.48
10:B:859:LEU:CB	10:B:874:CYS:O	2.59	0.48
4:C:690:PHE:C	4:C:692:GLU:N	2.70	0.48
2:J:70:ALA:O	2:J:134:ASN:HA	2.12	0.48
8:Y:95:ASP:CB	8:Y:98:ARG:CB	2.92	0.48
4:3:882:GLN:C	4:3:884:ARG:N	2.69	0.48
2:J:424:PHE:HA	2:J:429:ALA:O	2.13	0.48
3:K:29:ASN:HA	3:K:33:GLY:CA	2.42	0.48
2:1:70:ALA:O	2:1:134:ASN:HA	2.12	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
4:3:883:SER:N	4:3:926:ALA:CA	2.75	0.48
7:6:224:ILE:C	7:6:226:LEU:N	2.72	0.48
4:L:680:PRO:O	4:L:681:SER:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:106:VAL:HA	7:O:124:SER:HA	1.95	0.48
2:a:424:PHE:HA	2:a:429:ALA:O	2.13	0.48
4:C:882:GLN:C	4:C:884:ARG:N	2.69	0.48
8:7:189:SER:CA	8:7:195:ALA:H	2.27	0.48
8:G:95:ASP:CB	8:G:98:ARG:CB	2.92	0.48
8:P:95:ASP:CB	8:P:98:ARG:CB	2.92	0.48
2:1:589:ASP:CB	2:1:590:GLU:HA	2.44	0.48
2:a:589:ASP:CB	2:a:590:GLU:HA	2.44	0.48
7:6:274:ALA:O	7:6:275:ASN:CB	2.62	0.48
6:E:305:ALA:HA	6:E:317:HIS:O	2.14	0.48
3:T:29:ASN:HA	3:T:33:GLY:N	2.29	0.48
7:6:106:VAL:HA	7:6:124:SER:HA	1.95	0.47
6:W:305:ALA:HA	6:W:317:HIS:O	2.14	0.47
10:A:1311:ASP:CB	2:S:1009:LEU:N	2.77	0.47
7:F:274:ALA:O	7:F:275:ASN:CB	2.62	0.47
7:O:224:ILE:C	7:O:226:LEU:N	2.72	0.47
8:P:189:SER:CA	8:P:195:ALA:H	2.27	0.47
7:X:274:ALA:O	7:X:275:ASN:CB	2.62	0.47
10:B:1362:VAL:O	2:a:1108:LEU:CB	2.63	0.47
4:C:680:PRO:O	4:C:681:SER:C	2.56	0.47
2:S:424:PHE:HA	2:S:429:ALA:O	2.13	0.47
9:H:123:ALA:C	9:H:125:ASP:N	2.72	0.47
6:5:305:ALA:HA	6:5:317:HIS:O	2.15	0.47
8:7:95:ASP:CB	8:7:98:ARG:CB	2.92	0.47
8:G:189:SER:CA	8:G:195:ALA:H	2.27	0.47
7:O:274:ALA:O	7:O:275:ASN:CB	2.62	0.47
2:S:610:LEU:CB	2:S:733:ASP:CB	2.93	0.47
4:U:924:GLN:HA	4:U:927:ASN:CB	2.45	0.47
7:X:106:VAL:HA	7:X:124:SER:HA	1.95	0.47
2:a:610:LEU:CB	2:a:733:ASP:CB	2.93	0.47
3:2:274:GLY:HA2	3:2:277:ALA:HB2	1.96	0.47
6:5:489:GLN:C	6:5:491:VAL:H	2.20	0.47
9:8:123:ALA:C	9:8:125:ASP:N	2.72	0.47
10:A:856:SER:O	10:A:882:GLN:CB	2.63	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
3:b:29:ASN:HA	3:b:33:GLY:N	2.29	0.47
2:J:122:ASN:C	2:J:124:LEU:H	2.22	0.47
4:U:680:PRO:O	4:U:681:SER:C	2.56	0.47
9:Z:123:ALA:C	9:Z:125:ASP:N	2.72	0.47
4:3:680:PRO:O	4:3:681:SER:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:38:ARG:HA	10:A:484:THR:CB	2.45	0.47
4:U:882:GLN:C	4:U:884:ARG:N	2.69	0.47
2:a:122:ASN:C	2:a:124:LEU:H	2.22	0.47
8:Y:190:SER:HA	8:Y:219:THR:CB	2.45	0.47
2:1:292:CYS:HA	2:1:296:ASP:N	2.30	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
8:P:190:SER:HA	8:P:219:THR:CB	2.45	0.47
10:B:858:HIS:C	10:B:872:ALA:CA	2.86	0.46
8:G:190:SER:HA	8:G:219:THR:CB	2.45	0.46
9:Q:123:ALA:C	9:Q:125:ASP:N	2.72	0.46
2:1:610:LEU:CB	2:1:733:ASP:CB	2.93	0.46
4:3:924:GLN:HA	4:3:927:ASN:CB	2.45	0.46
8:7:322:ASN:CB	9:8:20:LYS:CB	2.94	0.46
7:F:106:VAL:HA	7:F:124:SER:HA	1.95	0.46
3:K:29:ASN:HA	3:K:33:GLY:N	2.29	0.46
2:S:122:ASN:C	2:S:124:LEU:H	2.22	0.46
4:U:699:ILE:C	4:U:701:GLU:H	2.24	0.46
6:N:305:ALA:HA	6:N:317:HIS:O	2.15	0.46
4:U:690:PHE:C	4:U:692:GLU:N	2.70	0.46
8:Y:189:SER:CA	8:Y:195:ALA:H	2.27	0.46
8:Y:322:ASN:CB	9:Z:20:LYS:CB	2.94	0.46
4:3:699:ILE:C	4:3:701:GLU:H	2.24	0.46
10:A:856:SER:CB	10:A:882:GLN:O	2.63	0.46
8:G:322:ASN:CB	9:H:20:LYS:CB	2.94	0.46
2:J:292:CYS:HA	2:J:296:ASP:N	2.30	0.46
4:C:1127:GLN:C	4:C:1129:ASP:N	2.74	0.46
3:K:274:GLY:HA2	3:K:277:ALA:HB2	1.96	0.46
4:C:924:GLN:HA	4:C:927:ASN:CB	2.45	0.46
2:S:292:CYS:HA	2:S:296:ASP:N	2.30	0.46
2:1:122:ASN:C	2:1:124:LEU:H	2.23	0.46
4:C:699:ILE:C	4:C:701:GLU:H	2.24	0.46
8:P:189:SER:CA	8:P:195:ALA:N	2.79	0.46
8:P:189:SER:C	8:P:220:ASP:N	2.74	0.46
10:B:1170:SER:C	10:B:1172:GLN:H	2.24	0.46
4:L:1119:LEU:C	4:L:1121:GLU:N	2.71	0.46
8:P:322:ASN:CB	9:Q:20:LYS:CB	2.94	0.46
2:S:70:ALA:HB1	2:S:133:GLN:O	2.16	0.46
8:7:190:SER:HA	8:7:219:THR:CB	2.45	0.45
10:B:856:SER:HA	10:B:878:ASN:N	2.31	0.45
10:B:856:SER:C	10:B:873:ILE:O	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:283:ASP:C	7:F:285:LYS:H	2.24	0.45
8:G:189:SER:C	8:G:220:ASP:N	2.74	0.45
2:a:292:CYS:HA	2:a:296:ASP:N	2.30	0.45
3:2:29:ASN:HA	3:2:33:GLY:N	2.29	0.45
4:3:690:PHE:C	4:3:692:GLU:N	2.70	0.45
10:A:942:PRO:HA	10:A:943:GLN:HA	1.48	0.45
8:G:189:SER:CA	8:G:195:ALA:N	2.79	0.45
3:b:284:HIS:CB	3:b:287:HIS:CB	2.94	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
7:O:283:ASP:C	7:O:285:LYS:H	2.23	0.45
4:U:1127:GLN:C	4:U:1129:ASP:N	2.74	0.45
8:Y:189:SER:CA	8:Y:195:ALA:N	2.79	0.45
3:b:29:ASN:CA	3:b:33:GLY:HA3	2.47	0.45
2:1:147:THR:C	2:1:149:ASN:H	2.25	0.45
4:3:682:ASN:HA	4:3:684:THR:HA	1.98	0.45
8:7:189:SER:CA	8:7:195:ALA:N	2.79	0.45
10:B:852:VAL:CB	10:B:879:GLU:CA	2.95	0.45
2:J:70:ALA:HB1	2:J:133:GLN:O	2.16	0.45
8:Y:189:SER:C	8:Y:220:ASP:N	2.74	0.45
2:a:590:GLU:N	2:a:591:THR:CA	2.79	0.45
4:3:1127:GLN:C	4:3:1129:ASP:N	2.74	0.45
4:C:626:SER:O	4:C:627:PHE:C	2.60	0.45
4:C:1143:VAL:HA	4:C:1146:ALA:CB	2.41	0.45
4:L:1127:GLN:C	4:L:1129:ASP:N	2.74	0.45
7:X:224:ILE:C	7:X:226:LEU:N	2.72	0.45
7:6:283:ASP:C	7:6:285:LYS:H	2.23	0.45
8:7:189:SER:C	8:7:220:ASP:N	2.74	0.45
2:S:477:GLN:HA	2:S:481:ARG:O	2.17	0.45
2:S:590:GLU:N	2:S:591:THR:CA	2.79	0.45
3:T:29:ASN:CA	3:T:33:GLY:HA3	2.47	0.45
2:a:367:GLN:HA	2:a:390:PHE:O	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
6:E:527:VAL:O	6:E:529:GLN:HA	2.17	0.45
8:G:116:VAL:HA	8:G:134:SER:HA	1.99	0.45
2:J:367:GLN:HA	2:J:390:PHE:O	2.17	0.45
4:L:690:PHE:C	4:L:692:GLU:N	2.70	0.45
2:a:70:ALA:HB1	2:a:133:GLN:O	2.16	0.45
2:1:590:GLU:N	2:1:591:THR:CA	2.79	0.45
2:1:849:GLN:C	2:1:851:GLY:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:860:GLN:N	10:B:872:ALA:C	2.74	0.45
2:J:590:GLU:N	2:J:591:THR:CA	2.79	0.45
3:K:29:ASN:CA	3:K:33:GLY:HA3	2.47	0.45
8:P:322:ASN:H	9:Q:18:SER:CB	2.30	0.45
2:S:147:THR:C	2:S:149:ASN:H	2.25	0.45
3:T:284:HIS:CB	3:T:287:HIS:CB	2.94	0.45
4:U:1143:VAL:HA	4:U:1146:ALA:CB	2.41	0.45
8:Y:116:VAL:HA	8:Y:134:SER:HA	1.99	0.45
2:a:477:GLN:HA	2:a:481:ARG:O	2.17	0.45
6:5:487:GLY:C	6:5:489:GLN:H	2.25	0.45
4:C:1149:GLU:C	4:C:1151:TYR:H	2.25	0.45
2:J:147:THR:C	2:J:149:ASN:H	2.25	0.45
2:S:367:GLN:HA	2:S:390:PHE:O	2.17	0.45
4:U:1149:GLU:C	4:U:1151:TYR:H	2.24	0.45
4:3:619:GLY:HA2	4:3:620:LEU:CB	2.47	0.45
4:3:1143:VAL:HA	4:3:1146:ALA:CB	2.41	0.45
4:3:1149:GLU:C	4:3:1151:TYR:H	2.24	0.45
8:7:116:VAL:HA	8:7:134:SER:HA	1.99	0.45
10:A:1170:SER:C	10:A:1172:GLN:H	2.24	0.45
8:G:322:ASN:H	9:H:18:SER:CB	2.30	0.45
6:N:487:GLY:C	6:N:489:GLN:H	2.25	0.45
4:3:626:SER:O	4:3:627:PHE:C	2.60	0.44
10:A:395:GLY:N	10:A:400:SER:CB	2.80	0.44
7:F:224:ILE:C	7:F:226:LEU:N	2.72	0.44
9:H:178:ASP:C	9:H:180:LEU:H	2.25	0.44
2:J:849:GLN:C	2:J:851:GLY:H	2.25	0.44
4:U:619:GLY:HA2	4:U:620:LEU:CB	2.47	0.44
6:W:527:VAL:O	6:W:529:GLN:HA	2.17	0.44
7:X:283:ASP:C	7:X:285:LYS:H	2.24	0.44
8:Y:322:ASN:H	9:Z:18:SER:CB	2.30	0.44
9:Z:178:ASP:C	9:Z:180:LEU:H	2.25	0.44
2:a:147:THR:C	2:a:149:ASN:H	2.25	0.44
4:C:619:GLY:HA2	4:C:620:LEU:CB	2.47	0.44
9:Q:244:SER:CA	9:Q:255:GLU:N	2.81	0.44
9:Q:335:PHE:C	9:Q:338:GLY:HA2	2.43	0.44
4:3:883:SER:CB	4:3:929:LEU:CB	2.95	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
9:H:335:PHE:C	9:H:338:GLY:HA2	2.43	0.44
4:L:682:ASN:HA	4:L:684:THR:HA	1.98	0.44
4:L:699:ILE:C	4:L:701:GLU:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:178:ASP:C	9:Q:180:LEU:H	2.25	0.44
4:U:682:ASN:HA	4:U:684:THR:HA	1.98	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
4:U:626:SER:O	4:U:627:PHE:C	2.60	0.44
3:b:230:ASN:CB	3:b:254:ALA:C	2.91	0.44
2:1:246:TYR:C	2:1:249:PRO:N	2.76	0.44
7:6:43:ARG:O	7:6:44:ASN:CB	2.66	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
9:Z:335:PHE:C	9:Z:338:GLY:HA2	2.43	0.44
2:1:167:PRO:C	2:1:169:PRO:N	2.76	0.44
2:1:477:GLN:HA	2:1:481:ARG:O	2.17	0.44
6:5:527:VAL:O	6:5:529:GLN:HA	2.17	0.44
9:8:335:PHE:C	9:8:338:GLY:HA2	2.43	0.44
4:C:615:ILE:O	4:C:620:LEU:CB	2.66	0.44
9:H:244:SER:CA	9:H:255:GLU:N	2.81	0.44
4:L:1149:GLU:C	4:L:1151:TYR:H	2.24	0.44
4:U:615:ILE:O	4:U:620:LEU:CB	2.66	0.44
3:2:29:ASN:CA	3:2:33:GLY:HA3	2.47	0.44
10:B:856:SER:O	10:B:874:CYS:N	2.49	0.44
3:T:230:ASN:CB	3:T:254:ALA:C	2.91	0.44
6:5:575:ASN:C	6:5:607:PRO:N	2.76	0.44
7:F:43:ARG:O	7:F:44:ASN:CB	2.66	0.44
4:L:626:SER:O	4:L:627:PHE:C	2.60	0.44
2:S:849:GLN:C	2:S:851:GLY:H	2.25	0.44
4:3:615:ILE:O	4:3:620:LEU:CB	2.66	0.43
9:8:244:SER:CA	9:8:255:GLU:N	2.81	0.43
2:J:167:PRO:C	2:J:169:PRO:N	2.76	0.43
7:X:43:ARG:O	7:X:44:ASN:CB	2.66	0.43
2:a:246:TYR:C	2:a:249:PRO:N	2.76	0.43
10:B:857:LEU:HA	10:B:873:ILE:HA	1.99	0.43
5:D:558:ARG:HA	5:D:561:GLY:O	2.18	0.43
4:L:619:GLY:HA2	4:L:620:LEU:CB	2.47	0.43
6:N:575:ASN:C	6:N:607:PRO:N	2.76	0.43
2:S:167:PRO:C	2:S:169:PRO:N	2.76	0.43
5:V:558:ARG:HA	5:V:561:GLY:O	2.18	0.43
9:H:367:ALA:C	9:H:370:ASN:N	2.77	0.43
2:a:167:PRO:C	2:a:169:PRO:N	2.76	0.43
2:a:849:GLN:C	2:a:851:GLY:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:193:ALA:O	8:7:194:MET:CB	2.66	0.43
2:J:246:TYR:C	2:J:249:PRO:N	2.76	0.43
9:Z:367:ALA:C	9:Z:370:ASN:N	2.77	0.43
10:B:859:LEU:CA	10:B:874:CYS:CB	2.96	0.43
6:E:487:GLY:C	6:E:489:GLN:H	2.25	0.43
4:L:615:ILE:O	4:L:620:LEU:CB	2.66	0.43
6:N:527:VAL:O	6:N:529:GLN:HA	2.17	0.43
2:S:246:TYR:C	2:S:249:PRO:N	2.76	0.43
3:2:230:ASN:CB	3:2:254:ALA:C	2.91	0.43
5:4:558:ARG:HA	5:4:561:GLY:O	2.18	0.43
9:8:178:ASP:C	9:8:180:LEU:H	2.25	0.43
9:8:367:ALA:C	9:8:370:ASN:N	2.77	0.43
10:B:863:CYS:H	10:B:871:ASP:CA	2.29	0.43
3:K:230:ASN:CB	3:K:254:ALA:C	2.91	0.43
4:U:536:HIS:O	4:U:537:ALA:C	2.62	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
2:a:220:TRP:C	2:a:225:GLY:CA	2.92	0.43
4:C:536:HIS:O	4:C:537:ALA:C	2.62	0.43
4:C:1119:LEU:C	4:C:1121:GLU:N	2.71	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
4:U:1069:LEU:C	4:U:1071:LEU:N	2.76	0.43
6:W:575:ASN:C	6:W:607:PRO:N	2.76	0.43
7:X:89:GLU:O	7:X:90:ASN:CB	2.66	0.43
7:X:289:TRP:HA	7:X:298:VAL:O	2.19	0.43
3:b:274:GLY:HA2	3:b:277:ALA:HB2	1.96	0.43
10:B:958:ASP:C	10:B:960:VAL:CA	2.92	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
6:W:487:GLY:C	6:W:489:GLN:H	2.25	0.43
9:Z:244:SER:CA	9:Z:255:GLU:N	2.81	0.43
7:F:289:TRP:HA	7:F: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
8:G:220:ASP:CB	8:G:243:LYS:CB	2.97	0.43
2:J:220:TRP:C	2:J:225:GLY:CA	2.92	0.43
2:J:413:ALA:O	2:J:415:ASN:HA	2.19	0.43
4:U:933:GLU:O	4:U:935:LEU:N	2.44	0.43
7:6:289:TRP:HA	7:6:298:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1355:ASP:CB	10:B:1358:CYS:CB	2.96	0.42
7:X:183:ALA:O	7:X:184:SER:CB	2.67	0.42
8:Y:220:ASP:CB	8:Y:243:LYS:CB	2.97	0.42
4:C:1021:SER:C	4:C:1023:MET:H	2.27	0.42
7:F:89:GLU:O	7:F:90:ASN:CB	2.67	0.42
9:Q:367:ALA:C	9:Q:370:ASN:N	2.77	0.42
8:Y:190:SER:N	8:Y:220:ASP:CA	2.82	0.42
2:1:413:ALA:O	2:1:415:ASN:HA	2.19	0.42
4:3:536:HIS:O	4:3:537:ALA:C	2.62	0.42
8:P:116:VAL:HA	8:P:134:SER:HA	1.99	0.42
8:Y:193:ALA:O	8:Y:194:MET:CB	2.67	0.42
2:a:292:CYS:CA	2:a:296:ASP:N	2.83	0.42
2:a:413:ALA:O	2:a:415:ASN:HA	2.19	0.42
7:6:89:GLU:O	7:6:90:ASN:CB	2.66	0.42
10:A:205:LEU:C	10:A:207:SER:CA	2.93	0.42
6:E:575:ASN:C	6:E:607:PRO:N	2.77	0.42
4:L:1119:LEU:O	4:L:1121:GLU:N	2.52	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
10:A:958:ASP:C	10:A:960:VAL:CA	2.92	0.42
10:B:942:PRO:HA	10:B:943:GLN:HA	1.48	0.42
8:G:189:SER:N	8:G:195:ALA:HB3	2.33	0.42
9:H:274:PHE:O	9:H:275:ALA:HB2	2.18	0.42
1:0:121:HIS:N	1:0:130:SER:O	2.51	0.42
2:1:292:CYS:CA	2:1:296:ASP:N	2.83	0.42
6:5:620:SER:C	6:5:622:ARG:H	2.28	0.42
7:F:195:LYS:O	7:F:202:TRP:HA	2.20	0.42
7:O:89:GLU:O	7:O:90:ASN:CB	2.66	0.42
8:P:189:SER:N	8:P:195:ALA:HB3	2.33	0.42
8:P:190:SER:N	8:P:194:MET:CB	2.83	0.42
7:X:195:LYS:O	7:X:202:TRP:HA	2.20	0.42
8:Y:190:SER:N	8:Y:194:MET:CB	2.83	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
3:K:274:GLY:CA	3:K:277:ALA:HB3	2.46	0.42
9:Q:274:PHE:O	9:Q:275:ALA:HB2	2.18	0.42
5:V:152:MET:C	5:V:154:MET:H	2.28	0.42
2:1:413:ALA:C	2:1:415:ASN:CA	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:183:ALA:O	7:F:184:SER:CB	2.67	0.42
1:R:106:ASN:O	1:R:107:GLN:C	2.63	0.42
5:4:191:ILE:CA	5:4:201:LYS:N	2.82	0.42
7:6:183:ALA:O	7:6:184:SER:CB	2.67	0.42
8:7:189:SER:N	8:7:195:ALA:HB3	2.33	0.42
10:A:584:PHE:C	10:A:586:THR:CA	2.93	0.42
4:C:933:GLU:O	4:C:935:LEU:N	2.44	0.42
8:G:190:SER:N	8:G:194:MET:CB	2.83	0.42
2:S:156:LEU:HA	2:S:160:THR:O	2.20	0.42
2:S:292:CYS:CA	2:S:296:ASP:N	2.83	0.42
6:W:620:SER:C	6:W:622:ARG:H	2.28	0.42
5:4:152:MET:C	5:4:154:MET:H	2.28	0.42
8:7:190:SER:N	8:7:220:ASP:CA	2.82	0.42
10:A:68:GLN:C	10:A:74:SER:CB	2.93	0.42
10:B:856:SER:O	10:B:872:ALA:O	2.38	0.42
10:B:1029:ARG:C	10:B:1034:LEU:N	2.78	0.42
5:D:152:MET:C	5:D:154:MET:H	2.28	0.42
4:L:531:ARG:O	4:L:535:GLY:O	2.38	0.42
9:Q:319:VAL:C	9:Q:322:ILE:N	2.78	0.42
2:S:75:GLY:C	2:S:78:LYS:H	2.28	0.42
1:0:121:HIS:CB	1:0:130:SER:CB	2.98	0.41
4:3:1119:LEU:O	4:3:1121:GLU:N	2.52	0.41
4:C:1124:ASP:O	4:C:1125:LEU:C	2.63	0.41
8:G:188:ASP:CA	8:G:195:ALA:HB3	2.50	0.41
2:a:156:LEU:HA	2:a:160:THR:O	2.20	0.41
1:0:106:ASN:O	1:0:107:GLN:C	2.63	0.41
4:3:1069:LEU:C	4:3:1071:LEU:N	2.76	0.41
10:B:584:PHE:C	10:B:586:THR:CA	2.93	0.41
8:G:190:SER:N	8:G:220:ASP:CA	2.82	0.41
2:J:292:CYS:CA	2:J:296:ASP:N	2.83	0.41
4:L:1124:ASP:O	4:L:1125:LEU:C	2.63	0.41
4:L:1143:VAL:HA	4:L:1146:ALA:CB	2.41	0.41
8:P:188:ASP:CA	8:P:195:ALA:HB3	2.50	0.41
1:R:121:HIS:CB	1:R:130:SER:CB	2.98	0.41
3:T:274:GLY:HA2	3:T:277:ALA:HB2	1.96	0.41
4:U:531:ARG:O	4:U:535:GLY:O	2.38	0.41
2:a:413:ALA:C	2:a:415:ASN:CA	2.93	0.41
2:1:75:GLY:C	2:1:78:LYS:H	2.28	0.41
4:3:881:ASN:CB	4:3:922:HIS:O	2.68	0.41
10:A:1029:ARG:C	10:A:1034:LEU:N	2.78	0.41
10:A:1309:SER:CA	2:S:1040:VAL:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:HIS:CB	1:I:130:SER:CB	2.98	0.41
2:J:755:LEU:C	2:J:762:LEU:N	2.79	0.41
5:M:152:MET:C	5:M:154:MET:H	2.28	0.41
5:M:282:GLY:CA	5:M:288:ILE:N	2.83	0.41
8:P:191:PRO:C	8:P:193:ALA:N	2.76	0.41
4:U:1119:LEU:C	4:U:1121:GLU:N	2.71	0.41
2:a:75:GLY:C	2:a:78:LYS:H	2.28	0.41
5:4:822:LEU:O	5:4:823:PHE:C	2.64	0.41
8:7:190:SER:N	8:7:194:MET:CB	2.83	0.41
10:B:842:ILE:CB	10:B:882:GLN:CB	2.92	0.41
10:B:859:LEU:C	10:B:874:CYS:CA	2.78	0.41
4:C:1069:LEU:C	4:C:1071:LEU:N	2.76	0.41
6:E:620:SER:C	6:E:622:ARG:H	2.27	0.41
7:F:283:ASP:C	7:F:285:LYS:N	2.79	0.41
1:I:106:ASN:O	1:I:107:GLN:C	2.63	0.41
2:J:413:ALA:C	2:J:415:ASN:CA	2.93	0.41
7:O:183:ALA:O	7:O:184:SER:CB	2.67	0.41
8:P:191:PRO:O	8:P:192:ASN:CB	2.69	0.41
8:P:320:LYS:O	9:Q:13:ILE:CB	2.69	0.41
2:S:349:SER:HA	2:S:401:LEU:O	2.20	0.41
7:X:283:ASP:C	7:X:285:LYS:N	2.79	0.41
9:8:274:PHE:O	9:8:275:ALA:HB2	2.18	0.41
9:8:319:VAL:C	9:8:322:ILE:N	2.78	0.41
1:9:106:ASN:O	1:9:107:GLN:C	2.63	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:L:1021:SER:C	4:L:1023:MET:H	2.27	0.41
6:N:620:SER:C	6:N:622:ARG:H	2.28	0.41
2:S:755:LEU:C	2:S:762:LEU:N	2.79	0.41
5:V:191:ILE:CA	5:V:201:LYS:N	2.82	0.41
9:Z:319:VAL:C	9:Z:322:ILE:N	2.78	0.41
4:3:531:ARG:O	4:3:535:GLY:O	2.38	0.41
4:3:933:GLU:O	4:3:935:LEU:N	2.44	0.41
10:B:68:GLN:C	10:B:74:SER:CB	2.93	0.41
1:I:121:HIS:N	1:I:130:SER:O	2.51	0.41
2:S:511:THR:HA	2:S:512:GLU:HA	1.86	0.41
4:U:1021:SER:C	4:U:1023:MET:H	2.27	0.41
8:Y:189:SER:C	8:Y:220:ASP:H	2.29	0.41
2:1:156:LEU:HA	2:1:160:THR:O	2.20	0.41
2:1:755:LEU:C	2:1:762:LEU:N	2.79	0.41
8:7:189:SER:C	8:7:220:ASP:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:A:221:THR:C	10:A:223:ASN:H	2.28	0.41
5:D:282:GLY:CA	5:D:288:ILE:N	2.82	0.41
5:D:822:LEU:O	5:D:823:PHE:C	2.64	0.41
9:H:319:VAL:C	9:H:322:ILE:N	2.78	0.41
4:L:1069:LEU:C	4:L:1071:LEU:N	2.76	0.41
5:V:822:LEU:O	5:V:823:PHE:C	2.64	0.41
8:Y:320:LYS:O	9:Z:13:ILE:CB	2.68	0.41
2:a:394:GLU:CB	2:a:410:TRP:CB	2.99	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
5:4:282:GLY:CA	5:4:288:ILE:N	2.82	0.41
8:G:189:SER:C	8:G:220:ASP:H	2.29	0.41
8:G:320:LYS:O	9:H:13:ILE:CB	2.69	0.41
4:L:536:HIS:O	4:L:537:ALA:C	2.62	0.41
8:P:189:SER:C	8:P:220:ASP:H	2.29	0.41
2:S:413:ALA:C	2:S:415:ASN:CA	2.93	0.41
8:Y:188:ASP:CA	8:Y:195:ALA:HB3	2.50	0.41
3:2:135:LYS:C	3:2:137:GLY:H	2.29	0.41
4:3:934:HIS:C	4:3:936:SER:N	2.78	0.41
4:3:1124:ASP:O	4:3:1125:LEU:C	2.63	0.41
9:8:335:PHE:C	9:8:338:GLY:CA	2.94	0.41
10:A:230:GLY:C	10:A:232:ASP:H	2.29	0.41
10:A:1311:ASP:H	2:S:1009:LEU:CB	2.33	0.41
10:A:1352:LEU:CB	2:S:1029:ARG:O	2.69	0.41
10:B:221:THR:C	10:B:223:ASN:H	2.28	0.41
10:B:326:ALA:CB	10:B:387:LEU:CB	2.95	0.41
4:C:896:ASN:O	4:C:900:PHE:N	2.52	0.41
5:D:191:ILE:CA	5:D:201:LYS:N	2.82	0.41
5:M:822:LEU:O	5:M:823:PHE:C	2.64	0.41
6:N:527:VAL:C	6:N:529:GLN:CA	2.94	0.41
4:U:693:VAL:C	4:U:695:GLN:N	2.79	0.41
4:U:896:ASN:O	4:U:900:PHE:N	2.52	0.41
9:Z:335:PHE:C	9:Z:338:GLY:CA	2.94	0.41
2:a:98:THR:HA	2:a:99:ARG:HA	1.51	0.41
3:b:10:ALA:HB1	3:b:321:PHE:O	2.21	0.41
10:A:1352:LEU:C	10:A:1354:LEU:N	2.79	0.41
10:B:350:ASN:HA	10:B:353:SER:O	2.21	0.41
2:S:590:GLU:CB	2:S:591:THR:C	2.94	0.41
2:a:755:LEU:C	2:a:762:LEU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:349:SER:HA	2:1:401:LEU:O	2.20	0.40
2:1:1013:HIS:O	2:1:1014:ASN:C	2.63	0.40
8:7:320:LYS:O	9:8:13:ILE:CB	2.69	0.40
10:B:230:GLY:C	10:B:232:ASP:H	2.29	0.40
3:T:10:ALA:HB1	3:T:321:PHE:O	2.21	0.40
3:2:10:ALA:HB1	3:2:321:PHE:O	2.21	0.40
4:3:1021:SER:C	4:3:1023:MET:H	2.27	0.40
8:7:191:PRO:C	8:7:193:ALA:N	2.76	0.40
3:T:135:LYS:C	3:T:137:GLY:H	2.28	0.40
10:B:376:ARG:C	10:B:380:ALA:CA	2.94	0.40
9:H:335:PHE:C	9:H:338:GLY:CA	2.94	0.40
4:L:934:HIS:C	4:L:936:SER:N	2.78	0.40
9:Q:335:PHE:C	9:Q:338:GLY:CA	2.94	0.40
6:W:527:VAL:C	6:W:529:GLN:CA	2.94	0.40
2:a:349:SER:HA	2:a:401:LEU:O	2.20	0.40
8:7:188:ASP:CA	8:7:195:ALA:HB3	2.51	0.40
10:B:340:LYS:C	10:B:342:ILE:N	2.80	0.40
2:J:590:GLU:CB	2:J:591:THR:C	2.95	0.40
3:K:135:LYS:C	3:K:137:GLY:H	2.29	0.40
2:a:395:THR:O	2:a:410:TRP:HA	2.22	0.40
2:1:331:LYS:O	2:1:341:GLY:HA2	2.22	0.40
2:1:599:ILE:C	2:1:601:ARG:N	2.80	0.40
10:A:326:ALA:CB	10:A:387:LEU:CB	2.95	0.40
10:A:340:LYS:C	10:A:342:ILE:N	2.80	0.40
10:B:861:ASP:N	10:B:872:ALA:C	2.34	0.40
3:K:10:ALA:HB1	3:K:321:PHE:O	2.21	0.40
4:L:1002:LEU:O	4:L:1004:HIS:N	2.55	0.40
4:U:934:HIS:C	4:U:936:SER:N	2.78	0.40
2:a:590:GLU:CB	2:a:591:THR:C	2.95	0.40
2:a:599:ILE:C	2:a:601:ARG:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	4	27
2	J	957/1436 (67%)	873 (91%)	62 (6%)	22 (2%)	5	28
2	S	957/1436 (67%)	873 (91%)	62 (6%)	22 (2%)	5	28
2	a	957/1436 (67%)	873 (91%)	62 (6%)	22 (2%)	5	28
3	2	316/326 (97%)	280 (89%)	15 (5%)	21 (7%)	1	12
3	K	316/326 (97%)	279 (88%)	16 (5%)	21 (7%)	1	12
3	T	316/326 (97%)	280 (89%)	15 (5%)	21 (7%)	1	12
3	b	316/326 (97%)	279 (88%)	16 (5%)	21 (7%)	1	12
4	3	508/1156 (44%)	437 (86%)	55 (11%)	16 (3%)	3	22
4	C	508/1156 (44%)	437 (86%)	56 (11%)	15 (3%)	3	23
4	L	508/1156 (44%)	437 (86%)	56 (11%)	15 (3%)	3	23
4	U	508/1156 (44%)	437 (86%)	56 (11%)	15 (3%)	3	23
5	4	636/925 (69%)	607 (95%)	25 (4%)	4 (1%)	21	59
5	D	640/925 (69%)	607 (95%)	28 (4%)	5 (1%)	16	54
5	M	636/925 (69%)	608 (96%)	24 (4%)	4 (1%)	21	59
5	V	640/925 (69%)	607 (95%)	27 (4%)	6 (1%)	14	51
6	5	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	4	24
6	E	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	4	24
6	N	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	4	24
6	W	393/937 (42%)	363 (92%)	19 (5%)	11 (3%)	4	24
7	6	281/322 (87%)	235 (84%)	38 (14%)	8 (3%)	4	24
7	F	281/322 (87%)	231 (82%)	42 (15%)	8 (3%)	4	24
7	O	281/322 (87%)	235 (84%)	38 (14%)	8 (3%)	4	24
7	X	281/322 (87%)	230 (82%)	43 (15%)	8 (3%)	4	24
8	7	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	3	21
8	G	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	P	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	3	21
8	Y	320/360 (89%)	288 (90%)	21 (7%)	11 (3%)	3	21
9	8	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	4	25
9	H	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	4	25
9	Q	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	4	25
9	Z	418/656 (64%)	379 (91%)	28 (7%)	11 (3%)	4	25
10	A	1043/1391 (75%)	961 (92%)	58 (6%)	24 (2%)	5	28
10	B	1043/1391 (75%)	961 (92%)	58 (6%)	24 (2%)	5	28
All	All	18636/28774 (65%)	16944 (91%)	1227 (7%)	465 (2%)	6	26

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	J	1
2	a	1
2	S	1
9	8	1
9	H	1
9	Q	1
9	Z	1

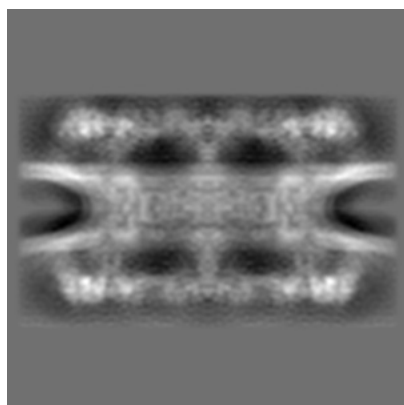
All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	1013:HIS	C	1014:ASN	N	6.20
1	a	1013:HIS	C	1014:ASN	N	6.01
1	S	1013:HIS	C	1014:ASN	N	4.29
1	8	64:TYR	C	65:SER	N	1.89
1	H	64:TYR	C	65:SER	N	1.89
1	Q	64:TYR	C	65:SER	N	1.89
1	Z	64:TYR	C	65:SER	N	1.89

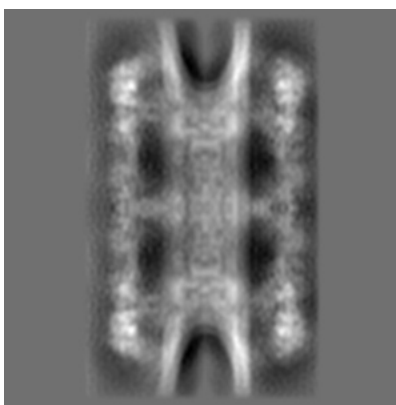
6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3103. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

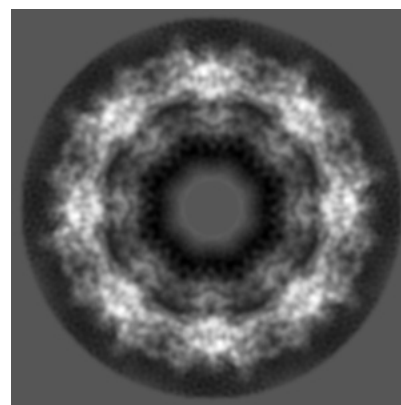
6.1 Orthogonal projections [i](#)



X



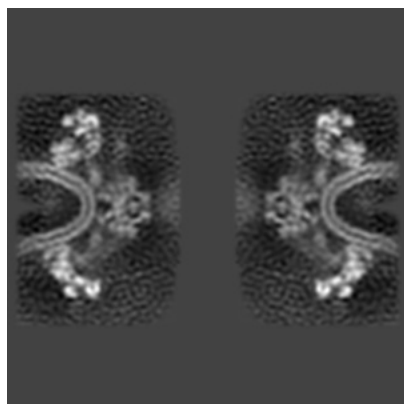
Y



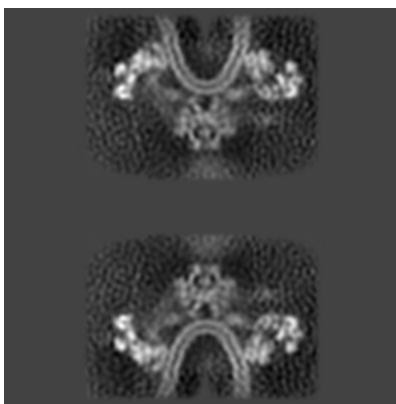
Z

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

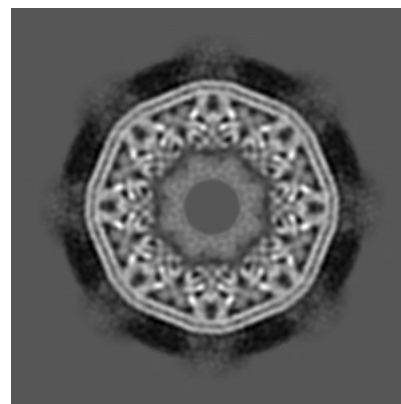
6.2 Central slices [i](#)



X Index: 104



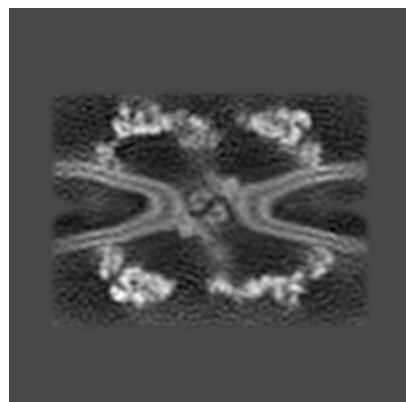
Y Index: 104



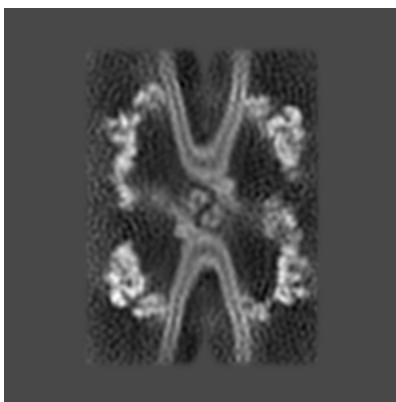
Z Index: 104

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

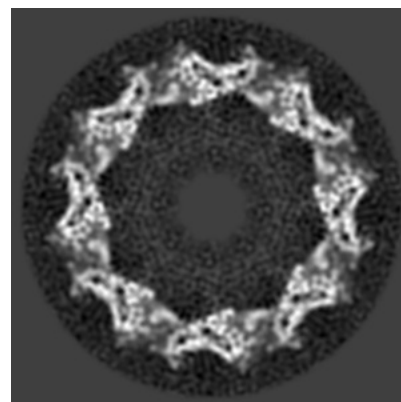
6.3 Largest variance slices [i](#)



X Index: 160



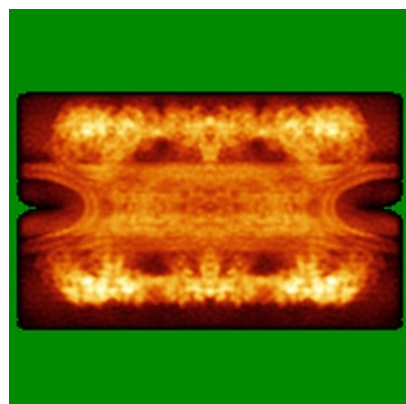
Y Index: 48



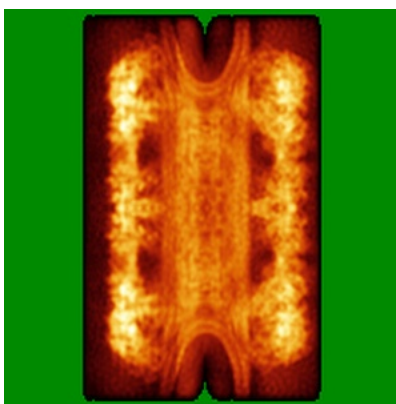
Z Index: 62

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

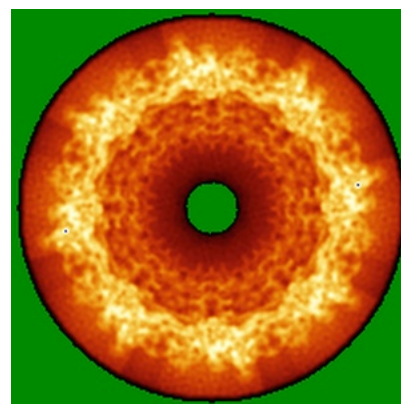
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

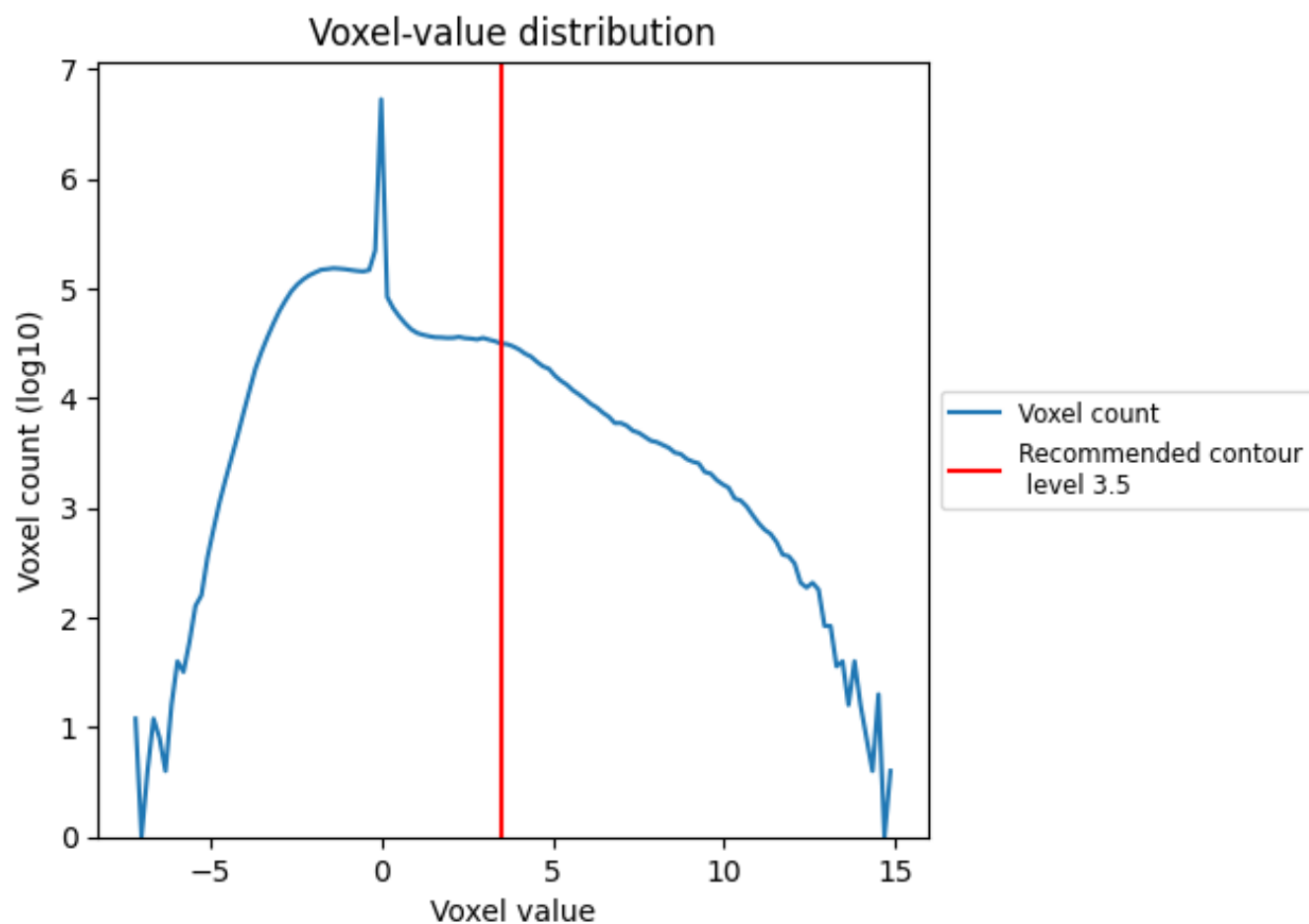
6.5 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

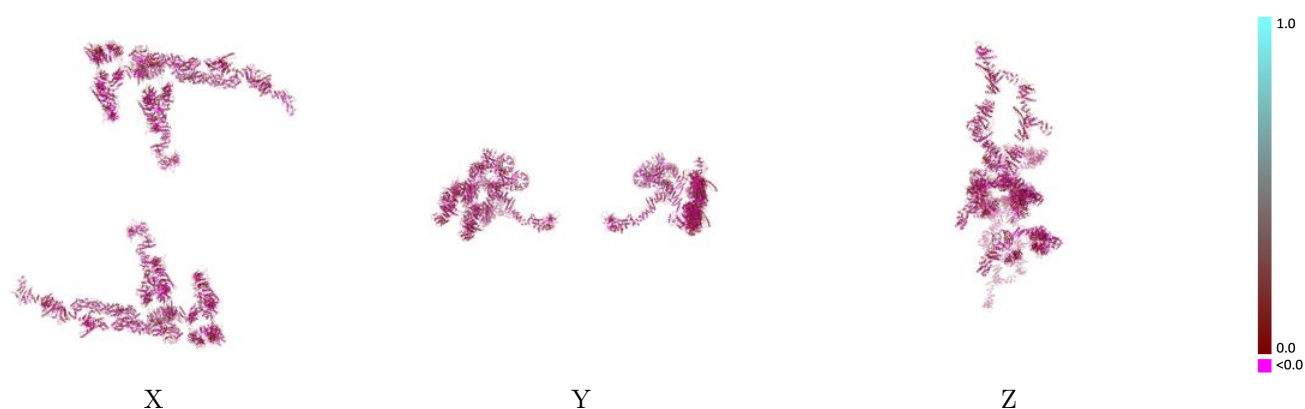
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3103 and PDB model 5A9Q. Per-residue inclusion information can be found in section 3 on page 8.

8.1 Map-model overlay [i](#)

This section was not generated.

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

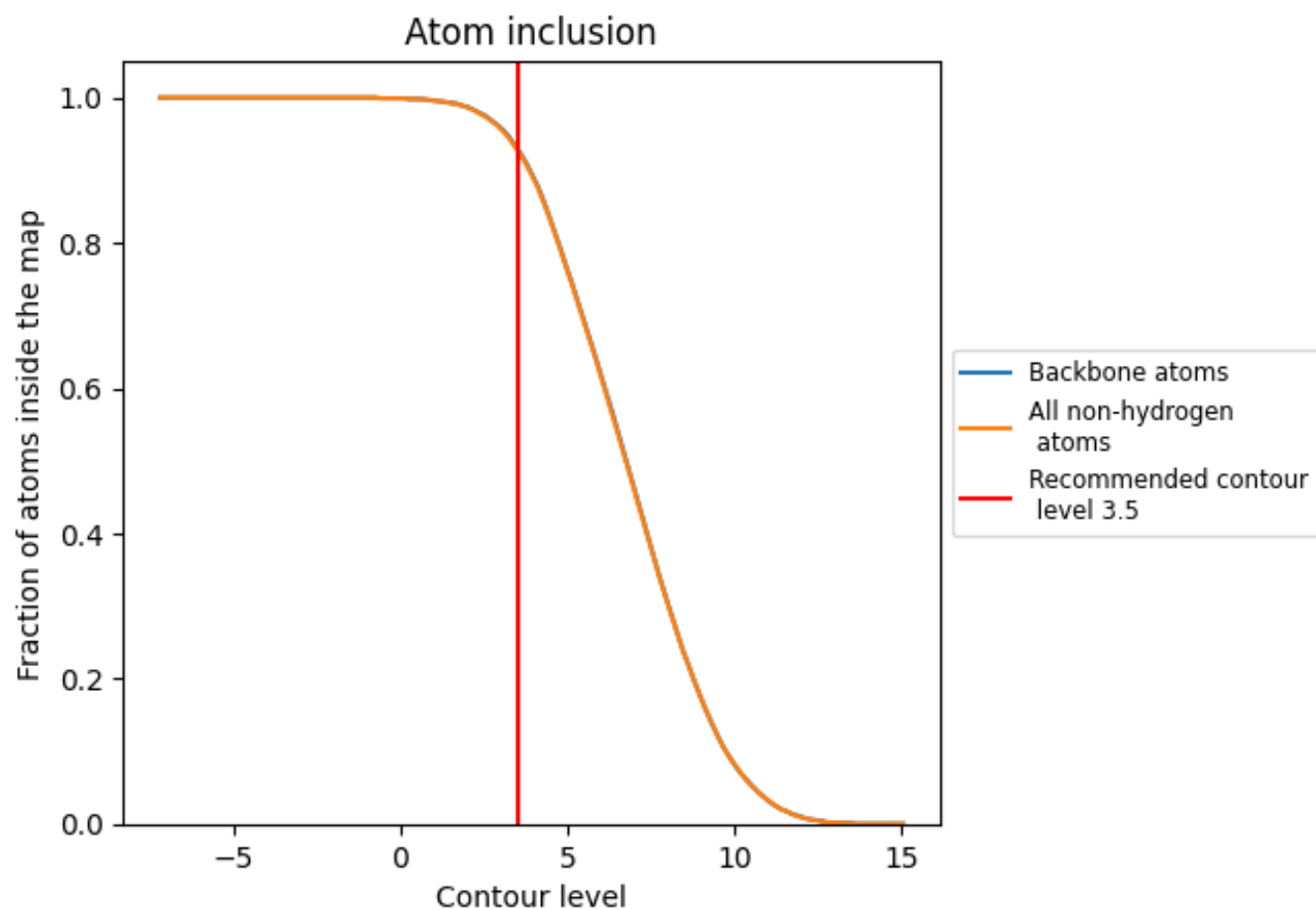


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9270	 0.0480
0	 0.9760	 0.0520
1	 0.8030	 0.0300
2	 0.8370	 0.0400
3	 0.8630	 0.0450
4	 0.9590	 0.0580
5	 0.9750	 0.0620
6	 0.9790	 0.0350
7	 0.9740	 0.0520
8	 0.9830	 0.0530
9	 0.9060	 0.0410
A	 0.8030	 0.0510
B	 0.8730	 0.0490
C	 0.8190	 0.0530
D	 0.9520	 0.0540
E	 0.9840	 0.0500
F	 0.9640	 0.0500
G	 0.9840	 0.0520
H	 0.9770	 0.0380
I	 0.9850	 0.0430
J	 0.9470	 0.0400
K	 0.9860	 0.0310
L	 0.9740	 0.0590
M	 0.9840	 0.0630
N	 0.9830	 0.0520
O	 0.9810	 0.0260
P	 0.9660	 0.0570
Q	 0.9920	 0.0490
R	 0.9930	 0.0490
S	 0.9500	 0.0410
T	 0.9720	 0.0500
U	 0.7690	 0.0600
V	 0.9260	 0.0510
W	 0.9930	 0.0550
X	 0.9230	 0.0440



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Chain	Atom inclusion	Q-score
Y	 0.9550	 0.0430
Z	 0.9760	 0.0550
a	 0.9450	 0.0430
b	 0.9270	 0.0400