



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:56 AM UTC

PDB ID : 3J1U / pdb_00003j1u
EMDB ID : EMD-5439
Title : Low affinity dynein microtubule binding domain - tubulin complex
Authors : Redwine, W.B.; Hernandez-Lopez, R.; Zou, S.; Huang, J.; Reck-Peterson, S.L.;
Leschziner, A.E.
Deposited on : 2012-06-25
Resolution : 9.70 Å (reported)
Based on initial models : 3ERR, 1JFF

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:

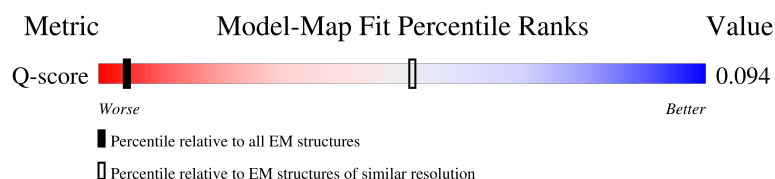
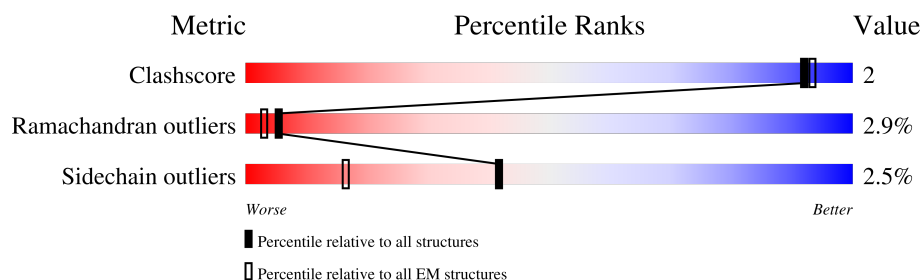
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 9.70 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	165 (9.20 - 10.20)

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	164	56% 49% 47% .
2	B	451	36% 42% 47% 8% ..
3	C	427	37% 44% 48% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8089 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 Cytoplasmic dynein 1 heavy chain 1, seryl t-RNA synthetase chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	164	Total	C	N	O	S	0	0
			1306	820	227	250	9		

- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	439	Total	C	N	O	S	0	0
			3423	2163	582	656	22		

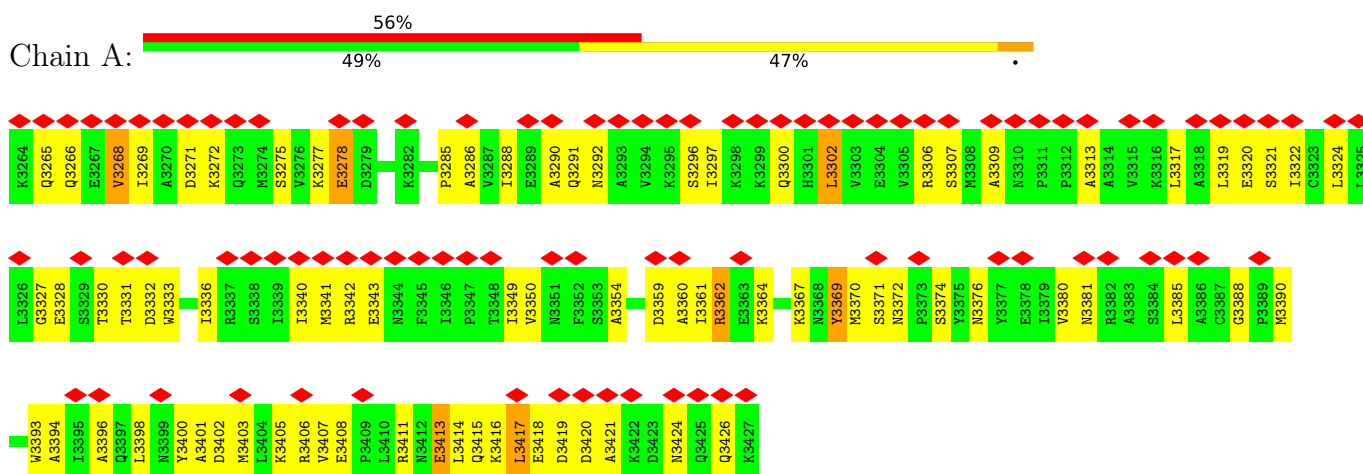
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	427	Total	C	N	O	S	0	0
			3360	2110	576	648	26		

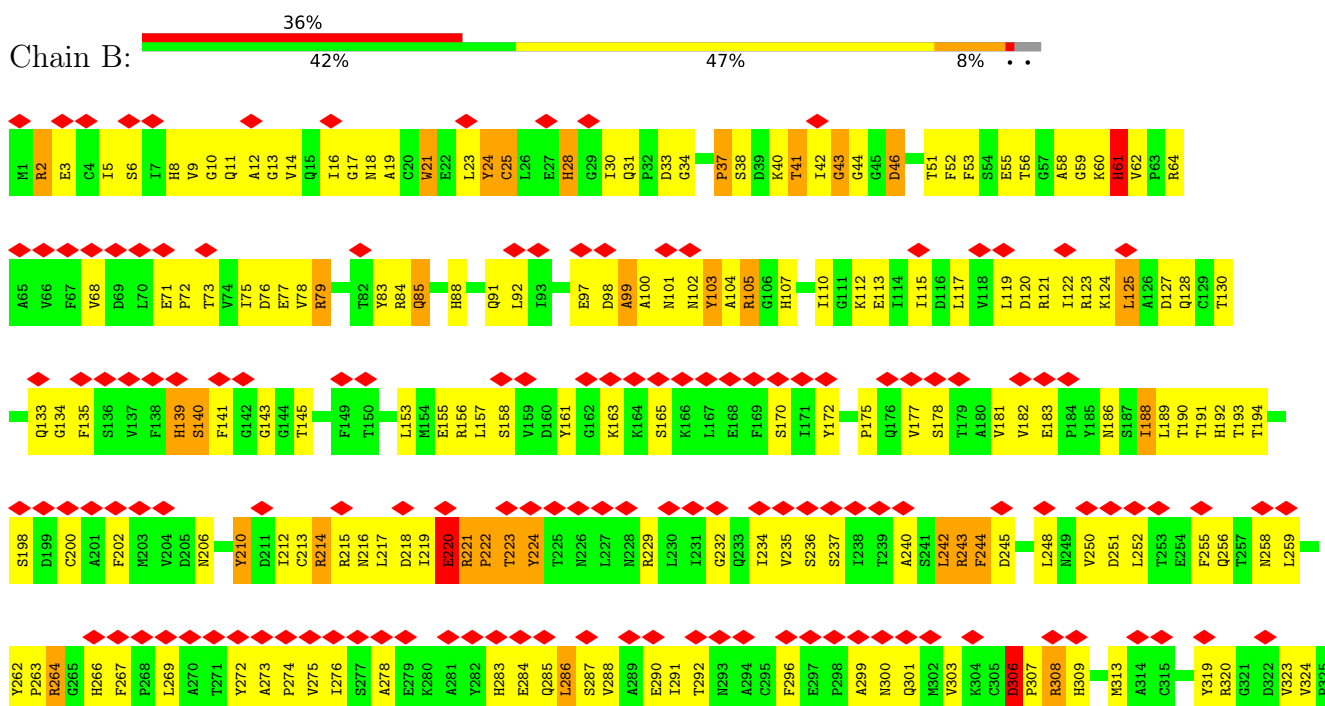
3 Residue-property plots

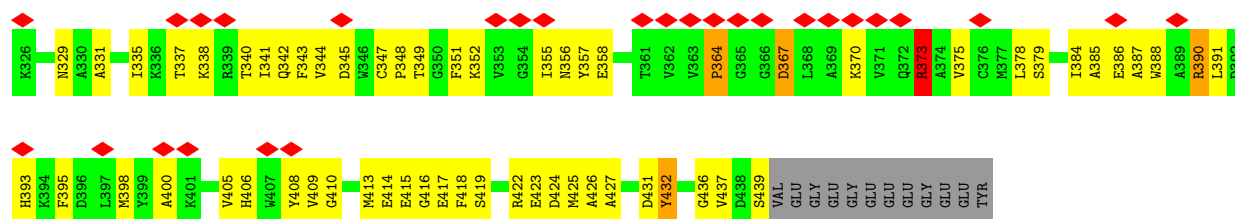
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cytoplasmic dynein 1 heavy chain 1, seryl t-RNA synthetase chimera

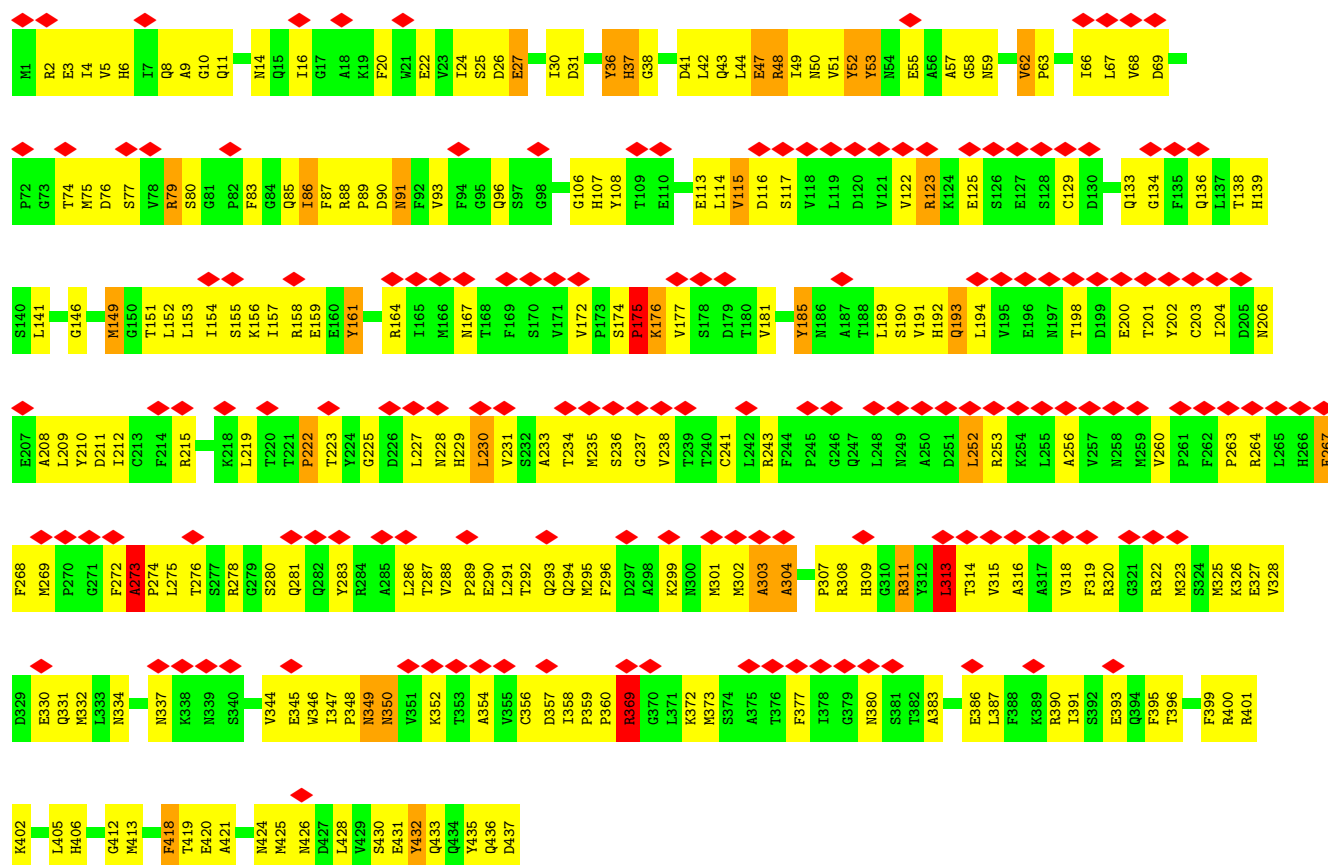
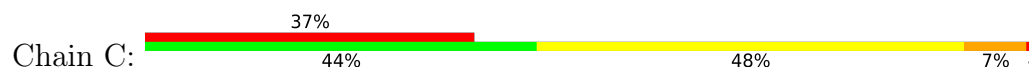


- Molecule 2: Tubulin alpha-1B chain





• Molecule 3: Tubulin beta-2B chain



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.76°, rise=9.26 Å, axial sym=C1	Depositor
Number of segments used	10419	Depositor
Resolution determination method	Not provided	
CTF correction method	phase and amplitude correction using Fre-align	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{Å}^2$)	15	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	63377	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.013	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0036	Depositor
Map size (Å)	109.340004, 77.532, 119.28	wwPDB
Map dimensions	55, 39, 60	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.988, 1.988, 1.988	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	2.13	33/1323 (2.5%)	2.43	82/1782 (4.6%)
2	B	2.16	103/3501 (2.9%)	2.57	297/4752 (6.2%)
3	C	2.17	113/3435 (3.3%)	2.51	250/4652 (5.4%)
All	All	2.16	249/8259 (3.0%)	2.53	629/11186 (5.6%)

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	6
2	B	0	20
3	C	0	18
All	All	0	44

All (249) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	439	SER	C-O	-11.55	1.00	1.23
3	C	437	ASP	C-OXT	-11.53	1.00	1.23
3	C	437	ASP	C-O	-11.53	1.00	1.23
3	C	237	GLY	CA-C	-9.56	1.41	1.52
3	C	172	VAL	CA-CB	-9.13	1.47	1.54
2	B	347	CYS	C-N	9.06	1.40	1.33
2	B	139	HIS	ND1-CE1	9.04	1.41	1.32
2	B	10	GLY	CA-C	-8.73	1.43	1.52
3	C	303	ALA	CA-C	8.51	1.64	1.52
3	C	37	HIS	CE1-NE2	8.43	1.41	1.32
3	C	323	MET	CA-C	8.28	1.62	1.52
1	A	3380	VAL	CA-C	8.10	1.62	1.52
2	B	77	GLU	N-CA	-8.00	1.36	1.46
3	C	44	LEU	CA-C	7.98	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	219	LEU	CA-C	-7.92	1.43	1.52
1	A	3362	ARG	CA-C	-7.79	1.43	1.52
2	B	68	VAL	CA-C	-7.65	1.43	1.52
2	B	340	THR	C-N	-7.50	1.25	1.33
1	A	3328	GLU	N-CA	-7.34	1.37	1.45
3	C	125	GLU	C-N	7.28	1.43	1.33
1	A	3390	MET	C-N	7.22	1.42	1.34
2	B	370	LYS	CA-CB	7.21	1.63	1.53
1	A	3343	GLU	C-N	7.20	1.43	1.33
1	A	3307	SER	CA-C	-7.19	1.43	1.52
3	C	48	ARG	CD-NE	7.19	1.56	1.46
3	C	299	LYS	C-O	-7.18	1.14	1.24
2	B	221	ARG	CD-NE	7.17	1.56	1.46
1	A	3364	LYS	N-CA	7.13	1.54	1.46
3	C	129	CYS	CA-C	7.06	1.62	1.53
3	C	383	ALA	CA-C	-7.04	1.44	1.53
2	B	16	ILE	CA-CB	7.04	1.62	1.54
3	C	181	VAL	CA-C	-7.02	1.43	1.52
2	B	99	ALA	CA-C	6.95	1.62	1.52
2	B	143	GLY	C-N	6.91	1.43	1.33
3	C	316	ALA	CA-C	6.84	1.61	1.52
2	B	21	TRP	NE1-CE2	6.82	1.45	1.37
3	C	359	PRO	CA-C	6.82	1.58	1.52
2	B	267	PHE	CA-C	6.81	1.60	1.52
3	C	192	HIS	CE1-NE2	6.80	1.39	1.32
3	C	352	LYS	CA-C	-6.79	1.44	1.52
2	B	101	ASN	CA-C	6.77	1.61	1.53
2	B	178	SER	N-CA	6.75	1.54	1.46
2	B	378	LEU	N-CA	-6.75	1.38	1.46
3	C	167	ASN	CA-C	-6.74	1.44	1.52
3	C	293	GLN	N-CA	-6.72	1.38	1.46
3	C	57	ALA	CA-C	6.71	1.61	1.53
2	B	357	TYR	C-O	-6.68	1.16	1.24
2	B	73	THR	C-N	6.67	1.42	1.33
3	C	96	GLN	CA-CB	6.66	1.64	1.53
1	A	3360	ALA	CA-C	-6.64	1.43	1.52
3	C	346	TRP	N-CA	-6.59	1.38	1.46
2	B	242	LEU	CA-CB	6.54	1.64	1.53
1	A	3396	ALA	N-CA	6.53	1.54	1.46
3	C	83	PHE	CA-CB	6.51	1.62	1.53
2	B	292	THR	CA-C	-6.42	1.44	1.52
1	A	3306	ARG	C-N	6.41	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	37	HIS	ND1-CE1	6.38	1.39	1.32
3	C	138	THR	CA-C	-6.38	1.44	1.52
3	C	294	GLN	N-CA	-6.37	1.38	1.46
1	A	3398	LEU	CA-C	6.36	1.60	1.52
2	B	181	VAL	C-N	6.34	1.40	1.34
2	B	58	ALA	CA-CB	6.32	1.64	1.53
3	C	24	ILE	CA-C	-6.31	1.44	1.52
3	C	241	CYS	CA-CB	6.31	1.63	1.53
2	B	285	GLN	CA-C	-6.28	1.45	1.52
3	C	47	GLU	C-N	6.27	1.42	1.33
2	B	306	ASP	CA-CB	6.27	1.63	1.53
2	B	121	ARG	CD-NE	6.24	1.54	1.46
2	B	300	ASN	CA-CB	6.23	1.63	1.53
2	B	237	SER	N-CA	6.23	1.54	1.46
2	B	79	ARG	C-O	-6.23	1.16	1.24
2	B	215	ARG	CD-NE	6.19	1.54	1.46
2	B	72	PRO	C-N	6.18	1.41	1.33
3	C	291	LEU	N-CA	6.17	1.53	1.46
1	A	3321	SER	N-CA	6.14	1.53	1.46
2	B	244	PHE	CA-CB	6.14	1.63	1.53
2	B	258	ASN	CA-C	6.13	1.60	1.52
2	B	217	LEU	CA-CB	6.11	1.63	1.53
2	B	283	HIS	ND1-CE1	6.10	1.38	1.32
2	B	194	THR	CA-C	-6.07	1.44	1.52
2	B	290	GLU	C-N	6.04	1.41	1.33
2	B	134	GLY	N-CA	6.03	1.52	1.45
3	C	79	ARG	CD-NE	6.03	1.54	1.46
3	C	372	LYS	CA-C	6.02	1.61	1.52
3	C	360	PRO	CA-C	6.01	1.59	1.52
2	B	319	TYR	CA-CB	6.01	1.61	1.52
3	C	48	ARG	C-N	6.00	1.41	1.33
3	C	47	GLU	N-CA	5.99	1.54	1.46
2	B	120	ASP	CA-CB	5.97	1.63	1.53
3	C	43	GLN	C-N	5.97	1.42	1.33
1	A	3350	VAL	CA-C	-5.97	1.45	1.52
3	C	345	GLU	CA-CB	5.96	1.62	1.53
2	B	24	TYR	CA-C	5.96	1.60	1.52
3	C	344	VAL	CA-CB	5.95	1.62	1.54
2	B	135	PHE	CA-C	5.94	1.60	1.52
3	C	16	ILE	CA-CB	-5.92	1.46	1.54
3	C	252	LEU	CA-C	5.89	1.60	1.52
3	C	90	ASP	CA-CB	5.88	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	296	PHE	CA-CB	5.87	1.61	1.53
3	C	177	VAL	CA-CB	-5.85	1.47	1.54
3	C	393	GLU	N-CA	-5.85	1.39	1.46
1	A	3369	TYR	CA-C	-5.83	1.47	1.52
1	A	3407	VAL	CA-C	5.83	1.60	1.52
3	C	406	HIS	CA-C	-5.82	1.45	1.52
3	C	123	ARG	CA-C	-5.82	1.44	1.52
2	B	356	ASN	N-CA	5.81	1.53	1.45
3	C	433	GLN	C-N	5.79	1.41	1.33
3	C	318	VAL	N-CA	-5.77	1.38	1.46
3	C	198	THR	CA-CB	-5.77	1.43	1.53
3	C	418	PHE	CA-C	5.77	1.60	1.52
3	C	354	ALA	C-N	5.76	1.41	1.33
1	A	3324	LEU	N-CA	-5.76	1.39	1.46
2	B	313	MET	CA-CB	5.76	1.62	1.53
2	B	30	ILE	CA-CB	-5.75	1.47	1.54
2	B	8	HIS	CA-CB	-5.75	1.44	1.53
3	C	203	CYS	N-CA	5.75	1.53	1.46
3	C	139	HIS	N-CA	-5.75	1.39	1.46
1	A	3286	ALA	N-CA	-5.74	1.39	1.46
1	A	3291	GLN	C-N	-5.74	1.26	1.33
2	B	223	THR	CA-C	-5.74	1.45	1.52
2	B	373	ARG	CD-NE	5.74	1.54	1.46
2	B	432	TYR	C-O	-5.74	1.16	1.24
3	C	301	MET	CA-C	5.73	1.60	1.53
3	C	320	ARG	C-N	5.72	1.39	1.32
2	B	97	GLU	N-CA	-5.71	1.38	1.45
1	A	3319	LEU	CA-C	-5.71	1.45	1.52
2	B	158	SER	C-O	-5.70	1.17	1.24
3	C	332	MET	C-N	5.70	1.41	1.33
2	B	431	ASP	CA-CB	5.69	1.62	1.53
2	B	122	ILE	C-N	5.67	1.41	1.33
2	B	375	VAL	CA-CB	5.67	1.61	1.55
2	B	243	ARG	CA-CB	5.66	1.62	1.53
3	C	68	VAL	CA-CB	-5.66	1.47	1.54
3	C	202	TYR	CA-C	5.66	1.59	1.52
1	A	3393	TRP	CA-CB	5.64	1.62	1.53
3	C	159	GLU	CA-C	5.64	1.60	1.52
3	C	151	THR	CA-C	5.63	1.60	1.52
1	A	3372	ASN	CA-C	5.63	1.58	1.53
2	B	193	THR	C-N	5.62	1.41	1.33
3	C	256	ALA	CA-CB	5.61	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	192	HIS	N-CA	-5.61	1.39	1.46
2	B	220	GLU	CA-C	-5.61	1.45	1.52
2	B	191	THR	C-N	5.60	1.41	1.33
2	B	222	PRO	N-CA	5.60	1.53	1.47
3	C	43	GLN	CA-CB	5.60	1.60	1.53
2	B	417	GLU	N-CA	5.59	1.53	1.46
2	B	215	ARG	C-N	5.58	1.41	1.33
3	C	337	ASN	CA-C	5.58	1.60	1.52
2	B	212	ILE	CA-CB	-5.57	1.47	1.54
1	A	3322	ILE	C-O	5.57	1.30	1.24
2	B	419	SER	N-CA	5.56	1.53	1.46
1	A	3381	ASN	N-CA	5.56	1.53	1.46
3	C	428	LEU	N-CA	-5.55	1.39	1.46
3	C	331	GLN	C-N	5.54	1.42	1.33
1	A	3320	GLU	C-N	5.54	1.40	1.33
2	B	56	THR	N-CA	5.53	1.53	1.46
2	B	9	VAL	C-O	-5.53	1.18	1.24
2	B	390	ARG	CD-NE	5.53	1.53	1.46
1	A	3302	LEU	CA-C	5.51	1.60	1.52
2	B	236	SER	N-CA	-5.50	1.39	1.46
2	B	198	SER	CA-CB	5.50	1.62	1.53
3	C	253	ARG	CD-NE	5.50	1.53	1.46
3	C	114	LEU	CA-CB	5.48	1.61	1.53
1	A	3268	VAL	C-N	5.46	1.40	1.33
2	B	296	PHE	CA-CB	5.45	1.61	1.53
3	C	10	GLY	N-CA	5.45	1.51	1.45
2	B	38	SER	N-CA	-5.44	1.39	1.46
3	C	405	LEU	CA-CB	5.44	1.63	1.53
2	B	193	THR	CA-C	5.44	1.59	1.52
3	C	43	GLN	N-CA	-5.43	1.39	1.46
1	A	3394	ALA	C-N	5.43	1.40	1.33
1	A	3419	ASP	C-N	5.43	1.41	1.33
2	B	384	ILE	CA-C	-5.40	1.45	1.52
3	C	191	VAL	CA-CB	-5.39	1.47	1.54
2	B	183	GLU	N-CA	5.39	1.51	1.46
3	C	5	VAL	N-CA	-5.38	1.39	1.46
2	B	264	ARG	C-N	5.38	1.41	1.33
3	C	208	ALA	C-N	5.38	1.40	1.33
2	B	413	MET	CA-C	-5.38	1.46	1.52
2	B	431	ASP	N-CA	5.37	1.52	1.46
2	B	141	PHE	CA-C	5.37	1.59	1.52
3	C	313	LEU	N-CA	5.36	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	63	PRO	N-CD	-5.36	1.40	1.47
2	B	189	LEU	CA-CB	5.35	1.61	1.53
3	C	198	THR	C-O	5.34	1.29	1.23
3	C	49	ILE	CA-C	5.33	1.59	1.52
3	C	67	LEU	CA-C	5.32	1.59	1.52
2	B	128	GLN	CA-CB	5.31	1.62	1.53
2	B	422	ARG	C-N	5.30	1.40	1.33
3	C	420	GLU	N-CA	-5.29	1.40	1.46
3	C	164	ARG	NE-CZ	5.28	1.38	1.33
3	C	420	GLU	CA-CB	5.28	1.61	1.53
1	A	3372	ASN	C-O	5.28	1.30	1.24
3	C	318	VAL	CA-C	5.28	1.59	1.52
2	B	123	ARG	C-N	5.27	1.41	1.33
1	A	3371	SER	N-CA	5.27	1.53	1.46
3	C	149	MET	CA-CB	5.26	1.61	1.53
3	C	89	PRO	C-N	5.26	1.40	1.33
2	B	214	ARG	NE-CZ	5.25	1.38	1.33
2	B	153	LEU	CA-C	5.25	1.59	1.52
3	C	155	SER	C-O	-5.25	1.18	1.24
3	C	319	PHE	CA-CB	5.24	1.61	1.53
2	B	240	ALA	CA-C	-5.24	1.45	1.52
2	B	393	HIS	C-N	5.23	1.41	1.33
3	C	358	ILE	C-N	5.23	1.39	1.33
3	C	129	CYS	CA-CB	5.23	1.61	1.53
3	C	11	GLN	CA-CB	5.23	1.61	1.53
1	A	3376	ASN	C-O	5.22	1.30	1.23
3	C	360	PRO	N-CA	5.22	1.52	1.47
3	C	267	PHE	CA-C	5.21	1.59	1.52
3	C	233	ALA	C-O	-5.21	1.18	1.24
2	B	31	GLN	CA-C	5.21	1.58	1.53
3	C	69	ASP	C-N	-5.21	1.26	1.33
3	C	344	VAL	CA-C	5.21	1.59	1.52
2	B	213	CYS	N-CA	-5.20	1.40	1.46
2	B	410	GLY	CA-C	-5.19	1.43	1.51
3	C	231	VAL	N-CA	5.19	1.52	1.46
1	A	3288	ILE	CB-CG1	5.18	1.63	1.53
3	C	201	THR	CA-C	-5.17	1.46	1.52
3	C	328	VAL	CA-CB	-5.16	1.48	1.54
2	B	117	LEU	C-N	5.15	1.40	1.33
2	B	344	VAL	C-N	5.15	1.41	1.33
2	B	356	ASN	CA-C	-5.15	1.46	1.52
3	C	204	ILE	C-N	5.15	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	346	TRP	C-N	5.15	1.39	1.33
3	C	322	ARG	CD-NE	5.13	1.53	1.46
3	C	354	ALA	CA-C	5.12	1.58	1.52
2	B	409	VAL	N-CA	5.11	1.52	1.46
3	C	360	PRO	C-N	5.11	1.40	1.33
3	C	393	GLU	C-N	5.10	1.40	1.34
3	C	192	HIS	CG-CD2	5.10	1.41	1.35
3	C	412	GLY	C-N	5.09	1.40	1.33
3	C	308	ARG	CD-NE	-5.08	1.39	1.46
3	C	52	TYR	CA-CB	5.08	1.62	1.54
3	C	431	GLU	CA-CB	5.08	1.61	1.53
2	B	84	ARG	C-O	5.07	1.30	1.24
2	B	104	ALA	CA-C	-5.07	1.45	1.52
2	B	100	ALA	CA-C	5.06	1.59	1.52
1	A	3403	MET	N-CA	5.06	1.52	1.46
2	B	370	LYS	N-CA	-5.05	1.40	1.46
3	C	215	ARG	NE-CZ	5.04	1.38	1.33
2	B	139	HIS	C-N	5.03	1.40	1.33
2	B	250	VAL	C-O	5.03	1.29	1.24
2	B	296	PHE	C-N	5.03	1.40	1.33
2	B	355	ILE	N-CA	-5.03	1.39	1.46
3	C	155	SER	CA-CB	5.03	1.61	1.53
2	B	183	GLU	CA-C	5.03	1.58	1.52
2	B	300	ASN	C-O	-5.01	1.18	1.24
3	C	8	GLN	N-CA	-5.01	1.40	1.46

All (629) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	288	VAL	O-C-N	-14.12	110.04	120.07
2	B	186	ASN	CA-CB-CG	10.78	123.38	112.60
3	C	43	GLN	CA-C-N	10.68	141.93	121.54
3	C	43	GLN	C-N-CA	10.68	141.93	121.54
2	B	224	TYR	CE1-CZ-CE2	-10.60	99.10	120.30
2	B	76	ASP	CA-C-N	10.60	134.22	120.44
2	B	76	ASP	C-N-CA	10.60	134.22	120.44
2	B	12	ALA	CA-C-N	10.24	131.26	120.00
2	B	12	ALA	C-N-CA	10.24	131.26	120.00
2	B	349	THR	N-CA-C	9.93	121.70	111.07
3	C	47	GLU	CA-C-O	-9.80	110.12	121.49
2	B	219	ILE	CA-C-N	9.73	133.67	120.44
2	B	219	ILE	C-N-CA	9.73	133.67	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	THR	N-CA-CB	9.72	124.41	110.12
3	C	359	PRO	O-C-N	-9.37	110.40	121.46
3	C	256	ALA	N-CA-C	9.34	121.46	111.28
1	A	3415	GLN	CA-C-N	9.32	132.55	120.44
1	A	3415	GLN	C-N-CA	9.32	132.55	120.44
1	A	3297	ILE	O-C-N	-9.30	112.53	122.67
2	B	78	VAL	N-CA-C	9.06	119.87	110.72
2	B	91	GLN	OE1-CD-NE2	-8.96	113.64	122.60
2	B	406	HIS	CA-CB-CG	8.95	122.75	113.80
3	C	193	GLN	CA-C-O	-8.84	111.59	120.70
2	B	252	LEU	CA-C-N	8.79	131.86	120.44
2	B	252	LEU	C-N-CA	8.79	131.86	120.44
3	C	43	GLN	O-C-N	8.75	133.92	122.20
3	C	327	GLU	N-CA-C	8.57	121.40	111.11
3	C	273	ALA	O-C-N	-8.50	111.55	121.32
2	B	303	VAL	CA-C-N	8.48	131.47	120.44
2	B	303	VAL	C-N-CA	8.48	131.47	120.44
2	B	60	LYS	CA-C-N	8.46	137.69	121.54
2	B	60	LYS	C-N-CA	8.46	137.69	121.54
2	B	348	PRO	N-CA-C	-8.41	103.92	114.68
2	B	224	TYR	CD1-CE1-CZ	8.36	134.65	119.60
2	B	427	ALA	CA-C-N	8.25	131.33	120.28
2	B	427	ALA	C-N-CA	8.25	131.33	120.28
3	C	75	MET	CA-C-N	8.24	131.67	120.38
3	C	75	MET	C-N-CA	8.24	131.67	120.38
2	B	104	ALA	CA-C-O	8.19	129.39	119.97
3	C	122	VAL	O-C-N	-8.16	113.95	121.87
3	C	85	GLN	CA-C-N	8.13	130.97	120.56
3	C	85	GLN	C-N-CA	8.13	130.97	120.56
3	C	11	GLN	N-CA-C	8.10	119.74	111.07
3	C	238	VAL	N-CA-C	8.08	118.02	110.42
3	C	330	GLU	N-CA-C	8.04	120.05	111.28
2	B	388	TRP	CA-C-N	8.04	131.37	120.44
2	B	388	TRP	C-N-CA	8.04	131.37	120.44
3	C	86	ILE	N-CA-C	8.03	118.08	110.53
3	C	319	PHE	CA-CB-CG	7.97	121.77	113.80
3	C	380	ASN	O-C-N	-7.93	113.59	123.27
2	B	255	PHE	CA-CB-CG	-7.93	105.87	113.80
3	C	115	VAL	CA-C-N	7.91	130.72	120.44
3	C	115	VAL	C-N-CA	7.91	130.72	120.44
3	C	264	ARG	N-CA-C	-7.90	95.62	109.06
3	C	154	ILE	CA-C-N	7.89	131.20	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	154	ILE	C-N-CA	7.89	131.20	120.54
3	C	421	ALA	CA-C-N	7.88	130.84	120.28
3	C	421	ALA	C-N-CA	7.88	130.84	120.28
3	C	228	ASN	N-CA-C	7.86	120.75	111.71
3	C	80	SER	O-C-N	-7.84	113.21	122.15
3	C	421	ALA	N-CA-C	7.82	119.80	111.28
3	C	236	SER	CA-C-N	7.82	128.65	119.98
3	C	236	SER	C-N-CA	7.82	128.65	119.98
1	A	3292	ASN	CA-CB-CG	-7.80	104.80	112.60
3	C	334	ASN	CA-CB-CG	-7.79	104.81	112.60
1	A	3354	ALA	N-CA-C	7.78	122.45	113.19
3	C	296	PHE	CA-CB-CG	-7.78	106.02	113.80
3	C	36	TYR	N-CA-C	7.77	121.78	110.28
2	B	288	VAL	CA-C-N	7.76	130.53	120.44
2	B	288	VAL	C-N-CA	7.76	130.53	120.44
3	C	134	GLY	N-CA-C	7.76	121.42	111.09
2	B	206	ASN	N-CA-C	7.74	119.72	111.28
3	C	337	ASN	CA-CB-CG	-7.69	104.91	112.60
2	B	262	TYR	O-C-N	-7.69	116.04	121.65
2	B	127	ASP	N-CA-C	7.69	119.66	111.28
2	B	172	TYR	CA-C-N	7.67	128.28	119.99
2	B	172	TYR	C-N-CA	7.67	128.28	119.99
2	B	133	GLN	N-CA-C	7.66	120.36	111.02
2	B	194	THR	O-C-N	-7.60	114.06	122.12
2	B	423	GLU	N-CA-C	7.58	119.55	111.28
1	A	3306	ARG	N-CA-C	7.58	119.63	111.36
3	C	156	LYS	O-C-N	-7.58	114.09	122.12
3	C	234	THR	CA-C-N	7.57	130.42	120.28
3	C	234	THR	C-N-CA	7.57	130.42	120.28
2	B	139	HIS	CE1-NE2-CD2	-7.53	101.47	109.00
3	C	3	GLU	CA-C-O	-7.53	112.80	122.14
2	B	202	PHE	CA-CB-CG	7.53	121.33	113.80
3	C	320	ARG	O-C-N	-7.51	114.49	123.27
3	C	37	HIS	CB-CG-CD2	-7.49	121.46	131.20
3	C	290	GLU	CA-C-O	7.48	128.48	120.55
2	B	28	HIS	ND1-CE1-NE2	7.47	115.87	108.40
3	C	288	VAL	CA-C-N	7.46	126.99	118.85
3	C	288	VAL	C-N-CA	7.46	126.99	118.85
2	B	273	ALA	N-CA-C	7.41	126.19	109.81
2	B	60	LYS	O-C-N	7.40	132.11	122.19
3	C	358	ILE	CA-C-N	7.36	127.96	120.38
3	C	358	ILE	C-N-CA	7.36	127.96	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3370	MET	N-CA-C	7.36	120.23	111.33
2	B	139	HIS	CA-C-N	7.35	134.94	121.70
2	B	139	HIS	C-N-CA	7.35	134.94	121.70
2	B	156	ARG	CA-C-N	7.32	130.42	120.54
2	B	156	ARG	C-N-CA	7.32	130.42	120.54
2	B	258	ASN	OD1-CG-ND2	-7.32	115.28	122.60
2	B	283	HIS	CA-CB-CG	7.29	121.09	113.80
1	A	3381	ASN	CA-C-O	7.29	128.35	119.97
2	B	405	VAL	CA-C-O	7.29	125.31	118.90
2	B	84	ARG	N-CA-C	7.28	120.14	111.33
3	C	74	THR	CA-C-N	7.28	130.37	120.54
3	C	74	THR	C-N-CA	7.28	130.37	120.54
3	C	155	SER	CA-C-N	7.26	130.01	120.28
3	C	155	SER	C-N-CA	7.26	130.01	120.28
3	C	37	HIS	CA-CB-CG	-7.24	106.56	113.80
3	C	253	ARG	NE-CZ-NH1	7.22	128.72	121.50
2	B	267	PHE	CA-CB-CG	7.21	121.01	113.80
2	B	391	LEU	N-CA-CB	7.20	120.45	110.01
2	B	426	ALA	N-CA-C	7.20	119.13	111.28
2	B	10	GLY	CA-C-O	-7.19	116.47	122.29
1	A	3394	ALA	CA-C-N	7.17	129.59	120.56
1	A	3394	ALA	C-N-CA	7.17	129.59	120.56
2	B	115	ILE	N-CA-C	7.16	117.30	110.42
3	C	117	SER	CA-C-N	7.13	129.69	120.56
3	C	117	SER	C-N-CA	7.13	129.69	120.56
3	C	401	ARG	NE-CZ-NH1	7.09	128.59	121.50
3	C	77	SER	CA-C-N	7.08	130.48	120.42
3	C	77	SER	C-N-CA	7.08	130.48	120.42
3	C	157	ILE	O-C-N	-7.07	114.55	121.90
3	C	87	PHE	CA-C-N	7.04	138.99	121.80
3	C	87	PHE	C-N-CA	7.04	138.99	121.80
3	C	269	MET	CB-CA-C	-7.03	102.36	110.17
3	C	209	LEU	CB-CA-C	7.01	121.89	110.88
2	B	31	GLN	CA-C-N	7.00	126.98	119.28
2	B	31	GLN	C-N-CA	7.00	126.98	119.28
2	B	431	ASP	CA-CB-CG	-7.00	105.60	112.60
1	A	3408	GLU	CA-C-N	6.99	126.81	119.05
1	A	3408	GLU	C-N-CA	6.99	126.81	119.05
3	C	337	ASN	CA-C-O	6.99	127.73	119.56
2	B	41	THR	CA-C-N	6.96	132.15	121.71
2	B	41	THR	C-N-CA	6.96	132.15	121.71
3	C	52	TYR	O-C-N	-6.96	114.64	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	175	PRO	CA-C-N	6.96	134.82	121.54
3	C	175	PRO	C-N-CA	6.96	134.82	121.54
3	C	176	LYS	CG-CD-CE	6.95	127.30	111.30
2	B	52	PHE	CA-C-N	6.95	132.90	122.68
2	B	52	PHE	C-N-CA	6.95	132.90	122.68
2	B	424	ASP	CA-CB-CG	6.95	119.55	112.60
3	C	309	HIS	CA-CB-CG	6.95	120.75	113.80
2	B	14	VAL	O-C-N	-6.94	114.68	121.83
2	B	425	MET	CA-C-N	6.93	129.56	120.28
2	B	425	MET	C-N-CA	6.93	129.56	120.28
2	B	439	SER	CA-C-O	-6.92	109.04	120.80
3	C	154	ILE	CB-CA-C	6.92	120.82	111.97
2	B	224	TYR	CE1-CZ-OH	6.91	140.63	119.90
2	B	384	ILE	N-CA-CB	6.88	122.59	111.23
3	C	235	MET	CA-C-N	6.88	129.49	120.28
3	C	235	MET	C-N-CA	6.88	129.49	120.28
2	B	145	THR	CA-C-N	6.83	127.68	120.03
2	B	145	THR	C-N-CA	6.83	127.68	120.03
3	C	383	ALA	O-C-N	-6.82	114.40	122.58
3	C	185	TYR	CB-CG-CD2	6.81	131.01	120.80
2	B	342	GLN	CA-C-O	6.80	127.79	120.38
2	B	51	THR	O-C-N	-6.78	114.62	122.89
2	B	24	TYR	CA-C-N	6.78	129.25	120.44
2	B	24	TYR	C-N-CA	6.78	129.25	120.44
3	C	51	VAL	N-CA-C	6.78	117.56	110.72
2	B	287	SER	O-C-N	-6.77	114.98	122.84
2	B	299	ALA	N-CA-CB	6.77	121.93	110.49
3	C	212	ILE	O-C-N	-6.75	115.32	121.87
2	B	234	ILE	CA-C-N	6.74	130.03	120.53
2	B	234	ILE	C-N-CA	6.74	130.03	120.53
2	B	347	CYS	O-C-N	-6.74	115.44	121.17
3	C	31	ASP	CB-CA-C	6.74	119.22	109.11
3	C	319	PHE	O-C-N	-6.74	115.31	123.19
3	C	356	CYS	N-CA-C	6.73	120.13	109.50
2	B	84	ARG	NE-CZ-NH2	-6.72	113.15	119.20
2	B	51	THR	CA-CB-OG1	6.71	119.67	109.60
1	A	3367	LYS	N-CA-C	6.69	118.57	111.28
3	C	426	ASN	O-C-N	-6.67	115.05	122.12
2	B	139	HIS	O-C-N	-6.65	115.49	122.94
3	C	349	ASN	OD1-CG-ND2	-6.65	115.95	122.60
3	C	272	PHE	CA-CB-CG	-6.65	107.15	113.80
3	C	20	PHE	N-CA-C	6.63	118.51	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	255	PHE	CA-C-N	6.62	129.15	120.28
2	B	255	PHE	C-N-CA	6.62	129.15	120.28
3	C	292	THR	OG1-CB-CG2	-6.61	96.09	109.30
3	C	357	ASP	N-CA-C	6.61	119.48	111.82
2	B	337	THR	CA-C-N	6.60	129.02	120.44
2	B	337	THR	C-N-CA	6.60	129.02	120.44
2	B	414	GLU	CA-C-N	6.57	128.98	120.44
2	B	414	GLU	C-N-CA	6.57	128.98	120.44
2	B	418	PHE	CA-CB-CG	-6.57	107.23	113.80
1	A	3372	ASN	CA-C-N	6.56	126.07	119.24
1	A	3372	ASN	C-N-CA	6.56	126.07	119.24
2	B	107	HIS	ND1-CE1-NE2	6.55	114.95	108.40
2	B	130	THR	CA-C-O	6.54	128.34	121.15
3	C	90	ASP	N-CA-C	6.54	120.72	112.87
1	A	3275	SER	CA-C-O	-6.53	113.92	120.90
2	B	308	ARG	NH1-CZ-NH2	-6.52	110.83	119.30
3	C	89	PRO	N-CA-C	6.51	122.31	113.84
3	C	136	GLN	O-C-N	-6.50	115.61	123.29
2	B	406	HIS	CE1-NE2-CD2	-6.50	102.50	109.00
2	B	124	LYS	CA-C-N	6.50	129.52	120.29
2	B	124	LYS	C-N-CA	6.50	129.52	120.29
1	A	3359	ASP	CA-CB-CG	6.50	119.10	112.60
3	C	396	THR	N-CA-C	6.49	118.90	111.11
3	C	27	GLU	CA-C-N	6.49	133.03	122.65
3	C	27	GLU	C-N-CA	6.49	133.03	122.65
2	B	216	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	3291	GLN	OE1-CD-NE2	-6.45	116.15	122.60
2	B	331	ALA	N-CA-C	6.45	119.14	111.33
3	C	432	TYR	N-CA-C	6.45	118.31	111.28
3	C	154	ILE	CA-C-O	-6.45	114.33	121.17
3	C	436	GLN	OE1-CD-NE2	-6.44	116.16	122.60
2	B	6	SER	O-C-N	-6.43	115.79	123.31
1	A	3374	SER	CB-CA-C	-6.42	101.35	111.17
3	C	138	THR	N-CA-CB	6.41	121.11	110.47
3	C	345	GLU	CA-C-N	6.37	128.82	120.28
3	C	345	GLU	C-N-CA	6.37	128.82	120.28
3	C	315	VAL	N-CA-C	6.36	117.04	107.75
3	C	323	MET	N-CA-C	6.35	118.73	109.07
2	B	422	ARG	CA-CB-CG	6.34	126.78	114.10
3	C	106	GLY	O-C-N	-6.32	115.39	122.28
2	B	324	VAL	CA-C-N	6.31	125.72	118.85
2	B	324	VAL	C-N-CA	6.31	125.72	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	175	PRO	O-C-N	6.31	129.86	122.98
2	B	182	VAL	CA-C-N	6.31	127.60	119.78
2	B	182	VAL	C-N-CA	6.31	127.60	119.78
2	B	177	VAL	CA-C-N	6.28	129.75	120.90
2	B	177	VAL	C-N-CA	6.28	129.75	120.90
2	B	301	GLN	OE1-CD-NE2	-6.26	116.34	122.60
2	B	276	ILE	CA-C-N	6.26	128.67	120.28
2	B	276	ILE	C-N-CA	6.26	128.67	120.28
2	B	320	ARG	N-CA-C	6.26	118.37	110.24
3	C	377	PHE	CA-CB-CG	-6.26	107.54	113.80
2	B	306	ASP	O-C-N	-6.25	114.13	121.32
3	C	41	ASP	O-C-N	-6.25	114.90	122.22
2	B	319	TYR	N-CA-C	6.25	119.40	108.52
1	A	3376	ASN	CA-CB-CG	6.23	118.83	112.60
2	B	119	LEU	CA-C-N	6.23	129.25	120.28
2	B	119	LEU	C-N-CA	6.23	129.25	120.28
2	B	153	LEU	O-C-N	6.21	128.71	122.12
2	B	385	ALA	CA-C-N	6.20	129.21	120.28
2	B	385	ALA	C-N-CA	6.20	129.21	120.28
2	B	273	ALA	CA-C-O	-6.20	111.67	120.16
2	B	423	GLU	CA-C-N	6.20	128.49	120.44
2	B	423	GLU	C-N-CA	6.20	128.49	120.44
3	C	399	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	3380	VAL	N-CA-C	6.19	116.35	110.53
2	B	188	ILE	N-CA-C	6.19	116.94	110.62
2	B	224	TYR	CZ-CE2-CD2	6.19	130.74	119.60
2	B	395	PHE	N-CA-C	-6.18	104.63	111.36
2	B	139	HIS	ND1-CE1-NE2	6.17	114.58	108.40
1	A	3271	ASP	N-CA-C	6.17	118.51	111.11
1	A	3416	LYS	CA-C-O	-6.16	114.36	120.82
2	B	215	ARG	NE-CZ-NH2	6.16	124.74	119.20
3	C	311	ARG	CG-CD-NE	-6.15	98.46	112.00
2	B	263	PRO	N-CA-CB	6.14	108.48	103.32
2	B	210	TYR	N-CA-C	6.12	117.95	111.28
1	A	3290	ALA	CB-CA-C	-6.11	99.52	110.70
3	C	200	GLU	CB-CG-CD	-6.11	102.22	112.60
3	C	294	GLN	OE1-CD-NE2	-6.11	116.49	122.60
3	C	49	ILE	CA-CB-CG1	6.10	120.78	110.40
2	B	103	TYR	CA-C-N	6.09	129.57	120.31
2	B	103	TYR	C-N-CA	6.09	129.57	120.31
2	B	112	LYS	O-C-N	-6.08	114.32	122.23
2	B	395	PHE	O-C-N	-6.08	115.22	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	HIS	ND1-CE1-NE2	6.08	114.47	108.40
3	C	347	ILE	O-C-N	-6.08	114.17	121.10
1	A	3388	GLY	CA-C-N	6.07	126.23	119.32
1	A	3388	GLY	C-N-CA	6.07	126.23	119.32
1	A	3405	LYS	O-C-N	-6.06	115.70	122.12
3	C	328	VAL	CB-CA-C	6.06	119.98	112.04
2	B	357	TYR	O-C-N	-6.06	115.09	122.05
3	C	243	ARG	NE-CZ-NH2	-6.05	113.75	119.20
2	B	309	HIS	CE1-NE2-CD2	-6.05	102.95	109.00
3	C	318	VAL	CB-CA-C	-6.04	103.54	110.73
3	C	91	ASN	N-CA-C	6.04	120.67	112.88
2	B	329	ASN	CA-CB-CG	-6.04	106.56	112.60
3	C	419	THR	CA-C-N	6.03	128.36	120.28
3	C	419	THR	C-N-CA	6.03	128.36	120.28
2	B	341	ILE	N-CA-C	6.03	119.31	109.78
2	B	105	ARG	O-C-N	-6.02	115.86	122.07
2	B	384	ILE	CA-C-N	6.02	128.94	120.28
2	B	384	ILE	C-N-CA	6.02	128.94	120.28
3	C	395	PHE	CA-C-O	-6.01	114.18	120.55
2	B	335	ILE	N-CA-C	6.01	116.75	110.62
3	C	337	ASN	O-C-N	-6.01	115.13	122.34
1	A	3424	ASN	N-CA-C	5.99	117.81	111.28
3	C	304	ALA	N-CA-C	5.99	123.55	110.80
1	A	3277	LYS	O-C-N	-5.98	115.78	122.12
1	A	3361	ILE	CA-C-N	5.98	128.22	120.44
1	A	3361	ILE	C-N-CA	5.98	128.22	120.44
2	B	309	HIS	CA-C-O	5.98	129.06	120.51
3	C	4	ILE	N-CA-CB	-5.98	102.31	110.56
2	B	324	VAL	O-C-N	-5.97	114.30	121.10
2	B	61	HIS	N-CA-CB	5.96	120.57	110.49
3	C	280	SER	CA-C-O	-5.96	115.06	121.38
3	C	295	MET	CG-SD-CE	-5.96	87.79	100.90
2	B	422	ARG	N-CA-C	5.96	117.45	111.07
2	B	367	ASP	N-CA-C	-5.96	106.06	113.38
1	A	3402	ASP	N-CA-C	5.95	117.44	111.07
3	C	229	HIS	CA-C-N	5.95	128.18	120.44
3	C	229	HIS	C-N-CA	5.95	128.18	120.44
2	B	194	THR	CB-CA-C	-5.94	100.92	110.79
3	C	433	GLN	CA-C-N	5.94	128.16	120.44
3	C	433	GLN	C-N-CA	5.94	128.16	120.44
2	B	212	ILE	CA-C-O	-5.93	114.88	121.17
2	B	278	ALA	N-CA-C	5.92	117.73	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	386	GLU	CA-C-N	5.92	128.22	120.28
3	C	386	GLU	C-N-CA	5.92	128.22	120.28
3	C	243	ARG	CA-C-O	5.92	125.79	119.34
2	B	194	THR	CA-C-N	5.91	128.51	120.54
2	B	194	THR	C-N-CA	5.91	128.51	120.54
3	C	206	ASN	N-CA-C	5.90	117.39	111.07
2	B	345	ASP	CA-C-N	5.90	128.77	120.28
2	B	345	ASP	C-N-CA	5.90	128.77	120.28
3	C	303	ALA	N-CA-CB	5.90	120.46	110.49
3	C	223	THR	N-CA-C	5.90	118.80	109.96
2	B	178	SER	O-C-N	-5.89	115.78	122.97
3	C	425	MET	CA-C-N	5.88	128.16	120.28
3	C	425	MET	C-N-CA	5.88	128.16	120.28
3	C	93	VAL	O-C-N	-5.88	116.81	123.10
3	C	294	GLN	CG-CD-OE1	5.88	132.55	120.80
3	C	139	HIS	O-C-N	-5.86	115.61	123.23
2	B	406	HIS	ND1-CE1-NE2	5.86	114.25	108.40
1	A	3372	ASN	OD1-CG-ND2	-5.84	116.76	122.60
3	C	191	VAL	CA-CB-CG1	5.84	120.33	110.40
2	B	46	ASP	CA-CB-CG	5.83	118.43	112.60
2	B	415	GLU	N-CA-C	5.82	117.30	111.07
3	C	80	SER	CA-C-O	5.82	126.59	120.42
2	B	248	LEU	CA-C-N	5.82	130.42	122.34
2	B	248	LEU	C-N-CA	5.82	130.42	122.34
3	C	430	SER	CA-C-N	5.81	128.38	120.54
3	C	430	SER	C-N-CA	5.81	128.38	120.54
3	C	401	ARG	CA-C-N	5.81	132.63	121.54
3	C	401	ARG	C-N-CA	5.81	132.63	121.54
3	C	9	ALA	N-CA-CB	-5.80	101.66	110.77
3	C	360	PRO	N-CA-C	5.80	119.78	111.13
2	B	55	GLU	CA-C-N	5.80	129.72	121.42
2	B	55	GLU	C-N-CA	5.80	129.72	121.42
1	A	3278	GLU	CA-C-O	5.79	126.69	120.55
3	C	210	TYR	CB-CG-CD1	5.79	129.49	120.80
2	B	175	PRO	CA-C-N	5.79	132.59	121.54
2	B	175	PRO	C-N-CA	5.79	132.59	121.54
2	B	120	ASP	O-C-N	-5.79	115.45	122.22
3	C	391	ILE	O-C-N	-5.78	116.26	121.87
2	B	251	ASP	CA-C-N	5.78	127.95	120.44
2	B	251	ASP	C-N-CA	5.78	127.95	120.44
3	C	278	ARG	O-C-N	-5.78	116.57	123.27
2	B	286	LEU	CA-C-O	5.78	128.77	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	ALA	N-CA-C	5.77	123.09	110.80
2	B	113	GLU	N-CA-C	5.75	117.23	111.07
1	A	3313	ALA	N-CA-C	5.75	118.33	111.71
2	B	158	SER	N-CA-C	5.74	117.34	111.14
1	A	3421	ALA	N-CA-C	5.73	117.61	111.36
3	C	149	MET	CA-C-N	5.73	126.19	119.94
3	C	149	MET	C-N-CA	5.73	126.19	119.94
3	C	289	PRO	CA-C-N	5.73	127.96	120.28
3	C	289	PRO	C-N-CA	5.73	127.96	120.28
3	C	390	ARG	CB-CG-CD	5.73	124.48	111.30
3	C	47	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	3332	ASP	CA-C-N	5.72	128.22	120.38
1	A	3332	ASP	C-N-CA	5.72	128.22	120.38
3	C	175	PRO	CA-C-O	-5.72	115.26	121.27
2	B	182	VAL	O-C-N	-5.72	115.78	122.07
1	A	3331	THR	CA-C-O	5.71	126.03	119.35
3	C	424	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	3300	GLN	CB-CG-CD	-5.69	102.93	112.60
3	C	149	MET	CA-C-O	5.69	126.58	120.55
1	A	3426	GLN	O-C-N	-5.68	114.81	122.43
1	A	3288	ILE	CA-C-N	5.67	127.88	120.28
1	A	3288	ILE	C-N-CA	5.67	127.88	120.28
3	C	154	ILE	N-CA-C	-5.67	104.98	110.42
2	B	341	ILE	CA-C-N	5.66	130.81	123.00
2	B	341	ILE	C-N-CA	5.66	130.81	123.00
3	C	288	VAL	CA-C-O	5.66	123.66	118.85
2	B	13	GLY	O-C-N	-5.66	116.70	122.19
3	C	14	ASN	CA-CB-CG	-5.66	106.94	112.60
3	C	302	MET	CA-CB-CG	5.65	125.41	114.10
1	A	3405	LYS	CA-C-N	5.65	128.90	120.31
1	A	3405	LYS	C-N-CA	5.65	128.90	120.31
3	C	318	VAL	CA-CB-CG2	-5.65	100.79	110.40
2	B	414	GLU	CA-C-O	5.64	127.40	121.19
3	C	50	ASN	O-C-N	-5.64	115.09	122.59
3	C	90	ASP	CA-CB-CG	-5.64	106.96	112.60
3	C	25	SER	N-CA-C	5.64	117.10	111.07
1	A	3317	LEU	N-CA-C	5.63	117.42	111.28
1	A	3309	ALA	CA-C-O	5.62	126.48	120.70
3	C	211	ASP	CA-C-O	5.61	126.89	121.00
2	B	37	PRO	O-C-N	-5.61	115.07	122.64
3	C	62	VAL	CA-C-N	5.61	125.89	119.83
3	C	62	VAL	C-N-CA	5.61	125.89	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	139	HIS	CG-CD2-NE2	5.60	112.80	107.20
2	B	133	GLN	O-C-N	-5.59	116.09	122.08
2	B	191	THR	CA-C-N	5.59	128.05	120.44
2	B	191	THR	C-N-CA	5.59	128.05	120.44
3	C	69	ASP	N-CA-C	-5.59	101.40	108.45
3	C	292	THR	CA-C-N	5.59	128.09	120.54
3	C	292	THR	C-N-CA	5.59	128.09	120.54
2	B	155	GLU	CB-CG-CD	-5.58	103.12	112.60
2	B	157	LEU	N-CA-CB	5.57	118.24	109.94
3	C	406	HIS	ND1-CG-CD2	5.56	111.66	106.10
3	C	25	SER	CB-CA-C	-5.55	102.17	110.88
1	A	3265	GLN	N-CA-C	5.55	117.41	111.36
2	B	130	THR	CA-C-N	5.54	131.02	122.20
2	B	130	THR	C-N-CA	5.54	131.02	122.20
2	B	21	TRP	CG-CD2-CE3	-5.53	128.37	133.90
3	C	133	GLN	N-CA-C	-5.53	106.20	113.17
3	C	307	PRO	CA-C-N	5.53	128.72	120.31
3	C	307	PRO	C-N-CA	5.53	128.72	120.31
3	C	136	GLN	N-CA-CB	-5.53	101.90	110.57
3	C	22	GLU	O-C-N	-5.52	115.48	122.27
2	B	110	ILE	CA-C-N	5.52	126.07	120.00
2	B	110	ILE	C-N-CA	5.52	126.07	120.00
3	C	6	HIS	CA-CB-CG	5.52	119.32	113.80
2	B	235	VAL	CA-C-N	5.51	127.93	120.44
2	B	235	VAL	C-N-CA	5.51	127.93	120.44
2	B	23	LEU	CB-CA-C	5.50	120.21	110.85
3	C	428	LEU	N-CA-C	5.50	117.28	111.28
1	A	3269	ILE	CA-C-N	5.50	128.44	120.79
1	A	3269	ILE	C-N-CA	5.50	128.44	120.79
2	B	153	LEU	CA-C-O	-5.50	114.72	120.55
3	C	76	ASP	O-C-N	-5.50	116.29	122.12
3	C	185	TYR	CB-CG-CD1	-5.50	112.55	120.80
3	C	146	GLY	O-C-N	-5.50	115.78	122.71
2	B	437	VAL	N-CA-C	-5.50	107.39	112.83
2	B	405	VAL	CA-C-N	5.47	129.03	120.82
2	B	405	VAL	C-N-CA	5.47	129.03	120.82
3	C	350	ASN	N-CA-CB	-5.46	101.26	110.49
3	C	406	HIS	CA-CB-CG	5.45	119.25	113.80
2	B	307	PRO	N-CA-C	5.45	121.87	113.75
2	B	379	SER	N-CA-CB	5.44	119.09	110.55
2	B	134	GLY	O-C-N	-5.44	117.37	123.62
2	B	418	PHE	O-C-N	-5.44	116.44	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	GLY	CA-C-O	5.43	126.48	121.76
3	C	227	LEU	CA-C-O	-5.42	114.67	120.42
2	B	18	ASN	O-C-N	-5.42	115.98	122.15
2	B	352	LYS	N-CA-C	5.41	116.94	109.15
2	B	390	ARG	N-CA-C	5.41	117.17	111.28
3	C	189	LEU	CA-C-O	-5.41	115.14	120.82
2	B	398	MET	CA-C-N	5.40	127.52	120.28
2	B	398	MET	C-N-CA	5.40	127.52	120.28
2	B	400	ALA	N-CA-C	5.40	116.85	111.07
2	B	431	ASP	N-CA-C	5.40	117.17	111.28
1	A	3418	GLU	CA-C-N	5.40	127.45	120.44
1	A	3418	GLU	C-N-CA	5.40	127.45	120.44
2	B	243	ARG	N-CA-C	5.40	117.24	111.36
3	C	53	TYR	O-C-N	5.40	129.76	122.96
2	B	73	THR	N-CA-CB	5.39	118.57	109.78
2	B	309	HIS	ND1-CE1-NE2	5.39	113.79	108.40
2	B	357	TYR	CA-C-O	5.39	124.74	119.08
2	B	43	GLY	O-C-N	-5.38	115.71	122.70
2	B	245	ASP	CA-CB-CG	-5.38	107.22	112.60
3	C	55	GLU	CA-C-O	5.38	126.51	120.70
3	C	387	LEU	O-C-N	-5.38	116.42	122.12
1	A	3272	LYS	N-CA-C	5.37	117.14	111.28
2	B	92	LEU	O-C-N	-5.37	115.37	122.57
3	C	325	MET	CA-C-N	5.37	127.42	120.44
3	C	325	MET	C-N-CA	5.37	127.42	120.44
2	B	17	GLY	CA-C-N	5.35	127.89	120.29
2	B	17	GLY	C-N-CA	5.35	127.89	120.29
2	B	358	GLU	CA-C-N	5.35	125.89	120.38
2	B	358	GLU	C-N-CA	5.35	125.89	120.38
2	B	88	HIS	CA-C-N	5.35	125.42	119.32
2	B	88	HIS	C-N-CA	5.35	125.42	119.32
2	B	244	PHE	CA-CB-CG	5.34	119.14	113.80
3	C	30	ILE	O-C-N	-5.34	117.10	123.03
1	A	3336	ILE	N-CA-C	5.34	117.76	111.09
3	C	113	GLU	CA-C-N	5.34	127.38	120.44
3	C	113	GLU	C-N-CA	5.34	127.38	120.44
3	C	238	VAL	CB-CA-C	-5.34	104.98	111.87
2	B	351	PHE	CA-CB-CG	-5.34	108.46	113.80
2	B	85	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	A	3401	ALA	O-C-N	-5.33	116.58	122.07
2	B	386	GLU	N-CA-C	5.33	117.84	111.71
3	C	24	ILE	CA-C-N	5.33	127.37	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	24	ILE	C-N-CA	5.33	127.37	120.44
2	B	52	PHE	CA-CB-CG	5.33	119.13	113.80
2	B	408	TYR	CA-CB-CG	-5.33	104.31	113.90
1	A	3413	GLU	N-CA-C	5.32	117.98	111.82
3	C	192	HIS	N-CA-C	5.32	117.07	111.28
1	A	3385	LEU	N-CA-CB	-5.31	101.57	110.39
2	B	16	ILE	CA-C-N	5.31	125.88	119.98
2	B	16	ILE	C-N-CA	5.31	125.88	119.98
2	B	243	ARG	NE-CZ-NH1	5.31	126.81	121.50
2	B	218	ASP	CA-CB-CG	5.30	117.91	112.60
1	A	3381	ASN	CA-C-N	5.30	127.39	120.28
1	A	3381	ASN	C-N-CA	5.30	127.39	120.28
2	B	25	CYS	CA-C-N	5.30	127.33	120.44
2	B	25	CYS	C-N-CA	5.30	127.33	120.44
2	B	416	GLY	CA-C-N	5.30	127.69	120.54
2	B	416	GLY	C-N-CA	5.30	127.69	120.54
2	B	75	ILE	CB-CA-C	-5.30	104.91	112.22
3	C	161	TYR	CB-CA-C	-5.29	102.88	111.14
1	A	3376	ASN	CA-C-O	-5.29	115.37	121.19
3	C	116	ASP	CA-C-O	5.29	126.37	120.82
2	B	218	ASP	O-C-N	-5.28	116.36	122.86
2	B	393	HIS	CB-CG-CD2	-5.28	124.33	131.20
3	C	390	ARG	CA-C-O	-5.28	114.95	120.55
2	B	291	ILE	N-CA-CB	5.28	117.72	110.54
2	B	170	SER	O-C-N	-5.28	116.37	123.23
3	C	190	SER	N-CA-C	5.28	116.72	111.07
3	C	287	THR	CA-CB-OG1	5.27	117.50	109.60
3	C	194	LEU	CD1-CG-CD2	-5.26	99.22	110.80
2	B	192	HIS	CA-CB-CG	5.26	119.06	113.80
2	B	34	GLY	O-C-N	-5.25	114.72	122.70
2	B	244	PHE	CB-CA-C	-5.25	99.97	110.42
2	B	338	LYS	O-C-N	5.25	127.48	122.07
2	B	220	GLU	N-CA-CB	5.25	117.68	110.07
3	C	141	LEU	O-C-N	-5.25	115.78	122.34
1	A	3407	VAL	CA-C-O	5.25	125.55	119.36
2	B	165	SER	CA-C-O	5.25	127.04	121.16
2	B	284	GLU	O-C-N	-5.24	115.62	122.59
1	A	3420	ASP	CB-CA-C	5.24	119.49	110.79
3	C	348	PRO	N-CA-CB	-5.24	98.46	103.33
2	B	19	ALA	CA-C-N	5.24	127.30	120.28
2	B	19	ALA	C-N-CA	5.24	127.30	120.28
2	B	436	GLY	O-C-N	-5.24	116.77	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	VAL	CA-C-N	5.23	130.26	122.99
2	B	275	VAL	C-N-CA	5.23	130.26	122.99
1	A	3297	ILE	N-CA-C	5.23	115.84	109.30
1	A	3349	ILE	CA-C-N	5.23	127.62	120.46
1	A	3349	ILE	C-N-CA	5.23	127.62	120.46
3	C	185	TYR	N-CA-C	5.23	116.98	111.28
2	B	99	ALA	O-C-N	-5.22	115.64	122.59
3	C	41	ASP	CA-CB-CG	-5.22	107.38	112.60
2	B	40	LYS	CA-C-N	5.22	131.51	121.54
2	B	40	LYS	C-N-CA	5.22	131.51	121.54
3	C	42	LEU	CA-C-O	5.22	125.59	119.28
3	C	313	LEU	CA-C-N	5.21	128.11	120.71
3	C	313	LEU	C-N-CA	5.21	128.11	120.71
3	C	369	ARG	N-CA-CB	5.21	119.30	110.49
3	C	281	GLN	N-CA-CB	5.21	119.29	110.49
2	B	256	GLN	N-CA-CB	5.20	117.76	110.12
3	C	301	MET	CA-C-O	-5.20	115.67	121.81
2	B	102	ASN	O-C-N	5.20	129.62	123.33
2	B	163	LYS	CA-C-N	5.20	128.09	120.71
2	B	163	LYS	C-N-CA	5.20	128.09	120.71
2	B	51	THR	N-CA-CB	5.19	117.60	109.97
2	B	269	LEU	CA-C-N	5.19	128.84	121.42
2	B	269	LEU	C-N-CA	5.19	128.84	121.42
3	C	222	PRO	N-CA-CB	5.19	108.70	103.25
3	C	74	THR	CA-C-O	-5.19	114.92	120.42
2	B	296	PHE	CA-C-N	5.18	127.59	120.39
2	B	296	PHE	C-N-CA	5.18	127.59	120.39
2	B	387	ALA	CA-C-O	5.18	126.09	120.55
2	B	256	GLN	OE1-CD-NE2	5.18	127.78	122.60
2	B	191	THR	CA-C-O	5.17	126.03	120.55
3	C	281	GLN	O-C-N	-5.17	115.71	122.59
1	A	3341	MET	N-CA-CB	-5.17	103.01	110.56
2	B	285	GLN	N-CA-C	5.17	116.72	111.14
3	C	151	THR	CA-C-N	5.17	127.51	120.54
3	C	151	THR	C-N-CA	5.17	127.51	120.54
3	C	210	TYR	N-CA-CB	5.16	117.71	110.12
3	C	230	LEU	CD1-CG-CD2	-5.16	99.45	110.80
2	B	223	THR	CA-C-O	-5.16	115.74	121.51
2	B	62	VAL	O-C-N	-5.15	117.09	121.57
2	B	143	GLY	O-C-N	-5.15	117.47	122.77
3	C	359	PRO	N-CD-CG	5.15	110.93	103.20
1	A	3271	ASP	CA-CB-CG	-5.15	107.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
1	A	3420	ASP	N-CA-CB	-5.13	102.57	110.12
2	B	393	HIS	ND1-CG-CD2	5.13	111.23	106.10
3	C	2	ARG	NE-CZ-NH2	-5.13	114.59	119.20
2	B	125	LEU	N-CA-C	-5.12	105.78	111.36
1	A	3296	SER	N-CA-CB	5.12	117.62	110.56
2	B	53	PHE	CA-C-N	5.12	132.54	122.61
2	B	53	PHE	C-N-CA	5.12	132.54	122.61
3	C	191	VAL	O-C-N	-5.12	116.91	121.87
3	C	405	LEU	CA-C-N	5.11	127.12	120.28
3	C	405	LEU	C-N-CA	5.11	127.12	120.28
1	A	3307	SER	CA-CB-OG	-5.11	100.89	111.10
2	B	13	GLY	N-CA-C	-5.11	106.23	112.77
2	B	18	ASN	N-CA-CB	-5.10	102.61	110.16
1	A	3321	SER	N-CA-C	5.10	117.23	111.11
2	B	243	ARG	CD-NE-CZ	-5.10	117.26	124.40
2	B	309	HIS	O-C-N	-5.10	115.81	122.59
3	C	96	GLN	N-CA-CB	5.10	119.11	110.49
3	C	373	MET	CG-SD-CE	-5.10	89.67	100.90
3	C	228	ASN	N-CA-CB	-5.10	102.37	110.22
1	A	3398	LEU	N-CA-C	-5.09	105.81	111.36
3	C	58	GLY	CA-C-N	5.09	131.25	121.54
3	C	58	GLY	C-N-CA	5.09	131.25	121.54
3	C	286	LEU	O-C-N	-5.08	115.83	122.59
2	B	409	VAL	CA-CB-CG2	-5.08	101.76	110.40
1	A	3414	LEU	CA-C-N	-5.08	112.24	120.72
1	A	3414	LEU	C-N-CA	-5.08	112.24	120.72
3	C	268	PHE	CB-CG-CD2	5.08	129.33	120.70
1	A	3417	LEU	CD1-CG-CD2	-5.07	99.64	110.80
3	C	373	MET	CA-C-O	5.07	126.77	120.54
2	B	163	LYS	O-C-N	-5.07	116.37	122.15
1	A	3285	PRO	CA-C-N	5.07	127.33	120.44
1	A	3285	PRO	C-N-CA	5.07	127.33	120.44
2	B	296	PHE	CA-CB-CG	5.06	118.86	113.80
2	B	214	ARG	N-CA-C	5.06	116.61	111.14
3	C	129	CYS	N-CA-CB	5.06	119.02	110.46
3	C	350	ASN	O-C-N	-5.06	115.86	122.59
2	B	8	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
3	C	223	THR	CA-CB-OG1	5.06	117.19	109.60
2	B	200	CYS	N-CA-C	5.06	116.55	107.80
2	B	71	GLU	CA-C-O	5.05	126.42	120.41
1	A	3333	TRP	CA-C-N	5.05	127.46	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3333	TRP	C-N-CA	5.05	127.46	120.29
3	C	106	GLY	CA-C-O	5.05	125.86	120.30
2	B	107	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
2	B	229	ARG	NE-CZ-NH1	-5.05	116.45	121.50
3	C	225	GLY	CA-C-O	5.05	126.55	120.90
3	C	123	ARG	N-CA-C	5.04	117.44	111.33
2	B	21	TRP	CE2-CD2-CE3	5.04	123.84	118.80
2	B	105	ARG	CG-CD-NE	-5.04	100.91	112.00
2	B	232	GLY	CA-C-O	5.04	125.94	120.75
3	C	3	GLU	N-CA-C	5.04	118.20	111.24
3	C	108	TYR	O-C-N	-5.04	116.17	120.71
3	C	151	THR	N-CA-CB	5.04	117.53	110.12
2	B	91	GLN	CG-CD-OE1	5.03	130.86	120.80
3	C	152	LEU	O-C-N	5.03	127.32	122.09
3	C	350	ASN	OD1-CG-ND2	-5.03	117.58	122.60
1	A	3381	ASN	N-CA-C	5.02	117.64	111.82
2	B	296	PHE	N-CA-C	-5.02	106.40	112.88
3	C	123	ARG	CA-C-O	-5.02	115.21	120.63
1	A	3266	GLN	CA-C-O	5.01	125.57	119.05
2	B	60	LYS	N-CA-CB	-5.01	104.27	111.54
2	B	33	ASP	CA-CB-CG	5.01	117.61	112.60
2	B	51	THR	CA-C-N	5.01	130.72	121.70
2	B	51	THR	C-N-CA	5.01	130.72	121.70
1	A	3330	THR	O-C-N	-5.00	117.61	123.27
2	B	2	ARG	O-C-N	-5.00	114.99	123.00
2	B	364	PRO	N-CA-C	5.00	122.78	112.47
3	C	215	ARG	N-CA-CB	-5.00	102.33	110.14
3	C	276	THR	N-CA-C	-5.00	107.34	113.50

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3342	ARG	Sidechain
1	A	3362	ARG	Sidechain
1	A	3369	TYR	Sidechain
1	A	3400	TYR	Sidechain
1	A	3406	ARG	Sidechain
1	A	3411	ARG	Sidechain
2	B	103	TYR	Sidechain
2	B	105	ARG	Sidechain
2	B	161	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	210	TYR	Sidechain
2	B	214	ARG	Sidechain
2	B	221	ARG	Sidechain
2	B	224	TYR	Sidechain
2	B	24	TYR	Sidechain
2	B	243	ARG	Sidechain
2	B	272	TYR	Sidechain
2	B	28	HIS	Sidechain
2	B	308	ARG	Sidechain
2	B	343	PHE	Sidechain
2	B	373	ARG	Sidechain
2	B	390	ARG	Sidechain
2	B	432	TYR	Sidechain
2	B	64	ARG	Sidechain
2	B	79	ARG	Sidechain
2	B	83	TYR	Sidechain
2	B	98	ASP	Peptide
3	C	123	ARG	Sidechain
3	C	158	ARG	Sidechain
3	C	161	TYR	Sidechain
3	C	185	TYR	Sidechain
3	C	263	PRO	Peptide
3	C	267	PHE	Sidechain
3	C	273	ALA	Peptide
3	C	283	TYR	Sidechain
3	C	36	TYR	Sidechain
3	C	369	ARG	Sidechain
3	C	37	HIS	Sidechain
3	C	400	ARG	Sidechain
3	C	432	TYR	Sidechain
3	C	435	TYR	Sidechain
3	C	52	TYR	Sidechain
3	C	53	TYR	Sidechain
3	C	79	ARG	Sidechain
3	C	88	ARG	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	1306	0	1342	2	0
2	B	3423	0	3324	12	0
3	C	3360	0	3241	11	0
All	All	8089	0	7907	24	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 (24) 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)
2:B:5:ILE:HG12	2:B:125:LEU:HD21	1.83	0.59
3:C:313:LEU:HG	3:C:314:THR:H	1.69	0.57
2:B:5:ILE:CG1	2:B:125:LEU:HD21	2.35	0.57
3:C:273:ALA:HB3	3:C:274:PRO:HD3	1.87	0.55
2:B:61:HIS:HB3	2:B:85:GLN:O	2.07	0.54
2:B:21:TRP:CD1	2:B:25:CYS:HG	2.28	0.52
3:C:107:HIS:CE1	3:C:193:GLN:OE1	2.64	0.51
3:C:230:LEU:HD23	3:C:230:LEU:C	2.40	0.47
2:B:259:LEU:O	2:B:266:HIS:CD2	2.68	0.47
3:C:26:ASP:CG	3:C:369:ARG:HH21	2.24	0.46
2:B:5:ILE:HG12	2:B:125:LEU:CD2	2.46	0.45
2:B:61:HIS:CB	2:B:85:GLN:O	2.66	0.44
2:B:139:HIS:HA	2:B:140:SER:HB3	2.01	0.43
2:B:220:GLU:H	2:B:220:GLU:CD	2.25	0.43
2:B:42:ILE:HG22	2:B:46:ASP:HA	2.01	0.43
1:A:3302:LEU:HD22	1:A:3340:ILE:HB	2.01	0.43
3:C:27:GLU:OE2	3:C:369:ARG:HB2	2.19	0.41
2:B:242:LEU:C	2:B:242:LEU:HD12	2.45	0.41
3:C:115:VAL:HG23	3:C:153:LEU:HD12	2.02	0.41
3:C:413:MET:HG2	3:C:418:PHE:CZ	2.56	0.41
1:A:3413:GLU:O	1:A:3417:LEU:HB2	2.20	0.40
3:C:47:GLU:O	3:C:48:ARG:HB2	2.21	0.40
3:C:174:SER:HA	3:C:175:PRO:HD3	1.95	0.40
2:B:222:PRO:HB2	3:C:326:LYS:HB2	2.04	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	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	21	59
2	B	437/451 (97%)	379 (87%)	43 (10%)	15 (3%)	3	21
3	C	425/427 (100%)	378 (89%)	33 (8%)	14 (3%)	3	21
All	All	1024/1042 (98%)	913 (89%)	81 (8%)	30 (3%)	5	23

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	252	LEU
3	C	273	ALA
3	C	349	ASN
3	C	369	ARG
2	B	2	ARG
2	B	61	HIS
2	B	244	PHE
3	C	59	ASN
3	C	303	ALA
3	C	304	ALA
1	A	3327	GLY
2	B	37	PRO
2	B	44	GLY
2	B	99	ALA
2	B	140	SER
2	B	264	ARG
2	B	274	PRO
2	B	364	PRO
3	C	313	LEU
3	C	402	LYS
2	B	41	THR
3	C	176	LYS
2	B	59	GLY
2	B	306	ASP

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Mol	Chain	Res	Type
3	C	311	ARG
2	B	286	LEU
2	B	43	GLY
3	C	66	ILE
3	C	38	GLY
3	C	222	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/146 (100%)	144 (99%)	2 (1%)	59	72
2	B	368/377 (98%)	358 (97%)	10 (3%)	39	61
3	C	368/368 (100%)	358 (97%)	10 (3%)	39	61
All	All	882/891 (99%)	860 (98%)	22 (2%)	42	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3268	VAL
1	A	3278	GLU
2	B	3	GLU
2	B	11	GLN
2	B	188	ILE
2	B	190	THR
2	B	220	GLU
2	B	223	THR
2	B	306	ASP
2	B	323	VAL
2	B	367	ASP
2	B	373	ARG
3	C	62	VAL
3	C	86	ILE
3	C	91	ASN
3	C	149	MET

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Mol	Chain	Res	Type
3	C	175	PRO
3	C	260	VAL
3	C	275	LEU
3	C	313	LEU
3	C	350	ASN
3	C	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3300	GLN
1	A	3335	GLN
1	A	3376	ASN
2	B	216	ASN
2	B	266	HIS
2	B	283	HIS
2	B	309	HIS
3	C	37	HIS
3	C	59	ASN
3	C	107	HIS
3	C	192	HIS
3	C	193	GLN
3	C	249	ASN
3	C	309	HIS
3	C	349	ASN
3	C	394	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 [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-5439. These allow visual inspection of the internal detail of the map and identification of artifacts.

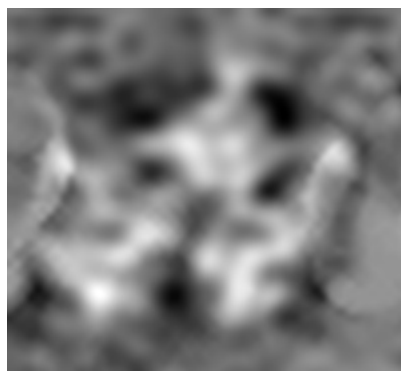
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 27



Y Index: 19



Z Index: 30

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: 32



Y Index: 20

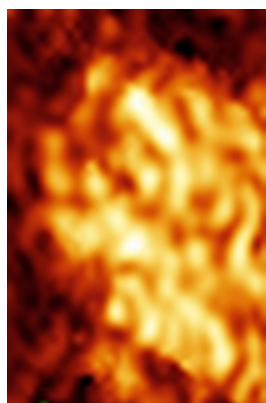


Z Index: 23

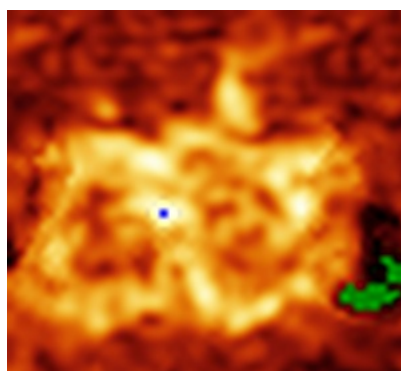
The images above show the largest variance slices of the map in three orthogonal directions.

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

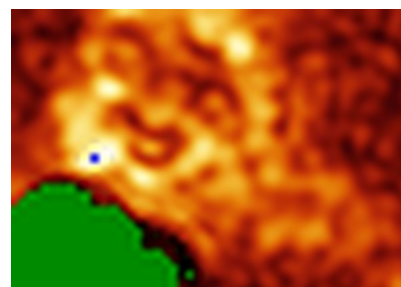
6.4.1 Primary map



X



Y

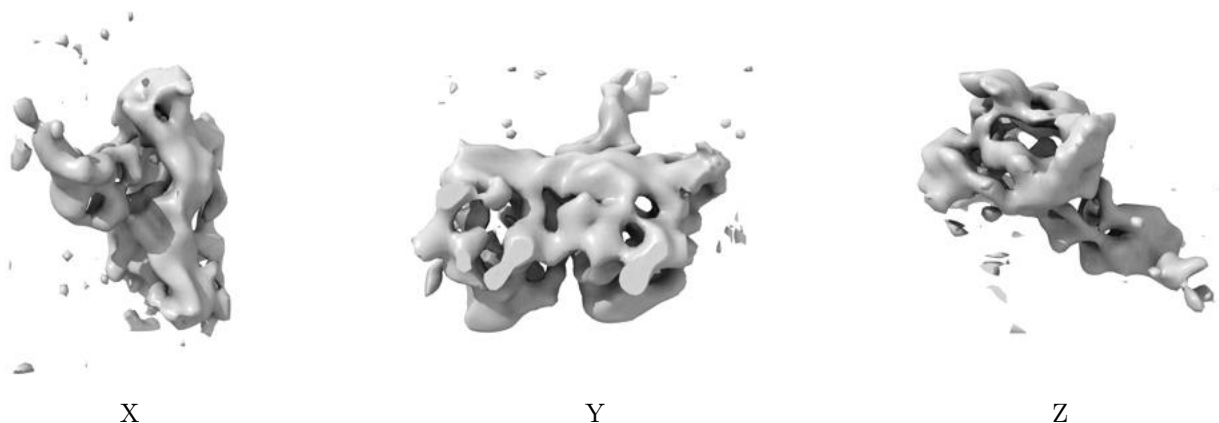


Z

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 0.0036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

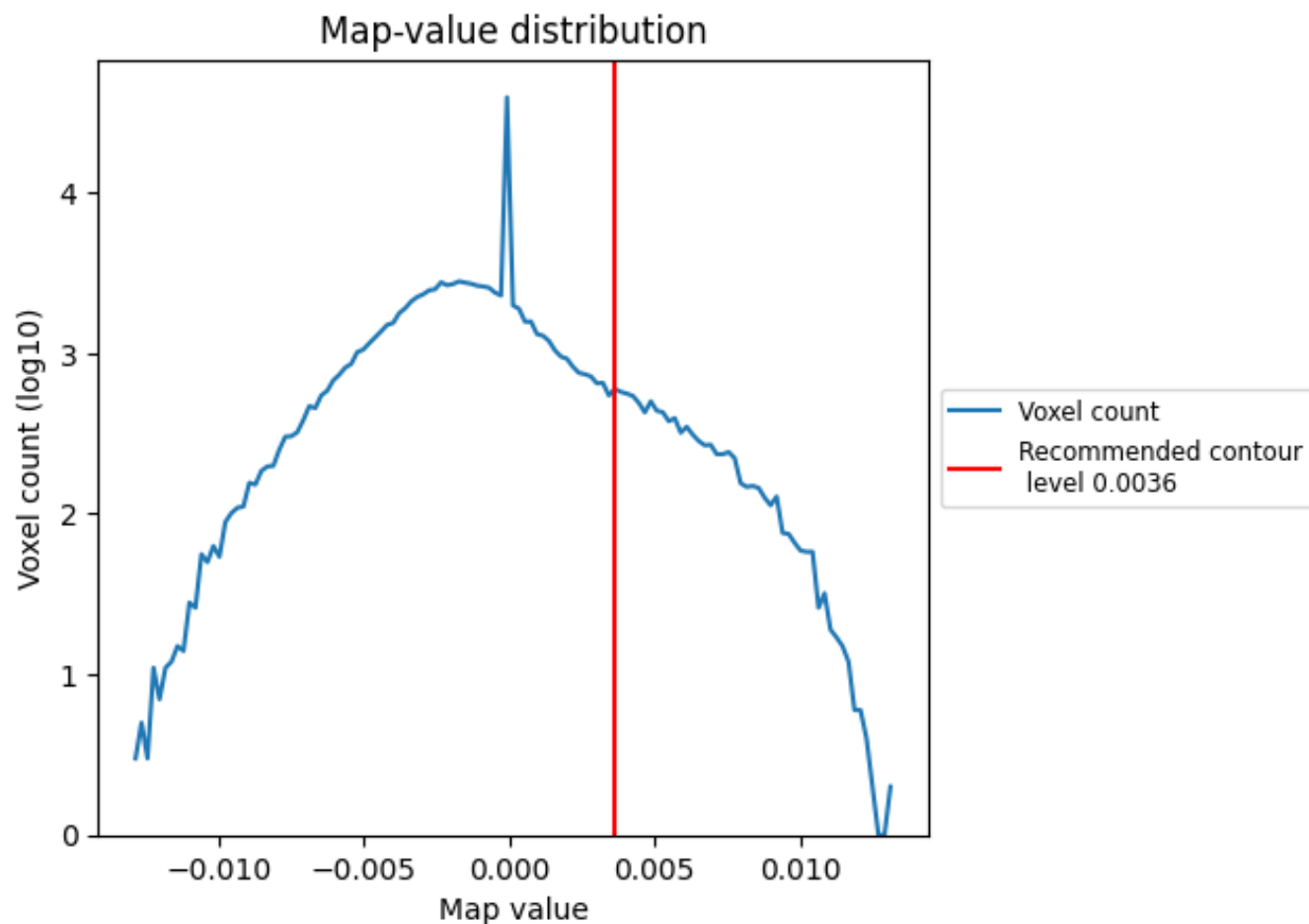
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

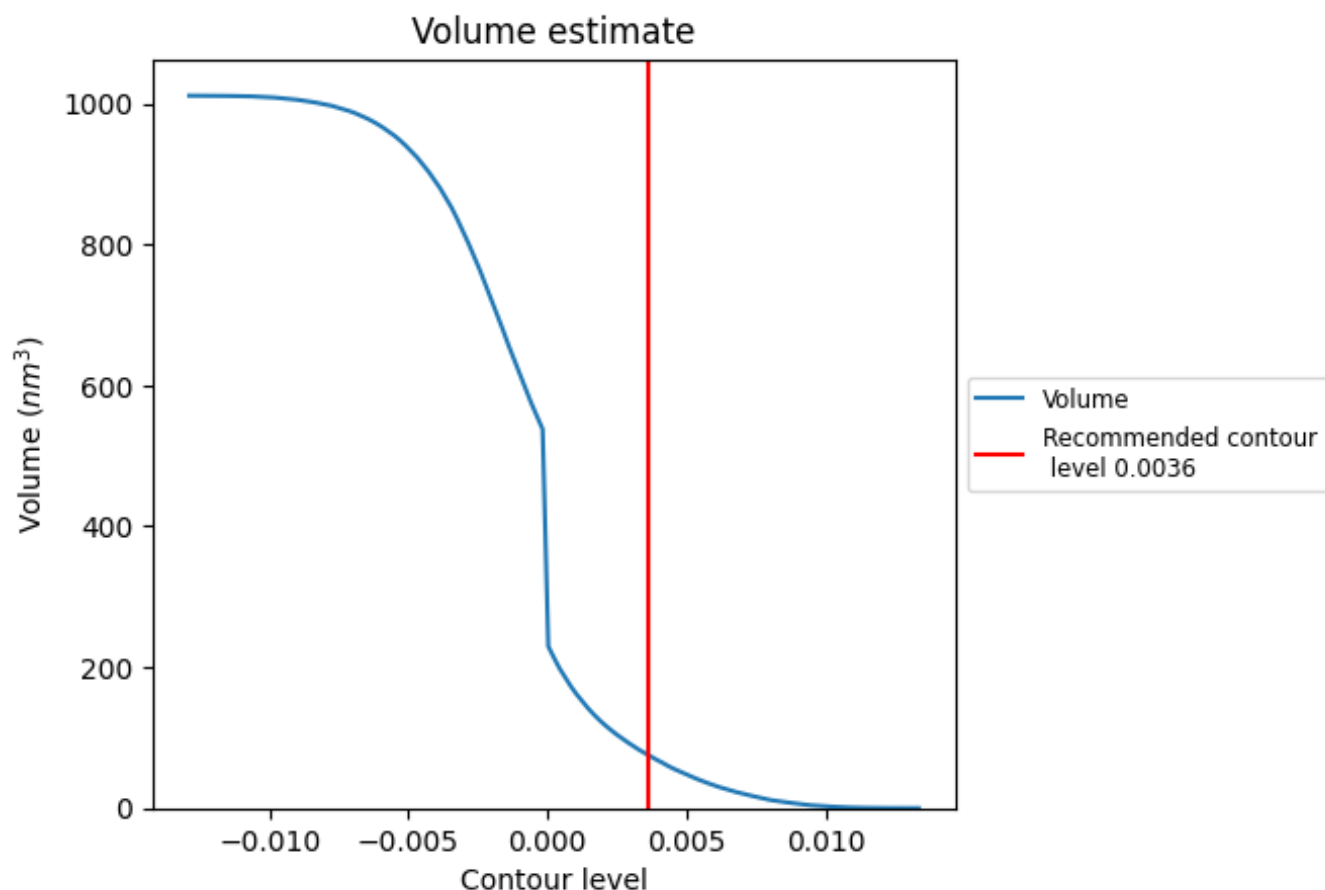
This section contains the results of statistical analysis of the map.

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 76 nm³; this corresponds to an approximate mass of 68 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

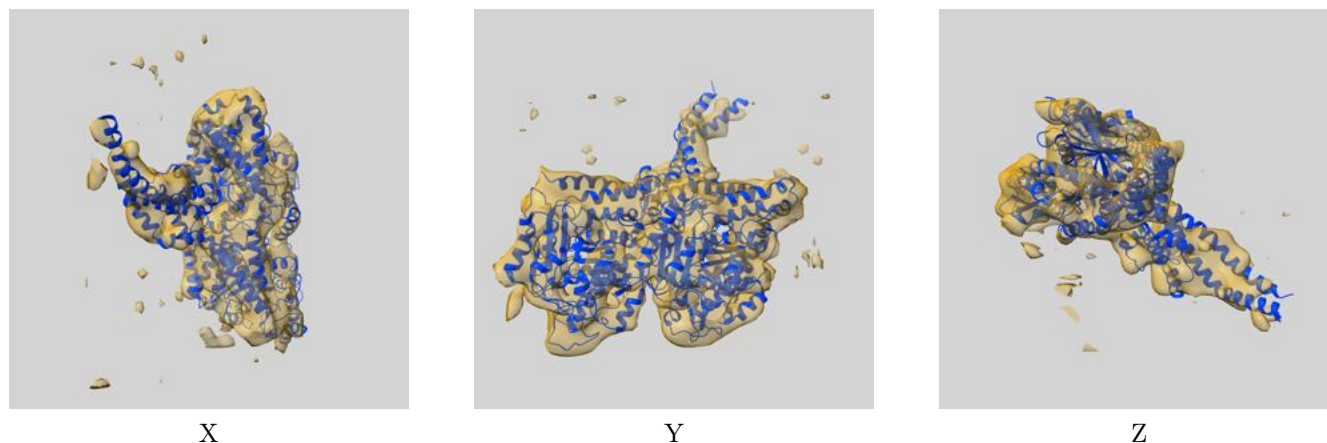
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

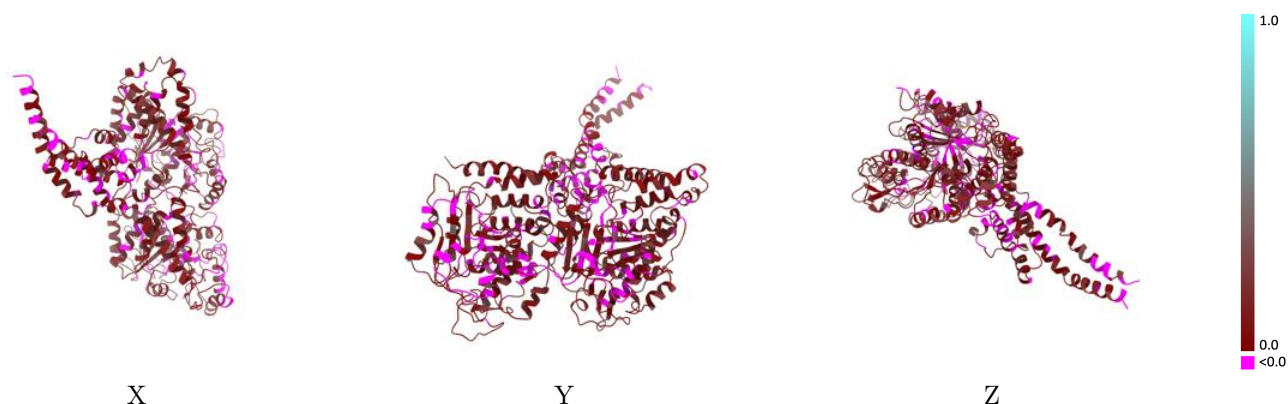
This section contains information regarding the fit between EMDB map EMD-5439 and PDB model 3J1U. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



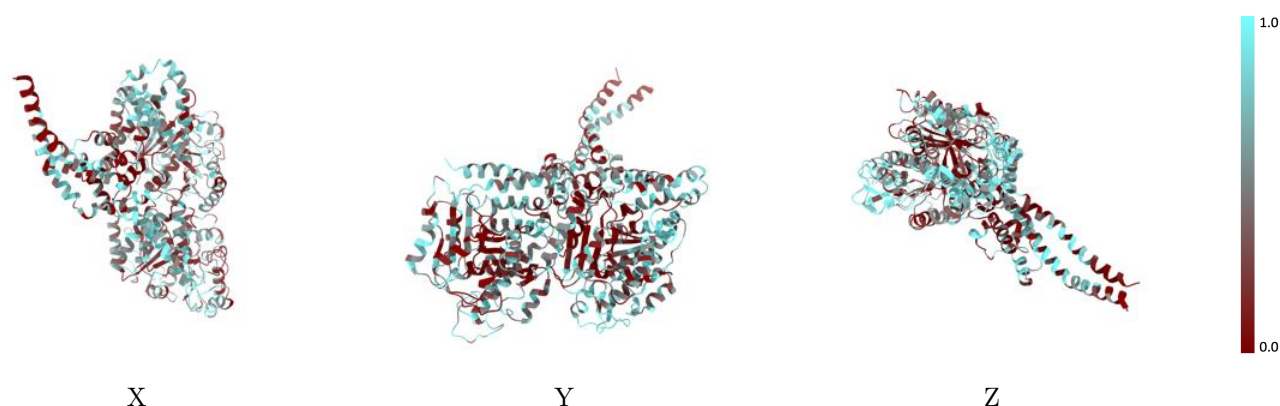
The images above show the 3D surface view of the map at the recommended contour level 0.0036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



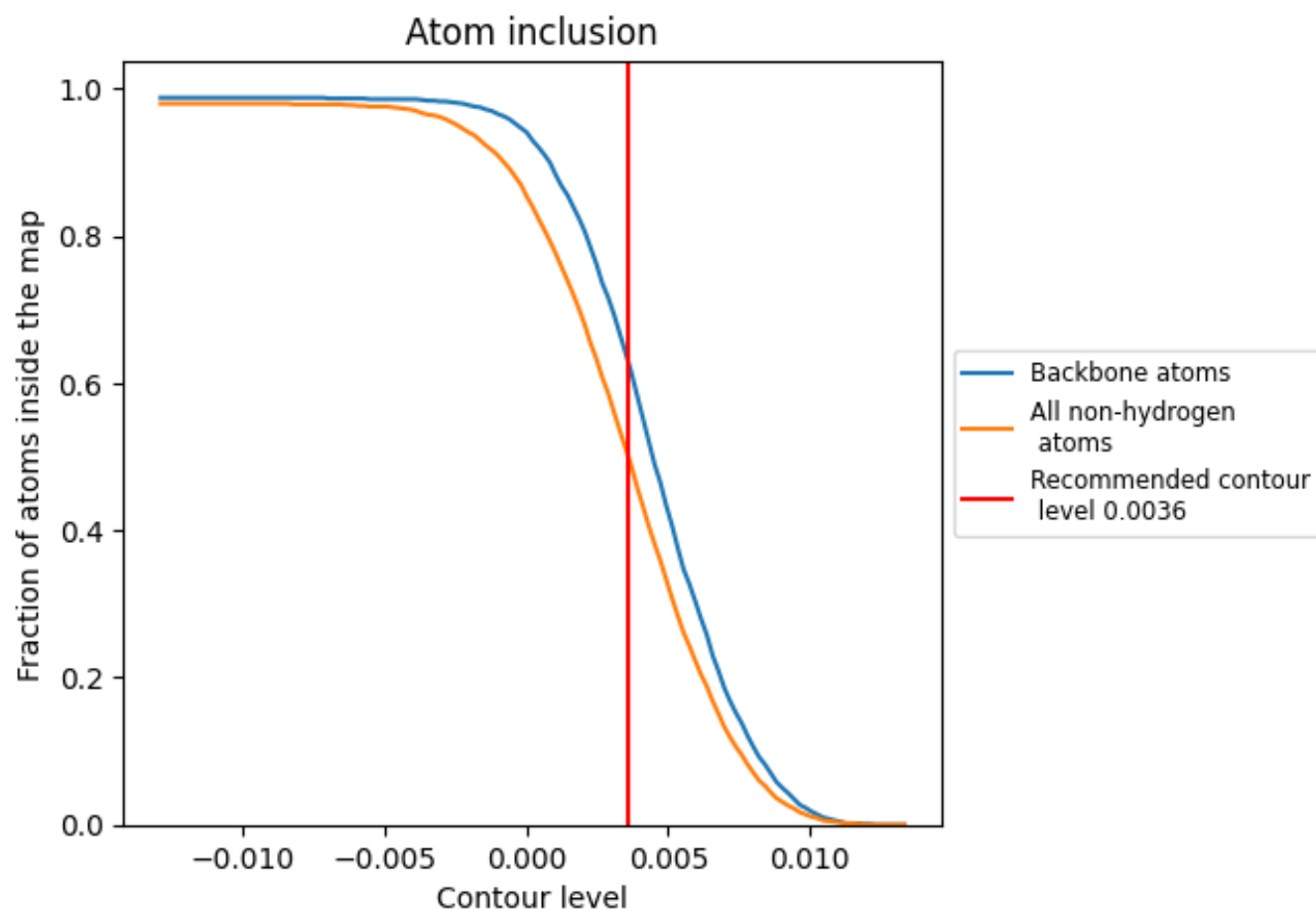
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 50% 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 (0.0036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5000	0.0940
A	0.3960	0.0560
B	0.5130	0.1010
C	0.5260	0.1030

