



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:10 AM UTC

PDB ID : 3J8Y / pdb_00003j8y
EMDB ID : EMD-6188
Title : High-resolution structure of ATP analog-bound 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:

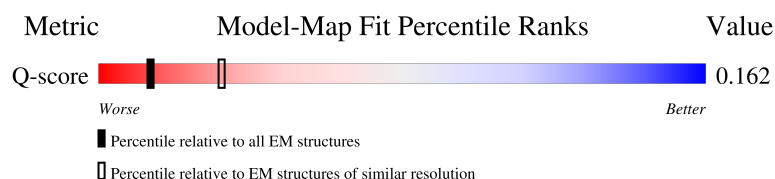
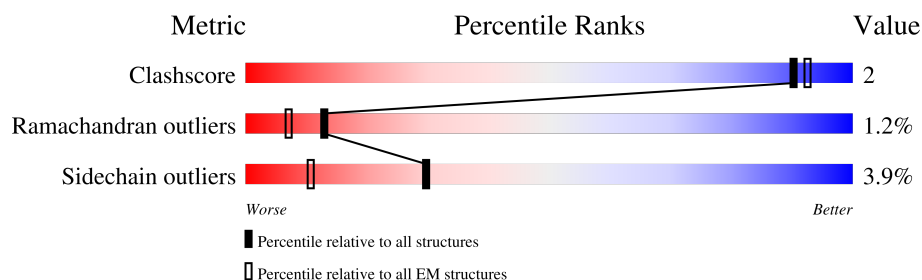
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	74% 47% 43% 5% 5%
2	A	451	53% 43% 44% 7% 5%
3	B	445	51% 48% 42% 6% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9435 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	330	Total	C	N	O	S	0	0
			2582	1609	444	519	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		

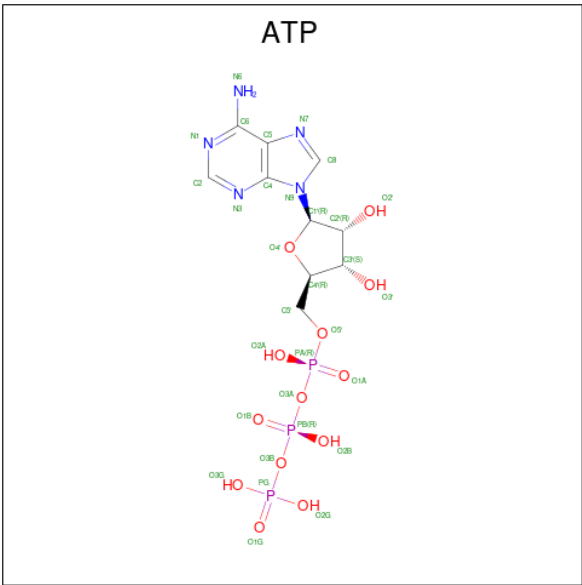
- Molecule 3 is a protein called Tubulin beta-2B chain.

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 ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

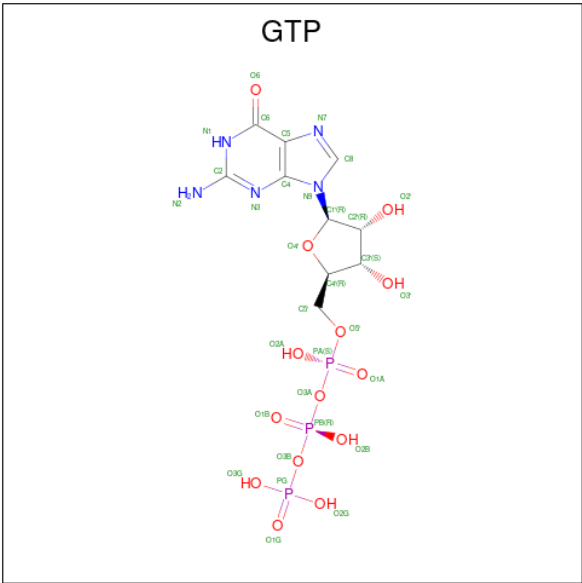


Mol	Chain	Residues	Atoms					AltConf
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

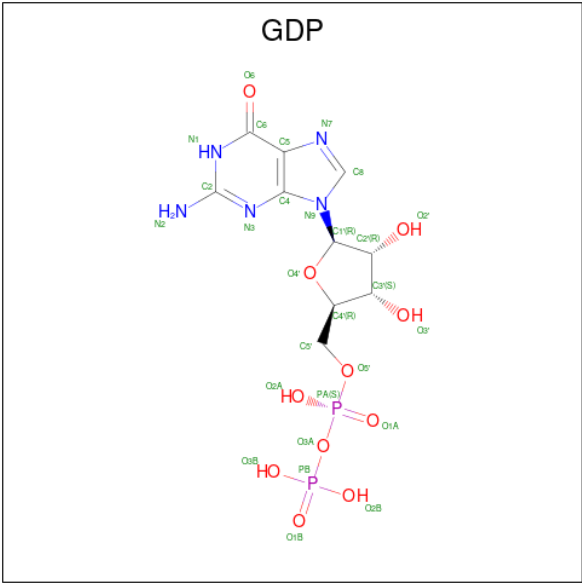
Mol	Chain	Residues	Atoms		AltConf
5	K	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

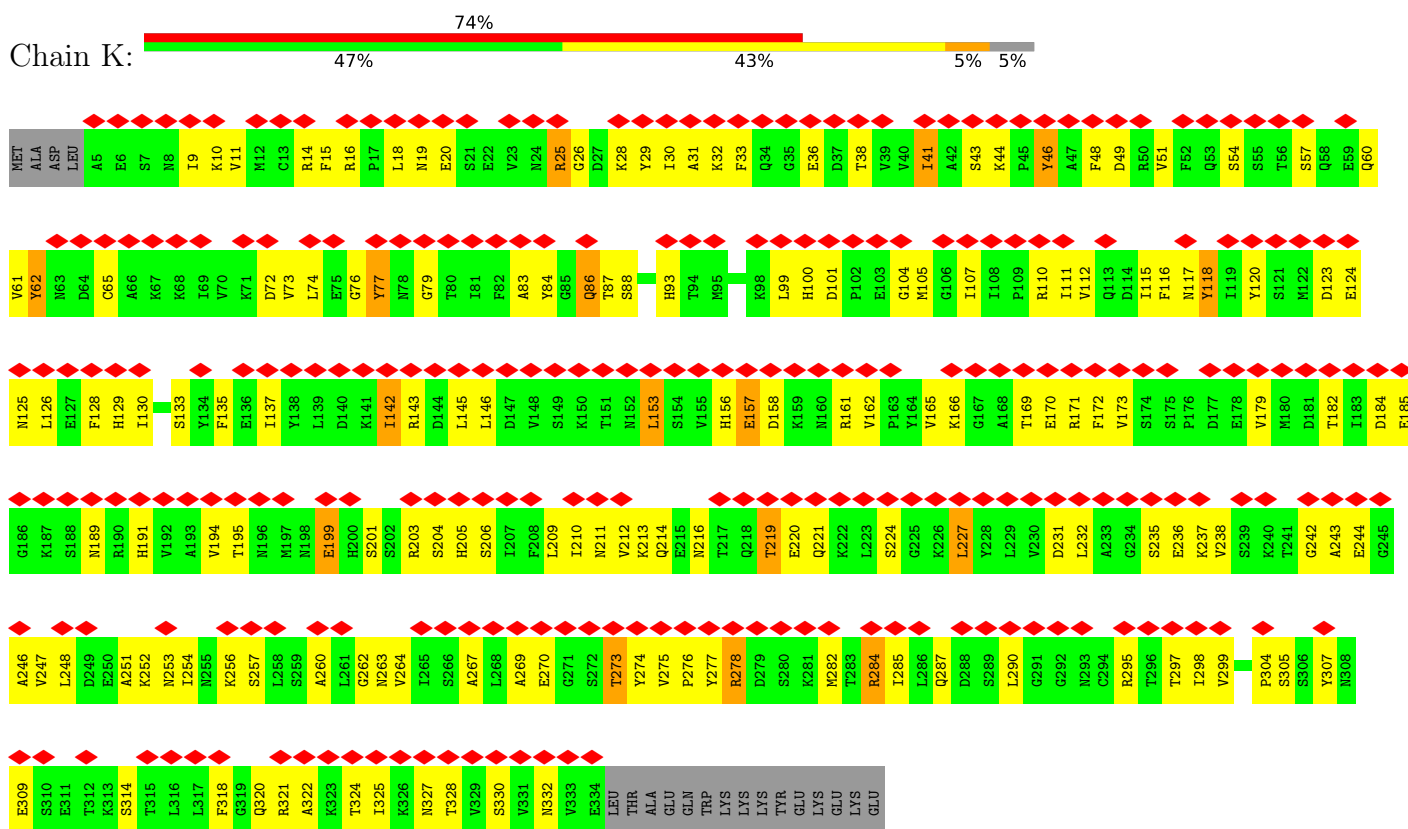


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

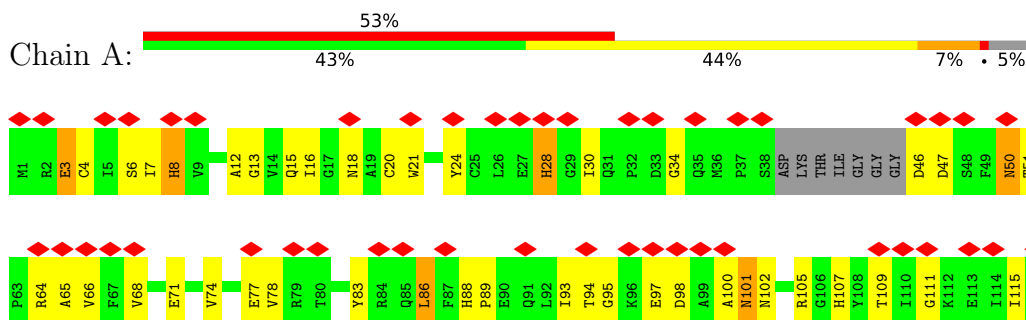
3 Residue-property plots

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.

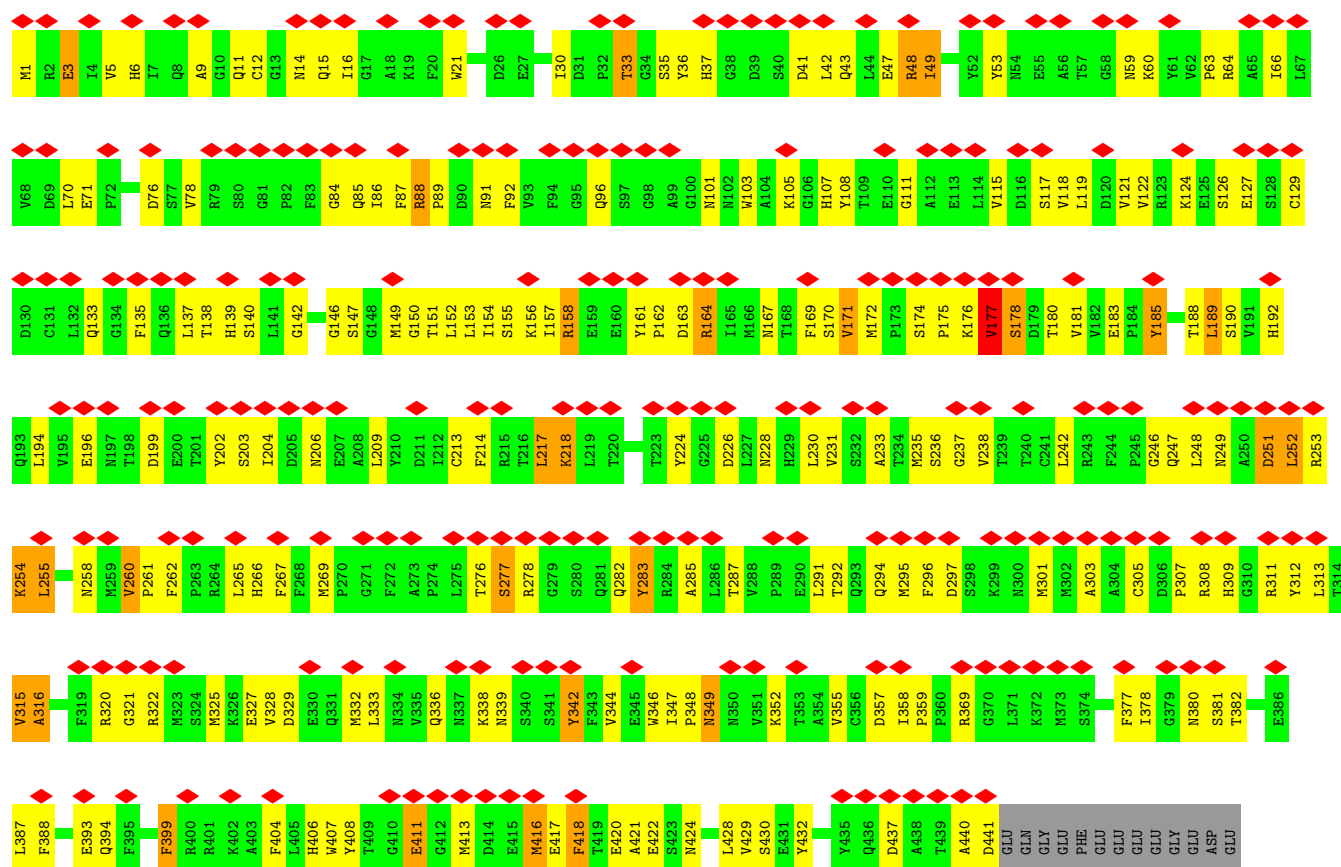
• Molecule 1: Kinesin-1 heavy chain



• Molecule 2: Tubulin alpha-1B chain



- Molecule 3: Tubulin beta-2B chain



ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=25.77°, rise=8.5215 Å, axial sym=C1	Depositor
Number of segments used	49961	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	done within FREALIGN	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	23859	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	671.04, 671.04, 190.827	wwPDB
Map dimensions	320, 320, 91	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.097, 2.097, 2.097	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GTP, MG, 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	2.04	57/2621 (2.2%)	2.46	165/3535 (4.7%)
2	A	2.11	91/3450 (2.6%)	2.46	235/4685 (5.0%)
3	B	2.10	88/3464 (2.5%)	2.40	228/4692 (4.9%)
All	All	2.09	236/9535 (2.5%)	2.44	628/12912 (4.9%)

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	13
2	A	0	19
3	B	0	16
All	All	0	48

All (236) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	145	THR	CA-C	-11.17	1.39	1.52
3	B	204	ILE	CA-C	-10.07	1.43	1.53
2	A	182	VAL	N-CA	-9.94	1.33	1.46
1	K	211	ASN	CA-CB	9.85	1.66	1.53
3	B	381	SER	CA-CB	9.66	1.70	1.53
2	A	160	ASP	CA-CB	8.83	1.67	1.53
3	B	253	ARG	CD-NE	8.66	1.58	1.46
2	A	95	GLY	N-CA	8.03	1.50	1.44
3	B	237	GLY	CA-C	-7.81	1.43	1.52
1	K	54	SER	N-CA	7.75	1.55	1.46
3	B	194	LEU	CA-C	-7.70	1.43	1.52
2	A	164	LYS	CA-C	7.69	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	364	PRO	N-CA	-7.59	1.37	1.47
3	B	294	GLN	N-CA	-7.49	1.37	1.46
2	A	202	PHE	CA-C	-7.49	1.43	1.53
3	B	339	ASN	C-N	7.48	1.43	1.33
3	B	92	PHE	CA-CB	7.46	1.62	1.53
3	B	64	ARG	CA-CB	-7.46	1.43	1.52
2	A	172	TYR	CA-C	7.35	1.61	1.52
2	A	377	MET	CA-C	-7.35	1.43	1.52
3	B	344	VAL	CA-C	7.35	1.61	1.52
2	A	221	ARG	CA-C	-7.32	1.43	1.52
1	K	133	SER	CA-C	-7.32	1.43	1.52
3	B	12	CYS	C-N	7.31	1.43	1.33
3	B	5	VAL	N-CA	7.26	1.55	1.46
2	A	93	ILE	CA-CB	-7.20	1.45	1.54
2	A	378	LEU	N-CA	-7.18	1.37	1.46
1	K	143	ARG	CD-NE	7.12	1.56	1.46
3	B	119	LEU	CA-CB	7.05	1.64	1.53
3	B	359	PRO	CA-C	-7.03	1.45	1.52
2	A	205	ASP	CA-CB	7.02	1.62	1.53
3	B	64	ARG	N-CA	-6.98	1.38	1.46
3	B	266	HIS	CD2-NE2	6.96	1.45	1.37
3	B	276	THR	CA-CB	6.93	1.63	1.53
3	B	92	PHE	C-N	6.87	1.42	1.33
1	K	209	LEU	N-CA	-6.82	1.37	1.46
3	B	320	ARG	NE-CZ	6.82	1.40	1.33
3	B	203	SER	C-N	6.81	1.41	1.33
1	K	100	HIS	CE1-NE2	6.79	1.39	1.32
2	A	100	ALA	CA-C	6.78	1.61	1.52
2	A	54	SER	CA-C	-6.77	1.44	1.52
3	B	177	VAL	CA-C	-6.74	1.44	1.52
3	B	258	ASN	CA-C	6.68	1.61	1.52
2	A	128	GLN	CA-CB	6.68	1.62	1.53
2	A	129	CYS	N-CA	-6.68	1.38	1.46
3	B	11	GLN	CA-C	-6.66	1.44	1.52
1	K	51	VAL	CA-C	-6.64	1.44	1.52
3	B	237	GLY	C-N	6.62	1.42	1.33
3	B	422	GLU	N-CA	-6.59	1.38	1.46
2	A	212	ILE	CA-CB	-6.58	1.46	1.54
1	K	107	ILE	C-N	6.53	1.40	1.33
3	B	218	LYS	C-N	6.53	1.42	1.33
1	K	321	ARG	CA-C	-6.51	1.44	1.52
1	K	307	TYR	CA-CB	6.50	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	406	HIS	CA-C	6.50	1.61	1.52
2	A	77	GLU	CA-CB	6.48	1.63	1.53
3	B	180	THR	C-O	-6.45	1.16	1.24
3	B	60	LYS	N-CA	-6.43	1.38	1.46
1	K	54	SER	CA-C	-6.42	1.44	1.52
2	A	192	HIS	N-CA	-6.41	1.38	1.46
2	A	177	VAL	CA-C	6.40	1.60	1.52
2	A	98	ASP	CA-CB	6.38	1.62	1.53
2	A	229	ARG	NE-CZ	6.37	1.40	1.33
3	B	437	ASP	CA-CB	6.37	1.63	1.53
2	A	306	ASP	N-CA	6.34	1.55	1.46
1	K	77	TYR	CA-C	-6.34	1.44	1.53
2	A	359	PRO	CA-C	6.33	1.58	1.52
2	A	248	LEU	N-CA	6.30	1.52	1.46
2	A	83	TYR	CA-C	-6.29	1.43	1.52
1	K	210	ILE	CA-C	-6.27	1.45	1.52
2	A	62	VAL	CA-C	6.26	1.58	1.52
3	B	71	GLU	C-N	-6.26	1.27	1.34
1	K	30	ILE	CA-C	6.25	1.59	1.52
3	B	235	MET	CA-C	6.23	1.60	1.52
2	A	253	THR	CA-C	-6.20	1.44	1.52
1	K	203	ARG	CD-NE	6.18	1.54	1.46
2	A	163	LYS	CA-CB	6.18	1.63	1.53
2	A	167	LEU	CA-C	-6.17	1.45	1.52
3	B	420	GLU	CA-C	-6.16	1.44	1.52
3	B	322	ARG	CA-C	-6.16	1.45	1.52
1	K	137	ILE	CA-C	-6.12	1.45	1.52
3	B	430	SER	CA-C	-6.10	1.44	1.52
1	K	115	ILE	N-CA	6.09	1.53	1.46
2	A	219	ILE	CA-C	-6.09	1.45	1.52
2	A	346	TRP	N-CA	-6.09	1.38	1.46
1	K	172	PHE	N-CA	-6.08	1.38	1.46
1	K	166	LYS	CA-C	-6.08	1.45	1.52
3	B	158	ARG	CD-NE	6.07	1.54	1.46
1	K	83	ALA	N-CA	6.06	1.53	1.46
3	B	36	TYR	CA-CB	6.05	1.60	1.52
2	A	201	ALA	CA-C	-6.04	1.45	1.52
2	A	370	LYS	CA-CB	-6.04	1.45	1.52
3	B	420	GLU	CA-CB	6.04	1.62	1.53
3	B	295	MET	CA-C	5.99	1.60	1.52
1	K	123	ASP	C-N	5.98	1.42	1.33
3	B	269	MET	N-CA	-5.95	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	315	VAL	CA-C	-5.95	1.45	1.52
3	B	339	ASN	CA-C	5.94	1.60	1.53
1	K	185	GLU	C-O	-5.94	1.17	1.24
1	K	74	LEU	N-CA	-5.93	1.38	1.46
2	A	222	PRO	CA-C	5.88	1.59	1.52
2	A	52	PHE	CA-C	5.86	1.60	1.52
2	A	219	ILE	N-CA	-5.86	1.39	1.46
1	K	10	LYS	N-CA	-5.85	1.38	1.46
3	B	406	HIS	ND1-CE1	-5.85	1.26	1.32
1	K	170	GLU	CA-CB	5.85	1.60	1.52
3	B	9	ALA	N-CA	5.85	1.53	1.46
2	A	416	GLY	C-N	5.84	1.41	1.33
3	B	411	GLU	CA-C	-5.83	1.44	1.52
1	K	274	TYR	C-O	-5.82	1.18	1.23
3	B	336	GLN	N-CA	-5.80	1.38	1.46
3	B	251	ASP	N-CA	-5.78	1.37	1.45
1	K	161	ARG	CD-NE	5.76	1.54	1.46
2	A	3	GLU	CA-CB	-5.75	1.44	1.53
2	A	314	ALA	N-CA	-5.74	1.38	1.46
2	A	140	SER	CA-CB	5.74	1.62	1.53
1	K	263	ASN	N-CA	5.74	1.53	1.46
3	B	37	HIS	C-N	5.73	1.41	1.33
2	A	68	VAL	CA-C	5.72	1.59	1.52
1	K	246	ALA	C-N	5.72	1.41	1.33
3	B	316	ALA	N-CA	-5.72	1.39	1.46
3	B	37	HIS	ND1-CE1	5.71	1.38	1.32
3	B	192	HIS	CB-CG	-5.70	1.42	1.50
3	B	183	GLU	N-CA	-5.70	1.40	1.46
2	A	327	ASP	CA-CB	5.69	1.62	1.53
2	A	197	HIS	CG-ND1	5.68	1.44	1.38
2	A	329	ASN	C-O	-5.68	1.17	1.24
1	K	274	TYR	CA-CB	5.66	1.60	1.53
2	A	266	HIS	CG-CD2	-5.66	1.29	1.35
2	A	161	TYR	N-CA	5.65	1.53	1.46
3	B	119	LEU	C-O	-5.64	1.17	1.24
2	A	309	HIS	CE1-NE2	5.63	1.38	1.32
1	K	201	SER	C-N	5.63	1.41	1.33
3	B	48	ARG	CD-NE	5.63	1.54	1.46
1	K	295	ARG	CD-NE	5.62	1.54	1.46
2	A	164	LYS	C-N	5.61	1.41	1.33
3	B	260	VAL	C-N	5.61	1.41	1.34
1	K	231	ASP	CA-C	5.57	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	PHE	CA-C	-5.57	1.45	1.52
3	B	177	VAL	C-O	-5.57	1.17	1.24
2	A	280	LYS	CA-CB	5.56	1.60	1.52
1	K	143	ARG	CA-CB	5.56	1.61	1.53
2	A	66	VAL	CA-CB	5.55	1.61	1.54
3	B	421	ALA	C-N	5.55	1.40	1.33
2	A	209	ILE	N-CA	-5.54	1.40	1.46
1	K	128	PHE	N-CA	-5.51	1.39	1.46
1	K	156	HIS	CA-C	-5.51	1.46	1.52
2	A	231	ILE	N-CA	-5.51	1.40	1.46
1	K	126	LEU	CA-CB	5.50	1.60	1.53
2	A	234	ILE	C-N	5.49	1.40	1.33
3	B	15	GLN	N-CA	5.48	1.53	1.46
1	K	93	HIS	CE1-NE2	5.45	1.38	1.32
1	K	214	GLN	N-CA	-5.44	1.39	1.45
2	A	173	PRO	CA-C	-5.44	1.46	1.52
2	A	139	HIS	CE1-NE2	5.44	1.38	1.32
2	A	397	LEU	CA-CB	5.43	1.61	1.53
3	B	175	PRO	C-N	5.42	1.40	1.33
3	B	111	GLY	CA-C	-5.42	1.45	1.51
2	A	168	GLU	N-CA	-5.42	1.39	1.45
3	B	127	GLU	CA-C	-5.41	1.45	1.52
2	A	162	GLY	CA-C	-5.41	1.44	1.51
3	B	231	VAL	N-CA	5.41	1.52	1.46
3	B	162	PRO	C-N	5.40	1.41	1.34
1	K	117	ASN	CA-CB	5.38	1.61	1.53
2	A	173	PRO	N-CD	5.37	1.55	1.47
2	A	311	LYS	C-N	5.37	1.40	1.33
1	K	204	SER	N-CA	-5.37	1.39	1.45
2	A	28	HIS	N-CA	-5.36	1.39	1.46
2	A	431	ASP	N-CA	-5.36	1.40	1.46
1	K	184	ASP	CA-CB	5.35	1.61	1.53
3	B	252	LEU	N-CA	-5.35	1.39	1.46
3	B	122	VAL	C-N	5.33	1.40	1.33
3	B	196	GLU	CA-C	5.33	1.60	1.52
3	B	196	GLU	N-CA	-5.33	1.39	1.46
3	B	406	HIS	CE1-NE2	5.33	1.37	1.32
3	B	137	LEU	C-N	5.33	1.40	1.33
1	K	99	LEU	CA-C	-5.32	1.45	1.52
2	A	176	GLN	CA-CB	5.32	1.62	1.53
2	A	326	LYS	C-O	-5.31	1.18	1.24
3	B	440	ALA	CA-CB	5.31	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	34	GLY	CA-C	-5.31	1.44	1.51
1	K	14	ARG	CD-NE	5.30	1.53	1.46
1	K	304	PRO	C-N	5.29	1.40	1.33
2	A	83	TYR	CA-CB	5.29	1.61	1.54
2	A	321	GLY	N-CA	5.28	1.53	1.45
2	A	71	GLU	C-O	5.28	1.30	1.24
2	A	428	LEU	C-N	5.28	1.40	1.33
1	K	20	GLU	C-O	-5.27	1.18	1.24
3	B	188	THR	CA-C	-5.25	1.46	1.52
2	A	348	PRO	CA-CB	5.25	1.61	1.53
2	A	351	PHE	C-O	-5.25	1.18	1.24
3	B	192	HIS	CE1-NE2	5.24	1.37	1.32
3	B	407	TRP	CA-C	-5.24	1.45	1.52
2	A	365	GLY	C-O	-5.23	1.19	1.24
2	A	394	LYS	CA-C	-5.23	1.46	1.52
2	A	435	VAL	CA-CB	-5.23	1.47	1.54
2	A	422	ARG	CD-NE	5.23	1.53	1.46
1	K	87	THR	N-CA	5.23	1.53	1.46
3	B	278	ARG	C-N	5.23	1.39	1.33
3	B	152	LEU	C-O	5.23	1.30	1.24
1	K	43	SER	CA-CB	5.22	1.62	1.53
2	A	268	PRO	CA-CB	5.22	1.61	1.53
2	A	16	ILE	CA-C	-5.22	1.46	1.52
1	K	79	GLY	N-CA	5.19	1.52	1.45
3	B	321	GLY	N-CA	-5.18	1.40	1.45
3	B	71	GLU	CA-C	-5.17	1.46	1.52
2	A	230	LEU	CA-CB	5.17	1.61	1.53
2	A	357	TYR	CA-C	5.16	1.59	1.52
2	A	308	ARG	C-N	5.15	1.40	1.33
3	B	89	PRO	C-O	-5.14	1.17	1.24
3	B	252	LEU	CA-C	-5.13	1.45	1.52
2	A	139	HIS	CD2-NE2	5.13	1.43	1.37
3	B	261	PRO	N-CD	-5.13	1.40	1.47
2	A	306	ASP	C-N	5.12	1.38	1.33
3	B	422	GLU	C-N	5.12	1.40	1.33
3	B	276	THR	C-N	5.12	1.40	1.33
1	K	146	LEU	C-N	5.11	1.40	1.33
1	K	32	LYS	CA-C	-5.11	1.46	1.52
1	K	309	GLU	C-N	5.11	1.40	1.33
3	B	139	HIS	N-CA	-5.10	1.40	1.46
1	K	107	ILE	CA-C	-5.09	1.46	1.52
3	B	153	LEU	CA-CB	5.06	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	358	GLN	C-N	5.05	1.39	1.33
3	B	63	PRO	C-N	5.05	1.40	1.33
2	A	240	ALA	CA-C	-5.05	1.46	1.52
2	A	353	VAL	CA-CB	-5.04	1.48	1.54
1	K	244	GLU	CA-C	5.04	1.59	1.52
3	B	181	VAL	N-CA	5.04	1.52	1.46
1	K	156	HIS	CE1-NE2	5.03	1.37	1.32
3	B	88	ARG	CD-NE	5.03	1.53	1.46
1	K	120	TYR	CA-CB	5.01	1.61	1.53
3	B	226	ASP	CA-CB	5.01	1.61	1.53
3	B	313	LEU	CA-C	-5.01	1.46	1.52
2	A	170	SER	N-CA	-5.00	1.40	1.46
1	K	252	LYS	N-CA	-5.00	1.40	1.46
2	A	355	ILE	CA-CB	5.00	1.60	1.54

All (628) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	158	ASP	CA-CB-CG	11.13	123.73	112.60
2	A	115	ILE	N-CA-C	10.81	121.71	110.36
2	A	98	ASP	N-CA-C	10.42	123.11	110.19
2	A	109	THR	N-CA-C	10.38	122.28	110.97
2	A	283	HIS	ND1-CE1-NE2	10.24	118.64	108.40
2	A	134	GLY	O-C-N	-10.22	115.32	123.80
3	B	247	GLN	CA-C-O	9.81	124.51	118.33
3	B	339	ASN	CA-CB-CG	-9.67	102.93	112.60
2	A	139	HIS	ND1-CG-CD2	9.62	115.72	106.10
2	A	171	ILE	CA-C-N	9.56	134.90	121.61
2	A	171	ILE	C-N-CA	9.56	134.90	121.61
1	K	49	ASP	CA-CB-CG	-9.47	103.13	112.60
1	K	309	GLU	N-CA-C	9.38	122.36	111.11
1	K	298	ILE	N-CA-CB	9.29	123.88	111.25
2	A	235	VAL	CB-CA-C	-9.03	97.64	112.26
2	A	284	GLU	N-CA-C	-8.99	102.44	113.41
1	K	237	LYS	CA-C-N	8.94	132.71	120.46
1	K	237	LYS	C-N-CA	8.94	132.71	120.46
3	B	96	GLN	N-CA-CB	-8.84	99.25	111.00
2	A	172	TYR	CA-C-O	-8.83	112.79	119.32
3	B	96	GLN	OE1-CD-NE2	-8.81	113.78	122.60
3	B	283	TYR	N-CA-CB	8.81	125.39	110.49
1	K	232	LEU	O-C-N	-8.80	111.82	122.65
3	B	260	VAL	O-C-N	-8.71	115.88	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	88	SER	O-C-N	-8.42	113.03	121.87
3	B	267	PHE	CA-CB-CG	-8.41	105.39	113.80
2	A	268	PRO	CA-C-N	8.37	134.27	122.72
2	A	268	PRO	C-N-CA	8.37	134.27	122.72
2	A	18	ASN	CA-CB-CG	-8.35	104.25	112.60
1	K	332	ASN	O-C-N	-8.34	112.08	122.68
2	A	244	PHE	CA-CB-CG	-8.30	105.50	113.80
2	A	262	TYR	O-C-N	-8.27	116.01	121.88
2	A	368	LEU	O-C-N	-8.27	113.36	122.79
2	A	183	GLU	O-C-N	-8.19	112.90	120.92
2	A	205	ASP	CA-CB-CG	8.18	120.78	112.60
3	B	126	SER	N-CA-C	8.16	124.83	111.37
2	A	94	THR	CA-C-N	8.13	131.15	122.69
2	A	94	THR	C-N-CA	8.13	131.15	122.69
1	K	184	ASP	CA-C-N	8.12	131.37	120.65
1	K	184	ASP	C-N-CA	8.12	131.37	120.65
3	B	309	HIS	O-C-N	-8.11	112.37	122.35
1	K	19	ASN	CA-CB-CG	8.08	120.68	112.60
2	A	159	VAL	N-CA-C	-8.02	103.45	110.74
1	K	130	ILE	O-C-N	-7.88	114.90	123.18
1	K	36	GLU	N-CA-C	-7.87	102.59	112.90
3	B	64	ARG	NE-CZ-NH2	7.82	126.24	119.20
2	A	382	THR	CA-CB-OG1	7.79	121.29	109.60
2	A	424	ASP	CA-CB-CG	-7.79	104.81	112.60
3	B	16	ILE	CA-CB-CG1	7.78	123.62	110.40
1	K	284	ARG	NE-CZ-NH2	-7.77	112.21	119.20
2	A	192	HIS	ND1-CG-CD2	7.74	113.84	106.10
2	A	156	ARG	O-C-N	-7.73	113.93	122.12
1	K	116	PHE	CA-C-N	7.72	130.96	120.38
1	K	116	PHE	C-N-CA	7.72	130.96	120.38
3	B	369	ARG	NE-CZ-NH1	-7.70	113.80	121.50
2	A	427	ALA	CA-C-N	7.67	130.41	120.44
2	A	427	ALA	C-N-CA	7.67	130.41	120.44
3	B	432	TYR	N-CA-CB	7.66	121.50	110.16
1	K	330	SER	O-C-N	-7.64	114.82	122.99
3	B	133	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	K	327	ASN	CA-CB-CG	7.62	120.22	112.60
2	A	267	PHE	CA-C-O	-7.61	110.21	120.64
3	B	172	MET	CA-C-N	7.61	127.54	119.85
3	B	172	MET	C-N-CA	7.61	127.54	119.85
3	B	309	HIS	CA-CB-CG	-7.61	106.19	113.80
2	A	233	GLN	O-C-N	-7.60	113.33	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	252	LEU	N-CA-CB	7.59	121.90	110.22
1	K	112	VAL	N-CA-C	7.58	118.32	110.36
1	K	260	ALA	N-CA-C	7.54	119.50	111.28
3	B	217	LEU	CA-C-N	7.50	135.86	121.54
3	B	217	LEU	C-N-CA	7.50	135.86	121.54
2	A	97	GLU	CA-C-O	-7.50	113.12	120.92
2	A	326	LYS	CA-C-N	7.48	130.30	120.28
2	A	326	LYS	C-N-CA	7.48	130.30	120.28
3	B	247	GLN	O-C-N	-7.47	115.45	121.65
2	A	323	VAL	O-C-N	-7.46	115.11	123.10
1	K	100	HIS	ND1-CG-CD2	7.45	113.55	106.10
2	A	387	ALA	CA-C-O	-7.44	113.03	120.70
3	B	91	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	K	248	LEU	N-CA-C	7.40	119.13	111.14
3	B	103	TRP	CA-C-N	7.39	130.18	120.28
3	B	103	TRP	C-N-CA	7.39	130.18	120.28
2	A	284	GLU	O-C-N	-7.36	111.92	122.36
2	A	239	THR	CA-C-O	7.33	127.90	119.18
2	A	256	GLN	CA-C-N	7.33	131.81	120.82
2	A	256	GLN	C-N-CA	7.33	131.81	120.82
1	K	123	ASP	CA-CB-CG	-7.32	105.28	112.60
3	B	127	GLU	CA-C-O	7.30	127.86	119.18
2	A	387	ALA	CA-C-N	7.29	130.38	120.54
2	A	387	ALA	C-N-CA	7.29	130.38	120.54
2	A	345	ASP	CA-CB-CG	-7.28	105.32	112.60
1	K	38	THR	N-CA-C	7.27	120.75	108.90
2	A	172	TYR	O-C-N	7.25	128.03	121.35
3	B	251	ASP	CA-C-N	7.25	133.00	120.68
3	B	251	ASP	C-N-CA	7.25	133.00	120.68
3	B	355	VAL	O-C-N	-7.25	115.64	123.18
3	B	421	ALA	CA-C-O	7.23	128.21	120.55
3	B	416	MET	CG-SD-CE	-7.22	85.02	100.90
1	K	332	ASN	CA-C-N	7.20	131.71	120.34
1	K	332	ASN	C-N-CA	7.20	131.71	120.34
3	B	322	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	K	110	ARG	NE-CZ-NH2	7.16	125.65	119.20
2	A	218	ASP	CA-CB-CG	-7.16	105.44	112.60
2	A	192	HIS	CA-CB-CG	7.14	120.94	113.80
3	B	92	PHE	CA-CB-CG	-7.13	106.67	113.80
1	K	142	ILE	O-C-N	-7.13	114.28	122.62
1	K	252	LYS	CB-CA-C	-7.12	99.41	110.81
3	B	41	ASP	CA-CB-CG	-7.12	105.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	251	ALA	CA-C-N	7.10	130.13	120.54
1	K	251	ALA	C-N-CA	7.10	130.13	120.54
3	B	332	MET	CG-SD-CE	-7.10	85.27	100.90
3	B	117	SER	CA-C-O	7.10	128.13	119.97
3	B	124	LYS	N-CA-C	7.10	119.87	111.71
1	K	184	ASP	N-CA-C	7.09	119.01	111.28
3	B	333	LEU	CA-C-N	7.09	130.64	120.79
3	B	333	LEU	C-N-CA	7.09	130.64	120.79
1	K	246	ALA	CA-C-O	7.08	128.11	119.97
1	K	118	TYR	O-C-N	-7.03	114.50	122.09
1	K	26	GLY	CA-C-O	7.02	125.37	118.77
3	B	236	SER	CA-C-N	7.02	127.73	119.94
3	B	236	SER	C-N-CA	7.02	127.73	119.94
2	A	231	ILE	N-CA-C	7.01	117.15	110.42
3	B	429	VAL	N-CA-C	7.00	117.14	110.42
2	A	302	MET	CA-C-N	-6.99	113.80	123.10
2	A	302	MET	C-N-CA	-6.99	113.80	123.10
3	B	183	GLU	CA-C-O	-6.98	111.91	118.33
3	B	87	PHE	O-C-N	-6.98	114.78	123.01
1	K	269	ALA	N-CA-C	6.97	118.96	111.36
3	B	192	HIS	N-CA-C	6.97	119.77	111.33
2	A	194	THR	CA-C-N	6.96	134.84	121.54
2	A	194	THR	C-N-CA	6.96	134.84	121.54
2	A	236	SER	CA-C-O	-6.94	113.06	120.42
3	B	177	VAL	CA-C-N	6.93	134.78	121.54
3	B	177	VAL	C-N-CA	6.93	134.78	121.54
1	K	44	LYS	O-C-N	-6.91	114.99	121.35
2	A	428	LEU	N-CA-C	-6.90	103.68	111.07
2	A	432	TYR	N-CA-C	6.89	119.64	111.71
2	A	88	HIS	CA-C-N	6.89	127.46	119.47
2	A	88	HIS	C-N-CA	6.89	127.46	119.47
3	B	189	LEU	O-C-N	-6.89	114.82	122.12
1	K	158	ASP	CA-C-O	6.88	130.11	121.50
2	A	102	ASN	CA-CB-CG	6.88	119.48	112.60
2	A	239	THR	N-CA-CB	6.87	121.25	110.46
3	B	381	SER	CA-C-O	6.87	128.00	120.71
1	K	60	GLN	CA-CB-CG	-6.86	100.37	114.10
3	B	394	GLN	N-CA-C	6.86	118.41	111.07
3	B	188	THR	N-CA-CB	6.84	119.93	110.01
3	B	118	VAL	CB-CA-C	-6.82	103.09	112.02
1	K	86	GLN	O-C-N	-6.81	114.10	122.82
3	B	249	ASN	CA-CB-CG	-6.81	105.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	192	HIS	CB-CG-CD2	-6.80	122.36	131.20
2	A	74	VAL	CA-C-O	6.79	128.01	120.95
2	A	93	ILE	CA-C-O	6.79	127.45	120.39
3	B	292	THR	N-CA-CB	6.78	120.05	109.94
2	A	175	PRO	N-CA-C	-6.77	103.23	114.75
3	B	181	VAL	CA-C-N	6.76	131.96	121.34
3	B	181	VAL	C-N-CA	6.76	131.96	121.34
1	K	157	GLU	O-C-N	-6.76	115.32	123.10
2	A	8	HIS	ND1-CE1-NE2	6.75	115.15	108.40
3	B	421	ALA	O-C-N	-6.73	114.99	122.12
3	B	204	ILE	N-CA-C	6.71	117.13	106.32
3	B	369	ARG	NE-CZ-NH2	6.71	125.23	119.20
1	K	104	GLY	N-CA-C	6.68	122.02	114.67
3	B	217	LEU	N-CA-CB	6.68	120.15	110.20
2	A	150	THR	O-C-N	-6.67	115.05	122.12
1	K	254	ILE	CA-C-N	6.64	130.03	120.79
1	K	254	ILE	C-N-CA	6.64	130.03	120.79
3	B	76	ASP	N-CA-C	6.64	119.08	111.11
2	A	109	THR	CB-CA-C	-6.64	100.73	110.96
1	K	156	HIS	CA-C-O	-6.61	113.56	121.56
2	A	234	ILE	CA-C-O	6.61	127.39	120.25
3	B	441	ASP	CA-CB-CG	6.60	119.20	112.60
3	B	138	THR	N-CA-C	-6.60	97.52	108.34
2	A	160	ASP	N-CA-C	6.58	119.05	111.02
2	A	359	PRO	O-C-N	-6.57	113.71	121.46
2	A	21	TRP	N-CA-CB	6.56	119.77	110.12
2	A	88	HIS	ND1-CG-CD2	6.56	112.66	106.10
1	K	251	ALA	N-CA-C	6.55	118.42	111.28
3	B	213	CYS	CA-C-N	6.55	131.65	120.71
3	B	213	CYS	C-N-CA	6.55	131.65	120.71
1	K	242	GLY	CA-C-O	6.54	128.07	119.58
2	A	189	LEU	N-CA-C	6.53	118.95	111.11
1	K	267	ALA	N-CA-C	6.53	118.94	111.11
2	A	156	ARG	CA-C-N	6.52	130.22	120.31
2	A	156	ARG	C-N-CA	6.52	130.22	120.31
1	K	31	ALA	N-CA-C	6.51	120.27	109.46
1	K	220	GLU	CA-C-O	6.51	128.00	120.32
3	B	37	HIS	O-C-N	-6.51	113.17	122.41
3	B	188	THR	CB-CA-C	-6.51	100.67	110.88
2	A	183	GLU	CA-C-N	6.50	126.43	119.28
2	A	183	GLU	C-N-CA	6.50	126.43	119.28
3	B	174	SER	N-CA-C	6.50	119.05	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	181	VAL	N-CA-C	6.47	118.06	111.00
2	A	164	LYS	N-CA-CB	6.46	119.65	109.71
2	A	197	HIS	O-C-N	-6.44	114.38	122.17
1	K	332	ASN	CA-C-O	6.41	127.59	120.92
3	B	43	GLN	N-CA-C	6.41	118.26	111.28
1	K	212	VAL	O-C-N	-6.40	115.61	123.10
1	K	305	SER	O-C-N	-6.39	115.47	123.01
1	K	162	VAL	N-CA-C	6.38	114.12	108.63
3	B	260	VAL	N-CA-C	6.37	113.86	107.55
2	A	24	TYR	CB-CG-CD1	-6.37	111.25	120.80
3	B	404	PHE	CA-C-N	6.36	128.71	120.44
3	B	404	PHE	C-N-CA	6.36	128.71	120.44
1	K	9	ILE	O-C-N	-6.35	115.35	122.66
1	K	101	ASP	CA-CB-CG	6.35	118.95	112.60
2	A	417	GLU	CA-C-N	6.33	129.09	120.54
2	A	417	GLU	C-N-CA	6.33	129.09	120.54
3	B	329	ASP	CA-C-N	6.32	129.27	120.29
3	B	329	ASP	C-N-CA	6.32	129.27	120.29
2	A	111	GLY	N-CA-C	6.32	120.54	112.83
1	K	262	GLY	N-CA-C	6.29	120.25	112.64
2	A	256	GLN	N-CA-C	-6.28	104.06	111.03
1	K	46	TYR	N-CA-CB	6.28	120.38	110.84
2	A	356	ASN	OD1-CG-ND2	6.27	128.87	122.60
3	B	135	PHE	CA-CB-CG	-6.27	107.53	113.80
3	B	406	HIS	ND1-CE1-NE2	6.23	114.63	108.40
3	B	278	ARG	CA-C-O	6.23	126.73	120.88
2	A	210	TYR	CA-CB-CG	6.22	125.10	113.90
3	B	33	THR	CA-CB-OG1	6.22	118.93	109.60
2	A	388	TRP	N-CA-CB	6.20	119.18	109.94
3	B	233	ALA	CA-C-N	6.20	128.50	120.44
3	B	233	ALA	C-N-CA	6.20	128.50	120.44
3	B	346	TRP	CD2-CE2-CZ2	-6.20	116.20	122.40
2	A	145	THR	CA-C-O	6.20	127.50	121.00
2	A	191	THR	CA-C-N	6.19	128.57	120.28
2	A	191	THR	C-N-CA	6.19	128.57	120.28
1	K	62	TYR	N-CA-C	6.18	118.53	111.11
1	K	76	GLY	CA-C-O	6.17	125.62	118.96
3	B	108	TYR	O-C-N	-6.16	113.65	122.03
3	B	64	ARG	NH1-CZ-NH2	-6.16	111.29	119.30
2	A	102	ASN	O-C-N	-6.16	115.01	123.01
1	K	276	PRO	N-CA-CB	6.15	106.72	102.35
2	A	318	LEU	CA-C-O	-6.15	113.94	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	378	LEU	N-CA-C	-6.14	99.19	109.07
1	K	273	THR	N-CA-C	6.13	118.05	111.36
1	K	11	VAL	CA-C-O	6.12	126.76	120.39
1	K	290	LEU	N-CA-C	-6.12	105.94	113.41
2	A	149	PHE	N-CA-CB	6.12	118.94	110.07
2	A	367	ASP	CA-CB-CG	-6.12	106.48	112.60
2	A	165	SER	N-CA-C	6.12	119.10	110.23
1	K	253	ASN	CA-C-N	6.11	128.34	120.88
1	K	253	ASN	C-N-CA	6.11	128.34	120.88
3	B	49	ILE	N-CA-C	6.07	116.82	110.62
3	B	101	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	K	107	ILE	N-CA-C	6.07	116.73	110.36
2	A	88	HIS	CA-C-O	-6.07	114.36	119.76
2	A	259	LEU	N-CA-C	-6.07	106.01	113.41
3	B	149	MET	CG-SD-CE	-6.06	87.57	100.90
2	A	343	PHE	N-CA-C	6.06	118.62	109.41
3	B	278	ARG	N-CA-C	6.05	119.59	110.64
1	K	120	TYR	CB-CG-CD1	6.04	129.86	120.80
1	K	129	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	K	101	ASP	CA-C-O	-6.03	114.72	119.66
1	K	33	PHE	CA-CB-CG	-6.02	107.78	113.80
1	K	278	ARG	O-C-N	-6.02	114.58	122.59
3	B	418	PHE	CA-CB-CG	-6.01	107.78	113.80
2	A	190	THR	N-CA-CB	6.00	118.72	110.01
2	A	13	GLY	CA-C-N	6.00	128.94	120.42
2	A	13	GLY	C-N-CA	6.00	128.94	120.42
2	A	412	GLY	O-C-N	-6.00	115.46	122.60
3	B	322	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	K	124	GLU	N-CA-CB	-5.99	99.91	110.39
2	A	192	HIS	CA-C-N	5.98	128.58	120.44
2	A	192	HIS	C-N-CA	5.98	128.58	120.44
2	A	46	ASP	CA-CB-CG	5.98	118.58	112.60
2	A	320	ARG	O-C-N	-5.98	116.32	123.31
1	K	72	ASP	O-C-N	-5.97	115.64	122.09
2	A	88	HIS	ND1-CE1-NE2	5.96	114.36	108.40
2	A	398	MET	CA-CB-CG	5.96	126.02	114.10
3	B	70	LEU	N-CA-C	-5.96	104.17	112.45
3	B	307	PRO	CA-C-N	5.96	130.67	120.72
3	B	307	PRO	C-N-CA	5.96	130.67	120.72
3	B	238	VAL	CB-CA-C	-5.96	102.45	112.16
3	B	137	LEU	O-C-N	-5.95	116.25	123.10
3	B	163	ASP	O-C-N	-5.95	114.95	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	21	TRP	CZ3-CH2-CZ2	-5.95	113.77	121.50
3	B	247	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	K	15	PHE	CA-CB-CG	-5.94	107.86	113.80
2	A	150	THR	N-CA-CB	5.94	118.97	110.06
2	A	428	LEU	O-C-N	-5.94	115.96	122.07
1	K	110	ARG	CA-C-N	5.92	128.23	120.60
1	K	110	ARG	C-N-CA	5.92	128.23	120.60
3	B	85	GLN	N-CA-CB	5.91	120.20	110.39
2	A	46	ASP	CA-C-N	5.91	132.82	121.54
2	A	46	ASP	C-N-CA	5.91	132.82	121.54
3	B	157	ILE	CA-C-O	5.90	127.11	120.85
3	B	190	SER	CB-CA-C	-5.90	100.82	110.85
3	B	378	ILE	O-C-N	-5.90	117.04	123.18
1	K	244	GLU	N-CA-C	-5.90	100.35	109.14
2	A	316	CYS	O-C-N	5.90	130.21	123.31
2	A	88	HIS	CA-CB-CG	-5.89	107.91	113.80
1	K	297	THR	N-CA-CB	5.88	119.81	110.57
2	A	15	GLN	N-CA-C	5.88	118.64	111.82
3	B	37	HIS	ND1-CG-CD2	5.88	111.98	106.10
3	B	213	CYS	O-C-N	-5.88	115.44	122.15
3	B	185	TYR	CA-C-N	5.88	128.43	120.38
3	B	185	TYR	C-N-CA	5.88	128.43	120.38
2	A	52	PHE	CA-C-O	-5.87	111.59	119.11
3	B	301	MET	CA-C-N	5.87	131.87	122.83
3	B	301	MET	C-N-CA	5.87	131.87	122.83
2	A	50	ASN	CA-CB-CG	5.86	118.46	112.60
3	B	147	SER	N-CA-C	5.86	118.80	111.24
2	A	54	SER	CA-C-O	5.85	126.68	120.36
3	B	155	SER	CA-C-N	5.85	128.12	120.28
3	B	155	SER	C-N-CA	5.85	128.12	120.28
2	A	151	SER	CA-C-O	5.85	126.73	120.24
2	A	194	THR	N-CA-C	5.85	117.65	111.28
2	A	220	GLU	N-CA-C	-5.84	104.91	112.68
1	K	297	THR	O-C-N	-5.84	116.40	123.29
1	K	125	ASN	CA-CB-CG	5.83	118.43	112.60
3	B	316	ALA	N-CA-CB	5.83	119.70	110.55
1	K	206	SER	CA-C-O	5.83	126.73	120.38
2	A	328	VAL	O-C-N	-5.83	116.20	121.91
1	K	25	ARG	N-CA-C	-5.82	104.36	112.45
2	A	266	HIS	CE1-NE2-CD2	-5.82	103.18	109.00
2	A	50	ASN	N-CA-C	5.82	123.19	110.80
1	K	282	MET	CA-C-N	5.80	128.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	282	MET	C-N-CA	5.80	128.06	120.28
1	K	199	GLU	O-C-N	-5.79	115.55	122.15
1	K	328	THR	CA-C-O	5.78	128.78	120.51
2	A	210	TYR	CA-C-N	5.78	128.50	120.29
2	A	210	TYR	C-N-CA	5.78	128.50	120.29
3	B	78	VAL	CB-CA-C	5.78	119.33	111.87
3	B	277	SER	CA-C-O	5.76	128.75	120.51
3	B	358	ILE	N-CA-CB	-5.76	103.14	111.21
2	A	51	THR	CA-CB-OG1	5.76	118.24	109.60
2	A	288	VAL	CA-C-N	5.76	127.93	120.44
2	A	288	VAL	C-N-CA	5.76	127.93	120.44
2	A	433	GLU	O-C-N	-5.76	116.14	122.07
1	K	62	TYR	O-C-N	-5.75	116.11	122.09
2	A	149	PHE	N-CA-C	-5.75	104.93	111.14
3	B	171	VAL	N-CA-CB	5.75	116.99	110.72
1	K	256	LYS	CA-C-N	5.75	129.05	120.31
1	K	256	LYS	C-N-CA	5.75	129.05	120.31
2	A	119	LEU	O-C-N	-5.74	115.60	122.15
3	B	206	ASN	OD1-CG-ND2	-5.74	116.86	122.60
2	A	28	HIS	CB-CG-ND1	-5.73	114.11	122.70
3	B	171	VAL	CB-CA-C	5.73	118.01	110.91
2	A	331	ALA	N-CA-C	5.72	117.52	111.28
3	B	59	ASN	O-C-N	-5.72	114.39	122.06
1	K	145	LEU	CA-C-O	5.72	125.43	119.14
2	A	64	ARG	NE-CZ-NH2	-5.72	114.05	119.20
2	A	160	ASP	CA-CB-CG	-5.72	106.88	112.60
2	A	7	ILE	N-CA-C	-5.72	99.40	107.75
2	A	229	ARG	N-CA-CB	5.71	119.02	110.22
1	K	274	TYR	N-CA-CB	-5.70	102.00	110.10
2	A	194	THR	N-CA-CB	5.70	118.50	110.12
2	A	400	ALA	CA-C-O	5.70	126.78	120.63
2	A	344	VAL	N-CA-CB	5.70	119.70	110.13
1	K	219	THR	N-CA-CB	5.69	119.83	110.39
2	A	396	ASP	N-CA-C	5.69	118.21	111.33
3	B	387	LEU	O-C-N	-5.69	116.18	122.09
1	K	246	ALA	O-C-N	-5.68	115.29	122.27
3	B	88	ARG	O-C-N	-5.67	115.41	121.42
2	A	123	ARG	N-CA-C	5.67	117.46	111.28
3	B	66	ILE	N-CA-CB	5.66	118.95	111.25
3	B	347	ILE	O-C-N	-5.66	117.53	121.55
1	K	299	VAL	CA-C-N	-5.65	115.31	122.37
1	K	299	VAL	C-N-CA	-5.65	115.31	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	84	GLY	CA-C-N	5.65	130.16	120.72
3	B	84	GLY	C-N-CA	5.65	130.16	120.72
3	B	59	ASN	CA-C-N	5.63	130.50	122.72
3	B	59	ASN	C-N-CA	5.63	130.50	122.72
3	B	291	LEU	CA-C-N	5.63	128.14	120.54
3	B	291	LEU	C-N-CA	5.63	128.14	120.54
3	B	107	HIS	CA-CB-CG	5.63	119.43	113.80
1	K	205	HIS	ND1-CG-CD2	5.62	111.72	106.10
1	K	216	ASN	CA-CB-CG	5.62	118.22	112.60
2	A	414	GLU	CB-CA-C	5.62	119.11	109.51
1	K	9	ILE	N-CA-CB	5.61	117.05	110.82
3	B	393	GLU	CA-C-N	5.61	127.73	120.44
3	B	393	GLU	C-N-CA	5.61	127.73	120.44
3	B	64	ARG	CB-CA-C	5.61	120.43	111.91
3	B	231	VAL	N-CA-C	5.60	116.24	110.36
2	A	139	HIS	CG-CD2-NE2	-5.60	101.60	107.20
3	B	246	GLY	CA-C-N	5.60	129.12	123.13
3	B	246	GLY	C-N-CA	5.60	129.12	123.13
1	K	195	THR	CA-CB-OG1	5.59	117.99	109.60
2	A	324	VAL	O-C-N	-5.59	114.72	121.10
1	K	117	ASN	CA-CB-CG	-5.59	107.01	112.60
2	A	386	GLU	CB-CG-CD	5.59	122.10	112.60
3	B	297	ASP	O-C-N	-5.58	116.52	123.04
3	B	325	MET	CA-C-N	5.57	127.69	120.44
3	B	325	MET	C-N-CA	5.57	127.69	120.44
3	B	238	VAL	CA-C-O	5.56	126.26	120.25
2	A	102	ASN	CA-C-N	5.56	132.17	121.54
2	A	102	ASN	C-N-CA	5.56	132.17	121.54
3	B	150	GLY	O-C-N	-5.56	116.62	122.13
3	B	231	VAL	O-C-N	5.56	127.50	121.94
2	A	292	THR	CA-C-N	5.55	127.66	120.44
2	A	292	THR	C-N-CA	5.55	127.66	120.44
2	A	386	GLU	CA-C-N	5.55	127.99	120.44
2	A	386	GLU	C-N-CA	5.55	127.99	120.44
1	K	165	VAL	N-CA-C	5.55	116.72	108.23
3	B	176	LYS	N-CA-C	5.55	117.19	111.03
1	K	269	ALA	O-C-N	5.54	128.46	122.15
3	B	262	PHE	CA-CB-CG	-5.54	108.26	113.80
2	A	20	CYS	O-C-N	-5.54	116.37	122.07
2	A	389	ALA	O-C-N	-5.54	116.25	122.12
2	A	380	ASN	CB-CA-C	5.53	119.46	110.22
3	B	328	VAL	CA-C-O	-5.53	115.31	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	229	ARG	NE-CZ-NH1	-5.53	115.97	121.50
3	B	199	ASP	N-CA-CB	5.52	118.07	110.07
3	B	16	ILE	CA-C-N	5.52	126.10	119.98
3	B	16	ILE	C-N-CA	5.52	126.10	119.98
3	B	432	TYR	CA-C-N	5.52	127.67	120.28
3	B	432	TYR	C-N-CA	5.52	127.67	120.28
2	A	313	MET	N-CA-CB	5.51	118.33	110.67
2	A	372	GLN	OE1-CD-NE2	-5.50	117.10	122.60
3	B	155	SER	CA-C-O	-5.49	115.04	120.70
3	B	349	ASN	O-C-N	-5.49	115.74	122.55
3	B	342	TYR	N-CA-C	5.48	119.96	113.16
1	K	165	VAL	CA-C-O	5.47	127.06	120.65
3	B	164	ARG	NE-CZ-NH1	5.47	126.97	121.50
3	B	178	SER	CA-C-N	5.47	132.24	122.06
3	B	178	SER	C-N-CA	5.47	132.24	122.06
3	B	327	GLU	N-CA-CB	-5.47	102.06	110.16
3	B	428	LEU	CA-C-N	5.47	127.45	120.56
3	B	428	LEU	C-N-CA	5.47	127.45	120.56
3	B	349	ASN	CA-CB-CG	5.47	118.07	112.60
3	B	5	VAL	O-C-N	-5.47	116.70	123.10
3	B	103	TRP	N-CA-C	5.46	117.93	111.33
1	K	191	HIS	CA-C-N	5.46	130.57	122.99
1	K	191	HIS	C-N-CA	5.46	130.57	122.99
2	A	231	ILE	N-CA-CB	5.46	116.93	110.55
2	A	346	TRP	CB-CG-CD2	-5.46	119.16	126.80
2	A	363	VAL	N-CA-CB	5.45	118.85	111.21
2	A	170	SER	O-C-N	-5.44	117.02	123.22
1	K	213	LYS	CA-C-O	5.44	127.25	121.11
2	A	12	ALA	N-CA-C	5.43	117.63	111.11
2	A	101	ASN	N-CA-C	5.42	122.35	110.80
2	A	258	ASN	CA-C-O	5.42	125.64	119.18
1	K	206	SER	CA-C-N	5.42	130.47	123.10
1	K	206	SER	C-N-CA	5.42	130.47	123.10
3	B	269	MET	N-CA-CB	-5.42	102.11	110.07
1	K	173	VAL	N-CA-C	5.42	116.78	108.71
2	A	296	PHE	CA-CB-CG	-5.42	108.38	113.80
3	B	382	THR	N-CA-CB	5.41	118.56	110.22
3	B	358	ILE	CA-C-N	5.41	125.95	120.38
3	B	358	ILE	C-N-CA	5.41	125.95	120.38
1	K	324	THR	CA-CB-OG1	5.40	117.71	109.60
3	B	137	LEU	CA-C-N	5.40	130.39	122.77
3	B	137	LEU	C-N-CA	5.40	130.39	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	238	ILE	O-C-N	5.39	127.38	121.83
1	K	153	LEU	N-CA-CB	5.39	118.72	110.70
3	B	167	ASN	CB-CG-ND2	5.38	124.48	116.40
2	A	239	THR	CA-C-N	5.38	127.75	120.38
2	A	239	THR	C-N-CA	5.38	127.75	120.38
3	B	169	PHE	CA-C-N	-5.38	115.52	123.05
3	B	169	PHE	C-N-CA	-5.38	115.52	123.05
2	A	225	THR	CA-CB-CG2	5.38	119.64	110.50
2	A	334	THR	CA-CB-OG1	5.38	117.67	109.60
1	K	28	LYS	CA-C-N	5.37	130.31	122.41
1	K	28	LYS	C-N-CA	5.37	130.31	122.41
1	K	235	SER	CA-C-O	5.37	126.60	120.80
1	K	242	GLY	CA-C-N	5.37	128.96	121.02
1	K	242	GLY	C-N-CA	5.37	128.96	121.02
1	K	191	HIS	CB-CG-CD2	-5.36	124.23	131.20
3	B	380	ASN	CB-CG-OD1	5.35	131.50	120.80
2	A	398	MET	CA-C-N	5.35	127.45	120.28
2	A	398	MET	C-N-CA	5.35	127.45	120.28
2	A	152	LEU	CA-C-N	5.35	127.39	120.44
2	A	152	LEU	C-N-CA	5.35	127.39	120.44
3	B	121	VAL	O-C-N	-5.33	114.04	122.04
3	B	14	ASN	N-CA-C	-5.33	105.13	111.69
3	B	146	GLY	O-C-N	-5.33	117.07	122.19
1	K	170	GLU	O-C-N	-5.33	115.91	122.68
2	A	283	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
2	A	259	LEU	O-C-N	-5.33	114.80	122.36
1	K	231	ASP	CA-CB-CG	5.32	117.92	112.60
3	B	154	ILE	CA-C-O	5.32	126.81	121.17
2	A	386	GLU	CA-C-O	5.32	126.19	120.55
3	B	214	PHE	O-C-N	-5.32	115.73	122.17
1	K	325	ILE	N-CA-CB	5.32	116.33	110.53
1	K	57	SER	N-CA-C	5.31	116.94	110.41
2	A	255	PHE	O-C-N	-5.31	116.50	122.12
2	A	305	CYS	O-C-N	-5.30	116.18	122.65
1	K	189	ASN	CA-CB-CG	-5.30	107.30	112.60
2	A	335	ILE	CA-C-N	5.29	127.90	120.28
2	A	335	ILE	C-N-CA	5.29	127.90	120.28
1	K	246	ALA	N-CA-C	5.29	117.95	111.82
2	A	21	TRP	CA-C-O	5.29	126.16	120.55
2	A	339	ARG	CA-C-N	5.29	131.64	121.54
2	A	339	ARG	C-N-CA	5.29	131.64	121.54
3	B	228	ASN	CA-CB-CG	-5.29	107.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	348	PRO	CA-C-O	-5.29	115.46	121.96
1	K	243	ALA	O-C-N	-5.28	115.99	123.01
1	K	61	VAL	CA-C-O	5.28	126.91	121.05
1	K	309	GLU	CA-C-O	5.27	126.54	120.90
2	A	429	GLU	CA-C-N	5.27	127.61	120.44
2	A	429	GLU	C-N-CA	5.27	127.61	120.44
2	A	199	ASP	CA-CB-CG	5.27	117.87	112.60
2	A	407	TRP	CA-CB-CG	5.27	123.62	113.60
3	B	163	ASP	CA-C-O	5.27	126.03	119.97
1	K	87	THR	N-CA-C	5.27	117.72	110.35
2	A	30	ILE	N-CA-C	5.27	115.94	107.73
2	A	382	THR	N-CA-C	-5.27	106.86	113.28
3	B	282	GLN	CB-CG-CD	5.26	121.55	112.60
3	B	255	LEU	CA-C-N	5.26	127.33	120.28
3	B	255	LEU	C-N-CA	5.26	127.33	120.28
3	B	262	PHE	O-C-N	-5.26	115.58	121.79
3	B	287	THR	CA-CB-OG1	5.26	117.49	109.60
2	A	144	GLY	CA-C-N	5.26	127.59	120.65
2	A	144	GLY	C-N-CA	5.26	127.59	120.65
1	K	179	VAL	CB-CA-C	-5.26	104.97	112.22
2	A	309	HIS	CB-CG-ND1	-5.25	114.82	122.70
2	A	326	LYS	CA-C-O	5.25	126.33	120.82
2	A	55	GLU	CB-CG-CD	-5.24	103.69	112.60
3	B	346	TRP	CE2-CD2-CE3	5.24	124.04	118.80
2	A	181	VAL	N-CA-C	-5.24	106.58	111.45
2	A	408	TYR	CA-C-N	5.24	127.64	120.46
2	A	408	TYR	C-N-CA	5.24	127.64	120.46
1	K	161	ARG	O-C-N	-5.24	115.45	122.00
1	K	320	GLN	OE1-CD-NE2	5.23	127.83	122.60
3	B	406	HIS	N-CA-C	5.23	118.44	111.75
3	B	107	HIS	CA-C-N	5.23	131.68	122.79
3	B	107	HIS	C-N-CA	5.23	131.68	122.79
1	K	322	ALA	CA-C-N	5.22	127.80	120.28
1	K	322	ALA	C-N-CA	5.22	127.80	120.28
3	B	357	ASP	CA-CB-CG	-5.22	107.38	112.60
3	B	71	GLU	O-C-N	-5.21	116.55	121.35
3	B	249	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	K	214	GLN	O-C-N	-5.21	117.44	123.33
3	B	21	TRP	N-CA-C	5.20	116.95	111.28
2	A	406	HIS	ND1-CG-CD2	5.20	111.30	106.10
2	A	367	ASP	CA-C-O	5.20	125.92	119.79
1	K	318	PHE	CA-C-O	5.20	126.06	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	328	VAL	CA-C-N	5.20	128.01	120.79
2	A	328	VAL	C-N-CA	5.20	128.01	120.79
3	B	129	CYS	N-CA-C	5.19	117.56	110.24
3	B	3	GLU	N-CA-CB	-5.19	101.59	110.16
3	B	309	HIS	N-CA-CB	5.19	118.28	110.65
2	A	146	GLY	N-CA-C	5.19	118.92	112.64
1	K	285	ILE	N-CA-C	-5.19	104.57	111.05
3	B	14	ASN	O-C-N	-5.18	115.49	122.23
2	A	93	ILE	O-C-N	-5.18	117.71	123.20
2	A	430	LYS	O-C-N	-5.18	116.50	122.09
3	B	328	VAL	N-CA-C	5.18	115.39	110.42
2	A	235	VAL	CA-C-N	5.17	127.64	120.29
2	A	235	VAL	C-N-CA	5.17	127.64	120.29
2	A	374	ALA	CA-C-O	5.17	126.77	121.23
1	K	287	GLN	CA-C-N	5.17	127.21	120.28
1	K	287	GLN	C-N-CA	5.17	127.21	120.28
2	A	285	GLN	O-C-N	5.17	129.54	122.41
2	A	283	HIS	CA-CB-CG	-5.16	108.64	113.80
2	A	434	GLU	N-CA-CB	5.16	118.28	110.28
2	A	329	ASN	CB-CA-C	5.16	119.12	110.92
3	B	175	PRO	CA-C-N	5.16	127.65	120.63
3	B	175	PRO	C-N-CA	5.16	127.65	120.63
3	B	35	SER	N-CA-CB	5.15	118.66	110.16
2	A	375	VAL	N-CA-C	5.15	115.15	108.35
3	B	417	GLU	CA-C-N	5.15	127.60	120.29
3	B	417	GLU	C-N-CA	5.15	127.60	120.29
3	B	140	SER	N-CA-CB	5.15	118.59	110.56
3	B	199	ASP	O-C-N	-5.15	116.53	122.09
1	K	86	GLN	CA-C-O	5.14	127.00	121.44
1	K	227	LEU	CA-C-N	-5.14	115.48	122.93
1	K	227	LEU	C-N-CA	-5.14	115.48	122.93
2	A	86	LEU	N-CA-C	-5.14	105.13	111.40
2	A	231	ILE	CB-CA-C	-5.14	105.39	111.97
3	B	156	LYS	N-CA-C	5.14	116.88	111.28
1	K	41	ILE	N-CA-C	-5.14	100.72	108.12
2	A	71	GLU	CB-CA-C	5.14	120.29	110.17
2	A	227	LEU	O-C-N	-5.14	116.54	122.09
2	A	4	CYS	CA-C-O	5.13	126.56	120.66
2	A	188	ILE	CA-CB-CG2	5.13	119.23	110.50
2	A	320	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	K	205	HIS	CB-CG-ND1	-5.13	115.00	122.70
1	K	18	LEU	O-C-N	-5.13	116.50	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	78	VAL	CA-CB-CG1	-5.12	101.69	110.40
2	A	314	ALA	N-CA-CB	5.12	119.15	110.49
2	A	185	TYR	CA-C-O	-5.12	115.63	120.90
1	K	314	SER	CA-C-N	5.12	127.14	120.28
1	K	314	SER	C-N-CA	5.12	127.14	120.28
1	K	224	SER	N-CA-C	-5.11	101.42	109.50
3	B	209	LEU	CA-C-N	5.11	127.40	120.65
3	B	209	LEU	C-N-CA	5.11	127.40	120.65
1	K	120	TYR	CB-CG-CD2	-5.10	113.15	120.80
1	K	162	VAL	CA-CB-CG2	-5.10	101.73	110.40
3	B	254	LYS	CA-CB-CG	5.10	124.30	114.10
1	K	84	TYR	N-CA-C	-5.10	101.33	109.23
2	A	102	ASN	CA-C-O	5.10	126.51	120.70
3	B	303	ALA	N-CA-C	-5.10	101.45	109.50
2	A	78	VAL	N-CA-CB	5.09	115.97	110.62
3	B	418	PHE	CA-C-N	5.09	127.06	120.44
3	B	418	PHE	C-N-CA	5.09	127.06	120.44
1	K	236	GLU	CA-C-O	5.09	126.86	121.11
2	A	107	HIS	O-C-N	-5.08	115.62	122.23
3	B	190	SER	N-CA-C	5.08	116.89	111.36
3	B	133	GLN	CB-CA-C	-5.07	102.89	110.90
3	B	388	PHE	CA-CB-CG	-5.07	108.73	113.80
3	B	394	GLN	CA-C-N	5.07	127.84	120.79
3	B	394	GLN	C-N-CA	5.07	127.84	120.79
1	K	88	SER	CA-C-O	5.07	125.90	119.16
2	A	197	HIS	CA-C-O	5.07	125.97	120.55
3	B	305	CYS	N-CA-CB	5.07	118.50	110.55
3	B	297	ASP	N-CA-C	5.07	117.81	109.76
3	B	301	MET	N-CA-C	5.06	118.20	110.20
2	A	414	GLU	O-C-N	-5.05	117.40	123.06
1	K	182	THR	N-CA-CB	5.05	118.08	110.30
1	K	269	ALA	N-CA-CB	-5.05	102.69	110.16
2	A	269	LEU	O-C-N	-5.05	117.56	123.27
1	K	297	THR	CA-C-O	5.05	125.88	120.38
2	A	334	THR	CA-CB-CG2	5.05	119.09	110.50
3	B	260	VAL	CA-C-N	5.05	124.54	119.19
3	B	260	VAL	C-N-CA	5.05	124.54	119.19
2	A	283	HIS	CG-ND1-CE1	-5.04	100.73	109.30
3	B	424	ASN	N-CA-CB	-5.04	102.54	110.30
1	K	105	MET	O-C-N	-5.03	116.92	122.86
2	A	18	ASN	CB-CG-ND2	5.03	123.94	116.40
2	A	249	ASN	N-CA-CB	5.03	119.72	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	212	ILE	N-CA-CB	-5.03	103.70	110.54
3	B	338	LYS	N-CA-C	5.03	116.84	111.36
3	B	115	VAL	N-CA-C	5.02	116.35	110.62
3	B	285	ALA	N-CA-C	5.02	116.69	108.55
1	K	264	VAL	CA-C-O	-5.02	116.19	121.41
2	A	373	ARG	CA-C-O	5.02	127.07	121.40
1	K	270	GLU	N-CA-C	5.01	119.10	112.89
3	B	170	SER	CB-CA-C	-5.01	101.97	110.19
1	K	257	SER	O-C-N	-5.01	116.11	122.27
1	K	238	VAL	CA-C-N	5.01	129.15	121.19
1	K	238	VAL	C-N-CA	5.01	129.15	121.19
3	B	11	GLN	CA-C-O	5.01	125.86	120.70
1	K	28	LYS	N-CA-C	5.00	117.16	110.35
3	B	339	ASN	N-CA-C	-5.00	105.66	112.26
1	K	209	LEU	CA-C-N	5.00	129.48	122.93
1	K	209	LEU	C-N-CA	5.00	129.48	122.93

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	105	ARG	Sidechain
2	A	156	ARG	Sidechain
2	A	161	TYR	Sidechain
2	A	185	TYR	Sidechain
2	A	210	TYR	Sidechain
2	A	215	ARG	Sidechain
2	A	255	PHE	Sidechain
2	A	264	ARG	Sidechain
2	A	272	TYR	Sidechain
2	A	28	HIS	Sidechain
2	A	308	ARG	Sidechain
2	A	351	PHE	Sidechain
2	A	357	TYR	Sidechain
2	A	373	ARG	Sidechain
2	A	390	ARG	Sidechain
2	A	402	ARG	Sidechain
2	A	408	TYR	Sidechain
2	A	422	ARG	Sidechain
2	A	65	ALA	Peptide
3	B	158	ARG	Sidechain
3	B	161	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	B	164	ARG	Sidechain
3	B	185	TYR	Sidechain
3	B	202	TYR	Sidechain
3	B	224	TYR	Sidechain
3	B	308	ARG	Sidechain
3	B	311	ARG	Sidechain
3	B	312	TYR	Sidechain
3	B	342	TYR	Sidechain
3	B	399	PHE	Sidechain
3	B	408	TYR	Sidechain
3	B	48	ARG	Sidechain
3	B	53	TYR	Sidechain
3	B	6	HIS	Sidechain
3	B	88	ARG	Sidechain
1	K	118	TYR	Sidechain
1	K	135	PHE	Sidechain
1	K	16	ARG	Sidechain
1	K	171	ARG	Sidechain
1	K	25	ARG	Sidechain
1	K	277	TYR	Sidechain
1	K	278	ARG	Sidechain
1	K	284	ARG	Sidechain
1	K	29	TYR	Sidechain
1	K	48	PHE	Sidechain
1	K	62	TYR	Sidechain
1	K	65	CYS	Mainchain
1	K	77	TYR	Sidechain

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	K	2582	0	2551	4	0
2	A	3372	0	3287	12	0
3	B	3389	0	3266	17	0
4	K	31	0	12	0	0
5	K	1	0	0	0	0
6	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	28	0	12	0	0
All	All	9435	0	9140	32	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 (32) 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:B:251:ASP:CG	3:B:252:LEU:H	2.17	0.52
1:K:142:ILE:HB	1:K:153:LEU:H	1.75	0.51
2:A:52:PHE:CD1	2:A:243:ARG:HD2	2.47	0.50
1:K:157:GLU:O	3:B:416:MET:HE2	2.13	0.49
3:B:189:LEU:HD22	3:B:413:MET:HE1	1.96	0.48
3:B:315:VAL:HG11	3:B:377:PHE:CE1	2.50	0.46
3:B:399:PHE:CE1	3:B:418:PHE:HB3	2.51	0.46
2:A:230:LEU:HD13	2:A:275:VAL:HG13	1.98	0.45
2:A:6:SER:HB3	2:A:8:HIS:CE1	2.50	0.45
3:B:255:LEU:HD11	3:B:316:ALA:HB1	1.99	0.45
3:B:242:LEU:HD21	3:B:252:LEU:HG	1.99	0.45
2:A:246:GLY:HA2	2:A:357:TYR:CZ	2.53	0.44
3:B:217:LEU:HG	3:B:230:LEU:HD21	2.00	0.44
3:B:105:LYS:HG3	3:B:411:GLU:HG3	2.00	0.43
2:A:119:LEU:HD11	2:A:156:ARG:HB3	2.00	0.43
2:A:274:PRO:HG2	2:A:371:VAL:HG11	2.00	0.43
3:B:315:VAL:CG1	3:B:377:PHE:CE1	3.01	0.43
1:K:194:VAL:HG13	1:K:199:GLU:HA	2.00	0.43
1:K:111:ILE:HG21	1:K:227:LEU:HD21	2.01	0.43
3:B:30:ILE:HD11	3:B:49:ILE:HD11	2.01	0.42
2:A:314:ALA:O	2:A:379:SER:HA	2.19	0.42
2:A:315:CYS:O	2:A:351:PHE:HA	2.18	0.42
3:B:189:LEU:HD11	3:B:418:PHE:CZ	2.54	0.42
2:A:208:ALA:HB2	2:A:304:LYS:HB2	2.01	0.42
3:B:177:VAL:HB	3:B:178:SER:H	1.61	0.42
2:A:140:SER:HA	2:A:171:ILE:HB	2.01	0.42
3:B:255:LEU:HD11	3:B:316:ALA:CB	2.50	0.42
2:A:174:ALA:HB1	2:A:175:PRO:HD2	2.02	0.41
3:B:251:ASP:CG	3:B:252:LEU:N	2.78	0.41
2:A:172:TYR:HB2	2:A:203:MET:HG3	2.02	0.41
3:B:242:LEU:HD23	3:B:251:ASP:HA	2.03	0.41
3:B:260:VAL:HG13	3:B:265:LEU:O	2.21	0.41

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	K	328/349 (94%)	306 (93%)	20 (6%)	2 (1%)	21	58
2	A	428/451 (95%)	376 (88%)	46 (11%)	6 (1%)	9	38
3	B	429/445 (96%)	392 (91%)	31 (7%)	6 (1%)	9	38
All	All	1185/1245 (95%)	1074 (91%)	97 (8%)	14 (1%)	13	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	47	ASP
2	A	50	ASN
3	B	283	TYR
2	A	162	GLY
3	B	218	LYS
2	A	58	ALA
2	A	261	PRO
3	B	47	GLU
3	B	277	SER
1	K	169	THR
3	B	142	GLY
1	K	275	VAL
2	A	265	ILE
3	B	177	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	292/311 (94%)	284 (97%)	8 (3%)	39	60
2	A	364/379 (96%)	344 (94%)	20 (6%)	19	42
3	B	372/383 (97%)	360 (97%)	12 (3%)	34	55
All	All	1028/1073 (96%)	988 (96%)	40 (4%)	30	50

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	41	ILE
1	K	46	TYR
1	K	73	VAL
1	K	86	GLN
1	K	219	THR
1	K	221	GLN
1	K	247	VAL
1	K	273	THR
2	A	3	GLU
2	A	86	LEU
2	A	89	PRO
2	A	101	ASN
2	A	138	PHE
2	A	160	ASP
2	A	170	SER
2	A	171	ILE
2	A	172	TYR
2	A	173	PRO
2	A	183	GLU
2	A	210	TYR
2	A	215	ARG
2	A	275	VAL
2	A	335	ILE
2	A	346	TRP
2	A	362	VAL
2	A	396	ASP
2	A	405	VAL
2	A	424	ASP
3	B	1	MET
3	B	3	GLU
3	B	33	THR

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Mol	Chain	Res	Type
3	B	42	LEU
3	B	86	ILE
3	B	151	THR
3	B	171	VAL
3	B	248	LEU
3	B	254	LYS
3	B	296	PHE
3	B	349	ASN
3	B	352	LYS

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

Mol	Chain	Res	Type
1	K	86	GLN
1	K	93	HIS
1	K	125	ASN
1	K	156	HIS
1	K	216	ASN
1	K	218	GLN
1	K	287	GLN
1	K	320	GLN
2	A	61	HIS
2	A	186	ASN
2	A	233	GLN
2	A	301	GLN
3	B	14	ASN
3	B	133	GLN
3	B	247	GLN
3	B	336	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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$
7	GDP	B	501	-	29,30,30	1.82	3 (10%)	45,47,47	1.26	6 (13%)
6	GTP	A	600	-	33,34,34	2.44	5 (15%)	50,54,54	1.49	6 (12%)
4	ATP	K	501	5	32,33,33	2.59	5 (15%)	48,52,52	1.40	4 (8%)

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
7	GDP	B	501	-	-	3/16/32/32	0/3/3/3
6	GTP	A	600	-	-	0/22/38/38	0/3/3/3
4	ATP	K	501	5	-	3/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	GTP	PA-O3A	-12.36	1.46	1.59
4	K	501	ATP	PA-O3A	-10.78	1.47	1.59
7	B	501	GDP	PA-O3A	-6.97	1.52	1.59
4	K	501	ATP	PB-O3A	-6.60	1.52	1.59
4	K	501	ATP	PB-O3B	-2.78	1.56	1.59
7	B	501	GDP	C2'-C3'	2.73	1.60	1.53
6	A	600	GTP	C2'-C3'	2.65	1.60	1.53
7	B	501	GDP	C5'-C4'	2.50	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	GTP	C4-N9	-2.46	1.31	1.38
4	K	501	ATP	C2-N3	2.38	1.38	1.33
4	K	501	ATP	C5-C6	-2.17	1.34	1.41
6	A	600	GTP	O6-C6	-2.10	1.19	1.23
6	A	600	GTP	PB-O3A	2.01	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	501	ATP	O2B-PB-O3A	5.17	121.24	107.27
6	A	600	GTP	O2B-PB-O3A	4.42	119.23	107.27
6	A	600	GTP	C5'-C4'-C3'	-3.53	102.49	115.21
6	A	600	GTP	O4'-C1'-N9	3.26	115.75	108.36
7	B	501	GDP	O2A-PA-O3A	3.12	115.70	107.27
4	K	501	ATP	O2G-PG-O3B	2.89	114.34	104.64
6	A	600	GTP	C8-N7-C5	-2.88	99.12	104.26
7	B	501	GDP	O6-C6-N1	-2.65	115.13	120.11
6	A	600	GTP	O3B-PB-O1B	-2.41	103.46	110.70
4	K	501	ATP	O3A-PB-O1B	-2.36	103.59	110.70
7	B	501	GDP	O5'-C5'-C4'	2.36	117.03	108.99
7	B	501	GDP	O2'-C2'-C3'	2.25	119.01	111.82
6	A	600	GTP	N2-C2-N1	-2.20	112.12	116.76
4	K	501	ATP	O4'-C4'-C5'	2.14	116.19	109.33
7	B	501	GDP	O5'-PA-O1A	-2.11	100.56	108.94
7	B	501	GDP	O2A-PA-O1A	2.05	122.00	112.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

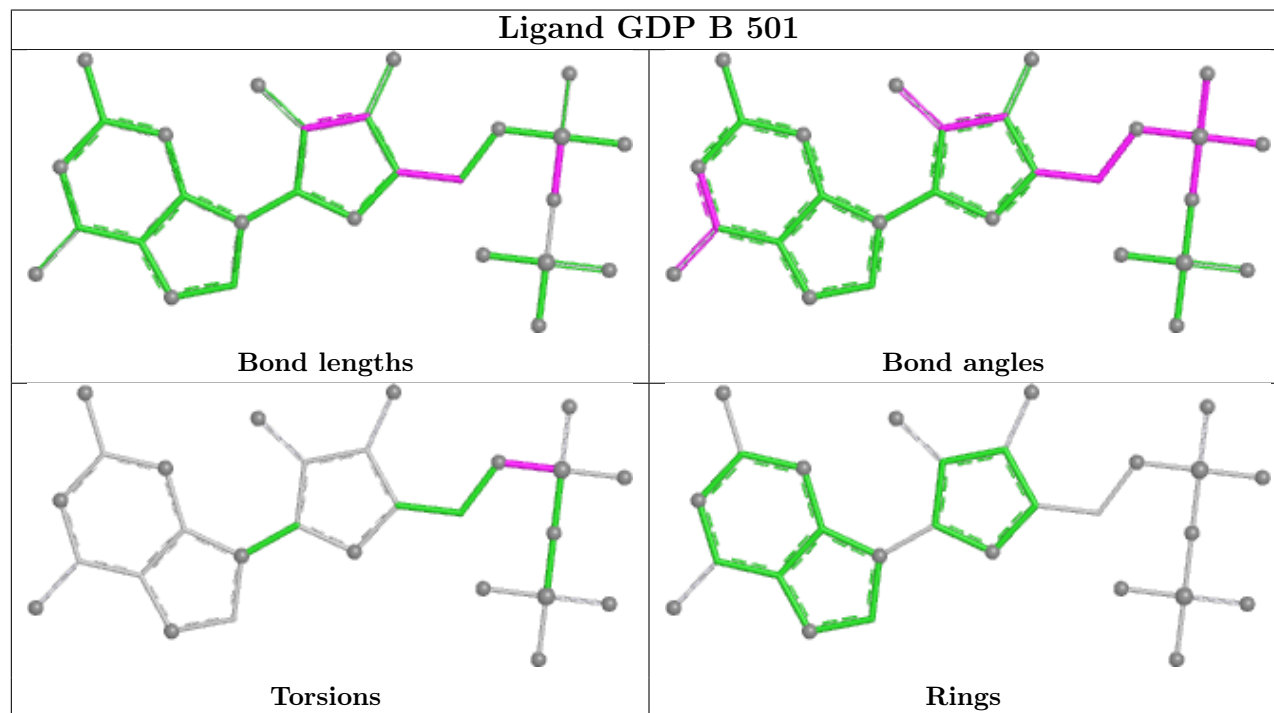
Mol	Chain	Res	Type	Atoms
4	K	501	ATP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
4	K	501	ATP	PA-O3A-PB-O2B
4	K	501	ATP	PA-O3A-PB-O1B

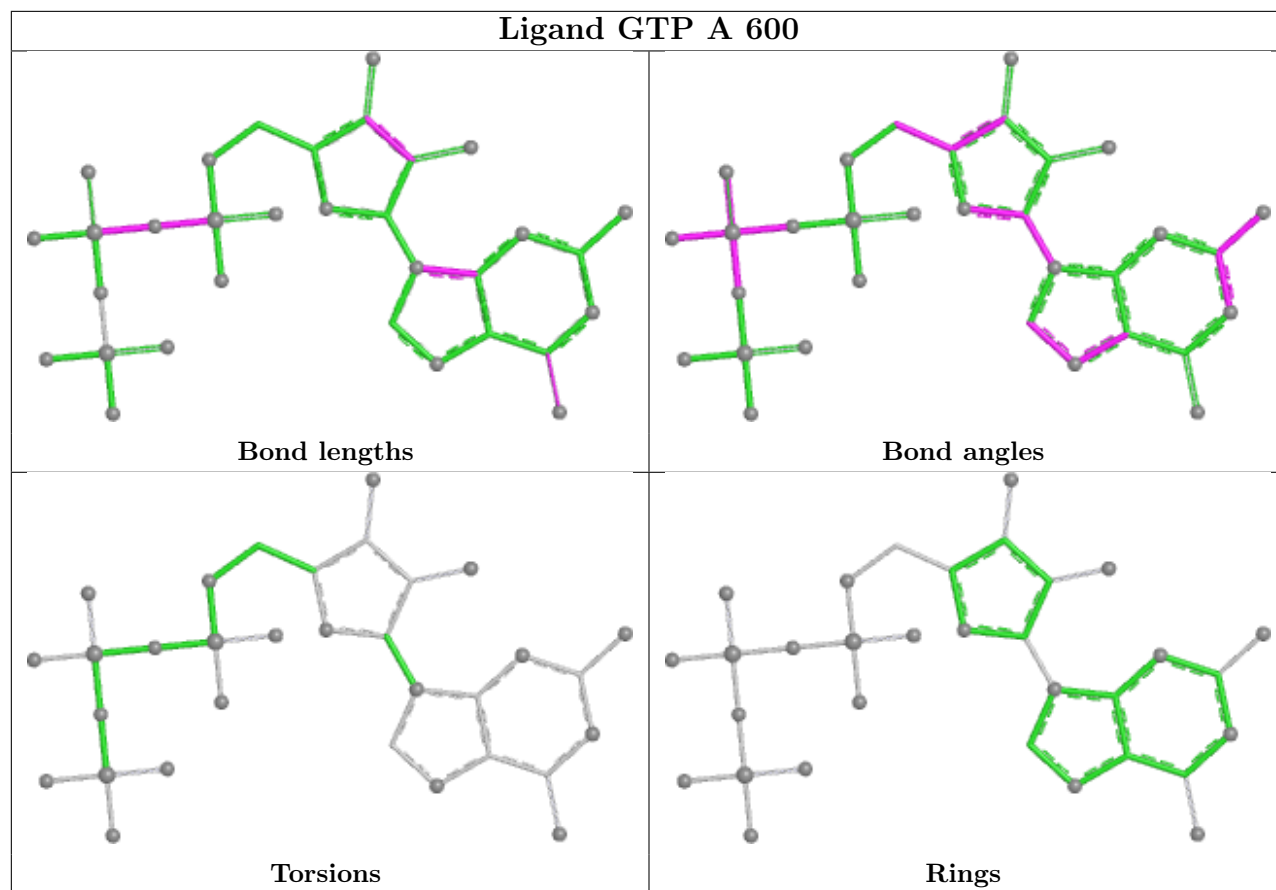
There are no ring outliers.

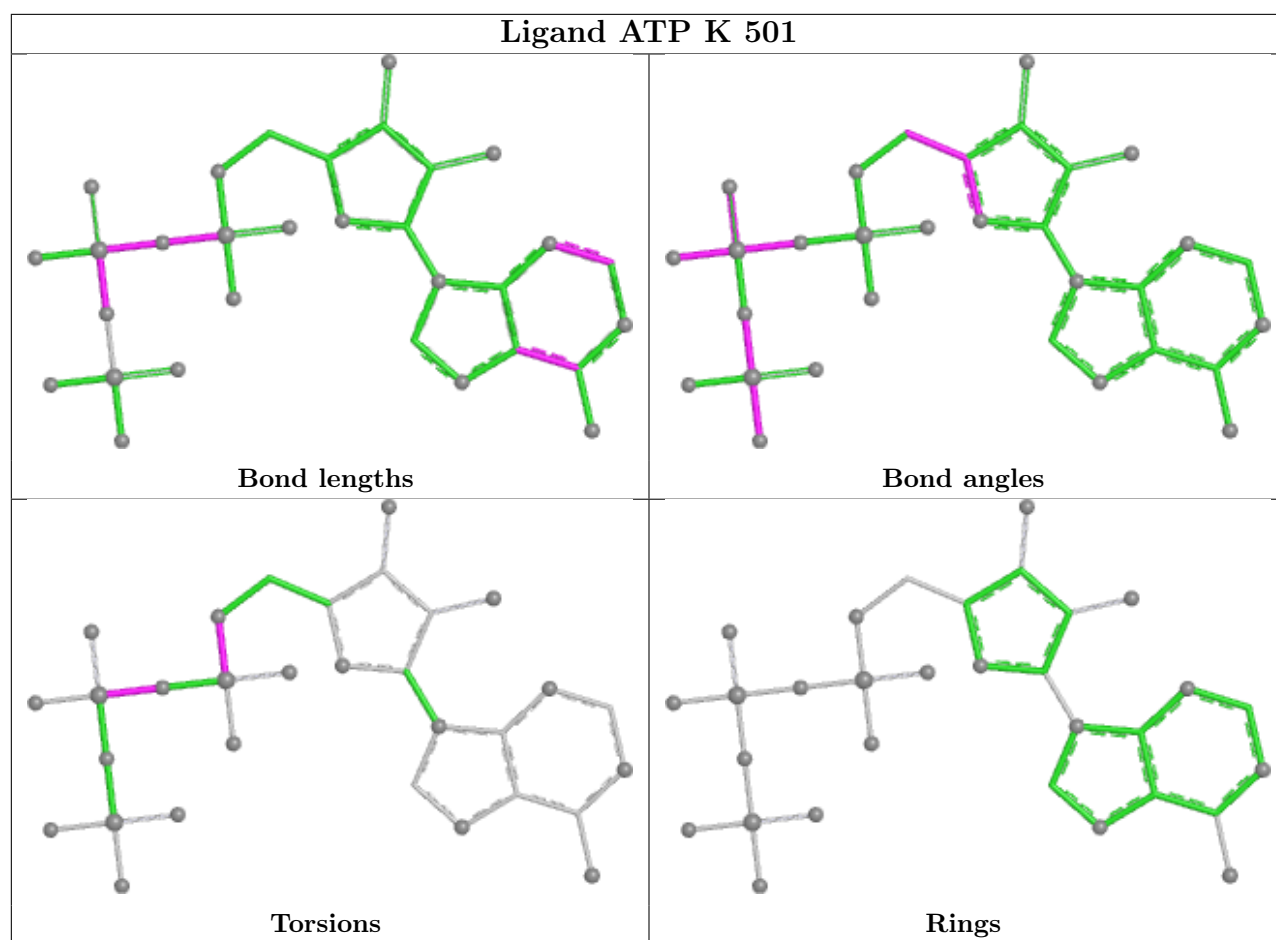
No monomer is involved in short contacts.

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 [i](#)

There are no chain breaks in this entry.

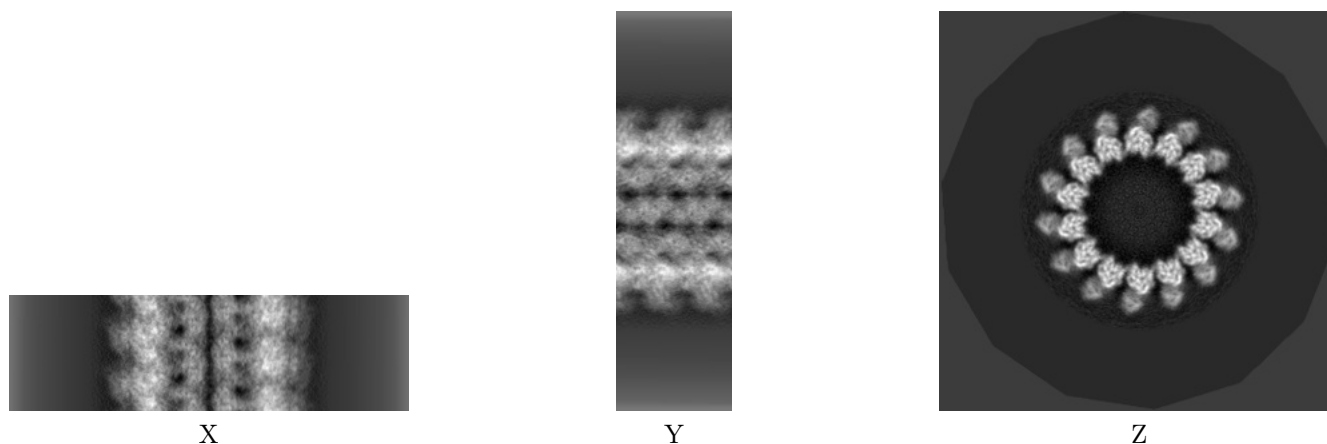
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6188. 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](#)

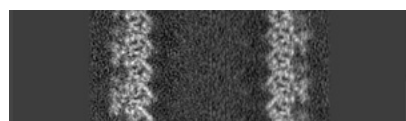
6.1.1 Primary map



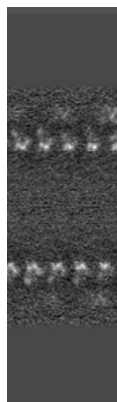
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

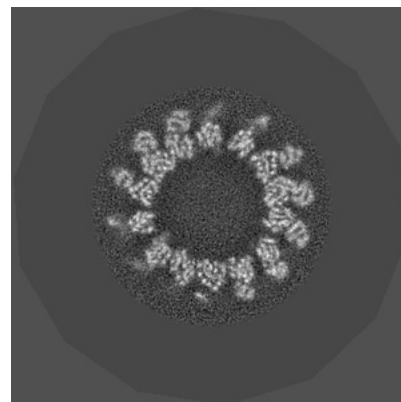
6.2.1 Primary map



X Index: 160



Y Index:
160

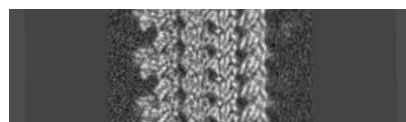


Z Index: 45

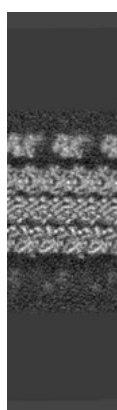
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

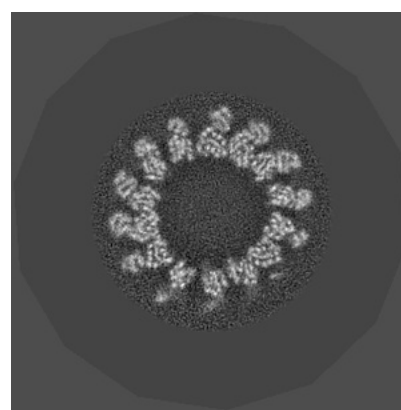
6.3.1 Primary map



X Index: 209



Y Index:
109

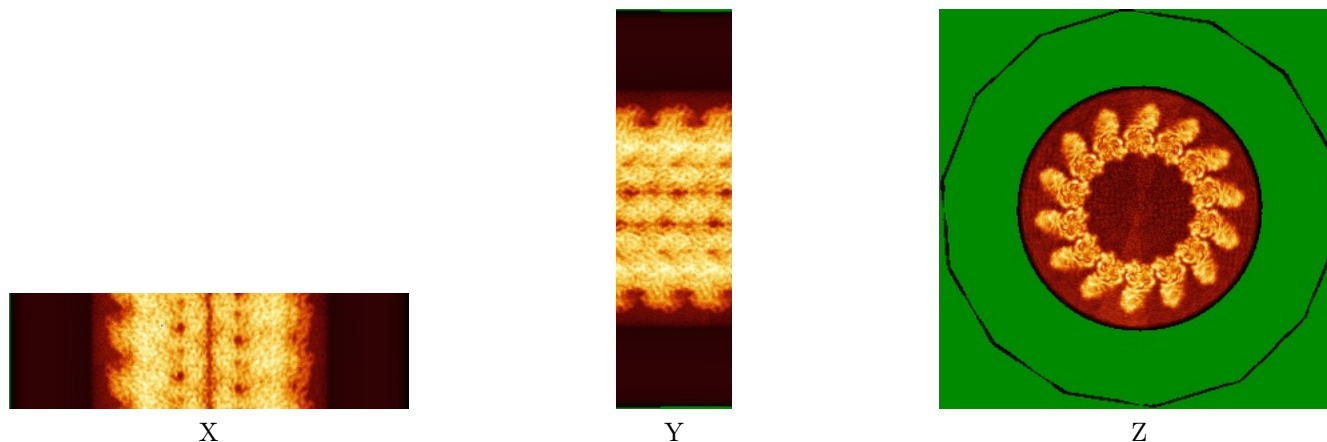


Z Index: 36

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

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

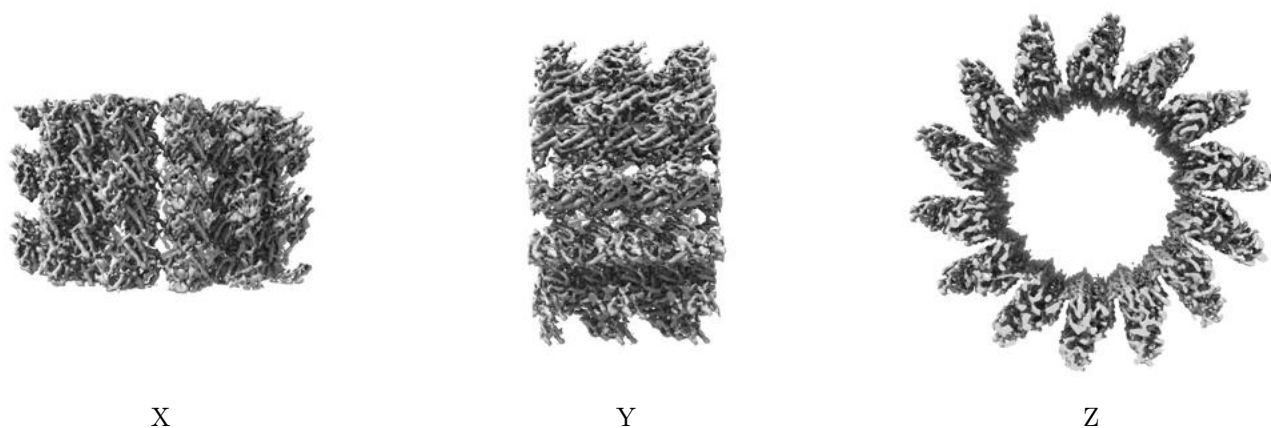
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

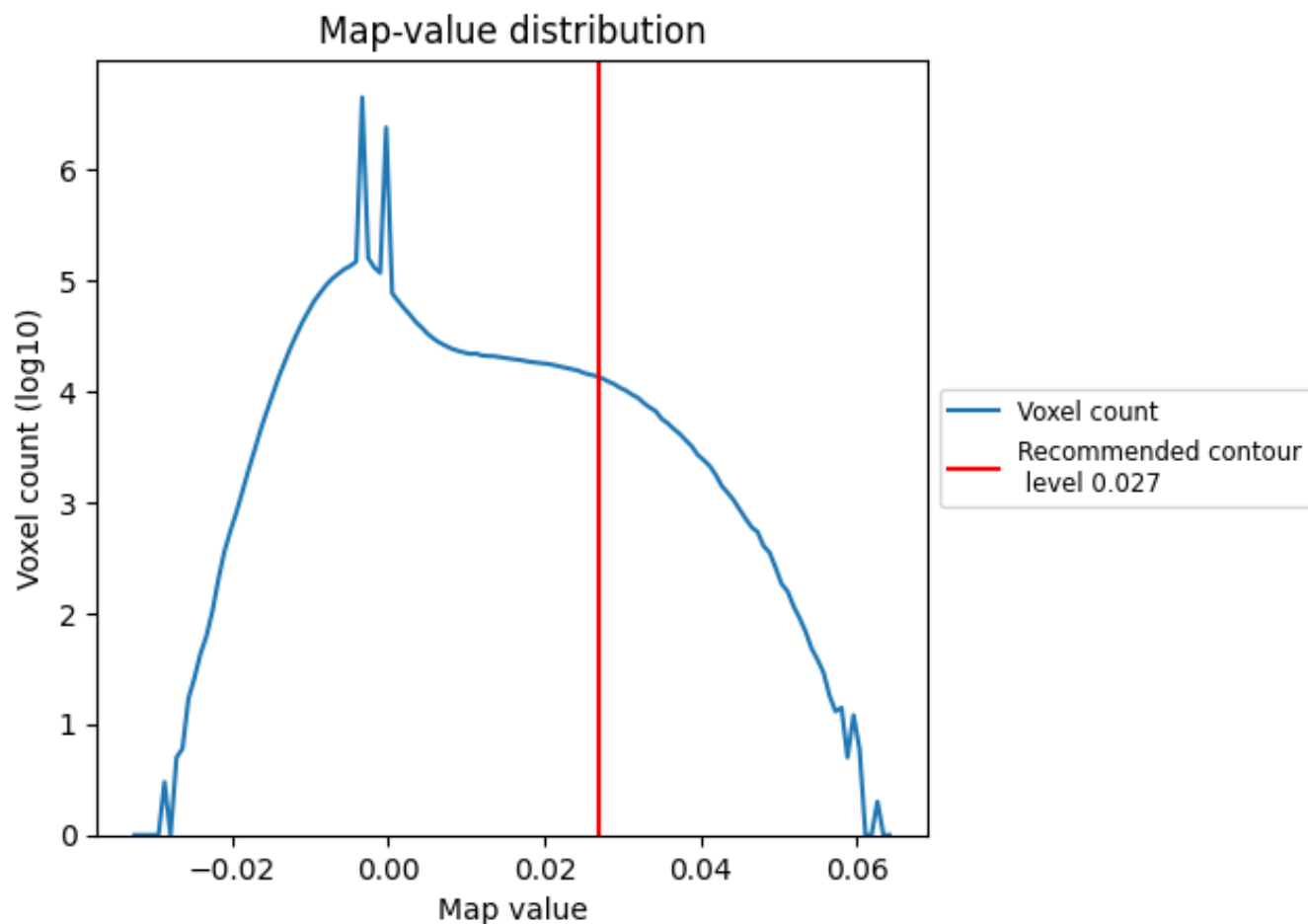
6.6 Mask visualisation

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

7 Map analysis [i](#)

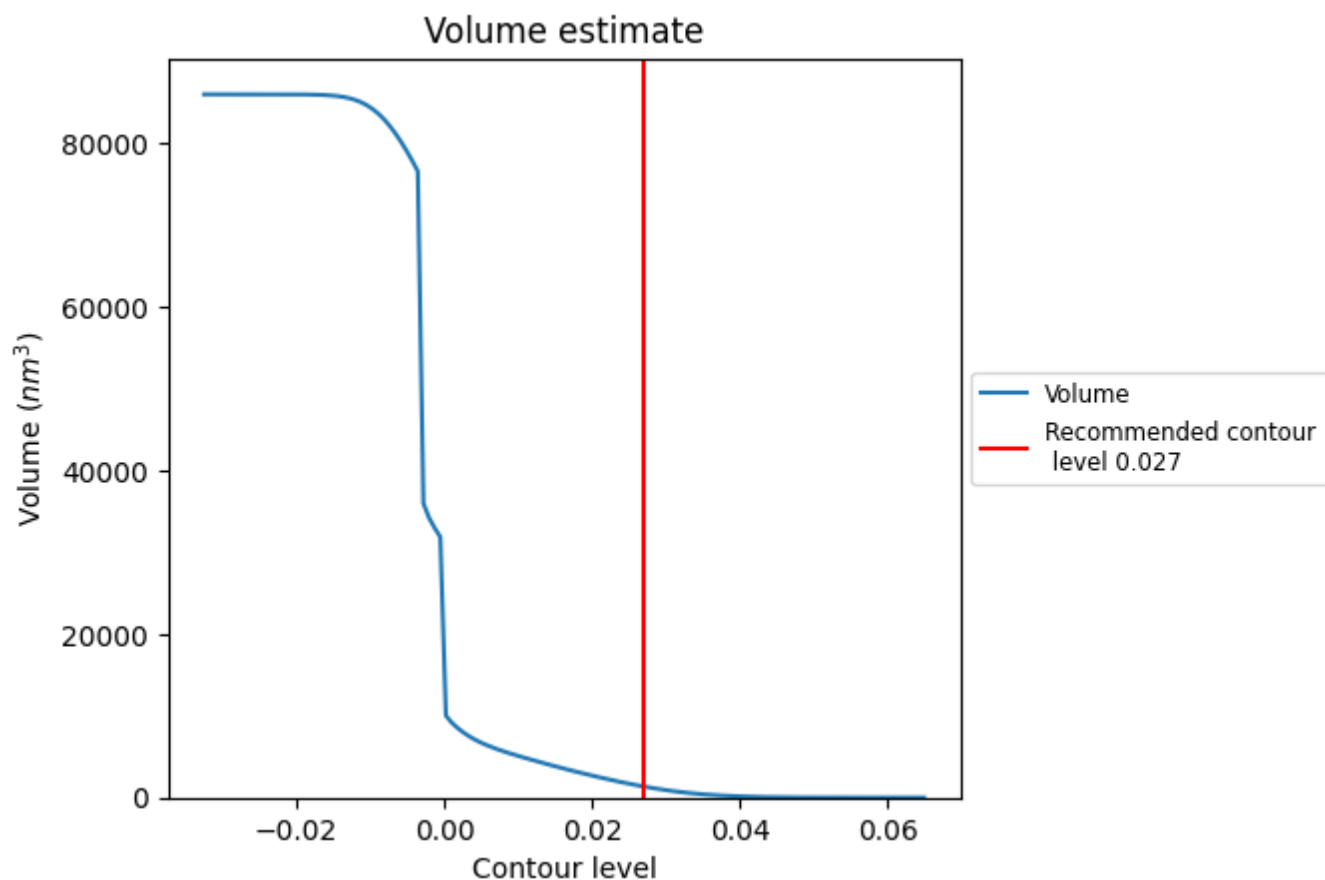
This section contains the results of statistical analysis of the map.

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 1350 nm³; this corresponds to an approximate mass of 1219 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.

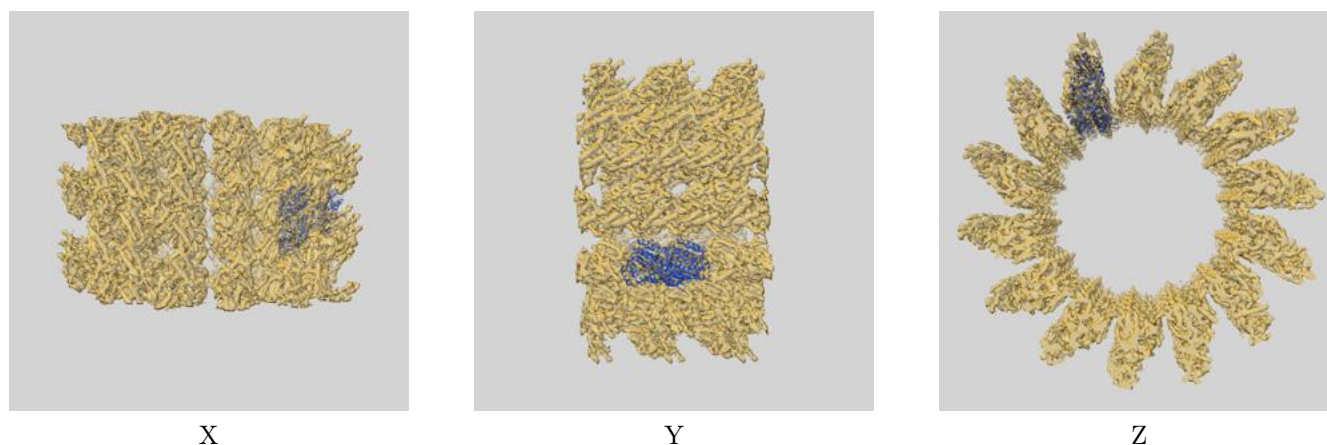
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

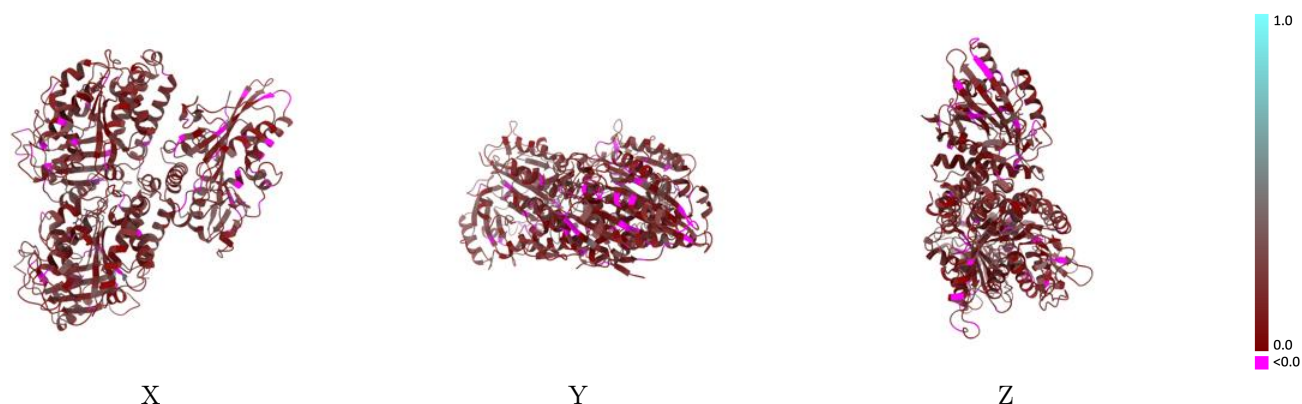
This section contains information regarding the fit between EMDB map EMD-6188 and PDB model 3J8Y. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



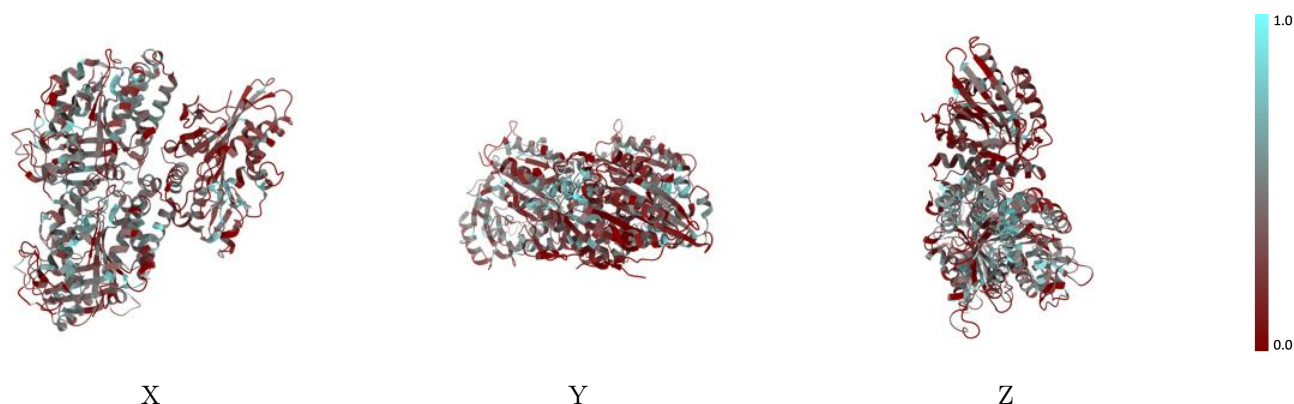
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



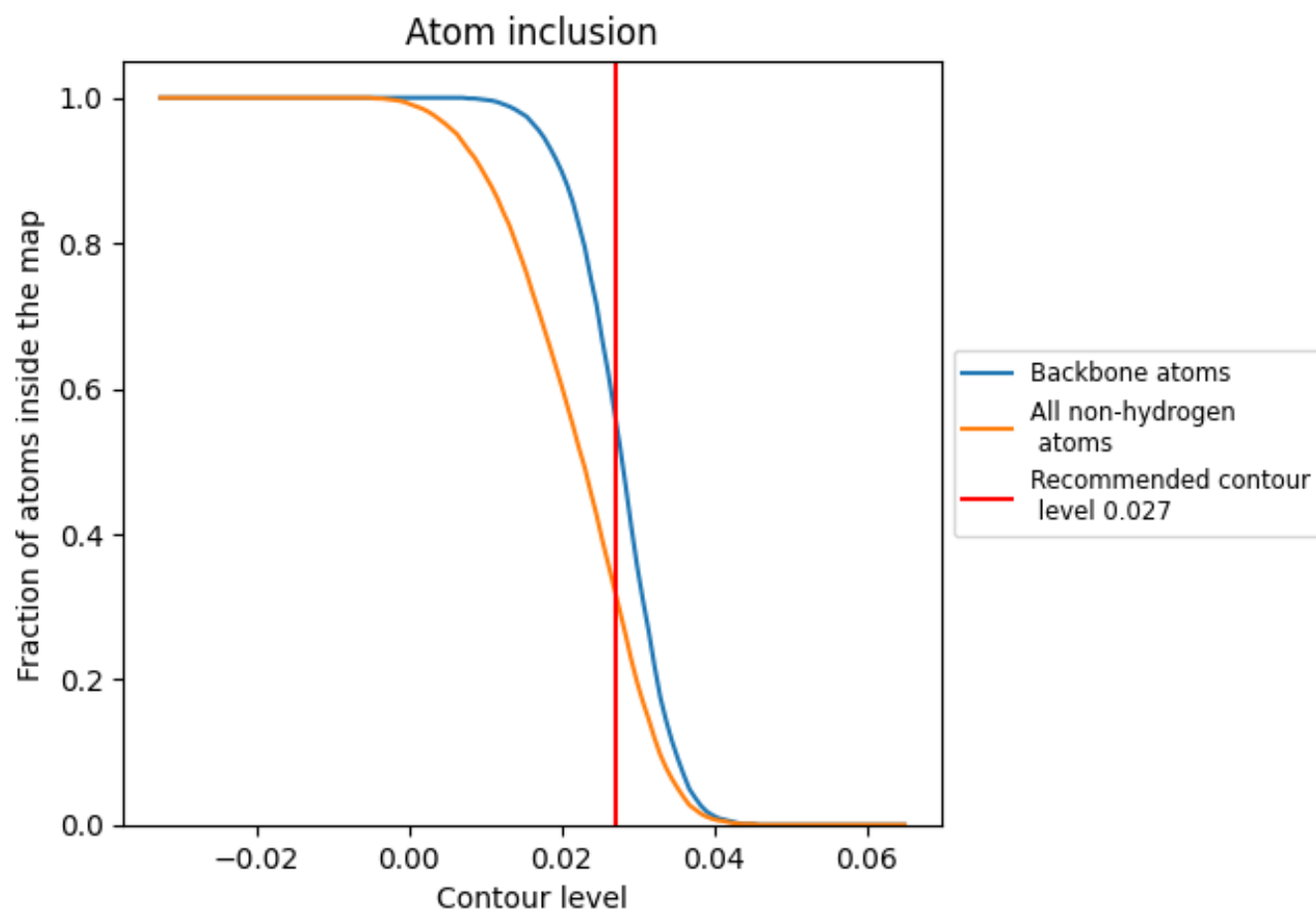
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 32% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3230	0.1620
A	0.3530	0.1710
B	0.3690	0.1630
K	0.2240	0.1500

