



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:07 AM UTC

PDB ID : 3J8X / pdb_00003j8x
EMDB ID : EMD-6187
Title : High-resolution structure of no-nucleotide kinesin on microtubules
Authors : Shang, Z.; Zhou, K.; Xu, C.; Csencsits, R.; Cochran, J.C.; Sindelar, C.V.
Deposited on : 2014-11-20
Resolution : 5.00 Å(reported)
Based on initial model : 4HNA

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:

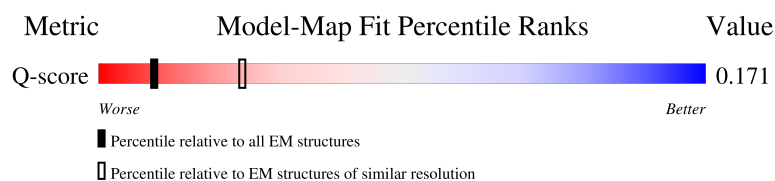
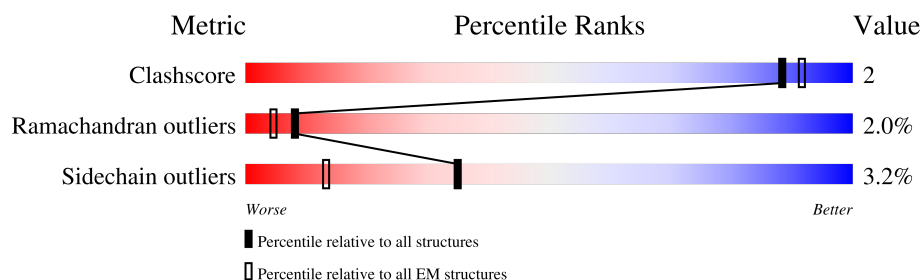
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1057 (4.50 - 5.50)

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

Mol	Chain	Length	Quality of chain
1	K	349	54% 45% 42% 9%
2	A	451	18% 43% 46% 6% 5%
3	B	445	19% 42% 46% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9295 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 Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	316	Total	C	N	O	S	0	0
			2474	1543	423	498	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	7	SER	CYS	conflict	UNP P33176
K	168	ALA	CYS	conflict	UNP P33176
K	174	SER	CYS	conflict	UNP P33176
K	330	SER	CYS	conflict	UNP P33176

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		

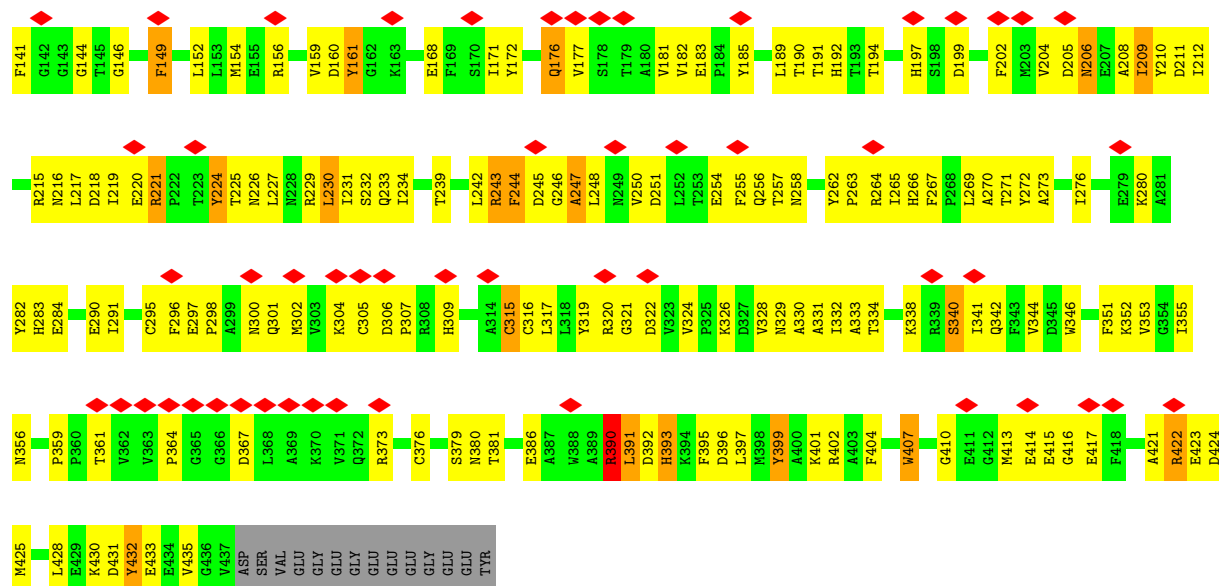
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	431	Total	C	N	O	S	0	0
			3389	2126	580	657	26		

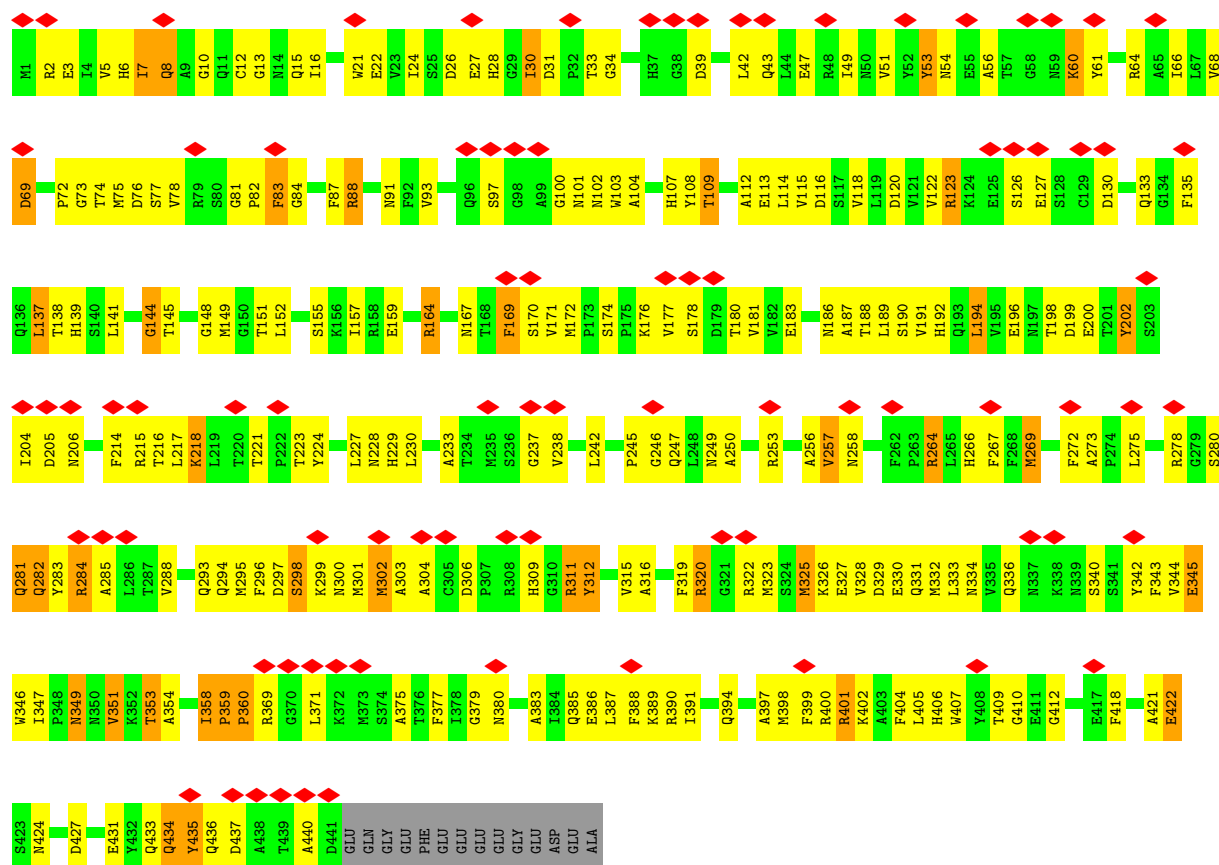
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	conflict	UNP F2Z5B2

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



• Molecule 3: Tubulin beta-2B chain



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=25.77°, rise=8.78 Å, axial sym=C1	Depositor
Number of segments used	120783	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	done within FREALIGN	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	509.44, 509.44, 191.04001	wwPDB
Map dimensions	256, 256, 96	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.99, 1.99, 1.9900001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP

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	K	2.16	74/2513 (2.9%)	2.42	159/3389 (4.7%)
2	A	2.15	92/3450 (2.7%)	2.43	219/4685 (4.7%)
3	B	2.13	98/3464 (2.8%)	2.48	238/4692 (5.1%)
All	All	2.14	264/9427 (2.8%)	2.45	616/12766 (4.8%)

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	K	0	10
2	A	1	19
3	B	0	18
All	All	1	47

All (264) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	11	VAL	CA-C	-11.38	1.40	1.53
1	K	96	GLU	CA-C	-11.11	1.42	1.52
2	A	10	GLY	N-CA	9.98	1.54	1.45
2	A	8	HIS	CE1-NE2	9.42	1.42	1.32
1	K	169	THR	CA-C	-9.38	1.41	1.52
2	A	10	GLY	CA-C	-9.28	1.42	1.52
3	B	407	TRP	N-CA	-8.94	1.34	1.46
1	K	106	GLY	C-N	8.65	1.44	1.33
3	B	39	ASP	CA-CB	8.36	1.66	1.53
3	B	412	GLY	CA-C	-8.27	1.39	1.51
2	A	114	ILE	CA-CB	-8.22	1.45	1.54
1	K	179	VAL	CA-C	-8.05	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	162	VAL	N-CA	8.02	1.53	1.46
3	B	406	HIS	CE1-NE2	7.90	1.40	1.32
2	A	224	TYR	CA-C	-7.89	1.42	1.52
3	B	227	LEU	CA-C	-7.66	1.42	1.52
1	K	286	LEU	C-N	7.60	1.43	1.33
1	K	108	ILE	CA-C	7.50	1.60	1.52
1	K	198	ASN	C-N	7.46	1.43	1.33
3	B	186	ASN	CA-C	7.45	1.62	1.52
2	A	295	CYS	N-CA	-7.37	1.36	1.46
2	A	254	GLU	CA-C	-7.36	1.42	1.52
2	A	202	PHE	CA-CB	7.29	1.62	1.52
1	K	51	VAL	CA-C	-7.25	1.46	1.53
2	A	19	ALA	CA-C	7.20	1.62	1.52
2	A	36	MET	C-N	-7.13	1.27	1.34
2	A	171	ILE	N-CA	7.12	1.55	1.46
2	A	306	ASP	CA-C	7.01	1.60	1.52
3	B	437	ASP	N-CA	-6.99	1.37	1.46
2	A	87	PHE	CA-C	6.97	1.62	1.52
3	B	266	HIS	CE1-NE2	6.94	1.39	1.32
2	A	69	ASP	CA-C	-6.88	1.44	1.52
3	B	380	ASN	N-CA	-6.86	1.36	1.46
1	K	276	PRO	N-CA	-6.79	1.39	1.46
1	K	200	HIS	CA-CB	6.78	1.63	1.53
1	K	144	ASP	C-N	6.74	1.43	1.33
1	K	63	ASN	CA-CB	6.71	1.63	1.53
3	B	237	GLY	CA-C	-6.70	1.42	1.51
2	A	266	HIS	CD2-NE2	6.68	1.45	1.37
3	B	230	LEU	N-CA	-6.67	1.37	1.46
2	A	99	ALA	CA-C	-6.66	1.43	1.52
2	A	176	GLN	CA-C	6.64	1.58	1.52
3	B	127	GLU	C-N	6.61	1.43	1.33
1	K	129	HIS	N-CA	-6.58	1.38	1.46
3	B	347	ILE	N-CA	6.54	1.51	1.46
2	A	7	ILE	CA-CB	-6.54	1.46	1.54
1	K	187	LYS	C-N	6.50	1.42	1.33
2	A	119	LEU	N-CA	-6.50	1.38	1.46
3	B	13	GLY	CA-C	6.48	1.59	1.52
3	B	215	ARG	C-N	6.48	1.41	1.33
3	B	135	PHE	N-CA	-6.46	1.38	1.46
1	K	16	ARG	NE-CZ	6.46	1.40	1.33
3	B	205	ASP	N-CA	6.46	1.53	1.46
3	B	138	THR	CA-C	-6.45	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	299	LYS	CA-CB	6.45	1.63	1.53
2	A	309	HIS	CA-C	6.43	1.61	1.52
3	B	422	GLU	CA-CB	6.43	1.63	1.53
3	B	329	ASP	CA-C	6.42	1.61	1.52
2	A	276	ILE	CA-C	-6.40	1.46	1.52
1	K	214	GLN	CA-C	-6.39	1.44	1.52
3	B	343	PHE	C-N	6.38	1.41	1.33
3	B	108	TYR	CA-C	-6.35	1.44	1.52
1	K	227	LEU	CA-CB	6.34	1.61	1.53
2	A	266	HIS	CA-CB	6.34	1.62	1.53
1	K	37	ASP	N-CA	-6.34	1.38	1.46
3	B	312	TYR	CA-C	-6.34	1.44	1.52
2	A	309	HIS	CE1-NE2	6.33	1.38	1.32
2	A	65	ALA	N-CA	-6.30	1.38	1.46
3	B	199	ASP	C-O	-6.29	1.18	1.23
2	A	291	ILE	CA-CB	-6.29	1.45	1.54
2	A	373	ARG	N-CA	-6.29	1.38	1.45
2	A	31	GLN	N-CA	-6.25	1.36	1.45
3	B	188	THR	CA-C	-6.23	1.45	1.52
1	K	41	ILE	CA-CB	6.23	1.61	1.53
3	B	390	ARG	CA-C	-6.22	1.44	1.52
1	K	25	ARG	CD-NE	6.20	1.54	1.46
2	A	376	CYS	C-O	-6.20	1.17	1.24
2	A	242	LEU	N-CA	6.20	1.53	1.46
2	A	113	GLU	N-CA	-6.18	1.38	1.46
2	A	321	GLY	N-CA	6.18	1.51	1.45
3	B	107	HIS	ND1-CE1	6.14	1.38	1.32
2	A	118	VAL	CA-CB	6.13	1.61	1.54
3	B	404	PHE	C-N	6.13	1.42	1.33
2	A	352	LYS	CA-CB	6.11	1.62	1.53
3	B	435	TYR	CA-C	-6.10	1.44	1.52
1	K	10	LYS	CA-CB	6.08	1.61	1.52
3	B	409	THR	CA-C	-6.05	1.44	1.52
2	A	199	ASP	CA-C	-6.03	1.45	1.52
1	K	17	PRO	CA-C	6.02	1.60	1.52
3	B	138	THR	C-N	-5.99	1.25	1.33
1	K	105	MET	CG-SD	5.97	1.95	1.80
2	A	331	ALA	N-CA	-5.97	1.39	1.46
3	B	278	ARG	CA-CB	5.94	1.60	1.53
3	B	107	HIS	CD2-NE2	5.93	1.44	1.37
3	B	379	GLY	N-CA	5.92	1.51	1.45
1	K	162	VAL	CA-C	-5.92	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ASN	CA-CB	5.92	1.63	1.53
1	K	187	LYS	CA-CB	-5.91	1.43	1.53
2	A	4	CYS	CA-CB	5.89	1.61	1.53
1	K	71	LYS	C-O	-5.86	1.17	1.24
3	B	345	GLU	C-N	5.85	1.42	1.33
2	A	417	GLU	CA-C	5.83	1.60	1.52
1	K	295	ARG	CD-NE	5.81	1.54	1.46
2	A	176	GLN	N-CA	-5.81	1.41	1.46
2	A	316	CYS	C-N	5.81	1.41	1.33
3	B	157	ILE	N-CA	-5.79	1.39	1.46
3	B	64	ARG	CD-NE	5.76	1.54	1.46
3	B	164	ARG	N-CA	-5.75	1.38	1.45
2	A	392	ASP	N-CA	-5.75	1.39	1.46
1	K	73	VAL	CA-CB	5.73	1.60	1.54
1	K	87	THR	N-CA	5.72	1.53	1.46
2	A	338	LYS	C-N	5.72	1.41	1.33
3	B	200	GLU	CA-C	-5.71	1.46	1.52
3	B	433	GLN	CA-CB	5.71	1.62	1.53
1	K	92	THR	N-CA	5.69	1.53	1.46
1	K	134	TYR	CA-C	-5.67	1.46	1.52
2	A	273	ALA	CA-C	5.66	1.59	1.52
1	K	285	ILE	N-CA	5.66	1.53	1.46
2	A	224	TYR	CA-CB	5.66	1.62	1.53
3	B	60	LYS	CA-C	-5.65	1.45	1.52
2	A	132	LEU	CA-CB	5.64	1.62	1.53
3	B	369	ARG	CD-NE	5.64	1.54	1.46
1	K	100	HIS	CE1-NE2	5.64	1.38	1.32
2	A	209	ILE	CA-CB	-5.63	1.48	1.54
2	A	144	GLY	CA-C	-5.62	1.44	1.51
3	B	329	ASP	CA-CB	5.62	1.62	1.53
3	B	133	GLN	CA-C	-5.60	1.46	1.52
2	A	340	SER	C-O	-5.59	1.17	1.24
2	A	346	TRP	CD2-CE3	-5.58	1.31	1.40
1	K	101	ASP	C-O	-5.58	1.17	1.24
2	A	35	GLN	CA-CB	5.58	1.62	1.53
2	A	181	VAL	C-N	-5.58	1.26	1.33
3	B	328	VAL	N-CA	-5.57	1.38	1.46
3	B	13	GLY	C-N	-5.56	1.26	1.33
2	A	386	GLU	CA-C	5.56	1.60	1.52
3	B	334	ASN	CA-C	-5.55	1.45	1.52
1	K	215	GLU	C-N	5.55	1.41	1.33
3	B	181	VAL	CA-CB	-5.55	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	391	ILE	CA-C	5.54	1.59	1.52
3	B	2	ARG	CD-NE	5.53	1.53	1.46
3	B	283	TYR	CA-CB	5.53	1.62	1.53
3	B	172	MET	CA-CB	5.53	1.60	1.53
3	B	135	PHE	CA-CB	5.51	1.61	1.53
3	B	139	HIS	CG-CD2	5.50	1.41	1.35
2	A	121	ARG	CD-NE	5.49	1.53	1.46
1	K	181	ASP	CA-C	5.49	1.59	1.52
1	K	43	SER	N-CA	-5.49	1.39	1.46
1	K	191	HIS	CE1-NE2	5.49	1.38	1.32
1	K	113	GLN	C-N	5.48	1.41	1.33
1	K	301	CYS	C-N	5.48	1.41	1.33
3	B	5	VAL	C-N	5.47	1.40	1.33
1	K	279	ASP	C-N	5.47	1.41	1.33
2	A	109	THR	CA-C	-5.46	1.46	1.52
3	B	100	GLY	C-N	5.44	1.41	1.33
1	K	264	VAL	CA-CB	5.44	1.61	1.54
3	B	303	ALA	N-CA	-5.44	1.39	1.46
3	B	327	GLU	N-CA	-5.43	1.39	1.46
3	B	280	SER	N-CA	5.42	1.53	1.46
2	A	297	GLU	CA-C	5.42	1.59	1.53
2	A	329	ASN	C-O	-5.41	1.17	1.24
2	A	191	THR	C-N	-5.41	1.27	1.33
2	A	239	THR	C-N	5.40	1.41	1.33
3	B	93	VAL	CA-C	-5.40	1.45	1.52
2	A	25	CYS	CA-C	-5.39	1.46	1.52
3	B	360	PRO	CA-C	-5.39	1.45	1.52
2	A	423	GLU	C-N	5.38	1.40	1.33
1	K	14	ARG	CA-C	-5.38	1.46	1.52
2	A	159	VAL	CA-CB	-5.37	1.47	1.54
1	K	13	CYS	C-O	-5.36	1.17	1.23
2	A	379	SER	CA-C	-5.36	1.46	1.52
3	B	107	HIS	CG-ND1	5.36	1.44	1.38
3	B	3	GLU	C-N	5.35	1.40	1.33
1	K	243	ALA	CA-C	-5.35	1.46	1.53
1	K	271	GLY	C-N	5.34	1.41	1.33
3	B	68	VAL	C-O	5.34	1.30	1.24
3	B	42	LEU	CA-CB	5.33	1.61	1.53
1	K	93	HIS	CE1-NE2	5.33	1.37	1.32
1	K	120	TYR	C-N	5.33	1.41	1.33
3	B	330	GLU	N-CA	-5.33	1.40	1.46
2	A	248	LEU	CA-C	5.33	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	107	ILE	C-N	5.32	1.39	1.33
3	B	190	SER	CA-CB	5.32	1.61	1.53
1	K	308	ASN	N-CA	5.32	1.52	1.46
2	A	9	VAL	CA-C	-5.31	1.46	1.52
2	A	332	ILE	N-CA	-5.31	1.40	1.46
1	K	168	ALA	N-CA	5.29	1.52	1.45
2	A	84	ARG	C-N	5.29	1.41	1.33
2	A	270	ALA	CA-CB	5.28	1.62	1.53
3	B	88	ARG	CD-NE	5.28	1.53	1.46
2	A	307	PRO	N-CA	5.28	1.54	1.47
2	A	321	GLY	CA-C	-5.28	1.46	1.51
3	B	436	GLN	CA-C	-5.28	1.46	1.52
2	A	428	LEU	CA-CB	5.27	1.61	1.53
2	A	6	SER	CA-CB	-5.26	1.46	1.53
2	A	298	PRO	C-O	-5.26	1.17	1.24
1	K	223	LEU	C-N	5.25	1.39	1.33
1	K	228	TYR	CA-CB	5.25	1.60	1.53
3	B	388	PHE	CA-CB	5.24	1.61	1.53
3	B	399	PHE	N-CA	-5.23	1.40	1.46
3	B	7	ILE	CA-C	-5.23	1.45	1.52
2	A	189	LEU	CB-CG	5.22	1.63	1.53
1	K	84	TYR	CA-C	-5.22	1.46	1.52
3	B	97	SER	CA-CB	5.22	1.61	1.53
3	B	272	PHE	C-N	5.21	1.40	1.33
2	A	333	ALA	CA-C	-5.20	1.46	1.52
2	A	52	PHE	N-CA	-5.20	1.39	1.46
3	B	266	HIS	CA-CB	-5.20	1.46	1.53
2	A	397	LEU	CA-C	-5.19	1.46	1.52
3	B	122	VAL	CA-C	-5.19	1.44	1.52
1	K	166	LYS	CA-CB	5.18	1.60	1.53
2	A	402	ARG	CA-C	-5.18	1.45	1.53
3	B	246	GLY	CA-C	5.17	1.59	1.51
2	A	301	GLN	C-N	5.16	1.41	1.33
2	A	185	TYR	CA-CB	5.16	1.61	1.53
2	A	256	GLN	CA-C	-5.15	1.46	1.52
2	A	77	GLU	CA-CB	5.15	1.61	1.53
3	B	294	GLN	CA-C	5.15	1.59	1.52
1	K	21	SER	C-O	-5.15	1.18	1.24
2	A	346	TRP	CA-C	5.14	1.59	1.52
2	A	84	ARG	CD-NE	5.14	1.53	1.46
3	B	369	ARG	NE-CZ	5.13	1.38	1.33
3	B	137	LEU	CA-CB	5.13	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	194	LEU	CA-CB	5.13	1.61	1.53
2	A	416	GLY	CA-C	-5.12	1.44	1.51
2	A	373	ARG	NE-CZ	5.12	1.38	1.33
1	K	292	GLY	N-CA	5.12	1.52	1.45
3	B	358	ILE	CA-CB	5.12	1.60	1.54
3	B	320	ARG	CA-CB	5.11	1.61	1.53
1	K	52	PHE	CA-CB	5.11	1.61	1.53
1	K	206	SER	CA-CB	5.11	1.63	1.53
1	K	129	HIS	CD2-NE2	5.11	1.43	1.37
1	K	139	LEU	CB-CG	5.10	1.63	1.53
1	K	223	LEU	N-CA	-5.10	1.39	1.46
1	K	263	ASN	C-N	5.10	1.40	1.33
1	K	310	SER	N-CA	5.10	1.52	1.46
3	B	284	ARG	N-CA	5.10	1.53	1.46
1	K	205	HIS	CA-CB	-5.09	1.44	1.53
3	B	304	ALA	CA-C	5.09	1.59	1.53
3	B	3	GLU	N-CA	5.08	1.52	1.46
3	B	21	TRP	N-CA	-5.08	1.40	1.46
1	K	139	LEU	CA-C	5.07	1.60	1.53
2	A	305	CYS	N-CA	-5.07	1.39	1.45
1	K	41	ILE	CA-C	-5.07	1.46	1.52
2	A	192	HIS	CG-CD2	-5.06	1.30	1.35
2	A	127	ASP	C-N	5.06	1.41	1.33
1	K	67	LYS	CA-CB	5.06	1.61	1.53
3	B	302	MET	N-CA	5.05	1.52	1.46
3	B	353	THR	CA-C	-5.04	1.46	1.52
1	K	256	LYS	CA-CB	5.04	1.61	1.53
3	B	346	TRP	CA-C	5.04	1.59	1.52
2	A	152	LEU	C-N	5.03	1.40	1.33
3	B	61	TYR	CA-C	-5.03	1.46	1.52
3	B	389	LYS	C-O	-5.03	1.18	1.24
1	K	205	HIS	CD2-NE2	-5.03	1.32	1.37
3	B	112	ALA	CA-CB	5.02	1.61	1.53
3	B	188	THR	CA-CB	-5.02	1.45	1.53
2	A	246	GLY	CA-C	5.02	1.58	1.51
1	K	241	THR	C-O	-5.01	1.17	1.24
2	A	407	TRP	CA-C	-5.01	1.46	1.52
2	A	396	ASP	CA-CB	5.01	1.61	1.53
3	B	174	SER	CA-C	5.01	1.59	1.52
1	K	231	ASP	CA-C	5.00	1.59	1.52
3	B	375	ALA	CA-C	-5.00	1.46	1.52
3	B	275	LEU	CA-CB	5.00	1.59	1.52

All (616) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	359	PRO	CA-C-N	13.53	133.52	119.85
3	B	359	PRO	C-N-CA	13.53	133.52	119.85
3	B	135	PHE	CA-CB-CG	-12.42	101.38	113.80
2	A	65	ALA	O-C-N	-10.54	111.20	123.22
2	A	211	ASP	CA-C-N	10.48	133.76	120.56
2	A	211	ASP	C-N-CA	10.48	133.76	120.56
2	A	415	GLU	N-CA-C	10.38	122.59	111.28
2	A	135	PHE	CA-CB-CG	-10.33	103.47	113.80
1	K	198	ASN	CA-CB-CG	-10.32	102.28	112.60
1	K	278	ARG	N-CA-C	10.17	123.31	111.11
2	A	433	GLU	CA-C-O	10.12	131.11	119.27
3	B	39	ASP	CA-CB-CG	-10.01	102.59	112.60
2	A	14	VAL	N-CA-C	9.97	119.97	110.30
3	B	322	ARG	NE-CZ-NH2	9.77	127.99	119.20
2	A	10	GLY	N-CA-C	-9.75	102.09	112.04
3	B	214	PHE	N-CA-C	9.49	121.39	111.14
3	B	344	VAL	N-CA-CB	9.40	122.73	110.13
3	B	102	ASN	CA-CB-CG	9.40	122.00	112.60
3	B	167	ASN	O-C-N	-9.38	111.89	123.05
2	A	301	GLN	OE1-CD-NE2	-9.29	113.31	122.60
2	A	110	ILE	CA-C-N	9.19	130.32	120.03
2	A	110	ILE	C-N-CA	9.19	130.32	120.03
1	K	308	ASN	OD1-CG-ND2	-9.10	113.50	122.60
2	A	212	ILE	CA-C-O	-9.01	111.62	121.17
3	B	109	THR	CA-C-N	8.98	132.65	120.44
3	B	109	THR	C-N-CA	8.98	132.65	120.44
1	K	69	ILE	N-CA-CB	8.88	120.37	110.51
2	A	49	PHE	CA-CB-CG	-8.80	105.00	113.80
1	K	304	PRO	N-CA-C	-8.77	102.18	114.98
1	K	30	ILE	N-CA-C	8.71	119.52	110.72
3	B	114	LEU	O-C-N	-8.69	112.24	122.15
1	K	278	ARG	NE-CZ-NH2	-8.64	111.43	119.20
1	K	205	HIS	N-CA-CB	8.63	122.65	109.97
2	A	297	GLU	O-C-N	-8.50	114.84	121.47
3	B	107	HIS	CA-CB-CG	8.49	122.29	113.80
2	A	226	ASN	CA-CB-CG	-8.46	104.14	112.60
2	A	401	LYS	N-CA-C	8.43	120.47	111.28
3	B	272	PHE	N-CA-CB	-8.36	97.00	111.55
1	K	180	MET	N-CA-C	8.32	120.13	111.14
1	K	108	ILE	O-C-N	-8.23	111.72	121.10
3	B	180	THR	CA-C-N	8.20	130.72	120.72
3	B	180	THR	C-N-CA	8.20	130.72	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	30	ILE	CA-C-N	8.19	132.12	120.49
3	B	30	ILE	C-N-CA	8.19	132.12	120.49
2	A	367	ASP	CA-CB-CG	-8.16	104.44	112.60
2	A	244	PHE	CA-CB-CG	-8.15	105.65	113.80
2	A	296	PHE	CA-CB-CG	-8.09	105.71	113.80
2	A	315	CYS	CA-C-O	8.09	130.07	120.20
3	B	24	ILE	N-CA-C	8.06	118.84	110.62
2	A	334	THR	O-C-N	-8.03	113.73	122.09
2	A	433	GLU	O-C-N	-8.04	111.45	122.46
1	K	196	ASN	CA-CB-CG	7.97	120.57	112.60
1	K	230	VAL	N-CA-CB	-7.95	100.43	111.25
2	A	161	TYR	CA-CB-CG	-7.95	99.58	113.90
3	B	351	VAL	O-C-N	-7.94	113.99	122.81
2	A	269	LEU	O-C-N	-7.80	112.34	122.72
3	B	75	MET	CG-SD-CE	-7.78	83.79	100.90
1	K	183	ILE	N-CA-CB	7.75	121.08	110.54
3	B	139	HIS	CA-CB-CG	-7.73	106.07	113.80
2	A	149	PHE	CA-CB-CG	-7.71	106.09	113.80
3	B	189	LEU	O-C-N	-7.70	113.96	122.12
1	K	253	ASN	OD1-CG-ND2	-7.69	114.91	122.60
3	B	281	GLN	CA-C-N	7.51	135.22	121.70
3	B	281	GLN	C-N-CA	7.51	135.22	121.70
3	B	431	GLU	O-C-N	-7.50	112.61	122.59
3	B	183	GLU	CA-C-N	7.48	127.19	119.56
3	B	183	GLU	C-N-CA	7.48	127.19	119.56
2	A	189	LEU	CA-C-N	7.43	130.56	120.38
2	A	189	LEU	C-N-CA	7.43	130.56	120.38
3	B	133	GLN	OE1-CD-NE2	-7.42	115.17	122.60
2	A	140	SER	CA-C-O	7.39	128.96	120.98
2	A	243	ARG	NE-CZ-NH1	7.38	128.88	121.50
3	B	178	SER	N-CA-C	7.37	120.37	110.35
2	A	395	PHE	CA-C-N	7.35	130.44	120.38
2	A	395	PHE	C-N-CA	7.35	130.44	120.38
1	K	96	GLU	CA-C-O	7.33	128.71	119.61
2	A	141	PHE	N-CA-C	7.33	118.91	111.07
1	K	60	GLN	OE1-CD-NE2	-7.32	115.28	122.60
3	B	399	PHE	CA-C-N	7.32	131.43	120.31
3	B	399	PHE	C-N-CA	7.32	131.43	120.31
2	A	326	LYS	CA-C-O	7.29	128.21	120.70
2	A	139	HIS	CB-CG-CD2	-7.29	121.72	131.20
1	K	35	GLY	CA-C-N	7.27	130.62	120.29
1	K	35	GLY	C-N-CA	7.27	130.62	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	205	ASP	CA-CB-CG	7.23	119.83	112.60
2	A	410	GLY	O-C-N	-7.19	115.20	122.17
2	A	424	ASP	N-CA-C	7.17	118.74	111.07
2	A	392	ASP	CA-CB-CG	7.17	119.77	112.60
3	B	300	ASN	CA-CB-CG	-7.17	105.43	112.60
3	B	388	PHE	CA-C-N	7.17	129.88	120.28
3	B	388	PHE	C-N-CA	7.17	129.88	120.28
1	K	21	SER	N-CA-CB	7.16	120.38	110.01
3	B	27	GLU	O-C-N	-7.13	113.57	122.20
2	A	141	PHE	CA-C-O	7.13	128.30	120.82
2	A	11	GLN	OE1-CD-NE2	7.10	129.70	122.60
3	B	206	ASN	CA-CB-CG	-7.09	105.51	112.60
1	K	60	GLN	CA-C-N	7.08	130.05	120.77
1	K	60	GLN	C-N-CA	7.08	130.05	120.77
2	A	245	ASP	O-C-N	-7.06	114.80	122.85
2	A	399	TYR	N-CA-C	7.06	118.97	111.28
2	A	34	GLY	CA-C-N	7.05	130.82	120.95
2	A	34	GLY	C-N-CA	7.05	130.82	120.95
2	A	334	THR	CA-C-O	7.04	128.43	120.90
3	B	409	THR	N-CA-CB	7.02	121.17	110.28
3	B	422	GLU	N-CA-C	-7.02	103.56	111.14
3	B	233	ALA	O-C-N	-6.99	114.71	122.12
3	B	196	GLU	CA-C-O	6.97	127.97	120.24
1	K	191	HIS	CA-CB-CG	-6.96	106.84	113.80
1	K	254	ILE	CA-C-N	6.96	129.93	120.54
1	K	254	ILE	C-N-CA	6.96	129.93	120.54
3	B	326	LYS	CA-C-N	6.93	130.85	120.31
3	B	326	LYS	C-N-CA	6.93	130.85	120.31
3	B	397	ALA	N-CA-CB	-6.92	99.30	109.82
1	K	21	SER	CB-CA-C	-6.92	100.02	110.88
2	A	272	TYR	CB-CG-CD2	-6.89	110.47	120.80
2	A	342	GLN	OE1-CD-NE2	-6.88	115.72	122.60
3	B	149	MET	O-C-N	-6.88	114.88	122.03
2	A	171	ILE	CA-C-N	6.83	130.76	121.20
2	A	171	ILE	C-N-CA	6.83	130.76	121.20
1	K	116	PHE	CA-CB-CG	-6.83	106.97	113.80
2	A	172	TYR	O-C-N	-6.81	115.52	121.31
1	K	298	ILE	CA-C-O	-6.79	113.26	120.53
3	B	405	LEU	CA-C-O	6.79	127.62	120.42
2	A	206	ASN	N-CA-C	-6.79	106.88	114.62
1	K	200	HIS	CA-CB-CG	-6.78	107.02	113.80
3	B	221	THR	CA-C-N	6.77	128.30	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	221	THR	C-N-CA	6.77	128.30	119.84
2	A	177	VAL	O-C-N	-6.76	114.12	122.57
2	A	156	ARG	CA-C-N	6.74	131.48	120.63
2	A	156	ARG	C-N-CA	6.74	131.48	120.63
1	K	101	ASP	O-C-N	-6.73	115.59	121.31
2	A	306	ASP	CB-CA-C	6.73	117.82	110.08
3	B	315	VAL	N-CA-C	-6.72	98.44	108.46
3	B	15	GLN	N-CA-CB	6.72	119.75	110.01
3	B	390	ARG	CB-CA-C	6.71	122.99	110.70
3	B	151	THR	N-CA-C	6.70	118.66	111.36
2	A	262	TYR	N-CA-C	-6.69	99.92	109.62
3	B	434	GLN	N-CA-C	-6.65	104.11	111.82
1	K	129	HIS	ND1-CG-CD2	6.64	112.74	106.10
1	K	31	ALA	N-CA-C	6.63	119.85	110.50
2	A	424	ASP	CA-C-O	6.63	127.78	120.82
2	A	257	THR	N-CA-CB	6.62	119.81	109.94
2	A	31	GLN	O-C-N	-6.61	114.12	121.53
3	B	242	LEU	N-CA-CB	6.61	120.25	110.33
3	B	230	LEU	N-CA-C	6.61	119.82	111.69
3	B	139	HIS	N-CA-CB	-6.60	100.81	110.84
3	B	266	HIS	CA-CB-CG	6.60	120.40	113.80
2	A	283	HIS	O-C-N	-6.60	115.13	122.12
3	B	108	TYR	CB-CG-CD1	6.58	130.68	120.80
3	B	410	GLY	O-C-N	-6.57	115.89	122.19
2	A	283	HIS	CA-CB-CG	6.56	120.36	113.80
1	K	25	ARG	NE-CZ-NH1	6.56	128.06	121.50
3	B	64	ARG	O-C-N	6.54	130.88	122.71
3	B	336	GLN	OE1-CD-NE2	6.53	129.13	122.60
3	B	406	HIS	ND1-CG-CD2	6.52	112.62	106.10
3	B	76	ASP	CA-C-O	6.52	127.33	120.42
1	K	284	ARG	NE-CZ-NH2	6.51	125.06	119.20
2	A	210	TYR	CA-C-N	6.51	129.53	120.29
2	A	210	TYR	C-N-CA	6.51	129.53	120.29
3	B	186	ASN	CA-CB-CG	-6.48	106.12	112.60
3	B	427	ASP	N-CA-CB	6.47	119.63	110.12
1	K	204	SER	O-C-N	-6.46	115.61	123.30
2	A	421	ALA	CA-C-N	6.46	128.93	120.28
2	A	421	ALA	C-N-CA	6.46	128.93	120.28
2	A	181	VAL	N-CA-C	-6.45	103.97	111.00
3	B	296	PHE	CA-C-O	6.44	127.36	119.11
1	K	19	ASN	CA-CB-CG	-6.44	106.16	112.60
3	B	421	ALA	CA-C-N	6.43	129.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	421	ALA	C-N-CA	6.43	129.19	120.44
1	K	96	GLU	O-C-N	-6.42	114.43	121.95
3	B	402	LYS	N-CA-CB	6.42	121.34	110.49
3	B	391	ILE	N-CA-CB	6.42	118.06	110.55
3	B	73	GLY	O-C-N	-6.42	116.74	122.77
3	B	159	GLU	CA-C-N	6.41	129.35	120.63
3	B	159	GLU	C-N-CA	6.41	129.35	120.63
2	A	264	ARG	NE-CZ-NH1	6.41	127.91	121.50
2	A	309	HIS	CE1-NE2-CD2	-6.41	102.59	109.00
3	B	167	ASN	CA-C-O	6.41	127.20	120.54
2	A	256	GLN	CA-C-N	6.38	129.16	120.54
2	A	256	GLN	C-N-CA	6.38	129.16	120.54
3	B	31	ASP	CA-CB-CG	-6.37	106.23	112.60
3	B	103	TRP	CG-CD2-CE3	-6.37	127.53	133.90
3	B	189	LEU	CA-C-O	6.37	127.30	120.55
3	B	285	ALA	N-CA-C	-6.37	103.41	112.13
3	B	216	THR	CA-C-O	-6.36	114.32	121.00
1	K	226	LYS	CA-C-O	-6.36	113.31	120.43
3	B	229	HIS	O-C-N	-6.35	115.49	122.09
3	B	16	ILE	CA-C-N	6.34	126.97	120.00
3	B	16	ILE	C-N-CA	6.34	126.97	120.00
1	K	69	ILE	CB-CA-C	-6.34	103.77	111.88
2	A	338	LYS	O-C-N	-6.32	114.52	122.17
1	K	252	LYS	CA-C-N	6.31	128.98	120.65
1	K	252	LYS	C-N-CA	6.31	128.98	120.65
3	B	257	VAL	CA-C-N	6.31	129.25	120.29
3	B	257	VAL	C-N-CA	6.31	129.25	120.29
1	K	288	ASP	CA-C-N	6.31	128.73	120.28
1	K	288	ASP	C-N-CA	6.31	128.73	120.28
2	A	402	ARG	CA-C-O	6.29	128.12	120.57
2	A	255	PHE	CB-CG-CD2	-6.26	110.05	120.70
3	B	169	PHE	CA-CB-CG	-6.26	107.54	113.80
2	A	243	ARG	CA-C-N	6.26	133.28	122.64
2	A	243	ARG	C-N-CA	6.26	133.28	122.64
3	B	170	SER	N-CA-CB	6.25	121.00	110.69
1	K	270	GLU	N-CA-C	-6.24	104.01	111.69
3	B	394	GLN	CA-C-N	6.24	128.56	120.44
3	B	394	GLN	C-N-CA	6.24	128.56	120.44
3	B	424	ASN	O-C-N	-6.24	115.64	122.07
3	B	88	ARG	CD-NE-CZ	-6.24	115.67	124.40
2	A	224	TYR	CA-C-N	6.24	131.10	121.19
2	A	224	TYR	C-N-CA	6.24	131.10	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	151	THR	CA-CB-OG1	6.24	118.95	109.60
3	B	282	GLN	OE1-CD-NE2	-6.23	116.37	122.60
1	K	106	GLY	CA-C-N	6.23	128.93	120.77
1	K	106	GLY	C-N-CA	6.23	128.93	120.77
1	K	31	ALA	N-CA-CB	-6.22	101.21	110.17
1	K	144	ASP	CA-C-N	6.21	131.08	120.72
1	K	144	ASP	C-N-CA	6.21	131.08	120.72
3	B	54	ASN	CA-CB-CG	-6.21	106.39	112.60
1	K	289	SER	CA-C-O	-6.20	113.97	120.55
2	A	199	ASP	CA-CB-CG	-6.19	106.41	112.60
2	A	229	ARG	CA-C-O	-6.19	112.00	119.49
1	K	182	THR	CA-C-N	6.19	128.94	120.46
1	K	182	THR	C-N-CA	6.19	128.94	120.46
3	B	427	ASP	CA-CB-CG	-6.18	106.42	112.60
1	K	160	ASN	CA-C-N	6.17	131.12	122.36
1	K	160	ASN	C-N-CA	6.17	131.12	122.36
2	A	402	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	K	78	ASN	CB-CG-ND2	-6.16	107.17	116.40
1	K	190	ARG	N-CA-C	6.15	118.71	110.35
3	B	51	VAL	O-C-N	6.15	128.11	121.90
3	B	418	PHE	CA-C-N	6.15	129.33	120.79
3	B	418	PHE	C-N-CA	6.15	129.33	120.79
3	B	177	VAL	CA-C-O	6.14	125.10	119.20
3	B	311	ARG	NH1-CZ-NH2	-6.14	111.31	119.30
2	A	233	GLN	CA-C-N	6.13	128.40	120.56
2	A	233	GLN	C-N-CA	6.13	128.40	120.56
2	A	78	VAL	O-C-N	-6.11	115.40	121.94
2	A	431	ASP	N-CA-CB	6.11	118.83	109.91
1	K	90	GLY	CA-C-N	6.10	128.78	120.54
1	K	90	GLY	C-N-CA	6.10	128.78	120.54
1	K	71	LYS	O-C-N	-6.10	115.79	122.07
3	B	340	SER	CA-C-N	6.09	128.72	120.38
3	B	340	SER	C-N-CA	6.09	128.72	120.38
3	B	306	ASP	CA-C-O	-6.09	113.54	119.51
1	K	201	SER	CA-C-N	6.08	131.15	121.66
1	K	201	SER	C-N-CA	6.08	131.15	121.66
2	A	26	LEU	CA-C-O	-6.07	114.44	120.70
1	K	58	GLN	O-C-N	6.07	128.56	122.12
1	K	302	CYS	CA-C-O	6.05	128.19	121.11
2	A	290	GLU	O-C-N	-6.05	115.80	122.09
1	K	227	LEU	N-CA-CB	6.05	120.28	110.42
3	B	228	ASN	OD1-CG-ND2	-6.05	116.55	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	234	ILE	N-CA-CB	6.04	118.30	110.57
2	A	254	GLU	O-C-N	-6.03	114.85	122.27
2	A	391	LEU	CA-C-N	6.03	129.17	120.79
2	A	391	LEU	C-N-CA	6.03	129.17	120.79
2	A	243	ARG	CG-CD-NE	-6.02	98.75	112.00
2	A	172	TYR	CA-C-N	6.01	126.35	119.92
2	A	172	TYR	C-N-CA	6.01	126.35	119.92
1	K	116	PHE	O-C-N	-6.01	114.28	122.33
1	K	151	THR	O-C-N	-6.01	115.89	122.38
3	B	200	GLU	N-CA-CB	6.01	120.02	110.65
2	A	60	LYS	CB-CA-C	-6.00	102.70	111.23
2	A	282	TYR	CA-C-N	6.00	128.32	120.28
2	A	282	TYR	C-N-CA	6.00	128.32	120.28
3	B	311	ARG	NE-CZ-NH2	6.00	124.60	119.20
2	A	232	SER	N-CA-CB	5.98	118.91	110.12
3	B	217	LEU	N-CA-CB	-5.98	101.28	110.13
3	B	16	ILE	CA-CB-CG1	5.97	120.56	110.40
1	K	169	THR	N-CA-C	-5.97	99.46	108.96
2	A	159	VAL	CA-CB-CG1	5.96	120.53	110.40
1	K	72	ASP	CA-C-N	5.96	128.29	120.60
1	K	72	ASP	C-N-CA	5.96	128.29	120.60
2	A	137	VAL	O-C-N	-5.95	116.62	122.99
3	B	21	TRP	CB-CG-CD1	5.93	135.80	126.90
2	A	204	VAL	O-C-N	-5.93	117.09	123.14
2	A	225	THR	CA-C-N	5.93	128.22	120.28
2	A	225	THR	C-N-CA	5.93	128.22	120.28
1	K	176	PRO	CA-C-N	5.92	130.74	120.68
1	K	176	PRO	C-N-CA	5.92	130.74	120.68
2	A	211	ASP	CA-C-O	5.91	126.68	120.42
3	B	398	MET	CA-C-N	5.91	128.68	120.29
3	B	398	MET	C-N-CA	5.91	128.68	120.29
1	K	202	SER	N-CA-CB	5.91	119.29	109.60
1	K	179	VAL	CA-C-O	5.88	128.13	120.78
3	B	424	ASN	CA-CB-CG	5.88	118.48	112.60
1	K	160	ASN	OD1-CG-ND2	-5.88	116.72	122.60
2	A	55	GLU	CA-CB-CG	5.88	125.85	114.10
3	B	267	PHE	CA-CB-CG	-5.86	107.94	113.80
1	K	145	LEU	N-CA-CB	5.85	120.11	110.39
1	K	191	HIS	ND1-CG-CD2	5.85	111.95	106.10
2	A	197	HIS	ND1-CE1-NE2	5.84	114.24	108.40
3	B	385	GLN	N-CA-C	5.83	118.41	111.71
2	A	112	LYS	CB-CA-C	-5.82	100.95	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	44	LYS	CA-C-N	5.82	125.72	119.85
1	K	44	LYS	C-N-CA	5.82	125.72	119.85
2	A	430	LYS	N-CA-C	5.81	118.40	111.71
3	B	181	VAL	N-CA-CB	5.81	117.22	110.65
3	B	218	LYS	CA-C-O	5.81	128.82	120.51
1	K	89	SER	CA-C-O	5.80	126.50	119.49
2	A	432	TYR	CA-CB-CG	-5.79	103.47	113.90
3	B	322	ARG	NH1-CZ-NH2	-5.79	111.77	119.30
2	A	84	ARG	N-CA-C	-5.79	104.94	112.23
1	K	92	THR	O-C-N	5.79	128.11	122.09
2	A	380	ASN	CB-CA-C	5.78	120.80	109.35
3	B	386	GLU	CA-C-N	5.78	128.50	120.29
3	B	386	GLU	C-N-CA	5.78	128.50	120.29
2	A	390	ARG	CA-C-N	5.78	128.28	120.65
2	A	390	ARG	C-N-CA	5.78	128.28	120.65
3	B	118	VAL	CB-CA-C	-5.78	104.34	112.14
1	K	73	VAL	CA-C-N	5.78	132.57	121.54
1	K	73	VAL	C-N-CA	5.78	132.57	121.54
1	K	118	TYR	CA-C-N	5.78	127.84	120.56
1	K	118	TYR	C-N-CA	5.78	127.84	120.56
3	B	16	ILE	CA-C-O	5.77	126.71	120.47
1	K	36	GLU	O-C-N	5.77	128.73	122.15
1	K	258	LEU	N-CA-C	5.77	117.24	111.07
1	K	238	VAL	O-C-N	-5.75	114.48	122.31
1	K	320	GLN	OE1-CD-NE2	-5.75	116.85	122.60
2	A	271	THR	N-CA-CB	5.75	120.48	111.56
3	B	43	GLN	N-CA-C	5.75	119.56	112.54
2	A	315	CYS	CB-CA-C	-5.75	101.28	110.14
3	B	298	SER	N-CA-C	5.74	123.03	110.80
3	B	264	ARG	O-C-N	-5.74	115.17	122.34
3	B	82	PRO	CB-CA-C	5.74	118.97	110.88
2	A	263	PRO	N-CA-CB	5.73	109.60	103.52
3	B	266	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
3	B	77	SER	O-C-N	-5.73	116.05	122.12
3	B	33	THR	O-C-N	-5.72	114.79	122.23
3	B	69	ASP	CA-CB-CG	-5.72	106.88	112.60
3	B	223	THR	CA-C-N	5.72	127.88	120.44
3	B	223	THR	C-N-CA	5.72	127.88	120.44
1	K	91	LYS	CA-C-O	-5.71	114.79	120.90
2	A	102	ASN	N-CA-C	5.70	117.36	109.15
2	A	355	ILE	CB-CA-C	-5.70	103.94	110.73
3	B	76	ASP	N-CA-CB	5.70	118.59	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	191	VAL	O-C-N	-5.70	116.14	121.90
3	B	43	GLN	CA-C-N	5.70	128.19	120.44
3	B	43	GLN	C-N-CA	5.70	128.19	120.44
2	A	54	SER	CA-C-N	5.69	129.98	121.72
2	A	54	SER	C-N-CA	5.69	129.98	121.72
3	B	343	PHE	O-C-N	-5.69	116.39	123.04
3	B	371	LEU	N-CA-C	-5.69	103.19	110.53
1	K	239	SER	CA-C-N	5.68	128.36	120.63
1	K	239	SER	C-N-CA	5.68	128.36	120.63
2	A	136	LEU	O-C-N	-5.68	116.74	123.22
3	B	388	PHE	N-CA-C	5.68	118.41	111.82
2	A	215	ARG	N-CA-CB	5.68	118.42	110.07
1	K	125	ASN	N-CA-C	5.67	118.31	111.40
1	K	215	GLU	CA-C-O	5.67	127.33	120.81
3	B	387	LEU	N-CA-C	-5.67	105.18	111.36
1	K	157	GLU	CB-CA-C	5.67	119.08	109.84
2	A	1	MET	CG-SD-CE	-5.67	88.43	100.90
1	K	165	VAL	CA-C-N	5.66	130.53	122.72
1	K	165	VAL	C-N-CA	5.66	130.53	122.72
3	B	120	ASP	CA-CB-CG	5.65	118.25	112.60
1	K	282	MET	N-CA-C	5.65	117.11	111.07
2	A	430	LYS	CA-C-N	5.64	128.09	120.65
2	A	430	LYS	C-N-CA	5.64	128.09	120.65
3	B	104	ALA	CA-C-O	5.63	126.58	120.55
3	B	47	GLU	CB-CA-C	5.63	121.62	110.42
3	B	300	ASN	CA-C-N	-5.62	114.51	122.94
3	B	300	ASN	C-N-CA	-5.62	114.51	122.94
1	K	277	TYR	CA-CB-CG	-5.60	103.82	113.90
3	B	21	TRP	CB-CG-CD2	-5.60	118.97	126.80
3	B	6	HIS	N-CA-CB	5.59	119.35	110.57
3	B	103	TRP	CB-CG-CD2	5.58	134.61	126.80
3	B	217	LEU	CB-CA-C	5.58	120.16	110.79
2	A	130	THR	N-CA-C	-5.58	103.03	111.56
3	B	192	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
1	K	277	TYR	CB-CA-C	-5.57	99.33	110.42
3	B	123	ARG	CA-C-N	5.57	127.68	120.44
3	B	123	ARG	C-N-CA	5.57	127.68	120.44
1	K	216	ASN	CA-C-N	5.56	128.76	120.31
1	K	216	ASN	C-N-CA	5.56	128.76	120.31
2	A	60	LYS	O-C-N	-5.56	116.03	123.14
2	A	258	ASN	CA-CB-CG	-5.55	107.05	112.60
2	A	32	PRO	N-CA-C	-5.55	106.92	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	354	ALA	CA-C-N	5.55	131.17	122.84
3	B	354	ALA	C-N-CA	5.55	131.17	122.84
2	A	227	LEU	CA-C-N	5.55	128.17	120.29
2	A	227	LEU	C-N-CA	5.55	128.17	120.29
3	B	152	LEU	CA-C-N	5.55	127.99	120.44
3	B	152	LEU	C-N-CA	5.55	127.99	120.44
2	A	330	ALA	N-CA-C	5.55	117.41	111.36
3	B	81	GLY	O-C-N	-5.55	116.22	121.77
1	K	43	SER	O-C-N	-5.55	115.21	122.59
1	K	301	CYS	CA-C-O	5.55	126.22	120.40
3	B	316	ALA	N-CA-CB	-5.54	101.90	111.55
2	A	322	ASP	N-CA-CB	-5.54	102.21	110.24
1	K	100	HIS	CA-C-N	5.54	128.96	121.20
1	K	100	HIS	C-N-CA	5.54	128.96	121.20
2	A	9	VAL	O-C-N	-5.54	116.90	123.05
3	B	297	ASP	N-CA-C	5.54	118.68	110.48
2	A	334	THR	N-CA-C	5.54	117.75	111.11
1	K	282	MET	O-C-N	-5.54	116.37	122.07
2	A	31	GLN	CA-C-N	5.54	125.15	119.56
2	A	31	GLN	C-N-CA	5.54	125.15	119.56
3	B	91	ASN	OD1-CG-ND2	-5.54	117.06	122.60
3	B	293	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	K	105	MET	N-CA-C	5.53	118.25	110.23
2	A	183	GLU	O-C-N	-5.53	115.23	120.70
2	A	424	ASP	O-C-N	-5.52	116.38	122.07
1	K	53	GLN	CB-CG-CD	5.52	121.98	112.60
1	K	88	SER	N-CA-C	5.52	122.56	110.80
3	B	159	GLU	CB-CG-CD	5.51	121.96	112.60
2	A	393	HIS	ND1-CE1-NE2	5.49	113.89	108.40
2	A	168	GLU	O-C-N	-5.49	116.77	123.19
1	K	204	SER	CA-C-O	5.48	126.28	120.36
2	A	331	ALA	N-CA-CB	5.48	118.15	109.82
2	A	297	GLU	CB-CG-CD	5.47	121.91	112.60
3	B	155	SER	N-CA-C	5.47	117.24	111.28
1	K	39	VAL	CA-C-O	5.47	127.63	121.28
2	A	256	GLN	CB-CA-C	-5.47	102.22	110.92
3	B	304	ALA	CA-C-N	5.47	129.95	122.84
3	B	304	ALA	C-N-CA	5.47	129.95	122.84
1	K	123	ASP	O-C-N	-5.47	116.83	122.84
2	A	356	ASN	CA-CB-CG	-5.47	107.13	112.60
3	B	349	ASN	OD1-CG-ND2	-5.46	117.14	122.60
2	A	24	TYR	CB-CG-CD1	-5.45	112.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	132	LEU	N-CA-C	5.45	118.48	110.30
2	A	206	ASN	CA-CB-CG	-5.45	107.15	112.60
2	A	353	VAL	O-C-N	-5.45	117.09	122.76
2	A	156	ARG	N-CA-CB	5.45	119.70	110.49
3	B	82	PRO	CA-C-O	-5.45	112.34	118.98
1	K	17	PRO	N-CA-C	5.44	119.57	111.41
1	K	125	ASN	OD1-CG-ND2	-5.44	117.16	122.60
2	A	320	ARG	CA-C-O	5.44	126.21	120.33
3	B	273	ALA	CA-C-O	-5.44	114.48	119.76
3	B	144	GLY	CA-C-N	5.44	127.84	120.44
3	B	144	GLY	C-N-CA	5.44	127.84	120.44
1	K	162	VAL	CA-C-N	5.43	126.63	119.84
1	K	162	VAL	C-N-CA	5.43	126.63	119.84
3	B	28	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
2	A	251	ASP	CA-C-N	5.42	127.55	120.28
2	A	251	ASP	C-N-CA	5.42	127.55	120.28
2	A	344	VAL	CB-CA-C	-5.42	103.79	111.28
2	A	422	ARG	CA-C-N	5.42	127.82	120.44
2	A	422	ARG	C-N-CA	5.42	127.82	120.44
3	B	245	PRO	O-C-N	-5.42	116.47	123.03
2	A	321	GLY	N-CA-C	-5.42	104.51	110.96
1	K	101	ASP	N-CA-C	5.42	117.44	109.42
1	K	272	SER	N-CA-C	5.39	118.20	109.79
2	A	160	ASP	CA-CB-CG	5.39	118.00	112.60
3	B	229	HIS	CB-CG-CD2	-5.39	124.19	131.20
3	B	282	GLN	CB-CG-CD	5.39	121.76	112.60
3	B	397	ALA	CB-CA-C	5.39	119.48	110.92
1	K	19	ASN	O-C-N	-5.38	115.49	122.97
1	K	262	GLY	N-CA-C	5.38	120.43	113.27
2	A	36	MET	N-CA-C	-5.38	102.99	109.72
2	A	209	ILE	N-CA-C	5.38	116.01	110.36
3	B	269	MET	N-CA-CB	-5.38	101.29	110.43
3	B	312	TYR	CB-CA-C	-5.37	100.42	109.50
2	A	84	ARG	CA-C-O	5.37	126.12	119.79
1	K	37	ASP	CA-CB-CG	5.37	117.97	112.60
3	B	217	LEU	CA-C-N	5.36	131.78	121.54
3	B	217	LEU	C-N-CA	5.36	131.78	121.54
2	A	22	GLU	O-C-N	-5.36	116.55	122.07
1	K	36	GLU	CA-C-N	5.36	129.66	120.71
1	K	36	GLU	C-N-CA	5.36	129.66	120.71
3	B	26	ASP	CA-C-O	5.36	126.44	120.82
3	B	436	GLN	CA-C-N	5.36	127.99	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	436	GLN	C-N-CA	5.36	127.99	120.28
1	K	63	ASN	N-CA-C	5.35	117.11	111.28
1	K	275	VAL	N-CA-CB	5.35	118.70	111.21
2	A	361	THR	O-C-N	-5.35	116.28	123.23
3	B	295	MET	O-C-N	-5.35	116.45	122.12
1	K	51	VAL	N-CA-CB	5.34	117.66	111.90
2	A	18	ASN	CB-CA-C	5.34	119.26	110.88
2	A	67	PHE	CA-CB-CG	-5.34	108.46	113.80
3	B	7	ILE	N-CA-C	5.33	115.54	107.75
2	A	118	VAL	CA-C-N	5.33	127.86	120.29
2	A	118	VAL	C-N-CA	5.33	127.86	120.29
3	B	296	PHE	CB-CA-C	-5.33	99.34	109.95
3	B	178	SER	CA-C-N	5.32	131.84	122.42
3	B	178	SER	C-N-CA	5.32	131.84	122.42
1	K	72	ASP	N-CA-C	5.32	117.99	111.82
1	K	78	ASN	CB-CG-OD1	5.32	131.43	120.80
2	A	324	VAL	CA-CB-CG1	5.32	119.44	110.40
3	B	148	GLY	O-C-N	-5.32	115.79	122.70
3	B	258	ASN	CA-C-O	-5.32	114.78	120.42
3	B	83	PHE	CA-C-N	5.31	131.82	121.41
3	B	83	PHE	C-N-CA	5.31	131.82	121.41
1	K	39	VAL	O-C-N	-5.31	117.32	123.00
3	B	322	ARG	N-CA-C	5.31	118.93	110.70
3	B	360	PRO	N-CA-C	-5.31	102.94	111.38
2	A	103	TYR	CA-C-N	5.30	127.82	120.29
2	A	103	TYR	C-N-CA	5.30	127.82	120.29
2	A	71	GLU	CB-CA-C	-5.30	101.00	109.69
1	K	195	THR	O-C-N	-5.30	115.44	122.59
2	A	234	ILE	CB-CA-C	-5.29	105.09	112.02
2	A	401	LYS	CA-C-N	5.29	130.36	122.74
2	A	401	LYS	C-N-CA	5.29	130.36	122.74
3	B	53	TYR	CB-CG-CD1	5.28	128.73	120.80
1	K	7	SER	CA-C-O	5.28	126.14	120.70
2	A	5	ILE	O-C-N	-5.28	116.50	122.94
3	B	88	ARG	NE-CZ-NH1	5.28	126.78	121.50
3	B	107	HIS	ND1-CE1-NE2	5.28	113.68	108.40
2	A	404	PHE	CA-CB-CG	-5.27	108.53	113.80
2	A	181	VAL	O-C-N	-5.27	114.89	121.84
2	A	154	MET	N-CA-CB	5.27	117.86	110.12
2	A	359	PRO	O-C-N	-5.26	115.26	121.46
3	B	347	ILE	CA-C-N	5.25	126.40	119.84
3	B	347	ILE	C-N-CA	5.25	126.40	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	82	PHE	N-CA-C	-5.25	101.14	109.59
3	B	309	HIS	O-C-N	-5.24	115.42	122.23
1	K	40	VAL	N-CA-CB	5.23	117.33	111.21
2	A	52	PHE	CA-CB-CG	-5.23	108.57	113.80
3	B	126	SER	CA-C-N	5.23	129.46	120.72
3	B	126	SER	C-N-CA	5.23	129.46	120.72
1	K	59	GLU	CA-C-N	5.23	127.24	120.44
1	K	59	GLU	C-N-CA	5.23	127.24	120.44
1	K	184	ASP	CA-C-N	5.22	127.55	120.44
1	K	184	ASP	C-N-CA	5.22	127.55	120.44
2	A	393	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
3	B	72	PRO	CA-C-N	5.22	129.66	123.44
3	B	72	PRO	C-N-CA	5.22	129.66	123.44
3	B	141	LEU	CA-C-O	-5.22	115.01	120.55
3	B	169	PHE	CA-C-O	5.22	125.97	120.54
3	B	12	CYS	CB-CA-C	-5.22	102.68	110.88
2	A	243	ARG	CA-CB-CG	-5.22	103.66	114.10
1	K	140	ASP	CA-C-N	5.22	129.13	120.94
1	K	140	ASP	C-N-CA	5.22	129.13	120.94
1	K	175	SER	CA-C-N	5.21	124.82	119.56
1	K	175	SER	C-N-CA	5.21	124.82	119.56
3	B	130	ASP	CA-CB-CG	-5.21	107.39	112.60
1	K	23	VAL	N-CA-C	5.21	115.42	110.53
3	B	247	GLN	OE1-CD-NE2	-5.21	117.39	122.60
2	A	182	VAL	N-CA-C	5.20	120.16	109.34
3	B	331	GLN	O-C-N	-5.20	116.22	122.15
2	A	121	ARG	N-CA-C	5.20	116.95	111.28
2	A	197	HIS	N-CA-C	5.20	116.68	110.44
1	K	300	ILE	N-CA-C	5.19	115.74	108.89
2	A	317	LEU	N-CA-CB	5.19	118.75	110.65
3	B	66	ILE	CA-C-O	5.19	125.51	120.27
3	B	294	GLN	CA-C-N	5.19	127.49	120.38
3	B	294	GLN	C-N-CA	5.19	127.49	120.38
2	A	88	HIS	CB-CG-ND1	-5.18	114.92	122.70
3	B	256	ALA	CA-C-O	-5.18	115.03	120.63
2	A	273	ALA	O-C-N	-5.18	117.00	121.71
1	K	226	LYS	CA-C-N	5.18	129.66	122.77
1	K	226	LYS	C-N-CA	5.18	129.66	122.77
2	A	171	ILE	N-CA-CB	5.17	119.76	111.23
2	A	380	ASN	CA-CB-CG	5.17	117.77	112.60
2	A	247	ALA	CB-CA-C	5.17	120.71	110.42
2	A	269	LEU	N-CA-C	-5.17	101.59	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	101	ASN	CA-C-O	-5.17	113.12	120.51
3	B	171	VAL	N-CA-CB	5.16	116.98	111.46
2	A	177	VAL	CA-C-N	5.16	129.66	121.72
2	A	177	VAL	C-N-CA	5.16	129.66	121.72
2	A	3	GLU	O-C-N	-5.15	117.34	123.22
2	A	230	LEU	CA-C-O	-5.14	115.60	120.90
1	K	278	ARG	NE-CZ-NH1	5.14	126.64	121.50
2	A	159	VAL	N-CA-CB	5.14	117.92	110.52
2	A	130	THR	N-CA-CB	5.14	118.15	110.14
2	A	197	HIS	ND1-CG-CD2	5.13	111.23	106.10
3	B	383	ALA	O-C-N	-5.13	115.60	122.43
3	B	401	ARG	CA-C-N	5.13	131.35	121.54
3	B	401	ARG	C-N-CA	5.13	131.35	121.54
2	A	414	GLU	O-C-N	-5.13	117.38	123.22
1	K	307	TYR	N-CA-CB	-5.13	102.42	109.91
2	A	20	CYS	N-CA-C	-5.13	105.58	111.07
2	A	341	ILE	CA-CB-CG1	5.12	119.11	110.40
3	B	191	VAL	CA-C-N	5.12	127.56	120.29
3	B	191	VAL	C-N-CA	5.12	127.56	120.29
3	B	187	ALA	N-CA-C	5.11	116.93	111.36
1	K	67	LYS	CA-C-N	5.10	127.54	120.29
1	K	67	LYS	C-N-CA	5.10	127.54	120.29
1	K	133	SER	CA-C-N	5.10	130.10	122.86
1	K	133	SER	C-N-CA	5.10	130.10	122.86
3	B	8	GLN	N-CA-C	5.09	116.61	108.41
3	B	78	VAL	N-CA-C	-5.09	105.58	110.72
3	B	288	VAL	N-CA-CB	5.09	118.34	111.21
2	A	216	ASN	OD1-CG-ND2	-5.09	117.51	122.60
3	B	224	TYR	CA-C-O	5.09	126.17	120.82
2	A	280	LYS	CB-CA-C	-5.09	100.91	110.67
3	B	202	TYR	CB-CG-CD2	-5.08	113.17	120.80
2	A	11	GLN	N-CA-CB	5.08	117.33	109.91
2	A	250	VAL	N-CA-C	-5.08	106.72	111.45
3	B	74	THR	N-CA-CB	5.08	117.44	110.07
2	A	28	HIS	CA-CB-CG	-5.08	108.72	113.80
3	B	389	LYS	CA-C-N	5.08	129.27	120.58
3	B	389	LYS	C-N-CA	5.08	129.27	120.58
3	B	264	ARG	CA-C-O	5.08	125.29	119.35
2	A	341	ILE	CA-CB-CG2	-5.08	101.87	110.50
1	K	242	GLY	CA-C-O	-5.07	113.53	119.72
3	B	116	ASP	N-CA-C	-5.07	105.67	111.14
2	A	76	ASP	CA-C-N	5.07	127.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	76	ASP	C-N-CA	5.07	127.57	120.28
2	A	67	PHE	CB-CA-C	-5.06	102.32	110.77
2	A	342	GLN	CG-CD-OE1	5.06	130.91	120.80
2	A	50	ASN	CB-CA-C	-5.05	102.07	110.81
1	K	217	THR	N-CA-CB	5.05	118.11	110.28
3	B	192	HIS	CA-CB-CG	-5.05	108.75	113.80
1	K	145	LEU	N-CA-C	-5.04	106.39	112.54
3	B	21	TRP	N-CA-CB	5.04	117.52	110.12
2	A	209	ILE	N-CA-CB	5.03	116.10	110.51
3	B	401	ARG	NH1-CZ-NH2	-5.03	112.76	119.30
3	B	113	GLU	N-CA-C	-5.03	105.51	111.69
2	A	34	GLY	O-C-N	5.02	126.73	122.71
3	B	228	ASN	CA-C-N	5.02	127.32	120.54
3	B	228	ASN	C-N-CA	5.02	127.32	120.54
1	K	181	ASP	CA-C-O	5.02	126.09	120.82
2	A	2	ARG	N-CA-C	-5.02	100.34	108.52
2	A	423	GLU	CA-C-O	-5.02	115.53	120.70
2	A	284	GLU	CB-CG-CD	5.02	121.13	112.60
2	A	97	GLU	CA-C-O	-5.01	116.27	121.99
2	A	231	ILE	N-CA-C	5.01	115.62	110.36
3	B	10	GLY	CA-C-N	5.01	127.31	120.54
3	B	10	GLY	C-N-CA	5.01	127.31	120.54
1	K	67	LYS	CA-C-O	-5.01	115.24	120.55
1	K	74	LEU	CA-C-N	5.01	129.59	122.08
1	K	74	LEU	C-N-CA	5.01	129.59	122.08
1	K	114	ASP	O-C-N	-5.00	116.81	122.12
1	K	285	ILE	CA-CB-CG1	5.00	118.90	110.40
3	B	306	ASP	CA-CB-CG	-5.00	107.60	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	46	ASP	CA

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	100	ALA	Peptide
2	A	101	ASN	Peptide
2	A	103	TYR	Sidechain
2	A	114	ILE	Peptide
2	A	123	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	A	146	GLY	Peptide
2	A	149	PHE	Sidechain
2	A	161	TYR	Sidechain
2	A	2	ARG	Sidechain
2	A	218	ASP	Peptide
2	A	224	TYR	Sidechain
2	A	243	ARG	Sidechain
2	A	267	PHE	Sidechain
2	A	28	HIS	Sidechain
2	A	390	ARG	Sidechain
2	A	399	TYR	Sidechain
2	A	422	ARG	Sidechain
2	A	83	TYR	Sidechain
2	A	84	ARG	Sidechain
3	B	123	ARG	Sidechain
3	B	164	ARG	Sidechain
3	B	169	PHE	Sidechain
3	B	202	TYR	Sidechain
3	B	250	ALA	Peptide
3	B	264	ARG	Sidechain
3	B	281	GLN	Peptide
3	B	284	ARG	Peptide
3	B	311	ARG	Sidechain
3	B	312	TYR	Sidechain
3	B	342	TYR	Sidechain
3	B	377	PHE	Sidechain
3	B	400	ARG	Sidechain
3	B	401	ARG	Sidechain
3	B	435	TYR	Sidechain
3	B	53	TYR	Sidechain
3	B	87	PHE	Sidechain
3	B	88	ARG	Sidechain
1	K	110	ARG	Sidechain
1	K	129	HIS	Sidechain
1	K	138	TYR	Sidechain
1	K	16	ARG	Sidechain
1	K	161	ARG	Sidechain
1	K	171	ARG	Sidechain
1	K	203	ARG	Sidechain
1	K	278	ARG	Sidechain
1	K	62	TYR	Sidechain
1	K	75	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2474	0	2434	6	0
2	A	3372	0	3287	17	0
3	B	3389	0	3266	15	0
4	A	32	0	12	0	0
5	B	28	0	12	0	0
All	All	9295	0	9011	34	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 (34) 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:A:36:MET:HE3	2:A:61:HIS:CE1	2.31	0.65
3:B:269:MET:HE3	3:B:301:MET:HG3	1.83	0.60
2:A:208:ALA:HB2	2:A:304:LYS:HB2	1.87	0.56
3:B:332:MET:HG3	3:B:351:VAL:HG11	1.87	0.56
2:A:407:TRP:CE3	3:B:257:VAL:HG22	2.41	0.55
3:B:69:ASP:HA	3:B:145:THR:HG21	1.87	0.55
3:B:30:ILE:HD11	3:B:49:ILE:HD11	1.90	0.53
2:A:407:TRP:CE2	3:B:257:VAL:HA	2.44	0.52
1:K:142:ILE:HD11	1:K:281:LYS:HE2	1.92	0.51
2:A:109:THR:HG22	2:A:110:ILE:HD13	1.92	0.51
2:A:265:ILE:HG23	2:A:432:TYR:CZ	2.47	0.49
2:A:217:LEU:HD23	2:A:217:LEU:O	2.14	0.48
3:B:319:PHE:HB3	3:B:323:MET:HE3	1.95	0.48
3:B:320:ARG:HB3	3:B:359:PRO:HA	1.96	0.47
2:A:190:THR:O	2:A:194:THR:HG23	2.15	0.47
2:A:18:ASN:HD21	2:A:82:THR:HG21	1.81	0.46
2:A:28:HIS:CE1	2:A:244:PHE:CZ	3.04	0.46
3:B:7:ILE:HD12	3:B:137:LEU:HD12	2.00	0.44
1:K:135:PHE:CZ	1:K:165:VAL:HG21	2.51	0.44
2:A:221:ARG:HH12	3:B:325:MET:HB2	1.83	0.44
2:A:315:CYS:HB2	2:A:351:PHE:CD1	2.52	0.44
3:B:253:ARG:HG3	3:B:257:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:VAL:HG11	1:K:226:LYS:NZ	2.32	0.43
2:A:176:GLN:HG2	3:B:333:LEU:HD22	2.00	0.43
3:B:194:LEU:HD22	3:B:198:THR:HG21	2.01	0.43
2:A:319:TYR:CE1	2:A:328:VAL:HG13	2.55	0.42
1:K:41:ILE:HD13	1:K:41:ILE:HA	1.87	0.41
2:A:208:ALA:HB3	2:A:302:MET:O	2.20	0.41
3:B:358:ILE:HG22	3:B:359:PRO:O	2.20	0.41
3:B:34:GLY:O	3:B:60:LYS:HA	2.21	0.41
1:K:81:ILE:HB	1:K:229:LEU:HD23	2.01	0.41
2:A:265:ILE:HG23	2:A:432:TYR:CE2	2.55	0.41
1:K:261:LEU:HD11	1:K:290:LEU:HD21	2.03	0.41
2:A:391:LEU:HD23	2:A:425:MET:HG3	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	K	314/349 (90%)	273 (87%)	39 (12%)	2 (1%)	21	58
2	A	428/451 (95%)	374 (87%)	44 (10%)	10 (2%)	5	27
3	B	429/445 (96%)	367 (86%)	51 (12%)	11 (3%)	4	25
All	All	1171/1245 (94%)	1014 (87%)	134 (11%)	23 (2%)	8	30

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	220	GLU
3	B	84	GLY
3	B	282	GLN
3	B	349	ASN
2	A	59	GLY

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Mol	Chain	Res	Type
2	A	247	ALA
3	B	325	MET
2	A	101	ASN
2	A	340	SER
3	B	109	THR
3	B	298	SER
3	B	440	ALA
2	A	70	LEU
3	B	56	ALA
3	B	218	LYS
3	B	249	ASN
2	A	81	GLY
2	A	364	PRO
3	B	144	GLY
2	A	393	HIS
2	A	435	VAL
1	K	225	GLY
1	K	275	VAL

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	K	279/311 (90%)	273 (98%)	6 (2%)	45	64
2	A	364/379 (96%)	351 (96%)	13 (4%)	31	52
3	B	372/383 (97%)	359 (96%)	13 (4%)	32	53
All	All	1015/1073 (95%)	983 (97%)	32 (3%)	35	55

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	56	THR
1	K	74	LEU
1	K	118	TYR
1	K	211	ASN

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Mol	Chain	Res	Type
1	K	279	ASP
1	K	298	ILE
2	A	8	HIS
2	A	33	ASP
2	A	51	THR
2	A	86	LEU
2	A	93	ILE
2	A	206	ASN
2	A	209	ILE
2	A	219	ILE
2	A	221	ARG
2	A	230	LEU
2	A	381	THR
2	A	390	ARG
2	A	413	MET
3	B	8	GLN
3	B	22	GLU
3	B	83	PHE
3	B	115	VAL
3	B	176	LYS
3	B	204	ILE
3	B	238	VAL
3	B	302	MET
3	B	345	GLU
3	B	353	THR
3	B	360	PRO
3	B	422	GLU
3	B	434	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	63	ASN
1	K	218	GLN
1	K	308	ASN
2	A	18	ASN
2	A	91	GLN
2	A	107	HIS
2	A	133	GLN
2	A	301	GLN
2	A	372	GLN
3	B	11	GLN

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Mol	Chain	Res	Type
3	B	91	ASN
3	B	102	ASN
3	B	266	HIS
3	B	309	HIS
3	B	434	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GDP	B	501	-	29,30,30	1.60	8 (27%)	45,47,47	1.43	6 (13%)
4	GTP	A	600	-	33,34,34	1.99	7 (21%)	50,54,54	1.58	12 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	B	501	-	-	5/16/32/32	0/3/3/3
4	GTP	A	600	-	-	7/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	PA-O3A	-7.33	1.51	1.59
4	A	600	GTP	C3'-C4'	4.61	1.64	1.53
4	A	600	GTP	O4'-C4'	3.42	1.52	1.45
5	B	501	GDP	C1'-N9	3.22	1.56	1.47
5	B	501	GDP	C2'-C1'	-3.14	1.43	1.53
5	B	501	GDP	C8-N9	2.98	1.44	1.37
5	B	501	GDP	O2'-C2'	2.64	1.49	1.43
4	A	600	GTP	PB-O3B	2.62	1.62	1.59
5	B	501	GDP	O4'-C4'	2.24	1.50	1.45
5	B	501	GDP	O6-C6	-2.20	1.19	1.23
4	A	600	GTP	PA-O2A	-2.15	1.45	1.55
5	B	501	GDP	PA-O3A	-2.11	1.57	1.59
4	A	600	GTP	C2'-C3'	2.10	1.59	1.53
5	B	501	GDP	C2-N2	-2.07	1.29	1.34
4	A	600	GTP	O6-C6	-2.07	1.19	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	GTP	O2B-PB-O3A	3.70	117.27	107.27
4	A	600	GTP	O4'-C1'-C2'	3.53	114.17	106.62
5	B	501	GDP	O4'-C4'-C3'	-3.52	98.17	105.15
4	A	600	GTP	C4-C5-N7	3.20	115.73	110.67
5	B	501	GDP	O3'-C3'-C2'	3.11	121.80	111.82
5	B	501	GDP	C2-N1-C6	2.94	130.46	125.11
4	A	600	GTP	C8-N7-C5	-2.53	99.76	104.26
4	A	600	GTP	O3A-PA-O1A	2.51	118.25	110.70
5	B	501	GDP	O4'-C1'-N9	2.47	113.97	108.36
4	A	600	GTP	C6-C5-C4	-2.43	115.18	118.83
4	A	600	GTP	N2-C2-N3	2.37	124.29	119.67
4	A	600	GTP	O2'-C2'-C3'	2.37	119.41	111.82
4	A	600	GTP	N2-C2-N1	-2.34	111.83	116.76
4	A	600	GTP	O2G-PG-O3B	2.28	112.28	104.64
5	B	501	GDP	O2A-PA-O3A	2.27	113.40	107.27
4	A	600	GTP	O4'-C1'-N9	2.21	113.37	108.36
5	B	501	GDP	O3B-PB-O3A	2.17	111.91	104.64
4	A	600	GTP	O3B-PB-O1B	-2.09	104.42	110.70

There are no chirality outliers.

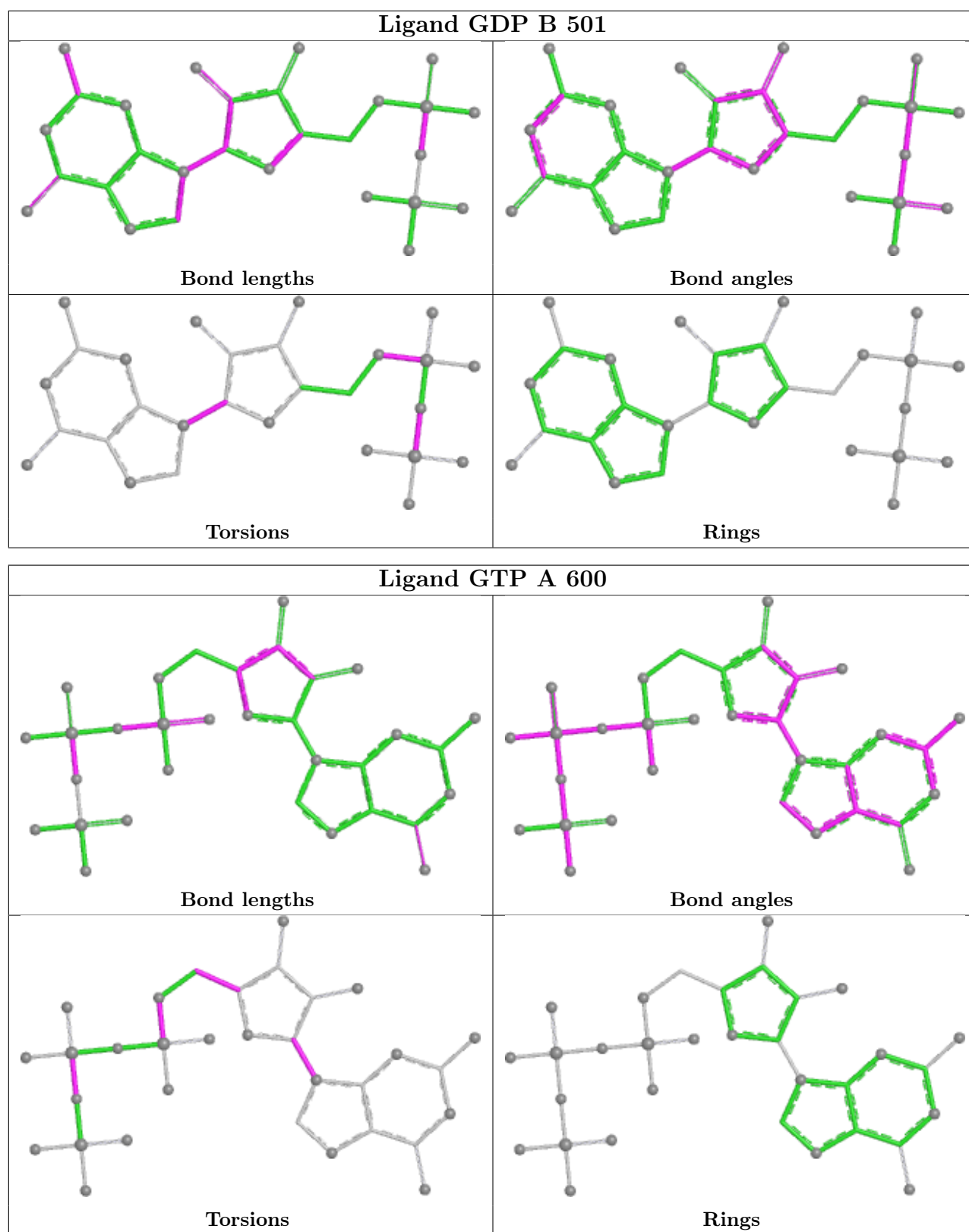
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GDP	PA-O3A-PB-O3B
5	B	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O2A
4	A	600	GTP	O4'-C4'-C5'-O5'
5	B	501	GDP	PA-O3A-PB-O1B
4	A	600	GTP	C5'-O5'-PA-O2A
4	A	600	GTP	PG-O3B-PB-O2B
4	A	600	GTP	C2'-C1'-N9-C8
4	A	600	GTP	C2'-C1'-N9-C4
5	B	501	GDP	C2'-C1'-N9-C4
4	A	600	GTP	PG-O3B-PB-O1B
4	A	600	GTP	O4'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

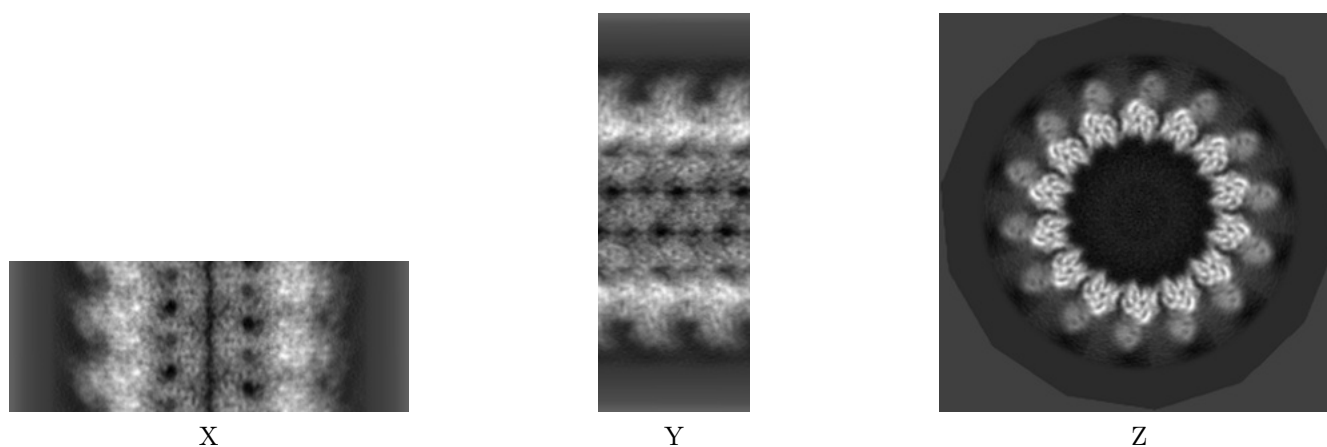
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6187. 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](#)

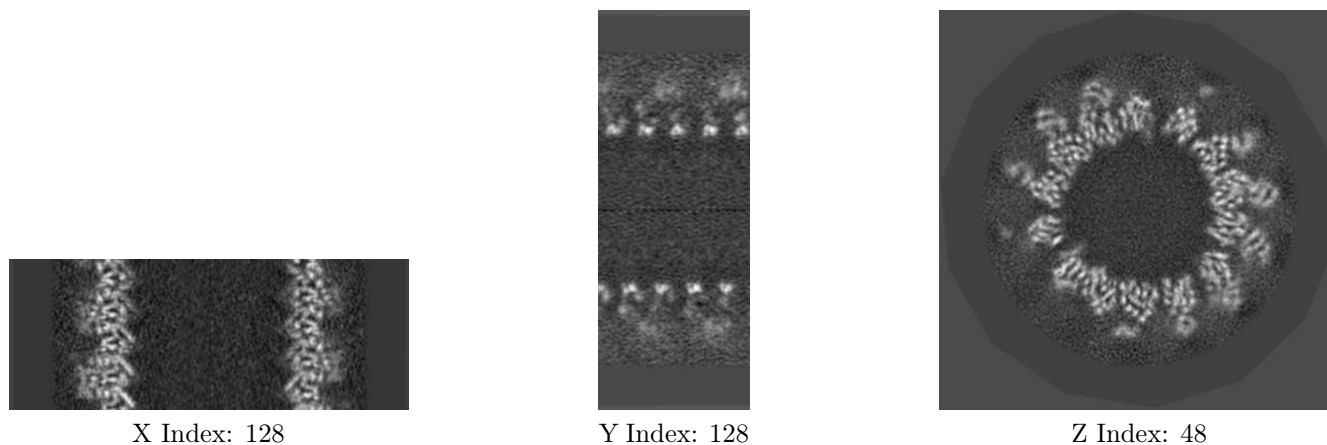
6.1.1 Primary map



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

6.2 Central slices [i](#)

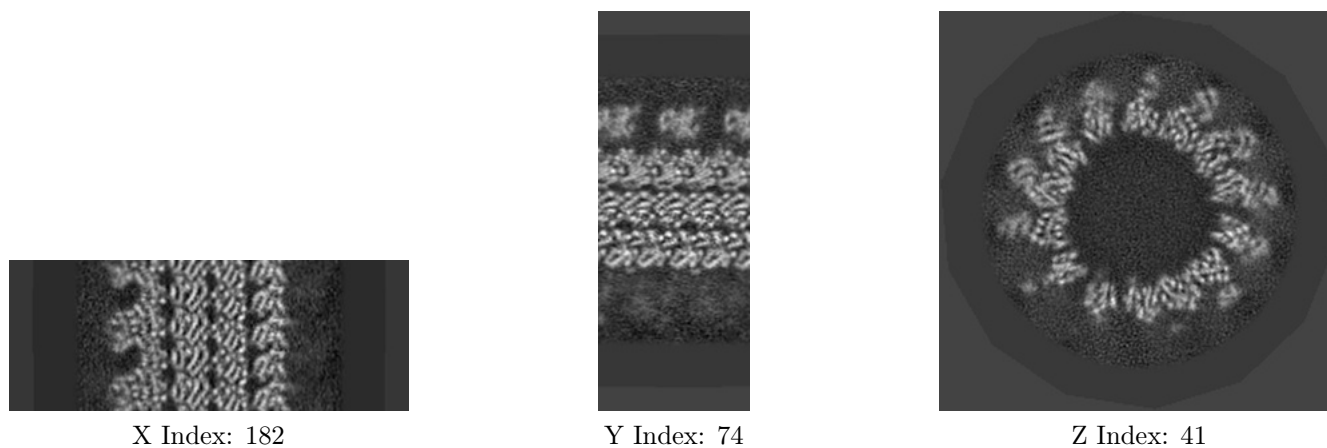
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

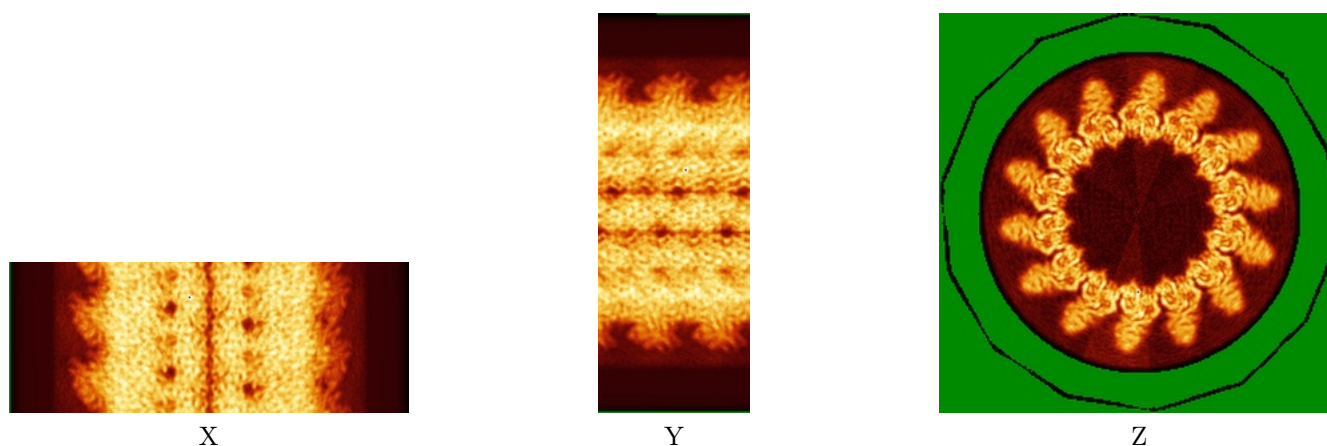
6.3.1 Primary map



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



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.

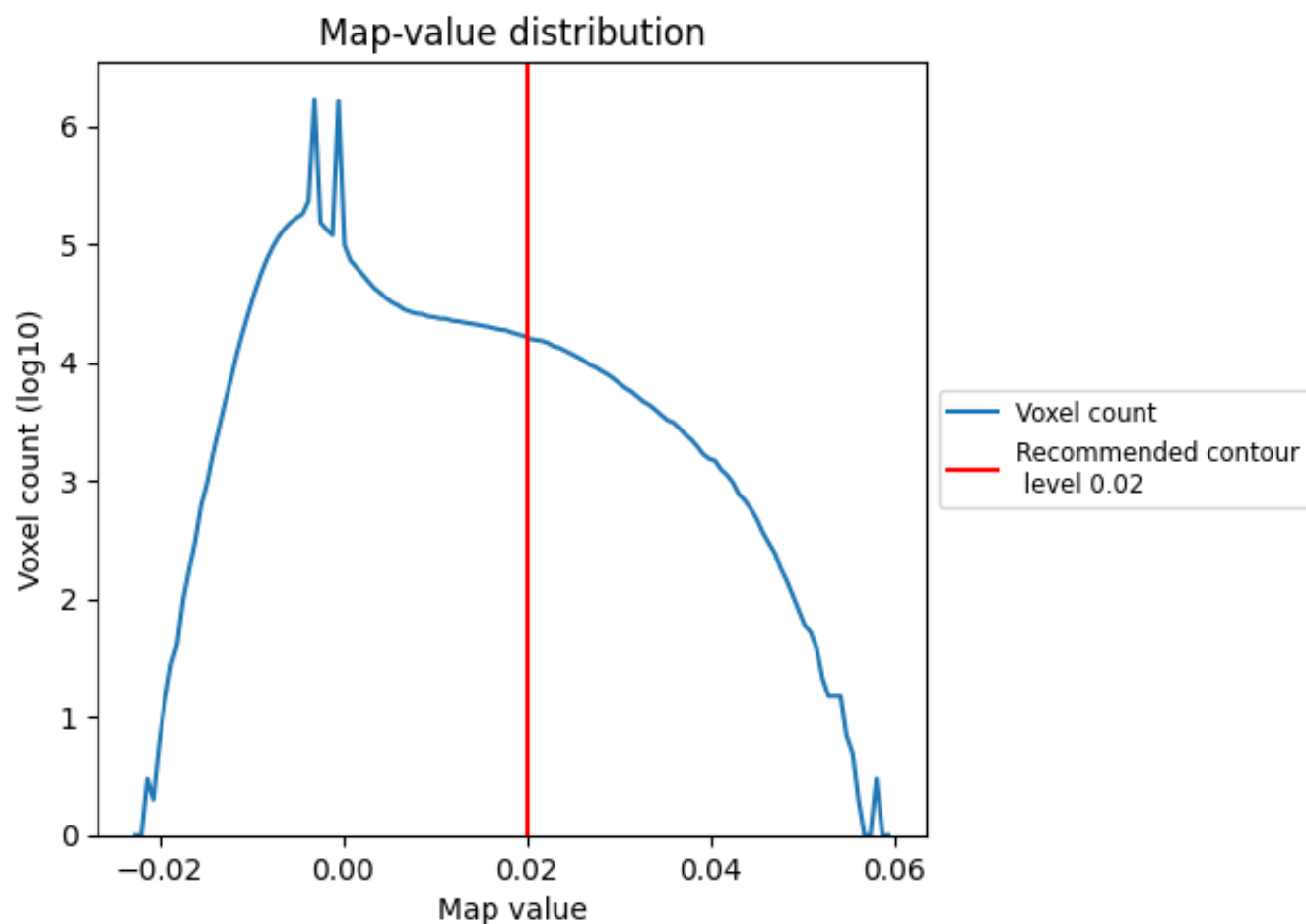
6.6 Mask visualisation

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

7 Map analysis [i](#)

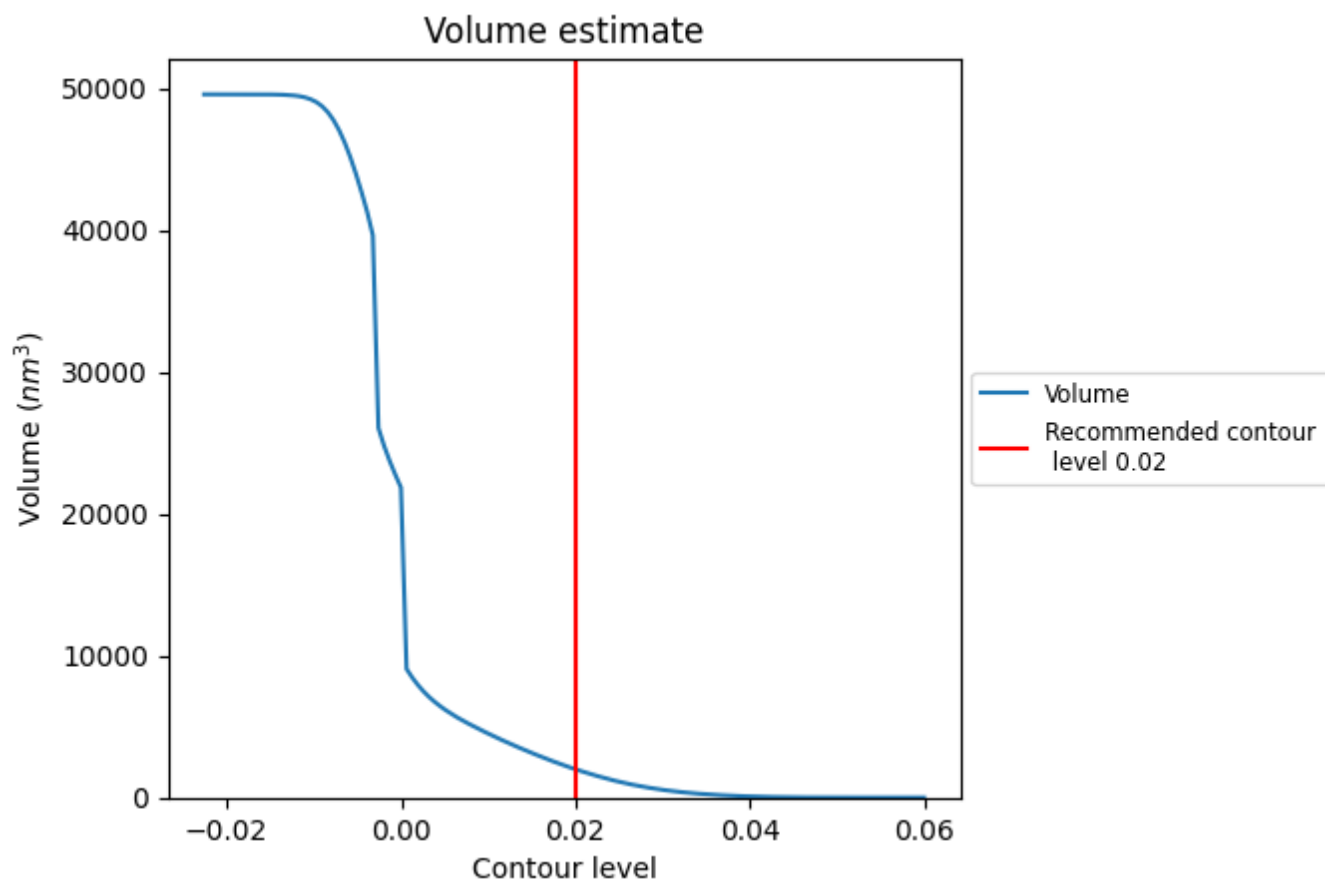
This section contains the results of statistical analysis of the map.

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 1994 nm³; this corresponds to an approximate mass of 1801 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.

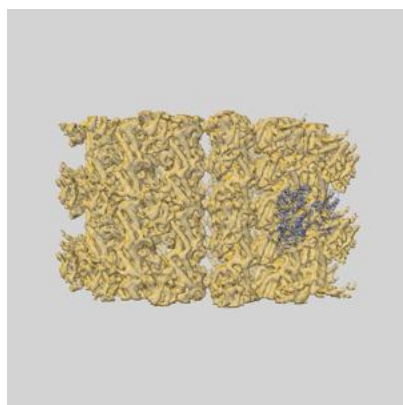
8 Fourier-Shell correlation ⓘ

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

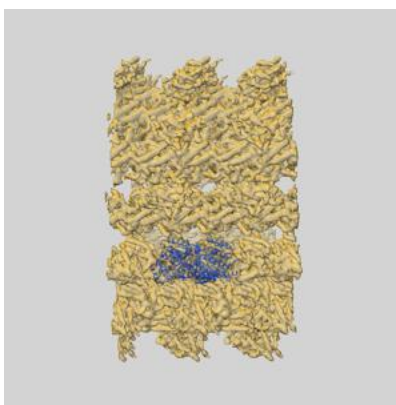
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6187 and PDB model 3J8X. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



X



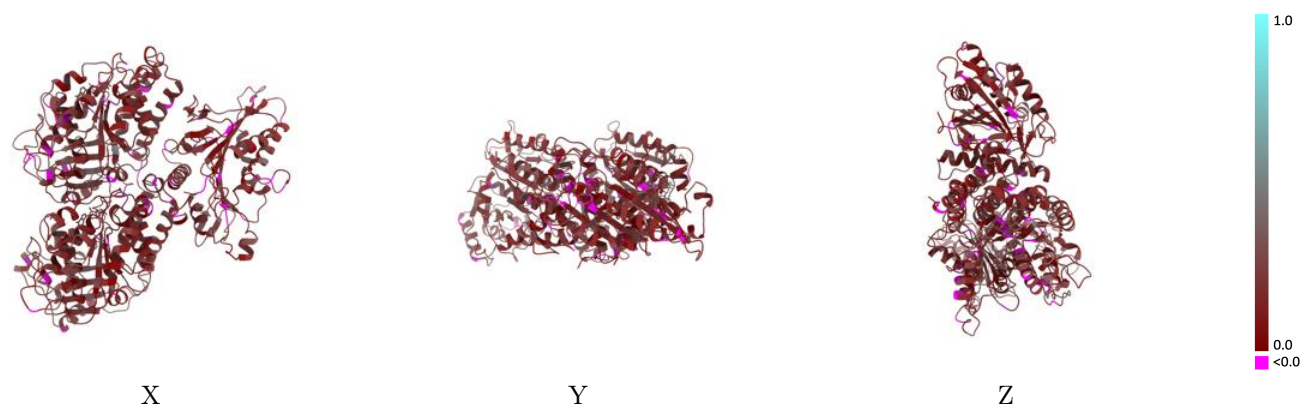
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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](#)

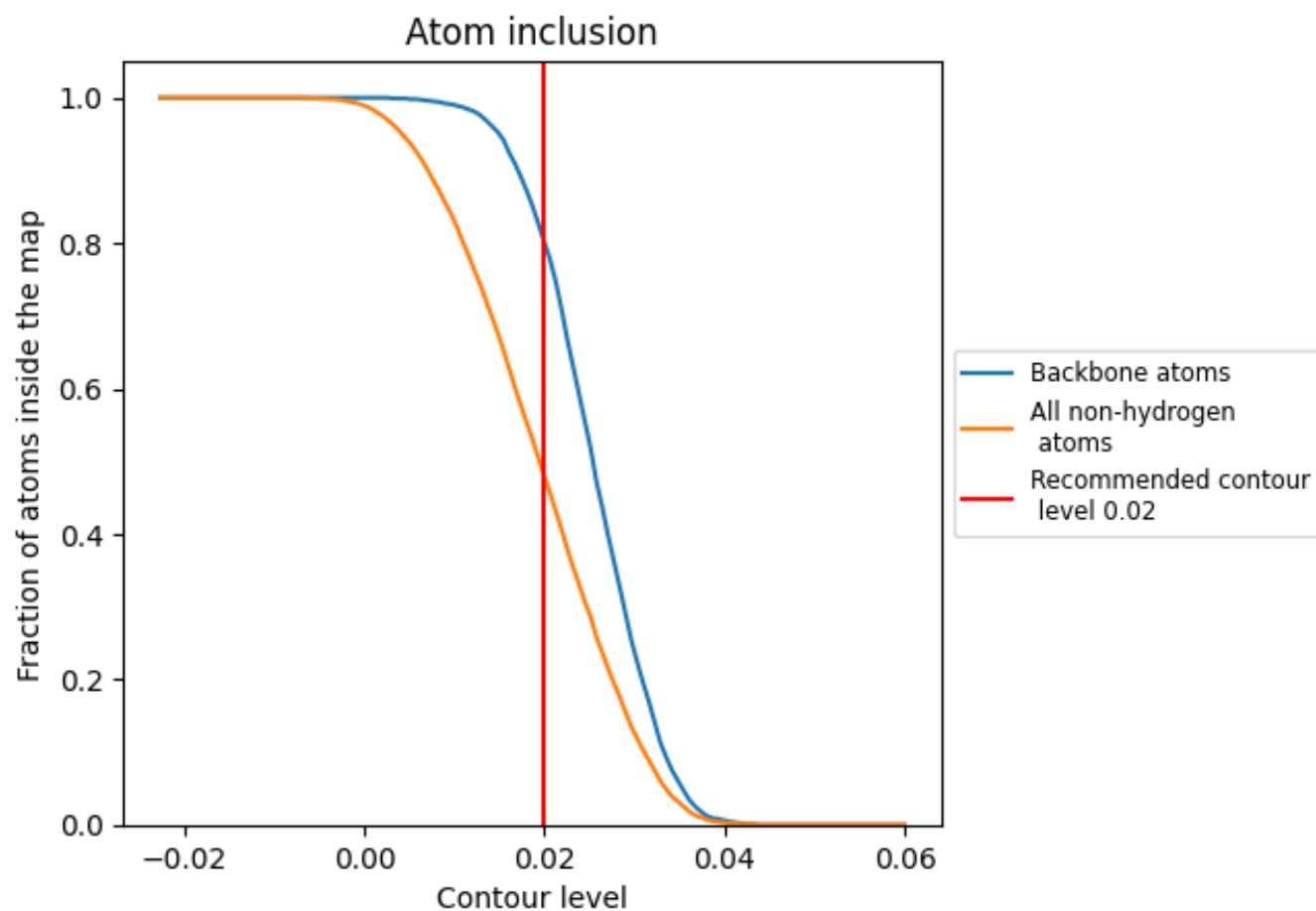


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 48% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4790	0.1710
A	0.5390	0.1760
B	0.5420	0.1770
K	0.3110	0.1560

