



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:44 AM UTC

PDB ID : 3J1T / pdb_00003j1t
EMDB ID : EMD-5439
Title : High 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:

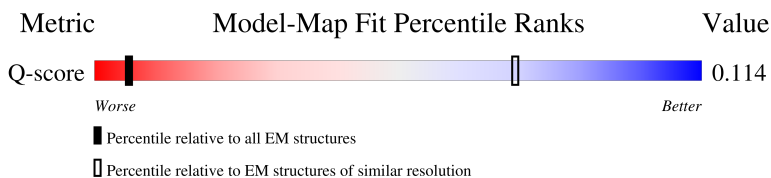
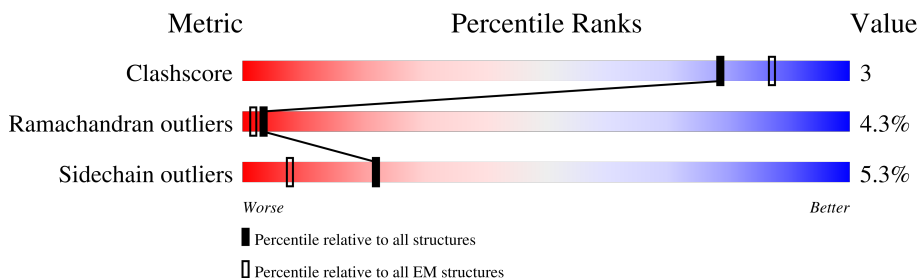
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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	42% 52% 44% .
2	B	451	33% 39% 49% 9% ..
3	C	427	34% 39% 48% 11% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8091 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
			1308	820	227	252	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		

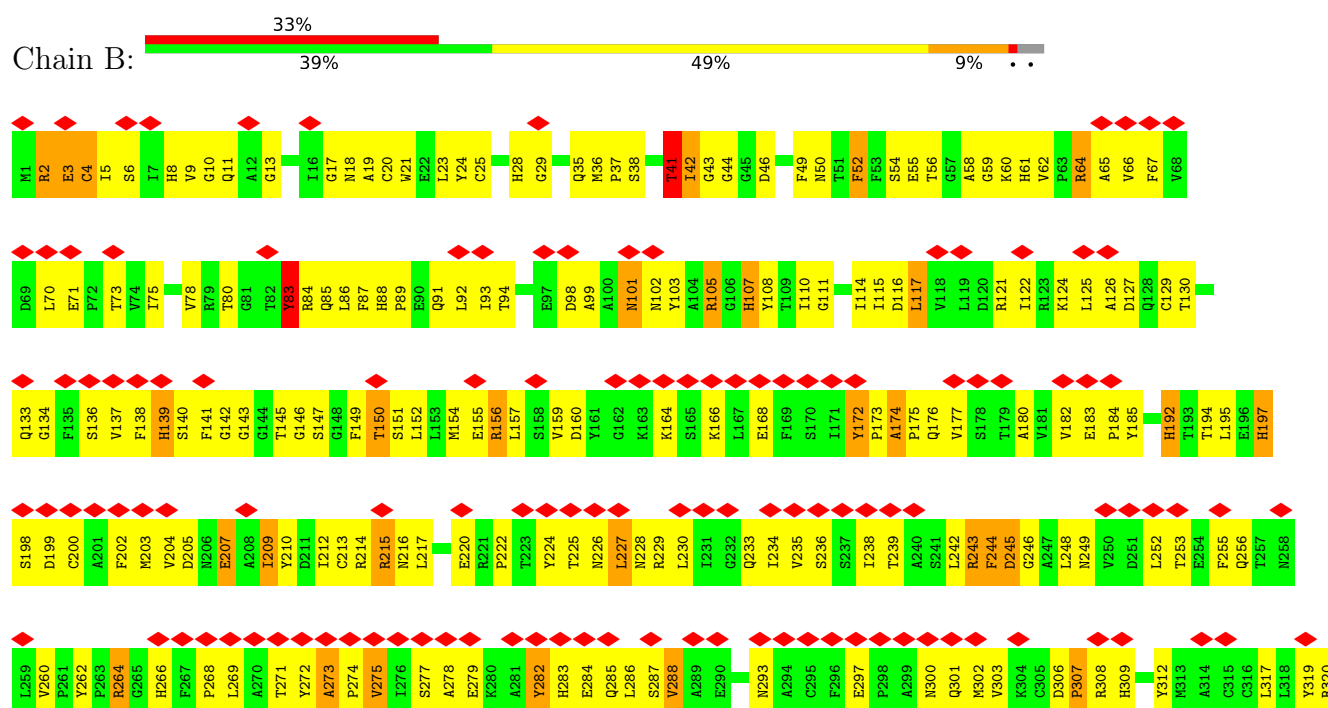
3 Residue-property plots

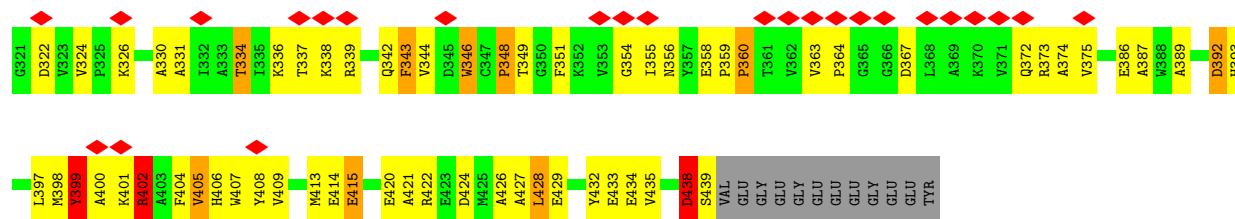
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

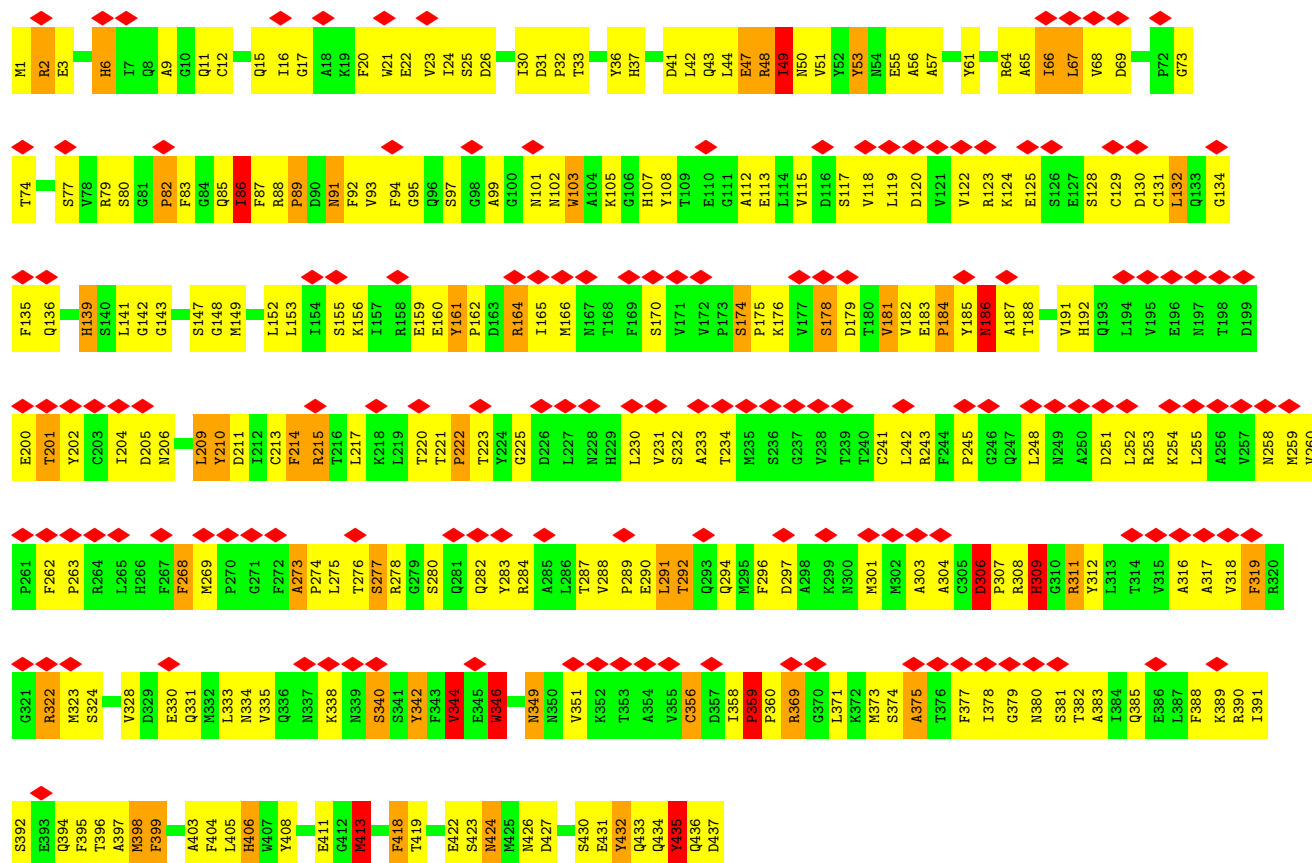


- Molecule 2: Tubulin alpha-1B chain





• 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	2.19	40/1325 (3.0%)	2.44	71/1783 (4.0%)
2	B	2.11	87/3501 (2.5%)	2.49	262/4752 (5.5%)
3	C	2.12	88/3435 (2.6%)	2.51	256/4652 (5.5%)
All	All	2.13	215/8261 (2.6%)	2.49	589/11187 (5.3%)

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	4
2	B	0	18
3	C	0	27
All	All	0	49

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3346	ILE	CA-CB	14.83	1.62	1.54
1	A	3427	LYS	C-OXT	-11.56	1.00	1.23
3	C	437	ASP	C-OXT	-11.56	1.00	1.23
1	A	3427	LYS	C-O	-11.55	1.00	1.23
3	C	437	ASP	C-O	-11.55	1.00	1.23
2	B	439	SER	C-O	-11.52	1.00	1.23
3	C	262	PHE	CA-C	-11.01	1.44	1.52
2	B	136	SER	N-CA	-9.68	1.34	1.46
3	C	113	GLU	C-O	-9.13	1.12	1.24
2	B	88	HIS	C-N	-9.09	1.22	1.34
2	B	245	ASP	CA-CB	8.63	1.68	1.53
3	C	26	ASP	N-CA	-8.45	1.36	1.46
3	C	30	ILE	CA-CB	-8.20	1.44	1.54
2	B	203	MET	CA-C	8.08	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3368	ASN	CA-C	-8.00	1.47	1.52
2	B	91	GLN	N-CA	-7.98	1.35	1.46
3	C	346	TRP	C-N	7.77	1.42	1.33
1	A	3424	ASN	C-N	7.73	1.44	1.33
2	B	308	ARG	CD-NE	7.67	1.56	1.46
2	B	360	PRO	N-CA	7.60	1.57	1.47
2	B	198	SER	N-CA	7.56	1.54	1.45
3	C	139	HIS	CE1-NE2	7.55	1.40	1.32
3	C	179	ASP	CA-C	7.52	1.62	1.52
3	C	99	ALA	CA-C	7.52	1.63	1.53
3	C	122	VAL	CA-CB	-7.35	1.45	1.54
1	A	3315	VAL	N-CA	-7.34	1.36	1.46
2	B	150	THR	C-N	7.34	1.42	1.33
3	C	37	HIS	CD2-NE2	7.23	1.45	1.37
2	B	266	HIS	CA-CB	7.22	1.62	1.52
2	B	192	HIS	ND1-CE1	7.21	1.39	1.32
1	A	3384	SER	CA-C	-7.18	1.43	1.52
3	C	134	GLY	C-N	7.14	1.42	1.33
3	C	51	VAL	N-CA	-6.92	1.38	1.46
2	B	275	VAL	CA-CB	6.92	1.63	1.54
3	C	360	PRO	CA-C	6.83	1.59	1.52
2	B	339	ARG	CD-NE	6.83	1.55	1.46
3	C	174	SER	CA-C	6.82	1.61	1.52
3	C	215	ARG	CD-NE	6.77	1.55	1.46
2	B	152	LEU	N-CA	-6.75	1.38	1.46
1	A	3382	ARG	NE-CZ	6.71	1.40	1.33
2	B	42	ILE	CA-C	-6.67	1.44	1.52
3	C	422	GLU	N-CA	-6.64	1.38	1.46
3	C	395	PHE	CA-C	6.63	1.61	1.52
3	C	258	ASN	C-N	6.60	1.42	1.33
1	A	3358	SER	CA-C	-6.53	1.44	1.52
1	A	3288	ILE	CA-CB	-6.52	1.45	1.54
3	C	206	ASN	CA-C	6.51	1.61	1.52
2	B	13	GLY	N-CA	6.51	1.54	1.45
2	B	302	MET	C-N	6.51	1.41	1.33
3	C	94	PHE	N-CA	6.44	1.54	1.45
3	C	308	ARG	CD-NE	6.44	1.55	1.46
1	A	3381	ASN	CA-CB	6.43	1.63	1.53
3	C	398	MET	CA-CB	6.41	1.62	1.53
3	C	317	ALA	CA-C	6.35	1.59	1.52
2	B	116	ASP	CA-CB	6.35	1.63	1.53
3	C	243	ARG	N-CA	-6.34	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	THR	N-CA	6.32	1.54	1.46
2	B	336	LYS	N-CA	-6.32	1.38	1.46
1	A	3281	ASP	CA-CB	6.31	1.63	1.53
3	C	65	ALA	N-CA	-6.30	1.38	1.46
3	C	297	ASP	N-CA	-6.30	1.39	1.46
1	A	3341	MET	CA-CB	6.30	1.62	1.53
3	C	340	SER	CA-CB	6.28	1.64	1.53
3	C	309	HIS	CG-ND1	-6.24	1.31	1.38
2	B	175	PRO	CA-C	-6.21	1.44	1.52
2	B	180	ALA	C-N	6.20	1.41	1.33
2	B	130	THR	C-N	6.17	1.42	1.33
3	C	288	VAL	CA-C	-6.17	1.47	1.52
2	B	397	LEU	CA-C	6.16	1.60	1.52
2	B	155	GLU	N-CA	-6.15	1.39	1.46
2	B	28	HIS	CE1-NE2	6.12	1.38	1.32
3	C	316	ALA	CA-C	-6.12	1.45	1.52
1	A	3314	ALA	CA-C	-6.12	1.44	1.52
3	C	6	HIS	CG-CD2	6.10	1.42	1.35
2	B	392	ASP	CA-CB	6.07	1.62	1.53
1	A	3264	LYS	N-CA	6.03	1.57	1.46
3	C	232	SER	CA-C	-6.03	1.45	1.52
3	C	22	GLU	CA-CB	6.02	1.62	1.53
3	C	11	GLN	C-N	6.02	1.42	1.33
1	A	3363	GLU	C-N	6.01	1.41	1.33
1	A	3337	ARG	CD-NE	6.00	1.54	1.46
2	B	432	TYR	N-CA	-5.98	1.38	1.46
2	B	235	VAL	N-CA	5.97	1.53	1.46
3	C	411	GLU	CA-CB	5.95	1.62	1.53
2	B	166	LYS	C-N	5.94	1.41	1.33
1	A	3265	GLN	CA-CB	5.92	1.62	1.53
2	B	300	ASN	CA-C	5.92	1.60	1.52
2	B	168	GLU	N-CA	-5.89	1.39	1.46
3	C	148	GLY	CA-C	-5.89	1.45	1.52
3	C	3	GLU	CA-C	5.89	1.60	1.53
3	C	403	ALA	CA-CB	5.89	1.61	1.53
1	A	3287	VAL	CA-CB	-5.88	1.46	1.54
2	B	428	LEU	N-CA	-5.86	1.39	1.46
3	C	252	LEU	CA-C	5.84	1.60	1.52
2	B	307	PRO	N-CA	-5.82	1.39	1.47
2	B	89	PRO	CA-CB	5.81	1.62	1.53
3	C	16	ILE	CA-C	-5.79	1.45	1.52
3	C	101	ASN	N-CA	5.78	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	91	ASN	CA-CB	5.78	1.62	1.53
1	A	3336	ILE	CA-CB	-5.77	1.47	1.54
2	B	160	ASP	CA-C	-5.76	1.44	1.52
3	C	210	TYR	CA-C	-5.75	1.45	1.52
3	C	118	VAL	N-CA	-5.73	1.39	1.46
2	B	434	GLU	C-O	-5.73	1.17	1.24
2	B	44	GLY	N-CA	5.72	1.53	1.45
3	C	290	GLU	CA-CB	5.72	1.63	1.53
3	C	66	ILE	CA-C	5.72	1.60	1.52
3	C	269	MET	CA-C	5.71	1.58	1.52
3	C	165	ILE	CA-C	5.71	1.59	1.52
3	C	233	ALA	CA-C	5.70	1.60	1.52
1	A	3359	ASP	CA-CB	5.69	1.62	1.53
2	B	346	TRP	NE1-CE2	5.68	1.43	1.37
2	B	114	ILE	C-O	-5.67	1.17	1.24
2	B	65	ALA	CA-C	-5.66	1.45	1.52
2	B	269	LEU	C-N	5.63	1.41	1.33
3	C	57	ALA	CA-C	5.63	1.60	1.52
2	B	262	TYR	N-CA	-5.62	1.40	1.46
2	B	93	ILE	CA-C	-5.62	1.45	1.52
2	B	253	THR	CA-C	5.62	1.60	1.52
2	B	54	SER	CA-C	-5.61	1.43	1.52
2	B	252	LEU	CA-C	5.61	1.60	1.52
3	C	399	PHE	CA-CB	-5.61	1.44	1.53
1	A	3334	LYS	CA-C	5.61	1.60	1.52
2	B	4	CYS	CA-C	-5.60	1.45	1.52
3	C	55	GLU	N-CA	5.59	1.52	1.46
2	B	20	CYS	CA-CB	5.58	1.62	1.53
3	C	330	GLU	CA-CB	5.57	1.62	1.53
1	A	3353	SER	CA-C	-5.56	1.45	1.52
2	B	222	PRO	N-CA	-5.56	1.40	1.47
2	B	142	GLY	C-N	5.56	1.39	1.33
3	C	248	LEU	CA-CB	5.55	1.62	1.53
3	C	381	SER	C-O	-5.54	1.17	1.24
2	B	424	ASP	C-N	5.52	1.41	1.33
2	B	9	VAL	N-CA	5.52	1.52	1.46
2	B	134	GLY	N-CA	-5.50	1.40	1.45
2	B	344	VAL	C-O	-5.50	1.17	1.24
1	A	3289	GLU	C-O	-5.49	1.17	1.24
3	C	85	GLN	CA-CB	5.49	1.61	1.53
2	B	271	THR	CA-C	5.47	1.59	1.52
3	C	125	GLU	C-O	-5.47	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	108	TYR	N-CA	-5.44	1.40	1.46
2	B	260	VAL	CA-C	-5.43	1.48	1.53
2	B	324	VAL	CA-CB	-5.43	1.47	1.54
3	C	319	PHE	C-N	5.43	1.41	1.33
3	C	243	ARG	CD-NE	5.43	1.53	1.46
3	C	152	LEU	C-N	5.42	1.40	1.33
3	C	358	ILE	C-N	5.42	1.39	1.33
3	C	289	PRO	N-CD	-5.41	1.40	1.47
1	A	3372	ASN	CA-C	-5.40	1.46	1.52
3	C	44	LEU	CA-C	5.39	1.59	1.52
3	C	82	PRO	C-N	5.37	1.41	1.33
3	C	418	PHE	CB-CG	5.37	1.62	1.50
2	B	59	GLY	N-CA	5.36	1.55	1.45
3	C	148	GLY	C-N	5.35	1.41	1.33
1	A	3292	ASN	C-N	5.35	1.41	1.33
1	A	3408	GLU	C-N	5.35	1.40	1.33
2	B	301	GLN	N-CA	5.34	1.53	1.46
2	B	62	VAL	CA-C	-5.34	1.47	1.52
2	B	180	ALA	CA-CB	5.33	1.61	1.53
1	A	3322	ILE	N-CA	5.33	1.52	1.46
2	B	336	LYS	CA-C	5.32	1.59	1.52
2	B	235	VAL	CA-C	5.31	1.59	1.52
1	A	3365	MET	N-CA	-5.31	1.40	1.46
2	B	10	GLY	N-CA	-5.31	1.39	1.45
2	B	420	GLU	CA-CB	5.31	1.61	1.53
2	B	139	HIS	CA-C	-5.30	1.46	1.52
3	C	53	TYR	CA-C	-5.28	1.46	1.52
3	C	378	ILE	CA-CB	-5.28	1.47	1.54
1	A	3266	GLN	CA-C	-5.25	1.46	1.52
3	C	397	ALA	CA-C	-5.25	1.46	1.52
3	C	53	TYR	N-CA	5.24	1.52	1.45
2	B	401	LYS	CA-C	5.24	1.58	1.52
2	B	136	SER	CA-CB	5.23	1.61	1.53
1	A	3317	LEU	N-CA	5.23	1.52	1.46
1	A	3294	VAL	CA-C	-5.23	1.46	1.52
2	B	317	LEU	CA-CB	5.23	1.62	1.53
2	B	164	LYS	CA-CB	5.22	1.61	1.53
3	C	213	CYS	CA-CB	5.21	1.61	1.53
2	B	284	GLU	CA-C	-5.21	1.46	1.52
2	B	127	ASP	CA-C	5.20	1.59	1.52
2	B	309	HIS	CG-CD2	5.20	1.41	1.35
2	B	204	VAL	C-O	-5.20	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	346	TRP	CD2-CE2	-5.18	1.32	1.41
2	B	139	HIS	N-CA	-5.17	1.39	1.45
2	B	233	GLN	C-N	5.17	1.40	1.33
1	A	3309	ALA	N-CA	5.17	1.52	1.46
3	C	164	ARG	C-N	5.17	1.40	1.33
3	C	276	THR	N-CA	5.16	1.52	1.45
1	A	3345	PHE	N-CA	5.16	1.52	1.46
2	B	402	ARG	CA-CB	5.14	1.62	1.53
3	C	21	TRP	N-CA	5.14	1.52	1.46
3	C	291	LEU	CA-C	5.14	1.59	1.52
3	C	423	SER	CA-C	-5.13	1.46	1.52
3	C	232	SER	CA-CB	5.13	1.61	1.53
2	B	98	ASP	C-N	5.12	1.40	1.33
2	B	207	GLU	N-CA	5.12	1.52	1.46
2	B	122	ILE	CA-CB	-5.12	1.47	1.54
2	B	297	GLU	CA-CB	5.12	1.60	1.53
3	C	404	PHE	CA-CB	5.11	1.62	1.53
3	C	166	MET	CA-CB	-5.10	1.45	1.53
3	C	184	PRO	CA-C	5.10	1.59	1.52
1	A	3273	GLN	CA-C	5.09	1.59	1.52
3	C	342	TYR	CB-CG	-5.09	1.40	1.51
1	A	3343	GLU	CA-C	5.09	1.59	1.52
2	B	215	ARG	NE-CZ	5.09	1.38	1.33
3	C	175	PRO	N-CA	-5.07	1.40	1.47
1	A	3287	VAL	CA-C	5.05	1.59	1.52
1	A	3412	ASN	C-N	5.05	1.40	1.33
3	C	294	GLN	CA-CB	5.05	1.61	1.53
3	C	356	CYS	C-N	5.04	1.40	1.34
2	B	117	LEU	N-CA	5.04	1.52	1.46
1	A	3339	ILE	CB-CG1	5.04	1.63	1.53
2	B	331	ALA	N-CA	-5.02	1.40	1.46
1	A	3368	ASN	CA-CB	5.02	1.60	1.53
3	C	245	PRO	CA-C	5.00	1.58	1.52

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	262	PHE	CA-C-O	-12.03	108.32	119.86
3	C	93	VAL	O-C-N	-10.80	111.53	123.20
2	B	2	ARG	NE-CZ-NH2	-10.43	109.81	119.20
2	B	110	ILE	CA-C-O	10.27	129.06	119.20
3	C	117	SER	N-CA-C	10.24	123.49	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	TRP	CB-CG-CD2	-10.21	112.50	126.80
2	B	202	PHE	CA-CB-CG	-9.91	103.89	113.80
3	C	108	TYR	CA-C-N	9.91	133.32	120.44
3	C	108	TYR	C-N-CA	9.91	133.32	120.44
3	C	287	THR	CA-C-N	9.89	126.47	120.24
3	C	287	THR	C-N-CA	9.89	126.47	120.24
2	B	66	VAL	CA-C-O	9.84	131.69	120.67
1	A	3313	ALA	N-CA-C	9.84	122.00	111.28
3	C	432	TYR	N-CA-C	9.64	121.87	111.36
1	A	3335	GLN	CA-C-N	9.28	132.25	120.56
1	A	3335	GLN	C-N-CA	9.28	132.25	120.56
1	A	3345	PHE	CA-CB-CG	9.26	123.06	113.80
3	C	349	ASN	CA-CB-CG	-9.20	103.40	112.60
2	B	262	TYR	CA-C-N	9.20	131.34	119.84
2	B	262	TYR	C-N-CA	9.20	131.34	119.84
2	B	49	PHE	CA-C-N	9.16	138.19	121.70
2	B	49	PHE	C-N-CA	9.16	138.19	121.70
2	B	213	CYS	CA-C-O	-9.08	111.19	120.90
3	C	141	LEU	N-CA-CB	8.95	123.45	110.47
1	A	3341	MET	N-CA-C	-8.88	102.98	112.93
3	C	427	ASP	CA-CB-CG	8.84	121.44	112.60
3	C	149	MET	CA-C-N	8.80	129.75	119.98
3	C	149	MET	C-N-CA	8.80	129.75	119.98
3	C	37	HIS	ND1-CE1-NE2	8.80	117.20	108.40
2	B	392	ASP	CA-CB-CG	8.72	121.32	112.60
1	A	3359	ASP	CA-CB-CG	-8.72	103.88	112.60
3	C	101	ASN	CA-CB-CG	-8.65	103.94	112.60
3	C	91	ASN	N-CA-C	8.64	121.85	111.82
3	C	129	CYS	CA-C-N	8.53	131.53	120.44
3	C	129	CYS	C-N-CA	8.53	131.53	120.44
3	C	73	GLY	CA-C-N	8.49	132.34	120.29
3	C	73	GLY	C-N-CA	8.49	132.34	120.29
2	B	320	ARG	N-CA-C	8.48	121.88	110.35
2	B	238	ILE	CA-C-N	8.40	131.89	120.38
2	B	238	ILE	C-N-CA	8.40	131.89	120.38
3	C	382	THR	O-C-N	-8.37	113.87	123.33
2	B	234	ILE	CA-C-O	8.33	130.00	121.17
3	C	179	ASP	CA-CB-CG	-8.29	104.31	112.60
2	B	227	LEU	CA-C-N	8.27	131.36	120.28
2	B	227	LEU	C-N-CA	8.27	131.36	120.28
3	C	275	LEU	CA-C-N	8.09	135.38	122.11
3	C	275	LEU	C-N-CA	8.09	135.38	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3379	ILE	N-CA-C	-8.08	103.01	111.58
3	C	253	ARG	CA-C-N	8.04	130.89	120.44
3	C	253	ARG	C-N-CA	8.04	130.89	120.44
2	B	422	ARG	NE-CZ-NH1	7.98	129.48	121.50
3	C	324	SER	CA-C-N	7.94	130.92	120.28
3	C	324	SER	C-N-CA	7.94	130.92	120.28
2	B	324	VAL	O-C-N	-7.90	112.10	121.10
2	B	239	THR	O-C-N	-7.88	113.77	122.12
3	C	334	ASN	CA-CB-CG	-7.86	104.74	112.60
2	B	197	HIS	CE1-NE2-CD2	-7.86	101.14	109.00
2	B	147	SER	N-CA-C	7.84	119.60	111.14
3	C	130	ASP	CA-CB-CG	7.83	120.43	112.60
3	C	51	VAL	N-CA-C	7.79	118.56	110.62
3	C	383	ALA	N-CA-C	7.73	121.82	111.30
3	C	221	THR	CA-C-O	-7.73	114.27	119.29
3	C	344	VAL	O-C-N	-7.72	112.91	122.57
2	B	41	THR	N-CA-CB	7.71	123.53	110.49
2	B	105	ARG	CA-C-N	7.71	128.50	119.94
2	B	105	ARG	C-N-CA	7.71	128.50	119.94
2	B	29	GLY	CA-C-N	7.70	131.05	120.35
2	B	29	GLY	C-N-CA	7.70	131.05	120.35
3	C	149	MET	CG-SD-CE	-7.70	83.97	100.90
2	B	11	GLN	OE1-CD-NE2	-7.66	114.94	122.60
2	B	326	LYS	CA-C-O	7.66	128.67	120.55
2	B	19	ALA	O-C-N	-7.65	114.01	122.12
2	B	21	TRP	CB-CG-CD1	7.62	138.34	126.90
2	B	139	HIS	O-C-N	-7.59	114.75	123.33
2	B	133	GLN	OE1-CD-NE2	7.59	130.19	122.60
1	A	3295	LYS	CA-C-O	7.59	128.69	119.97
3	C	83	PHE	CA-CB-CG	-7.58	106.22	113.80
3	C	139	HIS	ND1-CG-CD2	7.56	113.66	106.10
3	C	43	GLN	CA-C-N	7.56	135.97	121.54
3	C	43	GLN	C-N-CA	7.56	135.97	121.54
2	B	110	ILE	CA-C-N	7.53	128.34	119.98
2	B	110	ILE	C-N-CA	7.53	128.34	119.98
2	B	73	THR	O-C-N	-7.52	114.15	122.12
2	B	349	THR	N-CA-C	7.50	119.15	110.97
1	A	3303	VAL	N-CA-CB	7.49	119.32	110.55
3	C	356	CYS	CA-C-N	7.47	131.29	120.38
3	C	356	CYS	C-N-CA	7.47	131.29	120.38
3	C	427	ASP	CA-C-N	7.46	130.14	120.44
3	C	427	ASP	C-N-CA	7.46	130.14	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	176	LYS	CB-CA-C	7.44	121.83	111.86
2	B	200	CYS	CA-C-N	7.44	133.62	121.86
2	B	200	CYS	C-N-CA	7.44	133.62	121.86
1	A	3346	ILE	N-CA-CB	7.43	116.24	110.45
2	B	214	ARG	N-CA-C	7.42	119.45	111.36
1	A	3415	GLN	CA-C-N	7.41	130.21	120.28
1	A	3415	GLN	C-N-CA	7.41	130.21	120.28
2	B	271	THR	O-C-N	-7.39	114.60	123.10
2	B	438	ASP	CA-CB-CG	7.36	119.96	112.60
2	B	409	VAL	N-CA-C	-7.30	103.41	110.42
2	B	20	CYS	CA-C-N	7.30	130.07	120.28
2	B	20	CYS	C-N-CA	7.30	130.07	120.28
3	C	234	THR	CA-C-N	7.29	130.78	120.28
3	C	234	THR	C-N-CA	7.29	130.78	120.28
2	B	2	ARG	NE-CZ-NH1	7.28	128.78	121.50
3	C	174	SER	CA-C-O	-7.28	110.19	120.16
2	B	183	GLU	CA-C-N	7.27	126.94	119.82
2	B	183	GLU	C-N-CA	7.27	126.94	119.82
2	B	139	HIS	CE1-NE2-CD2	-7.27	101.73	109.00
2	B	18	ASN	CA-CB-CG	7.27	119.87	112.60
3	C	406	HIS	N-CA-C	7.23	121.20	112.38
2	B	111	GLY	O-C-N	-7.23	115.25	122.19
3	C	251	ASP	CA-CB-CG	7.23	119.83	112.60
3	C	398	MET	CG-SD-CE	-7.22	85.01	100.90
3	C	273	ALA	O-C-N	-7.18	113.06	121.32
3	C	419	THR	CA-C-N	7.18	129.90	120.28
3	C	419	THR	C-N-CA	7.18	129.90	120.28
2	B	320	ARG	CA-C-O	-7.17	113.94	121.55
2	B	392	ASP	N-CA-CB	-7.17	99.57	110.12
1	A	3283	VAL	N-CA-C	-7.16	105.80	112.96
3	C	288	VAL	CA-C-N	7.15	127.14	119.28
3	C	288	VAL	C-N-CA	7.15	127.14	119.28
3	C	132	LEU	CA-C-N	-7.13	108.66	121.14
3	C	132	LEU	C-N-CA	-7.13	108.66	121.14
2	B	407	TRP	N-CA-C	7.12	119.04	111.28
2	B	244	PHE	CA-C-N	7.11	135.12	121.54
2	B	244	PHE	C-N-CA	7.11	135.12	121.54
3	C	431	GLU	O-C-N	-7.10	112.81	122.33
2	B	408	TYR	CA-C-N	7.08	129.48	120.56
2	B	408	TYR	C-N-CA	7.08	129.48	120.56
2	B	414	GLU	N-CA-C	7.05	120.45	110.23
1	A	3276	VAL	CB-CA-C	7.05	121.68	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	391	ILE	CA-C-N	7.04	129.72	120.28
3	C	391	ILE	C-N-CA	7.04	129.72	120.28
2	B	52	PHE	CA-C-N	7.04	132.77	122.63
2	B	52	PHE	C-N-CA	7.04	132.77	122.63
2	B	226	ASN	CB-CG-ND2	-7.04	105.85	116.40
2	B	60	LYS	CA-C-N	7.03	134.97	121.54
2	B	60	LYS	C-N-CA	7.03	134.97	121.54
2	B	434	GLU	O-C-N	-7.03	114.83	122.07
3	C	328	VAL	O-C-N	-7.01	114.72	121.94
3	C	24	ILE	N-CA-C	7.00	117.76	110.62
3	C	115	VAL	O-C-N	7.00	128.66	121.87
3	C	430	SER	N-CA-C	6.99	118.90	111.28
2	B	25	CYS	N-CA-C	6.99	118.89	111.28
2	B	337	THR	N-CA-C	-6.97	104.58	113.23
2	B	230	LEU	O-C-N	-6.97	114.84	122.09
2	B	105	ARG	N-CA-C	6.96	118.52	111.07
2	B	303	VAL	N-CA-C	-6.94	106.05	112.43
2	B	439	SER	CA-C-O	-6.94	109.00	120.80
1	A	3277	LYS	N-CA-CB	-6.93	98.88	110.39
3	C	392	SER	O-C-N	-6.91	114.80	122.12
3	C	141	LEU	O-C-N	-6.88	113.51	122.39
1	A	3287	VAL	N-CA-C	6.88	117.66	110.72
3	C	260	VAL	CA-C-N	6.87	126.84	119.28
3	C	260	VAL	C-N-CA	6.87	126.84	119.28
2	B	405	VAL	CA-C-N	6.84	129.75	120.38
2	B	405	VAL	C-N-CA	6.84	129.75	120.38
3	C	124	LYS	N-CA-CB	-6.84	100.04	110.16
3	C	307	PRO	CA-C-N	6.83	129.74	120.38
3	C	307	PRO	C-N-CA	6.83	129.74	120.38
3	C	434	GLN	O-C-N	-6.83	114.88	122.12
2	B	38	SER	O-C-N	-6.82	116.12	123.42
2	B	88	HIS	CA-C-N	6.81	126.44	119.56
2	B	88	HIS	C-N-CA	6.81	126.44	119.56
1	A	3310	ASN	CA-C-O	-6.78	113.24	119.62
3	C	369	ARG	N-CA-C	6.78	125.24	110.80
2	B	363	VAL	CA-C-N	6.76	126.80	119.90
2	B	363	VAL	C-N-CA	6.76	126.80	119.90
3	C	186	ASN	OD1-CG-ND2	-6.72	115.88	122.60
2	B	399	TYR	CA-CB-CG	-6.71	101.81	113.90
3	C	312	TYR	CA-C-N	6.71	134.37	121.54
3	C	312	TYR	C-N-CA	6.71	134.37	121.54
3	C	56	ALA	CA-C-O	-6.70	114.14	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	91	ASN	CA-CB-CG	-6.69	105.91	112.60
2	B	339	ARG	CA-C-N	6.69	129.78	120.29
2	B	339	ARG	C-N-CA	6.69	129.78	120.29
3	C	86	ILE	N-CA-C	6.68	117.44	110.62
3	C	424	ASN	CA-CB-CG	6.67	119.28	112.60
3	C	41	ASP	CA-CB-CG	6.66	119.26	112.60
3	C	108	TYR	CA-C-O	6.64	123.56	119.77
1	A	3291	GLN	CA-C-O	6.63	127.59	119.97
2	B	174	ALA	N-CA-CB	6.62	119.78	110.11
2	B	160	ASP	N-CA-C	6.61	121.09	112.89
2	B	197	HIS	ND1-CE1-NE2	6.61	115.00	108.40
3	C	318	VAL	O-C-N	-6.57	113.11	122.76
1	A	3293	ALA	CA-C-N	6.55	129.44	120.46
1	A	3293	ALA	C-N-CA	6.55	129.44	120.46
3	C	181	VAL	CB-CA-C	6.52	121.98	111.29
2	B	359	PRO	CA-C-O	-6.51	111.11	120.56
2	B	67	PHE	O-C-N	-6.50	115.73	123.27
3	C	432	TYR	CA-C-N	6.50	129.31	120.54
3	C	432	TYR	C-N-CA	6.50	129.31	120.54
2	B	407	TRP	CG-CD2-CE3	-6.49	127.41	133.90
3	C	120	ASP	CA-CB-CG	6.49	119.09	112.60
3	C	186	ASN	N-CA-C	6.49	118.43	111.36
3	C	403	ALA	N-CA-CB	-6.47	104.02	111.79
1	A	3424	ASN	CA-CB-CG	-6.47	106.13	112.60
3	C	64	ARG	NE-CZ-NH1	6.46	127.95	121.50
3	C	50	ASN	CA-CB-CG	-6.42	106.18	112.60
3	C	192	HIS	ND1-CG-CD2	6.42	112.52	106.10
3	C	406	HIS	ND1-CE1-NE2	6.38	114.78	108.40
2	B	273	ALA	N-CA-C	6.37	120.88	112.35
2	B	23	LEU	O-C-N	-6.37	114.77	122.22
2	B	80	THR	N-CA-C	-6.33	104.71	112.88
3	C	241	CYS	CA-C-O	6.32	127.12	120.42
1	A	3368	ASN	CA-CB-CG	-6.32	106.28	112.60
2	B	427	ALA	CA-C-O	6.31	127.20	120.70
3	C	277	SER	O-C-N	-6.31	116.67	123.42
3	C	192	HIS	CB-CG-ND1	-6.30	113.25	122.70
3	C	220	THR	CA-C-N	6.30	130.06	121.74
3	C	220	THR	C-N-CA	6.30	130.06	121.74
3	C	263	PRO	CA-C-O	-6.30	110.04	119.86
2	B	400	ALA	N-CA-C	-6.28	104.87	112.54
3	C	201	THR	O-C-N	-6.26	115.26	123.21
2	B	102	ASN	CA-C-O	6.26	127.27	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	23	VAL	CA-C-O	-6.26	114.53	121.17
3	C	200	GLU	O-C-N	-6.24	115.29	123.28
2	B	141	PHE	CA-CB-CG	-6.22	107.58	113.80
3	C	191	VAL	CA-C-N	6.21	128.51	120.44
3	C	191	VAL	C-N-CA	6.21	128.51	120.44
3	C	230	LEU	CA-C-N	6.19	128.58	120.60
3	C	230	LEU	C-N-CA	6.19	128.58	120.60
2	B	115	ILE	N-CA-C	6.18	116.93	110.62
3	C	117	SER	O-C-N	-6.18	114.98	122.22
3	C	340	SER	CA-C-N	6.18	128.89	120.54
3	C	340	SER	C-N-CA	6.18	128.89	120.54
1	A	3411	ARG	NE-CZ-NH2	6.17	124.76	119.20
3	C	41	ASP	N-CA-C	6.17	117.67	111.07
2	B	393	HIS	ND1-CE1-NE2	6.16	114.56	108.40
3	C	296	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	3415	GLN	O-C-N	-6.15	115.73	122.07
2	B	372	GLN	CB-CA-C	-6.15	99.78	110.17
3	C	178	SER	N-CA-CB	6.15	120.88	110.49
2	B	91	GLN	N-CA-C	6.14	120.47	112.92
2	B	415	GLU	N-CA-C	6.13	118.94	111.82
3	C	103	TRP	N-CA-C	6.13	118.75	111.33
3	C	214	PHE	CB-CG-CD1	-6.13	110.28	120.70
1	A	3340	ILE	CA-CB-CG2	6.12	120.91	110.50
3	C	161	TYR	N-CA-C	6.12	120.44	108.21
2	B	331	ALA	N-CA-C	6.12	118.45	111.11
2	B	398	MET	CA-C-N	6.11	128.96	120.29
2	B	398	MET	C-N-CA	6.11	128.96	120.29
3	C	182	VAL	CA-C-N	6.10	128.63	120.58
3	C	182	VAL	C-N-CA	6.10	128.63	120.58
2	B	216	ASN	CA-C-O	6.10	127.01	120.24
2	B	387	ALA	N-CA-CB	-6.09	101.11	110.13
2	B	293	ASN	N-CA-CB	-6.09	100.52	110.14
1	A	3321	SER	O-C-N	-6.09	115.67	122.12
3	C	134	GLY	O-C-N	-6.07	116.63	123.67
3	C	64	ARG	NH1-CZ-NH2	-6.05	111.43	119.30
1	A	3406	ARG	CA-C-O	6.04	125.69	119.05
2	B	198	SER	N-CA-CB	6.03	120.14	110.85
3	C	406	HIS	CA-CB-CG	-6.03	107.77	113.80
1	A	3277	LYS	CA-C-N	6.03	129.48	120.31
1	A	3277	LYS	C-N-CA	6.03	129.48	120.31
2	B	6	SER	O-C-N	-6.02	116.14	123.30
2	B	50	ASN	CA-C-O	-6.02	110.57	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	221	THR	CB-CA-C	-6.01	103.17	110.08
2	B	322	ASP	CB-CA-C	6.00	119.36	109.70
3	C	131	CYS	CA-C-N	6.00	133.00	121.54
3	C	131	CYS	C-N-CA	6.00	133.00	121.54
2	B	182	VAL	CA-C-N	5.99	128.48	120.58
2	B	182	VAL	C-N-CA	5.99	128.48	120.58
3	C	107	HIS	CE1-NE2-CD2	-5.99	103.02	109.00
2	B	56	THR	CA-C-N	-5.98	112.05	121.37
2	B	56	THR	C-N-CA	-5.98	112.05	121.37
2	B	217	LEU	CA-C-O	5.96	126.24	119.27
3	C	338	LYS	N-CA-C	5.96	117.58	111.14
3	C	390	ARG	NE-CZ-NH2	5.96	124.56	119.20
3	C	15	GLN	CA-C-N	5.96	128.62	120.46
3	C	15	GLN	C-N-CA	5.96	128.62	120.46
3	C	49	ILE	O-C-N	-5.95	116.10	121.87
2	B	338	LYS	CA-C-N	5.93	130.79	122.36
2	B	338	LYS	C-N-CA	5.93	130.79	122.36
3	C	268	PHE	CA-CB-CG	-5.92	107.88	113.80
2	B	229	ARG	N-CA-C	-5.92	104.41	111.69
1	A	3284	GLU	O-C-N	-5.91	115.22	120.48
2	B	139	HIS	ND1-CE1-NE2	5.90	114.30	108.40
2	B	116	ASP	CA-C-O	5.90	127.01	120.82
3	C	379	GLY	O-C-N	-5.89	116.55	123.09
3	C	77	SER	CB-CA-C	-5.89	99.74	110.63
2	B	105	ARG	O-C-N	5.88	128.13	122.07
2	B	116	ASP	CA-C-N	5.87	128.08	120.44
2	B	116	ASP	C-N-CA	5.87	128.08	120.44
2	B	356	ASN	CA-C-O	-5.87	114.93	121.51
2	B	176	GLN	O-C-N	-5.87	114.78	122.59
2	B	86	LEU	CA-C-O	5.87	126.38	119.28
2	B	149	PHE	N-CA-CB	5.86	118.50	110.01
3	C	358	ILE	CA-C-O	-5.84	115.39	119.19
1	A	3307	SER	CA-C-O	-5.84	113.85	121.73
2	B	124	LYS	N-CA-C	5.83	117.63	111.28
3	C	225	GLY	CA-C-N	5.82	128.35	120.44
3	C	225	GLY	C-N-CA	5.82	128.35	120.44
3	C	318	VAL	CA-C-O	5.81	127.48	120.74
3	C	331	GLN	N-CA-C	-5.81	104.94	111.28
2	B	150	THR	O-C-N	-5.81	115.96	122.12
1	A	3280	LEU	CA-C-N	5.81	128.64	120.28
1	A	3280	LEU	C-N-CA	5.81	128.64	120.28
2	B	256	GLN	CA-C-N	5.80	128.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	GLN	C-N-CA	5.80	128.64	120.28
3	C	408	TYR	N-CA-C	-5.80	104.86	111.07
1	A	3282	LYS	N-CA-C	5.80	117.61	111.28
3	C	31	ASP	N-CA-C	-5.79	101.69	110.50
3	C	139	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	3290	ALA	N-CA-CB	-5.79	101.68	110.07
2	B	157	LEU	O-C-N	-5.79	115.55	122.15
2	B	217	LEU	N-CA-C	-5.79	106.06	113.23
3	C	112	ALA	O-C-N	-5.79	115.99	122.12
3	C	275	LEU	O-C-N	-5.77	116.51	123.03
2	B	205	ASP	CA-CB-CG	5.76	118.36	112.60
3	C	351	VAL	N-CA-C	5.76	117.05	108.46
2	B	324	VAL	CA-C-O	5.76	127.66	119.95
2	B	342	GLN	CB-CA-C	-5.75	101.17	110.77
3	C	153	LEU	N-CA-C	5.74	118.00	111.11
2	B	285	GLN	OE1-CD-NE2	-5.72	116.88	122.60
2	B	126	ALA	N-CA-C	5.71	117.58	111.36
3	C	113	GLU	CA-C-O	5.71	126.55	120.10
2	B	137	VAL	N-CA-C	5.71	116.33	108.12
2	B	108	TYR	CA-C-O	5.70	126.88	119.98
3	C	130	ASP	N-CA-C	5.70	117.17	111.07
3	C	381	SER	CA-C-N	5.70	131.94	121.85
3	C	381	SER	C-N-CA	5.70	131.94	121.85
2	B	138	PHE	CA-CB-CG	-5.70	108.10	113.80
3	C	122	VAL	CA-C-N	5.69	127.91	120.28
3	C	122	VAL	C-N-CA	5.69	127.91	120.28
2	B	348	PRO	CA-C-N	5.69	128.16	120.65
2	B	348	PRO	C-N-CA	5.69	128.16	120.65
2	B	42	ILE	CA-CB-CG1	5.68	120.06	110.40
3	C	21	TRP	O-C-N	5.68	128.14	122.12
3	C	23	VAL	N-CA-CB	5.67	117.18	110.55
3	C	323	MET	CG-SD-CE	-5.67	88.43	100.90
2	B	215	ARG	NE-CZ-NH2	5.66	124.30	119.20
3	C	388	PHE	CA-C-N	5.66	128.14	120.44
3	C	388	PHE	C-N-CA	5.66	128.14	120.44
3	C	258	ASN	CA-C-O	5.65	126.59	120.55
2	B	234	ILE	O-C-N	-5.64	116.38	121.91
3	C	21	TRP	CG-CD2-CE3	-5.64	128.26	133.90
1	A	3313	ALA	CA-C-N	5.64	130.14	120.72
1	A	3313	ALA	C-N-CA	5.64	130.14	120.72
3	C	380	ASN	N-CA-CB	-5.64	102.46	111.43
3	C	25	SER	N-CA-C	5.64	117.11	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3418	GLU	CA-C-N	5.63	128.29	120.29
1	A	3418	GLU	C-N-CA	5.63	128.29	120.29
3	C	231	VAL	N-CA-CB	5.63	116.76	110.51
1	A	3278	GLU	CA-C-O	5.62	126.44	119.97
3	C	143	GLY	CA-C-N	5.62	130.40	120.74
3	C	143	GLY	C-N-CA	5.62	130.40	120.74
3	C	37	HIS	CA-CB-CG	5.61	119.41	113.80
1	A	3283	VAL	CB-CA-C	-5.61	106.13	111.06
3	C	282	GLN	N-CA-C	-5.60	105.76	112.59
3	C	50	ASN	CA-C-N	5.60	128.13	120.46
3	C	50	ASN	C-N-CA	5.60	128.13	120.46
3	C	149	MET	N-CA-CB	5.58	118.42	110.16
3	C	182	VAL	N-CA-C	-5.58	106.36	113.22
3	C	283	TYR	O-C-N	-5.58	115.69	123.34
3	C	99	ALA	N-CA-C	5.58	119.39	112.58
2	B	192	HIS	CA-CB-CG	5.57	119.37	113.80
2	B	435	VAL	O-C-N	-5.56	114.44	122.12
2	B	139	HIS	CA-C-N	5.56	131.71	121.70
2	B	139	HIS	C-N-CA	5.56	131.71	121.70
2	B	386	GLU	CA-C-N	5.55	129.97	120.71
2	B	386	GLU	C-N-CA	5.55	129.97	120.71
1	A	3389	PRO	N-CA-C	5.54	121.05	113.84
3	C	397	ALA	N-CA-C	5.54	117.00	111.07
3	C	254	LYS	O-C-N	-5.54	116.36	122.07
2	B	93	ILE	N-CA-CB	-5.54	104.35	110.99
2	B	126	ALA	CA-C-O	5.54	126.29	120.42
3	C	102	ASN	CA-CB-CG	-5.53	107.07	112.60
2	B	64	ARG	O-C-N	-5.53	115.67	122.25
2	B	301	GLN	CG-CD-NE2	5.53	124.70	116.40
2	B	224	TYR	N-CA-C	-5.53	105.41	111.82
2	B	115	ILE	CA-C-N	5.53	127.62	120.44
2	B	115	ILE	C-N-CA	5.53	127.62	120.44
3	C	289	PRO	N-CD-CG	5.52	111.49	103.20
2	B	54	SER	CA-C-N	5.51	132.07	121.54
2	B	54	SER	C-N-CA	5.51	132.07	121.54
3	C	217	LEU	N-CA-CB	-5.51	102.01	110.44
3	C	204	ILE	CA-C-N	5.51	129.74	122.42
3	C	204	ILE	C-N-CA	5.51	129.74	122.42
2	B	287	SER	CA-C-N	5.50	129.16	120.47
2	B	287	SER	C-N-CA	5.50	129.16	120.47
3	C	47	GLU	CB-CG-CD	5.48	121.92	112.60
2	B	236	SER	N-CA-C	5.48	118.01	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	ASN	N-CA-C	-5.48	105.33	112.23
2	B	25	CYS	CA-C-N	5.47	128.06	120.29
2	B	25	CYS	C-N-CA	5.47	128.06	120.29
3	C	223	THR	O-C-N	-5.46	116.21	122.93
1	A	3346	ILE	O-C-N	-5.46	116.92	120.42
2	B	102	ASN	CA-C-N	5.45	129.00	120.82
2	B	102	ASN	C-N-CA	5.45	129.00	120.82
1	A	3351	ASN	N-CA-CB	5.45	118.75	110.14
2	B	243	ARG	CG-CD-NE	-5.45	100.01	112.00
2	B	407	TRP	CB-CG-CD1	5.45	135.07	126.90
2	B	279	GLU	N-CA-C	5.44	117.91	111.33
3	C	426	ASN	N-CA-C	5.44	118.13	111.82
2	B	156	ARG	N-CA-C	5.43	116.89	111.07
3	C	105	LYS	CB-CA-C	-5.43	102.35	110.88
3	C	260	VAL	O-C-N	-5.43	114.91	121.10
3	C	12	CYS	N-CA-C	5.42	117.26	111.36
2	B	264	ARG	N-CA-C	-5.41	99.27	110.80
2	B	334	THR	N-CA-C	5.41	117.18	111.28
1	A	3302	LEU	O-C-N	-5.41	116.39	122.12
3	C	37	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
3	C	136	GLN	OE1-CD-NE2	-5.41	117.19	122.60
2	B	228	ASN	CA-CB-CG	-5.40	107.20	112.60
3	C	68	VAL	CB-CA-C	5.40	118.67	110.62
2	B	84	ARG	CA-C-N	-5.40	114.12	122.49
2	B	84	ARG	C-N-CA	-5.40	114.12	122.49
2	B	422	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
3	C	405	LEU	CA-C-O	5.39	126.17	119.97
1	A	3375	TYR	CB-CG-CD2	5.39	128.89	120.80
3	C	103	TRP	CD2-CE2-CZ2	-5.39	117.01	122.40
3	C	283	TYR	N-CA-C	-5.39	98.86	108.13
3	C	436	GLN	CA-C-O	5.39	126.15	119.79
2	B	225	THR	O-C-N	-5.39	116.52	122.07
1	A	3353	SER	CA-C-O	-5.38	115.48	121.51
3	C	170	SER	O-C-N	-5.38	116.97	123.27
2	B	66	VAL	O-C-N	-5.38	117.35	123.10
2	B	374	ALA	O-C-N	-5.38	116.54	122.72
2	B	386	GLU	O-C-N	-5.37	116.08	122.20
3	C	89	PRO	N-CA-C	5.37	123.53	112.47
3	C	155	SER	CA-C-N	5.36	127.41	120.44
3	C	155	SER	C-N-CA	5.36	127.41	120.44
2	B	185	TYR	O-C-N	-5.36	116.44	122.12
2	B	301	GLN	OE1-CD-NE2	-5.36	117.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	242	LEU	CA-C-N	5.36	130.78	122.26
3	C	242	LEU	C-N-CA	5.36	130.78	122.26
2	B	87	PHE	CA-C-O	-5.35	115.55	121.33
1	A	3336	ILE	N-CA-CB	5.35	116.81	110.55
2	B	427	ALA	CA-C-N	5.35	127.45	120.28
2	B	427	ALA	C-N-CA	5.35	127.45	120.28
2	B	64	ARG	CA-C-O	5.35	125.90	119.59
2	B	413	MET	O-C-N	-5.35	116.96	123.16
3	C	159	GLU	CA-C-N	5.34	127.38	120.44
3	C	159	GLU	C-N-CA	5.34	127.38	120.44
2	B	184	PRO	CA-C-N	5.33	127.43	120.28
2	B	184	PRO	C-N-CA	5.33	127.43	120.28
2	B	399	TYR	CA-C-O	5.33	126.07	120.42
3	C	181	VAL	CA-CB-CG1	5.33	119.46	110.40
2	B	78	VAL	CA-C-N	5.33	129.74	120.68
2	B	78	VAL	C-N-CA	5.33	129.74	120.68
2	B	185	TYR	CB-CG-CD1	-5.32	112.81	120.80
3	C	389	LYS	CA-C-N	5.32	127.41	120.28
3	C	389	LYS	C-N-CA	5.32	127.41	120.28
3	C	21	TRP	N-CA-C	5.32	117.08	111.28
2	B	355	ILE	N-CA-C	-5.32	100.58	108.45
2	B	428	LEU	CA-C-O	5.32	126.19	120.55
3	C	69	ASP	O-C-N	-5.32	116.70	122.92
3	C	47	GLU	N-CA-CB	5.31	118.62	110.70
2	B	248	LEU	N-CA-C	-5.30	106.65	113.23
2	B	199	ASP	CA-CB-CG	-5.30	107.30	112.60
3	C	156	LYS	CA-C-O	-5.30	115.25	120.82
2	B	228	ASN	N-CA-CB	5.30	117.91	110.12
1	A	3400	TYR	N-CA-C	-5.30	105.59	111.36
2	B	151	SER	N-CA-C	5.30	117.48	111.02
2	B	204	VAL	CA-C-O	5.29	125.95	120.39
2	B	392	ASP	CA-C-N	5.29	127.64	120.44
2	B	392	ASP	C-N-CA	5.29	127.64	120.44
1	A	3303	VAL	CA-CB-CG1	5.29	119.38	110.40
2	B	89	PRO	CA-C-N	5.28	127.89	120.28
2	B	89	PRO	C-N-CA	5.28	127.89	120.28
2	B	215	ARG	O-C-N	-5.28	114.20	122.13
3	C	119	LEU	N-CA-C	5.28	117.04	111.28
3	C	311	ARG	N-CA-CB	5.28	119.42	110.49
3	C	322	ARG	CB-CA-C	5.28	118.34	109.89
2	B	125	LEU	N-CA-CB	-5.28	102.37	110.12
3	C	183	GLU	O-C-N	-5.28	115.48	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	MET	N-CA-CB	5.27	117.79	110.04
2	B	282	TYR	N-CA-CB	5.27	119.40	110.49
2	B	121	ARG	O-C-N	-5.27	116.40	122.09
2	B	343	PHE	O-C-N	-5.27	117.08	123.03
3	C	319	PHE	O-C-N	-5.27	117.08	123.03
2	B	262	TYR	N-CA-C	-5.26	101.33	108.11
2	B	46	ASP	CA-CB-CG	5.26	117.86	112.60
3	C	209	LEU	O-C-N	-5.26	115.80	122.27
2	B	288	VAL	CA-C-N	5.25	129.49	120.71
2	B	288	VAL	C-N-CA	5.25	129.49	120.71
2	B	212	ILE	CA-C-N	5.25	127.62	120.54
2	B	212	ILE	C-N-CA	5.25	127.62	120.54
2	B	194	THR	N-CA-C	-5.24	106.66	113.16
3	C	2	ARG	CA-C-N	5.24	129.63	122.34
3	C	2	ARG	C-N-CA	5.24	129.63	122.34
2	B	406	HIS	ND1-CG-CD2	5.24	111.34	106.10
2	B	66	VAL	CB-CA-C	5.24	118.56	110.50
2	B	330	ALA	N-CA-C	5.23	117.39	111.11
3	C	255	LEU	CA-C-O	5.23	125.98	119.97
2	B	145	THR	CA-C-N	5.23	131.66	121.41
2	B	145	THR	C-N-CA	5.23	131.66	121.41
3	C	36	TYR	N-CA-C	5.23	117.59	108.76
3	C	187	ALA	O-C-N	-5.23	115.32	122.33
3	C	230	LEU	CA-C-O	5.23	126.09	120.55
2	B	433	GLU	N-CA-C	-5.22	105.59	111.28
3	C	147	SER	O-C-N	-5.22	115.65	122.59
3	C	211	ASP	CA-C-N	5.21	127.82	120.42
3	C	211	ASP	C-N-CA	5.21	127.82	120.42
3	C	435	TYR	CA-C-O	5.21	125.79	119.38
2	B	235	VAL	N-CA-CB	5.21	118.40	110.58
3	C	135	PHE	CA-CB-CG	5.21	119.01	113.80
2	B	88	HIS	CA-CB-CG	5.20	119.00	113.80
2	B	249	ASN	O-C-N	-5.20	116.73	122.91
3	C	175	PRO	CA-C-N	5.20	129.56	122.34
3	C	175	PRO	C-N-CA	5.20	129.56	122.34
1	A	3340	ILE	CB-CA-C	-5.19	105.14	112.14
2	B	78	VAL	CA-C-O	-5.19	114.29	120.78
1	A	3411	ARG	CA-C-O	-5.19	114.92	120.42
2	B	28	HIS	CB-CG-ND1	-5.19	114.92	122.70
3	C	94	PHE	CA-C-O	-5.19	115.54	121.40
3	C	205	ASP	CA-C-O	5.19	126.13	120.58
2	B	322	ASP	CB-CG-OD2	5.18	130.32	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	364	PRO	CA-C-O	-5.18	115.50	121.36
2	B	349	THR	O-C-N	-5.18	116.64	122.03
3	C	389	LYS	N-CA-C	-5.18	105.54	111.14
2	B	243	ARG	CB-CG-CD	5.18	123.21	111.30
3	C	82	PRO	N-CA-CB	5.17	108.29	102.60
2	B	160	ASP	CA-C-O	5.17	125.72	119.31
2	B	83	TYR	CB-CG-CD1	-5.17	113.05	120.80
2	B	209	ILE	N-CA-C	5.16	117.54	111.09
1	A	3349	ILE	CB-CA-C	5.16	119.33	112.22
3	C	31	ASP	CA-CB-CG	5.16	117.75	112.60
2	B	152	LEU	CA-C-N	5.15	127.61	120.29
2	B	152	LEU	C-N-CA	5.15	127.61	120.29
1	A	3281	ASP	CA-C-N	5.15	127.18	120.28
1	A	3281	ASP	C-N-CA	5.15	127.18	120.28
1	A	3294	VAL	CA-C-N	5.14	128.13	120.31
1	A	3294	VAL	C-N-CA	5.14	128.13	120.31
3	C	103	TRP	CE2-CD2-CE3	5.14	123.94	118.80
3	C	394	GLN	CA-C-O	5.14	125.87	120.42
2	B	426	ALA	O-C-N	-5.13	115.55	122.43
3	C	252	LEU	N-CA-C	5.13	119.79	111.37
3	C	277	SER	N-CA-CB	5.13	119.51	111.56
2	B	307	PRO	CA-C-O	-5.13	111.27	120.60
3	C	95	GLY	CA-C-N	5.12	131.53	122.66
3	C	95	GLY	C-N-CA	5.12	131.53	122.66
3	C	359	PRO	N-CA-CB	-5.12	98.11	103.08
2	B	44	GLY	CA-C-N	5.12	130.91	121.70
2	B	44	GLY	C-N-CA	5.12	130.91	121.70
3	C	306	ASP	N-CA-C	5.12	121.12	109.81
3	C	33	THR	N-CA-C	-5.12	106.63	112.92
3	C	128	SER	CB-CA-C	-5.11	101.92	110.56
1	A	3376	ASN	CA-C-N	5.11	127.44	120.54
1	A	3376	ASN	C-N-CA	5.11	127.44	120.54
3	C	202	TYR	CB-CA-C	-5.11	102.27	110.14
2	B	94	THR	O-C-N	-5.10	117.30	123.27
2	B	224	TYR	CA-CB-CG	-5.10	104.72	113.90
1	A	3296	SER	N-CA-C	5.10	119.37	113.20
3	C	160	GLU	N-CA-C	5.10	116.52	111.07
1	A	3419	ASP	CA-C-N	5.09	127.53	120.29
1	A	3419	ASP	C-N-CA	5.09	127.53	120.29
2	B	426	ALA	CA-C-N	5.09	127.37	120.44
2	B	426	ALA	C-N-CA	5.09	127.37	120.44
1	A	3424	ASN	CA-C-N	5.09	127.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3424	ASN	C-N-CA	5.09	127.10	120.28
2	B	433	GLU	CA-C-N	5.09	127.06	120.44
2	B	433	GLU	C-N-CA	5.09	127.06	120.44
3	C	87	PHE	CA-C-O	5.09	126.69	120.99
2	B	421	ALA	CA-C-N	5.08	127.05	120.44
2	B	421	ALA	C-N-CA	5.08	127.05	120.44
1	A	3279	ASP	CA-CB-CG	-5.08	107.52	112.60
3	C	188	THR	CA-C-N	5.08	127.59	120.28
3	C	188	THR	C-N-CA	5.08	127.59	120.28
3	C	48	ARG	N-CA-C	5.08	121.61	110.80
2	B	336	LYS	O-C-N	-5.07	116.74	122.12
2	B	355	ILE	CA-CB-CG1	5.07	119.02	110.40
1	A	3342	ARG	CA-C-N	5.06	128.69	120.60
1	A	3342	ARG	C-N-CA	5.06	128.69	120.60
3	C	280	SER	N-CA-C	-5.06	101.21	108.60
2	B	407	TRP	CB-CA-C	-5.05	102.40	110.79
3	C	346	TRP	N-CA-C	5.05	117.52	111.71
3	C	375	ALA	CA-C-O	-5.05	115.90	121.31
2	B	101	ASN	N-CA-CB	-5.05	104.50	112.13
2	B	121	ARG	NE-CZ-NH1	5.05	126.55	121.50
2	B	277	SER	N-CA-C	5.05	116.78	111.28
2	B	36	MET	O-C-N	-5.04	116.64	121.94
3	C	204	ILE	CA-C-O	5.04	125.64	120.39
2	B	242	LEU	CA-C-O	-5.04	113.64	119.59
3	C	413	MET	N-CA-C	5.04	121.54	110.80
3	C	79	ARG	NE-CZ-NH2	-5.03	114.67	119.20
3	C	88	ARG	CA-C-N	5.03	126.13	119.84
3	C	88	ARG	C-N-CA	5.03	126.13	119.84
2	B	107	HIS	CG-CD2-NE2	5.03	112.23	107.20
2	B	354	GLY	O-C-N	-5.03	116.16	122.70
3	C	147	SER	CA-C-N	5.02	125.41	119.94
3	C	147	SER	C-N-CA	5.02	125.41	119.94
1	A	3278	GLU	CA-C-N	5.02	127.41	120.29
1	A	3278	GLU	C-N-CA	5.02	127.41	120.29
1	A	3360	ALA	CA-C-N	5.01	126.88	120.56
1	A	3360	ALA	C-N-CA	5.01	126.88	120.56
2	B	324	VAL	CA-CB-CG1	5.01	118.92	110.40
2	B	308	ARG	NH1-CZ-NH2	-5.00	112.80	119.30

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3337	ARG	Sidechain
1	A	3342	ARG	Sidechain
1	A	3356	GLU	Peptide
1	A	3362	ARG	Sidechain
2	B	103	TYR	Sidechain
2	B	105	ARG	Sidechain
2	B	107	HIS	Sidechain
2	B	156	ARG	Sidechain
2	B	172	TYR	Sidechain
2	B	210	TYR	Sidechain
2	B	215	ARG	Sidechain
2	B	220	GLU	Mainchain
2	B	24	TYR	Sidechain
2	B	255	PHE	Sidechain
2	B	272	TYR	Sidechain
2	B	312	TYR	Sidechain
2	B	343	PHE	Sidechain
2	B	399	TYR	Sidechain
2	B	402	ARG	Sidechain
2	B	52	PHE	Sidechain
2	B	64	ARG	Sidechain
2	B	83	TYR	Sidechain
3	C	123	ARG	Sidechain
3	C	161	TYR	Sidechain
3	C	164	ARG	Sidechain
3	C	2	ARG	Sidechain
3	C	20	PHE	Sidechain
3	C	215	ARG	Sidechain
3	C	274	PRO	Peptide
3	C	277	SER	Peptide
3	C	278	ARG	Sidechain
3	C	284	ARG	Sidechain
3	C	309	HIS	Sidechain
3	C	319	PHE	Sidechain
3	C	322	ARG	Sidechain
3	C	342	TYR	Sidechain
3	C	359	PRO	Peptide,Mainchain
3	C	377	PHE	Sidechain
3	C	398	MET	Peptide
3	C	399	PHE	Sidechain
3	C	406	HIS	Sidechain
3	C	418	PHE	Sidechain
3	C	432	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	C	435	TYR	Sidechain
3	C	48	ARG	Sidechain
3	C	53	TYR	Peptide
3	C	61	TYR	Sidechain
3	C	80	SER	Peptide

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	1308	0	1342	3	0
2	B	3423	0	3324	24	0
3	C	3360	0	3241	19	0
All	All	8091	0	7907	45	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 3.

All (45) 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)
3:C:259:MET:HB3	3:C:268:PHE:CZ	2.27	0.69
3:C:103:TRP:CG	3:C:186:ASN:HD21	2.19	0.61
3:C:6:HIS:HE1	3:C:17:GLY:HA2	1.65	0.60
1:A:3338:SER:HB2	3:C:162:PRO:HG3	1.88	0.55
3:C:6:HIS:CE1	3:C:17:GLY:HA2	2.42	0.54
3:C:86:ILE:H	3:C:86:ILE:HD13	1.73	0.54
2:B:61:HIS:HB3	2:B:85:GLN:O	2.08	0.54
3:C:306:ASP:O	3:C:309:HIS:CE1	2.60	0.54
1:A:3287:VAL:HG21	1:A:3400:TYR:CD1	2.43	0.52
2:B:139:HIS:CE1	2:B:150:THR:HG23	2.47	0.49
2:B:346:TRP:CH2	2:B:438:ASP:HA	2.47	0.49
3:C:42:LEU:HA	3:C:47:GLU:O	2.13	0.48
2:B:75:ILE:HD12	2:B:92:LEU:HB3	1.96	0.48
2:B:273:ALA:HB2	2:B:375:VAL:HG13	1.96	0.47
2:B:139:HIS:HE1	2:B:150:THR:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:HIS:CE1	2:B:150:THR:CG2	2.98	0.47
3:C:291:LEU:CD2	3:C:375:ALA:HB3	2.45	0.47
2:B:70:LEU:HD12	2:B:70:LEU:C	2.40	0.46
2:B:173:PRO:HB3	2:B:207:GLU:HG2	1.98	0.46
3:C:9:ALA:HB3	3:C:139:HIS:HA	1.98	0.46
2:B:2:ARG:HD2	2:B:55:GLU:HB2	1.98	0.45
3:C:346:TRP:CD1	3:C:346:TRP:H	2.34	0.45
2:B:243:ARG:HG3	2:B:244:PHE:H	1.82	0.45
1:A:3294:VAL:HG11	1:A:3393:TRP:CE2	2.53	0.44
2:B:154:MET:SD	2:B:197:HIS:HB2	2.58	0.43
2:B:195:LEU:HD21	2:B:428:LEU:HD22	1.99	0.43
2:B:58:ALA:O	2:B:61:HIS:HA	2.17	0.43
3:C:210:TYR:CD1	3:C:222:PRO:HB2	2.53	0.43
2:B:346:TRP:CZ3	2:B:438:ASP:HA	2.54	0.43
3:C:292:THR:HB	3:C:335:VAL:HG11	2.01	0.42
3:C:67:LEU:HD23	3:C:92:PHE:CE2	2.54	0.42
3:C:210:TYR:HB3	3:C:214:PHE:CZ	2.55	0.42
2:B:389:ALA:HB2	2:B:429:GLU:HG3	2.02	0.42
2:B:273:ALA:HB2	2:B:375:VAL:CG1	2.51	0.41
2:B:319:TYR:HB3	2:B:373:ARG:HH12	1.84	0.41
3:C:47:GLU:C	3:C:49:ILE:H	2.28	0.41
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.82	0.41
2:B:8:HIS:CE1	2:B:17:GLY:HA3	2.55	0.41
2:B:101:ASN:HD22	2:B:143:GLY:HA2	1.86	0.41
2:B:174:ALA:HB3	2:B:177:VAL:HG21	2.02	0.41
2:B:278:ALA:HB1	2:B:283:HIS:CD2	2.56	0.41
3:C:371:LEU:HD13	3:C:374:SER:HB2	2.03	0.41
2:B:172:TYR:HA	2:B:173:PRO:HD2	1.91	0.41
3:C:1:MET:CE	3:C:47:GLU:HA	2.50	0.40
3:C:344:VAL:HG22	3:C:346:TRP:CD2	2.57	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	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
2	B	437/451 (97%)	372 (85%)	42 (10%)	23 (5%)	1	15
3	C	425/427 (100%)	364 (86%)	40 (9%)	21 (5%)	1	16
All	All	1024/1042 (98%)	888 (87%)	92 (9%)	44 (4%)	3	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ALA
2	B	129	CYS
2	B	245	ASP
2	B	264	ARG
3	C	178	SER
3	C	304	ALA
3	C	344	VAL
3	C	369	ARG
2	B	4	CYS
2	B	5	ILE
2	B	282	TYR
3	C	66	ILE
3	C	97	SER
3	C	132	LEU
3	C	181	VAL
3	C	311	ARG
3	C	359	PRO
3	C	385	GLN
2	B	3	GLU
2	B	37	PRO
2	B	146	GLY
2	B	348	PRO
2	B	360	PRO
2	B	404	PHE
3	C	222	PRO
3	C	273	ALA
3	C	303	ALA
2	B	41	THR
2	B	246	GLY
2	B	274	PRO
2	B	286	LEU

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Mol	Chain	Res	Type
2	B	35	GLN
2	B	268	PRO
2	B	275	VAL
3	C	174	SER
3	C	413	MET
3	C	340	SER
3	C	349	ASN
2	B	43	GLY
3	C	306	ASP
3	C	142	GLY
2	B	159	VAL
2	B	306	ASP
3	C	82	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/146 (100%)	143 (98%)	3 (2%)	47	65
2	B	368/377 (98%)	347 (94%)	21 (6%)	18	40
3	C	368/368 (100%)	345 (94%)	23 (6%)	16	37
All	All	882/891 (99%)	835 (95%)	47 (5%)	22	41

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3297	ILE
1	A	3355	GLU
1	A	3363	GLU
2	B	3	GLU
2	B	41	THR
2	B	42	ILE
2	B	71	GLU
2	B	83	TYR
2	B	117	LEU

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Mol	Chain	Res	Type
2	B	140	SER
2	B	192	HIS
2	B	209	ILE
2	B	288	VAL
2	B	307	PRO
2	B	334	THR
2	B	351	PHE
2	B	358	GLU
2	B	367	ASP
2	B	392	ASP
2	B	399	TYR
2	B	402	ARG
2	B	405	VAL
2	B	415	GLU
2	B	438	ASP
3	C	32	PRO
3	C	49	ILE
3	C	67	LEU
3	C	74	THR
3	C	86	ILE
3	C	89	PRO
3	C	91	ASN
3	C	184	PRO
3	C	185	TYR
3	C	186	ASN
3	C	201	THR
3	C	209	LEU
3	C	292	THR
3	C	333	LEU
3	C	346	TRP
3	C	356	CYS
3	C	359	PRO
3	C	373	MET
3	C	396	THR
3	C	413	MET
3	C	424	ASN
3	C	433	GLN
3	C	435	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3291	GLN
1	A	3292	ASN
1	A	3335	GLN
1	A	3397	GLN
2	B	15	GLN
2	B	18	ASN
2	B	88	HIS
2	B	101	ASN
2	B	139	HIS
2	B	197	HIS
2	B	283	HIS
2	B	372	GLN
3	C	28	HIS
3	C	59	ASN
3	C	107	HIS
3	C	139	HIS
3	C	258	ASN
3	C	424	ASN
3	C	433	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.

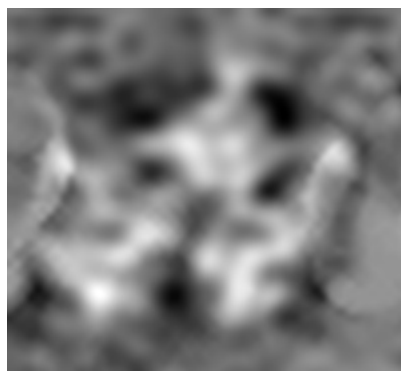
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

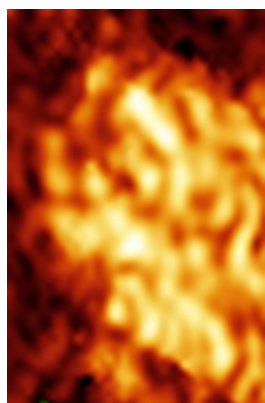


Z Index: 23

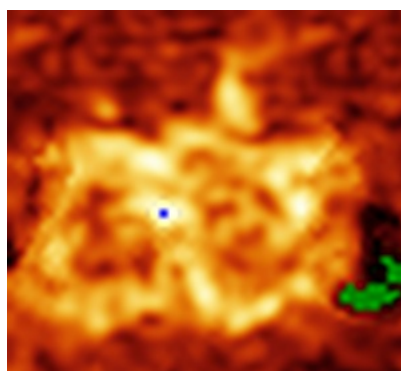
The images above show the largest variance slices of the map in three orthogonal directions.

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

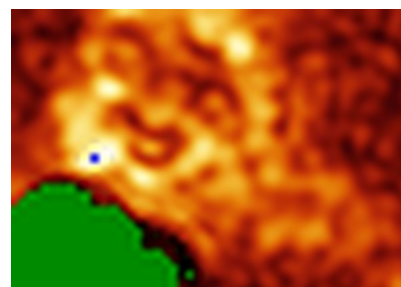
6.4.1 Primary map



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

This section was not generated.

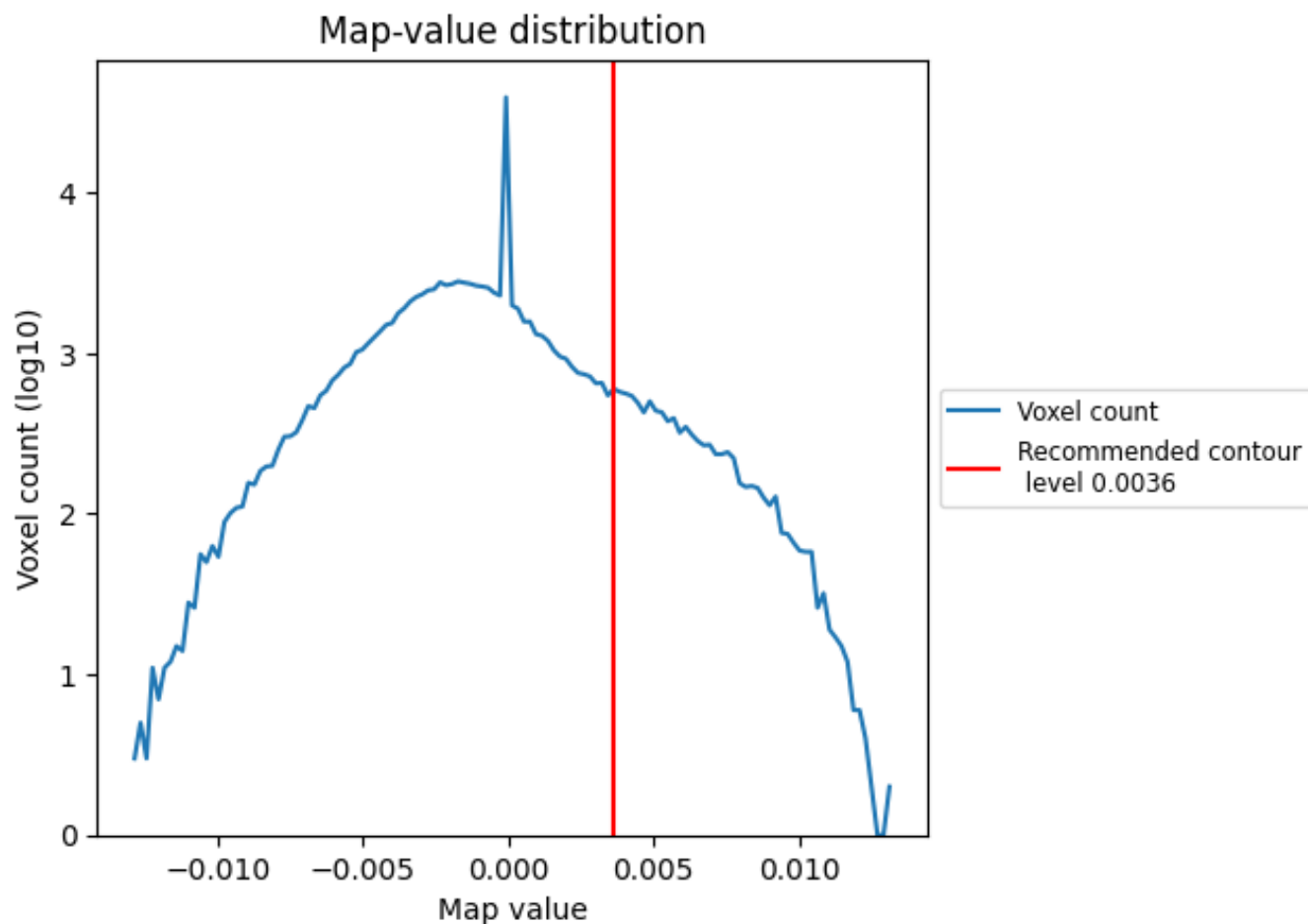
6.6 Mask visualisation

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

7 Map analysis [i](#)

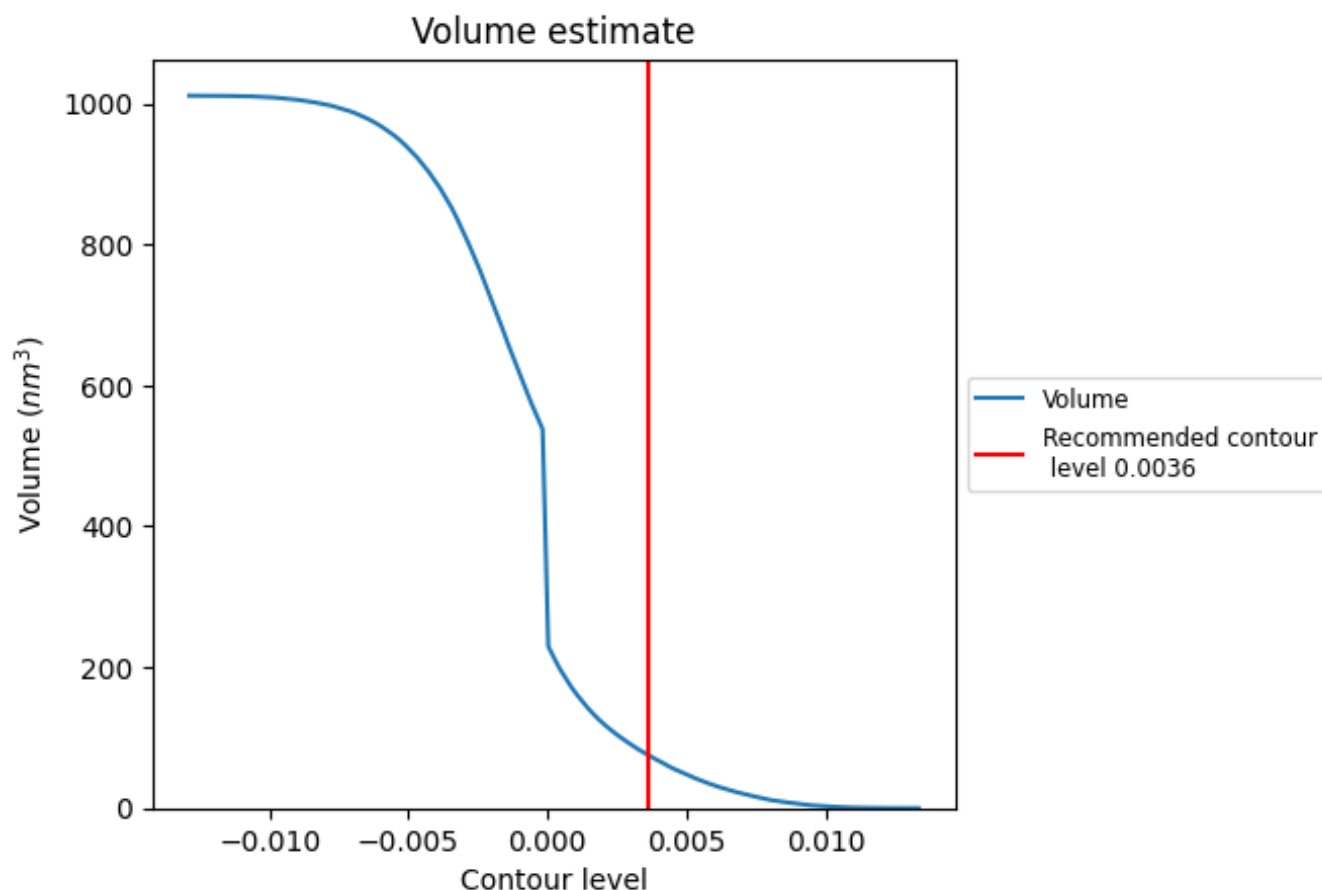
This section contains the results of statistical analysis of the map.

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.

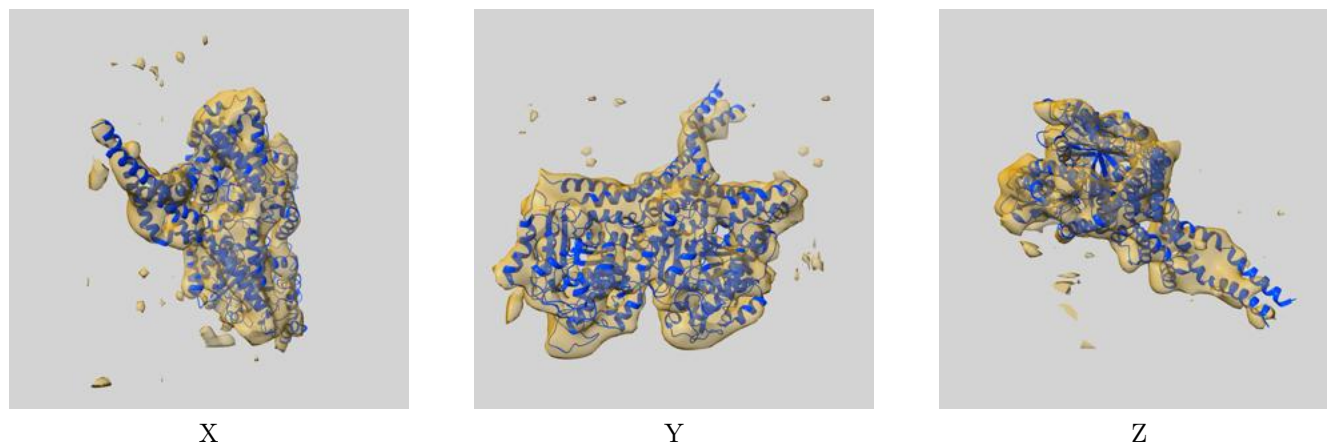
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

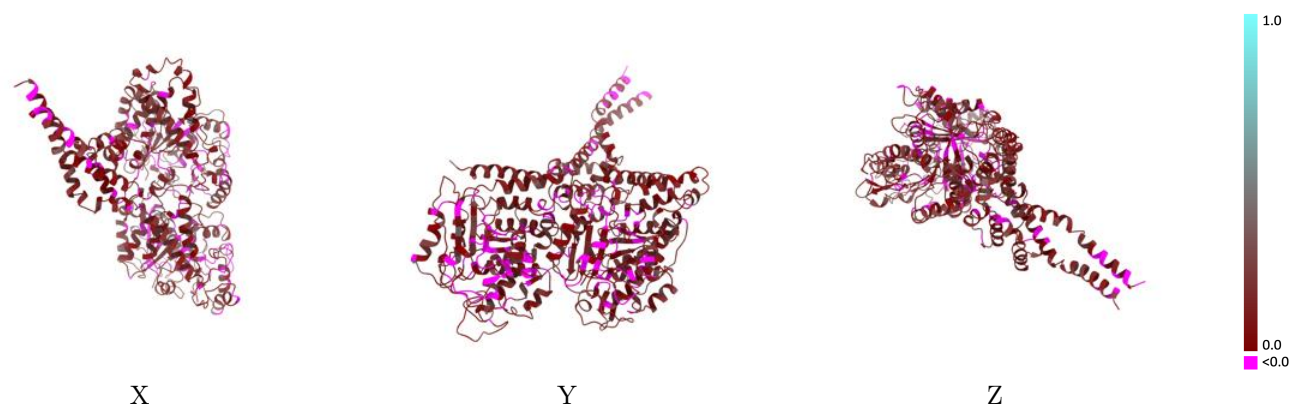
This section contains information regarding the fit between EMDB map EMD-5439 and PDB model 3J1T. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



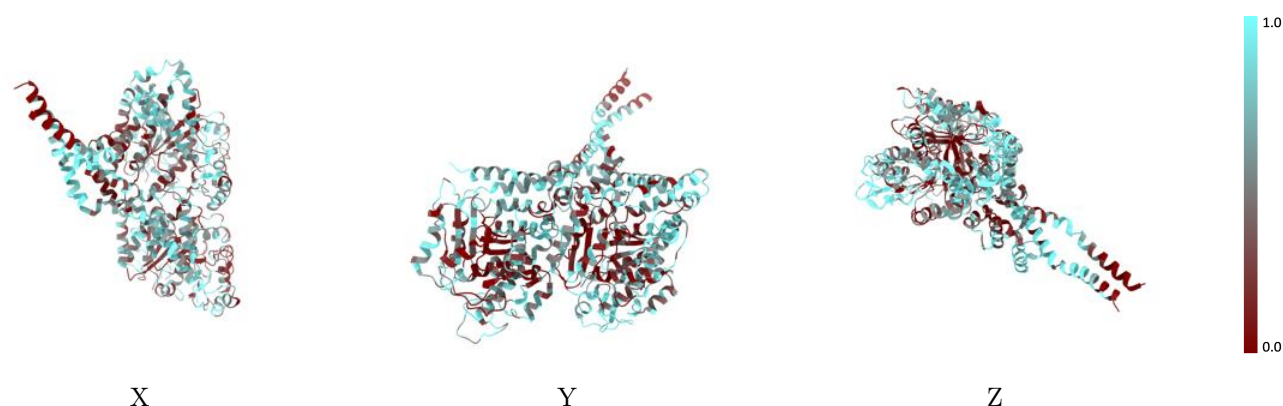
The images above show the 3D surface view of the map at the recommended contour level 0.0036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



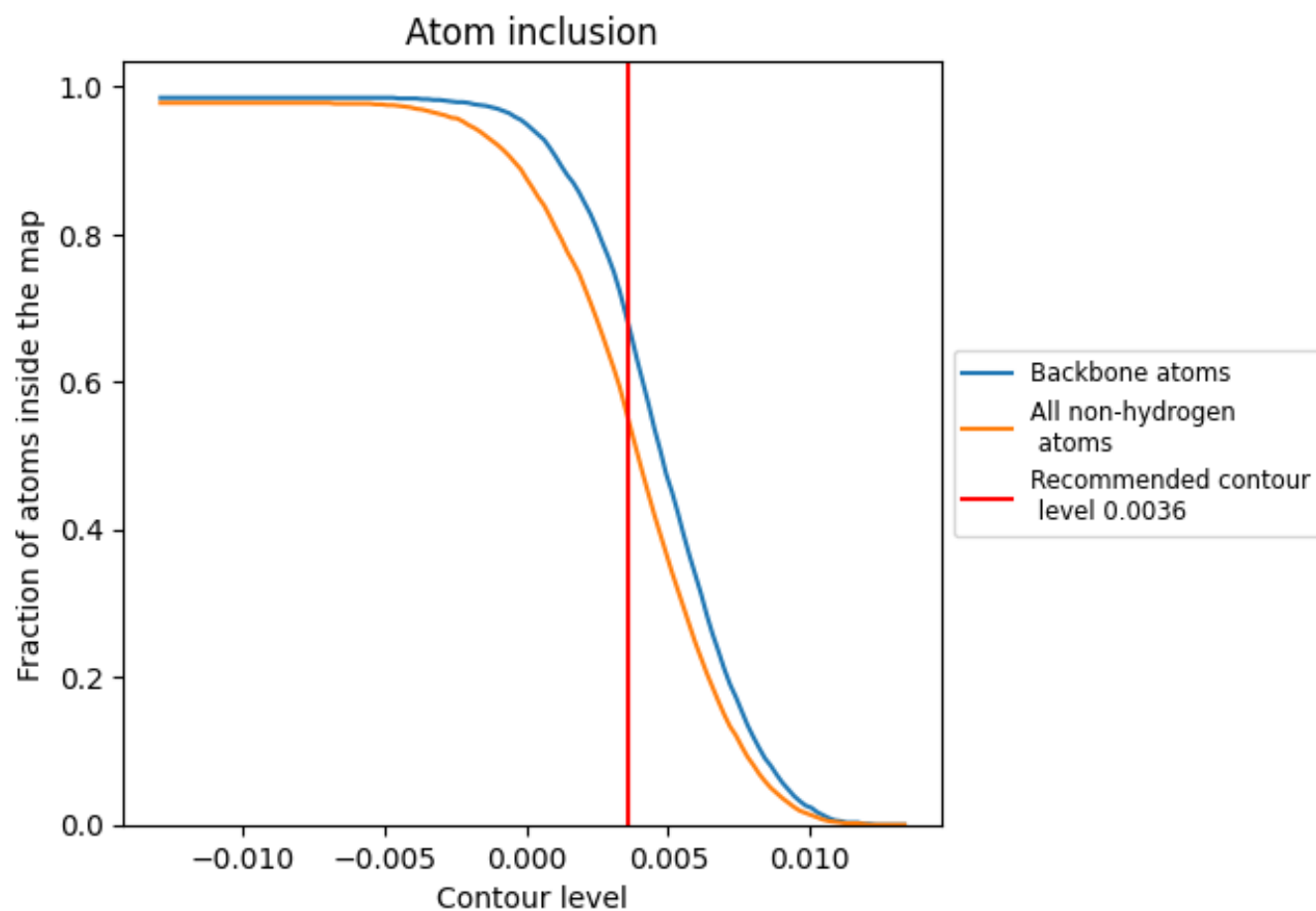
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 68% of all backbone atoms, 55% 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	0.5490	0.1140
A	0.5290	0.1140
B	0.5490	0.1150
C	0.5570	0.1130

