



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:44 AM UTC

PDB ID : 3J4J / pdb_00003j4j
EMDB ID : EMD-2448
Title : Model of full-length T. thermophilus Translation Initiation Factor 2 refined against its cryo-EM density from a 30S Initiation Complex map
Authors : Simonetti, A.; Marzi, S.; Billas, I.M.L.; Tsai, A.; Fabbretti, A.; Myasnikov, A.; Roblin, P.; Vaiana, A.C.; Hazemann, I.; Eiler, D.; Steitz, T.A.; Puglisi, J.D.; Gualerzi, C.O.; Klaholz, B.P.
Deposited on : 2013-08-26
Resolution : 11.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

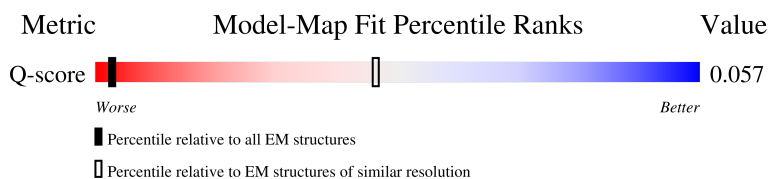
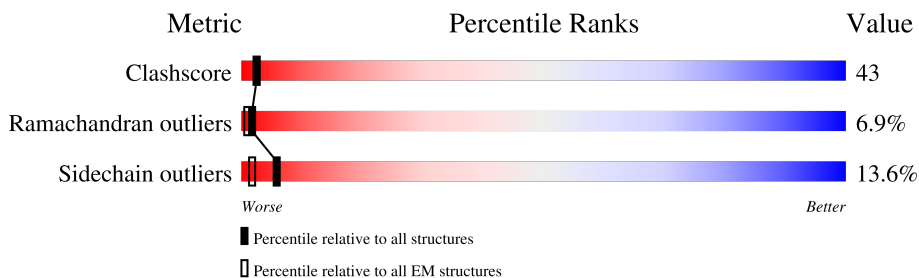
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	117 (11.00 - 12.00)

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

Mol	Chain	Length	Quality of chain
1	A	569	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4383 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 Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	569	Total	C	N	O	S	0	0
			4383	2747	778	841	17		

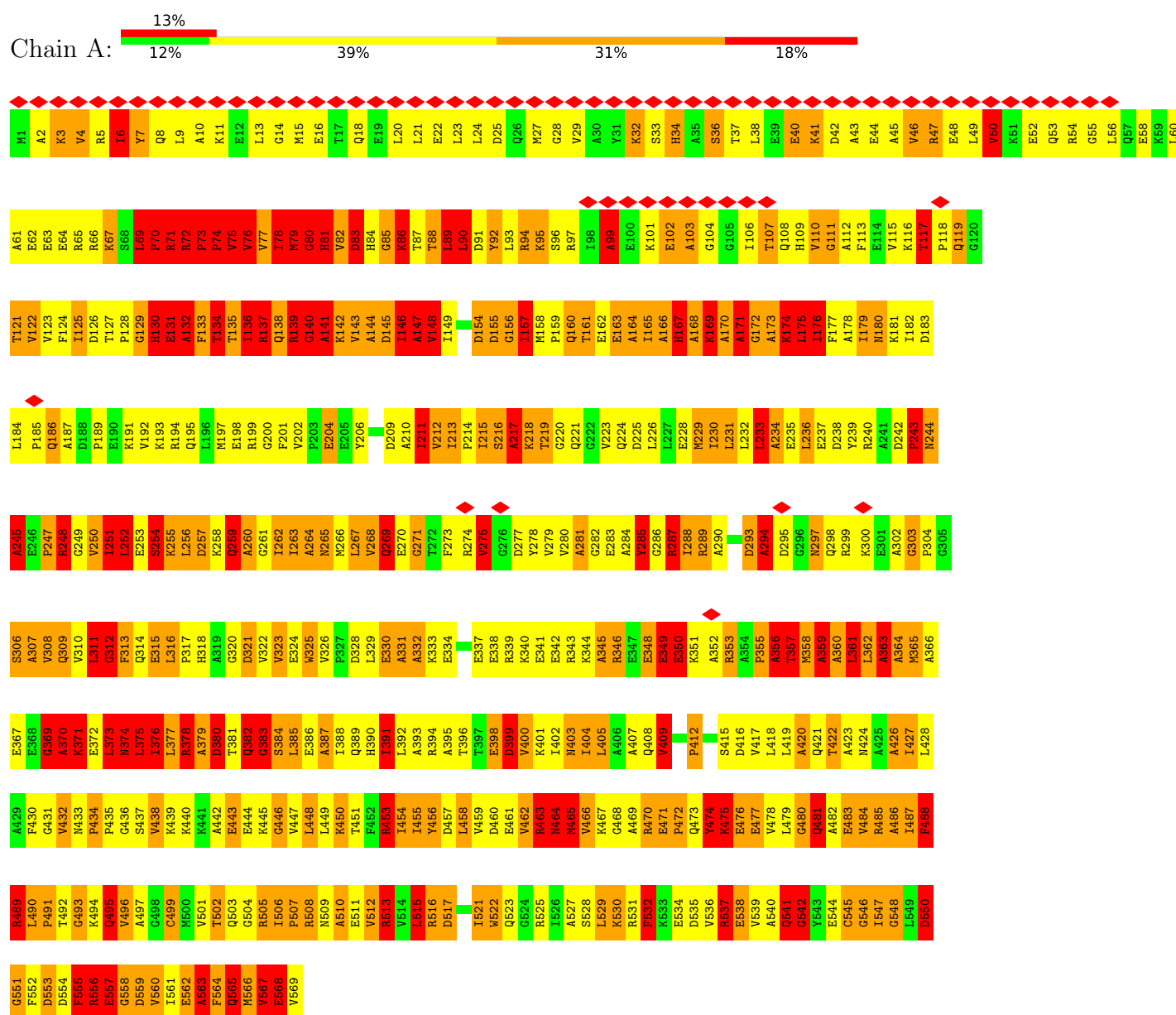
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	conflict	UNP P48515
A	356	ALA	ARG	conflict	UNP P48515
A	360	ALA	GLU	conflict	UNP P48515
A	363	ALA	ARG	conflict	UNP P48515
A	366	ALA	GLN	conflict	UNP P48515
A	370	ALA	ARG	conflict	UNP P48515
A	395	ALA	GLU	conflict	UNP P48515
A	396	THR	SER	conflict	UNP P48515
A	406	ALA	LEU	conflict	UNP P48515
A	469	ALA	GLN	conflict	UNP P48515

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: Translation initiation factor IF-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13000	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	150	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	3.606	Depositor
Minimum map value	-0.766	Depositor
Average map value	0.038	Depositor
Map value standard deviation	0.229	Depositor
Recommended contour level	0.169	Depositor
Map size ($\text{\AA}$)	378.56, 378.56, 378.56	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.8199999, 1.8199999, 1.8199999	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	2.24	118/4440 (2.7%)	3.61	930/5985 (15.5%)

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	177

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	PRO	CA-C	8.96	1.60	1.52
1	A	550	ASP	CA-C	8.85	1.61	1.53
1	A	69	LEU	CA-C	8.01	1.62	1.52
1	A	72	ARG	CA-C	7.90	1.61	1.52
1	A	353	ARG	CZ-NH2	-7.51	1.23	1.33
1	A	529	LEU	CA-C	7.25	1.60	1.53
1	A	64	GLU	CA-C	7.22	1.59	1.52
1	A	202	VAL	CA-C	7.07	1.60	1.52
1	A	400	VAL	CA-C	6.84	1.60	1.52
1	A	34	HIS	CG-ND1	6.71	1.45	1.38
1	A	29	VAL	C-O	-6.66	1.17	1.24
1	A	119	GLN	CA-C	6.62	1.61	1.52
1	A	97	ARG	CZ-NH2	-6.61	1.24	1.33
1	A	343	ARG	CZ-NH2	-6.57	1.25	1.33
1	A	531	ARG	N-CA	6.43	1.53	1.45
1	A	289	ARG	CZ-NH2	-6.37	1.25	1.33
1	A	242	ASP	CA-C	6.35	1.60	1.52
1	A	378	ARG	CA-CB	6.30	1.61	1.53
1	A	448	LEU	CA-CB	6.28	1.60	1.52
1	A	94	ARG	CZ-NH2	-6.22	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	THR	CA-C	6.20	1.60	1.52
1	A	191	LYS	N-CA	6.18	1.53	1.46
1	A	372	GLU	CA-C	6.15	1.60	1.52
1	A	127	THR	CA-C	6.13	1.60	1.52
1	A	130	HIS	CE1-NE2	6.12	1.38	1.32
1	A	339	ARG	NE-CZ	-6.08	1.26	1.33
1	A	253	GLU	C-O	-6.08	1.17	1.23
1	A	488	PHE	CA-CB	5.98	1.60	1.52
1	A	385	LEU	N-CA	5.96	1.53	1.46
1	A	362	LEU	CA-CB	5.96	1.60	1.52
1	A	270	GLU	CA-C	5.95	1.59	1.52
1	A	89	LEU	C-O	-5.94	1.17	1.24
1	A	496	VAL	N-CA	5.94	1.53	1.46
1	A	97	ARG	NE-CZ	-5.93	1.26	1.33
1	A	553	ASP	N-CA	5.88	1.53	1.46
1	A	471	GLU	CA-C	5.85	1.60	1.52
1	A	209	ASP	N-CA	5.83	1.51	1.46
1	A	242	ASP	N-CA	5.81	1.53	1.45
1	A	326	VAL	C-N	5.79	1.40	1.33
1	A	554	ASP	CA-C	5.79	1.60	1.53
1	A	402	ILE	C-O	-5.79	1.17	1.24
1	A	303	GLY	CA-C	5.78	1.59	1.51
1	A	82	VAL	N-CA	5.74	1.53	1.46
1	A	58	GLU	N-CA	5.73	1.53	1.46
1	A	427	ILE	CA-CB	5.72	1.60	1.53
1	A	343	ARG	N-CA	5.70	1.53	1.46
1	A	216	SER	N-CA	5.66	1.53	1.46
1	A	299	ARG	N-CA	5.62	1.53	1.46
1	A	537	ARG	N-CA	5.61	1.53	1.46
1	A	215	ILE	C-O	5.61	1.29	1.23
1	A	338	GLU	N-CA	5.60	1.53	1.46
1	A	200	GLY	CA-C	5.57	1.59	1.51
1	A	233	LEU	CA-C	5.57	1.60	1.52
1	A	186	GLN	N-CA	5.53	1.52	1.46
1	A	545	CYS	N-CA	5.52	1.52	1.45
1	A	71	ARG	N-CA	5.51	1.53	1.46
1	A	390	HIS	CD2-NE2	5.49	1.43	1.37
1	A	34	HIS	CA-C	5.49	1.60	1.52
1	A	99	ALA	CA-C	5.47	1.60	1.52
1	A	138	GLN	CA-C	5.47	1.60	1.52
1	A	512	VAL	C-O	-5.45	1.18	1.24
1	A	62	GLU	N-CA	5.45	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	VAL	CA-C	5.44	1.60	1.52
1	A	251	ILE	C-O	-5.43	1.18	1.24
1	A	181	LYS	CA-CB	5.43	1.61	1.53
1	A	220	GLY	N-CA	5.42	1.53	1.45
1	A	556	ARG	CD-NE	5.42	1.53	1.46
1	A	349	GLU	N-CA	5.41	1.53	1.46
1	A	352	ALA	N-CA	5.40	1.52	1.46
1	A	198	GLU	CA-C	5.38	1.60	1.52
1	A	467	LYS	C-O	-5.37	1.18	1.23
1	A	149	ILE	CA-C	5.36	1.59	1.52
1	A	109	HIS	N-CA	5.35	1.53	1.46
1	A	463	ARG	NE-CZ	-5.34	1.27	1.33
1	A	486	ALA	CA-C	5.34	1.59	1.52
1	A	130	HIS	CG-ND1	5.33	1.44	1.38
1	A	294	ALA	CA-C	5.33	1.59	1.52
1	A	76	VAL	N-CA	5.32	1.53	1.46
1	A	556	ARG	CZ-NH1	-5.32	1.25	1.32
1	A	109	HIS	CD2-NE2	-5.32	1.32	1.37
1	A	516	ARG	CD-NE	5.31	1.53	1.46
1	A	139	ARG	CZ-NH2	-5.30	1.26	1.33
1	A	101	LYS	N-CA	5.29	1.52	1.46
1	A	312	GLY	N-CA	5.28	1.53	1.45
1	A	78	ILE	CA-C	5.27	1.58	1.52
1	A	159	PRO	C-O	-5.26	1.17	1.24
1	A	256	LEU	N-CA	5.26	1.52	1.45
1	A	311	LEU	CA-C	5.25	1.59	1.52
1	A	359	ALA	CA-C	5.23	1.59	1.52
1	A	352	ALA	C-O	-5.23	1.18	1.24
1	A	109	HIS	CG-CD2	5.22	1.41	1.35
1	A	431	GLY	CA-C	5.22	1.59	1.51
1	A	83	ASP	N-CA	5.22	1.52	1.46
1	A	393	ALA	CA-C	5.20	1.60	1.52
1	A	418	LEU	N-CA	5.20	1.52	1.45
1	A	488	PHE	CA-C	5.20	1.59	1.52
1	A	459	VAL	C-O	-5.20	1.18	1.24
1	A	423	ALA	CA-C	5.19	1.60	1.52
1	A	32	LYS	N-CA	5.18	1.52	1.46
1	A	562	GLU	CA-CB	5.18	1.59	1.52
1	A	66	ARG	NE-CZ	5.16	1.38	1.33
1	A	537	ARG	CZ-NH2	-5.16	1.26	1.33
1	A	72	ARG	CZ-NH1	-5.12	1.25	1.32
1	A	540	ALA	C-O	5.12	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	ILE	N-CA	5.12	1.53	1.46
1	A	11	LYS	N-CA	5.12	1.52	1.46
1	A	46	VAL	C-O	5.10	1.29	1.24
1	A	378	ARG	NE-CZ	-5.09	1.27	1.33
1	A	41	LYS	C-O	-5.09	1.18	1.24
1	A	177	PHE	CA-C	5.09	1.58	1.52
1	A	531	ARG	CZ-NH1	-5.07	1.25	1.32
1	A	143	VAL	N-CA	5.07	1.52	1.46
1	A	147	ALA	C-O	5.05	1.29	1.23
1	A	371	LYS	C-O	-5.04	1.19	1.24
1	A	122	VAL	C-O	5.02	1.29	1.24
1	A	373	LEU	CA-C	5.02	1.58	1.52
1	A	550	ASP	C-O	-5.02	1.19	1.24
1	A	416	ASP	C-N	-5.01	1.29	1.34

All (930) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ARG	CD-NE-CZ	15.45	146.02	124.40
1	A	133	PHE	CA-C-N	15.07	140.03	120.44
1	A	133	PHE	C-N-CA	15.07	140.03	120.44
1	A	72	ARG	NE-CZ-NH1	13.85	135.35	121.50
1	A	505	ARG	NE-CZ-NH2	-13.73	106.84	119.20
1	A	275	VAL	O-C-N	-13.45	108.03	122.68
1	A	489	ARG	CD-NE-CZ	13.39	143.15	124.40
1	A	215	ILE	CA-C-O	-13.36	108.41	121.63
1	A	379	ALA	CA-C-O	-13.24	106.25	121.47
1	A	508	ARG	CD-NE-CZ	13.09	142.73	124.40
1	A	277	ASP	CA-CB-CG	13.00	125.60	112.60
1	A	394	ARG	NE-CZ-NH1	12.60	134.10	121.50
1	A	516	ARG	NE-CZ-NH2	12.58	130.52	119.20
1	A	464	ASN	OD1-CG-ND2	-12.30	110.30	122.60
1	A	369	GLY	CA-C-N	12.21	144.87	121.54
1	A	369	GLY	C-N-CA	12.21	144.87	121.54
1	A	285	TYR	CA-C-O	-12.21	107.85	121.40
1	A	555	PHE	CA-C-N	12.02	144.50	121.54
1	A	555	PHE	C-N-CA	12.02	144.50	121.54
1	A	72	ARG	CA-C-O	-11.92	107.16	120.03
1	A	11	LYS	CA-C-N	11.75	136.61	120.63
1	A	11	LYS	C-N-CA	11.75	136.61	120.63
1	A	149	ILE	N-CA-CB	11.69	124.33	111.00
1	A	470	ARG	NE-CZ-NH2	-11.68	108.68	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ASP	CA-CB-CG	11.52	124.12	112.60
1	A	235	GLU	N-CA-C	11.31	123.30	110.97
1	A	138	GLN	CA-C-N	11.26	141.97	121.70
1	A	138	GLN	C-N-CA	11.26	141.97	121.70
1	A	177	PHE	CA-CB-CG	-11.24	102.56	113.80
1	A	145	ASP	CA-C-N	11.15	138.44	121.71
1	A	145	ASP	C-N-CA	11.15	138.44	121.71
1	A	131	GLU	CA-C-N	11.04	142.63	121.54
1	A	131	GLU	C-N-CA	11.04	142.63	121.54
1	A	16	GLU	O-C-N	-10.97	109.50	122.89
1	A	490	LEU	CB-CA-C	10.94	122.32	109.85
1	A	231	LEU	CA-C-N	10.89	135.03	120.65
1	A	231	LEU	C-N-CA	10.89	135.03	120.65
1	A	134	THR	N-CA-CB	10.82	125.69	110.01
1	A	265	ASN	OD1-CG-ND2	-10.71	111.89	122.60
1	A	112	ALA	N-CA-C	10.69	122.96	107.88
1	A	133	PHE	CB-CA-C	10.63	125.43	111.82
1	A	145	ASP	CA-CB-CG	10.61	123.21	112.60
1	A	69	LEU	CA-C-N	10.60	133.09	119.84
1	A	69	LEU	C-N-CA	10.60	133.09	119.84
1	A	408	GLN	OE1-CD-NE2	-10.60	112.00	122.60
1	A	175	LEU	CA-C-O	-10.55	109.31	120.70
1	A	313	PHE	O-C-N	10.55	135.31	122.86
1	A	432	VAL	N-CA-CB	10.55	122.22	110.72
1	A	472	PRO	CA-C-N	10.54	134.76	120.54
1	A	472	PRO	C-N-CA	10.54	134.76	120.54
1	A	453	ARG	NE-CZ-NH2	10.43	128.59	119.20
1	A	74	PRO	N-CD-CG	10.43	116.31	103.80
1	A	439	LYS	CA-C-O	-10.42	109.96	120.70
1	A	330	GLU	O-C-N	-10.39	111.36	122.07
1	A	523	GLN	OE1-CD-NE2	-10.35	112.25	122.60
1	A	73	PRO	N-CA-C	10.32	123.29	110.70
1	A	470	ARG	CD-NE-CZ	10.31	138.83	124.40
1	A	548	GLY	CA-C-O	-10.30	110.11	121.23
1	A	248	ARG	CD-NE-CZ	10.26	138.76	124.40
1	A	234	ALA	O-C-N	-10.23	110.49	122.15
1	A	121	THR	CA-CB-OG1	10.22	124.94	109.60
1	A	541	GLN	OE1-CD-NE2	-10.22	112.38	122.60
1	A	72	ARG	NE-CZ-NH2	-10.20	110.02	119.20
1	A	102	GLU	O-C-N	-10.19	110.40	122.93
1	A	137	ARG	CA-C-O	-10.18	109.35	120.75
1	A	442	ALA	N-CA-C	10.17	123.31	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	VAL	N-CA-C	10.16	122.75	108.12
1	A	256	LEU	CA-C-N	10.15	137.08	122.77
1	A	256	LEU	C-N-CA	10.15	137.08	122.77
1	A	553	ASP	CA-C-O	-10.12	106.03	120.51
1	A	447	VAL	CA-C-O	-9.99	109.89	120.48
1	A	224	GLN	OE1-CD-NE2	-9.96	112.64	122.60
1	A	2	ALA	CA-C-N	9.94	139.60	121.70
1	A	2	ALA	C-N-CA	9.94	139.60	121.70
1	A	481	GLN	CA-C-N	9.91	140.46	121.54
1	A	481	GLN	C-N-CA	9.91	140.46	121.54
1	A	91	ASP	O-C-N	9.88	132.70	122.03
1	A	352	ALA	CA-C-N	9.86	139.44	121.70
1	A	352	ALA	C-N-CA	9.86	139.44	121.70
1	A	78	ILE	CA-C-O	-9.83	109.51	120.72
1	A	236	LEU	CA-C-O	-9.80	110.41	120.90
1	A	161	THR	CA-C-O	-9.78	108.72	119.97
1	A	117	THR	CA-C-N	9.76	129.89	119.05
1	A	117	THR	C-N-CA	9.76	129.89	119.05
1	A	535	ASP	CA-C-N	9.75	133.94	120.49
1	A	535	ASP	C-N-CA	9.75	133.94	120.49
1	A	448	LEU	CA-C-O	-9.74	110.46	122.64
1	A	409	VAL	CA-C-N	9.74	138.43	122.65
1	A	409	VAL	C-N-CA	9.74	138.43	122.65
1	A	231	LEU	N-CA-C	9.74	121.89	111.28
1	A	506	ILE	O-C-N	9.71	129.03	121.46
1	A	310	VAL	CA-C-N	9.70	136.80	121.66
1	A	310	VAL	C-N-CA	9.70	136.80	121.66
1	A	505	ARG	NH1-CZ-NH2	9.69	131.89	119.30
1	A	372	GLU	CA-C-O	-9.68	110.54	121.19
1	A	394	ARG	NE-CZ-NH2	-9.68	110.49	119.20
1	A	23	LEU	O-C-N	9.61	132.47	122.09
1	A	109	HIS	CB-CG-CD2	-9.56	118.77	131.20
1	A	325	TRP	O-C-N	-9.53	111.61	122.86
1	A	424	ASN	CA-CB-CG	9.51	122.11	112.60
1	A	134	THR	CA-CB-CG2	9.48	126.61	110.50
1	A	453	ARG	CD-NE-CZ	9.47	137.66	124.40
1	A	3	LYS	CA-C-N	9.46	136.13	122.99
1	A	3	LYS	C-N-CA	9.46	136.13	122.99
1	A	134	THR	CA-C-N	9.41	136.58	122.93
1	A	134	THR	C-N-CA	9.41	136.58	122.93
1	A	117	THR	O-C-N	-9.41	110.50	121.32
1	A	107	THR	N-CA-C	9.39	124.07	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	THR	N-CA-CB	9.37	126.32	110.49
1	A	321	ASP	CA-CB-CG	9.34	121.94	112.60
1	A	560	VAL	CA-C-N	9.34	136.68	122.68
1	A	560	VAL	C-N-CA	9.34	136.68	122.68
1	A	279	VAL	CA-C-N	9.33	135.36	123.14
1	A	279	VAL	C-N-CA	9.33	135.36	123.14
1	A	295	ASP	N-CA-C	-9.28	101.51	112.92
1	A	34	HIS	CG-CD2-NE2	-9.24	97.96	107.20
1	A	243	PRO	CA-C-N	9.19	139.09	121.54
1	A	243	PRO	C-N-CA	9.19	139.09	121.54
1	A	300	LYS	CA-C-N	9.12	137.34	122.29
1	A	300	LYS	C-N-CA	9.12	137.34	122.29
1	A	234	ALA	N-CA-C	9.08	121.26	111.36
1	A	97	ARG	O-C-N	-9.06	111.62	122.22
1	A	353	ARG	CD-NE-CZ	9.05	137.08	124.40
1	A	456	TYR	CA-C-O	-9.01	109.92	120.10
1	A	75	VAL	CA-C-O	-9.00	109.53	120.78
1	A	199	ARG	NE-CZ-NH1	8.99	130.49	121.50
1	A	168	ALA	O-C-N	-8.96	110.68	122.59
1	A	212	VAL	O-C-N	-8.95	113.64	123.03
1	A	174	LYS	O-C-N	-8.93	112.47	123.01
1	A	229	MET	CA-C-N	8.91	132.67	120.46
1	A	229	MET	C-N-CA	8.91	132.67	120.46
1	A	167	HIS	CA-C-O	-8.90	111.03	120.55
1	A	370	ALA	CA-C-N	8.90	135.15	121.53
1	A	370	ALA	C-N-CA	8.90	135.15	121.53
1	A	312	GLY	O-C-N	-8.84	111.20	122.70
1	A	167	HIS	CA-CB-CG	8.84	122.64	113.80
1	A	491	PRO	CA-C-N	8.83	136.36	122.49
1	A	491	PRO	C-N-CA	8.83	136.36	122.49
1	A	563	ALA	O-C-N	-8.83	112.71	123.04
1	A	230	ILE	O-C-N	-8.83	113.31	121.87
1	A	382	GLN	OE1-CD-NE2	-8.81	113.79	122.60
1	A	540	ALA	CA-C-N	8.80	138.34	121.54
1	A	540	ALA	C-N-CA	8.80	138.34	121.54
1	A	197	MET	O-C-N	-8.78	112.82	122.12
1	A	511	GLU	CA-C-O	-8.77	111.70	121.87
1	A	44	GLU	N-CA-C	8.76	120.91	111.36
1	A	547	ILE	CA-C-N	-8.75	112.93	122.38
1	A	547	ILE	C-N-CA	-8.75	112.93	122.38
1	A	127	THR	CA-C-O	-8.67	108.28	120.16
1	A	398	GLU	CA-C-O	-8.67	112.73	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	MET	N-CA-C	8.65	123.17	109.50
1	A	505	ARG	O-C-N	-8.65	112.59	123.24
1	A	248	ARG	NE-CZ-NH1	-8.65	112.85	121.50
1	A	567	VAL	CA-C-N	8.62	135.16	121.98
1	A	567	VAL	C-N-CA	8.62	135.16	121.98
1	A	341	GLU	CA-C-O	8.58	129.52	120.42
1	A	171	ALA	O-C-N	-8.56	112.06	122.25
1	A	494	LYS	O-C-N	8.55	133.97	122.59
1	A	341	GLU	N-CA-C	8.54	120.67	111.36
1	A	263	ILE	CB-CA-C	8.53	123.63	110.50
1	A	362	LEU	CA-C-N	8.52	137.82	121.54
1	A	362	LEU	C-N-CA	8.52	137.82	121.54
1	A	405	LEU	O-C-N	-8.48	112.83	122.75
1	A	362	LEU	N-CA-CB	-8.47	97.95	110.24
1	A	4	VAL	O-C-N	-8.47	114.05	123.20
1	A	564	PHE	CA-CB-CG	8.46	122.26	113.80
1	A	515	LEU	O-C-N	-8.45	113.30	123.27
1	A	156	GLY	O-C-N	-8.43	114.90	122.91
1	A	365	MET	CA-C-N	8.43	136.84	121.41
1	A	365	MET	C-N-CA	8.43	136.84	121.41
1	A	199	ARG	NE-CZ-NH2	-8.40	111.64	119.20
1	A	556	ARG	CA-C-N	8.39	137.57	121.54
1	A	556	ARG	C-N-CA	8.39	137.57	121.54
1	A	235	GLU	CA-C-N	8.39	131.87	120.54
1	A	235	GLU	C-N-CA	8.39	131.87	120.54
1	A	348	GLU	O-C-N	-8.39	112.38	122.11
1	A	378	ARG	NE-CZ-NH2	8.38	126.74	119.20
1	A	355	PRO	N-CD-CG	8.38	115.77	103.20
1	A	408	GLN	CA-C-N	8.35	133.54	123.19
1	A	408	GLN	C-N-CA	8.35	133.54	123.19
1	A	110	VAL	O-C-N	-8.34	112.14	122.57
1	A	443	GLU	CA-C-O	-8.31	109.98	119.79
1	A	461	GLU	CA-C-N	8.31	131.84	120.46
1	A	461	GLU	C-N-CA	8.31	131.84	120.46
1	A	192	VAL	CA-C-O	-8.31	112.63	121.27
1	A	325	TRP	CA-C-N	8.30	137.48	122.13
1	A	325	TRP	C-N-CA	8.30	137.48	122.13
1	A	248	ARG	O-C-N	-8.29	111.98	123.34
1	A	211	ILE	CA-C-O	-8.28	111.52	121.13
1	A	247	PRO	N-CA-C	8.24	124.22	111.11
1	A	125	ILE	CA-C-N	8.24	136.19	122.76
1	A	125	ILE	C-N-CA	8.24	136.19	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	THR	CA-CB-OG1	8.23	121.95	109.60
1	A	287	ARG	CA-C-O	-8.22	112.00	120.71
1	A	53	GLN	OE1-CD-NE2	-8.18	114.42	122.60
1	A	46	VAL	CA-CB-CG1	8.17	124.29	110.40
1	A	254	SER	O-C-N	-8.16	113.86	123.41
1	A	36	SER	N-CA-C	8.15	120.83	110.24
1	A	453	ARG	CA-C-O	-8.15	111.83	120.55
1	A	487	ILE	O-C-N	-8.13	115.39	123.19
1	A	213	ILE	N-CA-CB	8.12	122.58	111.21
1	A	137	ARG	NE-CZ-NH1	8.11	129.61	121.50
1	A	438	VAL	CA-C-O	-8.09	112.28	120.85
1	A	539	VAL	O-C-N	-8.06	114.49	123.20
1	A	474	TYR	CG-CD1-CE1	-8.05	109.12	121.20
1	A	509	ASN	CB-CA-C	8.03	124.17	112.12
1	A	511	GLU	CA-C-N	8.03	134.39	122.75
1	A	511	GLU	C-N-CA	8.03	134.39	122.75
1	A	462	VAL	O-C-N	-8.01	114.10	121.87
1	A	45	ALA	CA-C-O	-8.01	111.05	120.10
1	A	308	VAL	N-CA-C	7.98	121.74	108.81
1	A	85	GLY	O-C-N	-7.96	114.61	122.41
1	A	182	ILE	CA-C-N	7.95	133.99	120.72
1	A	182	ILE	C-N-CA	7.95	133.99	120.72
1	A	467	LYS	O-C-N	7.94	133.41	122.29
1	A	309	GLN	CA-C-O	-7.94	111.68	120.81
1	A	23	LEU	CA-C-O	-7.94	112.52	120.70
1	A	352	ALA	CA-C-O	7.93	129.13	120.32
1	A	565	GLN	O-C-N	-7.92	112.06	122.59
1	A	275	VAL	CB-CA-C	-7.92	102.68	111.23
1	A	391	ILE	CA-C-N	7.92	130.73	120.44
1	A	391	ILE	C-N-CA	7.92	130.73	120.44
1	A	326	VAL	CA-CB-CG2	7.90	123.83	110.40
1	A	90	LEU	O-C-N	-7.90	112.56	122.27
1	A	169	LYS	O-C-N	-7.90	112.09	122.59
1	A	297	ASN	CA-C-O	-7.89	112.41	121.72
1	A	25	ASP	CA-C-O	-7.86	109.71	119.38
1	A	214	PRO	CB-CA-C	7.86	120.12	111.56
1	A	43	ALA	O-C-N	7.84	131.09	122.15
1	A	206	TYR	CA-C-N	7.84	135.99	120.77
1	A	206	TYR	C-N-CA	7.84	135.99	120.77
1	A	294	ALA	CA-C-O	-7.82	111.26	120.10
1	A	269	GLN	CA-C-N	7.80	134.22	121.58
1	A	269	GLN	C-N-CA	7.80	134.22	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	GLU	CA-C-N	7.78	132.63	121.50
1	A	562	GLU	C-N-CA	7.78	132.63	121.50
1	A	277	ASP	CA-C-O	7.78	130.98	121.81
1	A	538	GLU	CA-C-N	7.74	133.74	122.99
1	A	538	GLU	C-N-CA	7.74	133.74	122.99
1	A	318	HIS	CA-CB-CG	7.73	121.53	113.80
1	A	343	ARG	O-C-N	-7.73	112.77	122.27
1	A	352	ALA	CB-CA-C	7.72	123.68	109.70
1	A	280	VAL	CB-CA-C	7.72	122.06	110.63
1	A	559	ASP	CA-C-N	7.70	130.81	120.50
1	A	559	ASP	C-N-CA	7.70	130.81	120.50
1	A	262	ILE	N-CA-CB	7.68	118.91	110.53
1	A	375	LEU	N-CA-C	7.66	121.85	108.75
1	A	334	GLU	CA-C-N	7.66	131.33	120.53
1	A	334	GLU	C-N-CA	7.66	131.33	120.53
1	A	303	GLY	CA-C-O	-7.65	115.04	122.46
1	A	245	ALA	N-CA-C	7.63	127.06	110.80
1	A	253	GLU	O-C-N	-7.61	116.10	123.26
1	A	154	ASP	CA-C-O	-7.60	111.69	120.20
1	A	487	ILE	CA-C-O	7.59	128.09	120.96
1	A	97	ARG	CD-NE-CZ	7.58	135.01	124.40
1	A	103	ALA	O-C-N	-7.56	110.91	123.00
1	A	66	ARG	NE-CZ-NH1	7.55	129.06	121.50
1	A	398	GLU	CA-C-N	7.54	135.95	121.54
1	A	398	GLU	C-N-CA	7.54	135.95	121.54
1	A	480	GLY	CA-C-N	7.53	135.93	121.54
1	A	480	GLY	C-N-CA	7.53	135.93	121.54
1	A	74	PRO	N-CA-CB	7.53	110.89	102.60
1	A	104	GLY	O-C-N	-7.53	110.95	123.00
1	A	529	LEU	CA-C-N	7.53	133.53	122.39
1	A	529	LEU	C-N-CA	7.53	133.53	122.39
1	A	187	ALA	N-CA-C	7.51	120.90	108.96
1	A	87	THR	CA-C-N	7.47	130.61	120.38
1	A	87	THR	C-N-CA	7.47	130.61	120.38
1	A	13	LEU	CA-C-N	7.45	136.01	121.41
1	A	13	LEU	C-N-CA	7.45	136.01	121.41
1	A	130	HIS	CA-C-O	7.44	128.48	119.10
1	A	313	PHE	CA-C-O	-7.44	113.45	121.56
1	A	70	PRO	CA-C-O	7.44	134.14	120.60
1	A	4	VAL	CA-CB-CG1	7.43	123.04	110.40
1	A	334	GLU	O-C-N	-7.42	114.25	122.12
1	A	40	GLU	CA-C-N	7.41	130.21	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLU	C-N-CA	7.41	130.21	120.28
1	A	259	GLN	CA-C-O	-7.38	112.59	120.42
1	A	295	ASP	O-C-N	-7.38	113.49	122.34
1	A	117	THR	CA-CB-OG1	7.37	120.65	109.60
1	A	535	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	399	ASP	N-CA-C	7.37	126.49	110.80
1	A	195	GLN	OE1-CD-NE2	-7.36	115.25	122.60
1	A	76	VAL	CA-CB-CG2	7.35	122.90	110.40
1	A	375	LEU	CA-C-N	7.35	135.02	122.67
1	A	375	LEU	C-N-CA	7.35	135.02	122.67
1	A	360	ALA	CA-C-N	7.34	135.56	121.54
1	A	360	ALA	C-N-CA	7.34	135.56	121.54
1	A	37	THR	CA-C-O	-7.33	113.04	121.47
1	A	78	ILE	CA-C-N	7.32	134.04	122.62
1	A	78	ILE	C-N-CA	7.32	134.04	122.62
1	A	121	THR	CA-C-O	-7.32	112.20	120.32
1	A	242	ASP	O-C-N	7.32	130.85	121.34
1	A	541	GLN	O-C-N	-7.29	112.89	122.59
1	A	46	VAL	CA-C-N	7.29	132.79	121.19
1	A	46	VAL	C-N-CA	7.29	132.79	121.19
1	A	186	GLN	CA-C-O	-7.29	110.62	119.59
1	A	390	HIS	ND1-CE1-NE2	7.26	115.66	108.40
1	A	324	GLU	CA-C-N	7.25	132.33	120.94
1	A	324	GLU	C-N-CA	7.25	132.33	120.94
1	A	157	ILE	CA-C-O	-7.25	111.72	120.78
1	A	81	HIS	CB-CG-CD2	-7.24	121.78	131.20
1	A	118	PRO	O-C-N	-7.23	113.56	122.23
1	A	345	ALA	CB-CA-C	7.21	122.07	110.96
1	A	3	LYS	CA-C-O	-7.19	108.58	120.80
1	A	401	LYS	O-C-N	-7.19	114.79	123.27
1	A	485	ARG	CA-C-O	-7.18	110.70	119.61
1	A	344	LYS	CA-C-O	-7.18	112.81	120.42
1	A	93	LEU	O-C-N	-7.16	113.99	122.15
1	A	562	GLU	CA-C-O	-7.16	111.40	120.27
1	A	289	ARG	NH1-CZ-NH2	-7.15	110.01	119.30
1	A	449	LEU	O-C-N	-7.13	114.04	122.81
1	A	248	ARG	NH1-CZ-NH2	7.13	128.57	119.30
1	A	463	ARG	CA-C-O	-7.13	110.31	120.51
1	A	341	GLU	CA-C-N	7.12	130.68	120.79
1	A	341	GLU	C-N-CA	7.12	130.68	120.79
1	A	5	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	A	70	PRO	O-C-N	-7.10	113.05	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	VAL	CA-C-N	7.09	134.56	122.37
1	A	143	VAL	C-N-CA	7.09	134.56	122.37
1	A	481	GLN	CA-C-O	-7.09	110.37	120.51
1	A	109	HIS	CB-CG-ND1	7.09	133.33	122.70
1	A	173	ALA	CA-C-N	7.08	131.54	121.42
1	A	173	ALA	C-N-CA	7.08	131.54	121.42
1	A	460	ASP	CA-C-N	7.05	134.12	121.92
1	A	460	ASP	C-N-CA	7.05	134.12	121.92
1	A	67	LYS	O-C-N	-7.03	111.95	122.28
1	A	293	ASP	CA-C-N	7.02	130.39	120.28
1	A	293	ASP	C-N-CA	7.02	130.39	120.28
1	A	138	GLN	OE1-CD-NE2	-7.00	115.60	122.60
1	A	73	PRO	CA-C-O	-7.00	110.42	120.56
1	A	259	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	A	453	ARG	NH1-CZ-NH2	-6.98	110.23	119.30
1	A	181	LYS	N-CA-C	6.97	121.16	112.24
1	A	84	HIS	CA-CB-CG	6.96	120.76	113.80
1	A	333	LYS	N-CA-C	6.96	118.75	111.03
1	A	258	LYS	CA-C-N	6.95	130.16	120.29
1	A	258	LYS	C-N-CA	6.95	130.16	120.29
1	A	316	LEU	CA-C-N	6.94	126.70	119.76
1	A	316	LEU	C-N-CA	6.94	126.70	119.76
1	A	176	ILE	CB-CA-C	6.93	119.50	110.91
1	A	357	THR	CA-C-O	-6.92	110.62	120.51
1	A	48	GLU	CA-C-O	-6.92	113.56	120.82
1	A	81	HIS	CA-C-O	-6.91	112.87	121.50
1	A	379	ALA	CA-C-N	6.89	134.70	121.54
1	A	379	ALA	C-N-CA	6.89	134.70	121.54
1	A	72	ARG	CD-NE-CZ	6.88	134.03	124.40
1	A	440	LYS	CA-C-N	6.87	129.72	120.65
1	A	440	LYS	C-N-CA	6.87	129.72	120.65
1	A	568	GLU	CA-C-N	-6.87	109.33	121.70
1	A	568	GLU	C-N-CA	-6.87	109.33	121.70
1	A	539	VAL	CA-C-O	6.86	127.63	120.36
1	A	317	PRO	O-C-N	-6.86	114.87	123.10
1	A	34	HIS	CE1-NE2-CD2	6.85	115.85	109.00
1	A	386	GLU	CA-C-O	6.85	127.76	120.70
1	A	523	GLN	CG-CD-NE2	6.84	126.67	116.40
1	A	536	VAL	O-C-N	-6.84	115.43	122.75
1	A	139	ARG	O-C-N	-6.84	112.06	123.00
1	A	171	ALA	CA-C-O	6.84	127.66	119.59
1	A	75	VAL	CA-CB-CG1	6.84	122.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	ALA	CA-C-O	-6.83	112.40	120.60
1	A	55	GLY	CA-C-O	6.83	127.82	120.30
1	A	80	GLY	O-C-N	-6.83	113.83	122.70
1	A	91	ASP	CA-C-O	-6.82	113.88	120.90
1	A	321	ASP	CA-C-O	6.81	128.65	120.81
1	A	357	THR	CA-C-N	6.81	134.55	121.54
1	A	357	THR	C-N-CA	6.81	134.55	121.54
1	A	350	GLU	N-CA-C	6.81	121.19	112.34
1	A	418	LEU	N-CA-CB	-6.81	101.21	110.67
1	A	475	LYS	CA-C-O	-6.80	113.55	120.96
1	A	409	VAL	CA-CB-CG2	6.80	121.95	110.40
1	A	65	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	A	123	VAL	CA-C-N	6.78	132.08	122.72
1	A	123	VAL	C-N-CA	6.78	132.08	122.72
1	A	400	VAL	CA-C-O	-6.78	113.31	121.04
1	A	290	ALA	N-CA-CB	-6.78	100.64	111.62
1	A	331	ALA	O-C-N	-6.78	114.29	122.22
1	A	380	ASP	CA-C-N	6.77	132.48	122.86
1	A	380	ASP	C-N-CA	6.77	132.48	122.86
1	A	375	LEU	O-C-N	-6.77	115.49	123.41
1	A	343	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	A	454	ILE	O-C-N	-6.73	116.28	123.14
1	A	530	LYS	N-CA-C	6.72	119.42	108.26
1	A	244	ASN	CA-C-N	6.71	134.35	121.54
1	A	244	ASN	C-N-CA	6.71	134.35	121.54
1	A	66	ARG	CA-C-O	-6.71	111.50	119.35
1	A	527	ALA	N-CA-CB	-6.71	101.67	110.59
1	A	304	PRO	CA-C-N	6.70	134.74	121.53
1	A	304	PRO	C-N-CA	6.70	134.74	121.53
1	A	401	LYS	CA-C-N	6.70	134.04	121.97
1	A	401	LYS	C-N-CA	6.70	134.04	121.97
1	A	182	ILE	CA-CB-CG1	6.70	121.79	110.40
1	A	316	LEU	CA-C-O	-6.70	110.98	120.16
1	A	229	MET	O-C-N	-6.70	115.12	122.09
1	A	297	ASN	OD1-CG-ND2	6.69	129.29	122.60
1	A	353	ARG	NH1-CZ-NH2	6.69	128.00	119.30
1	A	351	LYS	CA-C-O	-6.69	112.28	119.97
1	A	16	GLU	CA-C-O	6.69	128.65	121.16
1	A	485	ARG	NE-CZ-NH2	6.68	125.22	119.20
1	A	8	GLN	CA-C-N	6.68	129.53	120.38
1	A	8	GLN	C-N-CA	6.68	129.53	120.38
1	A	267	LEU	O-C-N	-6.68	115.61	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLU	CB-CG-CD	-6.66	101.27	112.60
1	A	407	ALA	CA-C-O	-6.66	113.65	121.44
1	A	143	VAL	N-CA-C	-6.66	102.77	111.09
1	A	313	PHE	CA-C-N	6.65	131.96	120.58
1	A	313	PHE	C-N-CA	6.65	131.96	120.58
1	A	134	THR	CA-CB-OG1	6.65	119.58	109.60
1	A	377	LEU	CA-C-N	6.65	132.45	122.67
1	A	377	LEU	C-N-CA	6.65	132.45	122.67
1	A	325	TRP	CZ3-CH2-CZ2	-6.64	112.86	121.50
1	A	462	VAL	CB-CA-C	6.64	121.11	112.14
1	A	516	ARG	CA-C-N	6.64	134.22	121.54
1	A	516	ARG	C-N-CA	6.64	134.22	121.54
1	A	277	ASP	O-C-N	-6.63	115.29	122.85
1	A	329	LEU	CA-C-N	6.61	129.04	120.44
1	A	329	LEU	C-N-CA	6.61	129.04	120.44
1	A	60	LEU	CA-C-N	6.61	136.26	122.58
1	A	60	LEU	C-N-CA	6.61	136.26	122.58
1	A	344	LYS	O-C-N	6.61	129.68	122.15
1	A	321	ASP	O-C-N	-6.61	114.80	122.93
1	A	464	ASN	CB-CG-ND2	6.60	126.30	116.40
1	A	560	VAL	CA-C-O	6.58	128.60	121.36
1	A	210	ALA	CA-C-N	6.57	129.37	120.63
1	A	210	ALA	C-N-CA	6.57	129.37	120.63
1	A	56	LEU	N-CA-C	6.57	118.52	111.36
1	A	81	HIS	N-CA-CB	-6.56	99.95	110.39
1	A	144	ALA	CA-C-O	-6.56	112.73	120.60
1	A	178	ALA	N-CA-C	6.56	119.29	109.25
1	A	66	ARG	CA-C-N	6.56	135.61	121.64
1	A	66	ARG	C-N-CA	6.56	135.61	121.64
1	A	264	ALA	N-CA-C	6.56	119.97	108.75
1	A	74	PRO	CA-N-CD	-6.56	102.32	111.50
1	A	325	TRP	CB-CG-CD2	6.55	135.97	126.80
1	A	333	LYS	O-C-N	6.54	129.09	122.03
1	A	362	LEU	O-C-N	-6.53	113.83	122.57
1	A	243	PRO	N-CA-CB	-6.51	96.41	103.25
1	A	47	ARG	O-C-N	-6.50	114.33	122.20
1	A	8	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	A	421	GLN	CA-C-N	6.50	130.18	120.31
1	A	421	GLN	C-N-CA	6.50	130.18	120.31
1	A	123	VAL	O-C-N	-6.49	114.40	122.97
1	A	392	LEU	N-CA-CB	6.49	119.43	110.01
1	A	361	LEU	N-CA-CB	6.49	121.46	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	ILE	CA-CB-CG1	6.49	121.43	110.40
1	A	204	GLU	N-CA-C	6.48	120.78	113.01
1	A	510	ALA	O-C-N	-6.47	116.71	123.56
1	A	554	ASP	CA-C-N	6.47	133.89	121.54
1	A	554	ASP	C-N-CA	6.47	133.89	121.54
1	A	165	ILE	CB-CA-C	6.46	121.88	111.29
1	A	77	VAL	O-C-N	-6.45	116.25	123.03
1	A	459	VAL	N-CA-C	6.44	117.97	110.62
1	A	248	ARG	CB-CA-C	6.44	119.65	110.24
1	A	440	LYS	CA-C-O	-6.44	112.83	120.10
1	A	562	GLU	O-C-N	6.44	130.67	123.40
1	A	217	ALA	CA-C-O	-6.43	111.31	120.51
1	A	136	ILE	O-C-N	-6.43	115.38	121.87
1	A	97	ARG	CA-C-N	6.43	133.54	121.97
1	A	97	ARG	C-N-CA	6.43	133.54	121.97
1	A	167	HIS	O-C-N	-6.42	114.40	122.17
1	A	294	ALA	N-CA-CB	-6.42	100.34	110.22
1	A	525	ARG	N-CA-C	6.42	118.70	109.14
1	A	24	LEU	O-C-N	-6.41	115.32	122.12
1	A	34	HIS	ND1-CG-CD2	6.39	112.50	106.10
1	A	381	THR	CA-CB-CG2	6.39	121.37	110.50
1	A	361	LEU	O-C-N	-6.39	114.09	122.59
1	A	315	GLU	O-C-N	-6.39	113.81	122.94
1	A	395	ALA	N-CA-C	6.38	120.80	112.89
1	A	374	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	A	251	ILE	CA-C-O	6.37	128.31	121.04
1	A	65	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	A	392	LEU	CA-C-O	-6.37	114.13	120.82
1	A	247	PRO	N-CA-CB	6.37	108.67	103.32
1	A	418	LEU	O-C-N	-6.36	114.78	122.48
1	A	483	GLU	O-C-N	-6.35	115.12	122.93
1	A	306	SER	N-CA-C	6.34	119.41	109.96
1	A	341	GLU	O-C-N	-6.34	114.92	122.15
1	A	7	TYR	CA-CB-CG	6.34	125.31	113.90
1	A	76	VAL	O-C-N	-6.33	114.65	122.57
1	A	346	ARG	O-C-N	-6.33	115.41	122.12
1	A	228	GLU	OE1-CD-OE2	6.33	138.10	122.90
1	A	288	ILE	CA-C-N	6.33	135.12	121.64
1	A	288	ILE	C-N-CA	6.33	135.12	121.64
1	A	328	ASP	O-C-N	-6.32	117.72	123.41
1	A	275	VAL	CA-C-O	-6.32	112.99	120.76
1	A	127	THR	CA-CB-OG1	6.31	119.06	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	ILE	CA-C-O	-6.31	114.59	119.20
1	A	317	PRO	CA-C-O	6.30	128.88	121.31
1	A	93	LEU	CA-C-N	6.29	130.66	120.60
1	A	93	LEU	C-N-CA	6.29	130.66	120.60
1	A	195	GLN	CA-C-N	6.29	128.99	120.44
1	A	195	GLN	C-N-CA	6.29	128.99	120.44
1	A	551	GLY	CA-C-N	6.29	134.31	123.05
1	A	551	GLY	C-N-CA	6.29	134.31	123.05
1	A	499	CYS	CA-C-O	-6.28	112.55	120.28
1	A	268	VAL	O-C-N	-6.28	115.79	122.95
1	A	177	PHE	CA-C-N	6.27	130.81	121.72
1	A	177	PHE	C-N-CA	6.27	130.81	121.72
1	A	244	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	491	PRO	N-CD-CG	6.25	112.58	103.20
1	A	421	GLN	CG-CD-NE2	-6.25	107.02	116.40
1	A	522	TRP	O-C-N	-6.22	117.30	123.46
1	A	382	GLN	O-C-N	-6.22	114.31	122.59
1	A	458	LEU	CD1-CG-CD2	-6.22	97.11	110.80
1	A	9	LEU	CA-C-N	6.21	128.52	120.44
1	A	9	LEU	C-N-CA	6.21	128.52	120.44
1	A	52	GLU	O-C-N	6.21	129.23	122.15
1	A	32	LYS	CB-CA-C	6.21	120.61	110.24
1	A	553	ASP	N-CA-CB	-6.20	100.00	110.49
1	A	225	ASP	CA-C-N	6.20	128.91	120.54
1	A	225	ASP	C-N-CA	6.20	128.91	120.54
1	A	84	HIS	CA-C-O	6.20	126.04	119.03
1	A	7	TYR	N-CA-C	6.20	119.69	111.75
1	A	454	ILE	CB-CA-C	6.20	120.23	110.81
1	A	283	GLU	CA-C-N	6.19	131.26	122.09
1	A	283	GLU	C-N-CA	6.19	131.26	122.09
1	A	224	GLN	N-CA-C	6.19	118.82	111.33
1	A	542	GLY	O-C-N	-6.19	114.66	122.70
1	A	446	GLY	CA-C-O	-6.18	109.81	120.57
1	A	163	GLU	O-C-N	6.18	129.20	122.15
1	A	225	ASP	N-CA-C	-6.18	104.08	111.69
1	A	490	LEU	CA-C-O	-6.18	112.40	119.32
1	A	173	ALA	CB-CA-C	6.17	120.96	109.86
1	A	187	ALA	CA-C-N	6.17	130.74	123.16
1	A	187	ALA	C-N-CA	6.17	130.74	123.16
1	A	139	ARG	CD-NE-CZ	6.16	133.02	124.40
1	A	453	ARG	O-C-N	-6.15	114.72	122.17
1	A	555	PHE	CA-C-O	6.15	129.31	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	GLY	CA-C-O	-6.15	115.00	120.53
1	A	379	ALA	O-C-N	6.15	129.91	122.96
1	A	10	ALA	N-CA-C	6.14	117.64	111.07
1	A	507	PRO	N-CD-CG	6.14	112.40	103.20
1	A	81	HIS	ND1-CE1-NE2	6.13	114.53	108.40
1	A	167	HIS	CB-CG-CD2	6.13	139.17	131.20
1	A	226	LEU	N-CA-C	6.13	118.47	111.11
1	A	81	HIS	ND1-CG-CD2	6.12	112.22	106.10
1	A	484	VAL	CA-CB-CG1	6.12	120.81	110.40
1	A	550	ASP	N-CA-C	6.12	117.62	108.31
1	A	421	GLN	CB-CA-C	6.11	120.37	110.96
1	A	158	MET	CA-C-N	6.11	126.29	119.32
1	A	158	MET	C-N-CA	6.11	126.29	119.32
1	A	142	LYS	N-CA-CB	-6.11	102.63	111.91
1	A	558	GLY	CA-C-O	-6.11	114.41	121.00
1	A	370	ALA	CB-CA-C	6.10	122.56	110.42
1	A	513	ARG	CB-CA-C	6.10	121.49	109.66
1	A	47	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	A	407	ALA	CA-C-N	6.09	133.86	123.01
1	A	407	ALA	C-N-CA	6.09	133.86	123.01
1	A	463	ARG	CD-NE-CZ	6.09	132.93	124.40
1	A	552	PHE	CD1-CE1-CZ	6.09	130.97	120.00
1	A	409	VAL	CB-CA-C	6.09	119.90	110.83
1	A	505	ARG	CA-C-N	6.08	129.34	123.02
1	A	505	ARG	C-N-CA	6.08	129.34	123.02
1	A	300	LYS	O-C-N	-6.07	115.11	122.22
1	A	160	GLN	N-CA-CB	6.07	119.57	110.22
1	A	374	ASN	CB-CG-ND2	6.07	125.50	116.40
1	A	46	VAL	CA-CB-CG2	6.05	120.69	110.40
1	A	154	ASP	N-CA-C	6.05	119.50	111.75
1	A	73	PRO	O-C-N	-6.05	114.32	121.46
1	A	140	GLY	CA-C-N	6.04	133.08	121.54
1	A	140	GLY	C-N-CA	6.04	133.08	121.54
1	A	294	ALA	O-C-N	-6.03	115.17	122.22
1	A	370	ALA	CA-C-O	-6.02	111.90	120.51
1	A	322	VAL	CG1-CB-CG2	-6.02	97.55	110.80
1	A	308	VAL	CA-C-N	6.02	129.38	120.95
1	A	308	VAL	C-N-CA	6.02	129.38	120.95
1	A	522	TRP	CH2-CZ2-CE2	6.02	125.33	117.50
1	A	434	PRO	CA-C-N	6.02	127.36	119.84
1	A	434	PRO	C-N-CA	6.02	127.36	119.84
1	A	236	LEU	O-C-N	6.02	128.35	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ARG	NE-CZ-NH1	6.01	127.51	121.50
1	A	365	MET	CB-CA-C	6.01	118.67	111.22
1	A	339	ARG	CA-C-N	6.01	128.82	120.29
1	A	339	ARG	C-N-CA	6.01	128.82	120.29
1	A	378	ARG	NH1-CZ-NH2	-6.00	111.50	119.30
1	A	537	ARG	N-CA-CB	-5.99	101.05	110.46
1	A	176	ILE	N-CA-CB	5.99	117.25	110.72
1	A	180	ASN	CB-CG-ND2	5.96	125.34	116.40
1	A	159	PRO	N-CA-CB	5.95	110.05	103.26
1	A	547	ILE	CA-C-O	-5.95	114.48	121.80
1	A	389	GLN	N-CA-C	5.95	117.43	111.07
1	A	449	LEU	CA-C-N	5.94	132.69	121.69
1	A	449	LEU	C-N-CA	5.94	132.69	121.69
1	A	285	TYR	CA-CB-CG	5.94	124.59	113.90
1	A	434	PRO	CA-C-O	-5.94	111.95	120.56
1	A	15	MET	CA-C-N	5.94	129.30	120.87
1	A	15	MET	C-N-CA	5.94	129.30	120.87
1	A	458	LEU	O-C-N	-5.94	115.73	122.08
1	A	88	THR	OG1-CB-CG2	-5.93	97.43	109.30
1	A	215	ILE	O-C-N	5.93	129.72	123.02
1	A	233	LEU	CA-C-O	-5.92	113.41	120.10
1	A	463	ARG	N-CA-CB	5.92	120.49	110.49
1	A	144	ALA	N-CA-CB	-5.91	100.54	111.13
1	A	528	SER	CA-C-N	5.91	129.60	121.33
1	A	528	SER	C-N-CA	5.91	129.60	121.33
1	A	457	ASP	CA-C-N	5.91	129.00	120.79
1	A	457	ASP	C-N-CA	5.91	129.00	120.79
1	A	443	GLU	CB-CG-CD	5.90	122.63	112.60
1	A	289	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	A	155	ASP	O-C-N	-5.89	114.75	122.59
1	A	118	PRO	N-CA-CB	5.89	109.81	103.33
1	A	496	VAL	N-CA-CB	-5.88	104.31	110.72
1	A	385	LEU	N-CA-C	-5.88	105.20	112.90
1	A	2	ALA	O-C-N	-5.88	115.63	122.86
1	A	517	ASP	CB-CA-C	5.87	122.11	110.42
1	A	453	ARG	N-CA-C	5.87	118.56	111.40
1	A	486	ALA	CA-C-N	5.87	130.93	121.95
1	A	486	ALA	C-N-CA	5.87	130.93	121.95
1	A	433	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	A	66	ARG	NE-CZ-NH2	-5.86	113.92	119.20
1	A	172	GLY	CA-C-N	5.86	132.54	121.69
1	A	172	GLY	C-N-CA	5.86	132.54	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	415	SER	N-CA-CB	5.86	118.83	110.16
1	A	91	ASP	N-CA-C	-5.86	104.53	111.03
1	A	545	CYS	CA-C-O	-5.86	115.18	121.45
1	A	382	GLN	N-CA-CB	5.85	120.38	110.49
1	A	162	GLU	CA-C-N	5.84	128.59	120.29
1	A	162	GLU	C-N-CA	5.84	128.59	120.29
1	A	173	ALA	O-C-N	5.84	130.14	123.48
1	A	65	ARG	O-C-N	5.84	129.98	122.39
1	A	109	HIS	CA-C-N	5.84	132.48	121.97
1	A	109	HIS	C-N-CA	5.84	132.48	121.97
1	A	69	LEU	O-C-N	-5.83	115.71	121.19
1	A	97	ARG	N-CA-CB	-5.83	101.24	110.22
1	A	213	ILE	O-C-N	-5.83	114.45	121.10
1	A	557	GLU	N-CA-CB	5.83	120.34	110.49
1	A	434	PRO	N-CA-CB	5.82	108.72	103.08
1	A	470	ARG	NH1-CZ-NH2	5.82	126.86	119.30
1	A	78	ILE	CA-CB-CG1	-5.81	100.52	110.40
1	A	445	LYS	N-CA-C	5.81	120.53	113.38
1	A	373	LEU	O-C-N	-5.80	116.31	123.33
1	A	448	LEU	CB-CA-C	-5.80	102.65	112.00
1	A	284	ALA	CA-C-O	-5.80	114.25	120.92
1	A	541	GLN	N-CA-C	5.80	123.16	110.80
1	A	265	ASN	CB-CG-OD1	5.80	132.40	120.80
1	A	537	ARG	CD-NE-CZ	5.80	132.52	124.40
1	A	528	SER	N-CA-C	5.80	118.22	109.41
1	A	184	LEU	CA-C-N	5.79	125.48	119.05
1	A	184	LEU	C-N-CA	5.79	125.48	119.05
1	A	95	LYS	CA-C-O	-5.79	112.87	119.41
1	A	206	TYR	CG-CD2-CE2	-5.79	112.52	121.20
1	A	321	ASP	CB-CG-OD2	5.79	131.71	118.40
1	A	481	GLN	N-CA-CB	5.79	120.27	110.49
1	A	38	LEU	O-C-N	-5.78	115.64	123.10
1	A	480	GLY	O-C-N	-5.78	115.19	122.70
1	A	209	ASP	CA-C-N	5.78	131.69	123.14
1	A	209	ASP	C-N-CA	5.78	131.69	123.14
1	A	355	PRO	CA-C-O	-5.77	110.77	119.55
1	A	62	GLU	O-C-N	-5.77	115.86	122.09
1	A	185	PRO	N-CA-CB	5.77	109.68	103.33
1	A	551	GLY	O-C-N	-5.76	115.21	122.70
1	A	99	ALA	N-CA-C	5.75	123.05	110.80
1	A	255	LYS	N-CA-C	5.75	115.43	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	GLU	CA-C-O	-5.75	112.28	120.16
1	A	273	PHE	CA-C-O	-5.75	114.31	120.92
1	A	219	THR	N-CA-CB	5.73	120.18	110.49
1	A	516	ARG	NH1-CZ-NH2	-5.73	111.85	119.30
1	A	433	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	485	ARG	NH1-CZ-NH2	-5.73	111.86	119.30
1	A	125	ILE	O-C-N	-5.72	116.84	122.67
1	A	63	GLU	CA-C-N	5.71	132.49	122.79
1	A	63	GLU	C-N-CA	5.71	132.49	122.79
1	A	374	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	472	PRO	N-CA-C	5.71	121.48	114.35
1	A	529	LEU	O-C-N	-5.71	117.80	123.62
1	A	146	ILE	CA-C-N	5.70	131.16	122.95
1	A	146	ILE	C-N-CA	5.70	131.16	122.95
1	A	546	GLY	CA-C-N	5.70	130.35	121.85
1	A	546	GLY	C-N-CA	5.70	130.35	121.85
1	A	180	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	A	332	ALA	N-CA-C	5.69	117.56	111.36
1	A	372	GLU	CB-CG-CD	-5.69	102.93	112.60
1	A	485	ARG	O-C-N	-5.67	115.31	121.95
1	A	359	ALA	N-CA-CB	-5.67	100.91	110.49
1	A	474	TYR	CA-C-N	5.67	129.15	121.05
1	A	474	TYR	C-N-CA	5.67	129.15	121.05
1	A	540	ALA	N-CA-C	5.66	118.69	109.06
1	A	8	GLN	CG-CD-NE2	5.66	124.89	116.40
1	A	179	ILE	CB-CG1-CD1	-5.66	101.92	113.80
1	A	499	CYS	N-CA-C	5.66	118.71	108.69
1	A	250	VAL	CA-C-O	-5.66	114.85	120.90
1	A	15	MET	O-C-N	-5.65	116.37	123.27
1	A	113	PHE	CA-C-O	5.65	127.03	120.14
1	A	273	PHE	CA-C-N	5.65	131.37	122.21
1	A	273	PHE	C-N-CA	5.65	131.37	122.21
1	A	164	ALA	N-CA-CB	5.64	118.15	109.91
1	A	248	ARG	CA-C-O	5.64	127.84	120.11
1	A	265	ASN	CA-C-N	5.64	130.94	122.99
1	A	265	ASN	C-N-CA	5.64	130.94	122.99
1	A	264	ALA	O-C-N	-5.64	116.81	123.41
1	A	133	PHE	O-C-N	5.64	129.04	122.67
1	A	323	VAL	CA-CB-CG2	-5.64	100.82	110.40
1	A	219	THR	CA-CB-OG1	5.63	118.05	109.60
1	A	386	GLU	CB-CG-CD	5.63	122.18	112.60
1	A	142	LYS	N-CA-C	5.63	119.40	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ILE	CB-CA-C	-5.62	102.26	110.81
1	A	58	GLU	CG-CD-OE2	5.61	131.31	118.40
1	A	495	GLN	O-C-N	-5.61	115.13	122.59
1	A	72	ARG	N-CA-CB	-5.61	98.34	110.95
1	A	49	LEU	N-CA-C	5.59	118.91	111.75
1	A	513	ARG	CG-CD-NE	5.59	124.29	112.00
1	A	343	ARG	NH1-CZ-NH2	5.58	126.56	119.30
1	A	537	ARG	CA-C-O	-5.58	112.54	119.18
1	A	274	ARG	N-CA-C	5.58	117.66	109.24
1	A	224	GLN	CG-CD-NE2	5.56	124.74	116.40
1	A	16	GLU	CB-CG-CD	5.55	122.04	112.60
1	A	189	PRO	N-CA-C	5.55	121.06	113.84
1	A	390	HIS	CE1-NE2-CD2	-5.55	103.44	109.00
1	A	512	VAL	CA-C-N	5.55	132.14	122.81
1	A	512	VAL	C-N-CA	5.55	132.14	122.81
1	A	133	PHE	CG-CD2-CE2	5.54	130.12	120.70
1	A	259	GLN	CB-CA-C	5.54	120.27	110.85
1	A	539	VAL	CA-CB-CG2	5.54	119.82	110.40
1	A	86	LYS	CA-C-O	-5.54	113.24	120.00
1	A	244	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	202	VAL	CA-C-O	-5.53	112.53	119.95
1	A	175	LEU	CA-C-N	5.53	129.50	122.37
1	A	175	LEU	C-N-CA	5.53	129.50	122.37
1	A	202	VAL	CA-C-N	5.53	125.51	120.03
1	A	202	VAL	C-N-CA	5.53	125.51	120.03
1	A	378	ARG	CA-CB-CG	-5.53	103.04	114.10
1	A	221	GLN	O-C-N	-5.53	116.75	123.16
1	A	473	GLN	CA-C-N	5.52	132.09	121.54
1	A	473	GLN	C-N-CA	5.52	132.09	121.54
1	A	566	MET	O-C-N	-5.52	115.98	123.10
1	A	450	LYS	O-C-N	-5.51	117.19	123.48
1	A	506	ILE	N-CA-C	5.51	113.94	107.77
1	A	33	SER	O-C-N	-5.51	117.47	123.26
1	A	455	ILE	CA-C-N	5.51	128.21	120.28
1	A	455	ILE	C-N-CA	5.51	128.21	120.28
1	A	47	ARG	NH1-CZ-NH2	-5.51	112.14	119.30
1	A	54	ARG	N-CA-C	5.50	117.28	111.28
1	A	378	ARG	CA-C-O	-5.50	114.01	122.32
1	A	218	LYS	CB-CA-C	5.50	121.37	110.42
1	A	130	HIS	CB-CA-C	5.49	122.24	110.21
1	A	522	TRP	CD2-CE2-CZ2	-5.49	116.91	122.40
1	A	369	GLY	O-C-N	-5.49	115.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	28	GLY	CA-C-N	5.49	129.48	121.80
1	A	28	GLY	C-N-CA	5.49	129.48	121.80
1	A	353	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	234	ALA	CA-C-O	5.48	126.23	120.42
1	A	461	GLU	CA-C-O	5.48	125.17	119.14
1	A	154	ASP	CB-CA-C	5.48	121.08	110.46
1	A	217	ALA	CA-C-N	5.47	132.00	121.54
1	A	217	ALA	C-N-CA	5.47	132.00	121.54
1	A	307	ALA	CB-CA-C	5.47	118.78	109.75
1	A	212	VAL	CA-C-N	5.47	132.24	122.13
1	A	212	VAL	C-N-CA	5.47	132.24	122.13
1	A	202	VAL	CG1-CB-CG2	-5.46	98.79	110.80
1	A	399	ASP	CA-C-N	5.46	128.40	120.98
1	A	399	ASP	C-N-CA	5.46	128.40	120.98
1	A	403	ASN	OD1-CG-ND2	5.46	128.06	122.60
1	A	512	VAL	N-CA-CB	5.46	120.42	111.58
1	A	146	ILE	N-CA-C	5.45	116.63	109.21
1	A	183	ASP	N-CA-C	5.45	119.19	112.54
1	A	568	GLU	N-CA-CB	5.45	118.18	110.98
1	A	149	ILE	CA-CB-CG2	5.45	119.77	110.50
1	A	343	ARG	N-CA-CB	-5.45	101.83	110.28
1	A	442	ALA	CB-CA-C	5.44	119.52	110.81
1	A	404	ILE	CA-C-O	-5.43	115.06	121.64
1	A	438	VAL	O-C-N	5.43	127.43	121.83
1	A	273	PHE	CB-CA-C	5.43	118.49	109.53
1	A	315	GLU	CA-C-O	-5.43	115.27	121.68
1	A	357	THR	CA-CB-CG2	5.42	119.72	110.50
1	A	444	GLU	CA-C-N	5.42	131.64	122.26
1	A	444	GLU	C-N-CA	5.42	131.64	122.26
1	A	36	SER	O-C-N	-5.42	115.88	122.82
1	A	52	GLU	N-CA-C	5.42	117.27	111.36
1	A	22	GLU	N-CA-C	5.42	117.89	111.33
1	A	252	LEU	N-CA-CB	-5.42	102.13	110.42
1	A	43	ALA	N-CA-C	5.41	117.26	111.36
1	A	109	HIS	CA-CB-CG	5.41	119.21	113.80
1	A	365	MET	N-CA-CB	-5.41	100.08	109.93
1	A	512	VAL	N-CA-C	5.41	116.07	108.17
1	A	528	SER	CB-CA-C	-5.41	99.59	110.30
1	A	381	THR	N-CA-C	5.41	117.64	108.02
1	A	42	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	209	ASP	O-C-N	-5.40	115.46	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ASP	N-CA-CB	5.40	117.81	109.98
1	A	234	ALA	N-CA-CB	5.40	118.15	110.16
1	A	231	LEU	CA-C-O	-5.39	114.84	120.55
1	A	206	TYR	CD1-CG-CD2	5.38	126.17	118.10
1	A	381	THR	CA-C-O	-5.38	114.52	120.33
1	A	92	TYR	N-CA-C	5.37	117.13	111.28
1	A	426	ALA	N-CA-CB	-5.37	101.88	110.63
1	A	250	VAL	N-CA-C	5.36	115.43	108.35
1	A	521	ILE	CA-C-O	-5.36	114.08	120.78
1	A	491	PRO	N-CA-C	5.35	123.49	112.47
1	A	232	LEU	O-C-N	-5.34	116.47	122.03
1	A	522	TRP	NE1-CE2-CZ2	5.34	138.12	130.10
1	A	547	ILE	CB-CA-C	5.34	118.86	111.49
1	A	115	VAL	CA-C-N	5.34	129.78	122.84
1	A	115	VAL	C-N-CA	5.34	129.78	122.84
1	A	380	ASP	CB-CA-C	5.34	121.04	110.42
1	A	21	LEU	CA-C-O	-5.33	115.21	120.70
1	A	50	VAL	CA-C-O	-5.33	112.82	119.70
1	A	394	ARG	N-CA-C	5.33	120.06	113.50
1	A	390	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	193	LYS	O-C-N	-5.32	116.56	122.09
1	A	566	MET	CA-C-N	5.32	131.54	121.97
1	A	566	MET	C-N-CA	5.32	131.54	121.97
1	A	420	ALA	CA-C-N	5.30	127.65	120.65
1	A	420	ALA	C-N-CA	5.30	127.65	120.65
1	A	186	GLN	N-CA-CB	-5.30	103.25	110.56
1	A	3	LYS	O-C-N	5.30	131.48	123.00
1	A	107	THR	OG1-CB-CG2	-5.30	98.70	109.30
1	A	170	ALA	CB-CA-C	5.30	120.55	110.27
1	A	387	ALA	CB-CA-C	5.29	119.19	110.88
1	A	303	GLY	CA-C-N	5.29	125.54	119.83
1	A	303	GLY	C-N-CA	5.29	125.54	119.83
1	A	481	GLN	O-C-N	5.29	129.62	122.59
1	A	510	ALA	CA-C-N	5.29	130.59	120.97
1	A	510	ALA	C-N-CA	5.29	130.59	120.97
1	A	194	ARG	CA-C-N	5.28	127.79	120.29
1	A	194	ARG	C-N-CA	5.28	127.79	120.29
1	A	544	GLU	N-CA-C	5.28	118.43	109.76
1	A	356	ALA	N-CA-CB	5.28	119.41	110.49
1	A	42	ASP	CA-C-O	-5.28	113.56	119.79
1	A	210	ALA	O-C-N	-5.27	116.16	123.01
1	A	243	PRO	O-C-N	-5.27	115.53	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLY	CA-C-N	5.27	132.86	121.64
1	A	85	GLY	C-N-CA	5.27	132.86	121.64
1	A	340	LYS	CA-C-O	-5.27	114.84	120.42
1	A	342	GLU	O-C-N	5.27	127.72	122.08
1	A	176	ILE	O-C-N	-5.26	116.95	122.95
1	A	18	GLN	CA-C-N	5.26	127.64	120.54
1	A	18	GLN	C-N-CA	5.26	127.64	120.54
1	A	412	PRO	N-CA-C	5.25	123.29	112.47
1	A	326	VAL	CA-C-O	-5.25	112.92	119.95
1	A	534	GLU	N-CA-C	5.24	116.11	108.14
1	A	109	HIS	CA-C-O	-5.24	116.08	122.41
1	A	185	PRO	CB-CA-C	5.24	121.26	112.62
1	A	465	MET	N-CA-C	5.24	119.42	113.19
1	A	382	GLN	CA-C-O	-5.22	113.04	120.51
1	A	467	LYS	CA-C-O	-5.22	116.04	122.36
1	A	126	ASP	CA-C-O	5.22	129.21	120.81
1	A	372	GLU	O-C-N	5.22	129.29	122.87
1	A	364	ALA	N-CA-C	5.22	121.91	110.80
1	A	258	LYS	CA-CB-CG	-5.21	103.69	114.10
1	A	547	ILE	CB-CG1-CD1	5.21	124.73	113.80
1	A	197	MET	N-CA-C	5.20	116.95	111.28
1	A	312	GLY	CA-C-N	5.20	129.10	120.94
1	A	312	GLY	C-N-CA	5.20	129.10	120.94
1	A	356	ALA	CA-C-N	5.20	131.47	121.54
1	A	356	ALA	C-N-CA	5.20	131.47	121.54
1	A	130	HIS	CB-CG-CD2	-5.20	124.45	131.20
1	A	148	VAL	CA-C-O	-5.20	114.14	120.69
1	A	130	HIS	O-C-N	-5.19	115.52	122.43
1	A	137	ARG	CB-CA-C	5.19	118.35	109.99
1	A	302	ALA	CA-C-O	-5.19	114.03	120.57
1	A	6	ILE	O-C-N	-5.18	116.09	122.57
1	A	461	GLU	N-CA-C	5.18	119.88	113.50
1	A	133	PHE	CA-C-O	-5.17	115.25	121.40
1	A	339	ARG	CD-NE-CZ	5.17	131.64	124.40
1	A	362	LEU	CA-C-O	5.17	126.56	120.98
1	A	159	PRO	CA-N-CD	-5.16	104.77	112.00
1	A	54	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	218	LYS	N-CA-CB	-5.16	101.77	110.49
1	A	376	ILE	CA-C-N	-5.16	114.72	122.81
1	A	376	ILE	C-N-CA	-5.16	114.72	122.81
1	A	34	HIS	O-C-N	5.15	129.09	122.39
1	A	326	VAL	CB-CA-C	5.15	120.73	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	VAL	CA-C-N	-5.15	116.31	122.90
1	A	122	VAL	C-N-CA	-5.15	116.31	122.90
1	A	287	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	366	ALA	CA-C-N	5.15	129.02	120.94
1	A	366	ALA	C-N-CA	5.15	129.02	120.94
1	A	412	PRO	CB-CA-C	5.14	120.04	111.56
1	A	155	ASP	N-CA-CB	5.14	119.17	110.49
1	A	306	SER	N-CA-CB	5.13	117.61	109.51
1	A	174	LYS	N-CA-CB	5.13	117.80	110.06
1	A	402	ILE	N-CA-CB	5.12	119.68	111.23
1	A	45	ALA	N-CA-C	5.12	117.60	111.71
1	A	250	VAL	N-CA-CB	-5.12	102.96	111.36
1	A	267	LEU	CD1-CG-CD2	-5.12	99.53	110.80
1	A	389	GLN	CA-C-N	5.11	127.38	120.38
1	A	389	GLN	C-N-CA	5.11	127.38	120.38
1	A	325	TRP	CE2-CD2-CE3	-5.11	113.69	118.80
1	A	438	VAL	CA-CB-CG2	5.11	119.08	110.40
1	A	531	ARG	CD-NE-CZ	5.11	131.55	124.40
1	A	233	LEU	CA-C-N	5.10	127.54	120.29
1	A	233	LEU	C-N-CA	5.10	127.54	120.29
1	A	447	VAL	CA-CB-CG2	5.10	119.07	110.40
1	A	168	ALA	CB-CA-C	5.10	120.56	110.42
1	A	231	LEU	O-C-N	-5.10	116.72	122.12
1	A	85	GLY	CA-C-O	-5.09	113.64	119.80
1	A	303	GLY	O-C-N	-5.09	116.22	122.03
1	A	71	ARG	O-C-N	-5.09	115.82	122.59
1	A	438	VAL	N-CA-C	5.09	115.86	110.72
1	A	24	LEU	CA-C-N	5.09	129.22	120.72
1	A	24	LEU	C-N-CA	5.09	129.22	120.72
1	A	530	LYS	O-C-N	-5.09	116.77	123.28
1	A	532	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	20	LEU	CD1-CG-CD2	-5.08	99.62	110.80
1	A	535	ASP	CB-CG-OD2	5.08	130.08	118.40
1	A	242	ASP	CA-C-O	-5.08	115.43	120.96
1	A	72	ARG	CA-C-N	5.07	125.61	120.38
1	A	72	ARG	C-N-CA	5.07	125.61	120.38
1	A	167	HIS	CB-CG-ND1	-5.07	115.09	122.70
1	A	247	PRO	CA-N-CD	-5.07	104.90	112.00
1	A	333	LYS	CA-C-O	-5.07	115.68	120.90
1	A	248	ARG	N-CA-C	5.07	116.84	108.13
1	A	34	HIS	CA-C-O	-5.06	113.36	119.49
1	A	300	LYS	CA-C-O	-5.06	114.38	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	LEU	CD1-CG-CD2	-5.05	99.69	110.80
1	A	431	GLY	O-C-N	5.05	129.27	122.70
1	A	14	GLY	CA-C-N	5.05	130.91	122.73
1	A	14	GLY	C-N-CA	5.05	130.91	122.73
1	A	141	ALA	O-C-N	-5.04	115.88	122.59
1	A	419	LEU	O-C-N	5.04	128.78	122.23
1	A	11	LYS	CA-C-O	-5.04	114.18	119.97
1	A	371	LYS	O-C-N	-5.04	117.19	122.18
1	A	253	GLU	CA-C-O	5.04	126.90	121.26
1	A	384	SER	CA-C-O	-5.04	113.31	120.51
1	A	141	ALA	CA-C-N	5.03	129.34	122.34
1	A	141	ALA	C-N-CA	5.03	129.34	122.34
1	A	268	VAL	CA-C-O	5.03	126.40	120.71
1	A	257	ASP	O-C-N	5.03	129.16	123.27
1	A	179	ILE	CA-CB-CG1	-5.03	101.85	110.40
1	A	464	ASN	N-CA-C	5.03	121.51	110.80
1	A	166	ALA	O-C-N	-5.03	115.86	122.39
1	A	111	GLY	CA-C-N	5.01	131.38	122.45
1	A	111	GLY	C-N-CA	5.01	131.38	122.45
1	A	37	THR	N-CA-C	5.01	117.90	110.48
1	A	139	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	442	ALA	N-CA-CB	-5.01	102.48	109.94
1	A	103	ALA	N-CA-CB	-5.01	102.89	110.40
1	A	403	ASN	CA-C-O	-5.00	115.11	120.46

There are no chirality outliers.

All (177) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	GLU	Peptide
1	A	103	ALA	Peptide,Mainchain
1	A	107	THR	Mainchain
1	A	116	LYS	Mainchain
1	A	117	THR	Mainchain
1	A	122	VAL	Mainchain
1	A	129	GLY	Mainchain
1	A	130	HIS	Peptide
1	A	132	ALA	Mainchain
1	A	134	THR	Peptide,Mainchain
1	A	136	ILE	Mainchain
1	A	137	ARG	Mainchain
1	A	138	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	139	ARG	Mainchain
1	A	140	GLY	Mainchain
1	A	141	ALA	Mainchain
1	A	142	LYS	Peptide
1	A	145	ASP	Peptide
1	A	146	ILE	Mainchain
1	A	147	ALA	Mainchain
1	A	154	ASP	Mainchain
1	A	155	ASP	Mainchain
1	A	156	GLY	Mainchain
1	A	157	ILE	Mainchain
1	A	161	THR	Mainchain
1	A	166	ALA	Mainchain
1	A	167	HIS	Mainchain
1	A	169	LYS	Mainchain
1	A	170	ALA	Mainchain
1	A	171	ALA	Mainchain
1	A	172	GLY	Mainchain
1	A	173	ALA	Peptide
1	A	174	LYS	Mainchain
1	A	175	LEU	Mainchain
1	A	179	ILE	Mainchain
1	A	186	GLN	Mainchain
1	A	204	GLU	Mainchain
1	A	212	VAL	Mainchain
1	A	216	SER	Mainchain
1	A	217	ALA	Mainchain
1	A	219	THR	Peptide,Mainchain
1	A	231	LEU	Mainchain
1	A	233	LEU	Mainchain
1	A	234	ALA	Mainchain
1	A	239	TYR	Sidechain
1	A	244	ASN	Peptide
1	A	245	ALA	Mainchain
1	A	248	ARG	Mainchain
1	A	252	LEU	Mainchain
1	A	254	SER	Mainchain
1	A	259	GLN	Mainchain
1	A	260	ALA	Mainchain
1	A	269	GLN	Mainchain
1	A	271	GLY	Mainchain
1	A	275	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	281	ALA	Mainchain
1	A	282	GLY	Mainchain
1	A	285	TYR	Mainchain
1	A	287	ARG	Mainchain
1	A	293	ASP	Mainchain
1	A	294	ALA	Mainchain
1	A	297	ASN	Mainchain
1	A	298	GLN	Mainchain
1	A	303	GLY	Mainchain
1	A	312	GLY	Mainchain
1	A	315	GLU	Mainchain
1	A	316	LEU	Mainchain
1	A	320	GLY	Mainchain
1	A	325	TRP	Mainchain
1	A	330	GLU	Mainchain
1	A	331	ALA	Mainchain
1	A	332	ALA	Mainchain
1	A	337	GLU	Mainchain
1	A	345	ALA	Mainchain
1	A	346	ARG	Mainchain
1	A	348	GLU	Peptide,Mainchain
1	A	349	GLU	Mainchain
1	A	350	GLU	Mainchain
1	A	355	PRO	Mainchain
1	A	356	ALA	Mainchain
1	A	358	MET	Mainchain
1	A	359	ALA	Peptide,Mainchain
1	A	36	SER	Mainchain
1	A	361	LEU	Peptide,Mainchain
1	A	362	LEU	Peptide
1	A	363	ALA	Mainchain
1	A	369	GLY	Peptide,Mainchain
1	A	370	ALA	Mainchain
1	A	374	ASN	Mainchain
1	A	375	LEU	Peptide
1	A	376	ILE	Mainchain
1	A	378	ARG	Mainchain
1	A	379	ALA	Peptide,Mainchain
1	A	380	ASP	Mainchain
1	A	382	GLN	Peptide,Mainchain
1	A	383	GLY	Peptide,Mainchain
1	A	391	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	40	GLU	Mainchain
1	A	404	ILE	Mainchain
1	A	409	VAL	Mainchain
1	A	422	THR	Mainchain
1	A	435	PRO	Mainchain
1	A	438	VAL	Mainchain
1	A	443	GLU	Mainchain
1	A	446	GLY	Mainchain
1	A	448	LEU	Mainchain
1	A	450	LYS	Mainchain
1	A	453	ARG	Mainchain
1	A	456	TYR	Mainchain
1	A	463	ARG	Mainchain
1	A	464	ASN	Mainchain
1	A	465	MET	Mainchain
1	A	469	ALA	Mainchain
1	A	47	ARG	Mainchain
1	A	470	ARG	Mainchain
1	A	476	GLU	Peptide
1	A	479	LEU	Peptide
1	A	480	GLY	Peptide,Mainchain
1	A	485	ARG	Mainchain
1	A	486	ALA	Mainchain
1	A	488	PHE	Peptide
1	A	493	GLY	Mainchain
1	A	495	GLN	Mainchain
1	A	499	CYS	Mainchain
1	A	50	VAL	Mainchain
1	A	502	THR	Mainchain
1	A	510	ALA	Mainchain
1	A	513	ARG	Mainchain
1	A	515	LEU	Mainchain
1	A	516	ARG	Mainchain
1	A	521	ILE	Mainchain
1	A	532	PHE	Mainchain
1	A	537	ARG	Mainchain
1	A	541	GLN	Mainchain
1	A	542	GLY	Mainchain
1	A	545	CYS	Mainchain
1	A	547	ILE	Mainchain
1	A	548	GLY	Mainchain
1	A	550	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	551	GLY	Mainchain
1	A	553	ASP	Mainchain
1	A	555	PHE	Mainchain
1	A	557	GLU	Mainchain
1	A	558	GLY	Mainchain
1	A	563	ALA	Mainchain
1	A	565	GLN	Mainchain
1	A	568	GLU	Peptide,Mainchain
1	A	61	ALA	Mainchain
1	A	67	LYS	Mainchain
1	A	69	LEU	Mainchain
1	A	71	ARG	Mainchain
1	A	72	ARG	Peptide
1	A	74	PRO	Peptide,Mainchain
1	A	75	VAL	Mainchain
1	A	76	VAL	Mainchain
1	A	78	ILE	Mainchain
1	A	80	GLY	Mainchain
1	A	81	HIS	Mainchain
1	A	83	ASP	Mainchain
1	A	85	GLY	Mainchain
1	A	90	LEU	Mainchain
1	A	96	SER	Mainchain
1	A	99	ALA	Peptide,Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4383	0	4465	381	0
All	All	4383	0	4465	381	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 43.

All (381) 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:A:556:ARG:HH11	1:A:556:ARG:CG	1.40	1.30
1:A:134:THR:HG23	1:A:382:GLN:CG	1.72	1.19
1:A:79:MET:HB2	1:A:164:ALA:CB	1.72	1.18
1:A:75:VAL:HB	1:A:144:ALA:CA	1.74	1.17
1:A:493:GLY:HA2	1:A:530:LYS:HE3	1.24	1.16
1:A:382:GLN:HG2	1:A:409:VAL:HG11	1.27	1.15
1:A:134:THR:HG23	1:A:382:GLN:CB	1.78	1.14
1:A:481:GLN:HG3	1:A:562:GLU:HG3	1.26	1.14
1:A:371:LYS:HB3	1:A:468:GLY:HA2	1.34	1.09
1:A:79:MET:HB2	1:A:164:ALA:HB2	1.31	1.09
1:A:72:ARG:HD2	1:A:74:PRO:HD3	1.35	1.07
1:A:75:VAL:CB	1:A:144:ALA:HA	1.85	1.06
1:A:371:LYS:HD3	1:A:468:GLY:HA3	1.31	1.06
1:A:488:PHE:HZ	1:A:532:PHE:HB2	1.13	1.06
1:A:92:TYR:CE2	1:A:223:VAL:HG21	1.90	1.06
1:A:76:VAL:HG13	1:A:147:ALA:HA	1.28	1.06
1:A:496:VAL:HG21	1:A:530:LYS:HB2	1.28	1.05
1:A:496:VAL:HG11	1:A:530:LYS:CG	1.87	1.05
1:A:373:LEU:HD12	1:A:465:MET:HE3	1.37	1.05
1:A:371:LYS:CD	1:A:468:GLY:HA3	1.86	1.04
1:A:496:VAL:HG11	1:A:530:LYS:HG3	1.40	1.03
1:A:108:GLN:HB2	1:A:294:ALA:C	1.82	1.03
1:A:373:LEU:HD12	1:A:465:MET:CE	1.88	1.02
1:A:496:VAL:HG11	1:A:530:LYS:CB	1.87	1.02
1:A:143:VAL:HG13	1:A:250:VAL:HG11	1.36	1.01
1:A:481:GLN:CG	1:A:562:GLU:HG3	1.91	1.01
1:A:76:VAL:HG11	1:A:148:VAL:HG13	1.44	1.00
1:A:263:ILE:HD12	1:A:309:GLN:NE2	1.77	1.00
1:A:382:GLN:CG	1:A:409:VAL:HG11	1.92	0.99
1:A:75:VAL:HB	1:A:144:ALA:HA	1.03	0.99
1:A:134:THR:HA	1:A:382:GLN:C	1.87	0.99
1:A:363:ALA:HB1	1:A:403:ASN:HA	1.45	0.99
1:A:380:ASP:HB2	1:A:432:VAL:HG13	1.44	0.99
1:A:453:ARG:HG3	1:A:453:ARG:O	1.58	0.98
1:A:375:LEU:HD23	1:A:426:ALA:HB3	1.44	0.98
1:A:556:ARG:HG3	1:A:556:ARG:NH1	1.34	0.97
1:A:124:PHE:HE1	1:A:148:VAL:HG11	1.27	0.97
1:A:496:VAL:HB	1:A:546:GLY:HA3	1.46	0.97
1:A:487:ILE:CG2	1:A:556:ARG:HD3	1.94	0.97
1:A:488:PHE:CZ	1:A:532:PHE:HB2	2.00	0.97
1:A:382:GLN:HG2	1:A:409:VAL:CG1	1.95	0.96
1:A:77:VAL:HG13	1:A:79:MET:HE3	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLY:CA	1:A:530:LYS:HE3	1.95	0.95
1:A:92:TYR:HE2	1:A:223:VAL:HG21	1.31	0.94
1:A:496:VAL:CG2	1:A:530:LYS:HB2	1.97	0.94
1:A:79:MET:HE2	1:A:131:GLU:CD	1.92	0.94
1:A:92:TYR:CG	1:A:217:ALA:HA	2.03	0.94
1:A:487:ILE:HG22	1:A:556:ARG:HD3	1.50	0.93
1:A:275:VAL:HG12	1:A:275:VAL:O	1.64	0.93
1:A:76:VAL:HG13	1:A:147:ALA:CA	1.97	0.93
1:A:92:TYR:CD2	1:A:217:ALA:HA	2.04	0.93
1:A:380:ASP:HB2	1:A:432:VAL:CG1	1.98	0.92
1:A:82:VAL:HG11	1:A:430:PHE:CZ	2.03	0.92
1:A:263:ILE:HB	1:A:309:GLN:CD	1.95	0.92
1:A:78:ILE:HD13	1:A:89:LEU:HD13	1.52	0.92
1:A:380:ASP:CB	1:A:432:VAL:HG13	1.98	0.92
1:A:80:GLY:HA2	1:A:160:GLN:HB2	1.52	0.91
1:A:496:VAL:HG11	1:A:530:LYS:HB2	1.51	0.90
1:A:80:GLY:HA2	1:A:160:GLN:CB	2.02	0.90
1:A:134:THR:HG23	1:A:382:GLN:HB2	1.52	0.90
1:A:398:GLU:HB2	1:A:466:VAL:HG12	1.55	0.88
1:A:134:THR:C	1:A:382:GLN:HB2	1.99	0.87
1:A:371:LYS:CB	1:A:468:GLY:HA2	2.04	0.87
1:A:134:THR:HG23	1:A:382:GLN:HG3	1.53	0.87
1:A:76:VAL:CG1	1:A:148:VAL:H	1.88	0.87
1:A:79:MET:HB2	1:A:164:ALA:HB1	1.55	0.86
1:A:481:GLN:HA	1:A:562:GLU:HA	1.54	0.86
1:A:72:ARG:HG3	1:A:72:ARG:O	1.73	0.86
1:A:92:TYR:HE2	1:A:223:VAL:CG2	1.88	0.85
1:A:380:ASP:CG	1:A:432:VAL:HG13	2.02	0.85
1:A:124:PHE:CE1	1:A:148:VAL:HG11	2.11	0.84
1:A:82:VAL:HG21	1:A:430:PHE:CZ	2.13	0.84
1:A:80:GLY:O	1:A:86:LYS:HE2	1.78	0.84
1:A:263:ILE:HB	1:A:309:GLN:OE1	1.78	0.83
1:A:82:VAL:HG22	1:A:130:HIS:CD2	2.13	0.83
1:A:79:MET:CB	1:A:164:ALA:HB2	2.10	0.82
1:A:82:VAL:HG11	1:A:430:PHE:CE1	2.14	0.81
1:A:108:GLN:HB2	1:A:294:ALA:O	1.80	0.81
1:A:376:ILE:HG22	1:A:405:LEU:HB2	1.61	0.81
1:A:76:VAL:CG1	1:A:147:ALA:HA	2.10	0.80
1:A:92:TYR:CE2	1:A:223:VAL:CG2	2.64	0.80
1:A:72:ARG:HD2	1:A:74:PRO:CD	2.10	0.80
1:A:124:PHE:HE1	1:A:148:VAL:CG1	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HB3	1:A:86:LYS:HZ2	1.46	0.79
1:A:248:ARG:O	1:A:269:GLN:HB2	1.82	0.79
1:A:134:THR:HA	1:A:383:GLY:CA	2.13	0.78
1:A:72:ARG:CD	1:A:74:PRO:HG3	2.13	0.78
1:A:380:ASP:HB2	1:A:432:VAL:HG22	1.66	0.77
1:A:483:GLU:HA	1:A:560:VAL:HA	1.66	0.77
1:A:134:THR:CG2	1:A:382:GLN:HB2	2.15	0.76
1:A:496:VAL:CG1	1:A:530:LYS:HB2	2.15	0.76
1:A:375:LEU:CD2	1:A:426:ALA:HB3	2.14	0.76
1:A:373:LEU:CD1	1:A:465:MET:HE3	2.15	0.76
1:A:82:VAL:HG22	1:A:130:HIS:HD2	1.50	0.75
1:A:380:ASP:HB2	1:A:432:VAL:CG2	2.16	0.75
1:A:92:TYR:CG	1:A:217:ALA:CA	2.69	0.75
1:A:76:VAL:N	1:A:144:ALA:HB1	2.01	0.75
1:A:78:ILE:CD1	1:A:89:LEU:HD13	2.17	0.75
1:A:165:ILE:HG21	1:A:201:PHE:CZ	2.22	0.75
1:A:496:VAL:CG1	1:A:530:LYS:HG3	2.16	0.74
1:A:82:VAL:CG1	1:A:430:PHE:CZ	2.70	0.74
1:A:263:ILE:HD12	1:A:309:GLN:CD	2.11	0.74
1:A:496:VAL:HG21	1:A:530:LYS:CB	2.12	0.74
1:A:75:VAL:HB	1:A:144:ALA:CB	2.17	0.74
1:A:92:TYR:HB2	1:A:217:ALA:O	1.87	0.74
1:A:78:ILE:HD13	1:A:89:LEU:CD1	2.18	0.73
1:A:453:ARG:O	1:A:453:ARG:CG	2.37	0.73
1:A:72:ARG:O	1:A:72:ARG:CG	2.37	0.73
1:A:512:VAL:HG12	1:A:563:ALA:HB2	1.70	0.72
1:A:487:ILE:HG22	1:A:556:ARG:CD	2.18	0.71
1:A:92:TYR:CB	1:A:217:ALA:HB1	2.21	0.70
1:A:82:VAL:CG2	1:A:430:PHE:CZ	2.73	0.70
1:A:260:ALA:O	1:A:311:LEU:HD11	1.92	0.70
1:A:134:THR:CA	1:A:382:GLN:C	2.63	0.70
1:A:132:ALA:HB1	1:A:383:GLY:C	2.17	0.70
1:A:380:ASP:H	1:A:432:VAL:HG22	1.57	0.70
1:A:373:LEU:HD12	1:A:465:MET:HE1	1.72	0.69
1:A:134:THR:HA	1:A:383:GLY:N	2.07	0.69
1:A:481:GLN:HG3	1:A:562:GLU:CG	2.15	0.69
1:A:71:ARG:HB3	1:A:71:ARG:CZ	2.21	0.69
1:A:487:ILE:HG23	1:A:556:ARG:HD3	1.73	0.69
1:A:81:HIS:CG	1:A:82:VAL:H	2.11	0.68
1:A:373:LEU:HD23	1:A:465:MET:O	1.93	0.68
1:A:211:ILE:HG13	1:A:233:LEU:HD22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LYS:HD3	1:A:468:GLY:CA	2.18	0.68
1:A:77:VAL:CG1	1:A:79:MET:HE3	2.23	0.68
1:A:82:VAL:HG21	1:A:430:PHE:CE2	2.30	0.67
1:A:398:GLU:HB2	1:A:466:VAL:CG1	2.23	0.67
1:A:79:MET:HE2	1:A:131:GLU:OE1	1.93	0.67
1:A:134:THR:CG2	1:A:382:GLN:CG	2.63	0.67
1:A:76:VAL:HA	1:A:146:ILE:O	1.96	0.66
1:A:496:VAL:HB	1:A:546:GLY:CA	2.25	0.65
1:A:289:ARG:NH2	1:A:311:LEU:HD22	2.11	0.65
1:A:371:LYS:HB3	1:A:468:GLY:CA	2.20	0.65
1:A:79:MET:SD	1:A:164:ALA:HB1	2.37	0.65
1:A:82:VAL:CG1	1:A:430:PHE:HZ	2.07	0.65
1:A:92:TYR:HB2	1:A:217:ALA:HB1	1.79	0.65
1:A:80:GLY:HA2	1:A:160:GLN:HB3	1.77	0.64
1:A:371:LYS:CB	1:A:468:GLY:CA	2.76	0.64
1:A:286:GLY:HA3	1:A:312:GLY:C	2.23	0.64
1:A:137:ARG:HH11	1:A:167:HIS:CD2	2.17	0.63
1:A:488:PHE:HZ	1:A:532:PHE:CB	2.02	0.63
1:A:522:TRP:CZ2	1:A:550:ASP:HB2	2.33	0.63
1:A:92:TYR:CD1	1:A:217:ALA:HA	2.34	0.63
1:A:86:LYS:HB3	1:A:86:LYS:NZ	2.11	0.63
1:A:75:VAL:HG21	1:A:143:VAL:O	1.98	0.62
1:A:490:LEU:HD12	1:A:491:PRO:CD	2.29	0.62
1:A:371:LYS:CE	1:A:468:GLY:HA3	2.29	0.62
1:A:134:THR:CG2	1:A:382:GLN:CB	2.66	0.62
1:A:365:MET:HB2	1:A:403:ASN:HD22	1.64	0.62
1:A:132:ALA:HB3	1:A:383:GLY:HA3	1.80	0.61
1:A:493:GLY:HA2	1:A:530:LYS:CE	2.16	0.61
1:A:266:MET:O	1:A:307:ALA:HA	2.01	0.61
1:A:496:VAL:CB	1:A:530:LYS:HB2	2.30	0.61
1:A:522:TRP:CH2	1:A:550:ASP:HB2	2.36	0.61
1:A:134:THR:O	1:A:382:GLN:HB2	2.01	0.60
1:A:92:TYR:CE2	1:A:217:ALA:HA	2.36	0.60
1:A:132:ALA:CB	1:A:383:GLY:C	2.74	0.60
1:A:134:THR:HG23	1:A:382:GLN:CD	2.24	0.60
1:A:376:ILE:HD11	1:A:420:ALA:HB2	1.82	0.60
1:A:92:TYR:CD1	1:A:217:ALA:C	2.80	0.60
1:A:278:TYR:CE1	1:A:287:ARG:HD2	2.37	0.60
1:A:111:GLY:HA3	1:A:252:LEU:HD13	1.84	0.59
1:A:363:ALA:O	1:A:403:ASN:HB2	2.02	0.59
1:A:384:SER:HA	1:A:455:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PHE:CE2	1:A:532:PHE:HA	2.37	0.59
1:A:131:GLU:C	1:A:133:PHE:H	2.11	0.59
1:A:263:ILE:HB	1:A:309:GLN:CG	2.32	0.59
1:A:134:THR:CG2	1:A:382:GLN:HG3	2.31	0.59
1:A:375:LEU:HD23	1:A:426:ALA:CB	2.27	0.58
1:A:487:ILE:CG2	1:A:556:ARG:CD	2.77	0.58
1:A:489:ARG:HG3	1:A:489:ARG:HH11	1.67	0.58
1:A:275:VAL:O	1:A:275:VAL:CG1	2.32	0.58
1:A:380:ASP:HB2	1:A:432:VAL:CB	2.33	0.58
1:A:77:VAL:HG23	1:A:125:ILE:HG21	1.85	0.58
1:A:133:PHE:HZ	1:A:160:GLN:O	1.86	0.58
1:A:79:MET:CB	1:A:164:ALA:CB	2.64	0.58
1:A:70:PRO:HG2	1:A:243:PRO:HG3	1.84	0.58
1:A:82:VAL:CG2	1:A:130:HIS:HD2	2.16	0.57
1:A:81:HIS:CG	1:A:82:VAL:N	2.71	0.57
1:A:72:ARG:HD2	1:A:74:PRO:CG	2.34	0.57
1:A:211:ILE:HD12	1:A:229:MET:CE	2.34	0.57
1:A:27:MET:SD	1:A:46:VAL:HG22	2.44	0.57
1:A:143:VAL:HA	1:A:269:GLN:NE2	2.18	0.57
1:A:76:VAL:CA	1:A:144:ALA:HB1	2.34	0.57
1:A:76:VAL:HG22	1:A:146:ILE:HB	1.85	0.57
1:A:146:ILE:CG2	1:A:176:ILE:HD12	2.34	0.57
1:A:80:GLY:CA	1:A:160:GLN:HB2	2.31	0.57
1:A:132:ALA:HB1	1:A:384:SER:N	2.20	0.57
1:A:373:LEU:HG	1:A:465:MET:HE3	1.86	0.56
1:A:380:ASP:CB	1:A:432:VAL:CG1	2.71	0.56
1:A:496:VAL:CG1	1:A:530:LYS:CG	2.73	0.56
1:A:380:ASP:CG	1:A:432:VAL:CG1	2.77	0.56
1:A:70:PRO:HG2	1:A:243:PRO:CG	2.34	0.56
1:A:503:GLN:HG3	1:A:504:GLY:H	1.70	0.56
1:A:522:TRP:CZ2	1:A:550:ASP:CB	2.88	0.56
1:A:75:VAL:CG2	1:A:144:ALA:HA	2.35	0.56
1:A:76:VAL:HG11	1:A:148:VAL:H	1.70	0.56
1:A:488:PHE:CZ	1:A:532:PHE:CB	2.82	0.56
1:A:70:PRO:HG2	1:A:243:PRO:CD	2.36	0.56
1:A:376:ILE:O	1:A:427:ILE:HA	2.06	0.55
1:A:211:ILE:HD12	1:A:229:MET:HE2	1.87	0.55
1:A:90:LEU:O	1:A:94:ARG:HB2	2.07	0.55
1:A:174:LYS:HG2	1:A:237:GLU:OE1	2.06	0.55
1:A:75:VAL:C	1:A:76:VAL:CG2	2.80	0.54
1:A:371:LYS:CG	1:A:468:GLY:HA3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:CD	1:A:74:PRO:CG	2.85	0.54
1:A:288:ILE:HA	1:A:311:LEU:O	2.08	0.54
1:A:143:VAL:CG1	1:A:250:VAL:HG11	2.24	0.54
1:A:134:THR:CG2	1:A:382:GLN:CD	2.80	0.54
1:A:92:TYR:CD2	1:A:217:ALA:CA	2.86	0.54
1:A:380:ASP:H	1:A:432:VAL:CG2	2.20	0.54
1:A:484:VAL:HB	1:A:561:ILE:HD11	1.90	0.54
1:A:481:GLN:CG	1:A:562:GLU:CG	2.78	0.54
1:A:72:ARG:HD3	1:A:74:PRO:HG3	1.89	0.54
1:A:515:LEU:HD11	1:A:562:GLU:OE1	2.07	0.53
1:A:262:ILE:C	1:A:263:ILE:HG23	2.33	0.53
1:A:133:PHE:HB3	1:A:136:ILE:HG12	1.90	0.53
1:A:371:LYS:O	1:A:400:VAL:HG22	2.08	0.53
1:A:483:GLU:HG2	1:A:560:VAL:CG2	2.38	0.53
1:A:168:ALA:HB1	1:A:175:LEU:CD2	2.38	0.53
1:A:278:TYR:CZ	1:A:287:ARG:HD2	2.44	0.53
1:A:252:LEU:HD11	1:A:267:LEU:HB2	1.91	0.52
1:A:483:GLU:HG2	1:A:560:VAL:HG13	1.91	0.52
1:A:75:VAL:C	1:A:76:VAL:HG23	2.34	0.52
1:A:75:VAL:HG12	1:A:144:ALA:HB2	1.92	0.52
1:A:76:VAL:CG1	1:A:148:VAL:N	2.67	0.52
1:A:143:VAL:HG13	1:A:250:VAL:CG1	2.24	0.52
1:A:556:ARG:HH11	1:A:556:ARG:HG3	0.49	0.52
1:A:289:ARG:NH2	1:A:311:LEU:CD2	2.72	0.52
1:A:75:VAL:C	1:A:144:ALA:HB1	2.35	0.51
1:A:289:ARG:CZ	1:A:311:LEU:HD22	2.40	0.51
1:A:249:GLY:HA2	1:A:269:GLN:CG	2.40	0.51
1:A:367:GLU:C	1:A:369:GLY:H	2.18	0.51
1:A:249:GLY:HA2	1:A:269:GLN:HB2	1.93	0.51
1:A:483:GLU:HG2	1:A:560:VAL:CG1	2.41	0.51
1:A:80:GLY:O	1:A:130:HIS:HB2	2.11	0.51
1:A:286:GLY:HA3	1:A:312:GLY:O	2.09	0.51
1:A:81:HIS:CD2	1:A:82:VAL:H	2.28	0.51
1:A:148:VAL:CG2	1:A:148:VAL:O	2.59	0.51
1:A:254:SER:HA	1:A:264:ALA:HA	1.93	0.51
1:A:285:TYR:CG	1:A:285:TYR:O	2.64	0.50
1:A:371:LYS:O	1:A:400:VAL:CG2	2.59	0.50
1:A:522:TRP:HZ2	1:A:550:ASP:CG	2.19	0.50
1:A:133:PHE:C	1:A:383:GLY:HA2	2.36	0.50
1:A:483:GLU:HG2	1:A:560:VAL:HG22	1.93	0.50
1:A:146:ILE:HG21	1:A:176:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:CD2	1:A:428:LEU:HB2	2.42	0.50
1:A:471:GLU:HB3	1:A:472:PRO:HD3	1.94	0.50
1:A:285:TYR:C	1:A:313:PHE:HA	2.37	0.50
1:A:373:LEU:HD23	1:A:465:MET:C	2.35	0.50
1:A:70:PRO:CG	1:A:243:PRO:HG3	2.41	0.50
1:A:133:PHE:CE1	1:A:163:GLU:OE1	2.65	0.49
1:A:365:MET:HB2	1:A:403:ASN:ND2	2.27	0.49
1:A:371:LYS:CD	1:A:468:GLY:CA	2.76	0.49
1:A:81:HIS:HB2	1:A:160:GLN:HG2	1.93	0.49
1:A:483:GLU:HA	1:A:560:VAL:CA	2.40	0.49
1:A:265:ASN:HA	1:A:308:VAL:O	2.12	0.49
1:A:378:ARG:HB2	1:A:427:ILE:HG22	1.95	0.49
1:A:471:GLU:O	1:A:474:TYR:CD2	2.65	0.49
1:A:76:VAL:HG13	1:A:147:ALA:N	2.26	0.49
1:A:483:GLU:CG	1:A:560:VAL:HG22	2.43	0.49
1:A:374:ASN:O	1:A:375:LEU:HD23	2.12	0.49
1:A:371:LYS:CG	1:A:468:GLY:CA	2.90	0.49
1:A:260:ALA:O	1:A:311:LEU:CD1	2.59	0.49
1:A:78:ILE:C	1:A:79:MET:HG3	2.37	0.48
1:A:128:PRO:HB2	1:A:130:HIS:CE1	2.47	0.48
1:A:80:GLY:O	1:A:130:HIS:CB	2.61	0.48
1:A:373:LEU:CG	1:A:465:MET:HE3	2.43	0.48
1:A:428:LEU:HD13	1:A:458:LEU:HD21	1.95	0.48
1:A:482:ALA:O	1:A:561:ILE:HB	2.12	0.48
1:A:505:ARG:HH21	1:A:569:VAL:C	2.21	0.48
1:A:79:MET:C	1:A:86:LYS:HD3	2.39	0.48
1:A:131:GLU:C	1:A:133:PHE:N	2.71	0.48
1:A:165:ILE:CG2	1:A:201:PHE:CZ	2.95	0.48
1:A:132:ALA:HB3	1:A:383:GLY:CA	2.44	0.48
1:A:176:ILE:HD13	1:A:230:ILE:HG12	1.95	0.48
1:A:513:ARG:HB2	1:A:564:PHE:CE1	2.49	0.48
1:A:75:VAL:HG12	1:A:76:VAL:H	1.79	0.47
1:A:79:MET:CB	1:A:164:ALA:HB1	2.38	0.47
1:A:387:ALA:O	1:A:391:ILE:HD12	2.14	0.47
1:A:458:LEU:C	1:A:458:LEU:HD23	2.38	0.47
1:A:82:VAL:CG2	1:A:130:HIS:CD2	2.93	0.47
1:A:83:ASP:OD2	1:A:453:ARG:HG2	2.15	0.47
1:A:363:ALA:HB1	1:A:403:ASN:CA	2.31	0.47
1:A:380:ASP:CB	1:A:432:VAL:HG22	2.41	0.47
1:A:513:ARG:HD2	1:A:564:PHE:HE1	1.79	0.47
1:A:481:GLN:HG2	1:A:562:GLU:HG3	1.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HG12	1:A:83:ASP:N	2.30	0.47
1:A:357:THR:C	1:A:359:ALA:H	2.24	0.46
1:A:378:ARG:HD2	1:A:412:PRO:HA	1.96	0.46
1:A:484:VAL:HG12	1:A:559:ASP:CA	2.45	0.46
1:A:249:GLY:HA2	1:A:269:GLN:HG3	1.97	0.46
1:A:363:ALA:HB3	1:A:403:ASN:OD1	2.16	0.46
1:A:484:VAL:HG12	1:A:559:ASP:C	2.40	0.46
1:A:568:GLU:H	1:A:569:VAL:HG13	1.80	0.46
1:A:481:GLN:N	1:A:562:GLU:HA	2.31	0.46
1:A:233:LEU:O	1:A:233:LEU:HG	2.16	0.46
1:A:259:GLN:OE1	1:A:259:GLN:HA	2.16	0.46
1:A:79:MET:SD	1:A:164:ALA:CB	3.03	0.45
1:A:76:VAL:HG13	1:A:146:ILE:C	2.41	0.45
1:A:508:ARG:HB2	1:A:537:ARG:O	2.16	0.45
1:A:490:LEU:HD12	1:A:491:PRO:HD3	1.99	0.45
1:A:86:LYS:NZ	1:A:130:HIS:HB3	2.31	0.45
1:A:148:VAL:O	1:A:148:VAL:HG23	2.17	0.45
1:A:559:ASP:OD1	1:A:560:VAL:HG23	2.17	0.45
1:A:371:LYS:HZ3	1:A:472:PRO:CD	2.30	0.44
1:A:130:HIS:HD1	1:A:130:HIS:H	1.66	0.44
1:A:134:THR:CG2	1:A:382:GLN:NE2	2.81	0.44
1:A:497:ALA:C	1:A:546:GLY:HA2	2.42	0.44
1:A:501:VAL:HG22	1:A:506:ILE:HG12	2.00	0.44
1:A:92:TYR:CD1	1:A:217:ALA:CA	3.00	0.44
1:A:251:ILE:HG12	1:A:323:VAL:CG2	2.48	0.44
1:A:522:TRP:CZ2	1:A:550:ASP:CG	2.96	0.44
1:A:483:GLU:CB	1:A:560:VAL:HG22	2.48	0.43
1:A:501:VAL:HG12	1:A:502:THR:N	2.33	0.43
1:A:257:ASP:HB3	1:A:260:ALA:HB3	2.00	0.43
1:A:505:ARG:NH2	1:A:569:VAL:C	2.76	0.43
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.18	0.43
1:A:75:VAL:CG1	1:A:144:ALA:HB2	2.49	0.43
1:A:119:GLN:OE1	1:A:119:GLN:N	2.50	0.43
1:A:490:LEU:HD12	1:A:491:PRO:HD2	2.00	0.43
1:A:46:VAL:O	1:A:50:VAL:HG23	2.18	0.43
1:A:484:VAL:HB	1:A:561:ILE:CD1	2.47	0.43
1:A:262:ILE:C	1:A:263:ILE:CG2	2.92	0.43
1:A:353:ARG:NH1	1:A:356:ALA:HB3	2.33	0.43
1:A:475:LYS:HZ2	1:A:477:GLU:CD	2.25	0.43
1:A:360:ALA:HB1	1:A:364:ALA:HB2	2.01	0.43
1:A:412:PRO:HG2	1:A:434:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HG13	1:A:34:HIS:O	2.18	0.43
1:A:143:VAL:HA	1:A:269:GLN:HE22	1.80	0.43
1:A:373:LEU:HB2	1:A:465:MET:O	2.19	0.43
1:A:513:ARG:HB3	1:A:562:GLU:O	2.18	0.43
1:A:130:HIS:C	1:A:132:ALA:H	2.27	0.43
1:A:180:ASN:HD21	1:A:217:ALA:HB3	1.84	0.43
1:A:92:TYR:CB	1:A:217:ALA:O	2.62	0.43
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.70	0.43
1:A:236:LEU:C	1:A:236:LEU:HD23	2.44	0.42
1:A:371:LYS:HE2	1:A:468:GLY:O	2.19	0.42
1:A:90:LEU:HD22	1:A:125:ILE:O	2.19	0.42
1:A:476:GLU:OE1	1:A:566:MET:HE2	2.19	0.42
1:A:505:ARG:HE	1:A:569:VAL:HG23	1.84	0.42
1:A:247:PRO:HG3	1:A:271:GLY:HA3	2.01	0.42
1:A:110:VAL:HB	1:A:307:ALA:CB	2.50	0.42
1:A:134:THR:CB	1:A:382:GLN:HB2	2.50	0.42
1:A:139:ARG:N	1:A:140:GLY:HA2	2.34	0.42
1:A:108:GLN:HB2	1:A:294:ALA:CA	2.48	0.42
1:A:567:VAL:HG13	1:A:567:VAL:O	2.19	0.42
1:A:86:LYS:HD2	1:A:129:GLY:O	2.19	0.42
1:A:266:MET:HE3	1:A:268:VAL:HG22	2.02	0.42
1:A:378:ARG:HD2	1:A:412:PRO:CA	2.50	0.42
1:A:169:LYS:C	1:A:171:ALA:H	2.28	0.42
1:A:27:MET:HE1	1:A:46:VAL:HG22	2.02	0.41
1:A:513:ARG:HB2	1:A:564:PHE:HE1	1.85	0.41
1:A:82:VAL:CG2	1:A:430:PHE:CE2	3.00	0.41
1:A:92:TYR:CG	1:A:217:ALA:CB	3.04	0.41
1:A:484:VAL:HG11	1:A:559:ASP:N	2.35	0.41
1:A:475:LYS:HZ2	1:A:475:LYS:HG2	1.71	0.41
1:A:388:ILE:CD1	1:A:458:LEU:HD13	2.50	0.41
1:A:281:ALA:CB	1:A:313:PHE:CE1	3.03	0.41
1:A:132:ALA:CB	1:A:384:SER:N	2.83	0.41
1:A:86:LYS:HZ1	1:A:130:HIS:HB3	1.85	0.41
1:A:143:VAL:HG22	1:A:250:VAL:HG21	2.02	0.41
1:A:281:ALA:HB3	1:A:313:PHE:CE1	2.56	0.41
1:A:371:LYS:C	1:A:400:VAL:HG22	2.44	0.41
1:A:388:ILE:HD11	1:A:458:LEU:HD13	2.03	0.41
1:A:481:GLN:CA	1:A:562:GLU:HA	2.38	0.41
1:A:69:LEU:HA	1:A:70:PRO:HD2	1.73	0.41
1:A:249:GLY:HA2	1:A:269:GLN:CB	2.51	0.41
1:A:287:ARG:O	1:A:312:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:C	1:A:86:LYS:HE2	2.46	0.40
1:A:238:ASP:OD1	1:A:240:ARG:NH2	2.54	0.40
1:A:357:THR:C	1:A:359:ALA:N	2.76	0.40
1:A:180:ASN:ND2	1:A:217:ALA:HB3	2.36	0.40
1:A:458:LEU:O	1:A:462:VAL:HG23	2.21	0.40
1:A:128:PRO:HB2	1:A:130:HIS:HE1	1.86	0.40
1:A:134:THR:CA	1:A:382:GLN:HB2	2.52	0.40
1:A:263:ILE:HB	1:A:309:GLN:HG3	2.03	0.40
1:A:82:VAL:HG13	1:A:430:PHE:HZ	1.84	0.40
1:A:110:VAL:HB	1:A:307:ALA:HB3	2.04	0.40
1:A:488:PHE:HE2	1:A:532:PHE:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	567/569 (100%)	436 (77%)	92 (16%)	39 (7%)	1 11

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	73	PRO
1	A	131	GLU
1	A	132	ALA
1	A	243	PRO
1	A	358	MET
1	A	363	ALA
1	A	369	GLY
1	A	370	ALA
1	A	382	GLN

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Mol	Chain	Res	Type
1	A	399	ASP
1	A	464	ASN
1	A	474	TYR
1	A	481	GLN
1	A	555	PHE
1	A	556	ARG
1	A	75	VAL
1	A	157	ILE
1	A	245	ALA
1	A	349	GLU
1	A	359	ALA
1	A	396	THR
1	A	517	ASP
1	A	99	ALA
1	A	141	ALA
1	A	507	PRO
1	A	541	GLN
1	A	557	GLU
1	A	567	VAL
1	A	74	PRO
1	A	169	LYS
1	A	350	GLU
1	A	478	VAL
1	A	542	GLY
1	A	71	ARG
1	A	463	ARG
1	A	357	THR
1	A	383	GLY
1	A	436	GLY

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	450/450 (100%)	389 (86%)	61 (14%)	3 14

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	VAL
1	A	6	ILE
1	A	7	TYR
1	A	32	LYS
1	A	41	LYS
1	A	72	ARG
1	A	73	PRO
1	A	79	MET
1	A	86	LYS
1	A	88	THR
1	A	89	LEU
1	A	95	LYS
1	A	106	ILE
1	A	117	THR
1	A	121	THR
1	A	130	HIS
1	A	135	THR
1	A	136	ILE
1	A	137	ARG
1	A	148	VAL
1	A	176	ILE
1	A	211	ILE
1	A	213	ILE
1	A	215	ILE
1	A	218	LYS
1	A	251	ILE
1	A	255	LYS
1	A	256	LEU
1	A	306	SER
1	A	311	LEU
1	A	314	GLN
1	A	321	ASP
1	A	349	GLU
1	A	350	GLU
1	A	361	LEU
1	A	371	LYS
1	A	373	LEU
1	A	378	ARG
1	A	385	LEU
1	A	399	ASP
1	A	409	VAL

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Mol	Chain	Res	Type
1	A	417	VAL
1	A	422	THR
1	A	437	SER
1	A	451	THR
1	A	454	ILE
1	A	463	ARG
1	A	464	ASN
1	A	475	LYS
1	A	477	GLU
1	A	489	ARG
1	A	492	THR
1	A	495	GLN
1	A	529	LEU
1	A	537	ARG
1	A	538	GLU
1	A	550	ASP
1	A	556	ARG
1	A	565	GLN
1	A	568	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	108	GLN
1	A	167	HIS
1	A	408	GLN
1	A	519	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

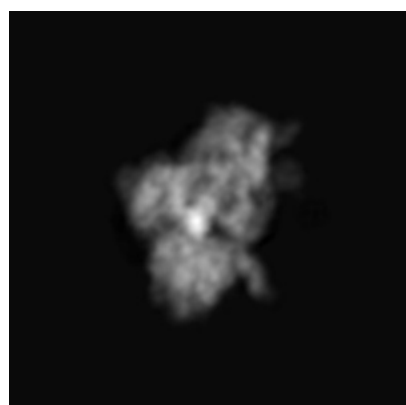
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2448. These allow visual inspection of the internal detail of the map and identification of artifacts.

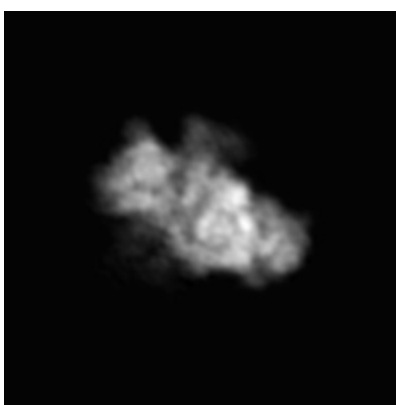
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

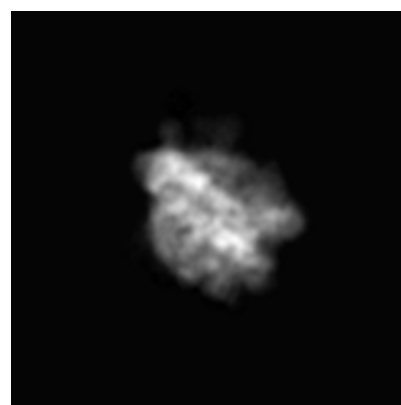
6.1.1 Primary map



X



Y

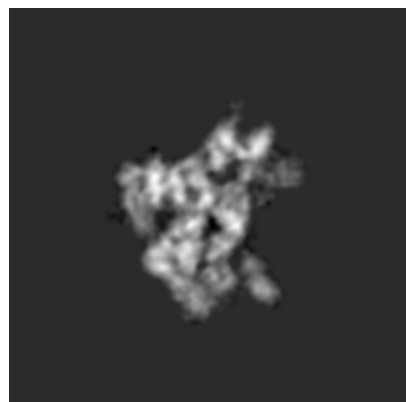


Z

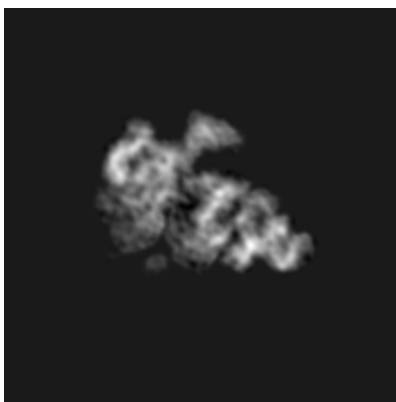
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

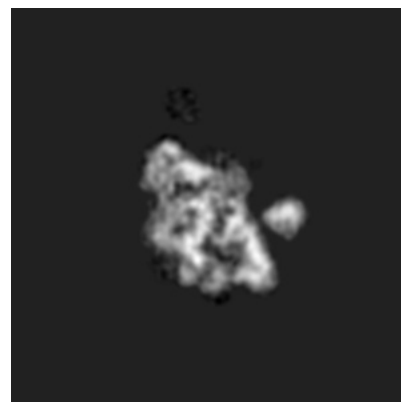
6.2.1 Primary map



X Index: 104



Y Index: 104

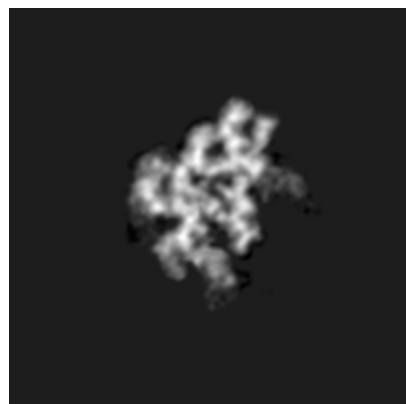


Z Index: 104

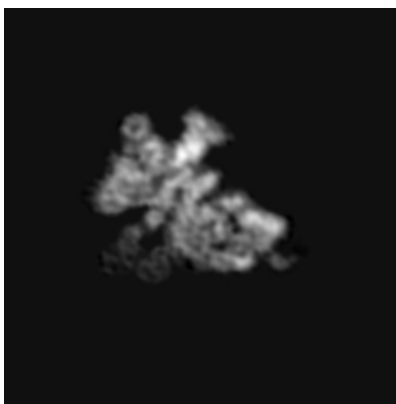
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

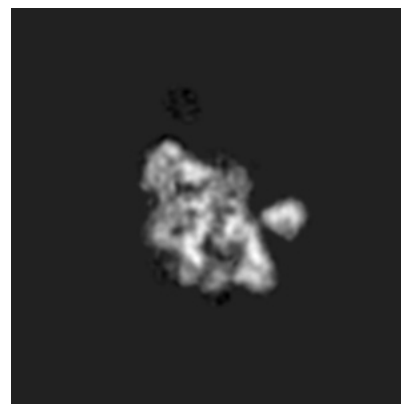
6.3.1 Primary map



X Index: 97



Y Index: 98

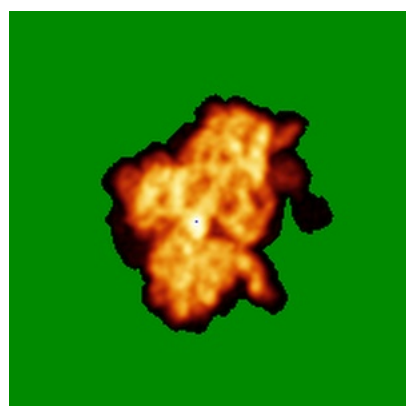


Z Index: 103

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

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

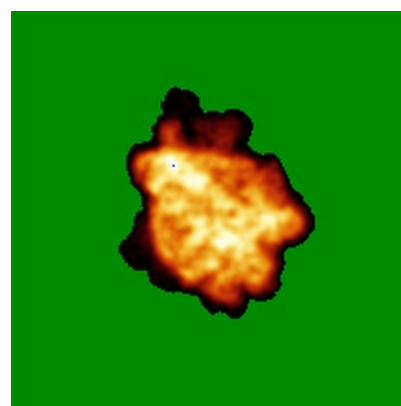
6.4.1 Primary map



X



Y

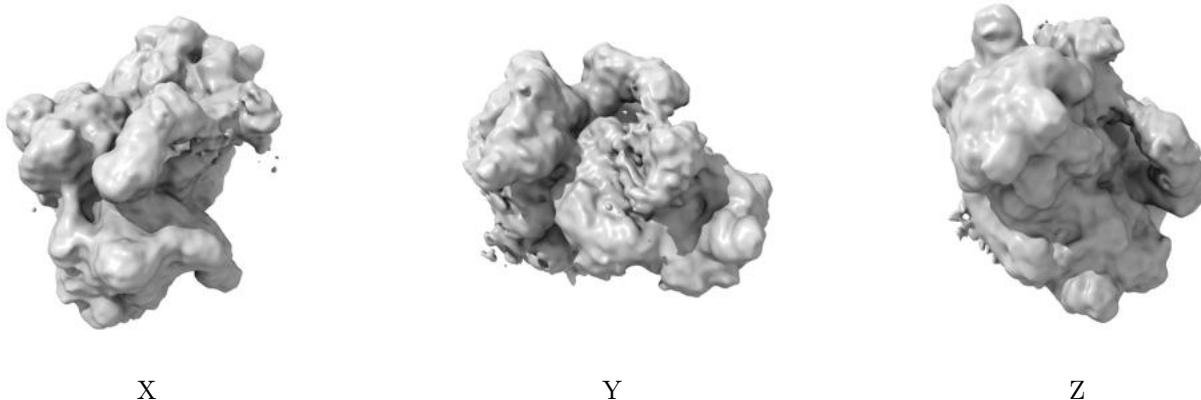


Z

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 0.169. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

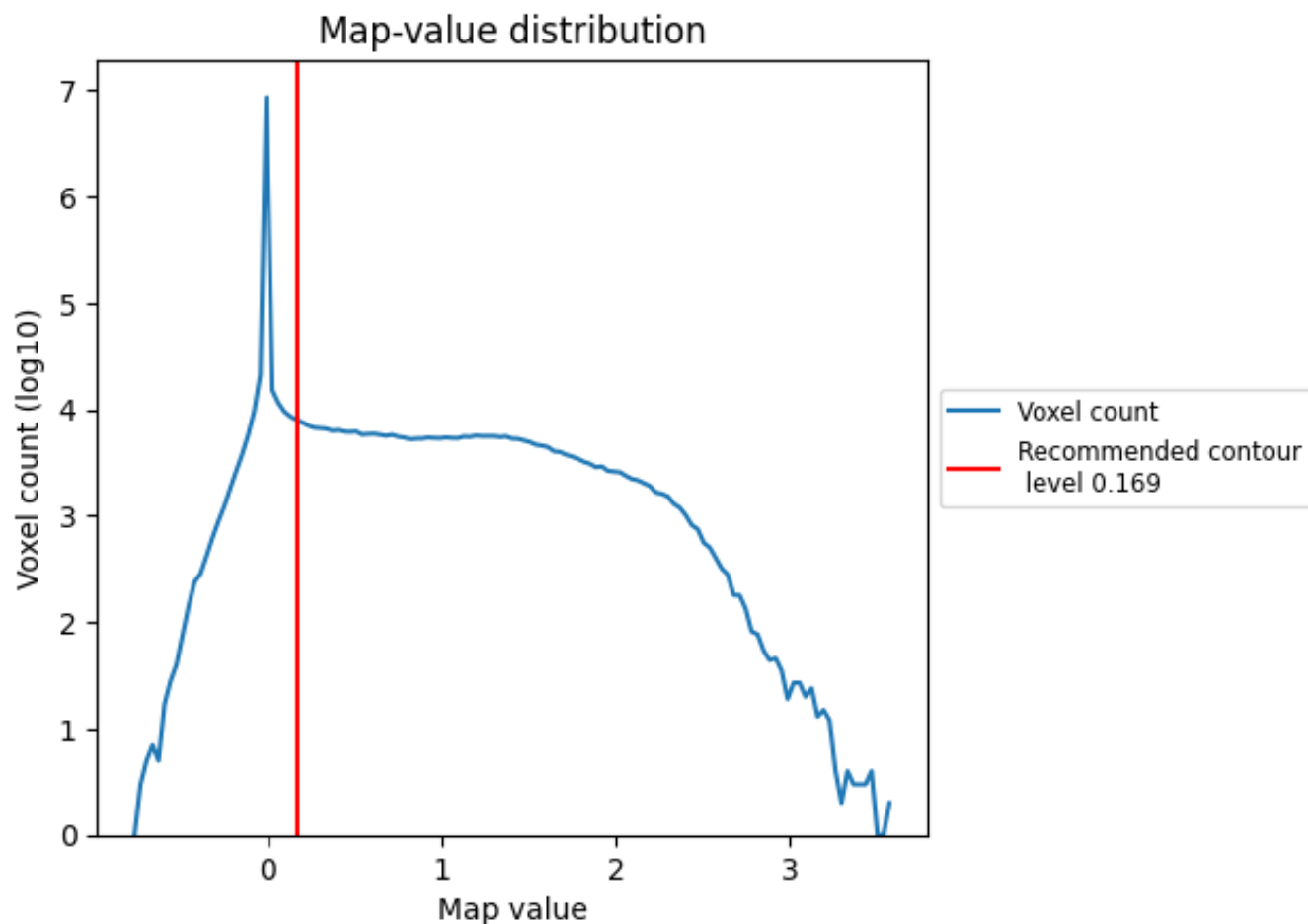
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

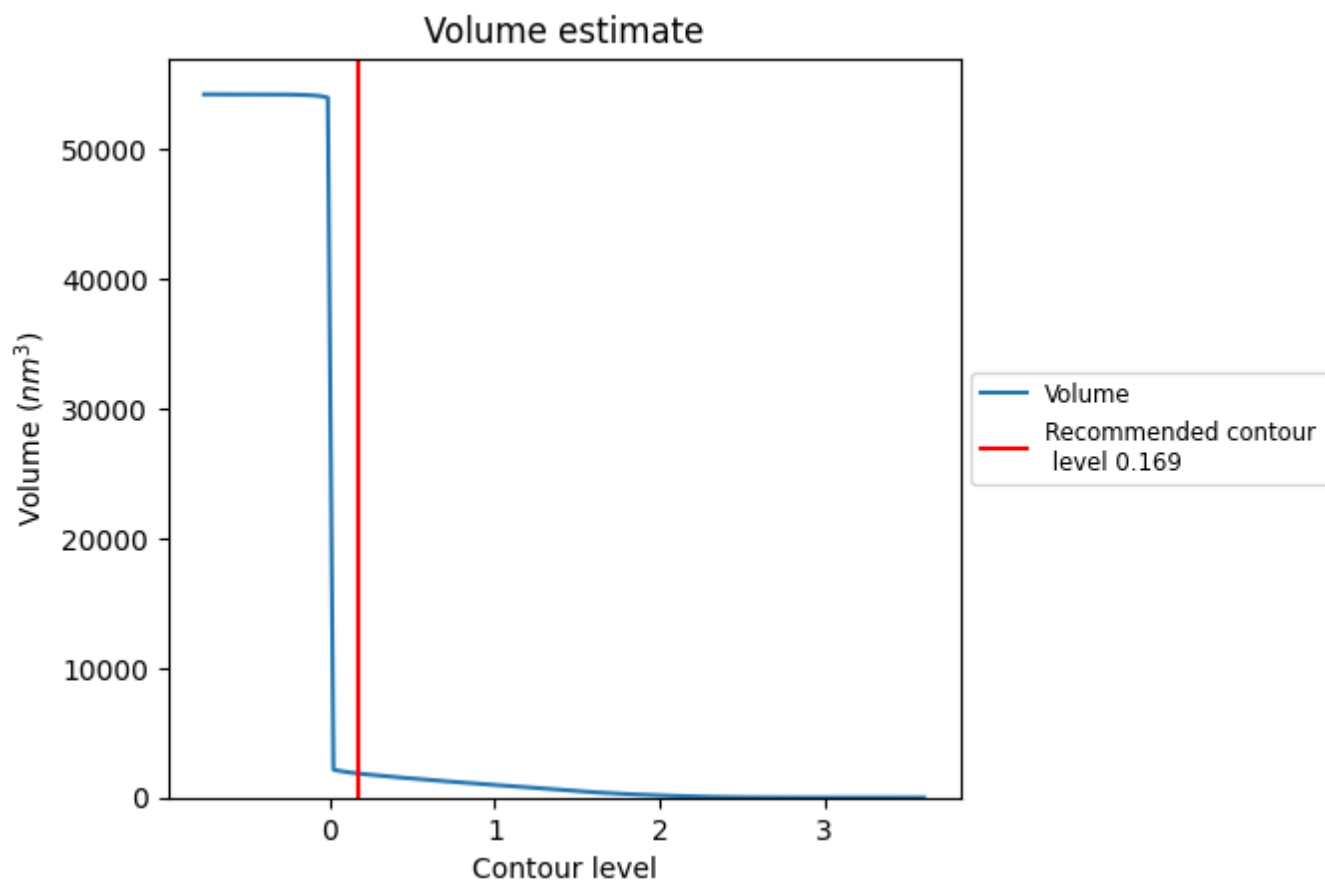
This section contains the results of statistical analysis of the map.

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.

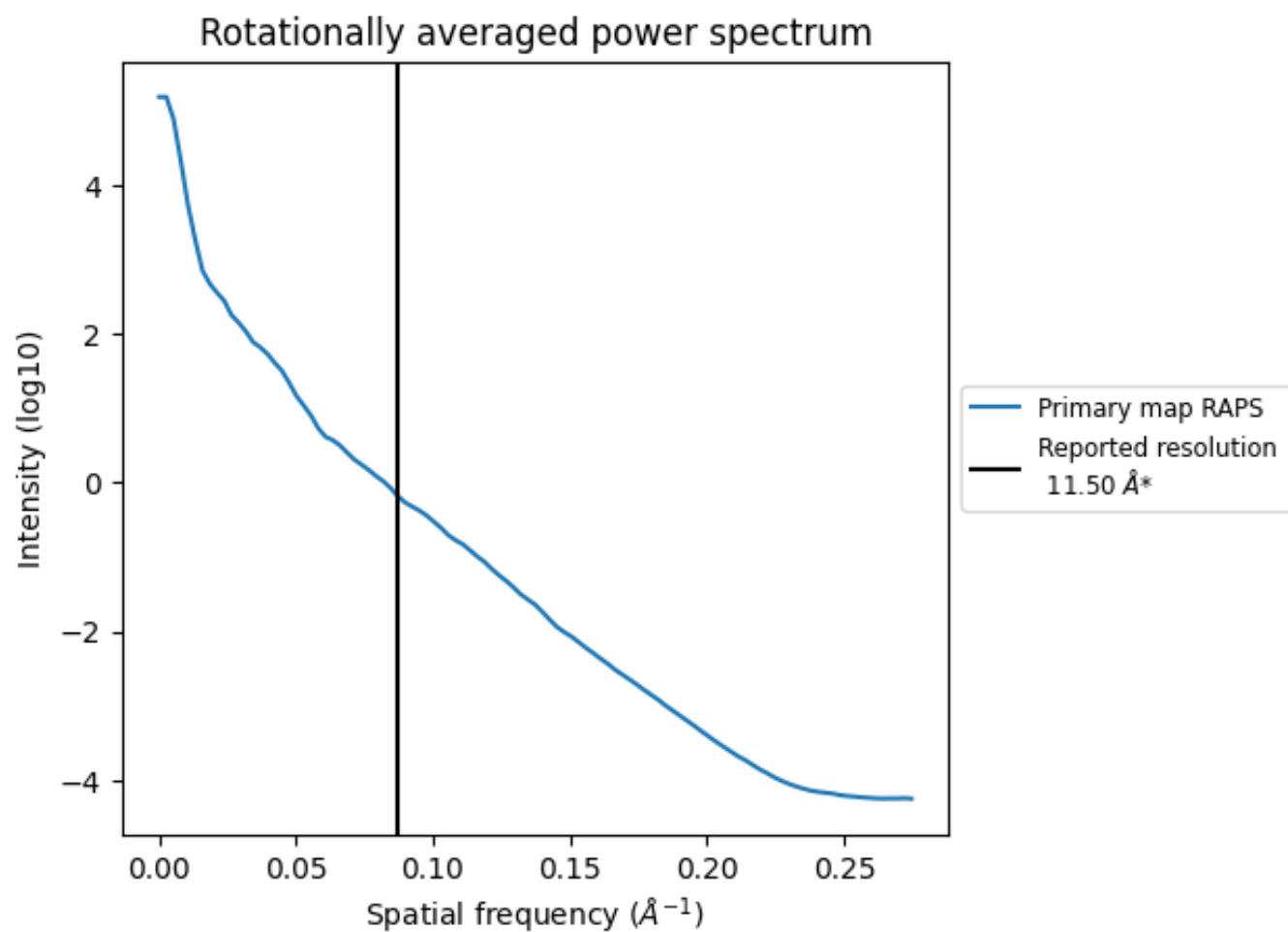
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1859 nm³; this corresponds to an approximate mass of 1680 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 0.087 Å⁻¹

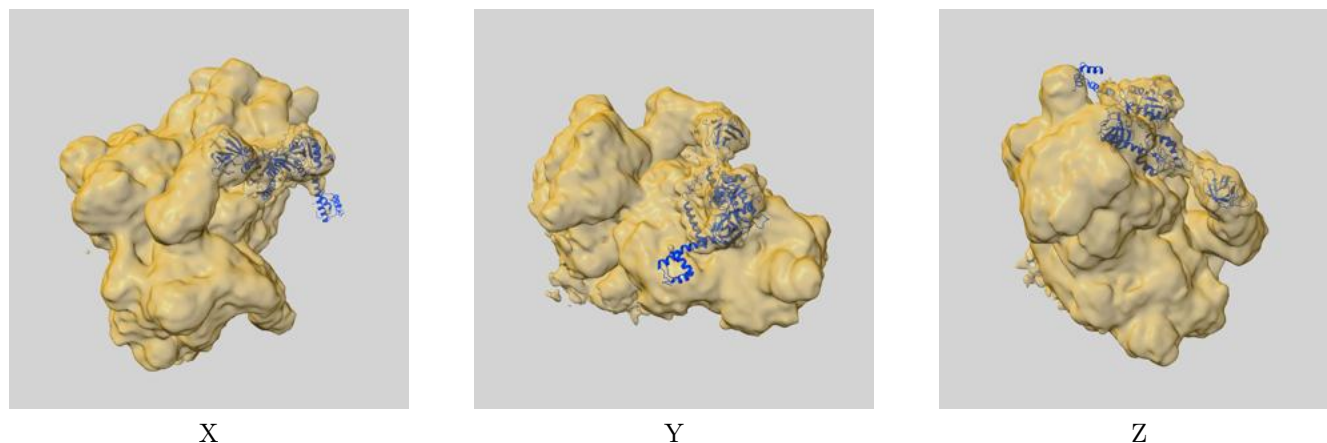
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

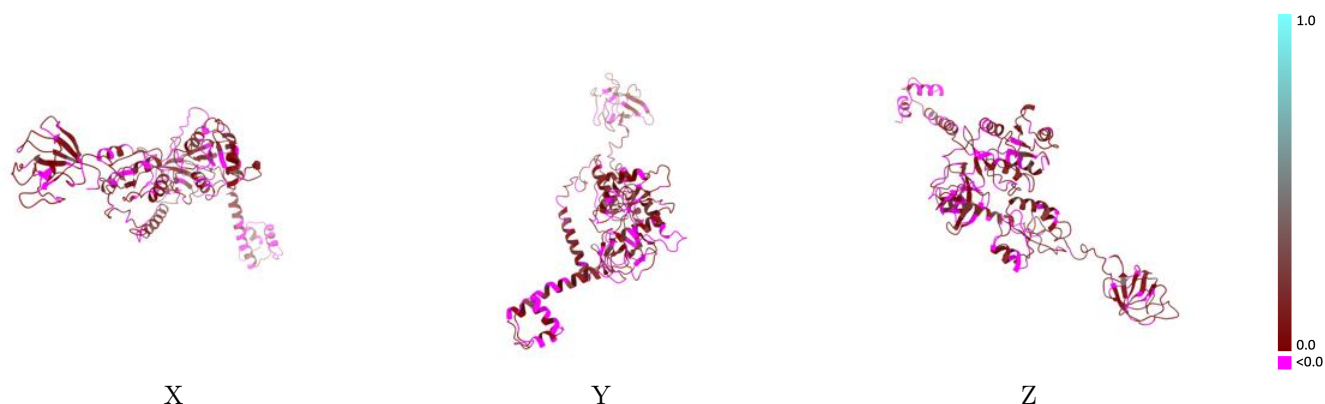
This section contains information regarding the fit between EMDB map EMD-2448 and PDB model 3J4J. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



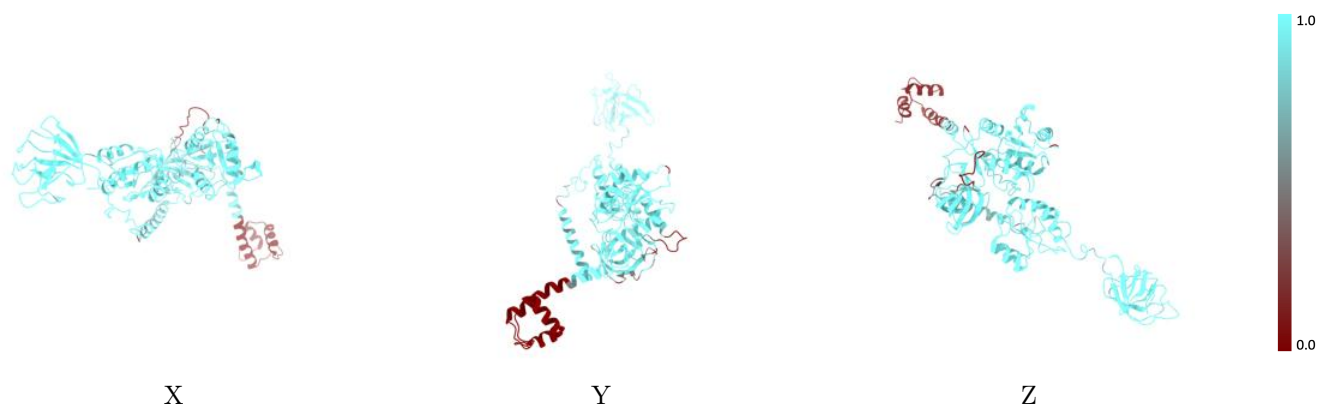
The images above show the 3D surface view of the map at the recommended contour level 0.169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



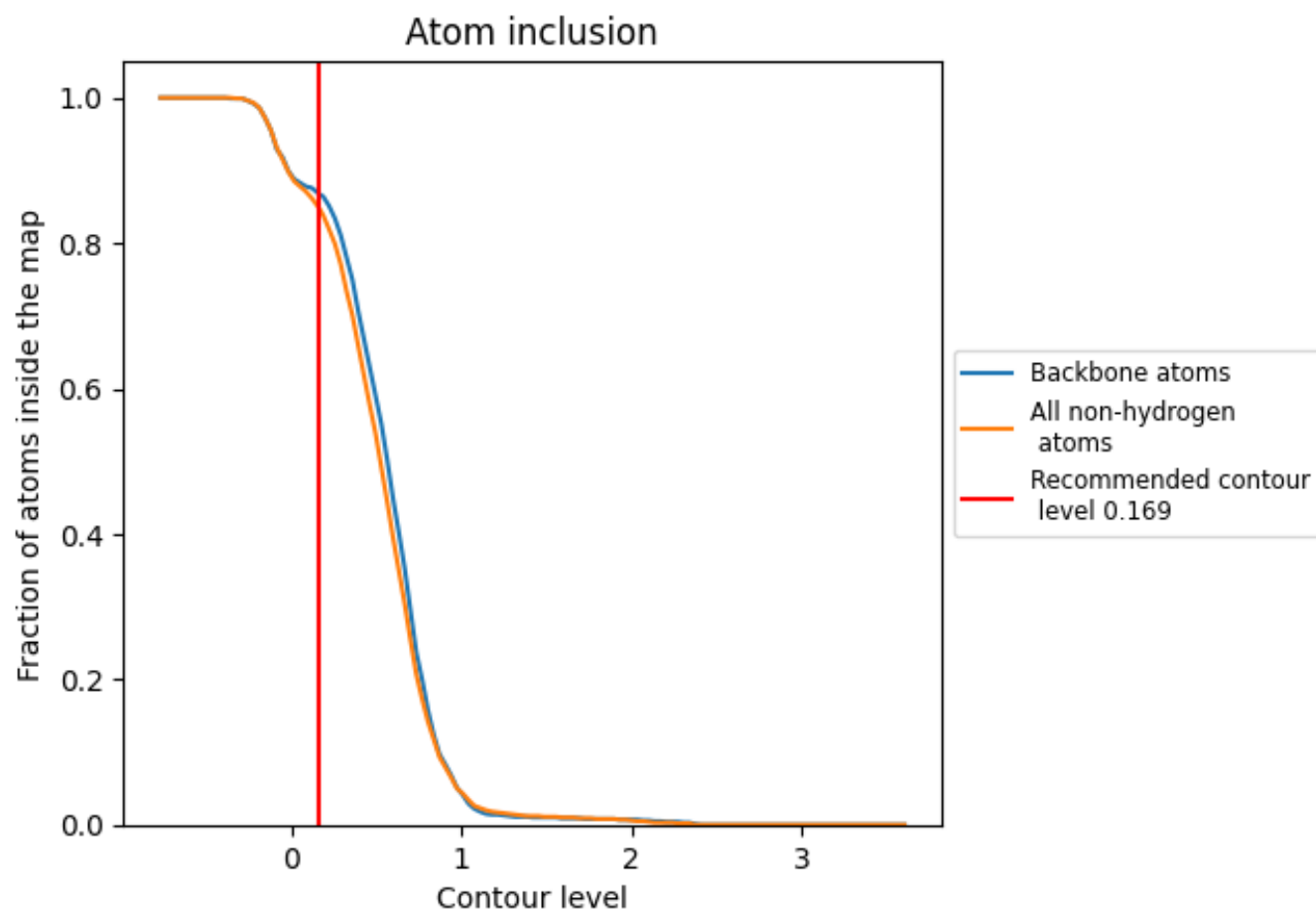
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.169).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.0570
A	0.8470	0.0570

