



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 09:58 PM EDT

PDB ID : 8QOX / pdb\_00008qox  
EMDB ID : EMD-18127  
Title : Two-component assembly of SlaA and SlaB S-layer proteins of *Sulfolobus acidocaldarius*  
Authors : Gambelli, L.; McLaren, M.; Isupov, M.; Conners, R.; Daum, B.  
Deposited on : 2023-09-29  
Resolution : 11.20 Å (reported)  
Based on initial models : 7ZCX, .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

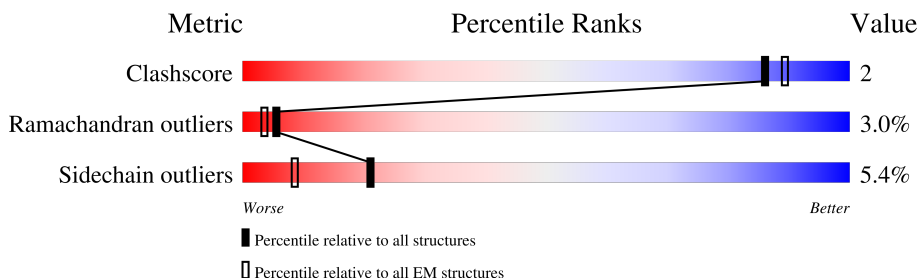
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 11.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	A	1424	
1	V	1424	
1	W	1424	
1	Z	1424	
2	B	475	
2	C	475	
2	X	475	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 51848 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 S-layer protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	V	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	W	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	Z	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		

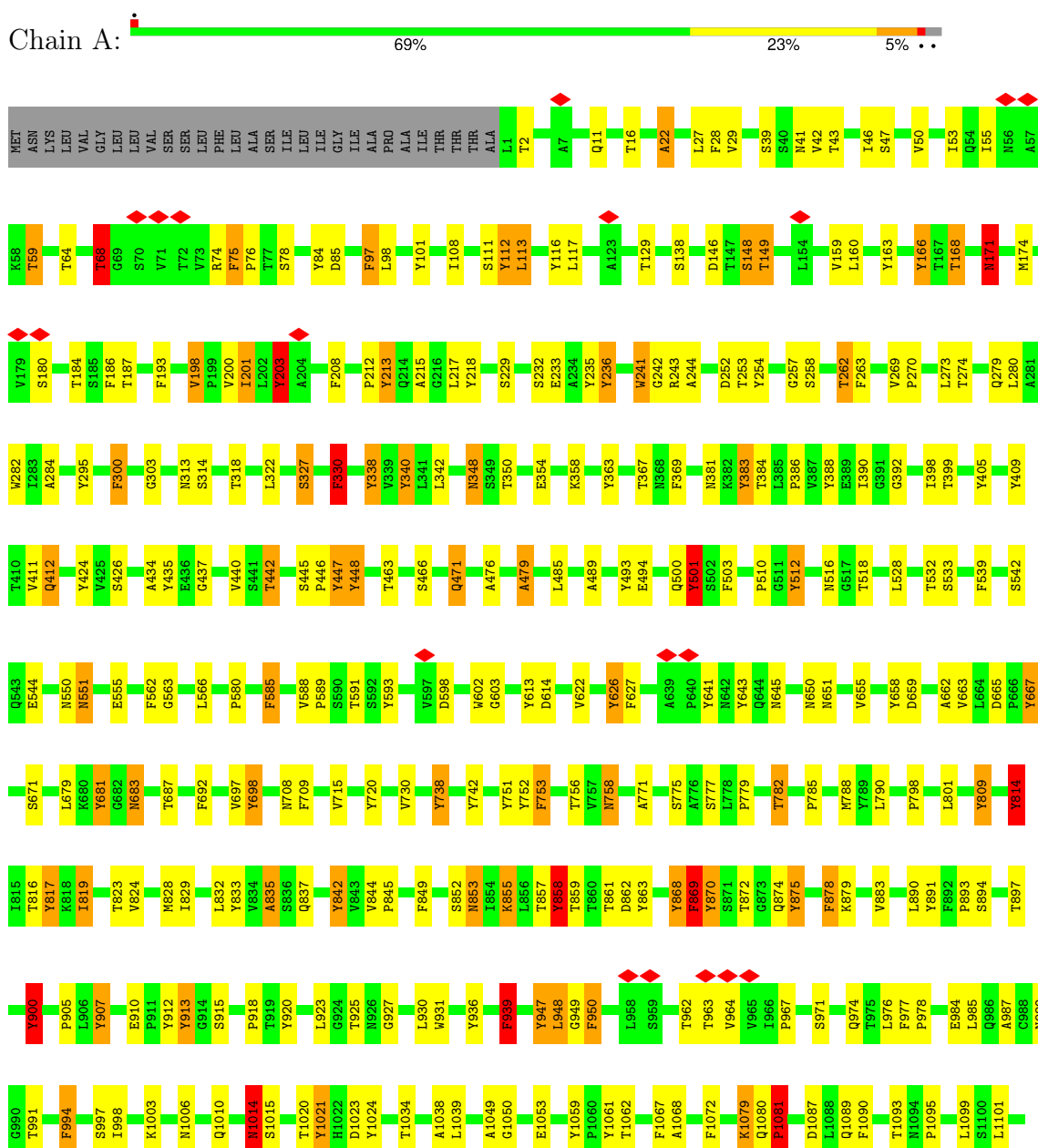
- Molecule 2 is a protein called Conserved membrane protein.

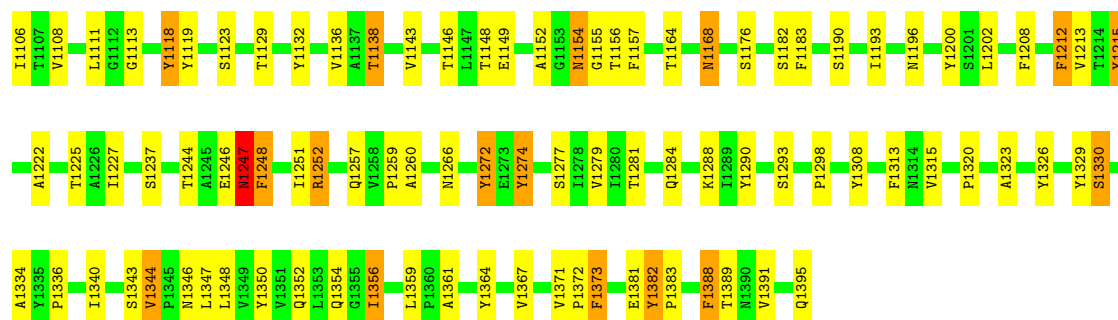
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		
2	C	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		
2	X	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		

### 3 Residue-property plots

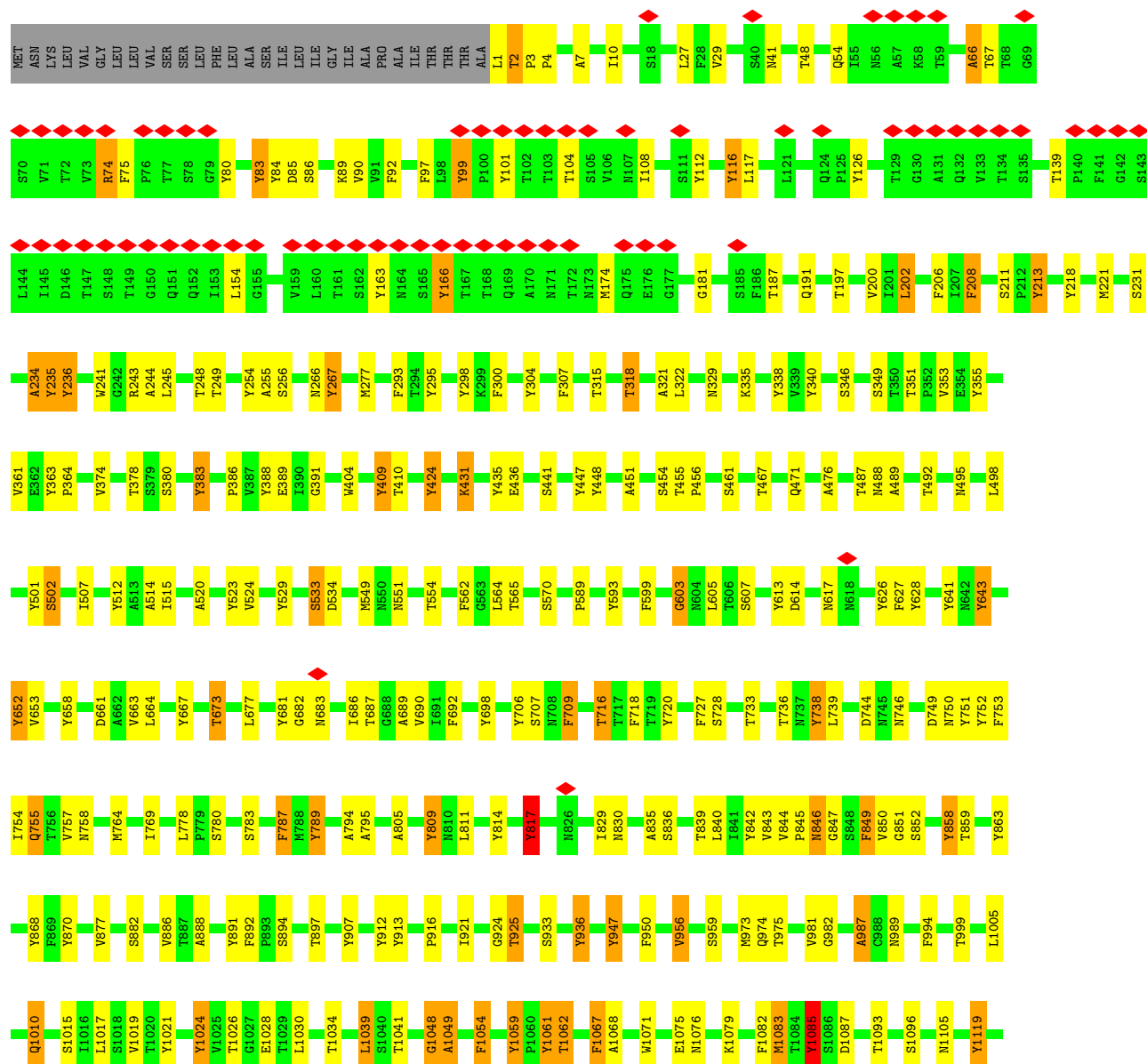
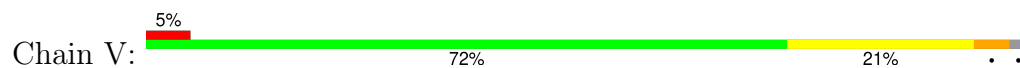
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

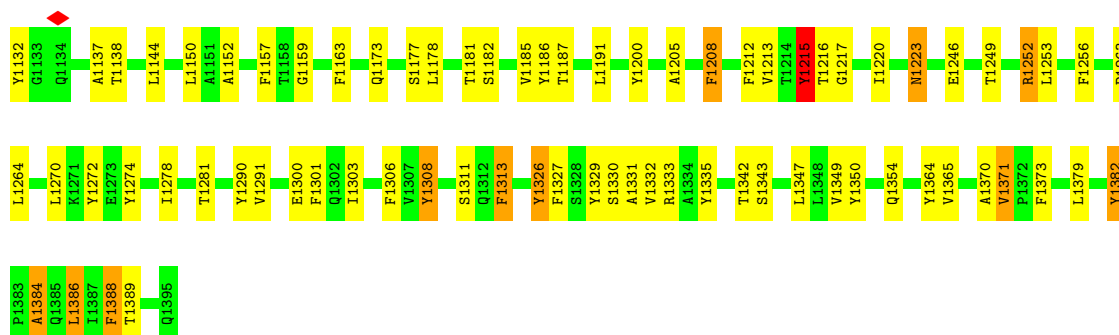
#### • Molecule 1: S-layer protein A



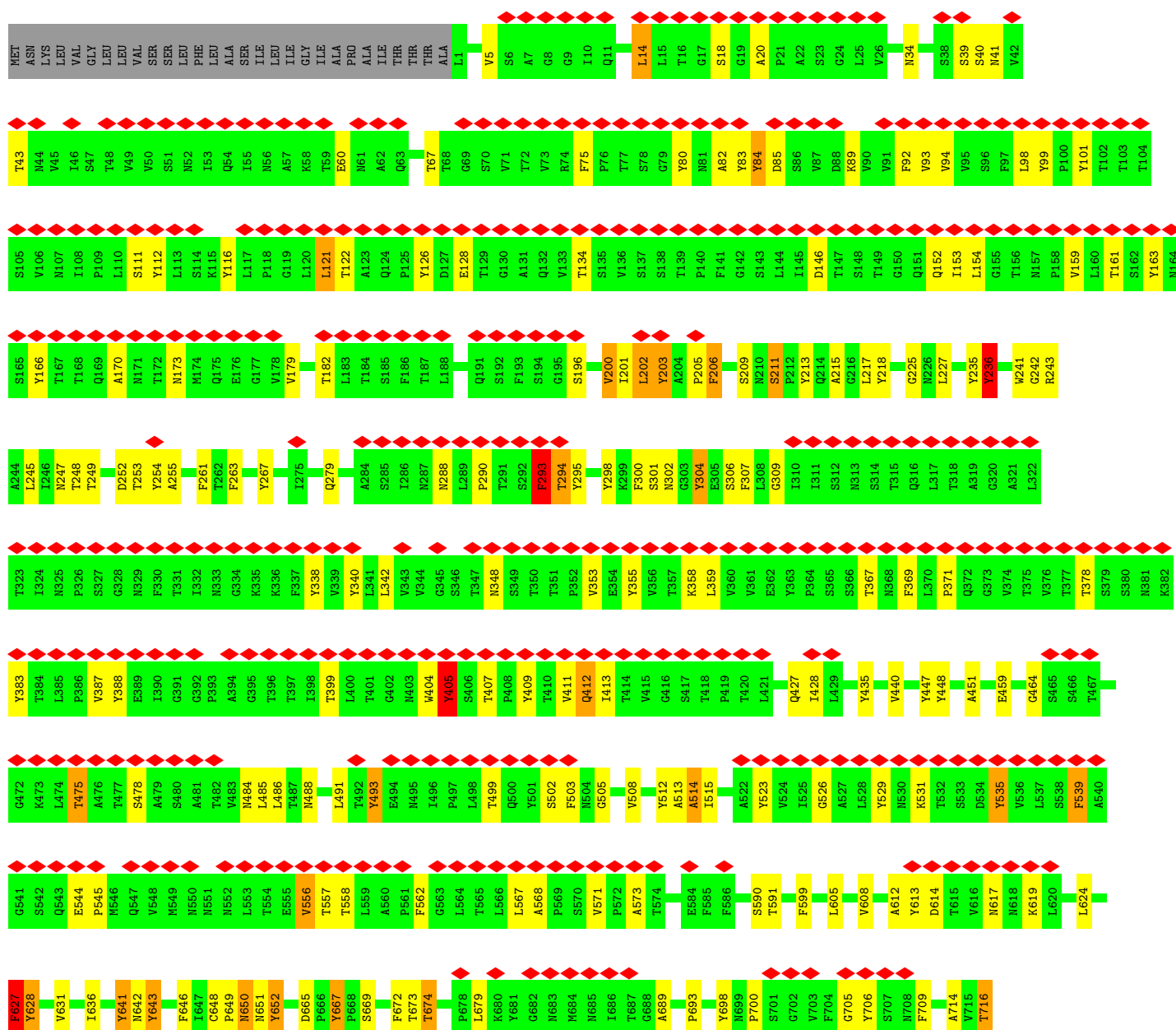


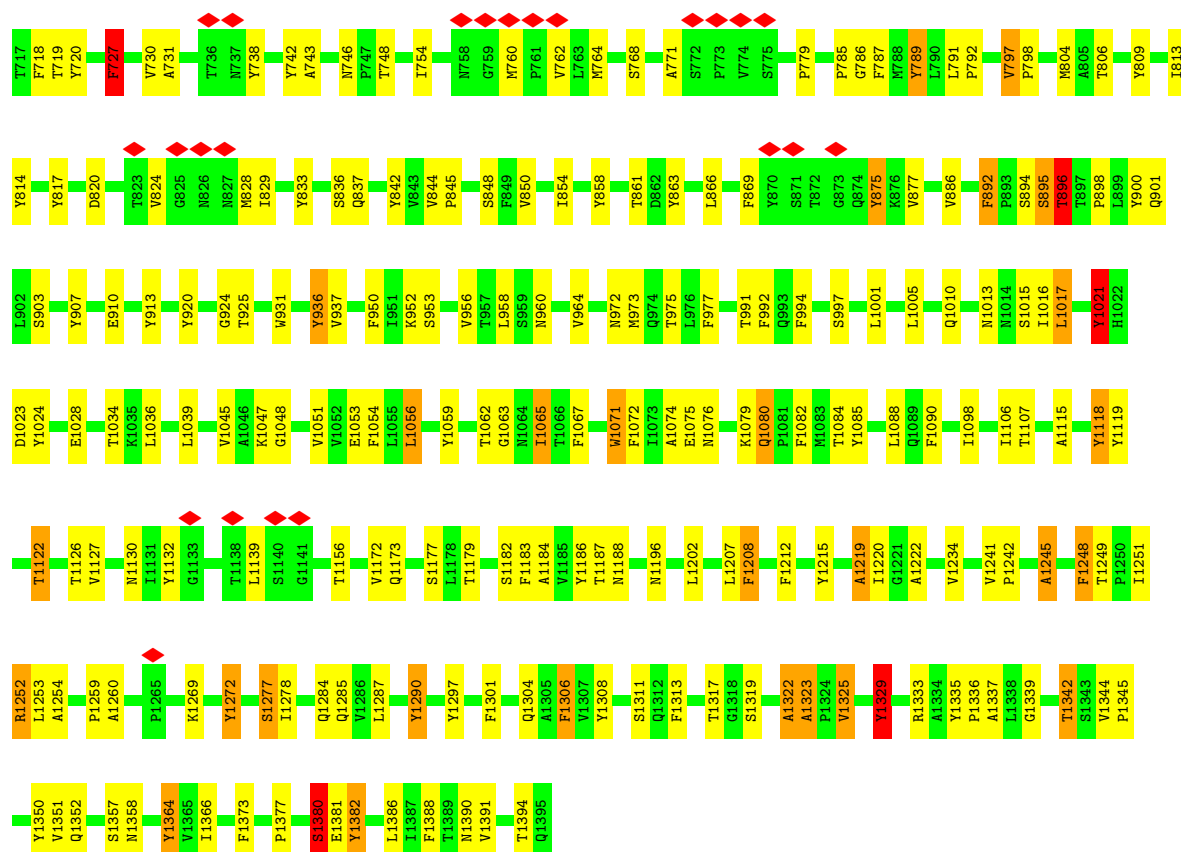
• Molecule 1: S-layer protein A



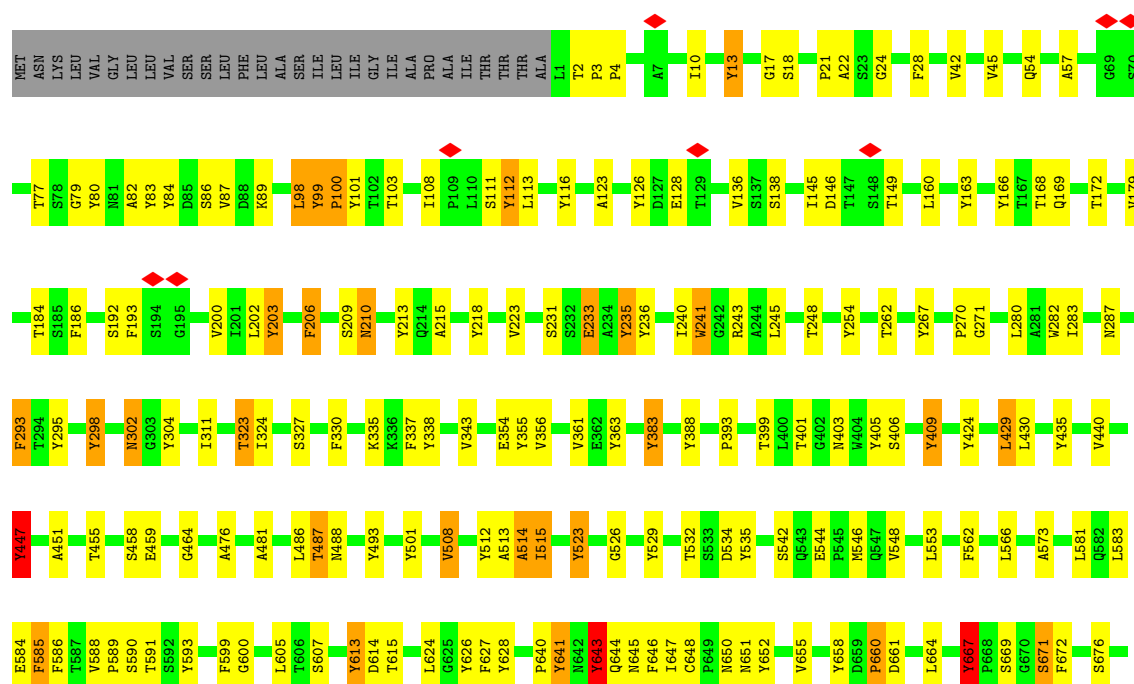


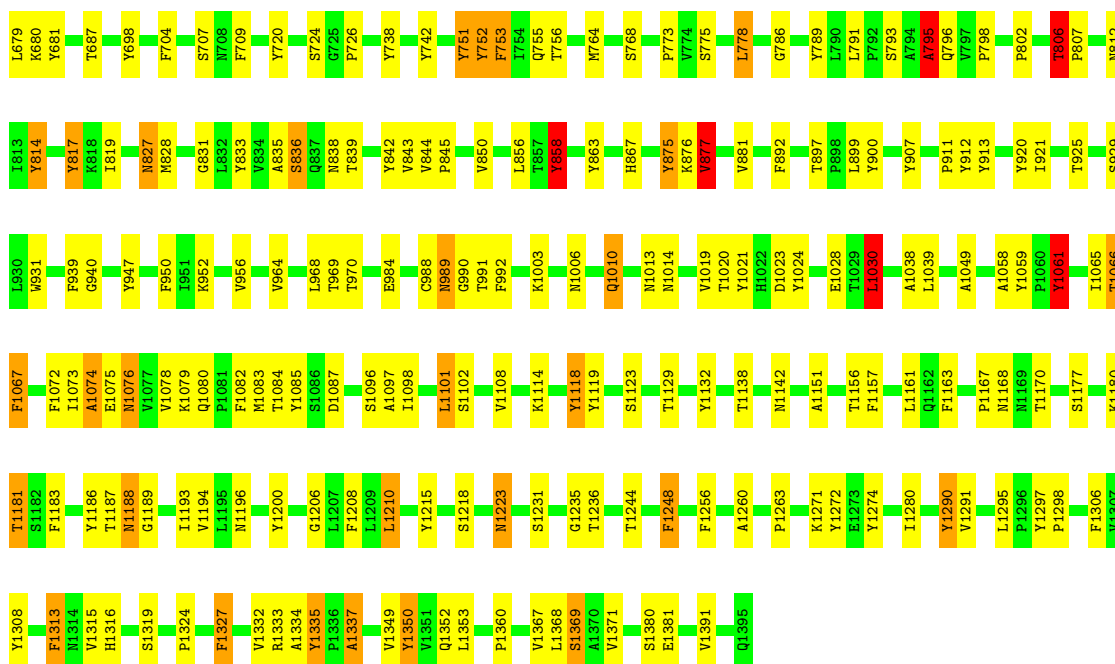
• Molecule 1: S-layer protein A



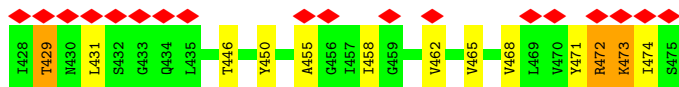
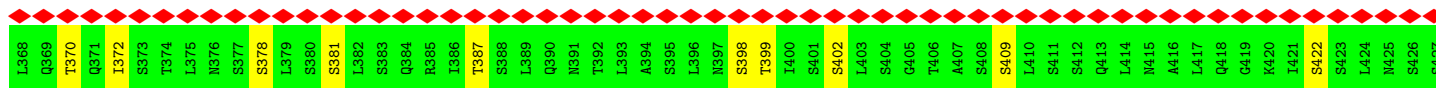
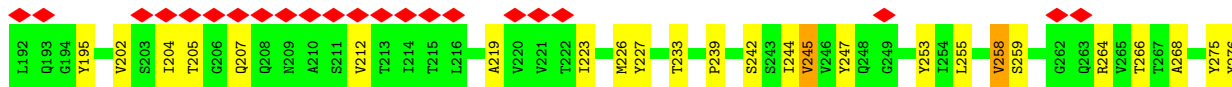
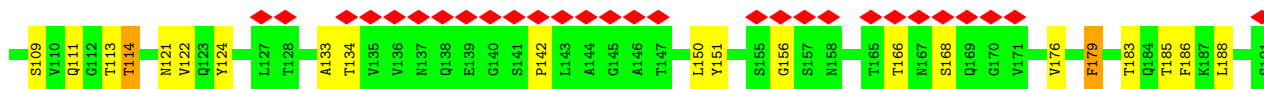


• Molecule 1: S-layer protein A





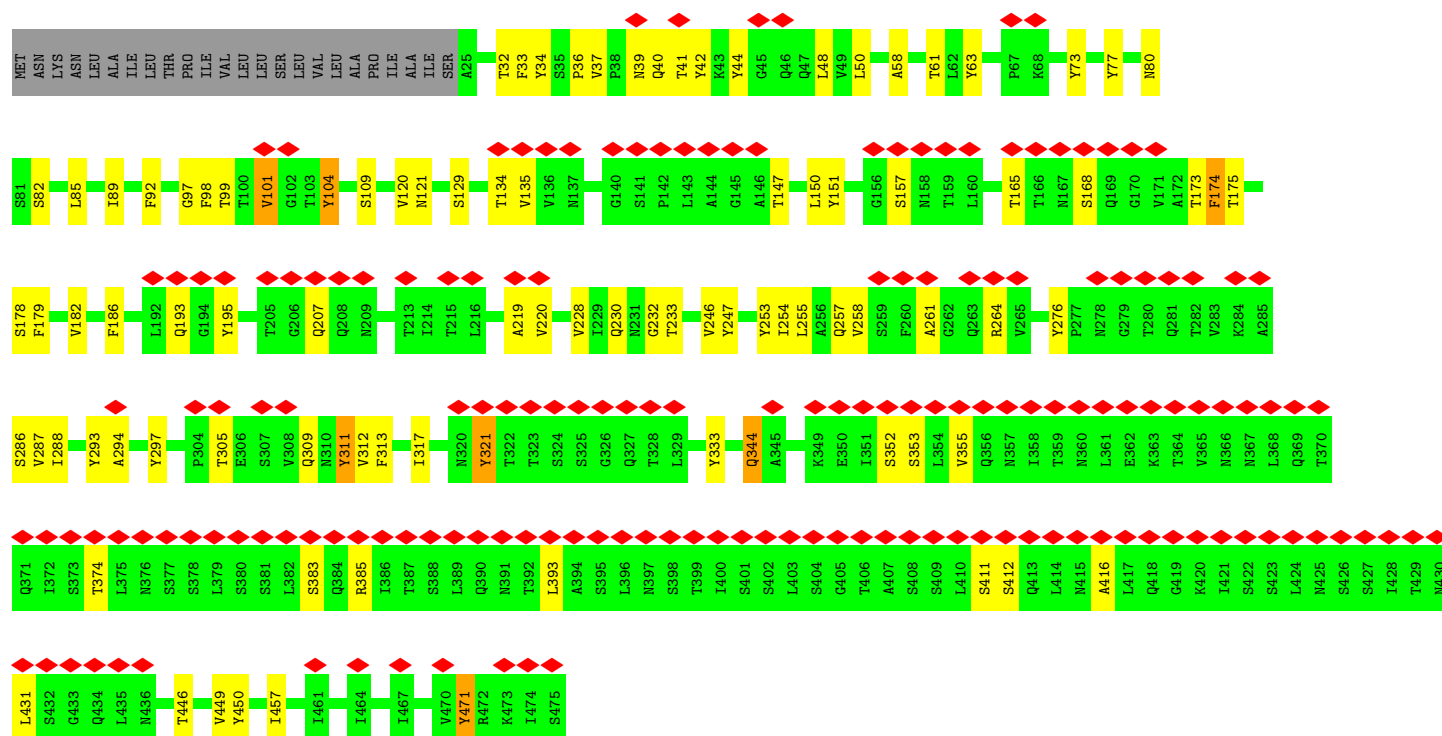
• Molecule 2: Conserved membrane protein



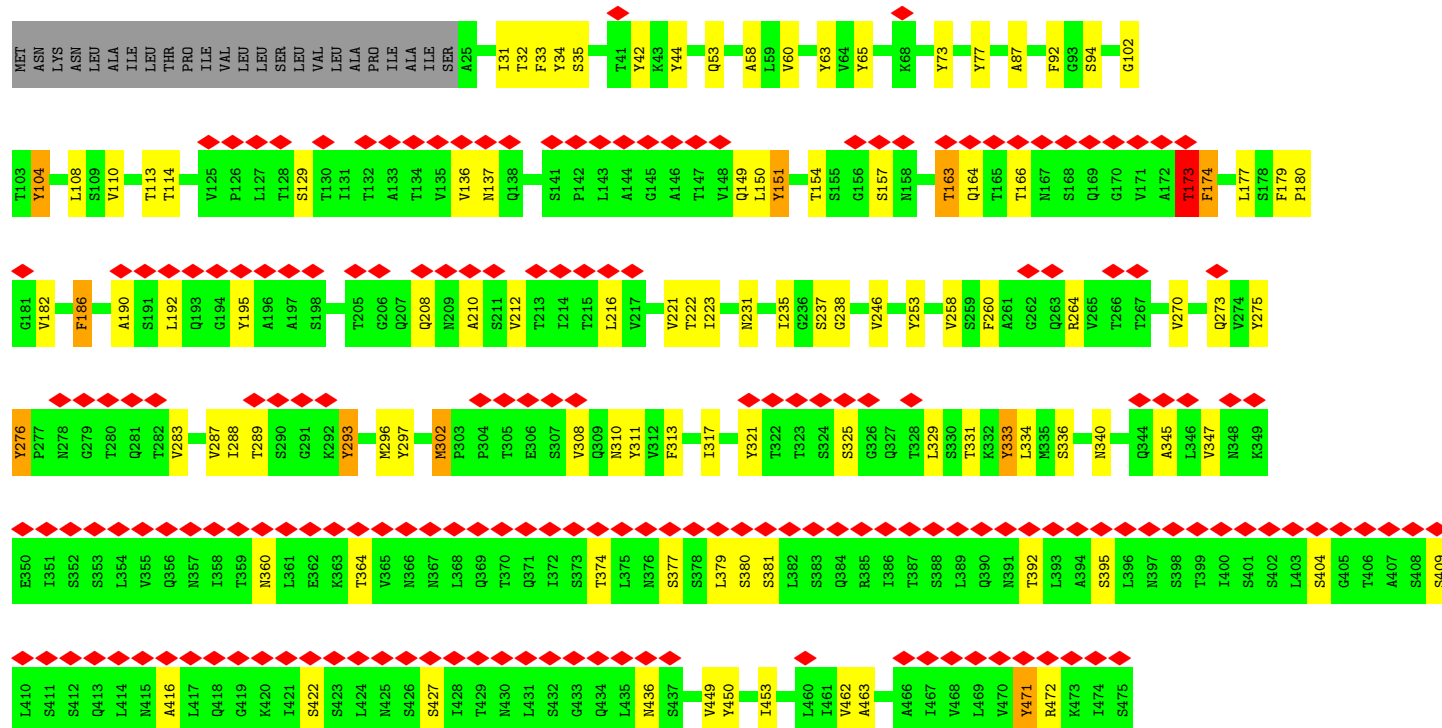
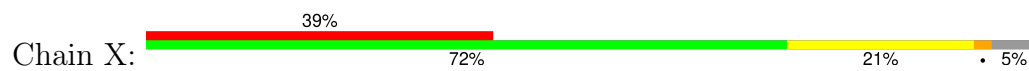
• Molecule 2: Conserved membrane protein







• Molecule 2: Conserved membrane protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	2771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, TFS TALOS	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	83, 83	Depositor
Minimum defocus (nm)	4000, 4000	Depositor
Maximum defocus (nm)	6000, 6000	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	TFS FALCON 4i (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00509	Depositor
Map size (Å)	700.0, 700.0, 700.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.5, 3.5, 3.5	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	A	1.71	74/10749 (0.7%)	1.97	257/14803 (1.7%)
1	V	1.73	79/10749 (0.7%)	1.93	260/14803 (1.8%)
1	W	1.72	90/10749 (0.8%)	1.96	274/14803 (1.9%)
1	Z	1.69	78/10749 (0.7%)	1.91	229/14803 (1.5%)
2	B	1.68	25/3359 (0.7%)	1.86	66/4606 (1.4%)
2	C	1.66	19/3359 (0.6%)	1.81	62/4606 (1.3%)
2	X	1.69	32/3359 (1.0%)	1.89	68/4606 (1.5%)
All	All	1.71	397/53073 (0.7%)	1.93	1216/73030 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	60
1	V	0	40
1	W	0	47
1	Z	0	53
2	B	0	11
2	C	0	8
2	X	0	7
All	All	0	226

All (397) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	1326	TYR	CE2-CZ	9.60	1.51	1.38
1	Z	1119	TYR	CG-CD1	9.42	1.51	1.39
1	W	464	GLY	CA-C	-9.24	1.37	1.51
1	A	39	SER	CA-CB	9.04	1.66	1.52
1	V	1096	SER	CA-CB	8.38	1.65	1.52
2	B	398	SER	CA-CB	8.29	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	129	SER	CA-CB	8.07	1.65	1.52
2	X	157	SER	CA-CB	8.06	1.65	1.52
1	W	206	PHE	CG-CD1	8.04	1.50	1.38
1	Z	900	TYR	CE1-CZ	7.96	1.49	1.38
1	V	388	TYR	CE2-CZ	7.94	1.48	1.38
1	A	555	GLU	CG-CD	7.85	1.63	1.51
1	V	728	SER	CA-CB	7.79	1.64	1.52
1	V	1217	GLY	N-CA	-7.75	1.34	1.46
1	V	1311	SER	CA-CB	7.73	1.64	1.52
1	W	116	TYR	CG-CD1	7.73	1.49	1.39
1	W	1297	TYR	CG-CD1	7.69	1.49	1.39
1	V	1048	GLY	CA-C	-7.67	1.39	1.51
1	V	346	SER	CA-CB	7.53	1.64	1.52
1	Z	1028	GLU	CD-OE1	7.49	1.33	1.25
1	W	60	GLU	CG-CD	7.46	1.63	1.51
1	W	18	SER	CB-OG	7.43	1.51	1.42
1	Z	798	PRO	N-CD	-7.42	1.37	1.47
1	Z	1274	TYR	CE2-CZ	7.39	1.48	1.38
2	X	180	PRO	N-CD	-7.26	1.37	1.47
1	Z	789	TYR	CE1-CZ	7.25	1.48	1.38
1	A	1293	SER	CA-CB	7.23	1.63	1.52
1	A	580	PRO	N-CD	-7.14	1.37	1.47
1	V	870	TYR	CE2-CZ	7.12	1.47	1.38
1	V	894	SER	CA-CB	7.05	1.63	1.52
1	A	327	SER	CA-CB	6.98	1.63	1.52
1	W	40	SER	CA-CB	6.98	1.63	1.52
1	W	203	TYR	CE1-CZ	6.97	1.47	1.38
1	V	780	SER	CA-CB	6.91	1.63	1.52
1	W	1364	TYR	CG-CD1	6.90	1.48	1.39
1	Z	751	TYR	CB-CG	6.89	1.61	1.51
2	X	409	SER	CA-CB	6.89	1.63	1.52
2	C	293	TYR	CE1-CZ	6.88	1.47	1.38
2	B	409	SER	CA-CB	6.85	1.63	1.52
1	W	1297	TYR	CE1-CZ	6.84	1.47	1.38
1	V	603	GLY	CA-C	-6.83	1.41	1.51
1	A	108	ILE	N-CA	-6.83	1.32	1.46
1	V	1177	SER	CA-CB	6.80	1.63	1.52
1	W	1118	TYR	CD2-CE2	6.78	1.49	1.39
1	Z	988	CYS	CB-SG	-6.77	1.70	1.82
1	V	1119	TYR	CE2-CZ	6.74	1.47	1.38
1	W	1272	TYR	CE2-CZ	6.70	1.47	1.38
1	W	203	TYR	CZ-OH	6.70	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	533	SER	CA-CB	6.69	1.62	1.52
1	W	1325	VAL	CB-CG2	6.63	1.66	1.52
1	Z	707	SER	CA-CB	6.59	1.62	1.52
1	V	80	TYR	CE1-CZ	6.58	1.47	1.38
2	B	422	SER	CA-CB	6.55	1.62	1.52
1	W	544	GLU	CB-CG	6.54	1.64	1.52
1	W	842	TYR	N-CA	-6.53	1.33	1.46
2	C	168	SER	CA-CB	6.50	1.62	1.52
1	A	878	PHE	CB-CG	6.50	1.62	1.51
1	W	306	SER	CA-CB	6.50	1.62	1.52
2	X	33	PHE	CE2-CZ	6.48	1.49	1.37
1	A	254	TYR	CZ-OH	6.45	1.48	1.37
1	A	893	PRO	N-CD	-6.45	1.38	1.47
1	W	235	TYR	CE2-CZ	6.41	1.46	1.38
2	X	63	TYR	CG-CD2	6.39	1.47	1.39
1	W	1333	ARG	NE-CZ	6.38	1.41	1.33
2	X	151	TYR	CE1-CZ	6.38	1.46	1.38
2	B	450	TYR	CE1-CZ	6.37	1.46	1.38
1	W	1380	SER	CA-CB	6.37	1.62	1.52
1	W	112	TYR	CE1-CZ	6.37	1.46	1.38
1	A	1388	PHE	CG-CD1	6.34	1.48	1.38
1	A	437	GLY	CA-C	-6.33	1.41	1.51
2	C	383	SER	CB-OG	6.33	1.50	1.42
1	Z	600	GLY	CA-C	-6.32	1.41	1.51
2	C	104	TYR	CE2-CZ	6.31	1.46	1.38
1	A	858	TYR	CG-CD1	6.30	1.47	1.39
2	X	104	TYR	CB-CG	6.30	1.61	1.51
1	W	203	TYR	CG-CD2	6.29	1.47	1.39
2	X	336	SER	CA-CB	6.27	1.62	1.52
2	X	422	SER	CA-CB	6.26	1.62	1.52
1	A	1329	TYR	CE2-CZ	6.26	1.46	1.38
1	V	4	PRO	N-CD	-6.25	1.39	1.47
1	A	533	SER	CA-CB	6.23	1.62	1.52
2	C	276	TYR	CE1-CZ	6.23	1.46	1.38
1	A	593	TYR	CG-CD1	6.22	1.47	1.39
1	A	180	SER	CA-CB	6.22	1.62	1.52
1	Z	169	GLN	N-CA	-6.22	1.33	1.46
1	Z	337	PHE	CG-CD2	6.22	1.48	1.38
1	W	1311	SER	CA-CB	6.21	1.62	1.52
1	Z	562	PHE	CG-CD1	6.21	1.48	1.38
1	A	1237	SER	CA-CB	6.21	1.62	1.52
1	A	479	ALA	CA-CB	6.20	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	TYR	CG-CD1	6.20	1.47	1.39
1	A	891	TYR	CE2-CZ	6.19	1.46	1.38
1	W	1319	SER	CA-CB	6.18	1.62	1.52
1	A	405	TYR	CD1-CE1	6.17	1.48	1.39
2	B	168	SER	CA-CB	6.17	1.62	1.52
1	W	1053	GLU	CD-OE1	6.17	1.32	1.25
1	A	978	PRO	N-CD	-6.17	1.39	1.47
1	W	236	TYR	CE2-CZ	6.16	1.46	1.38
1	W	388	TYR	CE2-CZ	6.16	1.46	1.38
1	A	236	TYR	CE2-CZ	6.15	1.46	1.38
1	W	112	TYR	CB-CG	-6.14	1.42	1.51
1	Z	235	TYR	CG-CD1	6.14	1.47	1.39
2	X	276	TYR	CG-CD2	6.13	1.47	1.39
1	A	213	TYR	CG-CD2	6.13	1.47	1.39
1	W	1130	ASN	CA-CB	6.12	1.69	1.53
2	B	124	TYR	CG-CD2	6.11	1.47	1.39
1	V	851	GLY	N-CA	-6.11	1.36	1.46
1	Z	209	SER	CA-CB	6.10	1.62	1.52
1	W	409	TYR	CG-CD1	6.10	1.47	1.39
1	W	863	TYR	CG-CD1	6.10	1.47	1.39
1	Z	667	TYR	CG-CD1	6.10	1.47	1.39
1	A	426	SER	CA-CB	6.08	1.62	1.52
2	C	385	ARG	CZ-NH2	6.08	1.41	1.33
1	Z	1123	SER	CA-CB	6.07	1.62	1.52
1	W	590	SER	CB-OG	6.07	1.50	1.42
2	B	67	PRO	N-CD	-6.06	1.39	1.47
1	W	545	PRO	N-CD	-6.04	1.39	1.47
1	V	461	SER	CA-CB	6.04	1.62	1.52
1	V	1059	TYR	CG-CD1	6.03	1.47	1.39
1	Z	1335	TYR	CG-CD1	6.03	1.47	1.39
1	A	494	GLU	CD-OE2	6.02	1.32	1.25
1	W	643	TYR	CB-CG	6.02	1.60	1.51
2	B	179	PHE	CE2-CZ	5.99	1.48	1.37
1	V	83	TYR	CD2-CE2	5.99	1.48	1.39
1	V	116	TYR	CG-CD1	5.99	1.47	1.39
1	W	99	TYR	CZ-OH	5.99	1.48	1.37
1	W	895	SER	CA-CB	5.98	1.61	1.52
1	Z	101	TYR	CE1-CZ	5.98	1.46	1.38
1	V	101	TYR	CZ-OH	5.97	1.48	1.37
1	V	471	GLN	C-N	5.97	1.43	1.33
1	V	1327	PHE	CG-CD2	5.97	1.47	1.38
1	Z	1215	TYR	CB-CG	5.96	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	260	PHE	CG-CD2	5.95	1.47	1.38
1	W	1373	PHE	CG-CD1	5.95	1.47	1.38
1	Z	1118	TYR	CG-CD2	5.92	1.46	1.39
2	C	286	SER	CA-CB	5.91	1.61	1.52
1	W	1048	GLY	N-CA	-5.91	1.37	1.46
1	V	97	PHE	CG-CD2	5.90	1.47	1.38
1	V	847	GLY	CA-C	-5.90	1.42	1.51
1	A	74	ARG	NE-CZ	5.89	1.40	1.33
1	W	1021	TYR	CG-CD2	5.88	1.46	1.39
2	X	381	SER	CA-CB	5.88	1.61	1.52
2	B	253	TYR	CE2-CZ	5.88	1.46	1.38
2	X	73	TYR	CG-CD2	5.88	1.46	1.39
1	V	882	SER	CA-CB	5.88	1.61	1.52
1	V	340	TYR	CG-CD2	5.88	1.46	1.39
1	V	441	SER	CA-CB	5.86	1.61	1.52
2	X	395	SER	CA-CB	5.86	1.61	1.52
1	Z	913	TYR	CG-CD2	5.86	1.46	1.39
1	Z	988	CYS	CA-CB	5.85	1.66	1.53
1	Z	203	TYR	CZ-OH	5.85	1.47	1.37
1	Z	724	SER	CA-CB	5.84	1.61	1.52
1	V	613	TYR	CG-CD1	5.83	1.46	1.39
1	W	814	TYR	CG-CD1	5.83	1.46	1.39
1	Z	751	TYR	CG-CD1	-5.82	1.31	1.39
1	Z	401	THR	C-N	5.78	1.43	1.33
2	C	157	SER	CA-CB	5.78	1.61	1.52
1	W	196	SER	CA-CB	5.77	1.61	1.52
1	V	593	TYR	CE2-CZ	5.76	1.46	1.38
1	W	953	SER	CB-OG	5.76	1.49	1.42
1	V	1215	TYR	CG-CD2	5.76	1.46	1.39
1	Z	526	GLY	CA-C	-5.76	1.42	1.51
1	A	1248	PHE	CE2-CZ	5.75	1.48	1.37
1	A	1313	PHE	CE2-CZ	5.75	1.48	1.37
2	B	402	SER	CA-CB	5.75	1.61	1.52
1	A	113	LEU	CA-CB	5.73	1.67	1.53
1	A	913	TYR	CG-CD1	5.73	1.46	1.39
1	V	959	SER	CB-OG	5.72	1.49	1.42
2	X	325	SER	C-N	5.72	1.43	1.33
1	A	383	TYR	CB-CG	-5.70	1.43	1.51
1	W	858	TYR	CE2-CZ	5.70	1.46	1.38
2	C	411	SER	CA-CB	5.70	1.61	1.52
1	V	117	LEU	CA-CB	5.69	1.66	1.53
1	W	1339	GLY	N-CA	-5.69	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	471	TYR	CG-CD2	5.69	1.46	1.39
1	A	1308	TYR	CA-CB	5.68	1.66	1.53
2	B	455	ALA	N-CA	-5.68	1.34	1.46
1	V	454	SER	CA-CB	5.68	1.61	1.52
1	V	83	TYR	CE1-CZ	5.66	1.46	1.38
1	V	692	PHE	CB-CG	5.66	1.60	1.51
1	W	950	PHE	CE2-CZ	5.66	1.48	1.37
2	C	195	TYR	CE1-CZ	5.66	1.46	1.38
1	W	338	TYR	CE2-CZ	5.66	1.46	1.38
1	W	209	SER	CA-CB	5.65	1.61	1.52
1	Z	628	TYR	CD1-CE1	5.65	1.47	1.39
1	Z	267	TYR	CG-CD1	5.63	1.46	1.39
1	V	1021	TYR	CG-CD2	5.62	1.46	1.39
1	W	994	PHE	CG-CD1	5.62	1.47	1.38
2	X	333	TYR	CG-CD2	5.62	1.46	1.39
1	W	652	TYR	CE2-CZ	5.62	1.45	1.38
2	X	237	SER	CA-CB	5.61	1.61	1.52
1	Z	192	SER	CA-CB	5.61	1.61	1.52
1	W	301	SER	CB-OG	5.61	1.49	1.42
1	V	447	TYR	CE2-CZ	5.60	1.45	1.38
1	Z	3	PRO	N-CD	-5.60	1.40	1.47
1	Z	218	TYR	CG-CD2	5.59	1.46	1.39
2	C	321	TYR	CD1-CE1	-5.58	1.30	1.39
1	Z	913	TYR	CZ-OH	5.58	1.47	1.37
1	Z	355	TYR	CZ-OH	5.58	1.47	1.37
1	W	1059	TYR	CE2-CZ	5.57	1.45	1.38
2	X	293	TYR	CE1-CZ	5.57	1.45	1.38
1	A	585	PHE	CG-CD2	5.56	1.47	1.38
1	V	687	THR	N-CA	-5.56	1.35	1.46
1	A	868	TYR	CE2-CZ	5.56	1.45	1.38
1	Z	1218	SER	CA-CB	5.55	1.61	1.52
1	A	303	GLY	CA-C	-5.55	1.43	1.51
1	A	829	ILE	N-CA	-5.54	1.35	1.46
2	X	73	TYR	CZ-OH	5.53	1.47	1.37
2	X	44	TYR	CD1-CE1	5.52	1.47	1.39
1	V	641	TYR	CE1-CZ	5.52	1.45	1.38
2	X	347	VAL	CB-CG1	5.52	1.64	1.52
1	Z	409	TYR	CE2-CZ	-5.51	1.31	1.38
1	W	627	PHE	CD1-CE1	5.51	1.50	1.39
1	W	203	TYR	CB-CG	-5.50	1.43	1.51
2	X	195	TYR	CE1-CZ	5.50	1.45	1.38
1	V	213	TYR	CG-CD2	5.49	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	1300	GLU	CD-OE1	5.49	1.31	1.25
1	W	101	TYR	CE2-CZ	5.49	1.45	1.38
1	W	700	PRO	N-CD	-5.48	1.40	1.47
1	A	1183	PHE	CE2-CZ	5.48	1.47	1.37
2	C	34	TYR	CE2-CZ	5.47	1.45	1.38
1	Z	13	TYR	CD1-CE1	5.47	1.47	1.39
1	Z	947	TYR	CE1-CZ	5.47	1.45	1.38
2	X	471	TYR	CD1-CE1	5.46	1.47	1.39
1	Z	920	TYR	CE2-CZ	5.46	1.45	1.38
1	Z	218	TYR	CE2-CZ	5.46	1.45	1.38
1	Z	1024	TYR	CG-CD1	5.46	1.46	1.39
1	Z	80	TYR	CG-CD2	5.45	1.46	1.39
1	W	1024	TYR	CG-CD2	5.44	1.46	1.39
1	A	1157	PHE	CG-CD2	5.43	1.46	1.38
1	W	628	TYR	CD1-CE1	5.43	1.47	1.39
1	V	836	SER	CA-CB	5.43	1.61	1.52
2	B	472	ARG	CA-CB	5.43	1.65	1.53
1	W	1132	TYR	CE1-CZ	5.43	1.45	1.38
2	C	97	GLY	CA-C	-5.42	1.43	1.51
1	A	163	TYR	CE1-CZ	5.42	1.45	1.38
1	V	456	PRO	N-CD	-5.42	1.40	1.47
1	W	924	GLY	CA-C	-5.42	1.43	1.51
2	X	53	GLN	CG-CD	5.42	1.63	1.51
1	W	705	GLY	CA-C	-5.40	1.43	1.51
1	V	256	SER	CB-OG	-5.39	1.35	1.42
1	A	1364	TYR	CG-CD2	-5.39	1.32	1.39
1	A	1383	PRO	N-CD	-5.39	1.40	1.47
1	W	1015	SER	CA-CB	5.39	1.61	1.52
2	B	450	TYR	CE2-CZ	-5.38	1.31	1.38
1	W	1177	SER	CA-CB	5.38	1.61	1.52
1	Z	1059	TYR	CE2-CZ	5.38	1.45	1.38
1	Z	1352	GLN	CA-CB	5.38	1.65	1.53
1	V	795	ALA	CA-CB	5.37	1.63	1.52
1	W	669	SER	C-N	5.37	1.42	1.33
1	W	447	TYR	CZ-OH	5.37	1.47	1.37
1	Z	501	TYR	CB-CG	5.37	1.59	1.51
1	A	409	TYR	CD2-CE2	5.37	1.47	1.39
1	V	1021	TYR	CE2-CZ	5.36	1.45	1.38
1	V	912	TYR	CG-CD1	5.36	1.46	1.39
1	V	166	TYR	CA-CB	5.36	1.65	1.53
1	A	907	TYR	CG-CD2	5.35	1.46	1.39
1	W	254	TYR	CE1-CZ	5.35	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	GLY	N-CA	-5.34	1.38	1.46
1	V	1333	ARG	CZ-NH1	5.34	1.40	1.33
2	X	102	GLY	CA-C	-5.34	1.43	1.51
2	X	231	ASN	C-N	5.33	1.42	1.33
1	V	706	TYR	CD1-CE1	5.33	1.47	1.39
1	V	1067	PHE	CE1-CZ	5.33	1.47	1.37
1	Z	1319	SER	CA-CB	5.33	1.60	1.52
2	B	156	GLY	N-CA	5.33	1.54	1.46
2	X	377	SER	CA-CB	5.33	1.60	1.52
1	W	526	GLY	N-CA	-5.32	1.38	1.46
1	Z	17	GLY	CA-C	-5.32	1.43	1.51
1	Z	768	SER	CB-OG	5.32	1.49	1.42
1	A	1119	TYR	CZ-OH	5.32	1.46	1.37
1	V	652	TYR	CE2-CZ	5.32	1.45	1.38
1	V	1246	GLU	CD-OE1	5.30	1.31	1.25
1	A	849	PHE	CE1-CZ	5.30	1.47	1.37
1	W	742	TYR	CE2-CZ	5.30	1.45	1.38
1	Z	940	GLY	CA-C	5.29	1.60	1.51
1	W	771	ALA	N-CA	-5.29	1.35	1.46
2	B	242	SER	CA-CB	5.28	1.60	1.52
2	C	129	SER	CA-CB	5.28	1.60	1.52
1	A	947	TYR	CG-CD2	5.27	1.46	1.39
1	Z	508	VAL	CB-CG1	5.27	1.64	1.52
1	V	1075	GLU	CG-CD	5.26	1.59	1.51
2	B	239	PRO	CA-CB	5.26	1.64	1.53
1	V	794	ALA	CA-CB	5.26	1.63	1.52
1	V	1015	SER	CB-OG	-5.26	1.35	1.42
1	Z	641	TYR	CZ-OH	5.26	1.46	1.37
1	W	505	GLY	CA-C	-5.25	1.43	1.51
1	V	974	GLN	CG-CD	5.25	1.63	1.51
1	W	649	PRO	N-CD	-5.24	1.40	1.47
2	B	42	TYR	CZ-OH	5.24	1.46	1.37
1	V	80	TYR	CA-CB	5.24	1.65	1.53
1	V	74	ARG	CZ-NH1	5.24	1.39	1.33
1	V	266	ASN	CA-CB	5.24	1.66	1.53
1	A	471	GLN	N-CA	-5.23	1.35	1.46
1	Z	1235	GLY	CA-C	-5.22	1.43	1.51
1	W	1172	VAL	CB-CG1	5.22	1.63	1.52
1	W	1183	PHE	CD2-CE2	5.22	1.49	1.39
1	A	1157	PHE	CG-CD1	5.22	1.46	1.38
2	X	404	SER	CA-CB	5.22	1.60	1.52
1	W	1252	ARG	CD-NE	5.22	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	380	SER	CA-CB	5.21	1.60	1.52
1	Z	101	TYR	CG-CD2	5.21	1.46	1.39
1	Z	1315	VAL	CB-CG2	5.21	1.63	1.52
2	C	457	ILE	N-CA	5.21	1.56	1.46
1	A	655	VAL	CA-CB	-5.20	1.43	1.54
1	A	1123	SER	CA-CB	5.20	1.60	1.52
1	A	1132	TYR	CB-CG	-5.20	1.43	1.51
2	B	212	VAL	CB-CG2	5.19	1.63	1.52
1	V	787	PHE	CE1-CZ	5.19	1.47	1.37
1	V	907	TYR	CB-CG	-5.18	1.43	1.51
1	W	213	TYR	CG-CD2	5.18	1.45	1.39
1	A	1095	PRO	N-CD	5.18	1.55	1.47
1	Z	435	TYR	CE2-CZ	5.18	1.45	1.38
2	B	297	TYR	CG-CD2	5.18	1.45	1.39
2	C	352	SER	CA-CB	5.17	1.60	1.52
1	W	211	SER	CA-CB	5.17	1.60	1.52
1	V	607	SER	CA-CB	5.17	1.60	1.52
2	X	270	VAL	CA-CB	-5.17	1.43	1.54
1	Z	775	SER	CA-CB	5.17	1.60	1.52
1	V	1308	TYR	CG-CD1	5.17	1.45	1.39
1	W	1241	VAL	CB-CG2	5.17	1.63	1.52
1	Z	1327	PHE	CG-CD1	5.17	1.46	1.38
1	W	768	SER	CB-OG	5.16	1.49	1.42
1	Z	338	TYR	CE2-CZ	5.16	1.45	1.38
1	W	562	PHE	C-N	5.16	1.42	1.33
2	C	257	GLN	CG-CD	5.16	1.62	1.51
1	V	858	TYR	CE2-CZ	-5.16	1.31	1.38
2	X	321	TYR	CE2-CZ	5.15	1.45	1.38
1	A	870	TYR	CA-CB	5.15	1.65	1.53
2	X	151	TYR	CZ-OH	5.15	1.46	1.37
1	Z	669	SER	C-N	5.14	1.42	1.33
1	Z	186	PHE	CA-CB	5.14	1.65	1.53
1	V	1212	PHE	CG-CD1	5.14	1.46	1.38
1	W	894	SER	CB-OG	5.14	1.49	1.42
1	Z	687	THR	C-N	5.14	1.42	1.33
1	A	1090	PHE	CG-CD1	5.14	1.46	1.38
1	A	166	TYR	CE2-CZ	5.14	1.45	1.38
1	V	1252	ARG	NE-CZ	5.12	1.39	1.33
1	W	92	PHE	CA-CB	5.12	1.65	1.53
1	Z	84	TYR	CE2-CZ	5.12	1.45	1.38
1	A	542	SER	CB-OG	5.12	1.49	1.42
1	V	870	TYR	CG-CD2	5.12	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	49	VAL	CB-CG1	5.12	1.63	1.52
1	W	355	TYR	CG-CD2	5.12	1.45	1.39
1	Z	875	TYR	CB-CG	5.11	1.59	1.51
1	V	389	GLU	CD-OE2	-5.11	1.20	1.25
1	Z	643	TYR	CE1-CZ	5.11	1.45	1.38
2	B	293	TYR	CG-CD1	5.11	1.45	1.39
1	A	1119	TYR	CE2-CZ	5.10	1.45	1.38
1	W	225	GLY	CA-C	-5.10	1.43	1.51
1	A	180	SER	CB-OG	-5.10	1.35	1.42
1	W	448	TYR	CE2-CZ	5.10	1.45	1.38
1	Z	523	TYR	CD1-CE1	5.10	1.47	1.39
1	A	501	TYR	CE2-CZ	5.09	1.45	1.38
1	A	1272	TYR	CZ-OH	5.09	1.46	1.37
1	V	295	TYR	CE2-CZ	5.09	1.45	1.38
1	Z	535	TYR	CE2-CZ	5.08	1.45	1.38
1	Z	681	TYR	CG-CD2	5.08	1.45	1.39
2	B	65	TYR	CE2-CZ	5.08	1.45	1.38
1	W	1269	LYS	CD-CE	5.08	1.64	1.51
1	W	338	TYR	CG-CD2	5.08	1.45	1.39
2	B	247	TYR	CG-CD1	5.07	1.45	1.39
1	W	975	THR	N-CA	-5.07	1.36	1.46
1	V	236	TYR	CG-CD1	5.07	1.45	1.39
1	A	74	ARG	CZ-NH2	5.06	1.39	1.33
1	W	627	PHE	CB-CG	5.06	1.59	1.51
1	A	229	SER	CA-CB	5.05	1.60	1.52
1	Z	1335	TYR	CB-CG	5.05	1.59	1.51
1	A	28	PHE	CG-CD1	5.05	1.46	1.38
1	W	1297	TYR	CG-CD2	5.05	1.45	1.39
1	Z	584	GLU	CD-OE2	5.05	1.31	1.25
1	Z	681	TYR	CE2-CZ	5.05	1.45	1.38
1	Z	83	TYR	CZ-OH	5.05	1.46	1.37
1	A	539	PHE	CG-CD1	5.05	1.46	1.38
1	A	493	TYR	CG-CD1	5.04	1.45	1.39
1	A	1279	VAL	CB-CG1	5.04	1.63	1.52
1	V	1290	TYR	CE2-CZ	5.04	1.45	1.38
2	B	409	SER	CB-OG	5.04	1.48	1.42
1	W	1350	TYR	CE1-CZ	5.04	1.45	1.38
1	Z	236	TYR	CZ-OH	5.04	1.46	1.37
1	V	523	TYR	CE2-CZ	5.03	1.45	1.38
2	C	109	SER	CA-CB	5.03	1.60	1.52
1	A	75	PHE	CG-CD1	5.03	1.46	1.38
1	V	1028	GLU	CD-OE2	5.03	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	1030	LEU	CA-CB	5.03	1.65	1.53
1	A	1072	PHE	CG-CD2	5.02	1.46	1.38
1	W	1350	TYR	CG-CD1	5.02	1.45	1.39
1	A	563	GLY	N-CA	-5.02	1.38	1.46
1	A	1246	GLU	CB-CG	5.02	1.61	1.52
1	Z	786	GLY	CA-C	-5.02	1.43	1.51
1	Z	858	TYR	CB-CG	5.02	1.59	1.51
1	A	111	SER	CB-OG	5.02	1.48	1.42
1	Z	1215	TYR	CE1-CZ	-5.01	1.32	1.38
1	A	1072	PHE	CE2-CZ	5.01	1.46	1.37
1	Z	613	TYR	CE2-CZ	5.01	1.45	1.38
1	A	868	TYR	CD1-CE1	5.00	1.46	1.39
1	V	1062	THR	C-N	5.00	1.42	1.33

All (1216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	1252	ARG	NE-CZ-NH2	-20.21	110.19	120.30
1	A	1364	TYR	CB-CG-CD1	-17.88	110.28	121.00
1	Z	512	TYR	CB-CG-CD2	-16.12	111.33	121.00
1	V	1024	TYR	CB-CG-CD2	-16.02	111.39	121.00
1	V	789	TYR	CB-CG-CD2	-15.91	111.46	121.00
1	V	752	TYR	CB-CG-CD2	-15.28	111.83	121.00
1	A	243	ARG	NE-CZ-NH2	-14.88	112.86	120.30
2	B	264	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	A	338	TYR	CB-CG-CD2	-14.41	112.36	121.00
2	X	450	TYR	CB-CG-CD2	-14.23	112.46	121.00
2	X	472	ARG	NE-CZ-NH2	-14.11	113.25	120.30
1	A	447	TYR	CB-CG-CD2	-14.05	112.57	121.00
2	X	276	TYR	CB-CG-CD2	13.96	129.37	121.00
1	A	295	TYR	CB-CG-CD2	-13.54	112.88	121.00
1	A	738	TYR	CB-CG-CD2	-13.49	112.91	121.00
1	A	1132	TYR	CB-CG-CD1	-13.29	113.02	121.00
2	B	65	TYR	CB-CG-CD2	13.29	128.97	121.00
1	W	1333	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	V	298	TYR	CB-CG-CD1	13.17	128.90	121.00
1	Z	817	TYR	CB-CG-CD2	-13.08	113.15	121.00
1	A	1252	ARG	NE-CZ-NH1	13.07	126.83	120.30
2	X	276	TYR	CB-CG-CD1	-12.95	113.23	121.00
1	W	789	TYR	CB-CG-CD2	-12.94	113.23	121.00
1	A	447	TYR	CB-CG-CD1	12.85	128.71	121.00
1	V	243	ARG	NE-CZ-NH1	12.75	126.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	295	TYR	CB-CG-CD1	-12.56	113.46	121.00
1	W	641	TYR	CB-CG-CD2	12.44	128.47	121.00
1	W	613	TYR	CB-CG-CD2	-12.43	113.54	121.00
2	X	34	TYR	CB-CG-CD1	-12.40	113.56	121.00
1	Z	512	TYR	CB-CG-CD1	12.39	128.44	121.00
2	X	450	TYR	CB-CG-CD1	12.33	128.40	121.00
1	A	1208	PHE	CB-CG-CD2	12.30	129.41	120.80
1	A	112	TYR	CB-CG-CD2	-12.23	113.66	121.00
1	W	613	TYR	CB-CG-CD1	12.22	128.33	121.00
1	Z	206	PHE	CB-CG-CD2	12.02	129.21	120.80
2	B	65	TYR	CB-CG-CD1	-12.01	113.80	121.00
1	W	1272	TYR	CB-CG-CD1	-11.99	113.81	121.00
1	Z	355	TYR	CB-CG-CD2	11.94	128.16	121.00
2	X	92	PHE	CB-CG-CD2	11.92	129.15	120.80
1	W	1272	TYR	CB-CG-CD2	11.88	128.13	121.00
2	B	311	TYR	CB-CG-CD2	11.83	128.10	121.00
1	Z	1215	TYR	CB-CG-CD1	-11.82	113.91	121.00
1	A	1208	PHE	CB-CG-CD1	-11.60	112.68	120.80
1	W	1090	PHE	CB-CG-CD1	11.59	128.92	120.80
1	W	992	PHE	CB-CG-CD2	11.52	128.86	120.80
2	X	34	TYR	CB-CG-CD2	11.51	127.91	121.00
1	W	163	TYR	CB-CG-CD1	11.50	127.90	121.00
1	V	817	TYR	CB-CG-CD1	11.47	127.89	121.00
1	W	1215	TYR	CB-CG-CD1	-11.45	114.13	121.00
1	W	599	PHE	CB-CG-CD2	-11.44	112.79	120.80
1	Z	858	TYR	CB-CG-CD1	11.42	127.85	121.00
1	V	1061	TYR	CB-CG-CD2	-11.40	114.16	121.00
1	W	243	ARG	NE-CZ-NH1	11.35	125.98	120.30
1	A	1132	TYR	CB-CG-CD2	11.33	127.80	121.00
1	V	338	TYR	CB-CG-CD1	-11.21	114.27	121.00
1	V	243	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	V	1373	PHE	CB-CG-CD2	11.17	128.62	120.80
1	W	1333	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	Z	116	TYR	CB-CG-CD1	11.10	127.66	121.00
1	V	112	TYR	CB-CG-CD1	-10.87	114.48	121.00
1	A	1350	TYR	CB-CG-CD1	-10.85	114.49	121.00
1	W	267	TYR	CB-CG-CD1	-10.79	114.53	121.00
1	V	814	TYR	CB-CG-CD1	10.71	127.43	121.00
1	A	448	TYR	CB-CG-CD1	-10.68	114.59	121.00
2	C	264	ARG	NE-CZ-NH2	10.66	125.63	120.30
1	A	501	TYR	CB-CG-CD2	-10.66	114.61	121.00
1	W	1208	PHE	CB-CG-CD1	10.62	128.23	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1364	TYR	CB-CG-CD2	10.56	127.34	121.00
2	C	276	TYR	CB-CG-CD2	10.55	127.33	121.00
1	A	1024	TYR	CB-CG-CD1	-10.54	114.67	121.00
1	V	523	TYR	CB-CG-CD1	10.52	127.31	121.00
1	Z	613	TYR	CB-CG-CD1	-10.51	114.70	121.00
1	W	1208	PHE	CB-CG-CD2	-10.50	113.45	120.80
1	V	523	TYR	CB-CG-CD2	-10.50	114.70	121.00
1	W	950	PHE	CB-CG-CD2	-10.44	113.49	120.80
1	V	809	TYR	CB-CG-CD2	-10.36	114.78	121.00
1	W	1252	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	A	101	TYR	CB-CG-CD1	10.31	127.19	121.00
1	Z	585	PHE	CB-CG-CD1	-10.29	113.59	120.80
1	Z	355	TYR	CB-CG-CD1	-10.26	114.84	121.00
1	A	842	TYR	CB-CG-CD1	-10.25	114.85	121.00
1	Z	720	TYR	CB-CG-CD2	-10.21	114.87	121.00
2	B	264	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	W	1382	TYR	CB-CG-CD1	-10.12	114.93	121.00
1	A	338	TYR	CB-CG-CD1	10.11	127.06	121.00
1	W	435	TYR	CG-CD2-CE2	-10.05	113.26	121.30
1	A	97	PHE	CB-CG-CD2	-10.05	113.76	120.80
1	A	751	TYR	CB-CG-CD2	-10.05	114.97	121.00
1	V	218	TYR	CB-CG-CD2	10.04	127.03	121.00
1	V	1329	TYR	CB-CG-CD1	10.02	127.01	121.00
1	A	738	TYR	CB-CG-CD1	10.01	127.00	121.00
1	W	163	TYR	CB-CG-CD2	-9.99	115.01	121.00
1	W	1382	TYR	CB-CG-CD2	9.94	126.96	121.00
1	W	448	TYR	CB-CG-CD2	9.93	126.96	121.00
1	V	698	TYR	CB-CG-CD1	-9.92	115.05	121.00
1	W	523	TYR	CB-CG-CD1	-9.90	115.06	121.00
1	Z	1118	TYR	CG-CD2-CE2	-9.90	113.38	121.30
1	W	1184	ALA	N-CA-CB	9.88	123.93	110.10
1	V	208	PHE	CB-CG-CD2	-9.85	113.90	120.80
1	V	749	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	V	789	TYR	CB-CG-CD1	9.74	126.84	121.00
1	A	1308	TYR	CB-CG-CD2	9.74	126.84	121.00
1	Z	628	TYR	CB-CG-CD1	-9.70	115.18	121.00
2	X	77	TYR	CB-CG-CD1	-9.66	115.20	121.00
1	W	727	PHE	CB-CG-CD1	-9.65	114.04	120.80
2	B	63	TYR	CG-CD1-CE1	-9.64	113.59	121.30
1	Z	193	PHE	CB-CG-CD1	-9.61	114.07	120.80
2	X	253	TYR	CB-CG-CD2	9.60	126.76	121.00
1	W	1215	TYR	CB-CG-CD2	9.59	126.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	44	TYR	CB-CG-CD1	-9.59	115.25	121.00
1	V	99	TYR	CB-CG-CD1	-9.54	115.28	121.00
1	W	727	PHE	CB-CG-CD2	9.52	127.46	120.80
1	W	388	TYR	CB-CG-CD1	9.48	126.69	121.00
2	B	297	TYR	CB-CG-CD2	9.37	126.62	121.00
1	W	1308	TYR	CB-CG-CD2	-9.35	115.39	121.00
1	V	338	TYR	CB-CG-CD2	9.35	126.61	121.00
1	Z	1333	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	Z	1215	TYR	CB-CG-CD2	9.33	126.60	121.00
1	A	448	TYR	CB-CG-CD2	9.28	126.57	121.00
1	A	939	PHE	CB-CG-CD1	9.27	127.29	120.80
1	V	613	TYR	CG-CD1-CE1	-9.26	113.89	121.30
1	V	1067	PHE	CB-CG-CD1	9.24	127.27	120.80
1	V	613	TYR	CB-CG-CD2	-9.23	115.46	121.00
1	V	817	TYR	CB-CG-CD2	-9.23	115.46	121.00
1	A	503	PHE	CB-CG-CD1	-9.22	114.35	120.80
1	V	1373	PHE	CB-CG-CD1	-9.21	114.35	120.80
1	W	1119	TYR	CB-CG-CD1	-9.21	115.47	121.00
1	Z	1157	PHE	CB-CG-CD1	-9.21	114.35	120.80
1	Z	206	PHE	CB-CG-CD1	-9.19	114.36	120.80
1	Z	652	TYR	CB-CG-CD2	9.17	126.50	121.00
2	C	92	PHE	CB-CG-CD2	9.17	127.22	120.80
1	V	448	TYR	CB-CG-CD2	-9.13	115.52	121.00
1	V	1061	TYR	CB-CG-CD1	9.09	126.45	121.00
1	W	858	TYR	CB-CG-CD1	-9.08	115.55	121.00
1	Z	99	TYR	CB-CG-CD1	9.07	126.44	121.00
1	W	1329	TYR	CG-CD1-CE1	-9.06	114.05	121.30
1	V	307	PHE	CB-CG-CD1	-8.94	114.54	120.80
1	Z	817	TYR	CB-CG-CD1	8.94	126.36	121.00
1	A	1152	ALA	N-CA-CB	8.92	122.59	110.10
1	A	236	TYR	CB-CG-CD1	-8.90	115.66	121.00
1	Z	1308	TYR	CB-CG-CD2	8.89	126.34	121.00
1	W	409	TYR	CG-CD1-CE1	-8.88	114.19	121.30
1	W	599	PHE	CB-CG-CD1	8.87	127.01	120.80
1	V	718	PHE	CB-CG-CD2	-8.87	114.59	120.80
1	W	842	TYR	CB-CG-CD1	-8.85	115.69	121.00
1	V	868	TYR	CB-CG-CD2	8.84	126.31	121.00
1	V	614	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	1373	PHE	CB-CG-CD1	-8.82	114.62	120.80
1	W	405	TYR	CB-CG-CD2	-8.78	115.73	121.00
2	C	247	TYR	CB-CG-CD1	-8.72	115.77	121.00
1	V	1327	PHE	CB-CG-CD2	8.72	126.91	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	TYR	CB-CG-CD2	-8.68	115.79	121.00
1	W	435	TYR	CB-CG-CD2	-8.68	115.79	121.00
2	C	92	PHE	CB-CG-CD1	-8.68	114.72	120.80
1	A	912	TYR	CB-CG-CD1	-8.66	115.81	121.00
1	W	1186	TYR	CB-CG-CD2	8.65	126.19	121.00
1	W	535	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	V	1215	TYR	CG-CD1-CE1	-8.63	114.40	121.30
1	Z	82	ALA	N-CA-CB	8.62	122.16	110.10
1	W	1342	THR	CA-CB-CG2	-8.61	100.35	112.40
1	W	1329	TYR	CD1-CE1-CZ	8.60	127.54	119.80
1	A	1157	PHE	CB-CG-CD2	8.60	126.82	120.80
1	V	706	TYR	CG-CD1-CE1	-8.60	114.42	121.30
2	B	275	TYR	CB-CG-CD1	-8.59	115.84	121.00
1	A	405	TYR	CZ-CE2-CD2	-8.59	112.07	119.80
2	X	313	PHE	CB-CG-CD1	-8.56	114.81	120.80
1	Z	1290	TYR	CB-CG-CD1	-8.53	115.88	121.00
1	V	383	TYR	CB-CG-CD1	8.51	126.10	121.00
1	A	1326	TYR	CB-CG-CD1	-8.49	115.90	121.00
1	A	163	TYR	CB-CG-CD2	-8.49	115.91	121.00
1	A	330	PHE	CB-CG-CD1	8.48	126.74	120.80
1	A	698	TYR	CB-CG-CD1	8.47	126.08	121.00
1	Z	672	PHE	CB-CG-CD2	-8.47	114.87	120.80
1	V	1274	TYR	CB-CG-CD2	8.45	126.07	121.00
1	W	304	TYR	CB-CG-CD2	8.45	126.07	121.00
1	Z	1072	PHE	CB-CG-CD2	-8.43	114.90	120.80
1	A	663	VAL	CA-CB-CG2	-8.40	98.30	110.90
1	A	388	TYR	CB-CG-CD1	8.38	126.03	121.00
1	A	900	TYR	CB-CG-CD1	8.38	126.03	121.00
1	A	1330	SER	N-CA-CB	8.34	123.01	110.50
1	A	74	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	W	405	TYR	CB-CG-CD1	8.31	125.99	121.00
1	V	206	PHE	CB-CG-CD2	-8.30	114.99	120.80
1	A	720	TYR	CB-CG-CD1	-8.28	116.03	121.00
2	C	313	PHE	CB-CG-CD2	8.26	126.58	120.80
1	V	673	THR	CA-CB-CG2	-8.25	100.84	112.40
2	C	253	TYR	CZ-CE2-CD2	8.25	127.23	119.80
1	Z	84	TYR	CB-CG-CD2	-8.24	116.05	121.00
2	B	297	TYR	CB-CG-CD1	-8.22	116.07	121.00
1	Z	1119	TYR	CB-CG-CD2	8.20	125.92	121.00
1	Z	833	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	V	75	PHE	CB-CG-CD2	8.17	126.52	120.80
1	W	267	TYR	CB-CG-CD2	8.17	125.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	1364	TYR	CB-CG-CD1	8.16	125.90	121.00
2	X	186	PHE	CB-CG-CD2	8.16	126.51	120.80
2	X	73	TYR	CB-CG-CD1	8.14	125.88	121.00
1	V	512	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	V	126	TYR	CB-CG-CD1	8.10	125.86	121.00
1	W	1364	TYR	CB-CG-CD2	8.10	125.86	121.00
1	V	501	TYR	CB-CG-CD2	8.07	125.84	121.00
1	V	1067	PHE	CB-CG-CD2	-8.07	115.15	120.80
1	A	116	TYR	CB-CG-CD2	-8.03	116.18	121.00
2	B	34	TYR	CB-CG-CD1	8.03	125.82	121.00
2	B	63	TYR	CD1-CE1-CZ	8.01	127.01	119.80
1	A	1215	TYR	CB-CG-CD1	8.00	125.80	121.00
2	X	65	TYR	CB-CG-CD1	7.98	125.79	121.00
1	A	411	VAL	CA-CB-CG2	7.94	122.81	110.90
2	B	73	TYR	CB-CG-CD2	7.92	125.75	121.00
1	W	263	PHE	CB-CG-CD1	7.91	126.34	120.80
1	Z	424	TYR	CB-CG-CD2	-7.91	116.25	121.00
1	W	627	PHE	CB-CG-CD2	-7.90	115.27	120.80
1	A	1118	TYR	CB-CG-CD1	-7.90	116.26	121.00
2	X	313	PHE	CB-CG-CD2	7.89	126.32	120.80
1	A	97	PHE	CB-CG-CD1	7.87	126.31	120.80
1	Z	405	TYR	CB-CG-CD1	7.86	125.72	121.00
1	Z	752	TYR	CB-CG-CD1	-7.86	116.28	121.00
1	V	487	THR	CA-CB-CG2	-7.85	101.41	112.40
1	Z	599	PHE	CB-CG-CD1	7.84	126.29	120.80
1	Z	875	TYR	CB-CG-CD1	7.83	125.70	121.00
2	X	471	TYR	CB-CG-CD1	-7.82	116.31	121.00
1	W	83	TYR	CB-CG-CD1	7.82	125.69	121.00
1	Z	752	TYR	CG-CD1-CE1	-7.80	115.06	121.30
1	A	698	TYR	CB-CG-CD2	-7.78	116.33	121.00
1	V	809	TYR	CB-CG-CD1	7.78	125.67	121.00
1	W	814	TYR	CB-CG-CD1	7.77	125.66	121.00
1	W	1313	PHE	CB-CG-CD2	7.77	126.24	120.80
1	V	752	TYR	CG-CD2-CE2	-7.76	115.09	121.30
1	Z	203	TYR	CB-CG-CD1	-7.75	116.35	121.00
1	W	112	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	V	1024	TYR	CB-CG-CD1	7.74	125.64	121.00
1	A	753	PHE	CB-CG-CD1	7.73	126.21	120.80
1	Z	1290	TYR	CB-CG-CD2	7.72	125.63	121.00
1	W	1119	TYR	CB-CG-CD2	7.71	125.63	121.00
1	A	658	TYR	CB-CG-CD1	7.70	125.62	121.00
1	V	811	LEU	CB-CG-CD1	7.70	124.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	1118	TYR	CD1-CE1-CZ	-7.70	112.87	119.80
1	A	116	TYR	CB-CG-CD1	7.70	125.62	121.00
1	W	448	TYR	CB-CG-CD1	-7.68	116.39	121.00
1	W	1059	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	Z	116	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	Z	267	TYR	CB-CG-CD2	7.67	125.60	121.00
1	A	858	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	W	1306	PHE	CB-CG-CD2	-7.66	115.44	120.80
1	Z	330	PHE	CB-CG-CD2	7.65	126.16	120.80
1	A	658	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	Z	646	PHE	CB-CG-CD2	-7.64	115.45	120.80
2	X	104	TYR	CB-CG-CD1	-7.64	116.42	121.00
1	W	787	PHE	CB-CG-CD2	7.64	126.15	120.80
1	W	235	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	W	493	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	A	681	TYR	CB-CG-CD2	7.61	125.57	121.00
2	C	471	TYR	CB-CG-CD2	-7.61	116.43	121.00
2	X	179	PHE	CB-CG-CD2	7.61	126.13	120.80
1	A	977	PHE	CB-CG-CD1	-7.60	115.48	120.80
1	Z	435	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	A	593	TYR	CB-CG-CD1	7.60	125.56	121.00
1	W	261	PHE	CB-CG-CD2	-7.58	115.49	120.80
1	W	99	TYR	CB-CG-CD1	-7.57	116.46	121.00
2	B	133	ALA	N-CA-CB	7.54	120.66	110.10
1	V	1083	MET	CG-SD-CE	-7.53	88.14	100.20
1	A	777	SER	N-CA-CB	7.53	121.80	110.50
1	W	760	MET	CG-SD-CE	-7.53	88.16	100.20
1	A	663	VAL	CA-CB-CG1	7.53	122.19	110.90
1	W	75	PHE	CB-CG-CD2	7.51	126.06	120.80
1	Z	435	TYR	CB-CG-CD2	7.50	125.50	121.00
1	Z	613	TYR	CB-CG-CD2	7.50	125.50	121.00
1	Z	112	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	300	PHE	CB-CG-CD2	7.49	126.05	120.80
1	A	627	PHE	CB-CG-CD2	-7.49	115.56	120.80
1	W	493	TYR	CB-CG-CD1	7.49	125.50	121.00
1	Z	858	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	Z	1183	PHE	CB-CG-CD1	-7.47	115.57	120.80
1	A	626	TYR	CB-CG-CD1	-7.45	116.53	121.00
1	A	720	TYR	CG-CD2-CE2	-7.43	115.36	121.30
1	A	1382	TYR	CG-CD1-CE1	-7.42	115.37	121.30
1	A	1329	TYR	CD1-CE1-CZ	7.42	126.48	119.80
1	V	1087	ASP	CB-CG-OD1	7.41	124.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	83	TYR	CB-CG-CD2	-7.41	116.56	121.00
1	Z	892	PHE	CB-CG-CD2	7.39	125.97	120.80
1	W	14	LEU	CB-CG-CD2	7.39	123.56	111.00
1	A	641	TYR	CB-CG-CD1	7.37	125.42	121.00
1	W	126	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	W	1054	PHE	CB-CG-CD2	7.37	125.96	120.80
1	A	1215	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	V	593	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	W	203	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	Z	1334	ALA	N-CA-CB	7.36	120.41	110.10
1	A	503	PHE	CB-CG-CD2	7.35	125.95	120.80
1	Z	989	ASN	N-CA-CB	7.34	123.82	110.60
1	W	1284	GLN	N-CA-C	-7.34	91.18	111.00
1	W	698	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	V	409	TYR	CB-CG-CD1	-7.33	116.60	121.00
1	A	203	TYR	N-CA-CB	7.32	123.78	110.60
2	B	42	TYR	CG-CD2-CE2	-7.32	115.44	121.30
1	W	205	PRO	N-CD-CG	7.31	114.17	103.20
1	W	539	PHE	CB-CG-CD2	-7.30	115.69	120.80
1	V	501	TYR	CG-CD2-CE2	7.30	127.14	121.30
1	W	842	TYR	CG-CD1-CE1	-7.30	115.46	121.30
1	W	405	TYR	N-CA-CB	7.29	123.73	110.60
1	Z	588	VAL	CA-CB-CG1	7.29	121.83	110.90
1	V	448	TYR	CB-CG-CD1	7.28	125.37	121.00
1	Z	168	THR	CA-CB-CG2	-7.26	102.23	112.40
1	V	67	THR	CA-CB-CG2	-7.25	102.25	112.40
2	C	312	VAL	CA-CB-CG1	7.25	121.77	110.90
1	V	520	ALA	CB-CA-C	7.25	120.97	110.10
2	X	151	TYR	CB-CG-CD1	-7.24	116.65	121.00
1	V	1087	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	V	643	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	A	313	ASN	N-CA-CB	-7.21	97.61	110.60
1	Z	166	TYR	CB-CG-CD2	-7.21	116.68	121.00
1	W	298	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	Z	806	THR	CA-CB-CG2	-7.19	102.34	112.40
1	V	7	ALA	N-CA-CB	7.18	120.16	110.10
1	A	479	ALA	N-CA-CB	7.17	120.14	110.10
1	Z	842	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	Z	950	PHE	CB-CG-CD2	7.16	125.81	120.80
1	Z	1098	ILE	N-CA-C	-7.16	91.68	111.00
1	Z	907	TYR	CB-CG-CD2	-7.14	116.71	121.00
1	A	948	LEU	CB-CG-CD1	7.14	123.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	363	TYR	CB-CG-CD2	-7.13	116.72	121.00
2	B	387	THR	CA-CB-CG2	-7.13	102.42	112.40
1	A	243	ARG	NH1-CZ-NH2	7.12	127.23	119.40
1	W	833	TYR	CB-CG-CD1	7.12	125.27	121.00
2	B	205	THR	CA-CB-CG2	-7.11	102.44	112.40
1	Z	789	TYR	CG-CD1-CE1	7.11	126.99	121.30
1	V	97	PHE	CB-CG-CD1	7.10	125.77	120.80
1	W	1297	TYR	CZ-CE2-CD2	7.09	126.18	119.80
2	X	104	TYR	CB-CG-CD2	7.08	125.25	121.00
1	W	1115	ALA	N-CA-CB	7.08	120.01	110.10
1	A	112	TYR	CB-CG-CD1	7.08	125.25	121.00
2	B	34	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	V	254	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	A	1024	TYR	CG-CD1-CE1	-7.06	115.65	121.30
2	C	42	TYR	CB-CG-CD2	7.06	125.24	121.00
1	W	146	ASP	CB-CG-OD2	7.06	124.65	118.30
1	A	1260	ALA	N-CA-CB	7.04	119.95	110.10
1	W	535	TYR	CG-CD1-CE1	-7.04	115.67	121.30
1	Z	493	TYR	CB-CG-CD2	7.04	125.22	121.00
2	X	65	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	A	330	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	Z	241	TRP	N-CA-CB	7.01	123.21	110.60
2	C	297	TYR	CB-CG-CD1	-7.00	116.80	121.00
1	Z	753	PHE	CB-CG-CD1	6.99	125.69	120.80
1	A	814	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	A	920	TYR	CB-CG-CD1	6.98	125.19	121.00
1	V	300	PHE	CB-CG-CD1	-6.98	115.91	120.80
1	W	706	TYR	CD1-CE1-CZ	6.97	126.08	119.80
2	C	37	VAL	CA-CB-CG1	6.97	121.36	110.90
1	Z	652	TYR	CB-CG-CD1	-6.97	116.82	121.00
1	Z	641	TYR	CB-CG-CD1	-6.97	116.82	121.00
1	A	613	TYR	CB-CG-CD1	6.96	125.18	121.00
1	W	1021	TYR	CG-CD2-CE2	-6.95	115.74	121.30
1	V	1208	PHE	CB-CG-CD2	6.95	125.66	120.80
1	Z	863	TYR	CB-CG-CD2	-6.95	116.83	121.00
2	X	174	PHE	CB-CG-CD2	6.94	125.66	120.80
1	A	117	LEU	CB-CG-CD2	6.93	122.79	111.00
1	V	658	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	W	252	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	709	PHE	CB-CG-CD2	6.93	125.65	120.80
1	Z	751	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	A	580	PRO	N-CA-CB	6.93	111.61	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	44	TYR	CB-CG-CD1	-6.92	116.85	121.00
2	C	33	PHE	CB-CG-CD1	-6.92	115.96	120.80
1	V	112	TYR	CG-CD1-CE1	-6.91	115.77	121.30
1	V	643	TYR	CB-CG-CD1	6.91	125.14	121.00
1	W	1306	PHE	CB-CG-CD1	6.90	125.63	120.80
1	V	1329	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	A	950	PHE	CB-CG-CD2	6.88	125.62	120.80
1	W	1059	TYR	CB-CG-CD1	6.88	125.13	121.00
1	V	388	TYR	CZ-CE2-CD2	-6.88	113.61	119.80
2	B	378	SER	N-CA-CB	6.87	120.80	110.50
1	V	1105	ASN	CB-CG-OD1	-6.85	107.90	121.60
2	C	321	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	1087	ASP	CB-CG-OD1	6.83	124.45	118.30
1	V	388	TYR	CG-CD2-CE2	6.83	126.76	121.30
1	V	913	TYR	CB-CG-CD1	6.82	125.09	121.00
1	V	1215	TYR	CD1-CE1-CZ	6.82	125.94	119.80
2	C	416	ALA	N-CA-CB	6.80	119.62	110.10
1	V	1384	ALA	N-CA-CB	6.79	119.60	110.10
1	Z	992	PHE	CB-CG-CD1	6.78	125.55	120.80
1	Z	435	TYR	CZ-CE2-CD2	-6.75	113.73	119.80
1	V	690	VAL	CA-CB-CG2	-6.74	100.78	110.90
1	A	235	TYR	CB-CG-CD1	6.74	125.05	121.00
1	A	254	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	A	235	TYR	CZ-CE2-CD2	6.73	125.86	119.80
1	V	749	ASP	CB-CG-OD1	6.72	124.35	118.30
1	V	778	LEU	CA-C-N	6.72	135.91	117.10
1	A	1024	TYR	CG-CD2-CE2	-6.71	115.93	121.30
1	A	369	PHE	CG-CD2-CE2	6.71	128.18	120.80
1	A	28	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	Z	1223	ASN	N-CA-CB	6.70	122.65	110.60
2	C	58	ALA	N-CA-CB	6.69	119.47	110.10
1	W	388	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	W	435	TYR	CZ-CE2-CD2	6.69	125.82	119.80
1	A	842	TYR	CG-CD2-CE2	-6.67	115.96	121.30
1	V	174	MET	CG-SD-CE	-6.67	89.52	100.20
1	A	405	TYR	CG-CD2-CE2	6.67	126.64	121.30
2	C	355	VAL	CA-CB-CG2	-6.67	100.89	110.90
1	A	875	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	V	1326	TYR	CG-CD2-CE2	-6.66	115.97	121.30
1	A	858	TYR	CB-CG-CD1	6.66	124.99	121.00
1	W	568	ALA	N-CA-CB	6.65	119.41	110.10
1	A	1336	PRO	N-CA-CB	6.64	111.27	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	44	TYR	CB-CG-CD2	6.64	124.99	121.00
1	Z	1297	TYR	CB-CG-CD1	-6.64	117.02	121.00
1	Z	614	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	C	42	TYR	CB-CG-CD1	-6.63	117.02	121.00
1	W	20	ALA	CB-CA-C	-6.63	100.16	110.10
2	X	73	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	A	1111	LEU	CB-CG-CD2	6.62	122.26	111.00
1	V	1215	TYR	CB-CG-CD1	6.62	124.97	121.00
2	X	297	TYR	CB-CG-CD1	-6.62	117.03	121.00
2	C	412	SER	N-CA-CB	6.60	120.40	110.50
1	V	1163	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	V	1200	TYR	N-CA-CB	6.57	122.43	110.60
1	Z	1181	THR	CA-CB-CG2	-6.57	103.21	112.40
2	C	450	TYR	CB-CG-CD1	6.56	124.94	121.00
1	W	556	VAL	CA-CB-CG1	-6.55	101.07	110.90
1	V	84	TYR	CB-CG-CD2	6.55	124.93	121.00
1	A	1248	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	A	512	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	V	554	THR	CA-CB-CG2	-6.53	103.26	112.40
1	W	227	LEU	CB-CG-CD2	6.53	122.10	111.00
1	W	248	THR	CA-CB-CG2	-6.53	103.26	112.40
1	V	1326	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	A	74	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	327	SER	N-CA-CB	6.52	120.28	110.50
2	C	165	THR	CA-CB-CG2	-6.52	103.28	112.40
1	A	681	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	A	252	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	434	ALA	N-CA-CB	6.51	119.21	110.10
1	V	363	TYR	CB-CG-CD1	6.51	124.91	121.00
1	Z	361	VAL	CA-CB-CG1	6.51	120.66	110.90
1	W	1313	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	V	652	TYR	CG-CD1-CE1	6.50	126.50	121.30
2	C	311	TYR	CB-CG-CD1	-6.49	117.10	121.00
1	V	318	THR	CA-CB-CG2	-6.49	103.31	112.40
1	W	101	TYR	CB-CG-CD2	-6.49	117.11	121.00
1	Z	833	TYR	CB-CG-CD1	6.49	124.89	121.00
1	V	764	MET	N-CA-C	-6.49	93.49	111.00
2	C	471	TYR	CB-CG-CD1	6.48	124.89	121.00
1	V	1071	TRP	CH2-CZ2-CE2	6.48	123.88	117.40
1	W	674	THR	CA-CB-CG2	-6.48	103.33	112.40
1	Z	599	PHE	CB-CG-CD2	-6.48	116.26	120.80
1	W	571	VAL	CA-CB-CG2	-6.48	101.18	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	903	SER	N-CA-CB	6.48	120.21	110.50
1	Z	1215	TYR	CG-CD1-CE1	-6.47	116.12	121.30
1	A	68	THR	CA-CB-CG2	6.47	121.46	112.40
1	W	804	MET	CA-CB-CG	-6.47	102.31	113.30
1	A	771	ALA	N-CA-CB	6.46	119.14	110.10
1	W	491	LEU	CB-CG-CD2	6.46	121.98	111.00
1	A	208	PHE	CB-CG-CD2	-6.46	116.28	120.80
1	V	1082	PHE	CB-CG-CD1	6.45	125.32	120.80
1	W	850	VAL	CA-CB-CG2	-6.45	101.22	110.90
2	C	333	TYR	CG-CD2-CE2	-6.45	116.14	121.30
1	A	1212	PHE	CB-CG-CD1	6.45	125.31	120.80
1	A	369	PHE	CB-CG-CD1	6.45	125.31	120.80
1	W	1242	PRO	N-CA-CB	6.44	111.03	103.30
1	A	598	ASP	CB-CG-OD2	6.44	124.10	118.30
2	C	253	TYR	CG-CD2-CE2	-6.44	116.15	121.30
1	W	1090	PHE	CB-CG-CD2	-6.44	116.29	120.80
1	A	235	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	Z	383	TYR	CB-CG-CD2	6.42	124.85	121.00
1	Z	1074	ALA	N-CA-CB	6.42	119.09	110.10
1	A	842	TYR	CB-CG-CD2	6.42	124.85	121.00
1	A	295	TYR	CG-CD1-CE1	-6.41	116.17	121.30
2	X	449	VAL	CG1-CB-CG2	6.41	121.16	110.90
1	V	512	TYR	CB-CG-CD1	6.40	124.84	121.00
1	V	1085	TYR	CB-CG-CD2	6.39	124.84	121.00
1	W	514	ALA	N-CA-CB	6.39	119.05	110.10
1	V	738	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	Z	241	TRP	C-N-CA	6.39	135.72	122.30
2	X	311	TYR	CG-CD2-CE2	-6.39	116.19	121.30
2	C	247	TYR	CB-CG-CD2	6.39	124.83	121.00
1	W	748	THR	CA-CB-CG2	-6.39	103.46	112.40
1	W	738	TYR	CB-CG-CD2	6.38	124.83	121.00
1	V	913	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	930	LEU	CB-CG-CD2	6.38	121.84	111.00
2	B	176	VAL	CG1-CB-CG2	-6.38	100.70	110.90
1	A	112	TYR	CG-CD1-CE1	-6.37	116.20	121.30
1	V	1252	ARG	N-CA-CB	6.37	122.07	110.60
1	Z	1082	PHE	CB-CG-CD2	-6.37	116.34	120.80
1	A	1248	PHE	CB-CG-CD1	6.36	125.25	120.80
1	W	435	TYR	CD1-CG-CD2	6.36	124.89	117.90
1	V	982	GLY	N-CA-C	-6.35	97.22	113.10
1	W	742	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	A	1136	VAL	CA-CB-CG1	6.35	120.42	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	111	SER	O-C-N	6.35	132.86	122.70
1	V	1274	TYR	CB-CG-CD1	-6.34	117.19	121.00
1	W	1082	PHE	CB-CG-CD2	-6.34	116.36	120.80
1	W	409	TYR	CD1-CE1-CZ	6.33	125.50	119.80
1	Z	111	SER	N-CA-CB	6.33	119.99	110.50
1	W	977	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	W	1122	THR	CA-CB-CG2	-6.32	103.56	112.40
1	Z	1196	ASN	CB-CG-OD1	-6.31	108.98	121.60
1	W	243	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
1	V	307	PHE	CB-CG-CD2	6.29	125.20	120.80
2	X	210	ALA	N-CA-CB	6.29	118.91	110.10
2	X	427	SER	N-CA-CB	6.29	119.94	110.50
1	Z	897	THR	CA-CB-CG2	-6.29	103.60	112.40
1	W	293	PHE	CB-CG-CD1	6.28	125.20	120.80
1	Z	1157	PHE	CB-CG-CD2	6.27	125.19	120.80
1	A	409	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	1212	PHE	CB-CG-CD2	-6.27	116.41	120.80
2	C	311	TYR	O-C-N	6.26	132.72	122.70
1	W	789	TYR	CB-CG-CD1	6.26	124.76	121.00
1	W	67	THR	CA-CB-CG2	-6.26	103.64	112.40
1	Z	529	TYR	CG-CD1-CE1	6.26	126.31	121.30
2	X	311	TYR	CZ-CE2-CD2	6.26	125.43	119.80
1	W	369	PHE	CD1-CE1-CZ	6.25	127.60	120.10
1	V	1085	TYR	CB-CG-CD1	-6.25	117.25	121.00
2	X	34	TYR	CD1-CE1-CZ	-6.25	114.18	119.80
1	Z	236	TYR	CG-CD1-CE1	-6.24	116.31	121.30
1	W	1290	TYR	CG-CD2-CE2	-6.24	116.31	121.30
1	W	447	TYR	CB-CG-CD1	6.23	124.74	121.00
2	B	321	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	V	388	TYR	CB-CG-CD1	6.23	124.74	121.00
1	W	1186	TYR	CB-CG-CD1	-6.23	117.26	121.00
2	X	472	ARG	NH1-CZ-NH2	6.22	126.24	119.40
1	V	757	VAL	CA-CB-CG1	-6.22	101.57	110.90
2	X	182	VAL	N-CA-C	-6.22	94.21	111.00
2	X	416	ALA	CB-CA-C	-6.22	100.77	110.10
2	B	311	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	Z	828	MET	CG-SD-CE	-6.21	90.26	100.20
2	B	311	TYR	CG-CD2-CE2	6.21	126.27	121.30
1	A	388	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	V	1205	ALA	N-CA-CB	6.20	118.78	110.10
1	W	910	GLU	N-CA-CB	6.20	121.76	110.60
1	W	170	ALA	N-CA-CB	6.20	118.78	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	V	947	TYR	CB-CG-CD1	6.18	124.71	121.00
1	W	651	ASN	N-CA-CB	6.18	121.73	110.60
2	X	264	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	987	ALA	N-CA-CB	6.18	118.75	110.10
1	Z	383	TYR	CG-CD1-CE1	6.17	126.24	121.30
1	Z	881	VAL	CA-CB-CG2	-6.17	101.64	110.90
1	A	146	ASP	CB-CG-OD1	6.17	123.85	118.30
1	Z	643	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	Z	1085	TYR	CB-CG-CD2	-6.17	117.30	121.00
2	B	365	VAL	CA-CB-CG1	6.17	120.15	110.90
1	A	22	ALA	N-CA-CB	6.16	118.73	110.10
2	B	276	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	V	627	PHE	CB-CG-CD1	-6.16	116.49	120.80
1	A	849	PHE	CB-CG-CD2	-6.16	116.49	120.80
1	A	977	PHE	CB-CG-CD2	6.16	125.11	120.80
1	V	1331	ALA	CB-CA-C	-6.16	100.86	110.10
1	W	964	VAL	CA-CB-CG2	-6.16	101.67	110.90
1	V	565	THR	N-CA-CB	6.15	121.99	110.30
1	Z	363	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	W	789	TYR	N-CA-C	-6.14	94.42	111.00
1	Z	514	ALA	N-CA-CB	6.14	118.70	110.10
1	W	641	TYR	CG-CD1-CE1	6.14	126.21	121.30
1	Z	667	TYR	CB-CG-CD2	6.14	124.68	121.00
1	Z	1236	THR	CA-CB-CG2	6.14	120.99	112.40
1	A	539	PHE	N-CA-CB	6.13	121.64	110.60
2	B	450	TYR	CZ-CE2-CD2	6.13	125.32	119.80
1	A	442	THR	N-CA-C	-6.13	94.46	111.00
1	V	752	TYR	CB-CG-CD1	6.12	124.67	121.00
1	W	1339	GLY	N-CA-C	-6.12	97.80	113.10
1	V	975	THR	CA-CB-CG2	-6.12	103.84	112.40
1	A	824	VAL	CA-CB-CG1	6.11	120.07	110.90
1	A	295	TYR	CD1-CG-CD2	6.11	124.61	117.90
1	Z	343	VAL	CA-CB-CG1	6.11	120.06	110.90
1	A	512	TYR	CG-CD2-CE2	-6.10	116.42	121.30
1	V	956	VAL	CA-CB-CG1	-6.10	101.75	110.90
1	Z	57	ALA	N-CA-CB	6.10	118.64	110.10
1	A	1354	GLN	CA-CB-CG	6.09	126.81	113.40
1	W	203	TYR	CG-CD2-CE2	-6.09	116.42	121.30
1	W	1065	ILE	O-C-N	-6.09	112.95	122.70
1	A	1118	TYR	CZ-CE2-CD2	-6.09	114.32	119.80
1	W	85	ASP	N-CA-CB	6.09	121.56	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	720	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	Z	293	PHE	CG-CD2-CE2	-6.09	114.10	120.80
1	V	295	TYR	CG-CD1-CE1	-6.09	116.43	121.30
1	V	84	TYR	CB-CG-CD1	-6.08	117.35	121.00
2	B	306	GLU	OE1-CD-OE2	6.08	130.60	123.30
1	Z	435	TYR	CG-CD2-CE2	6.08	126.17	121.30
2	X	392	THR	CA-CB-CG2	-6.08	103.89	112.40
1	V	66	ALA	N-CA-CB	6.08	118.61	110.10
1	Z	1151	ALA	N-CA-CB	6.08	118.61	110.10
2	C	40	GLN	N-CA-CB	6.08	121.54	110.60
1	W	267	TYR	N-CA-CB	6.07	121.52	110.60
1	A	193	PHE	CB-CG-CD2	-6.05	116.56	120.80
1	V	48	THR	CA-CB-CG2	6.05	120.88	112.40
2	C	77	TYR	CB-CG-CD1	-6.05	117.37	121.00
2	C	179	PHE	CZ-CE2-CD2	-6.05	112.84	120.10
1	V	340	TYR	CG-CD1-CE1	6.05	126.14	121.30
1	V	744	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	V	1182	SER	N-CA-CB	6.04	119.56	110.50
1	W	806	THR	CA-CB-CG2	-6.03	103.95	112.40
2	B	321	TYR	CB-CG-CD2	6.03	124.62	121.00
1	A	1061	TYR	CB-CG-CD2	-6.03	117.39	121.00
2	X	311	TYR	N-CA-CB	6.02	121.44	110.60
1	Z	1337	ALA	N-CA-CB	6.02	118.52	110.10
1	A	193	PHE	CB-CG-CD1	6.01	125.01	120.80
2	X	92	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	A	994	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	V	947	TYR	CB-CG-CD2	-6.01	117.39	121.00
2	C	276	TYR	CG-CD2-CE2	6.01	126.11	121.30
2	B	296	MET	CG-SD-CE	-6.01	90.59	100.20
1	Z	1210	LEU	N-CA-C	-6.01	94.78	111.00
2	B	349	LYS	CA-CB-CG	6.00	126.60	113.40
1	W	1127	VAL	CA-CB-CG2	6.00	119.90	110.90
1	W	1054	PHE	CB-CG-CD1	-6.00	116.60	120.80
2	B	242	SER	O-C-N	-5.99	113.11	122.70
1	W	387	VAL	N-CA-C	-5.99	94.82	111.00
1	Z	1313	PHE	CG-CD1-CE1	5.99	127.39	120.80
1	A	868	TYR	CZ-CE2-CD2	5.98	125.18	119.80
1	V	628	TYR	CB-CG-CD1	-5.98	117.41	121.00
2	X	374	THR	CA-CB-CG2	-5.98	104.03	112.40
1	Z	819	ILE	CA-CB-CG1	5.98	122.36	111.00
1	A	295	TYR	CG-CD2-CE2	-5.98	116.52	121.30
1	W	295	TYR	CB-CG-CD1	-5.97	117.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	165	THR	CA-CB-OG1	5.97	121.53	109.00
1	V	830	ASN	N-CA-C	-5.96	94.91	111.00
1	Z	1291	VAL	N-CA-C	-5.95	94.92	111.00
1	A	146	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	891	TYR	CG-CD1-CE1	-5.95	116.54	121.30
1	W	411	VAL	CA-CB-CG1	5.95	119.83	110.90
1	V	236	TYR	CD1-CE1-CZ	-5.95	114.45	119.80
1	A	869	PHE	N-CA-C	-5.94	94.96	111.00
1	V	1327	PHE	CG-CD1-CE1	5.94	127.33	120.80
1	V	754	ILE	N-CA-C	-5.93	94.98	111.00
1	W	267	TYR	CD1-CE1-CZ	-5.93	114.46	119.80
1	Z	223	VAL	CA-CB-CG2	-5.93	102.00	110.90
1	V	410	THR	CA-CB-CG2	-5.93	104.10	112.40
2	C	220	VAL	CA-CB-CG2	-5.93	102.01	110.90
1	V	355	TYR	CZ-CE2-CD2	5.93	125.14	119.80
1	A	1146	THR	CA-CB-CG2	-5.92	104.11	112.40
1	Z	1306	PHE	CD1-CE1-CZ	-5.92	112.99	120.10
2	C	321	TYR	CB-CG-CD1	5.92	124.55	121.00
1	V	166	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	V	447	TYR	CB-CG-CD1	5.91	124.55	121.00
1	V	987	ALA	N-CA-CB	5.91	118.37	110.10
1	W	539	PHE	CB-CG-CD1	5.91	124.94	120.80
2	C	135	VAL	CA-CB-CG1	-5.91	102.04	110.90
1	V	846	ASN	N-CA-CB	5.91	121.23	110.60
1	A	340	TYR	CG-CD1-CE1	-5.90	116.58	121.30
2	B	349	LYS	N-CA-CB	5.90	121.22	110.60
1	A	1350	TYR	CB-CG-CD2	5.90	124.54	121.00
2	B	114	THR	N-CA-C	-5.90	95.08	111.00
1	W	673	THR	CA-CB-CG2	-5.89	104.15	112.40
1	W	931	TRP	CB-CG-CD1	5.89	134.66	127.00
1	Z	283	ILE	N-CA-C	-5.89	95.09	111.00
2	C	411	SER	N-CA-CB	5.89	119.34	110.50
1	V	1223	ASN	N-CA-CB	5.89	121.20	110.60
2	B	50	LEU	O-C-N	-5.88	113.29	122.70
1	A	1168	ASN	N-CA-CB	5.88	121.18	110.60
1	W	789	TYR	CG-CD1-CE1	-5.88	116.60	121.30
1	Z	123	ALA	N-CA-CB	5.88	118.33	110.10
2	B	402	SER	N-CA-CB	5.87	119.31	110.50
1	W	828	MET	CG-SD-CE	-5.87	90.80	100.20
1	V	363	TYR	CZ-CE2-CD2	-5.87	114.52	119.80
1	W	792	PRO	N-CA-CB	5.87	110.34	103.30
1	Z	1186	TYR	CB-CG-CD2	-5.87	117.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	972	ASN	O-C-N	-5.86	113.32	122.70
1	V	436	GLU	N-CA-CB	5.86	121.15	110.60
1	V	298	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	V	1371	VAL	CA-CB-CG2	-5.86	102.11	110.90
1	A	782	THR	CA-CB-CG2	-5.86	104.20	112.40
1	Z	1061	TYR	CB-CG-CD1	5.86	124.51	121.00
1	A	667	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	W	672	PHE	CB-CG-CD1	5.85	124.90	120.80
1	W	1085	TYR	CG-CD2-CE2	-5.85	116.62	121.30
1	V	1138	THR	N-CA-C	-5.85	95.20	111.00
1	V	933	SER	N-CA-CB	5.85	119.27	110.50
1	A	708	ASN	CB-CA-C	-5.84	98.71	110.40
1	W	1056	LEU	CB-CG-CD1	5.84	120.94	111.00
1	Z	112	TYR	CG-CD2-CE2	-5.84	116.63	121.30
1	W	992	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	Z	877	VAL	CA-CB-CG1	-5.84	102.14	110.90
2	C	182	VAL	CA-CB-CG1	5.83	119.65	110.90
2	X	166	THR	CA-CB-CG2	-5.83	104.24	112.40
2	C	276	TYR	CD1-CE1-CZ	5.83	125.05	119.80
2	B	212	VAL	CA-CB-CG2	5.83	119.64	110.90
1	Z	1118	TYR	CG-CD1-CE1	5.83	125.96	121.30
1	A	1371	VAL	CA-CB-CG2	-5.82	102.16	110.90
1	W	407	THR	CA-CB-CG2	-5.82	104.25	112.40
1	Z	698	TYR	CB-CG-CD2	5.82	124.49	121.00
1	V	728	SER	N-CA-CB	5.81	119.22	110.50
1	W	1156	THR	CA-CB-CG2	-5.81	104.26	112.40
1	A	1364	TYR	CZ-CE2-CD2	-5.81	114.57	119.80
1	W	844	VAL	CA-CB-CG2	5.81	119.61	110.90
1	V	92	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	V	863	TYR	CD1-CE1-CZ	-5.81	114.58	119.80
1	A	386	PRO	N-CA-CB	-5.80	96.22	102.60
1	W	84	TYR	CA-CB-CG	5.80	124.43	113.40
1	Z	1087	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	W	1132	TYR	CD1-CE1-CZ	-5.80	114.58	119.80
1	Z	1186	TYR	CB-CG-CD1	5.80	124.48	121.00
1	Z	18	SER	N-CA-CB	5.80	119.20	110.50
1	Z	1132	TYR	CD1-CE1-CZ	-5.79	114.58	119.80
2	B	195	TYR	N-CA-CB	5.79	121.02	110.60
1	W	937	VAL	CA-CB-CG2	5.79	119.59	110.90
1	V	1163	PHE	CB-CG-CD1	5.79	124.85	120.80
1	V	218	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	V	727	PHE	CB-CG-CD2	-5.79	116.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	355	TYR	CB-CG-CD2	5.79	124.47	121.00
1	W	1080	GLN	N-CA-CB	5.79	121.01	110.60
1	A	900	TYR	CB-CG-CD2	-5.78	117.53	121.00
2	X	77	TYR	CG-CD2-CE2	-5.78	116.68	121.30
1	W	1219	ALA	N-CA-CB	5.78	118.19	110.10
1	Z	964	VAL	CA-CB-CG2	-5.78	102.23	110.90
1	W	709	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	Z	287	ASN	N-CA-CB	5.77	120.98	110.60
1	Z	323	THR	CA-CB-CG2	-5.76	104.33	112.40
1	Z	1256	PHE	C-N-CA	5.76	136.10	121.70
1	A	1367	VAL	CA-CB-CG1	5.76	119.53	110.90
2	B	35	SER	N-CA-CB	5.75	119.13	110.50
1	W	154	LEU	CB-CG-CD1	5.75	120.78	111.00
1	Z	388	TYR	CD1-CE1-CZ	-5.75	114.62	119.80
2	X	347	VAL	CA-CB-CG2	-5.75	102.27	110.90
1	V	738	TYR	CG-CD2-CE2	-5.75	116.70	121.30
2	X	63	TYR	CZ-CE2-CD2	5.75	124.97	119.80
1	A	47	SER	N-CA-CB	5.74	119.11	110.50
1	Z	907	TYR	N-CA-CB	5.74	120.94	110.60
1	V	753	PHE	CB-CG-CD1	-5.74	116.78	120.80
2	X	179	PHE	CG-CD1-CE1	5.74	127.11	120.80
1	V	1252	ARG	CD-NE-CZ	5.74	131.63	123.60
1	V	1264	LEU	CB-CG-CD2	5.73	120.74	111.00
1	Z	126	TYR	N-CA-CB	5.73	120.92	110.60
1	W	1351	VAL	CA-CB-CG2	-5.73	102.31	110.90
1	Z	337	PHE	CB-CG-CD1	5.73	124.81	120.80
1	V	994	PHE	CB-CG-CD1	-5.72	116.79	120.80
1	W	126	TYR	CG-CD1-CE1	-5.72	116.72	121.30
2	X	35	SER	N-CA-CB	5.72	119.09	110.50
1	V	549	MET	CG-SD-CE	-5.72	91.05	100.20
1	V	805	ALA	O-C-N	5.71	131.84	122.70
1	A	193	PHE	N-CA-CB	5.70	120.86	110.60
1	A	931	TRP	NE1-CE2-CZ2	5.70	136.67	130.40
1	W	1323	ALA	N-CA-CB	5.70	118.07	110.10
1	V	1076	ASN	N-CA-C	-5.69	95.63	111.00
2	B	27	THR	CA-CB-CG2	5.69	120.36	112.40
2	C	317	ILE	CA-CB-CG1	5.69	121.80	111.00
2	C	353	SER	N-CA-CB	5.68	119.02	110.50
1	A	872	THR	CA-CB-CG2	-5.68	104.45	112.40
1	V	213	TYR	CB-CG-CD1	5.68	124.41	121.00
1	V	1354	GLN	N-CA-CB	5.67	120.82	110.60
1	Z	1367	VAL	CA-CB-CG2	-5.67	102.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	THR	CA-CB-CG2	-5.67	104.47	112.40
1	A	160	LEU	CB-CG-CD2	5.66	120.63	111.00
1	A	626	TYR	CB-CG-CD2	5.66	124.40	121.00
2	B	399	THR	CA-CB-CG2	-5.66	104.47	112.40
1	W	886	VAL	CA-CB-CG1	-5.65	102.42	110.90
1	W	253	THR	CA-CB-CG2	-5.64	104.50	112.40
2	C	174	PHE	CB-CA-C	-5.64	99.11	110.40
1	A	1138	THR	CA-CB-CG2	-5.64	104.51	112.40
1	Z	1006	ASN	N-CA-CB	5.63	120.74	110.60
1	A	962	THR	N-CA-C	-5.63	95.80	111.00
1	A	367	THR	CA-CB-CG2	-5.62	104.52	112.40
1	W	218	TYR	CB-CG-CD1	-5.62	117.62	121.00
1	W	484	ASN	N-CA-C	-5.62	95.81	111.00
1	W	743	ALA	CB-CA-C	-5.62	101.66	110.10
1	W	1308	TYR	CB-CG-CD1	5.62	124.38	121.00
1	V	1335	TYR	CB-CG-CD2	5.62	124.37	121.00
1	W	742	TYR	CG-CD2-CE2	-5.62	116.80	121.30
1	W	1059	TYR	CA-CB-CG	5.62	124.08	113.40
1	Z	447	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	697	VAL	CA-CB-CG2	-5.62	102.47	110.90
2	B	446	THR	CA-CB-CG2	-5.61	104.54	112.40
1	W	997	SER	C-N-CA	5.61	135.73	121.70
1	W	1183	PHE	CB-CG-CD1	-5.61	116.87	120.80
1	V	925	THR	N-CA-CB	5.61	120.95	110.30
1	V	1278	ILE	C-N-CA	5.61	135.71	121.70
2	C	73	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	W	628	TYR	CG-CD1-CE1	-5.60	116.82	121.30
2	X	186	PHE	CD1-CG-CD2	-5.60	111.02	118.30
1	W	1118	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	W	513	ALA	C-N-CA	5.60	135.70	121.70
1	A	1277	SER	N-CA-CB	5.60	118.89	110.50
2	X	60	VAL	CG1-CB-CG2	5.60	119.85	110.90
1	V	404	TRP	N-CA-CB	5.59	120.67	110.60
1	V	936	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	W	116	TYR	CG-CD2-CE2	-5.59	116.83	121.30
1	W	896	THR	N-CA-CB	5.59	120.92	110.30
1	A	963	THR	CA-CB-CG2	-5.58	104.58	112.40
1	Z	720	TYR	CG-CD1-CE1	-5.58	116.83	121.30
1	Z	920	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	V	888	ALA	N-CA-CB	5.58	117.92	110.10
1	W	173	ASN	C-N-CA	5.58	135.66	121.70
1	W	338	TYR	CB-CG-CD1	-5.58	117.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	1084	THR	N-CA-C	-5.58	95.93	111.00
1	Z	54	GLN	N-CA-C	-5.58	95.93	111.00
1	A	1308	TYR	CG-CD2-CE2	5.58	125.76	121.30
1	W	1107	THR	CA-CB-CG2	-5.57	104.60	112.40
1	A	1182	SER	N-CA-CB	5.57	118.86	110.50
1	Z	641	TYR	CB-CG-CD2	5.57	124.34	121.00
1	A	855	LYS	N-CA-CB	5.57	120.62	110.60
2	B	111	GLN	N-CA-CB	5.57	120.62	110.60
1	Z	600	GLY	N-CA-C	-5.57	99.18	113.10
1	W	1350	TYR	CG-CD1-CE1	-5.57	116.85	121.30
1	V	234	ALA	N-CA-CB	5.56	117.89	110.10
1	V	689	ALA	CB-CA-C	-5.56	101.76	110.10
1	A	405	TYR	CD1-CE1-CZ	-5.55	114.80	119.80
1	V	778	LEU	O-C-N	-5.55	110.55	121.10
1	V	1159	GLY	N-CA-C	-5.55	99.22	113.10
1	A	78	SER	N-CA-CB	5.55	118.83	110.50
1	V	197	THR	CA-CB-OG1	5.55	120.66	109.00
1	V	1389	THR	CA-CB-CG2	-5.55	104.63	112.40
1	V	4	PRO	N-CD-CG	5.55	111.52	103.20
1	Z	900	TYR	CB-CG-CD2	5.55	124.33	121.00
1	Z	920	TYR	CZ-CE2-CD2	-5.55	114.81	119.80
1	V	921	ILE	N-CA-C	-5.55	96.02	111.00
1	W	641	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	Z	481	ALA	N-CA-CB	5.54	117.86	110.10
1	W	652	TYR	N-CA-CB	5.54	120.57	110.60
2	B	25	ALA	CB-CA-C	5.54	118.41	110.10
1	V	764	MET	CG-SD-CE	5.54	109.06	100.20
1	V	1144	LEU	CB-CG-CD2	5.54	120.41	111.00
2	C	297	TYR	CA-CB-CG	-5.53	102.89	113.40
1	V	754	ILE	N-CA-CB	5.53	123.52	110.80
1	Z	566	LEU	CB-CG-CD2	5.53	120.40	111.00
1	A	76	PRO	N-CA-CB	5.53	109.93	103.30
1	W	485	LEU	N-CA-CB	5.53	121.46	110.40
1	W	1085	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	Z	627	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	A	489	ALA	N-CA-CB	5.53	117.84	110.10
2	B	245	VAL	CA-CB-CG2	-5.53	102.61	110.90
1	W	693	PRO	N-CD-CG	5.53	111.49	103.20
1	V	355	TYR	CG-CD2-CE2	-5.53	116.88	121.30
1	Z	13	TYR	CB-CG-CD1	-5.53	117.69	121.00
1	A	282	TRP	CE2-CD2-CG	-5.52	102.88	107.30
1	A	862	ASP	CB-CG-OD2	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	SER	N-CA-C	-5.52	96.09	111.00
1	A	1087	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	W	101	TYR	CB-CG-CD1	5.52	124.31	121.00
1	W	89	LYS	CB-CG-CD	5.52	125.95	111.60
1	A	890	LEU	CB-CG-CD1	5.51	120.37	111.00
2	B	219	ALA	N-CA-CB	5.51	117.82	110.10
1	A	823	THR	CA-CB-CG2	-5.51	104.69	112.40
1	V	628	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
1	Z	236	TYR	CD1-CE1-CZ	5.51	124.76	119.80
1	Z	1353	LEU	N-CA-CB	5.51	121.42	110.40
1	V	431	LYS	N-CA-CB	5.51	120.51	110.60
1	W	383	TYR	CB-CG-CD2	5.51	124.30	121.00
1	W	742	TYR	CD1-CG-CD2	5.51	123.96	117.90
1	A	1196	ASN	N-CA-CB	5.50	120.51	110.60
1	A	257	GLY	N-CA-C	-5.50	99.34	113.10
1	Z	907	TYR	CB-CG-CD1	5.50	124.30	121.00
2	B	370	THR	N-CA-CB	5.50	120.74	110.30
1	V	1342	THR	CA-CB-CG2	-5.50	104.71	112.40
1	V	1343	SER	N-CA-C	-5.50	96.16	111.00
1	V	501	TYR	CB-CG-CD1	-5.49	117.70	121.00
2	X	302	MET	CG-SD-CE	-5.49	91.42	100.20
2	C	195	TYR	CG-CD1-CE1	5.48	125.68	121.30
1	V	235	TYR	CG-CD1-CE1	-5.48	116.92	121.30
2	X	58	ALA	N-CA-CB	5.48	117.77	110.10
1	Z	850	VAL	CA-CB-CG2	-5.48	102.68	110.90
1	Z	203	TYR	CB-CG-CD2	5.48	124.29	121.00
1	A	687	THR	O-C-N	-5.48	113.89	123.20
1	Z	814	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	967	PRO	N-CD-CG	5.47	111.41	103.20
1	A	1323	ALA	N-CA-CB	5.47	117.76	110.10
1	Z	856	LEU	N-CA-C	-5.47	96.23	111.00
1	A	1251	ILE	O-C-N	-5.47	113.95	122.70
1	V	304	TYR	CB-CG-CD2	5.47	124.28	121.00
1	W	764	MET	CG-SD-CE	-5.47	91.45	100.20
1	W	809	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	Z	1038	ALA	N-CA-CB	5.47	117.75	110.10
2	C	264	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	V	1152	ALA	CB-CA-C	-5.46	101.91	110.10
1	W	731	ALA	N-CA-CB	5.46	117.75	110.10
1	W	950	PHE	N-CA-CB	5.46	120.43	110.60
1	Z	646	PHE	CB-CG-CD1	5.46	124.62	120.80
1	A	218	TYR	CB-CG-CD2	-5.46	117.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	929	SER	N-CA-CB	5.46	118.69	110.50
1	A	939	PHE	N-CA-CB	5.46	120.42	110.60
1	V	892	PHE	CB-CG-CD2	5.46	124.62	120.80
1	W	920	TYR	CZ-CE2-CD2	-5.46	114.89	119.80
1	Z	1368	LEU	N-CA-CB	5.46	121.31	110.40
2	C	293	TYR	CB-CG-CD2	5.46	124.27	121.00
1	A	544	GLU	O-C-N	-5.45	110.74	121.10
1	W	936	TYR	CD1-CE1-CZ	5.45	124.71	119.80
1	W	1344	VAL	CB-CA-C	-5.45	101.05	111.40
1	A	984	GLU	CA-CB-CG	5.45	125.38	113.40
1	A	1320	PRO	N-CD-CG	5.45	111.37	103.20
1	A	1388	PHE	CB-CG-CD2	5.44	124.61	120.80
2	C	297	TYR	CB-CG-CD2	5.44	124.27	121.00
1	W	665	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	W	475	THR	CA-CB-CG2	-5.44	104.78	112.40
1	A	698	TYR	CG-CD2-CE2	5.44	125.65	121.30
2	C	287	VAL	CA-CB-CG2	-5.44	102.74	110.90
2	C	313	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	Z	1118	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	Z	802	PRO	N-CD-CG	5.44	111.36	103.20
1	A	186	PHE	CB-CG-CD2	5.43	124.60	120.80
1	V	891	TYR	CG-CD1-CE1	-5.43	116.95	121.30
1	W	300	PHE	CB-CG-CD2	5.43	124.60	120.80
1	W	1350	TYR	CD1-CE1-CZ	5.43	124.69	119.80
2	B	342	ASN	C-N-CA	5.42	135.26	121.70
2	X	293	TYR	CB-CG-CD2	5.42	124.25	121.00
1	Z	236	TYR	CB-CG-CD2	5.42	124.25	121.00
1	Z	1013	ASN	N-CA-CB	-5.42	100.84	110.60
2	B	381	SER	N-CA-CB	5.42	118.63	110.50
1	V	1388	PHE	CG-CD1-CE1	5.42	126.76	120.80
2	B	90	ALA	CB-CA-C	-5.41	101.98	110.10
1	W	1336	PRO	C-N-CA	5.41	135.24	121.70
2	X	42	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	Z	900	TYR	CB-CG-CD1	-5.41	117.75	121.00
2	B	233	THR	N-CA-CB	5.41	120.57	110.30
1	W	861	THR	N-CA-C	-5.41	96.40	111.00
1	W	235	TYR	CG-CD2-CE2	-5.40	116.98	121.30
1	A	566	LEU	N-CA-CB	5.40	121.20	110.40
1	V	787	PHE	CZ-CE2-CD2	5.40	126.58	120.10
2	X	273	GLN	N-CA-C	-5.40	96.42	111.00
2	C	32	THR	N-CA-CB	5.40	120.56	110.30
1	Z	86	SER	CB-CA-C	-5.40	99.85	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	836	SER	N-CA-CB	5.40	118.60	110.50
1	Z	838	ASN	N-CA-CB	5.40	120.32	110.60
1	W	5	VAL	CA-CB-CG1	-5.39	102.81	110.90
1	W	535	TYR	CD1-CE1-CZ	5.39	124.65	119.80
2	B	473	LYS	CA-CB-CG	5.39	125.25	113.40
1	V	293	PHE	CB-CG-CD1	5.39	124.57	120.80
1	W	779	PRO	C-N-CA	5.39	135.17	121.70
1	W	833	TYR	CD1-CE1-CZ	-5.39	114.95	119.80
1	A	971	SER	N-CA-CB	-5.38	102.42	110.50
1	V	92	PHE	CA-CB-CG	5.38	126.81	113.90
1	V	1290	TYR	CG-CD1-CE1	-5.38	117.00	121.30
1	A	985	LEU	CB-CG-CD2	5.38	120.15	111.00
1	V	2	THR	CA-CB-CG2	-5.38	104.87	112.40
1	V	99	TYR	CG-CD1-CE1	-5.38	117.00	121.30
2	B	212	VAL	CA-CB-CG1	-5.38	102.84	110.90
1	W	371	PRO	N-CD-CG	5.38	111.26	103.20
1	Z	900	TYR	CG-CD2-CE2	5.38	125.60	121.30
1	W	716	THR	CA-CB-CG2	-5.37	104.88	112.40
1	Z	627	PHE	CG-CD2-CE2	-5.37	114.89	120.80
1	Z	112	TYR	CA-CB-CG	-5.37	103.20	113.40
1	W	448	TYR	CG-CD2-CE2	5.37	125.59	121.30
1	W	1024	TYR	CG-CD1-CE1	-5.37	117.00	121.30
2	C	276	TYR	N-CA-CB	5.37	120.26	110.60
1	V	54	GLN	N-CA-CB	5.37	120.26	110.60
1	V	716	THR	N-CA-CB	5.37	120.50	110.30
1	A	424	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	X	190	ALA	CB-CA-C	5.37	118.15	110.10
1	A	1119	TYR	CG-CD1-CE1	-5.36	117.01	121.30
1	Z	1306	PHE	CG-CD1-CE1	5.36	126.70	120.80
1	A	667	TYR	CB-CG-CD1	5.36	124.22	121.00
1	V	850	VAL	N-CA-C	-5.36	96.53	111.00
1	Z	1119	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	V	523	TYR	N-CA-CB	5.35	120.23	110.60
1	Z	403	ASN	N-CA-CB	5.35	120.23	110.60
2	C	179	PHE	CG-CD2-CE2	5.35	126.69	120.80
1	A	217	LEU	N-CA-CB	5.35	121.10	110.40
1	W	206	PHE	N-CA-C	-5.35	96.56	111.00
1	W	787	PHE	CG-CD1-CE1	5.35	126.69	120.80
1	Z	1023	ASP	CB-CG-OD1	5.35	123.11	118.30
1	W	255	ALA	N-CA-CB	5.35	117.58	110.10
1	V	1330	SER	N-CA-CB	5.34	118.52	110.50
1	W	20	ALA	N-CA-CB	5.34	117.58	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	718	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	V	1071	TRP	CD2-CE2-CZ2	-5.34	115.89	122.30
1	W	1071	TRP	CB-CG-CD1	-5.34	120.06	127.00
1	A	1015	SER	N-CA-CB	5.34	118.51	110.50
1	A	809	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	Z	1327	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	A	659	ASP	N-CA-CB	5.33	120.20	110.60
1	V	467	THR	O-C-N	5.33	131.23	122.70
1	V	907	TYR	CB-CG-CD2	5.33	124.20	121.00
1	A	1129	THR	N-CA-CB	5.33	120.43	110.30
2	B	259	SER	CB-CA-C	-5.33	99.97	110.10
1	Z	184	THR	CA-CB-CG2	-5.33	104.94	112.40
1	Z	1316	HIS	CA-CB-CG	-5.33	104.55	113.60
1	Z	113	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	V	1291	VAL	CA-CB-CG2	-5.32	102.92	110.90
1	A	1281	THR	CA-CB-CG2	-5.32	104.95	112.40
2	X	380	SER	N-CA-CB	5.32	118.48	110.50
1	W	833	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	W	1126	THR	N-CA-C	-5.31	96.65	111.00
1	W	1045	VAL	CA-CB-CG2	5.31	118.87	110.90
1	Z	1324	PRO	N-CD-CG	5.31	111.17	103.20
1	A	936	TYR	CG-CD1-CE1	5.31	125.55	121.30
1	W	435	TYR	CG-CD1-CE1	-5.31	117.05	121.30
1	A	424	TYR	CG-CD1-CE1	-5.31	117.05	121.30
1	A	354	GLU	CG-CD-OE2	-5.31	107.69	118.30
1	V	1187	THR	CA-CB-CG2	-5.31	104.97	112.40
2	X	364	THR	N-CA-CB	5.31	120.39	110.30
1	Z	671	SER	N-CA-CB	5.31	118.46	110.50
1	V	404	TRP	CB-CG-CD2	5.31	133.50	126.60
1	Z	87	VAL	CG1-CB-CG2	5.31	119.39	110.90
1	Z	1280	ILE	N-CA-C	-5.31	96.67	111.00
2	B	142	PRO	N-CA-CB	5.30	109.67	103.30
2	C	135	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	W	309	GLY	N-CA-C	-5.30	99.85	113.10
2	B	381	SER	CB-CA-C	-5.30	100.03	110.10
1	V	83	TYR	CB-CG-CD1	5.30	124.18	121.00
2	B	316	LEU	CB-CG-CD2	5.30	120.00	111.00
1	W	1028	GLU	CG-CD-OE1	-5.29	107.71	118.30
1	W	1329	TYR	CB-CG-CD1	-5.29	117.82	121.00
2	B	95	THR	N-CA-CB	5.29	120.35	110.30
1	V	814	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	V	248	THR	CA-CB-CG2	-5.29	104.99	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	1216	THR	CA-CB-CG2	-5.29	104.99	112.40
1	V	90	VAL	CA-CB-CG1	5.29	118.83	110.90
1	Z	112	TYR	CZ-CE2-CD2	5.29	124.56	119.80
1	A	501	TYR	CG-CD2-CE2	-5.29	117.07	121.30
2	B	113	THR	CA-CB-CG2	-5.29	105.00	112.40
2	B	166	THR	CA-CB-CG2	-5.29	105.00	112.40
1	Z	812	ASN	N-CA-CB	5.29	120.12	110.60
2	C	385	ARG	CD-NE-CZ	-5.29	116.20	123.60
1	Z	1248	PHE	CB-CG-CD2	5.28	124.50	120.80
1	V	1132	TYR	CB-CG-CD1	-5.28	117.83	121.00
2	B	429	THR	CA-CB-CG2	-5.28	105.01	112.40
1	W	1322	ALA	N-CA-CB	5.28	117.48	110.10
1	W	459	GLU	OE1-CD-OE2	5.27	129.63	123.30
1	V	1347	LEU	CB-CG-CD2	5.27	119.97	111.00
1	W	369	PHE	CG-CD1-CE1	-5.27	115.00	120.80
2	X	379	LEU	O-C-N	-5.27	114.27	122.70
1	A	1329	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	279	GLN	CG-CD-OE1	5.27	132.13	121.60
1	A	1119	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	1382	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	V	512	TYR	N-CA-C	-5.26	96.81	111.00
2	B	188	LEU	N-CA-CB	5.25	120.91	110.40
1	V	181	GLY	N-CA-C	-5.25	99.97	113.10
1	Z	163	TYR	CB-CG-CD1	5.25	124.15	121.00
1	A	284	ALA	CB-CA-C	-5.25	102.23	110.10
2	C	121	ASN	N-CA-CB	5.25	120.05	110.60
1	A	987	ALA	CB-CA-C	-5.25	102.23	110.10
1	Z	1194	VAL	CA-CB-CG1	5.25	118.77	110.90
1	A	424	TYR	CD1-CE1-CZ	5.24	124.52	119.80
2	C	431	LEU	O-C-N	-5.24	114.32	122.70
1	Z	363	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	Z	585	PHE	CB-CG-CD2	5.23	124.46	120.80
2	X	87	ALA	N-CA-CB	5.23	117.42	110.10
1	Z	939	PHE	CB-CG-CD1	-5.23	117.14	120.80
1	A	201	ILE	N-CA-C	-5.23	96.89	111.00
2	C	333	TYR	CG-CD1-CE1	-5.23	117.12	121.30
1	V	86	SER	N-CA-CB	5.23	118.34	110.50
1	A	258	SER	O-C-N	-5.22	114.34	122.70
1	W	535	TYR	CG-CD2-CE2	-5.22	117.12	121.30
1	W	730	VAL	CA-CB-CG1	5.22	118.73	110.90
1	Z	593	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	V	1256	PHE	CD1-CE1-CZ	5.22	126.36	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	1272	TYR	CB-CG-CD2	5.22	124.13	121.00
1	V	1215	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	Z	1118	TYR	CZ-CE2-CD2	5.21	124.49	119.80
1	A	817	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	W	667	TYR	N-CA-C	-5.21	96.94	111.00
1	A	1014	ASN	N-CA-C	-5.21	96.95	111.00
1	V	191	GLN	CB-CA-C	-5.20	100.00	110.40
1	V	1054	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	W	771	ALA	N-CA-CB	5.20	117.38	110.10
1	Z	218	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	466	SER	N-CA-C	-5.20	96.96	111.00
2	X	334	LEU	CB-CA-C	-5.20	100.32	110.20
1	Z	1208	PHE	N-CA-CB	5.20	119.96	110.60
1	Z	1308	TYR	C-N-CA	5.19	134.69	121.70
1	V	391	GLY	N-CA-C	-5.19	100.12	113.10
1	V	613	TYR	CD1-CE1-CZ	5.19	124.47	119.80
1	Z	1142	ASN	N-CA-CB	5.19	119.94	110.60
1	A	853	ASN	CB-CG-OD1	-5.19	111.22	121.60
1	A	1215	TYR	CG-CD1-CE1	-5.19	117.15	121.30
2	X	163	THR	O-C-N	5.19	131.00	122.70
1	Z	877	VAL	CA-CB-CG2	5.19	118.68	110.90
1	V	783	SER	N-CA-C	-5.18	97.01	111.00
1	Z	709	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	V	1005	LEU	O-C-N	-5.18	114.41	122.70
1	W	1139	LEU	N-CA-CB	5.18	120.76	110.40
1	A	1053	GLU	CB-CA-C	-5.18	100.04	110.40
1	W	1202	LEU	CB-CG-CD2	5.18	119.80	111.00
2	X	463	ALA	CB-CA-C	-5.18	102.33	110.10
1	Z	875	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	1344	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	W	1072	PHE	CB-CG-CD2	-5.17	117.18	120.80
2	X	173	THR	N-CA-CB	5.17	120.12	110.30
2	X	283	VAL	CA-CB-CG2	-5.17	103.15	110.90
1	W	1352	GLN	CB-CA-C	-5.17	100.07	110.40
1	W	353	VAL	CG1-CB-CG2	5.17	119.17	110.90
1	W	448	TYR	CZ-CE2-CD2	-5.17	115.15	119.80
1	A	318	THR	N-CA-C	-5.16	97.06	111.00
1	A	1154	ASN	N-CA-C	-5.16	97.06	111.00
2	X	275	TYR	CD1-CE1-CZ	5.16	124.45	119.80
1	V	628	TYR	CB-CG-CD2	5.16	124.09	121.00
1	W	348	ASN	CB-CG-OD1	-5.16	111.28	121.60
1	A	59	THR	CA-CB-CG2	-5.16	105.18	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	862	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	X	462	VAL	CA-CB-CG2	5.16	118.63	110.90
1	Z	1097	ALA	N-CA-CB	5.16	117.32	110.10
1	Z	1349	VAL	CG1-CB-CG2	5.15	119.15	110.90
1	A	1279	VAL	CA-CB-CG1	-5.15	103.17	110.90
1	V	1144	LEU	N-CA-CB	5.15	120.69	110.40
1	A	562	PHE	CB-CG-CD2	5.15	124.40	120.80
2	B	73	TYR	N-CA-CB	5.14	119.85	110.60
1	V	29	VAL	N-CA-C	-5.14	97.12	111.00
1	W	820	ASP	N-CA-C	-5.14	97.13	111.00
1	A	85	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	897	THR	CA-CB-CG2	-5.13	105.21	112.40
2	B	258	VAL	N-CA-C	-5.13	97.14	111.00
1	W	646	PHE	O-C-N	-5.13	114.49	122.70
1	W	892	PHE	CD1-CE1-CZ	5.13	126.26	120.10
1	W	1284	GLN	N-CA-CB	5.13	119.84	110.60
1	A	1272	TYR	CB-CG-CD2	5.13	124.08	121.00
1	W	294	THR	CA-CB-CG2	-5.13	105.22	112.40
1	Z	624	LEU	N-CA-C	-5.13	97.16	111.00
1	Z	1308	TYR	CG-CD1-CE1	5.13	125.40	121.30
1	A	1024	TYR	CD1-CG-CD2	5.12	123.53	117.90
1	A	435	TYR	CG-CD1-CE1	-5.12	117.20	121.30
1	V	409	TYR	CG-CD1-CE1	-5.12	117.20	121.30
2	X	321	TYR	O-C-N	5.12	130.89	122.70
1	A	1079	LYS	C-N-CA	5.12	134.50	121.70
1	W	412	GLN	CB-CA-C	5.12	120.64	110.40
1	V	353	VAL	CA-CB-CG2	-5.12	103.23	110.90
1	V	1005	LEU	CB-CA-C	-5.11	100.49	110.20
1	Z	1367	VAL	N-CA-CB	5.11	122.75	111.50
1	A	883	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	Z	298	TYR	CG-CD2-CE2	-5.11	117.21	121.30
2	X	253	TYR	CG-CD2-CE2	5.11	125.39	121.30
1	V	892	PHE	N-CA-C	-5.11	97.21	111.00
1	V	1157	PHE	CG-CD2-CE2	5.11	126.42	120.80
1	Z	791	LEU	CB-CG-CD1	5.11	119.68	111.00
1	Z	795	ALA	C-N-CA	5.11	134.47	121.70
1	Z	424	TYR	CB-CG-CD1	5.10	124.06	121.00
1	Z	1023	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	435	TYR	CG-CD2-CE2	-5.10	117.22	121.30
1	V	652	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
1	V	1384	ALA	CB-CA-C	-5.10	102.45	110.10
2	X	453	ILE	CG1-CB-CG2	-5.10	100.17	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1274	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	X	212	VAL	N-CA-C	-5.10	97.23	111.00
1	V	1386	LEU	N-CA-CB	5.10	120.60	110.40
1	A	29	VAL	CA-CB-CG2	5.10	118.54	110.90
1	W	1056	LEU	N-CA-C	-5.10	97.24	111.00
1	A	424	TYR	CB-CG-CD1	5.09	124.06	121.00
1	W	1053	GLU	CB-CA-C	-5.09	100.21	110.40
1	A	1021	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	W	814	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	W	869	PHE	CB-CG-CD1	5.09	124.36	120.80
1	V	41	ASN	N-CA-CB	5.09	119.76	110.60
1	W	925	THR	CA-CB-CG2	-5.09	105.28	112.40
1	Z	1108	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	A	1108	VAL	CA-CB-CG1	-5.08	103.27	110.90
1	V	315	THR	CA-CB-CG2	-5.08	105.28	112.40
1	V	67	THR	CA-CB-OG1	5.08	119.68	109.00
1	V	950	PHE	CB-CG-CD1	-5.08	117.24	120.80
1	Z	655	VAL	N-CA-C	-5.08	97.27	111.00
2	C	450	TYR	CG-CD1-CE1	5.08	125.36	121.30
1	V	163	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	V	304	TYR	CG-CD1-CE1	5.08	125.36	121.30
1	W	972	ASN	CB-CA-C	-5.08	100.24	110.40
1	V	10	ILE	CA-CB-CG1	5.08	120.65	111.00
1	V	534	ASP	N-CA-C	-5.08	97.29	111.00
1	W	1173	GLN	CA-CB-CG	5.08	124.57	113.40
1	Z	311	ILE	N-CA-C	-5.08	97.29	111.00
2	B	109	SER	CB-CA-C	5.08	119.74	110.10
1	V	981	VAL	CA-CB-CG2	-5.07	103.29	110.90
1	Z	939	PHE	CB-CG-CD2	5.07	124.35	120.80
1	W	1106	ILE	N-CA-C	-5.07	97.30	111.00
1	V	298	TYR	CG-CD2-CE2	5.07	125.36	121.30
1	V	507	ILE	N-CA-C	-5.07	97.31	111.00
2	X	345	ALA	N-CA-CB	5.07	117.20	110.10
1	A	602	TRP	N-CA-CB	5.07	119.72	110.60
1	V	277	MET	O-C-N	5.07	130.81	122.70
2	C	98	PHE	CZ-CE2-CD2	-5.07	114.02	120.10
1	Z	282	TRP	NE1-CE2-CD2	5.07	112.37	107.30
1	V	1093	THR	N-CA-CB	5.07	119.93	110.30
1	Z	573	ALA	N-CA-CB	5.07	117.19	110.10
1	V	211	SER	N-CA-CB	5.06	118.09	110.50
1	V	267	TYR	N-CA-CB	5.06	119.71	110.60
1	W	714	ALA	O-C-N	5.06	130.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	791	LEU	N-CA-CB	5.06	120.52	110.40
1	Z	493	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	Z	542	SER	N-CA-CB	5.06	118.09	110.50
1	Z	1332	VAL	C-N-CA	5.06	134.36	121.70
1	Z	128	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	V	3	PRO	N-CD-CG	5.06	110.79	103.20
1	W	1182	SER	N-CA-CB	5.06	118.09	110.50
1	V	752	TYR	CD1-CG-CD2	5.06	123.46	117.90
1	Z	534	ASP	CB-CA-C	-5.06	100.28	110.40
2	C	309	GLN	CA-CB-CG	5.06	124.52	113.40
1	W	34	ASN	C-N-CA	5.05	134.34	121.70
1	W	642	ASN	CB-CG-OD1	-5.05	111.49	121.60
1	Z	1369	SER	N-CA-CB	5.05	118.08	110.50
1	W	900	TYR	CG-CD2-CE2	-5.05	117.26	121.30
1	A	879	LYS	CA-CB-CG	5.05	124.51	113.40
1	W	1245	ALA	N-CA-CB	5.05	117.17	110.10
1	Z	1014	ASN	N-CA-C	-5.05	97.36	111.00
1	A	1348	LEU	N-CA-C	-5.05	97.37	111.00
1	V	1181	THR	CA-CB-OG1	5.04	119.59	109.00
1	Z	262	THR	N-CA-C	-5.04	97.38	111.00
1	A	363	TYR	N-CA-CB	5.04	119.67	110.60
2	C	294	ALA	C-N-CA	5.04	132.89	122.30
1	A	1359	LEU	N-CA-CB	5.04	120.48	110.40
1	V	1313	PHE	CB-CG-CD2	5.04	124.33	120.80
1	A	1227	ILE	CA-CB-CG2	-5.04	100.83	110.90
1	W	159	VAL	CA-CB-CG2	5.03	118.45	110.90
1	W	573	ALA	CB-CA-C	-5.03	102.55	110.10
1	V	1354	GLN	N-CA-C	-5.03	97.42	111.00
1	W	99	TYR	CB-CG-CD2	5.03	124.02	121.00
1	W	646	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	Z	1085	TYR	CA-CB-CG	-5.03	103.84	113.40
1	A	708	ASN	N-CA-CB	5.03	119.65	110.60
2	B	287	VAL	CA-CB-CG1	5.03	118.44	110.90
1	Z	658	TYR	CB-CG-CD1	5.03	124.02	121.00
1	Z	1295	LEU	N-CA-C	-5.03	97.43	111.00
1	W	1139	LEU	N-CA-C	-5.02	97.44	111.00
1	W	845	PRO	N-CA-CB	5.02	109.33	103.30
1	W	973	MET	CG-SD-CE	-5.02	92.16	100.20
1	W	631	VAL	O-C-N	5.02	130.73	122.70
1	Z	827	ASN	CB-CG-OD1	-5.02	111.56	121.60
1	Z	1231	SER	CA-C-O	5.02	130.64	120.10
1	V	85	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	848	SER	N-CA-CB	5.02	118.03	110.50
1	Z	1170	THR	O-C-N	5.02	130.73	122.70
1	Z	1391	VAL	CA-CB-CG1	5.02	118.43	110.90
1	A	500	GLN	CG-CD-OE1	-5.01	111.58	121.60
1	V	1137	ALA	CB-CA-C	5.01	117.61	110.10
1	Z	98	LEU	CB-CG-CD1	5.01	119.52	111.00
1	A	1382	TYR	N-CA-CB	5.01	119.61	110.60
1	V	86	SER	CB-CA-C	-5.01	100.59	110.10
1	V	256	SER	O-C-N	-5.01	114.69	123.20
1	V	562	PHE	CD1-CE1-CZ	5.01	126.11	120.10
1	V	502	SER	N-CA-CB	5.00	118.01	110.50
1	Z	607	SER	N-CA-CB	5.00	118.01	110.50
1	Z	523	TYR	N-CA-CB	5.00	119.61	110.60
1	A	859	THR	CA-CB-CG2	5.00	119.40	112.40
1	V	455	THR	N-CA-CB	5.00	119.80	110.30

There are no chirality outliers.

All (226) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1081	PRO	Peptide
1	A	1101	LEU	Peptide
1	A	1118	TYR	Sidechain
1	A	112	TYR	Sidechain
1	A	1143	VAL	Peptide
1	A	1200	TYR	Sidechain
1	A	1215	TYR	Sidechain
1	A	1247	ASN	Peptide
1	A	1252	ARG	Sidechain
1	A	1272	TYR	Sidechain
1	A	1274	TYR	Sidechain
1	A	1290	TYR	Sidechain
1	A	1373	PHE	Peptide
1	A	138	SER	Peptide
1	A	1381	GLU	Peptide
1	A	1388	PHE	Sidechain
1	A	171	ASN	Peptide
1	A	198	VAL	Peptide
1	A	236	TYR	Sidechain
1	A	241	TRP	Peptide
1	A	244	ALA	Peptide
1	A	253	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	330	PHE	Sidechain
1	A	338	TYR	Sidechain
1	A	340	TYR	Sidechain
1	A	383	TYR	Sidechain
1	A	448	TYR	Sidechain
1	A	501	TYR	Sidechain
1	A	512	TYR	Sidechain
1	A	55	ILE	Peptide
1	A	551	ASN	Peptide
1	A	603	GLY	Peptide
1	A	626	TYR	Sidechain
1	A	643	TYR	Sidechain
1	A	692	PHE	Sidechain
1	A	698	TYR	Sidechain
1	A	715	VAL	Peptide
1	A	738	TYR	Sidechain
1	A	742	TYR	Sidechain
1	A	75	PHE	Sidechain
1	A	752	TYR	Sidechain
1	A	753	PHE	Sidechain
1	A	756	THR	Peptide
1	A	775	SER	Peptide
1	A	785	PRO	Peptide
1	A	809	TYR	Sidechain
1	A	814	TYR	Sidechain
1	A	817	TYR	Sidechain
1	A	828	MET	Peptide
1	A	835	ALA	Peptide
1	A	84	TYR	Sidechain
1	A	842	TYR	Sidechain
1	A	858	TYR	Sidechain
1	A	869	PHE	Sidechain
1	A	907	TYR	Sidechain
1	A	927	GLY	Peptide
1	A	947	TYR	Sidechain
1	A	97	PHE	Sidechain
1	A	991	THR	Peptide
1	A	997	SER	Peptide
2	B	151	TYR	Sidechain
2	B	179	PHE	Sidechain
2	B	186	PHE	Sidechain
2	B	227	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	28	ILE	Peptide
2	B	311	TYR	Sidechain
2	B	321	TYR	Sidechain
2	B	42	TYR	Sidechain
2	B	44	TYR	Sidechain
2	B	471	TYR	Sidechain
2	B	472	ARG	Sidechain
2	C	101	VAL	Peptide
2	C	104	TYR	Sidechain
2	C	151	TYR	Sidechain
2	C	186	PHE	Sidechain
2	C	311	TYR	Sidechain
2	C	321	TYR	Sidechain
2	C	471	TYR	Sidechain
2	C	63	TYR	Sidechain
1	V	1024	TYR	Sidechain
1	V	1059	TYR	Sidechain
1	V	1061	TYR	Sidechain
1	V	1085	TYR	Sidechain
1	V	1119	TYR	Sidechain
1	V	116	TYR	Sidechain
1	V	1281	THR	Peptide
1	V	1306	PHE	Sidechain
1	V	1308	TYR	Sidechain
1	V	1326	TYR	Sidechain
1	V	1382	TYR	Sidechain
1	V	1388	PHE	Sidechain
1	V	208	PHE	Sidechain
1	V	213	TYR	Sidechain
1	V	235	TYR	Sidechain
1	V	267	TYR	Sidechain
1	V	383	TYR	Sidechain
1	V	409	TYR	Sidechain
1	V	424	TYR	Sidechain
1	V	599	PHE	Sidechain
1	V	626	TYR	Sidechain
1	V	643	TYR	Sidechain
1	V	652	TYR	Sidechain
1	V	677	LEU	Peptide
1	V	681	TYR	Sidechain
1	V	709	PHE	Sidechain
1	V	720	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	V	733	THR	Peptide
1	V	738	TYR	Sidechain
1	V	74	ARG	Sidechain
1	V	751	TYR	Sidechain
1	V	787	PHE	Peptide
1	V	789	TYR	Sidechain
1	V	809	TYR	Sidechain
1	V	83	TYR	Sidechain
1	V	835	ALA	Peptide
1	V	842	TYR	Sidechain
1	V	858	TYR	Sidechain
1	V	947	TYR	Sidechain
1	V	99	TYR	Sidechain
1	W	1021	TYR	Sidechain
1	W	1074	ALA	Peptide
1	W	1076	ASN	Peptide
1	W	1118	TYR	Sidechain
1	W	1187	THR	Peptide
1	W	1208	PHE	Sidechain
1	W	1252	ARG	Sidechain
1	W	1277	SER	Peptide
1	W	1290	TYR	Sidechain
1	W	1329	TYR	Sidechain
1	W	1335	TYR	Sidechain
1	W	1364	TYR	Sidechain
1	W	1380	SER	Peptide
1	W	1381	GLU	Peptide
1	W	1388	PHE	Sidechain
1	W	166	TYR	Sidechain
1	W	200	VAL	Peptide
1	W	203	TYR	Sidechain
1	W	236	TYR	Sidechain
1	W	293	PHE	Sidechain
1	W	304	TYR	Sidechain
1	W	307	PHE	Sidechain
1	W	340	TYR	Sidechain
1	W	404	TRP	Peptide
1	W	405	TYR	Sidechain,Peptide
1	W	493	TYR	Sidechain
1	W	503	PHE	Sidechain
1	W	512	TYR	Sidechain
1	W	529	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	W	535	TYR	Sidechain
1	W	539	PHE	Sidechain
1	W	627	PHE	Sidechain
1	W	628	TYR	Sidechain
1	W	641	TYR	Sidechain
1	W	652	TYR	Sidechain
1	W	667	TYR	Sidechain
1	W	789	TYR	Sidechain
1	W	80	TYR	Sidechain
1	W	817	TYR	Sidechain
1	W	836	SER	Peptide
1	W	84	TYR	Sidechain
1	W	875	TYR	Sidechain
1	W	892	PHE	Sidechain
1	W	907	TYR	Sidechain
1	W	913	TYR	Sidechain
1	W	936	TYR	Sidechain
2	X	104	TYR	Sidechain
2	X	151	TYR	Sidechain
2	X	186	PHE	Sidechain
2	X	276	TYR	Sidechain
2	X	293	TYR	Sidechain
2	X	333	TYR	Sidechain
2	X	471	TYR	Sidechain
1	Z	1021	TYR	Sidechain
1	Z	1030	LEU	Peptide
1	Z	1061	TYR	Sidechain
1	Z	1073	ILE	Peptide
1	Z	1076	ASN	Peptide
1	Z	1078	VAL	Peptide
1	Z	1118	TYR	Sidechain
1	Z	112	TYR	Sidechain
1	Z	1167	PRO	Peptide
1	Z	1187	THR	Peptide
1	Z	1200	TYR	Sidechain
1	Z	1248	PHE	Sidechain
1	Z	1272	TYR	Sidechain
1	Z	13	TYR	Sidechain
1	Z	1327	PHE	Sidechain
1	Z	1335	TYR	Sidechain
1	Z	1350	TYR	Sidechain
1	Z	146	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	Z	2	THR	Peptide
1	Z	203	TYR	Sidechain
1	Z	213	TYR	Sidechain
1	Z	243	ARG	Sidechain
1	Z	254	TYR	Sidechain
1	Z	295	TYR	Sidechain
1	Z	298	TYR	Sidechain
1	Z	327	SER	Peptide
1	Z	383	TYR	Sidechain
1	Z	4	PRO	Peptide
1	Z	409	TYR	Sidechain
1	Z	440	VAL	Peptide
1	Z	447	TYR	Sidechain
1	Z	458	SER	Peptide
1	Z	544	GLU	Peptide
1	Z	613	TYR	Sidechain
1	Z	641	TYR	Sidechain
1	Z	643	TYR	Sidechain
1	Z	667	TYR	Sidechain
1	Z	680	LYS	Peptide
1	Z	704	PHE	Sidechain
1	Z	738	TYR	Sidechain
1	Z	742	TYR	Sidechain
1	Z	751	TYR	Sidechain
1	Z	752	TYR	Sidechain
1	Z	753	PHE	Sidechain
1	Z	756	THR	Peptide
1	Z	778	LEU	Peptide
1	Z	79	GLY	Mainchain
1	Z	814	TYR	Sidechain
1	Z	835	ALA	Peptide
1	Z	858	TYR	Sidechain
1	Z	876	LYS	Peptide
1	Z	877	VAL	Peptide
1	Z	912	TYR	Sidechain

## 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	A	10478	0	10402	48	0
1	V	10478	0	10402	31	0
1	W	10478	0	10402	40	0
1	Z	10478	0	10402	49	0
2	B	3312	0	3388	9	0
2	C	3312	0	3388	15	0
2	X	3312	0	3388	17	0
All	All	51848	0	51772	203	0

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

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:255:ALA:HB2	1:V:617:ASN:HD21	1.59	0.66
2:C:344:GLN:H	2:C:344:GLN:HE21	1.43	0.65
1:V:1215:TYR:CD1	1:V:1371:VAL:HG13	2.33	0.64
2:X:288:ILE:HD12	2:X:296:MET:HB2	1.80	0.63
1:V:1010:GLN:HE22	1:V:1039:LEU:HD23	1.62	0.63
2:C:233:THR:HG21	2:X:310:ASN:HB2	1.79	0.62
1:A:342:LEU:HD22	1:A:390:ILE:HG23	1.81	0.62
1:V:1303:ILE:HD13	1:V:1370:ALA:HA	1.81	0.61
2:X:223:ILE:HD12	2:X:258:VAL:HG22	1.84	0.60
1:A:269:VAL:HG11	1:A:273:LEU:HD21	1.84	0.58
1:Z:245:LEU:HD13	1:Z:451:ALA:HB1	1.85	0.58
1:A:683:ASN:HD22	1:A:683:ASN:H	1.49	0.58
1:A:269:VAL:HG12	1:A:270:PRO:O	2.03	0.58
2:B:244:ILE:HD12	2:B:245:VAL:H	1.69	0.58
1:V:1017:LEU:HD21	1:V:1019:VAL:HG23	1.85	0.58
1:W:1188:ASN:HD22	1:W:1220:ILE:HA	1.70	0.57
1:A:918:PRO:HA	1:Z:210:ASN:HD22	1.70	0.56
1:V:244:ALA:HA	1:V:664:LEU:HA	1.88	0.56
1:Z:1260:ALA:HB2	1:Z:1290:TYR:CD1	2.40	0.56
1:Z:179:VAL:H	1:Z:202:LEU:HD21	1.70	0.56
1:Z:523:TYR:CE1	1:Z:581:LEU:HD11	2.42	0.55
1:W:813:ILE:HG23	1:W:854:ILE:HD12	1.88	0.55
2:C:36:PRO:HB2	2:C:120:VAL:HG11	1.90	0.54
1:Z:1101:LEU:HD13	1:Z:1102:SER:H	1.70	0.54
1:W:1251:ILE:H	1:W:1380:SER:H	1.55	0.54
2:C:230:GLN:HE22	2:C:246:VAL:HB	1.73	0.54
1:Z:1188:ASN:HD21	1:Z:1206:GLY:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HE22	1:A:198:VAL:H	1.54	0.53
2:X:221:VAL:HG13	2:X:331:THR:HB	1.90	0.53
1:A:910:GLU:HG2	1:A:913:TYR:HB2	1.90	0.53
1:W:1207:LEU:HA	1:W:1219:ALA:HB3	1.91	0.52
1:Z:24:GLY:HA3	1:Z:98:LEU:HD22	1.92	0.52
2:B:103:THR:CG2	2:B:121:ASN:HB3	2.40	0.52
1:W:428:ILE:HD11	1:W:486:LEU:HD22	1.92	0.52
1:W:1088:LEU:HD12	1:W:1088:LEU:H	1.74	0.52
1:V:1332:VAL:HG13	1:V:1349:VAL:HG11	1.91	0.52
1:W:1207:LEU:HD12	1:W:1207:LEU:H	1.73	0.52
1:Z:795:ALA:HA	1:Z:806:THR:HG23	1.92	0.51
1:A:894:SER:HB2	1:Z:233:GLU:HB3	1.91	0.51
1:Z:202:LEU:H	1:Z:202:LEU:HD23	1.76	0.51
1:W:1253:LEU:HD23	1:W:1386:LEU:HB3	1.92	0.51
2:C:36:PRO:CB	2:C:120:VAL:HG11	2.41	0.51
1:Z:1074:ALA:HB2	1:Z:1210:LEU:HD21	1.92	0.51
1:A:588:VAL:HG13	1:A:589:PRO:HD2	1.92	0.51
1:Z:660:PRO:HA	1:Z:807:PRO:HG2	1.91	0.51
2:X:108:LEU:HB3	2:X:110:VAL:HG23	1.92	0.51
1:W:82:ALA:HA	1:W:93:VAL:HG12	1.93	0.50
1:Z:546:MET:HB2	1:Z:553:LEU:HD11	1.93	0.50
1:V:1253:LEU:HD22	1:V:1370:ALA:HB2	1.93	0.50
1:Z:583:LEU:HD11	1:Z:585:PHE:CZ	2.47	0.50
1:W:288:ASN:HD21	1:W:502:SER:HB2	1.74	0.50
1:Z:304:TYR:CD1	1:Z:354:GLU:HG2	2.47	0.50
1:W:952:LYS:H	1:W:1021:TYR:HA	1.76	0.50
1:W:1212:PHE:HB2	1:W:1219:ALA:HB1	1.94	0.49
2:B:65:TYR:CE1	2:B:71:VAL:HG13	2.47	0.49
1:V:924:GLY:HA2	1:V:973:MET:HB2	1.94	0.49
1:A:1284:GLN:OE1	1:A:1284:GLN:HA	2.12	0.49
1:V:349:SER:HB3	1:V:351:THR:H	1.77	0.49
2:X:235:ILE:HD11	2:X:246:VAL:HG12	1.93	0.49
1:Z:952:LYS:O	1:Z:968:LEU:HD11	2.13	0.49
1:A:923:LEU:HD11	1:A:994:PHE:CE1	2.47	0.49
1:W:1254:ALA:HB3	1:W:1260:ALA:HA	1.95	0.49
1:Z:356:VAL:HA	1:Z:553:LEU:HB3	1.94	0.49
1:V:424:TYR:CE1	1:V:489:ALA:HB2	2.48	0.49
1:A:816:THR:HG21	1:A:819:ILE:HD11	1.94	0.49
1:V:498:LEU:HD23	1:V:529:TYR:CD2	2.47	0.49
1:Z:99:TYR:CD2	1:Z:100:PRO:HA	2.47	0.48
1:W:608:VAL:HG21	1:W:627:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:PRO:HG3	2:C:48:LEU:HD11	1.96	0.48
2:X:177:LEU:HD23	2:X:177:LEU:H	1.79	0.48
1:W:179:VAL:H	1:W:201:ILE:CD1	2.27	0.48
1:A:1081:PRO:HB3	1:A:1106:ILE:HA	1.95	0.48
1:Z:302:ASN:OD1	1:Z:548:VAL:HG12	2.14	0.48
1:A:392:GLY:H	1:A:398:ILE:HD12	1.78	0.48
1:A:501:TYR:CE2	1:A:528:LEU:HD13	2.49	0.48
1:A:844:VAL:HG21	1:A:852:SER:HB3	1.95	0.48
1:V:844:VAL:HG11	1:V:852:SER:CB	2.44	0.47
1:A:50:VAL:HA	1:A:53:ILE:HG22	1.97	0.47
1:A:832:LEU:HD12	1:A:833:TYR:H	1.79	0.47
1:Z:831:GLY:H	1:Z:843:VAL:HB	1.78	0.47
1:Z:921:ILE:HA	1:Z:931:TRP:HA	1.96	0.47
2:C:228:VAL:HG22	2:C:254:ILE:HG23	1.95	0.47
1:Z:755:GLN:NE2	1:Z:755:GLN:HA	2.30	0.47
1:A:949:GLY:HA3	1:A:1023:ASP:HA	1.97	0.47
1:W:206:PHE:CE1	1:W:612:ALA:HB1	2.50	0.47
1:A:510:PRO:HD3	1:A:585:PHE:CZ	2.49	0.47
2:C:178:SER:HB3	2:C:207:GLN:HE22	1.80	0.46
1:Z:1168:ASN:H	1:Z:1189:GLY:HA2	1.79	0.46
2:X:192:LEU:HD23	2:X:216:LEU:CD1	2.46	0.46
1:V:108:ILE:N	1:V:108:ILE:HD12	2.31	0.46
1:W:727:PHE:CE2	1:W:829:ILE:HD12	2.51	0.46
2:X:31:ILE:HG12	2:X:110:VAL:HG21	1.98	0.46
2:B:458:ILE:O	2:B:462:VAL:HG23	2.15	0.46
2:X:287:VAL:O	2:X:289:THR:HG23	2.15	0.46
1:A:1361:ALA:HB2	1:A:1395:GLN:H	1.80	0.46
1:W:797:VAL:H	1:W:798:PRO:HD3	1.81	0.46
1:A:976:LEU:HA	1:Z:271:GLY:H	1.80	0.45
1:Z:42:VAL:HA	1:Z:45:VAL:HG22	1.97	0.45
1:A:42:VAL:HG22	1:A:46:ILE:HD13	1.98	0.45
1:V:245:LEU:HB3	1:V:451:ALA:HB1	1.98	0.45
1:Z:10:ILE:HD11	1:Z:28:PHE:HB3	1.97	0.45
1:A:1154:ASN:HD21	1:A:1156:THR:HB	1.81	0.45
1:A:280:LEU:HD12	1:A:300:PHE:CE2	2.51	0.45
2:C:255:LEU:HB3	2:C:288:ILE:HD11	1.99	0.45
1:V:1270:LEU:HA	1:V:1384:ALA:HB3	1.99	0.45
1:V:1213:VAL:HB	1:V:1379:LEU:H	1.82	0.45
2:C:50:LEU:CB	2:C:89:ILE:HD11	2.47	0.45
1:W:1098:ILE:N	1:W:1098:ILE:HD12	2.31	0.45
1:W:1285:GLN:HB2	1:W:1394:THR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:280:LEU:HD11	1:Z:304:TYR:CD2	2.52	0.45
1:V:435:TYR:CD1	1:V:686:ILE:HG21	2.52	0.45
1:W:1071:TRP:CZ3	1:W:1222:ALA:HB3	2.52	0.45
2:B:258:VAL:HG11	2:B:268:ALA:HB3	1.99	0.45
1:V:1313:PHE:CD2	1:V:1365:VAL:HG11	2.51	0.45
1:V:361:VAL:HG12	1:V:524:VAL:HG11	1.99	0.44
1:A:159:VAL:H	1:A:159:VAL:HG23	1.53	0.44
1:A:322:LEU:HD22	1:A:348:ASN:HB3	1.98	0.44
2:C:50:LEU:HB3	2:C:89:ILE:HD11	1.99	0.44
2:X:136:VAL:HG22	2:X:137:ASN:H	1.83	0.44
1:V:221:MET:HE2	1:V:663:VAL:HG11	1.98	0.44
1:W:98:LEU:HD21	1:W:202:LEU:HD13	2.00	0.44
1:Z:726:PRO:HG3	1:Z:827:ASN:HB3	1.98	0.44
1:A:1193:ILE:HB	1:A:1202:LEU:HD11	1.98	0.44
1:A:1257:GLN:HG2	1:W:1234:VAL:HG11	2.00	0.44
1:A:1344:VAL:HG12	1:A:1346:ASN:H	1.81	0.44
1:A:1050:GLY:HA3	1:A:1081:PRO:HG2	2.00	0.44
1:Z:645:ASN:HA	1:Z:651:ASN:HB3	2.00	0.44
1:A:645:ASN:HA	1:A:651:ASN:HB2	1.99	0.43
1:V:886:VAL:O	1:V:1026:THR:HG21	2.18	0.43
2:X:149:GLN:HG2	2:X:163:THR:HG23	1.99	0.43
1:A:1213:VAL:HG21	1:A:1372:PRO:HG3	2.00	0.43
2:X:223:ILE:HD13	2:X:317:ILE:CG2	2.49	0.43
2:X:310:ASN:HD22	2:X:340:ASN:HA	1.83	0.43
1:Z:486:LEU:CD1	1:Z:508:VAL:HG11	2.48	0.43
1:W:245:LEU:HB3	1:W:451:ALA:HB1	1.99	0.43
1:W:591:THR:HG22	1:W:591:THR:O	2.18	0.43
1:Z:108:ILE:HD11	1:Z:138:SER:HB3	2.01	0.43
1:Z:108:ILE:HD13	1:Z:136:VAL:HG12	2.00	0.43
2:X:221:VAL:HG12	2:X:329:LEU:HD23	2.01	0.43
1:A:1062:THR:HG21	1:A:1068:ALA:HA	2.00	0.43
1:A:1099:LEU:H	1:A:1149:GLU:HB2	1.83	0.43
1:W:636:ILE:HG22	1:W:877:VAL:HB	2.00	0.43
1:W:797:VAL:H	1:W:798:PRO:CD	2.32	0.43
1:Z:430:LEU:HD23	1:Z:464:GLY:HA3	2.00	0.43
1:A:835:ALA:HB1	1:A:939:PHE:CD1	2.54	0.43
1:A:1222:ALA:CA	1:A:1247:ASN:HD22	2.32	0.42
1:V:1048:GLY:O	1:V:1049:ALA:HB2	2.20	0.42
1:Z:984:GLU:HG2	1:Z:991:THR:H	1.84	0.42
1:A:816:THR:HG21	1:A:819:ILE:CD1	2.49	0.42
1:Z:911:PRO:HA	1:Z:990:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:VAL:HA	2:B:468:VAL:HG22	2.00	0.42
1:W:1277:SER:HA	1:W:1390:ASN:HB3	2.01	0.42
1:Z:899:LEU:HD12	1:Z:1010:GLN:HB3	2.02	0.42
1:A:27:LEU:HD13	1:A:113:LEU:HG	2.02	0.42
1:Z:245:LEU:HD21	1:Z:664:LEU:HD12	2.02	0.42
1:Z:1369:SER:O	1:Z:1371:VAL:HG23	2.20	0.42
1:A:801:LEU:HD23	1:A:801:LEU:HA	1.93	0.42
1:A:1334:ALA:HB1	1:A:1347:LEU:HD11	2.02	0.42
2:B:204:ILE:O	2:B:204:ILE:HG13	2.19	0.42
1:Z:245:LEU:HD13	1:Z:451:ALA:CB	2.49	0.42
1:V:1313:PHE:CE2	1:V:1365:VAL:HG11	2.55	0.42
1:W:247:ASN:HA	1:W:451:ALA:HA	2.01	0.42
1:Z:77:THR:H	1:Z:145:ILE:HD12	1.85	0.42
1:Z:1066:THR:O	1:Z:1067:PHE:CB	2.67	0.42
2:C:219:ALA:HB1	2:C:261:ALA:HB2	2.01	0.41
1:A:857:THR:HA	1:A:878:PHE:HA	2.02	0.41
1:V:707:SER:HA	1:V:709:PHE:CE1	2.55	0.41
1:V:829:ILE:HG22	1:V:843:VAL:HG21	2.02	0.41
1:Z:429:LEU:N	1:Z:429:LEU:HD22	2.36	0.41
1:Z:1188:ASN:ND2	1:Z:1206:GLY:H	2.17	0.41
2:X:164:GLN:HG2	2:X:173:THR:H	1.85	0.41
1:Z:430:LEU:HA	1:Z:464:GLY:HA3	2.01	0.41
2:B:50:LEU:HD23	2:B:85:LEU:HD21	2.02	0.41
1:W:648:CYS:HB2	1:W:650:ASN:HD21	1.84	0.41
1:W:674:THR:CG2	1:W:689:ALA:HB1	2.51	0.41
1:A:900:TYR:HB2	1:A:1093:THR:HG21	2.02	0.41
1:W:1366:ILE:HD12	1:W:1391:VAL:HG11	2.02	0.41
1:Z:1058:ALA:HA	1:Z:1163:PHE:CD1	2.55	0.41
1:A:399:THR:HA	1:A:412:GLN:HA	2.02	0.41
2:C:255:LEU:HD22	2:C:288:ILE:CD1	2.51	0.41
2:C:446:THR:HA	2:C:449:VAL:HB	2.03	0.41
1:V:840:LEU:HD23	1:V:840:LEU:HA	1.79	0.41
1:V:1185:VAL:HG21	1:V:1220:ILE:HG12	2.03	0.41
1:Z:644:GLN:HA	1:Z:647:ILE:CD1	2.50	0.41
1:A:1020:THR:HG22	1:A:1021:TYR:N	2.36	0.41
2:C:61:THR:HG21	1:W:1322:ALA:HA	2.03	0.41
1:W:958:LEU:HD21	1:W:1005:LEU:HD22	2.02	0.41
2:X:150:LEU:HD13	2:X:174:PHE:CD2	2.56	0.41
1:A:1330:SER:HB3	1:A:1352:GLN:H	1.86	0.41
1:V:844:VAL:HG11	1:V:852:SER:HB2	2.02	0.41
1:Z:487:THR:HG22	1:Z:487:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:O	1:A:149:THR:HB	2.21	0.40
1:A:262:THR:HG22	1:A:263:PHE:H	1.86	0.40
1:W:614:ASP:HB2	1:W:619:LYS:H	1.85	0.40
1:W:746:ASN:HD21	1:W:786:GLY:HA2	1.86	0.40
1:W:1251:ILE:HD13	1:W:1301:PHE:CZ	2.56	0.40
1:V:1191:LEU:HD22	1:V:1208:PHE:CG	2.56	0.40
1:W:1005:LEU:HD13	1:W:1013:ASN:HD21	1.87	0.40
1:W:1304:GLN:HA	1:W:1329:TYR:HB3	2.03	0.40
1:Z:1061:TYR:CD1	1:Z:1065:ILE:HD13	2.56	0.40
1:V:664:LEU:HD13	1:V:750:ASN:ND2	2.37	0.40
1:W:1016:ILE:HG23	1:W:1017:LEU:N	2.37	0.40
2:B:223:ILE:HD12	2:B:258:VAL:HG22	2.01	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	A	1393/1424 (98%)	1150 (83%)	177 (13%)	66 (5%)	2	16
1	V	1393/1424 (98%)	1218 (87%)	137 (10%)	38 (3%)	4	25
1	W	1393/1424 (98%)	1209 (87%)	135 (10%)	49 (4%)	3	20
1	Z	1393/1424 (98%)	1187 (85%)	158 (11%)	48 (3%)	3	21
2	B	449/475 (94%)	424 (94%)	24 (5%)	1 (0%)	44	78
2	C	449/475 (94%)	420 (94%)	24 (5%)	5 (1%)	12	47
2	X	449/475 (94%)	414 (92%)	32 (7%)	3 (1%)	19	57
All	All	6919/7121 (97%)	6022 (87%)	687 (10%)	210 (3%)	5	23

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	THR
1	A	166	TYR
1	A	171	ASN
1	A	200	VAL
1	A	203	TYR
1	A	358	LYS
1	A	476	ALA
1	A	479	ALA
1	A	662	ALA
1	A	779	PRO
1	A	798	PRO
1	A	869	PHE
1	A	900	TYR
1	A	989	ASN
1	A	1039	LEU
1	A	1059	TYR
1	A	1067	PHE
1	A	1080	GLN
1	A	1356	ILE
1	A	1382	TYR
1	V	66	ALA
1	V	234	ALA
1	V	488	ASN
1	V	495	ASN
1	V	755	GLN
1	V	758	ASN
1	V	925	THR
1	V	987	ALA
1	V	989	ASN
1	V	1049	ALA
1	W	39	SER
1	W	200	VAL
1	W	302	ASN
1	W	358	LYS
1	W	405	TYR
1	W	837	GLN
1	W	1047	LYS
1	W	1080	GLN
1	W	1245	ALA
1	W	1248	PHE
1	W	1272	TYR
1	W	1323	ALA
1	W	1357	SER

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Mol	Chain	Res	Type
2	X	94	SER
1	Z	235	TYR
1	Z	459	GLU
1	Z	487	THR
1	Z	845	PRO
1	Z	925	THR
1	Z	989	ASN
1	Z	1067	PHE
1	Z	1076	ASN
1	Z	1337	ALA
1	Z	1381	GLU
1	A	16	THR
1	A	129	THR
1	A	148	SER
1	A	201	ILE
1	A	242	GLY
1	A	314	SER
1	A	550	ASN
1	A	551	ASN
1	A	758	ASN
1	A	837	GLN
1	A	868	TYR
1	A	870	TYR
1	A	939	PHE
1	A	1014	ASN
1	A	1190	SER
1	A	1343	SER
1	V	89	LYS
1	V	200	VAL
1	V	202	LEU
1	V	231	SER
1	V	476	ALA
1	V	514	ALA
1	V	515	ILE
1	V	533	SER
1	V	849	PHE
1	V	1010	GLN
1	V	1186	TYR
1	V	1223	ASN
1	V	1382	TYR
1	W	121	LEU
1	W	215	ALA

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Mol	Chain	Res	Type
1	W	236	TYR
1	W	875	TYR
1	W	896	THR
1	W	960	ASN
1	W	1036	LEU
1	W	1039	LEU
1	W	1079	LYS
1	W	1337	ALA
2	X	308	VAL
1	Z	172	THR
1	Z	200	VAL
1	Z	210	ASN
1	Z	476	ALA
1	Z	488	ASN
1	Z	514	ALA
1	Z	661	ASP
1	Z	671	SER
1	Z	796	GLN
1	Z	867	HIS
1	Z	1096	SER
1	Z	1188	ASN
1	Z	1223	ASN
1	A	22	ALA
1	A	232	SER
1	A	381	ASN
1	A	905	PRO
1	A	915	SER
1	A	1010	GLN
1	A	1049	ALA
1	A	1248	PHE
2	C	85	LEU
2	C	101	VAL
1	V	322	LEU
1	V	1039	LEU
1	V	1068	ALA
1	W	41	ASN
1	W	290	PRO
1	W	727	PHE
1	W	754	ILE
1	W	1010	GLN
1	W	1063	GLY
1	W	1075	GLU

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Mol	Chain	Res	Type
1	W	1377	PRO
1	Z	21	PRO
1	Z	215	ALA
1	Z	650	ASN
1	Z	793	SER
1	Z	795	ALA
1	Z	1177	SER
1	Z	1360	PRO
1	A	215	ALA
1	A	665	ASP
1	A	863	TYR
1	A	1038	ALA
1	A	1259	PRO
2	C	39	ASN
2	C	82	SER
2	C	232	GLY
1	V	321	ALA
1	V	603	GLY
1	V	817	TYR
1	V	1067	PHE
1	V	1249	THR
1	W	211	SER
1	W	488	ASN
1	W	514	ALA
1	W	617	ASN
1	W	1380	SER
1	Z	22	ALA
1	Z	231	SER
1	Z	513	ALA
1	Z	615	THR
1	Z	667	TYR
1	Z	836	SER
1	Z	1010	GLN
1	Z	1049	ALA
1	Z	1080	GLN
1	Z	1380	SER
1	A	68	THR
1	A	1006	ASN
1	A	1081	PRO
1	A	1247	ASN
1	V	551	ASN
1	V	605	LEU

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Mol	Chain	Res	Type
1	W	217	LEU
1	W	515	ILE
1	W	797	VAL
1	W	895	SER
1	W	1017	LEU
1	W	1034	THR
1	W	1358	ASN
1	Z	89	LYS
1	Z	1039	LEU
1	A	98	LEU
1	A	174	MET
1	A	445	SER
1	A	1079	LYS
1	A	1113	GLY
2	B	304	PRO
1	W	1249	THR
1	Z	1079	LYS
1	Z	393	PRO
1	A	622	VAL
1	W	153	ILE
1	W	1345	PRO
1	W	1382	TYR
1	A	845	PRO
1	V	386	PRO
1	V	682	GLY
1	V	1263	PRO
2	X	238	GLY
1	Z	515	ILE
1	Z	1298	PRO
1	V	364	PRO
1	W	242	GLY
1	W	898	PRO
1	A	667	TYR
1	A	1155	GLY
1	A	1298	PRO
1	A	1315	VAL
1	V	667	TYR
1	Z	660	PRO
1	A	212	PRO
1	A	446	PRO
1	Z	773	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1189/1212 (98%)	1116 (94%)	73 (6%)	15	37
1	V	1189/1212 (98%)	1128 (95%)	61 (5%)	20	41
1	W	1189/1212 (98%)	1120 (94%)	69 (6%)	17	38
1	Z	1189/1212 (98%)	1123 (94%)	66 (6%)	17	38
2	B	386/407 (95%)	361 (94%)	25 (6%)	14	35
2	C	386/407 (95%)	371 (96%)	15 (4%)	27	48
2	X	386/407 (95%)	376 (97%)	10 (3%)	41	59
All	All	5914/6069 (97%)	5595 (95%)	319 (5%)	21	40

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	41	ASN
1	A	43	THR
1	A	59	THR
1	A	64	THR
1	A	68	THR
1	A	168	THR
1	A	171	ASN
1	A	184	THR
1	A	187	THR
1	A	203	TYR
1	A	213	TYR
1	A	233	GLU
1	A	241	TRP
1	A	262	THR
1	A	274	THR
1	A	327	SER
1	A	330	PHE
1	A	348	ASN
1	A	350	THR

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Mol	Chain	Res	Type
1	A	384	THR
1	A	412	GLN
1	A	440	VAL
1	A	442	THR
1	A	447	TYR
1	A	463	THR
1	A	471	GLN
1	A	485	LEU
1	A	516	ASN
1	A	518	THR
1	A	532	THR
1	A	591	THR
1	A	650	ASN
1	A	679	LEU
1	A	681	TYR
1	A	683	ASN
1	A	730	VAL
1	A	758	ASN
1	A	782	THR
1	A	788	MET
1	A	790	LEU
1	A	814	TYR
1	A	819	ILE
1	A	853	ASN
1	A	855	LYS
1	A	858	TYR
1	A	861	THR
1	A	874	GLN
1	A	875	TYR
1	A	925	THR
1	A	948	LEU
1	A	950	PHE
1	A	964	VAL
1	A	974	GLN
1	A	998	ILE
1	A	1003	LYS
1	A	1014	ASN
1	A	1034	THR
1	A	1089	GLN
1	A	1138	THR
1	A	1148	THR
1	A	1164	THR

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Mol	Chain	Res	Type
1	A	1168	ASN
1	A	1176	SER
1	A	1212	PHE
1	A	1225	THR
1	A	1244	THR
1	A	1266	ASN
1	A	1288	LYS
1	A	1340	ILE
1	A	1356	ILE
1	A	1389	THR
1	A	1391	VAL
2	B	91	THR
2	B	95	THR
2	B	105	THR
2	B	114	THR
2	B	122	VAL
2	B	134	THR
2	B	150	LEU
2	B	183	THR
2	B	185	THR
2	B	202	VAL
2	B	207	GLN
2	B	226	MET
2	B	255	LEU
2	B	266	THR
2	B	283	VAL
2	B	328	THR
2	B	334	LEU
2	B	337	VAL
2	B	349	LYS
2	B	367	ASN
2	B	372	ILE
2	B	429	THR
2	B	431	LEU
2	B	473	LYS
2	B	474	ILE
2	C	41	THR
2	C	80	ASN
2	C	99	THR
2	C	134	THR
2	C	147	THR
2	C	150	LEU

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Mol	Chain	Res	Type
2	C	173	THR
2	C	174	PHE
2	C	175	THR
2	C	193	GLN
2	C	258	VAL
2	C	305	THR
2	C	344	GLN
2	C	374	THR
2	C	393	LEU
1	V	1	LEU
1	V	2	THR
1	V	27	LEU
1	V	104	THR
1	V	139	THR
1	V	154	LEU
1	V	166	TYR
1	V	187	THR
1	V	202	LEU
1	V	236	TYR
1	V	241	TRP
1	V	249	THR
1	V	318	THR
1	V	329	ASN
1	V	335	LYS
1	V	374	VAL
1	V	378	THR
1	V	431	LYS
1	V	492	THR
1	V	502	SER
1	V	564	LEU
1	V	570	SER
1	V	589	PRO
1	V	653	VAL
1	V	661	ASP
1	V	673	THR
1	V	683	ASN
1	V	716	THR
1	V	736	THR
1	V	739	LEU
1	V	746	ASN
1	V	755	GLN
1	V	769	ILE

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Mol	Chain	Res	Type
1	V	817	TYR
1	V	839	THR
1	V	845	PRO
1	V	846	ASN
1	V	849	PHE
1	V	859	THR
1	V	877	VAL
1	V	897	THR
1	V	916	PRO
1	V	936	TYR
1	V	956	VAL
1	V	999	THR
1	V	1030	LEU
1	V	1034	THR
1	V	1041	THR
1	V	1054	PHE
1	V	1062	THR
1	V	1079	LYS
1	V	1083	MET
1	V	1085	TYR
1	V	1150	LEU
1	V	1173	GLN
1	V	1178	LEU
1	V	1215	TYR
1	V	1252	ARG
1	V	1301	PHE
1	V	1350	TYR
1	V	1386	LEU
1	W	14	LEU
1	W	43	THR
1	W	94	VAL
1	W	121	LEU
1	W	122	THR
1	W	128	GLU
1	W	134	THR
1	W	152	GLN
1	W	161	THR
1	W	182	THR
1	W	202	LEU
1	W	241	TRP
1	W	249	THR
1	W	279	GLN

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Mol	Chain	Res	Type
1	W	293	PHE
1	W	294	THR
1	W	342	LEU
1	W	359	LEU
1	W	367	THR
1	W	378	THR
1	W	399	THR
1	W	412	GLN
1	W	413	ILE
1	W	427	GLN
1	W	440	VAL
1	W	475	THR
1	W	478	SER
1	W	499	THR
1	W	508	VAL
1	W	531	LYS
1	W	556	VAL
1	W	557	THR
1	W	558	THR
1	W	567	LEU
1	W	605	LEU
1	W	624	LEU
1	W	643	TYR
1	W	650	ASN
1	W	679	LEU
1	W	716	THR
1	W	719	THR
1	W	762	VAL
1	W	785	PRO
1	W	824	VAL
1	W	866	LEU
1	W	896	THR
1	W	901	GLN
1	W	956	VAL
1	W	991	THR
1	W	1001	LEU
1	W	1021	TYR
1	W	1023	ASP
1	W	1051	VAL
1	W	1056	LEU
1	W	1062	THR
1	W	1065	ILE

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Mol	Chain	Res	Type
1	W	1067	PHE
1	W	1084	THR
1	W	1122	THR
1	W	1179	THR
1	W	1196	ASN
1	W	1248	PHE
1	W	1259	PRO
1	W	1278	ILE
1	W	1287	LEU
1	W	1306	PHE
1	W	1317	THR
1	W	1325	VAL
1	W	1342	THR
2	X	32	THR
2	X	113	THR
2	X	114	THR
2	X	154	THR
2	X	173	THR
2	X	208	GLN
2	X	222	THR
2	X	302	MET
2	X	360	ASN
2	X	436	ASN
1	Z	100	PRO
1	Z	103	THR
1	Z	149	THR
1	Z	160	LEU
1	Z	206	PHE
1	Z	233	GLU
1	Z	240	ILE
1	Z	241	TRP
1	Z	248	THR
1	Z	270	PRO
1	Z	293	PHE
1	Z	302	ASN
1	Z	323	THR
1	Z	324	ILE
1	Z	335	LYS
1	Z	399	THR
1	Z	406	SER
1	Z	429	LEU
1	Z	447	TYR

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Mol	Chain	Res	Type
1	Z	455	THR
1	Z	515	ILE
1	Z	532	THR
1	Z	586	PHE
1	Z	589	PRO
1	Z	590	SER
1	Z	591	THR
1	Z	605	LEU
1	Z	626	TYR
1	Z	640	PRO
1	Z	643	TYR
1	Z	648	CYS
1	Z	676	SER
1	Z	679	LEU
1	Z	764	MET
1	Z	778	LEU
1	Z	806	THR
1	Z	817	TYR
1	Z	839	THR
1	Z	844	VAL
1	Z	858	TYR
1	Z	875	TYR
1	Z	877	VAL
1	Z	956	VAL
1	Z	969	THR
1	Z	970	THR
1	Z	1003	LYS
1	Z	1019	VAL
1	Z	1020	THR
1	Z	1030	LEU
1	Z	1066	THR
1	Z	1075	GLU
1	Z	1083	MET
1	Z	1101	LEU
1	Z	1114	LYS
1	Z	1129	THR
1	Z	1138	THR
1	Z	1156	THR
1	Z	1161	LEU
1	Z	1180	LYS
1	Z	1181	THR
1	Z	1193	ILE

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Mol	Chain	Res	Type
1	Z	1244	THR
1	Z	1263	PRO
1	Z	1271	LYS
1	Z	1313	PHE
1	Z	1350	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	41	ASN
1	A	329	ASN
1	A	427	GLN
1	A	444	GLN
1	A	471	GLN
1	A	516	ASN
1	A	551	ASN
1	A	644	GLN
1	A	683	ASN
1	A	1014	ASN
1	A	1080	GLN
1	A	1154	ASN
1	A	1261	GLN
2	B	46	GLN
2	B	70	ASN
2	B	75	ASN
2	B	281	GLN
2	B	338	GLN
2	B	369	GLN
2	B	371	GLN
2	B	390	GLN
2	B	418	GLN
2	C	78	GLN
2	C	207	GLN
2	C	230	GLN
2	C	309	GLN
2	C	344	GLN
2	C	425	ASN
1	V	54	GLN
1	V	81	ASN
1	V	157	ASN
1	V	175	GLN

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Mol	Chain	Res	Type
1	V	214	GLN
1	V	516	ASN
1	V	617	ASN
1	V	645	ASN
1	V	750	ASN
1	V	758	ASN
1	V	846	ASN
1	V	901	GLN
1	V	983	GLN
1	V	1010	GLN
1	V	1285	GLN
1	V	1314	ASN
1	W	124	GLN
1	W	288	ASN
1	W	651	ASN
1	W	710	ASN
1	W	746	ASN
1	W	812	ASN
1	W	945	GLN
1	W	1013	ASN
1	W	1014	ASN
1	W	1094	ASN
1	W	1257	GLN
1	W	1346	ASN
2	X	74	ASN
2	X	278	ASN
2	X	310	ASN
1	Z	41	ASN
1	Z	157	ASN
1	Z	169	GLN
1	Z	329	ASN
1	Z	651	ASN
1	Z	737	ASN
1	Z	755	GLN
1	Z	1080	GLN
1	Z	1188	ASN
1	Z	1302	GLN

### 5.3.3 RNA ⓘ

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](#)

There are no chain breaks in this entry.

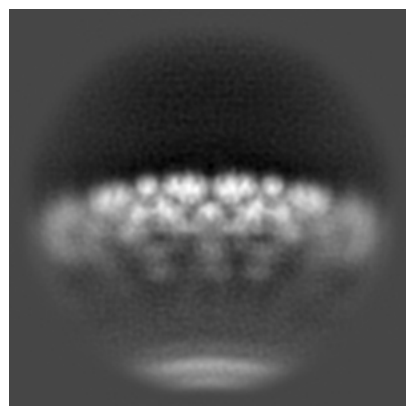
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18127. These allow visual inspection of the internal detail of the map and identification of artifacts.

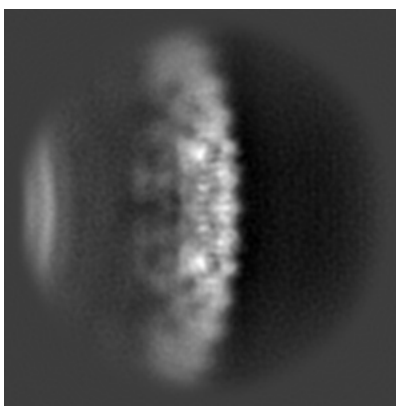
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

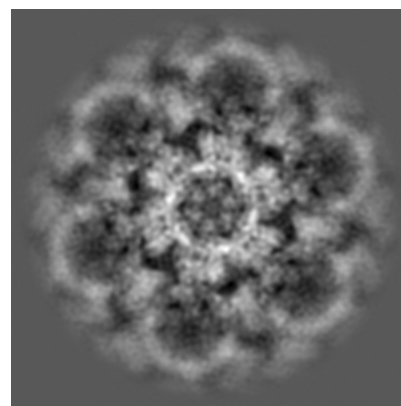
#### 6.1.1 Primary map



X

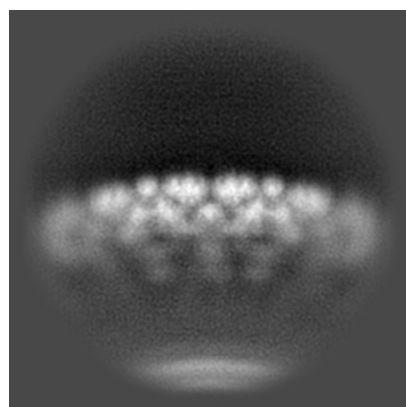


Y

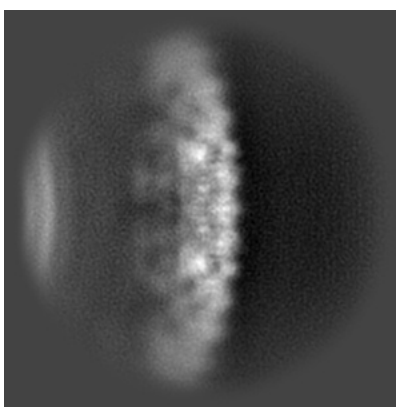


Z

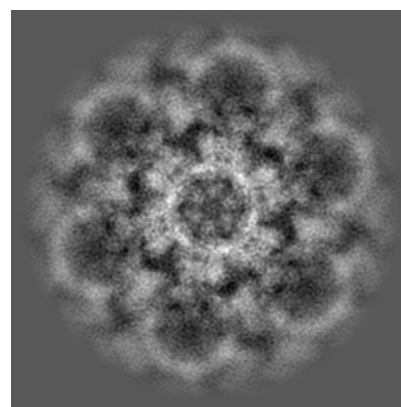
#### 6.1.2 Raw map



X



Y

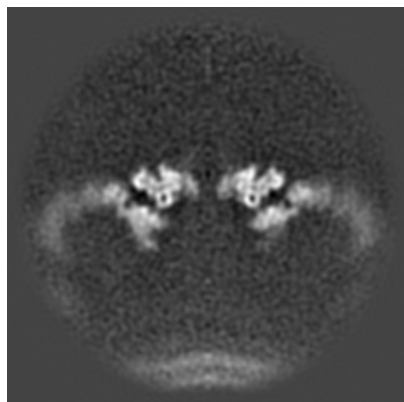


Z

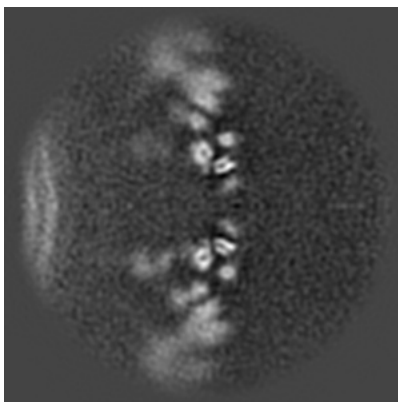
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

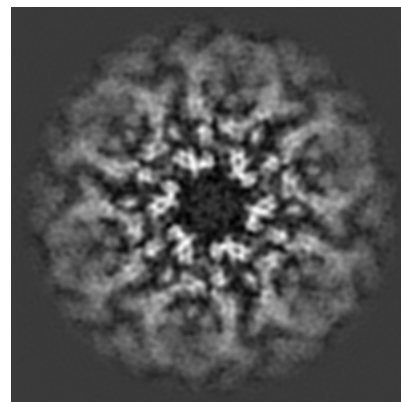
### 6.2.1 Primary map



X Index: 100

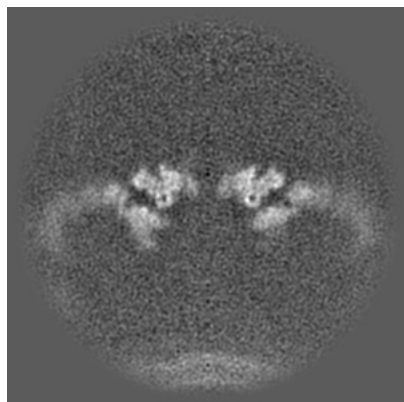


Y Index: 100

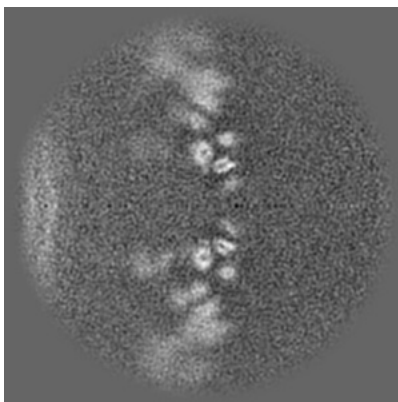


Z Index: 100

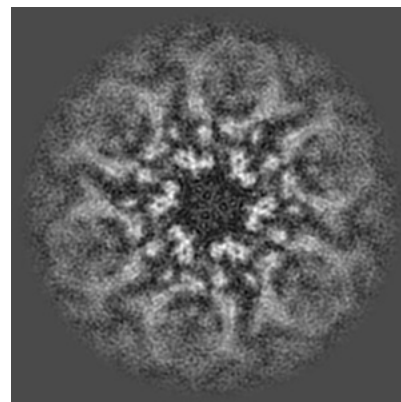
### 6.2.2 Raw map



X Index: 100



Y Index: 100



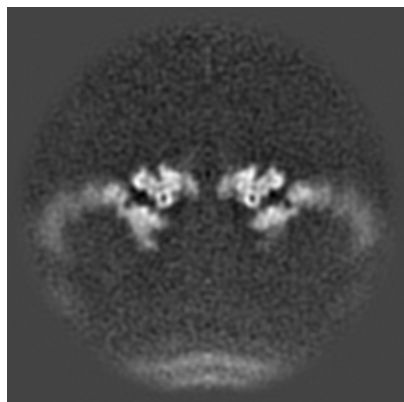
Z Index: 100

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

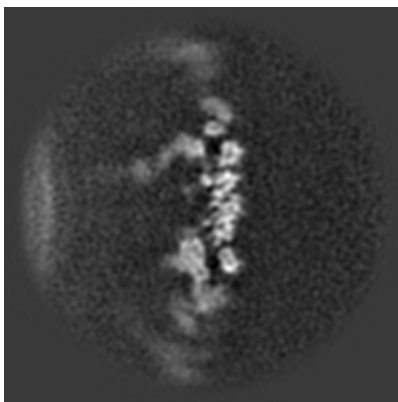


## 6.3 Largest variance slices [i](#)

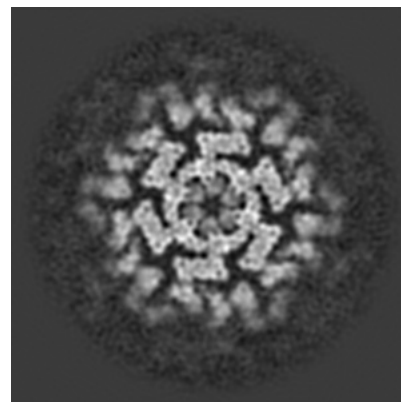
### 6.3.1 Primary map



X Index: 100

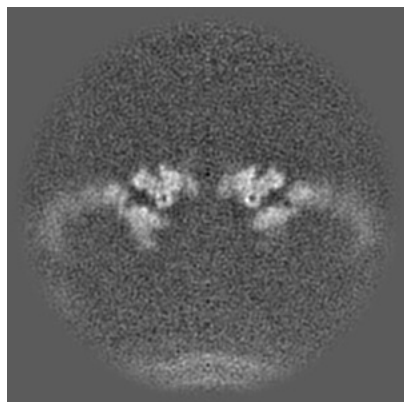


Y Index: 117

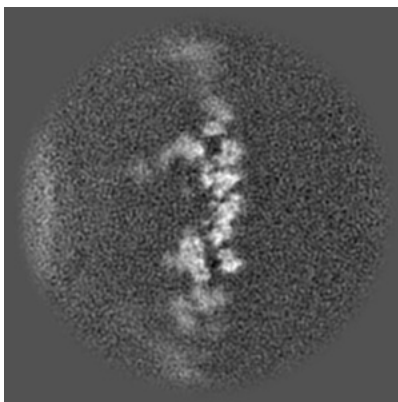


Z Index: 110

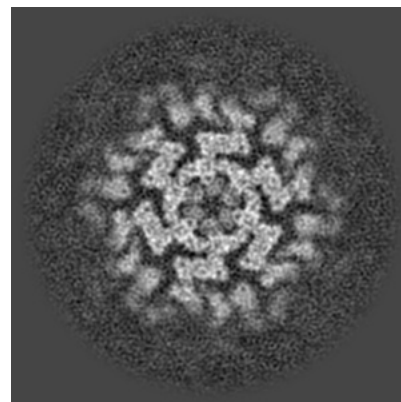
### 6.3.2 Raw map



X Index: 100



Y Index: 116

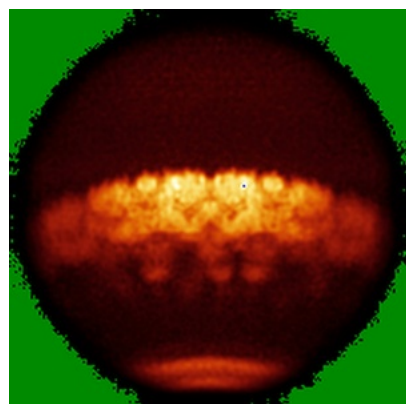


Z Index: 110

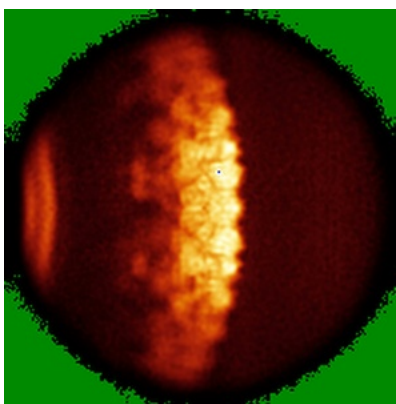
The images above show the largest variance slices of the map in three orthogonal directions.

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

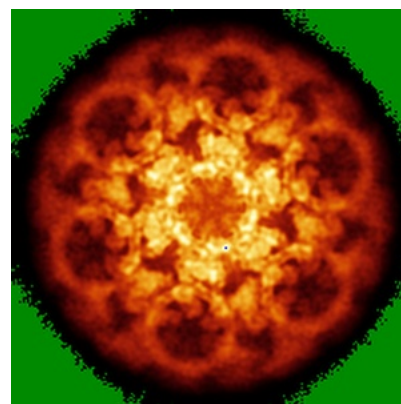
### 6.4.1 Primary map



X

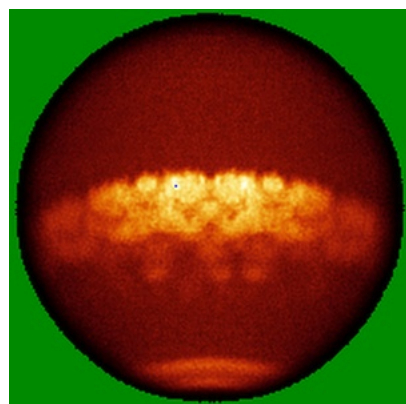


Y

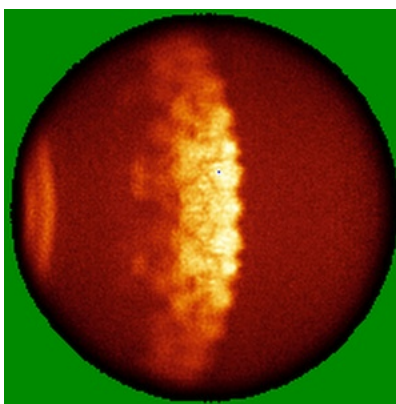


Z

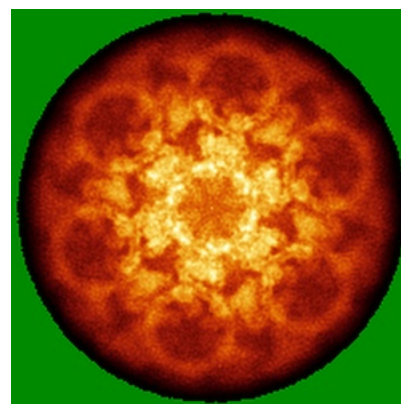
### 6.4.2 Raw map



X



Y

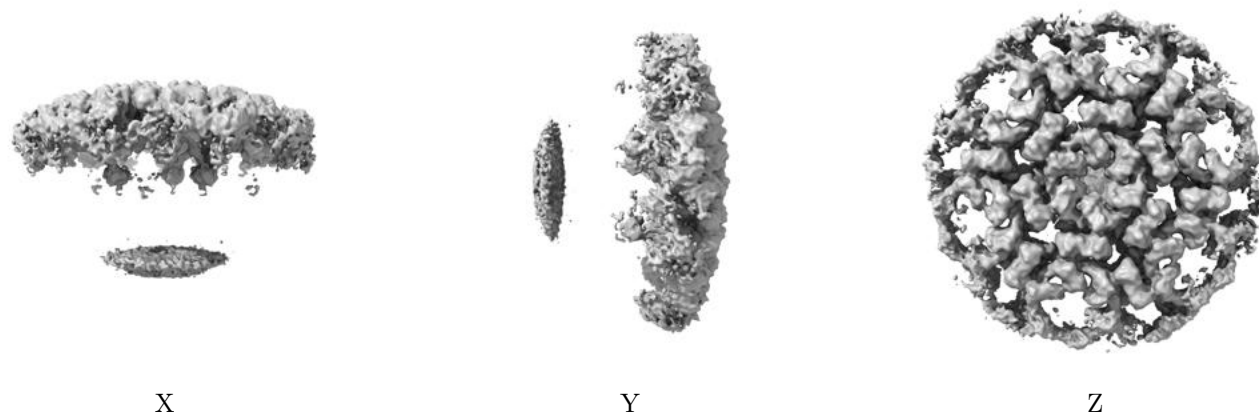


Z

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

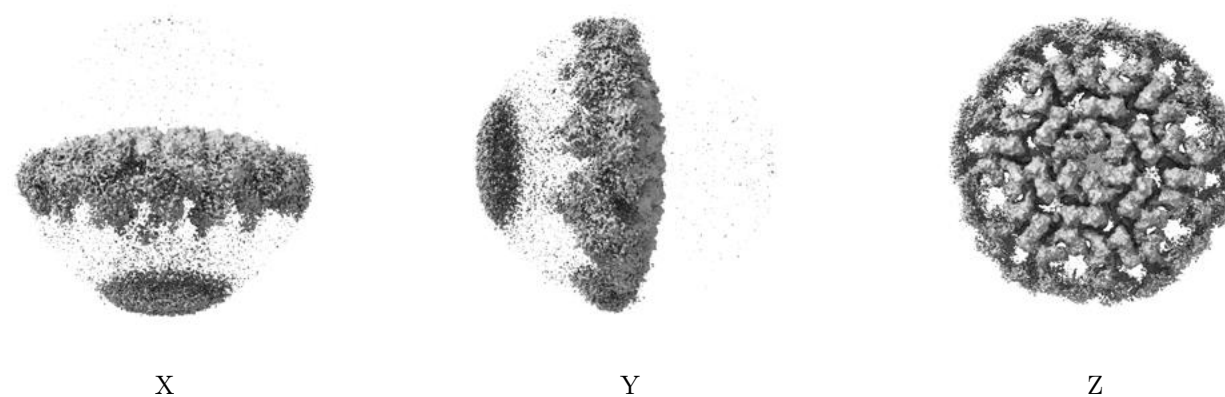
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00509. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

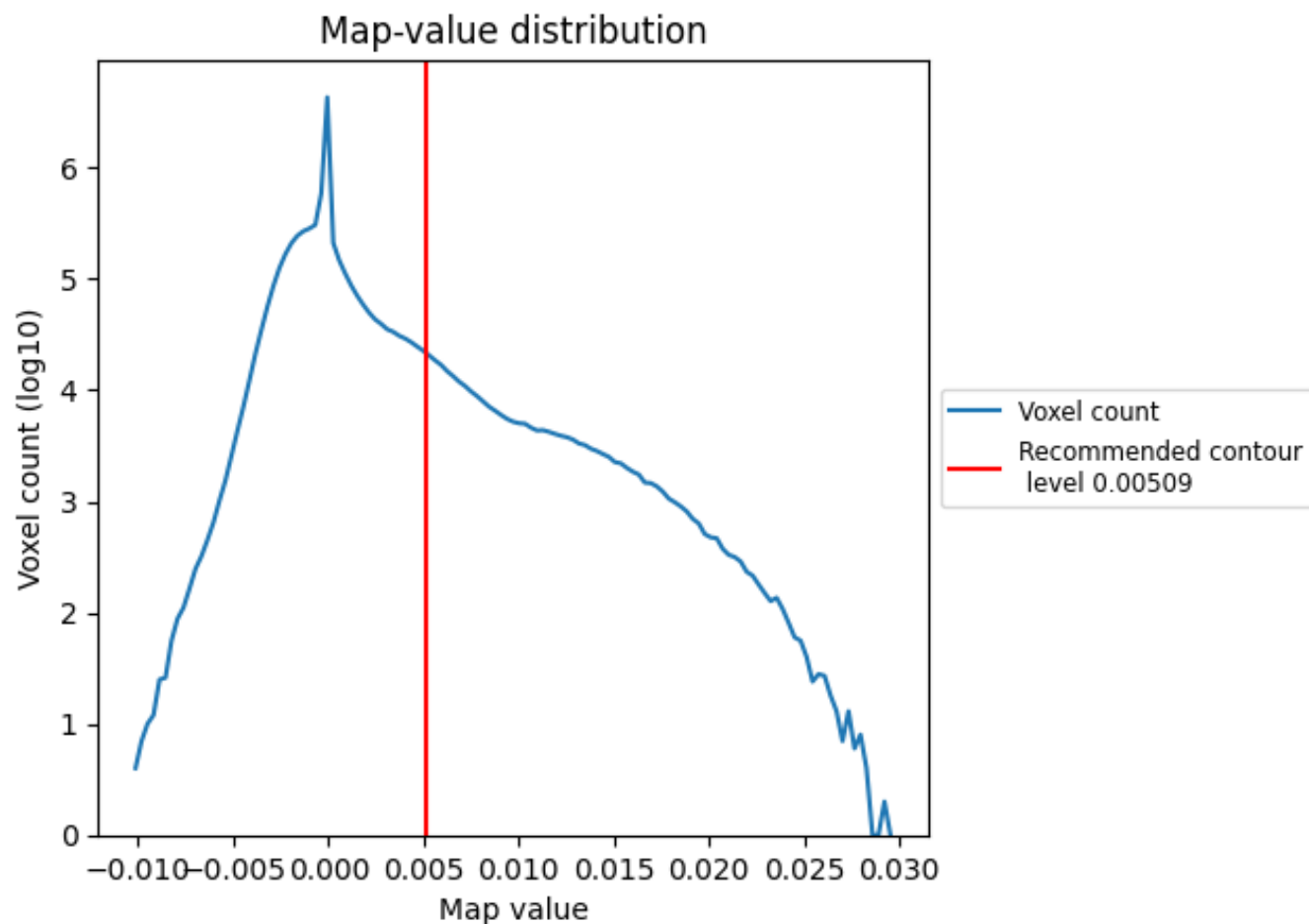
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

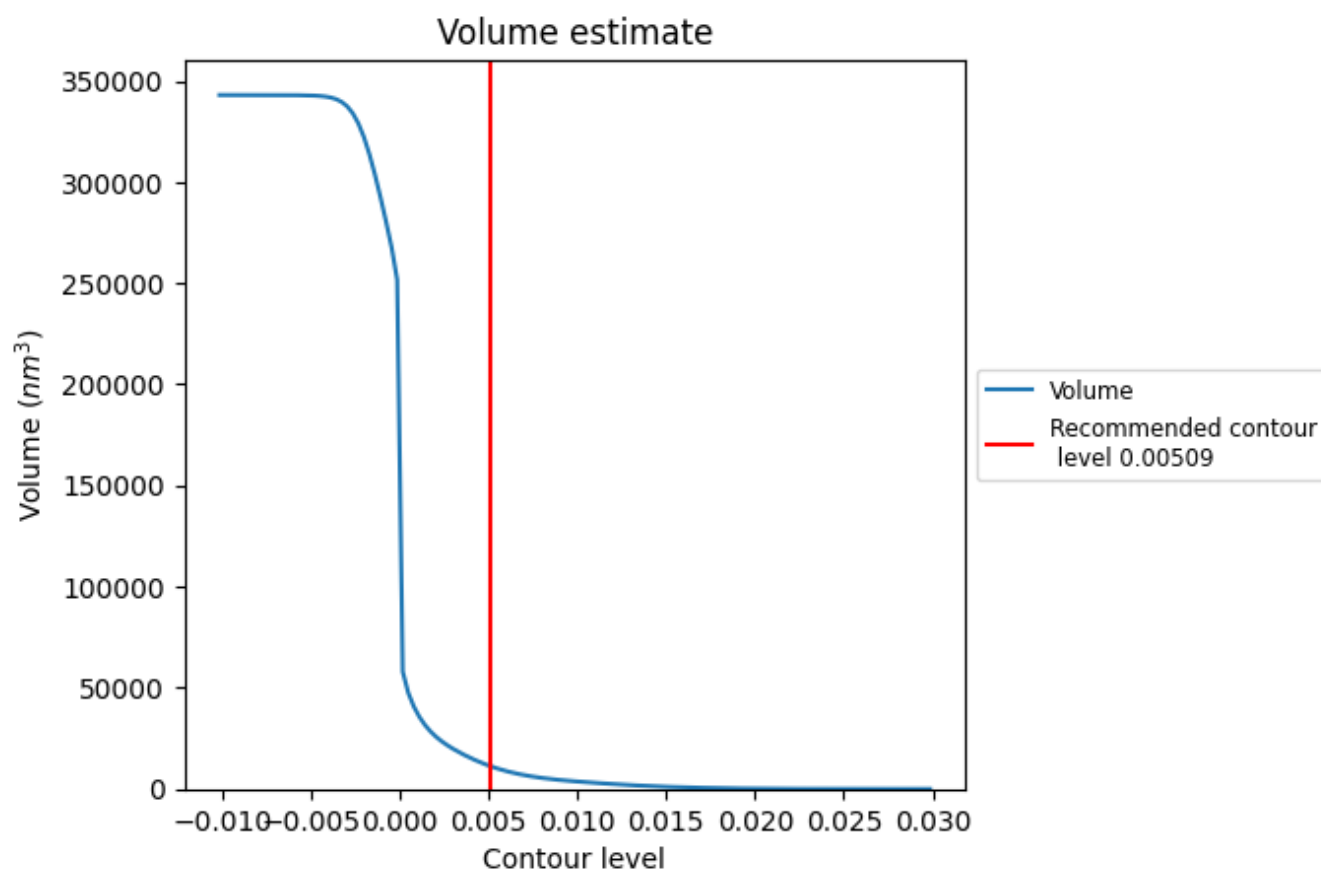
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

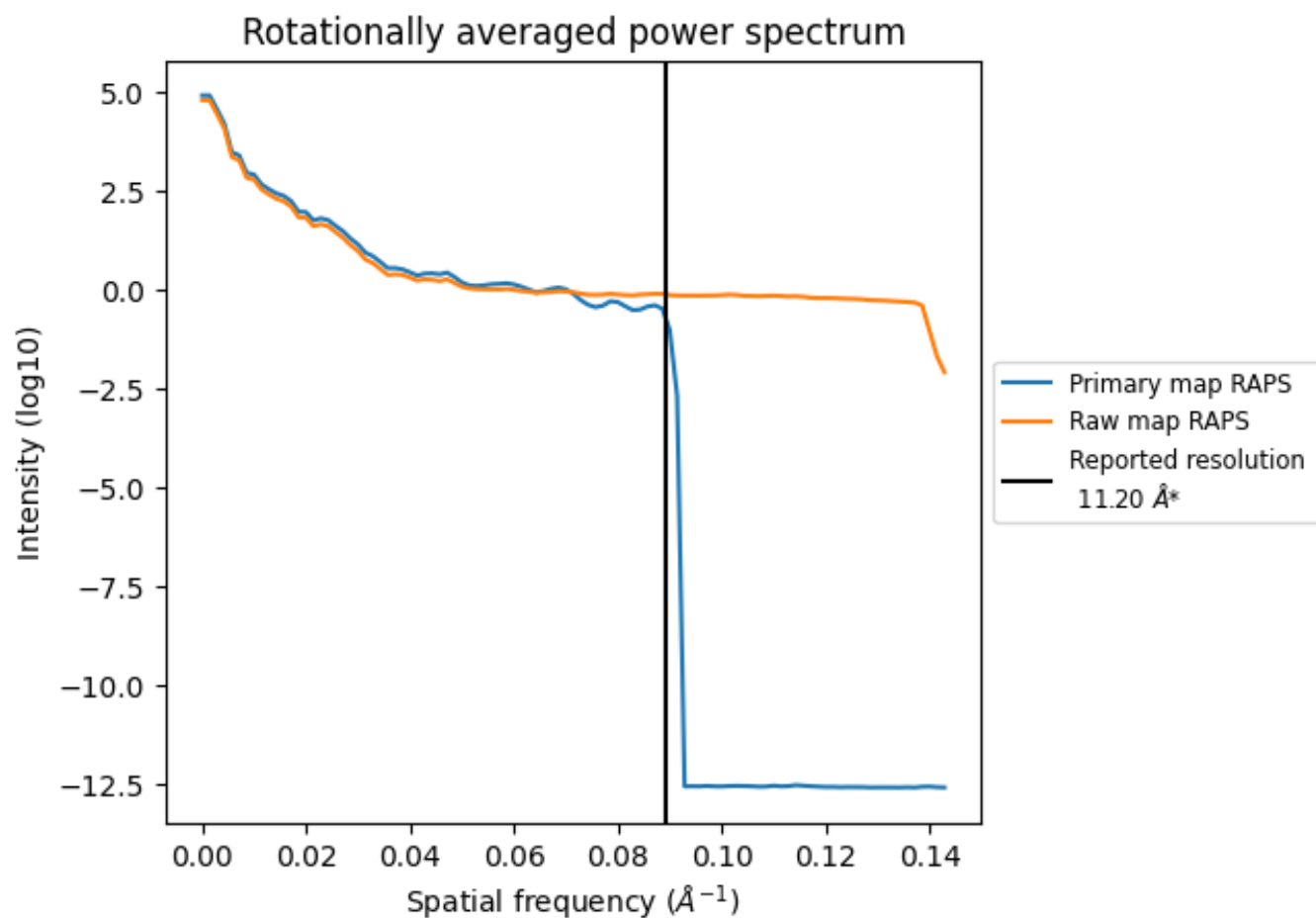
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11315  $\text{nm}^3$ ; this corresponds to an approximate mass of 10221 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

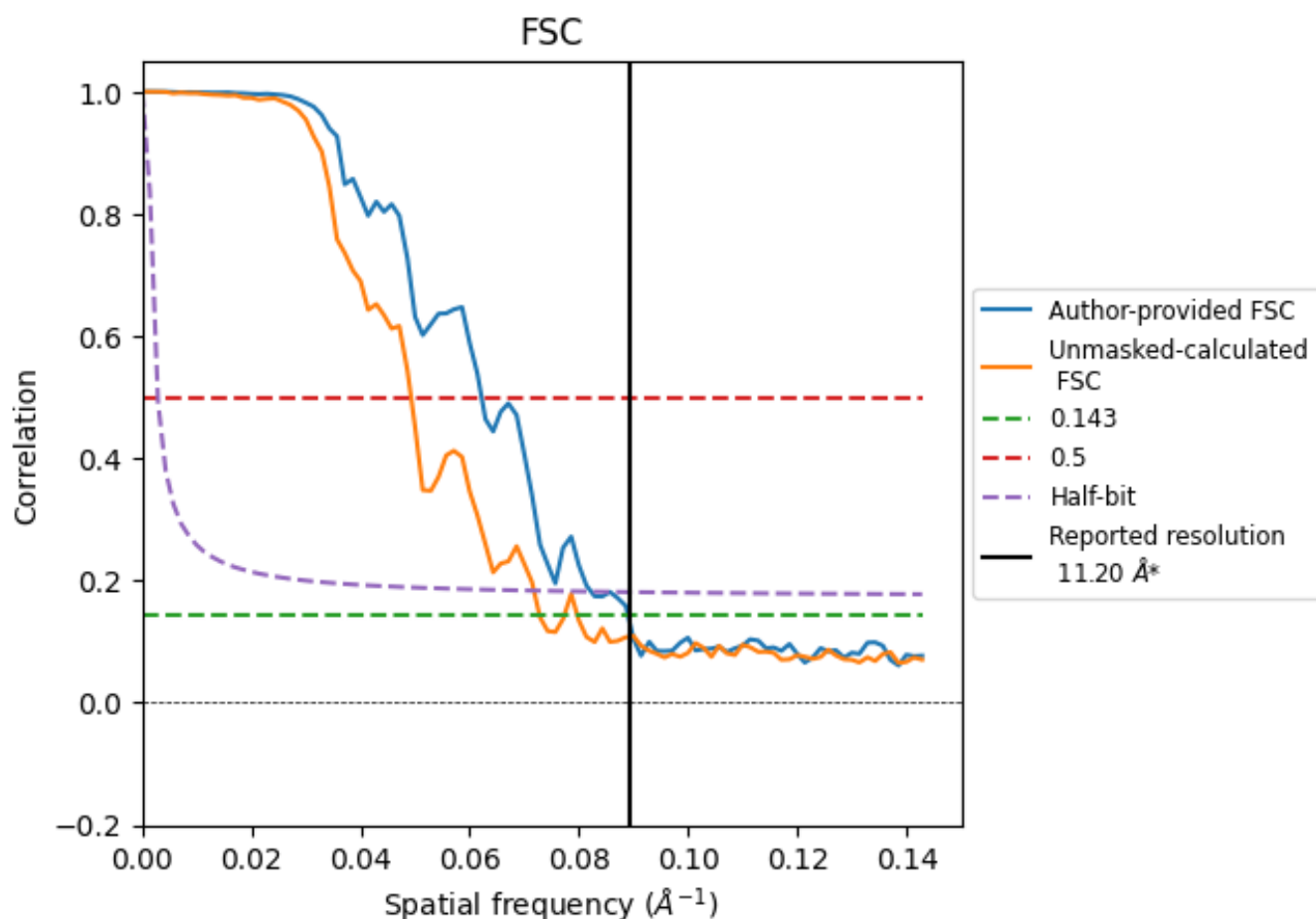


\*Reported resolution corresponds to spatial frequency of 0.089 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.089  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.20	-	-
Author-provided FSC curve	11.24	16.08	12.17
Unmasked-calculated*	13.74	20.33	13.93

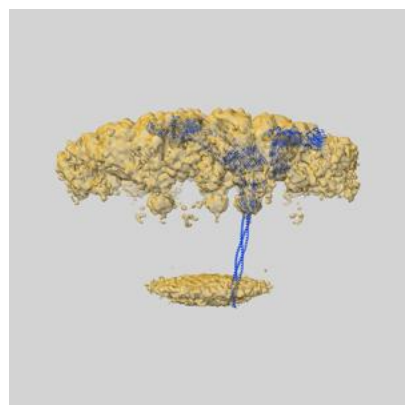
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.74 differs from the reported value 11.2 by more than 10 %



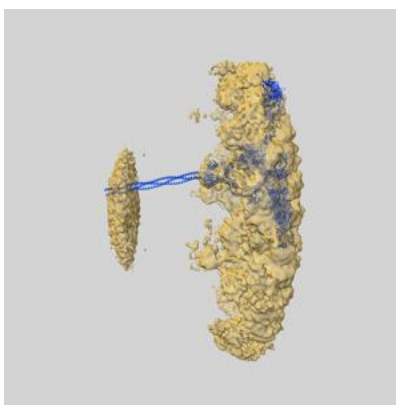
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18127 and PDB model 8QOX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

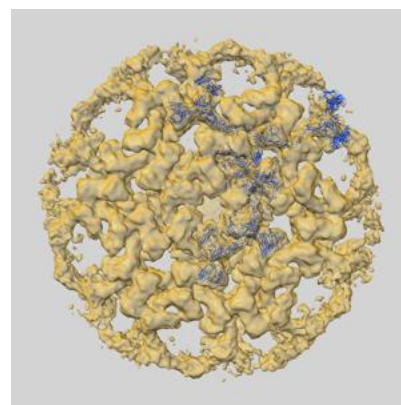
### 9.1 Map-model overlay [i](#)



X



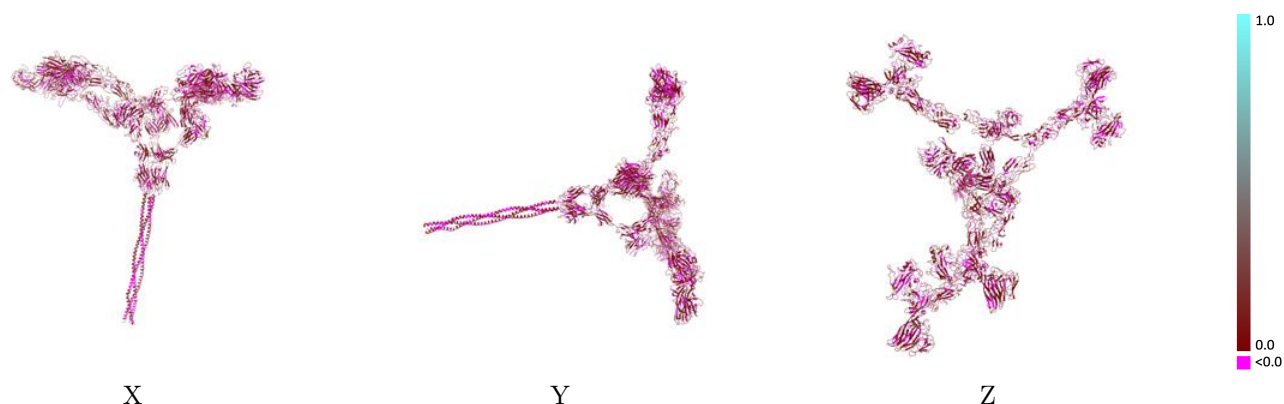
Y



Z

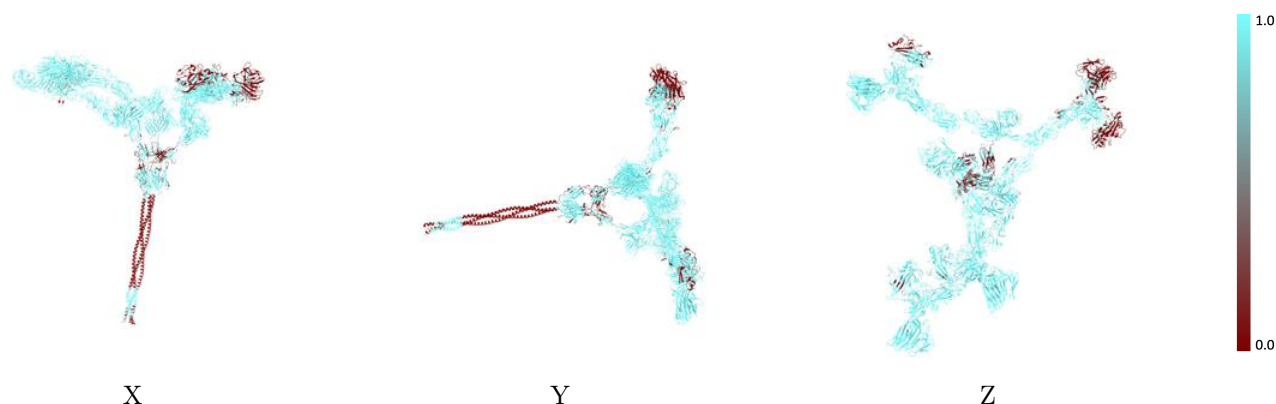
The images above show the 3D surface view of the map at the recommended contour level 0.00509 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



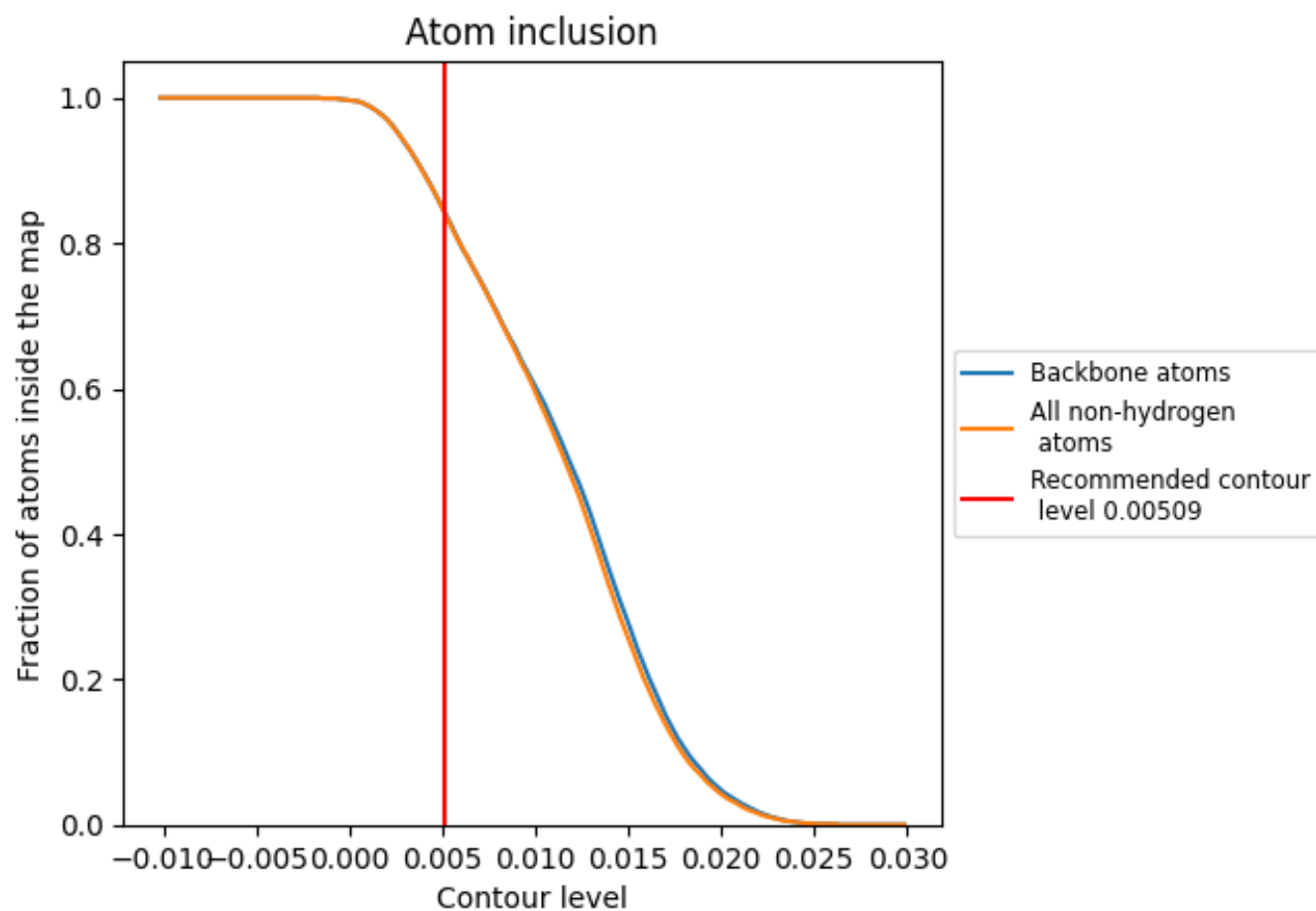
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00509).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00509) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8440</div>	<div><div></div>0.0660</div>
A	<div><div></div>0.9780</div>	<div><div></div>0.0790</div>
B	<div><div></div>0.6270</div>	<div><div></div>0.0550</div>
C	<div><div></div>0.6100</div>	<div><div></div>0.0560</div>
V	<div><div></div>0.9390</div>	<div><div></div>0.0660</div>
W	<div><div></div>0.6970</div>	<div><div></div>0.0510</div>
X	<div><div></div>0.5710</div>	<div><div></div>0.0460</div>
Z	<div><div></div>0.9890</div>	<div><div></div>0.0810</div>

1.0

0.0

<0.0