Full wwPDB EM Validation Report ⓘ

Feb 12, 2024 – 07:47 PM EST

PDB ID	:	3J8Y
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:

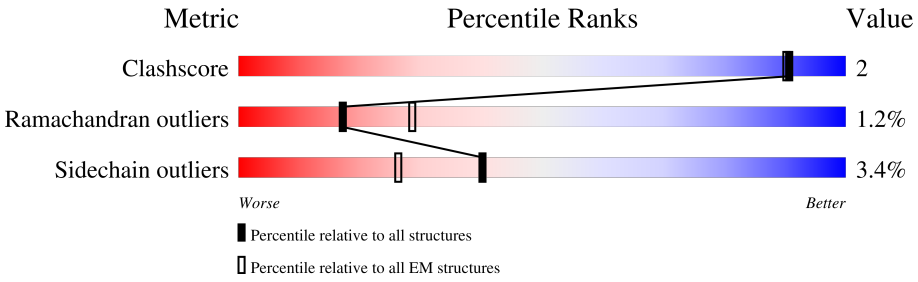
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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% 72% 18% • 5%
2	A	451	53% 67% 24% • • 5%
3	B	445	51% 71% 22% • •

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
			Total	C	N	O	S		
1	K	330	2582	1609	444	519	10	0	0

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
			Total	C	N	O	S		
2	A	430	3372	2137	573	640	22	0	0

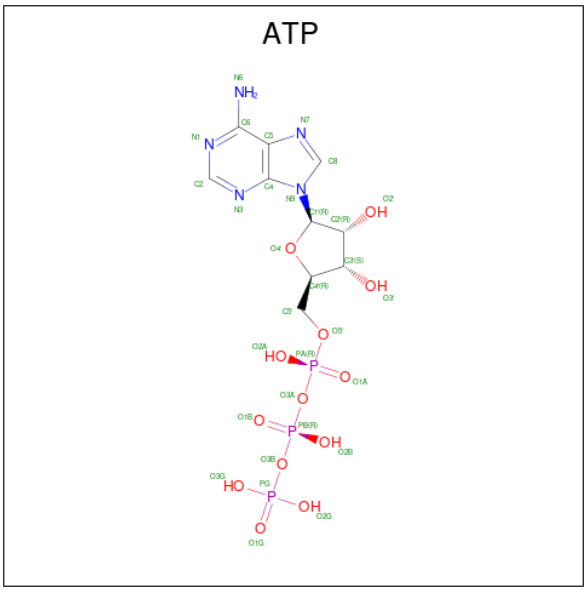
- Molecule 3 is a protein called Tubulin beta-2B chain.

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

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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

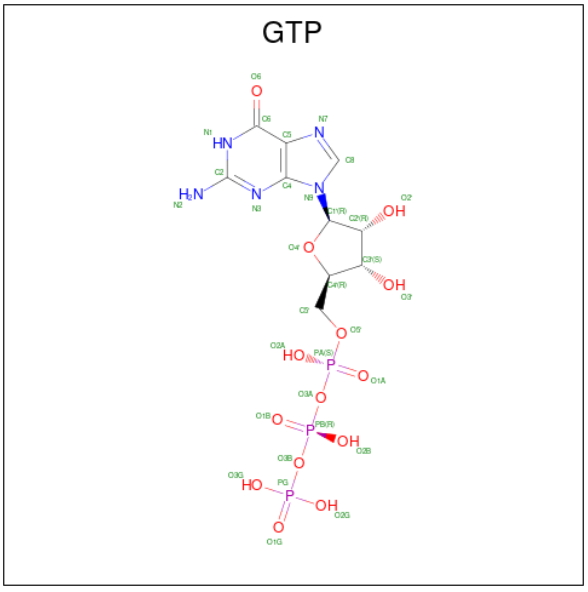


Mol	Chain	Residues	Atoms					AltConf
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

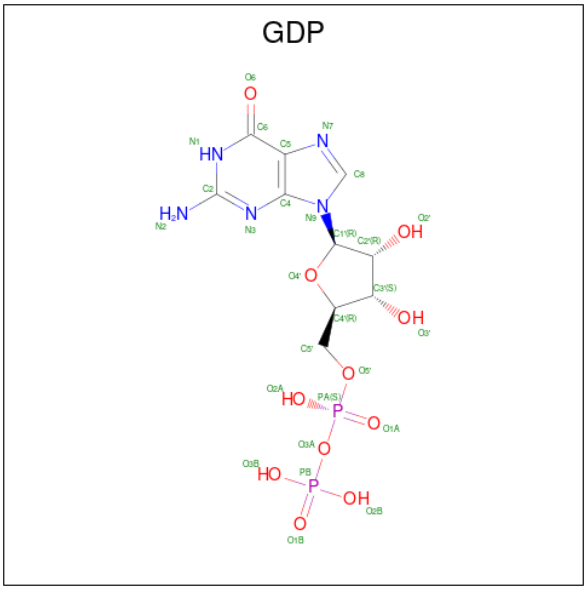
Mol	Chain	Residues	Atoms		AltConf
5	K	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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 (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



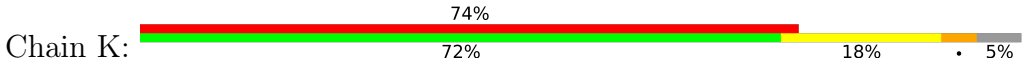
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

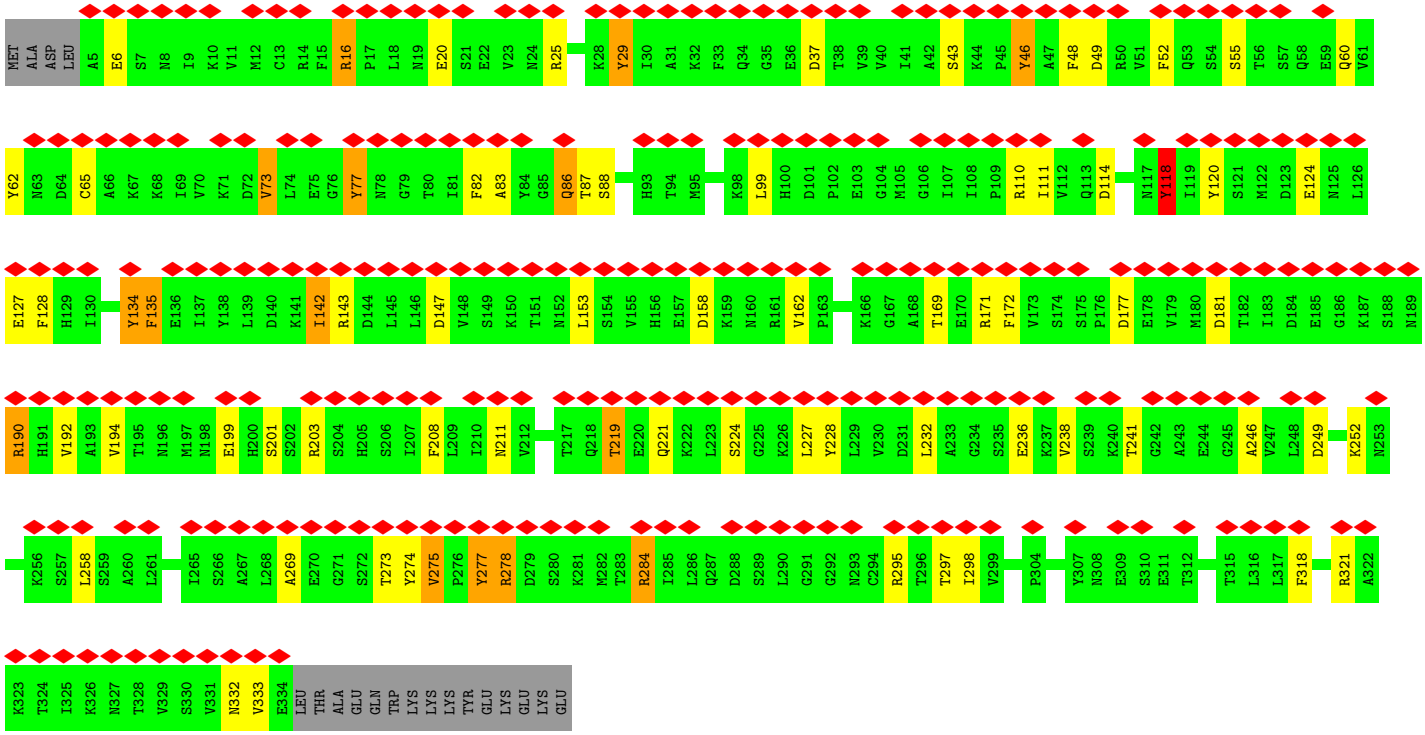
3 Residue-property plots (i)

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

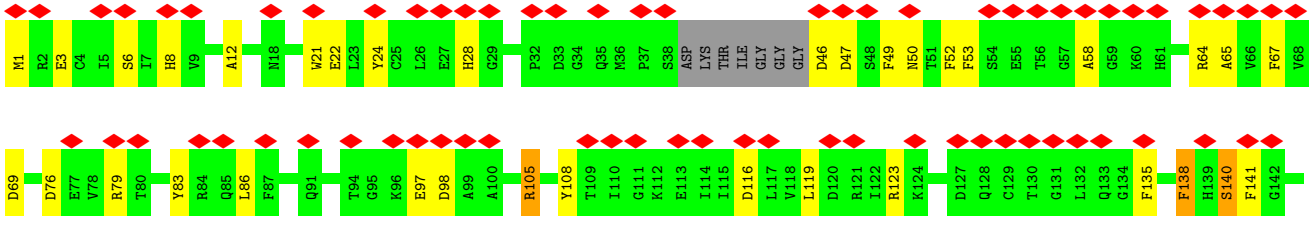
Chain K:

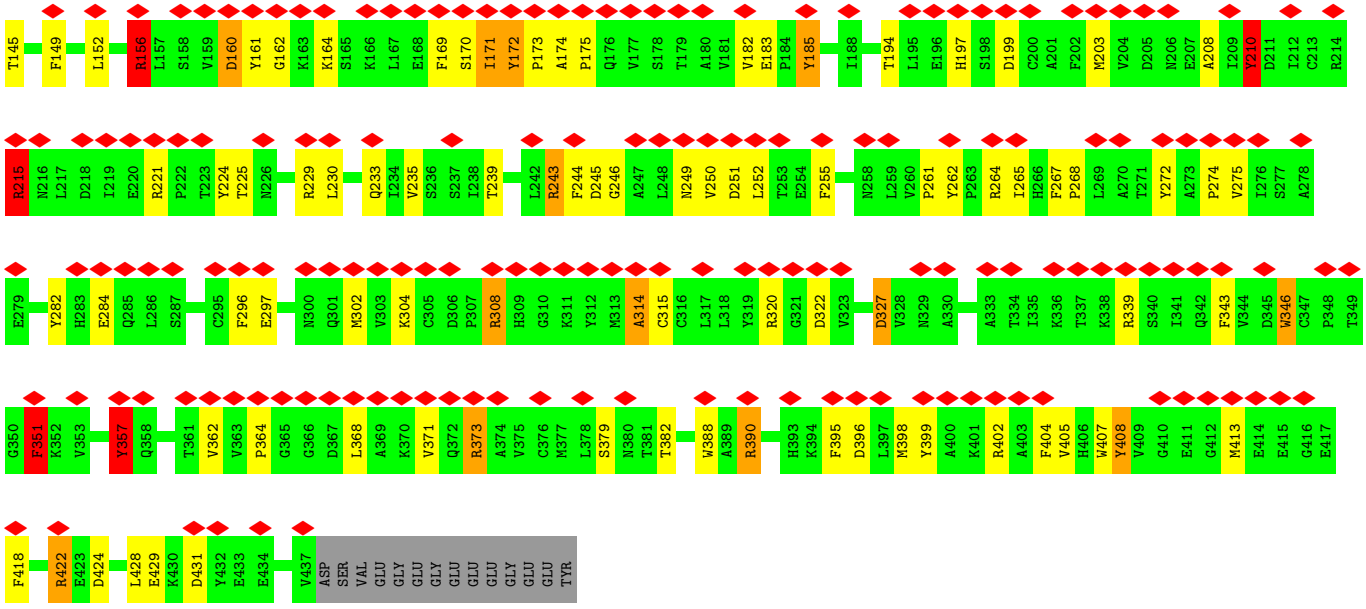




• Molecule 2: Tubulin alpha-1B chain

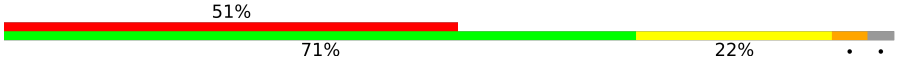
Chain A:

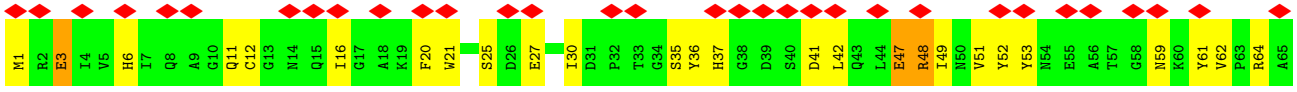


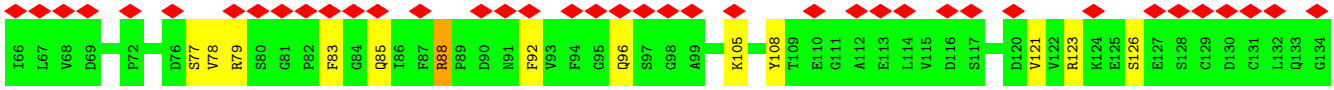


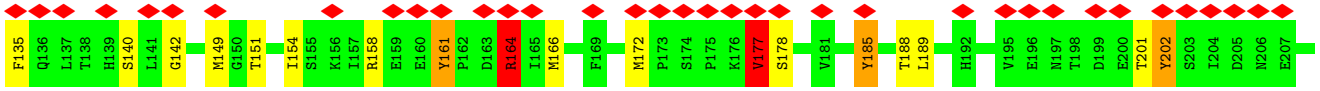
- Molecule 3: Tubulin beta-2B chain

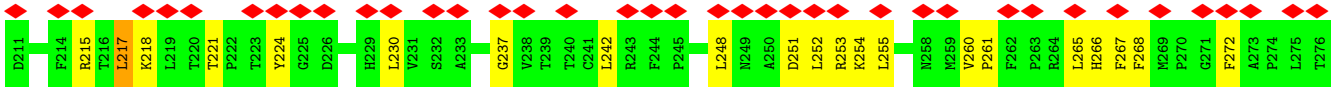
Chain B:

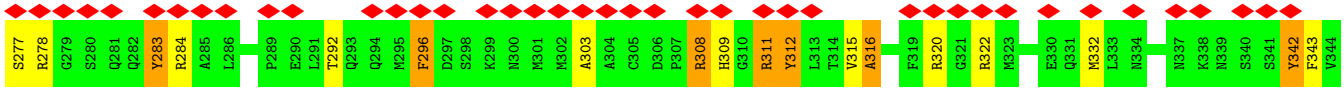


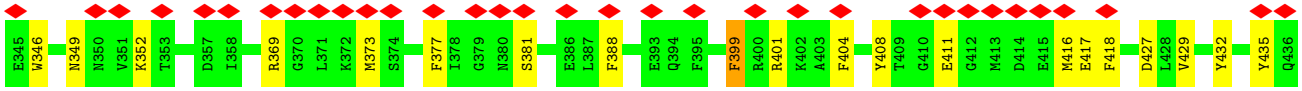


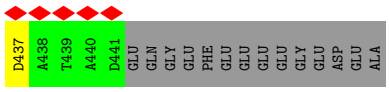












4 Experimental information (i)

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 ($e^-/Å^2$)	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: GTP, ATP, 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	1.59	13/2621 (0.5%)	2.01	73/3535 (2.1%)
2	A	1.58	19/3450 (0.6%)	2.03	99/4685 (2.1%)
3	B	1.60	16/3464 (0.5%)	1.97	102/4692 (2.2%)
All	All	1.59	48/9535 (0.5%)	2.00	274/12912 (2.1%)

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 (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	381	SER	CA-CB	11.64	1.70	1.52
3	B	435	TYR	CE1-CZ	7.77	1.48	1.38
3	B	47	GLU	CB-CG	7.27	1.66	1.52
3	B	253	ARG	CD-NE	7.02	1.58	1.46
1	K	228	TYR	CG-CD1	6.48	1.47	1.39
2	A	108	TYR	CG-CD2	6.34	1.47	1.39
3	B	381	SER	CB-OG	6.31	1.50	1.42
1	K	29	TYR	CE2-CZ	6.31	1.46	1.38
2	A	140	SER	CA-CB	6.24	1.62	1.52
1	K	43	SER	CA-CB	6.23	1.62	1.52
2	A	182	VAL	N-CA	-6.21	1.33	1.46
2	A	160	ASP	CA-CB	6.13	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	342	TYR	CG-CD1	5.97	1.47	1.39
1	K	55	SER	CB-OG	5.86	1.49	1.42
1	K	118	TYR	CG-CD2	5.81	1.46	1.39
3	B	320	ARG	NE-CZ	5.77	1.40	1.33
1	K	143	ARG	CD-NE	5.75	1.56	1.46
2	A	364	PRO	N-CA	-5.73	1.37	1.47
1	K	224	SER	CB-OG	5.67	1.49	1.42
2	A	53	PHE	CG-CD2	5.62	1.47	1.38
3	B	12	CYS	C-N	5.59	1.43	1.33
3	B	77	SER	CA-CB	5.55	1.61	1.52
1	K	127	GLU	CD-OE1	5.50	1.31	1.25
2	A	343	PHE	CB-CG	-5.46	1.42	1.51
1	K	118	TYR	CE2-CZ	-5.46	1.31	1.38
2	A	3	GLU	CG-CD	5.44	1.60	1.51
2	A	229	ARG	NE-CZ	5.39	1.40	1.33
2	A	145	THR	CA-C	-5.36	1.39	1.52
2	A	351	PHE	CE1-CZ	5.33	1.47	1.37
2	A	408	TYR	CE1-CZ	5.31	1.45	1.38
2	A	173	PRO	N-CD	5.30	1.55	1.47
1	K	201	SER	CA-CB	5.27	1.60	1.52
3	B	52	TYR	CG-CD1	5.21	1.46	1.39
3	B	261	PRO	N-CD	-5.20	1.40	1.47
3	B	237	GLY	CA-C	-5.18	1.43	1.51
1	K	118	TYR	CD1-CE1	5.15	1.47	1.39
2	A	229	ARG	CZ-NH1	5.15	1.39	1.33
1	K	211	ASN	CA-CB	5.14	1.66	1.53
2	A	22	GLU	CB-CG	5.14	1.61	1.52
1	K	275	VAL	CB-CG1	5.13	1.63	1.52
2	A	429	GLU	CB-CG	5.12	1.61	1.52
2	A	267	PHE	CG-CD2	5.11	1.46	1.38
2	A	408	TYR	CG-CD1	5.10	1.45	1.39
3	B	312	TYR	CZ-OH	5.09	1.46	1.37
3	B	25	SER	CB-OG	5.09	1.48	1.42
3	B	20	PHE	CG-CD2	5.06	1.46	1.38
2	A	97	GLU	CD-OE1	5.01	1.31	1.25
3	B	202	TYR	CE2-CZ	5.01	1.45	1.38

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	24	TYR	CB-CG-CD1	-16.25	111.25	121.00
1	K	284	ARG	NE-CZ-NH2	-16.19	112.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	120	TYR	CB-CG-CD1	14.77	129.86	121.00
3	B	164	ARG	NE-CZ-NH1	13.35	126.97	120.30
1	K	120	TYR	CB-CG-CD2	-13.08	113.15	121.00
3	B	369	ARG	NE-CZ-NH1	-12.99	113.80	120.30
2	A	64	ARG	NE-CZ-NH2	-12.49	114.05	120.30
2	A	79	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	K	284	ARG	NE-CZ-NH1	12.31	126.46	120.30
2	A	67	PHE	CB-CG-CD2	-12.08	112.34	120.80
2	A	373	ARG	NE-CZ-NH1	12.00	126.30	120.30
3	B	64	ARG	NE-CZ-NH2	11.88	126.24	120.30
3	B	388	PHE	CB-CG-CD2	-11.84	112.51	120.80
2	A	408	TYR	CB-CG-CD1	11.71	128.03	121.00
2	A	67	PHE	CB-CG-CD1	11.50	128.85	120.80
2	A	320	ARG	NE-CZ-NH2	-11.44	114.58	120.30
3	B	388	PHE	CB-CG-CD1	11.18	128.62	120.80
3	B	164	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	K	134	TYR	CB-CG-CD1	10.88	127.53	121.00
3	B	322	ARG	NE-CZ-NH2	10.73	125.66	120.30
1	K	110	ARG	NE-CZ-NH2	10.69	125.65	120.30
2	A	149	PHE	CB-CG-CD2	-10.61	113.37	120.80
2	A	83	TYR	CB-CG-CD1	-10.09	114.94	121.00
1	K	177	ASP	CB-CG-OD1	10.03	127.32	118.30
3	B	369	ARG	NE-CZ-NH2	9.87	125.23	120.30
1	K	321	ARG	NE-CZ-NH1	9.62	125.11	120.30
3	B	401	ARG	NE-CZ-NH2	-9.62	115.49	120.30
3	B	322	ARG	NE-CZ-NH1	-9.59	115.50	120.30
2	A	64	ARG	NE-CZ-NH1	9.54	125.07	120.30
3	B	416	MET	CG-SD-CE	-9.49	85.02	100.20
3	B	88	ARG	NE-CZ-NH2	-9.46	115.57	120.30
3	B	161	TYR	CB-CG-CD2	9.42	126.65	121.00
3	B	267	PHE	CB-CG-CD2	9.41	127.39	120.80
2	A	320	ARG	NE-CZ-NH1	9.39	124.99	120.30
3	B	332	MET	CG-SD-CE	-9.33	85.27	100.20
3	B	92	PHE	CB-CG-CD2	9.33	127.33	120.80
2	A	215	ARG	NE-CZ-NH2	-9.20	115.70	120.30
2	A	399	TYR	CB-CG-CD2	-9.16	115.50	121.00
1	K	158	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	K	295	ARG	NE-CZ-NH1	8.95	124.78	120.30
2	A	141	PHE	CB-CG-CD1	-8.85	114.61	120.80
2	A	418	PHE	CB-CG-CD1	-8.81	114.63	120.80
2	A	399	TYR	CB-CG-CD1	8.76	126.25	121.00
3	B	342	TYR	CG-CD2-CE2	8.75	128.30	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	404	PHE	CB-CG-CD2	-8.73	114.69	120.80
2	A	229	ARG	NE-CZ-NH1	-8.65	115.97	120.30
1	K	147	ASP	CB-CG-OD1	8.64	126.07	118.30
1	K	77	TYR	CB-CG-CD2	8.61	126.17	121.00
2	A	83	TYR	CB-CG-CD2	8.57	126.14	121.00
3	B	41	ASP	CB-CG-OD1	8.47	125.93	118.30
1	K	208	PHE	CB-CG-CD2	-8.44	114.89	120.80
2	A	135	PHE	CB-CG-CD2	-8.43	114.90	120.80
2	A	49	PHE	CB-CG-CD1	-8.40	114.92	120.80
1	K	46	TYR	CB-CG-CD2	-8.34	115.99	121.00
1	K	158	ASP	CB-CG-OD1	8.33	125.80	118.30
2	A	24	TYR	CB-CG-CD2	8.26	125.95	121.00
2	A	395	PHE	CB-CG-CD2	-8.21	115.05	120.80
3	B	283	TYR	N-CA-CB	8.21	125.39	110.60
1	K	277	TYR	CB-CG-CD1	-8.13	116.12	121.00
2	A	138	PHE	CB-CG-CD1	8.10	126.47	120.80
2	A	244	PHE	CB-CG-CD2	-8.10	115.13	120.80
2	A	418	PHE	CB-CG-CD2	8.09	126.46	120.80
1	K	208	PHE	CB-CG-CD1	8.07	126.45	120.80
2	A	339	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	A	141	PHE	CB-CG-CD2	8.03	126.42	120.80
2	A	408	TYR	CB-CG-CD2	-8.02	116.19	121.00
3	B	149	MET	CG-SD-CE	-7.90	87.57	100.20
1	K	82	PHE	CB-CG-CD2	-7.89	115.28	120.80
1	K	128	PHE	CB-CG-CD1	-7.88	115.28	120.80
3	B	308	ARG	NE-CZ-NH2	-7.78	116.41	120.30
3	B	83	PHE	CB-CG-CD1	-7.73	115.39	120.80
3	B	123	ARG	NE-CZ-NH1	7.67	124.13	120.30
3	B	202	TYR	CB-CG-CD1	-7.62	116.43	121.00
1	K	77	TYR	CG-CD2-CE2	7.62	127.39	121.30
3	B	278	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	A	431	ASP	CB-CG-OD2	7.55	125.09	118.30
2	A	398	MET	CA-CB-CG	7.48	126.02	113.30
1	K	318	PHE	CB-CG-CD1	7.47	126.03	120.80
2	A	215	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	K	274	TYR	CB-CG-CD2	-7.39	116.57	121.00
3	B	108	TYR	CB-CG-CD1	7.37	125.42	121.00
3	B	64	ARG	NH1-CZ-NH2	-7.37	111.29	119.40
3	B	151	THR	CA-CB-CG2	-7.29	102.19	112.40
2	A	235	VAL	CB-CA-C	-7.25	97.64	111.40
1	K	128	PHE	CB-CG-CD2	7.24	125.87	120.80
2	A	243	ARG	NE-CZ-NH2	-7.21	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	149	PHE	CB-CG-CD1	7.15	125.80	120.80
2	A	422	ARG	NE-CZ-NH2	-7.11	116.75	120.30
2	A	390	ARG	NE-CZ-NH1	7.01	123.81	120.30
2	A	327	ASP	CB-CG-OD2	7.01	124.61	118.30
1	K	29	TYR	CB-CG-CD1	6.92	125.15	121.00
1	K	16	ARG	NE-CZ-NH1	6.92	123.76	120.30
3	B	221	THR	CA-CB-CG2	-6.90	102.73	112.40
3	B	316	ALA	N-CA-CB	6.86	119.70	110.10
2	A	224	TYR	CB-CG-CD1	-6.86	116.89	121.00
1	K	181	ASP	CB-CG-OD1	6.85	124.47	118.30
1	K	134	TYR	CB-CG-CD2	-6.85	116.89	121.00
3	B	135	PHE	CB-CG-CD2	-6.84	116.01	120.80
2	A	373	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	K	232	LEU	O-C-N	-6.80	111.82	122.70
3	B	20	PHE	CB-CG-CD2	6.79	125.56	120.80
3	B	92	PHE	CB-CG-CD1	-6.78	116.06	120.80
1	K	192	VAL	CG1-CB-CG2	-6.75	100.10	110.90
2	A	284	GLU	O-C-N	-6.74	111.92	122.70
3	B	253	ARG	NE-CZ-NH1	6.67	123.63	120.30
3	B	16	ILE	CA-CB-CG1	6.64	123.62	111.00
1	K	332	ASN	O-C-N	-6.63	112.08	122.70
2	A	105	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	A	243	ARG	NE-CZ-NH1	6.62	123.61	120.30
3	B	272	PHE	CB-CG-CD1	6.62	125.43	120.80
3	B	342	TYR	CB-CG-CD2	6.62	124.97	121.00
2	A	250	VAL	CG1-CB-CG2	-6.58	100.36	110.90
1	K	274	TYR	CB-CG-CD1	6.58	124.95	121.00
3	B	432	TYR	CB-CG-CD2	6.56	124.94	121.00
2	A	123	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	A	296	PHE	CB-CG-CD2	-6.54	116.22	120.80
3	B	283	TYR	CB-CG-CD1	-6.54	117.08	121.00
3	B	346	TRP	CE2-CD2-CG	-6.53	102.08	107.30
3	B	21	TRP	CZ3-CH2-CZ2	-6.53	113.77	121.60
3	B	161	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	K	190	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	A	221	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	A	314	ALA	N-CA-CB	6.46	119.15	110.10
3	B	284	ARG	NE-CZ-NH1	-6.46	117.07	120.30
3	B	36	TYR	CG-CD2-CE2	-6.41	116.17	121.30
1	K	37	ASP	CB-CG-OD2	6.40	124.06	118.30
3	B	267	PHE	CG-CD2-CE2	6.39	127.83	120.80
1	K	190	ARG	NE-CZ-NH1	6.38	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	311	ARG	NE-CZ-NH1	6.38	123.49	120.30
3	B	309	HIS	O-C-N	-6.37	112.37	123.20
1	K	114	ASP	CB-CG-OD1	6.36	124.02	118.30
2	A	1	MET	CG-SD-CE	-6.36	90.03	100.20
3	B	311	ARG	NE-CZ-NH2	-6.34	117.13	120.30
3	B	96	GLN	N-CA-CB	-6.31	99.25	110.60
2	A	116	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	K	318	PHE	CB-CG-CD2	-6.28	116.40	120.80
3	B	108	TYR	CZ-CE2-CD2	-6.25	114.17	119.80
2	A	123	ARG	NE-CZ-NH1	6.25	123.42	120.30
3	B	427	ASP	CB-CG-OD1	6.25	123.92	118.30
2	A	357	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	K	87	THR	CA-CB-CG2	-6.22	103.69	112.40
2	A	199	ASP	CB-CG-OD1	6.21	123.89	118.30
2	A	408	TYR	CD1-CE1-CZ	-6.19	114.23	119.80
2	A	210	TYR	CA-CB-CG	6.16	125.10	113.40
3	B	78	VAL	CA-CB-CG1	-6.14	101.69	110.90
1	K	135	PHE	CB-CG-CD2	-6.14	116.50	120.80
3	B	437	ASP	CB-CG-OD2	6.12	123.81	118.30
1	K	162	VAL	CA-CB-CG2	-6.11	101.73	110.90
2	A	98	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	K	238	VAL	CG1-CB-CG2	-6.08	101.17	110.90
1	K	228	TYR	CB-CG-CD1	6.08	124.65	121.00
1	K	49	ASP	CB-CG-OD1	6.08	123.77	118.30
3	B	432	TYR	N-CA-CB	6.06	121.50	110.60
2	A	404	PHE	CB-CG-CD1	6.05	125.04	120.80
1	K	88	SER	O-C-N	-6.05	113.03	122.70
3	B	52	TYR	CB-CG-CD2	6.04	124.62	121.00
2	A	169	PHE	CB-CG-CD2	-6.03	116.58	120.80
3	B	185	TYR	CB-CG-CD1	-6.00	117.40	121.00
2	A	282	TYR	CG-CD2-CE2	-5.98	116.52	121.30
3	B	108	TYR	CG-CD2-CE2	5.96	126.06	121.30
1	K	124	GLU	N-CA-CB	-5.94	99.91	110.60
3	B	343	PHE	CB-CG-CD2	5.94	124.95	120.80
2	A	413	MET	CG-SD-CE	-5.92	90.72	100.20
3	B	161	TYR	CD1-CE1-CZ	-5.92	114.47	119.80
1	K	60	GLN	CA-CB-CG	-5.92	100.37	113.40
3	B	161	TYR	CG-CD1-CE1	5.92	126.03	121.30
3	B	37	HIS	O-C-N	-5.90	113.17	123.20
3	B	429	VAL	CG1-CB-CG2	-5.89	101.47	110.90
2	A	108	TYR	CG-CD2-CE2	-5.87	116.60	121.30
2	A	233	GLN	O-C-N	-5.86	113.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	27	GLU	OE1-CD-OE2	-5.85	116.28	123.30
2	A	382	THR	CA-CB-OG1	5.85	121.29	109.00
2	A	368	LEU	O-C-N	-5.84	113.36	122.70
3	B	48	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	K	203	ARG	NE-CZ-NH2	5.81	123.21	120.30
3	B	166	MET	CG-SD-CE	-5.78	90.95	100.20
2	A	239	THR	N-CA-CB	5.76	121.25	110.30
3	B	61	TYR	CB-CG-CD2	-5.76	117.55	121.00
2	A	252	LEU	N-CA-CB	5.75	121.90	110.40
3	B	296	PHE	CB-CG-CD2	-5.73	116.79	120.80
2	A	346	TRP	CB-CG-CD2	-5.72	119.16	126.60
3	B	215	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	A	49	PHE	CB-CG-CD2	5.72	124.81	120.80
2	A	135	PHE	CB-CG-CD1	5.72	124.80	120.80
1	K	298	ILE	N-CA-CB	5.69	123.88	110.80
3	B	217	LEU	C-N-CA	5.66	135.86	121.70
3	B	435	TYR	CZ-CE2-CD2	-5.66	114.70	119.80
2	A	46	ASP	CB-CG-OD1	-5.66	113.21	118.30
3	B	108	TYR	O-C-N	-5.66	113.65	122.70
3	B	21	TRP	CH2-CZ2-CE2	5.64	123.04	117.40
1	K	295	ARG	NE-CZ-NH2	-5.63	117.48	120.30
3	B	342	TYR	CD1-CG-CD2	-5.62	111.71	117.90
1	K	6	GLU	OE1-CD-OE2	5.60	130.02	123.30
2	A	428	LEU	CB-CG-CD2	-5.56	101.54	111.00
3	B	51	VAL	CA-CB-CG2	-5.55	102.58	110.90
1	K	241	THR	CA-CB-CG2	-5.55	104.63	112.40
2	A	245	ASP	CB-CG-OD1	5.51	123.26	118.30
1	K	333	VAL	CG1-CB-CG2	5.50	119.71	110.90
2	A	322	ASP	CB-CG-OD2	5.50	123.25	118.30
1	K	252	LYS	CB-CA-C	-5.49	99.41	110.40
2	A	156	ARG	O-C-N	-5.48	113.93	122.70
2	A	185	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	K	172	PHE	CG-CD2-CE2	5.46	126.80	120.80
3	B	154	ILE	CG1-CB-CG2	-5.46	99.39	111.40
2	A	69	ASP	CB-CG-OD1	5.45	123.20	118.30
3	B	35	SER	N-CA-CB	5.44	118.66	110.50
1	K	46	TYR	N-CA-CB	5.43	120.38	110.60
1	K	110	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
2	A	12	ALA	N-CA-CB	-5.42	102.52	110.10
3	B	121	VAL	O-C-N	-5.41	114.04	122.70
3	B	140	SER	N-CA-CB	5.39	118.59	110.50
2	A	262	TYR	CG-CD1-CE1	5.39	125.61	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	29	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	K	86	GLN	O-C-N	-5.37	114.10	122.70
2	A	244	PHE	CB-CG-CD1	5.34	124.54	120.80
3	B	303	ALA	N-CA-CB	5.34	117.58	110.10
3	B	85	GLN	N-CA-CB	5.33	120.20	110.60
2	A	388	TRP	CG-CD2-CE3	-5.33	129.10	133.90
3	B	36	TYR	CZ-CE2-CD2	5.32	124.59	119.80
2	A	152	LEU	CB-CG-CD1	5.31	120.03	111.00
1	K	249	ASP	CB-CG-OD1	5.30	123.07	118.30
1	K	269	ALA	N-CA-CB	-5.30	102.69	110.10
1	K	258	LEU	CB-CG-CD2	5.29	119.98	111.00
3	B	62	VAL	CA-CB-CG2	-5.28	102.98	110.90
2	A	171	ILE	C-N-CA	5.28	134.90	121.70
1	K	142	ILE	O-C-N	-5.26	114.28	122.70
2	A	194	THR	C-N-CA	5.26	134.84	121.70
3	B	41	ASP	CB-CG-OD2	-5.23	113.59	118.30
3	B	177	VAL	C-N-CA	5.23	134.78	121.70
3	B	373	MET	CG-SD-CE	-5.23	91.83	100.20
2	A	160	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	A	407	TRP	CA-CB-CG	5.22	123.62	113.70
3	B	417	GLU	OE1-CD-OE2	-5.21	117.04	123.30
2	A	297	GLU	OE1-CD-OE2	5.21	129.55	123.30
2	A	197	HIS	O-C-N	-5.20	114.38	122.70
3	B	373	MET	CA-CB-CG	5.20	122.14	113.30
2	A	346	TRP	CE2-CD2-CG	-5.20	103.14	107.30
3	B	59	ASN	O-C-N	-5.19	114.39	122.70
1	K	52	PHE	CB-CG-CD1	-5.19	117.17	120.80
2	A	225	THR	CA-CB-CG2	5.17	119.64	112.40
3	B	268	PHE	CG-CD1-CE1	5.17	126.48	120.80
1	K	83	ALA	N-CA-CB	5.16	117.33	110.10
3	B	404	PHE	CB-CG-CD1	5.15	124.41	120.80
3	B	292	THR	N-CA-CB	5.13	120.05	110.30
2	A	408	TYR	CG-CD1-CE1	5.13	125.40	121.30
2	A	346	TRP	CB-CG-CD1	5.13	133.67	127.00
1	K	118	TYR	O-C-N	-5.12	114.50	122.70
3	B	126	SER	N-CA-C	5.12	124.83	111.00
2	A	302	MET	CA-CB-CG	5.12	122.00	113.30
3	B	172	MET	CG-SD-CE	-5.11	92.02	100.20
1	K	73	VAL	CA-CB-CG2	-5.11	103.24	110.90
2	A	308	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
3	B	36	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	A	21	TRP	N-CA-CB	5.09	119.77	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	K	277	TYR	CB-CG-CD2	5.09	124.06	121.00
3	B	346	TRP	CD2-CE2-CZ2	-5.08	116.20	122.30
3	B	320	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	K	278	ARG	O-C-N	-5.07	114.58	122.70
3	B	435	TYR	CG-CD2-CE2	5.07	125.36	121.30
3	B	188	THR	N-CA-CB	5.07	119.93	110.30
2	A	249	ASN	N-CA-CB	5.07	119.72	110.60
1	K	236	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	K	275	VAL	CA-CB-CG1	-5.04	103.34	110.90
1	K	99	LEU	CB-CG-CD1	-5.03	102.44	111.00
2	A	164	LYS	N-CA-CB	5.03	119.65	110.60
2	A	268	PRO	C-N-CA	5.03	134.27	121.70
1	K	219	THR	N-CA-CB	5.02	119.83	110.30
3	B	64	ARG	CB-CA-C	5.01	120.43	110.40
1	K	246	ALA	CB-CA-C	-5.01	102.59	110.10
2	A	76	ASP	CB-CG-OD1	-5.01	113.79	118.30
3	B	79	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	K	297	THR	N-CA-CB	5.00	119.81	110.30
3	B	3	GLU	N-CA-CB	-5.00	101.59	110.60

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

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Mol	Chain	Res	Type	Group
2	A	422	ARG	Sidechain
2	A	65	ALA	Peptide
3	B	158	ARG	Sidechain
3	B	161	TYR	Sidechain
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	3	0
2	A	3372	0	3287	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3389	0	3266	15	0
4	K	31	0	12	0	0
5	K	1	0	0	0	0
6	A	32	0	12	0	0
7	B	28	0	12	0	0
All	All	9435	0	9140	30	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 (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
3:B:251:ASP:CG	3:B:252:LEU:H	2.17	0.47
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
3:B:201:THR:HG1	3:B:266:HIS:CE1	2.36	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
2:A:172:TYR:HB2	2:A:203:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	25	65
2	A	428/451 (95%)	376 (88%)	46 (11%)	6 (1%)	11	46
3	B	429/445 (96%)	392 (91%)	31 (7%)	6 (1%)	11	46
All	All	1185/1245 (95%)	1074 (91%)	97 (8%)	14 (1%)	17	50

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%)	282 (97%)	10 (3%)	37	60
2	A	364/379 (96%)	349 (96%)	15 (4%)	30	55
3	B	372/383 (97%)	362 (97%)	10 (3%)	44	65
All	All	1028/1073 (96%)	993 (97%)	35 (3%)	40	60

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	20	GLU
1	K	46	TYR
1	K	73	VAL
1	K	86	GLN
1	K	118	TYR
1	K	134	TYR
1	K	190	ARG
1	K	219	THR
1	K	221	GLN
1	K	273	THR
2	A	86	LEU
2	A	138	PHE
2	A	160	ASP
2	A	170	SER
2	A	172	TYR
2	A	183	GLU
2	A	210	TYR
2	A	215	ARG
2	A	251	ASP
2	A	327	ASP
2	A	346	TRP
2	A	362	VAL
2	A	396	ASP
2	A	405	VAL
2	A	424	ASP
3	B	1	MET

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Mol	Chain	Res	Type
3	B	3	GLU
3	B	11	GLN
3	B	42	LEU
3	B	164	ARG
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	93	HIS
1	K	129	HIS
1	K	191	HIS
2	A	61	HIS

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 monosaccharides 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	$\#\|Z\| > 2$
4	ATP	K	501	5	26,33,33	1.48	4 (15%)	31,52,52	1.55	5 (16%)
6	GTP	A	600	-	26,34,34	1.38	3 (11%)	32,54,54	2.17	6 (18%)
7	GDP	B	501	-	24,30,30	1.37	3 (12%)	30,47,47	2.08	6 (20%)

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
4	ATP	K	501	5	-	3/18/38/38	0/3/3/3
6	GTP	A	600	-	-	0/18/38/38	0/3/3/3
7	GDP	B	501	-	-	4/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	501	ATP	C2-N3	3.76	1.38	1.32
6	A	600	GTP	C5-C6	-3.74	1.39	1.47
4	K	501	ATP	C2'-C1'	3.31	1.58	1.53
7	B	501	GDP	C2'-C1'	2.89	1.58	1.53
7	B	501	GDP	C2'-C3'	2.71	1.60	1.53
6	A	600	GTP	C2'-C3'	2.64	1.60	1.53
4	K	501	ATP	O4'-C1'	2.59	1.44	1.41
7	B	501	GDP	C5'-C4'	2.40	1.59	1.51
4	K	501	ATP	C6-C5	-2.25	1.34	1.43
6	A	600	GTP	C5-C4	-2.07	1.37	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	600	GTP	PA-O3A-PB	-8.39	104.04	132.83
7	B	501	GDP	PA-O3A-PB	-7.54	106.94	132.83
4	K	501	ATP	PA-O3A-PB	-5.03	115.58	132.83
6	A	600	GTP	PB-O3B-PG	-4.94	115.87	132.83
7	B	501	GDP	O6-C6-N1	-4.68	115.13	120.65
6	A	600	GTP	C5'-C4'-C3'	-3.39	102.49	115.18
7	B	501	GDP	O6-C6-C5	3.02	130.27	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	501	ATP	O2G-PG-O3B	2.89	114.34	104.64
4	K	501	ATP	PB-O3B-PG	-2.76	123.37	132.83
6	A	600	GTP	O4'-C1'-C2'	2.59	110.71	106.93
7	B	501	GDP	O5'-C5'-C4'	2.34	117.03	108.99
7	B	501	GDP	O2'-C2'-C3'	2.22	119.01	111.82
7	B	501	GDP	O5'-PA-O1A	-2.18	100.56	109.07
6	A	600	GTP	N2-C2-N1	-2.16	112.12	116.71
4	K	501	ATP	O4'-C4'-C5'	2.07	116.19	109.37
6	A	600	GTP	C8-N7-C5	-2.03	99.12	102.99
4	K	501	ATP	C4-C5-N7	2.02	111.50	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

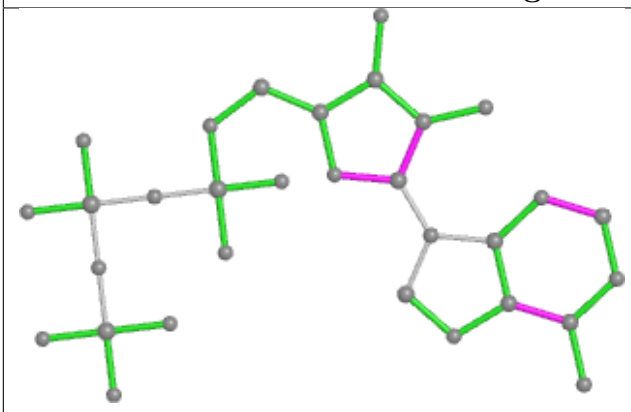
Mol	Chain	Res	Type	Atoms
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
4	K	501	ATP	C5'-O5'-PA-O1A
4	K	501	ATP	PA-O3A-PB-O2B
7	B	501	GDP	C5'-O5'-PA-O3A
7	B	501	GDP	O4'-C4'-C5'-O5'
4	K	501	ATP	PA-O3A-PB-O1B

There are no ring outliers.

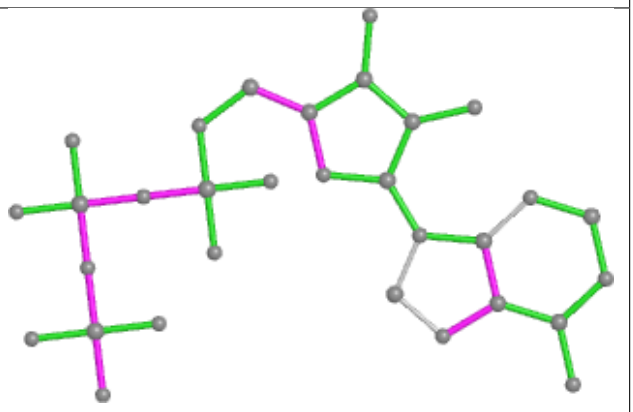
No monomer is involved in short contacts.

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 then 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.

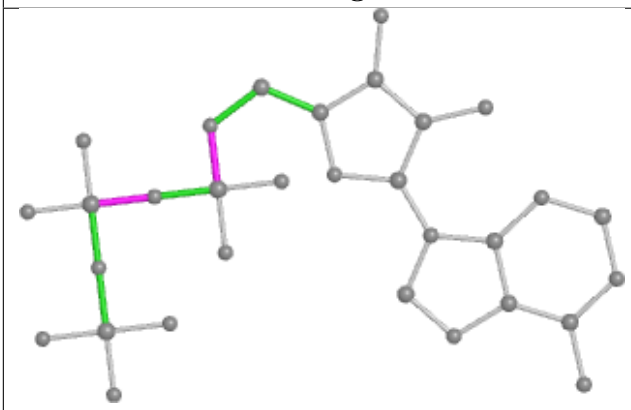
Ligand ATP K 501



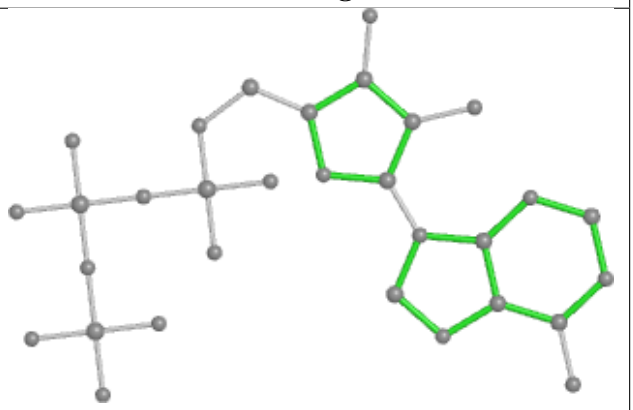
Bond lengths



Bond angles

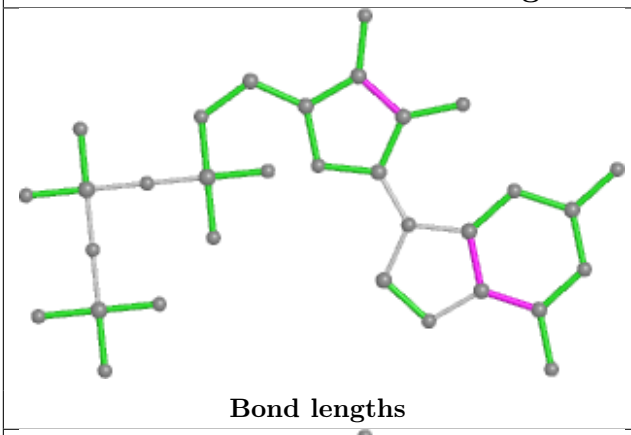


Torsions

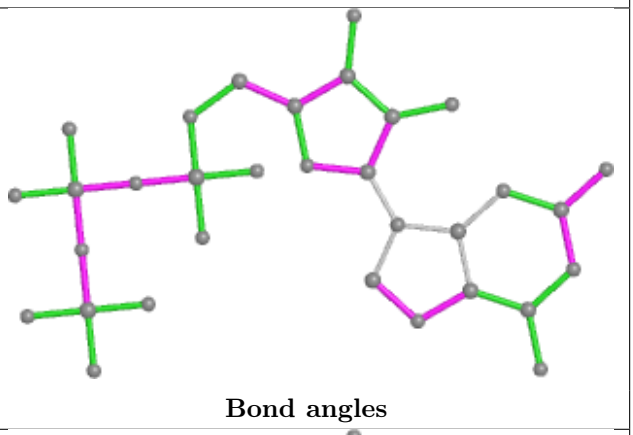


Rings

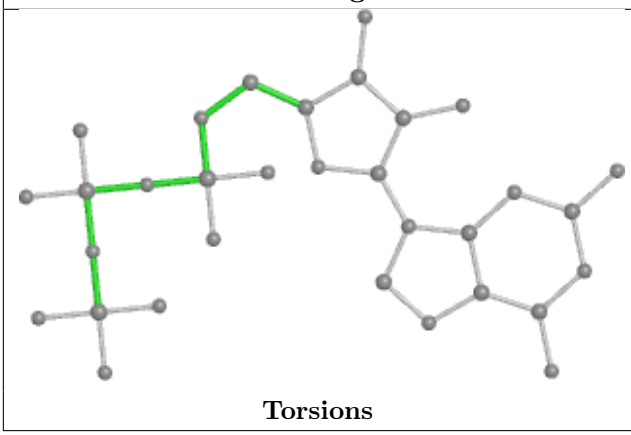
Ligand GTP A 600



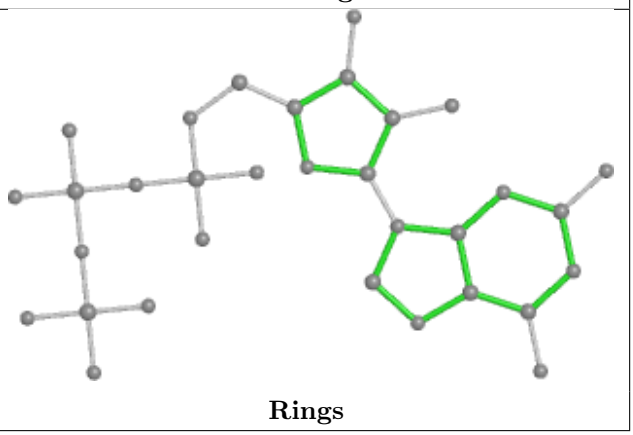
Bond lengths



Bond angles

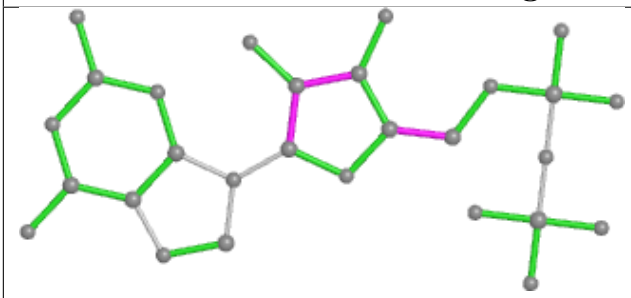


Torsions

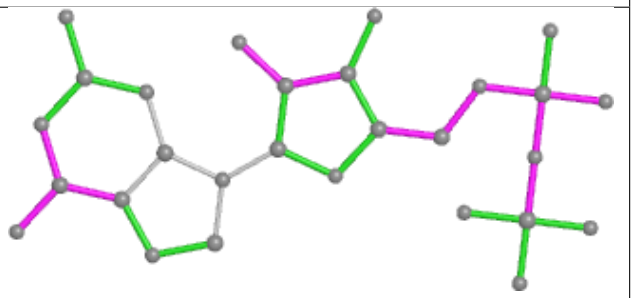


Rings

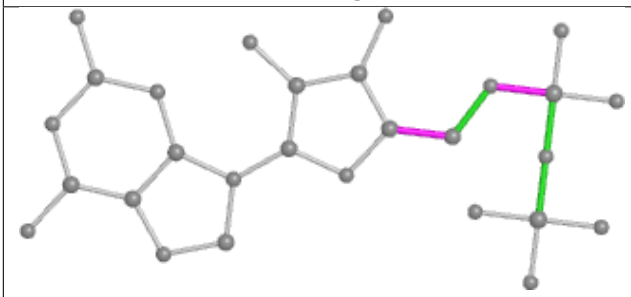
Ligand GDP B 501



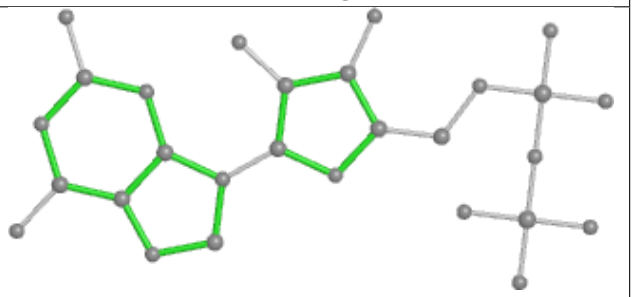
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

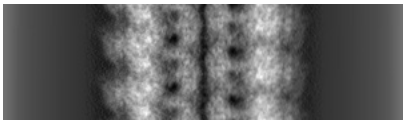
6 Map visualisation

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.

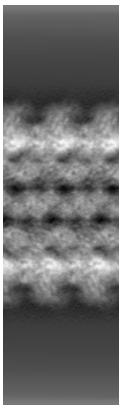
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

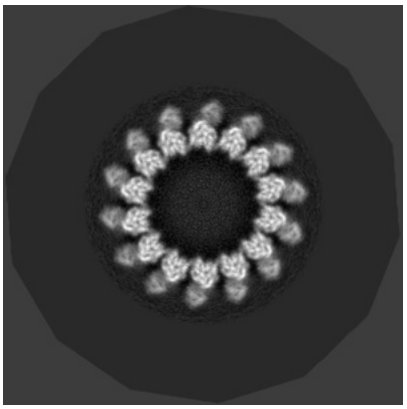
6.1.1 Primary map



X



Y

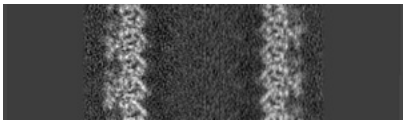


Z

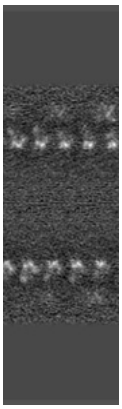
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

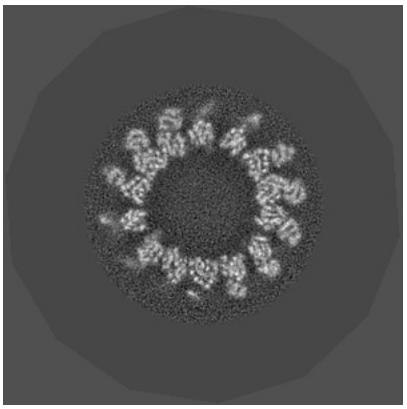
6.2.1 Primary map



X Index: 160



Y Index: 160

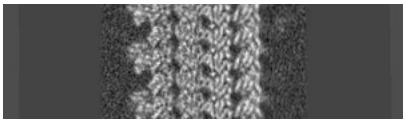


Z Index: 45

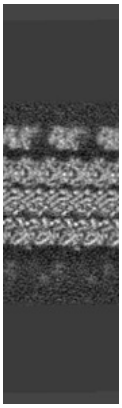
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

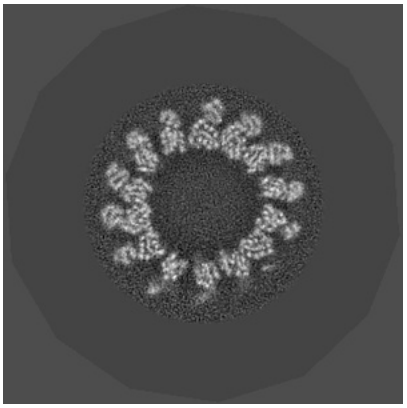
6.3.1 Primary map



X Index: 209



Y Index: 109

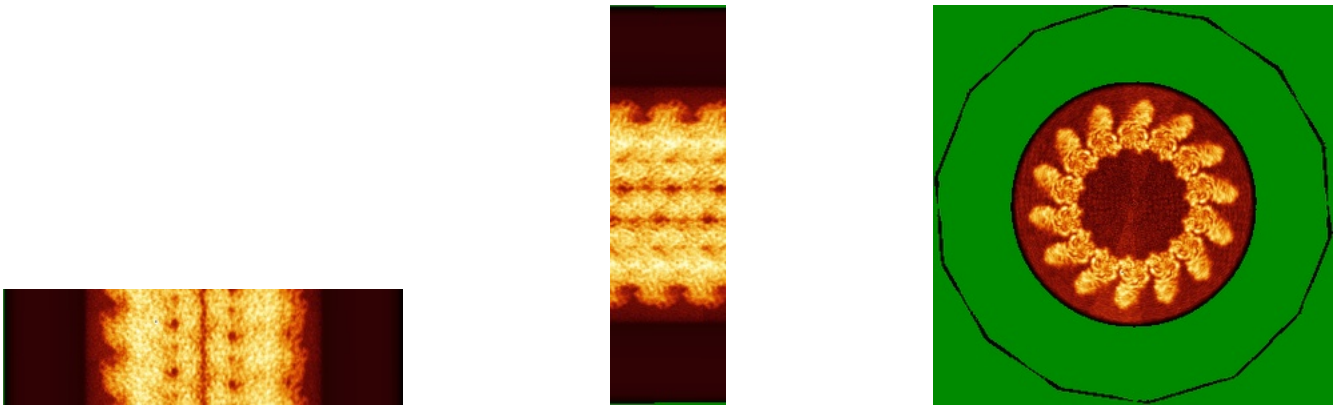


Z Index: 36

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

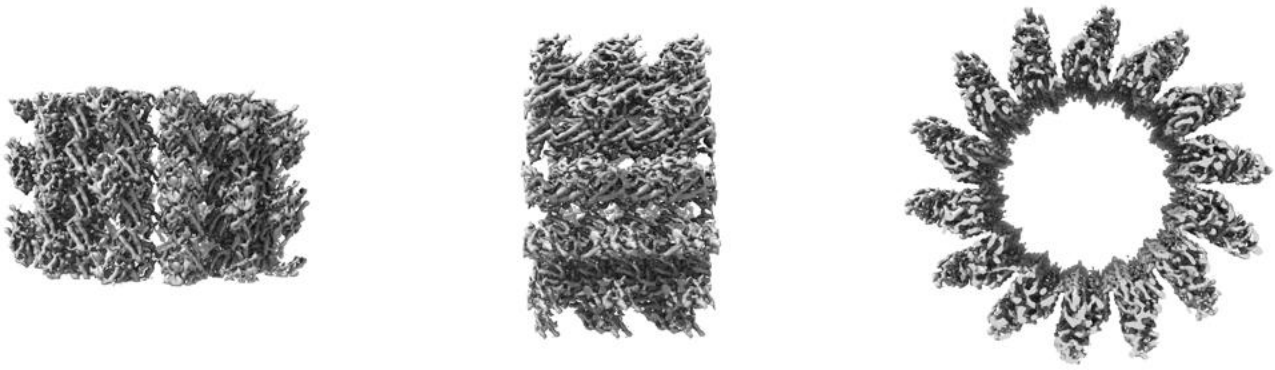


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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.

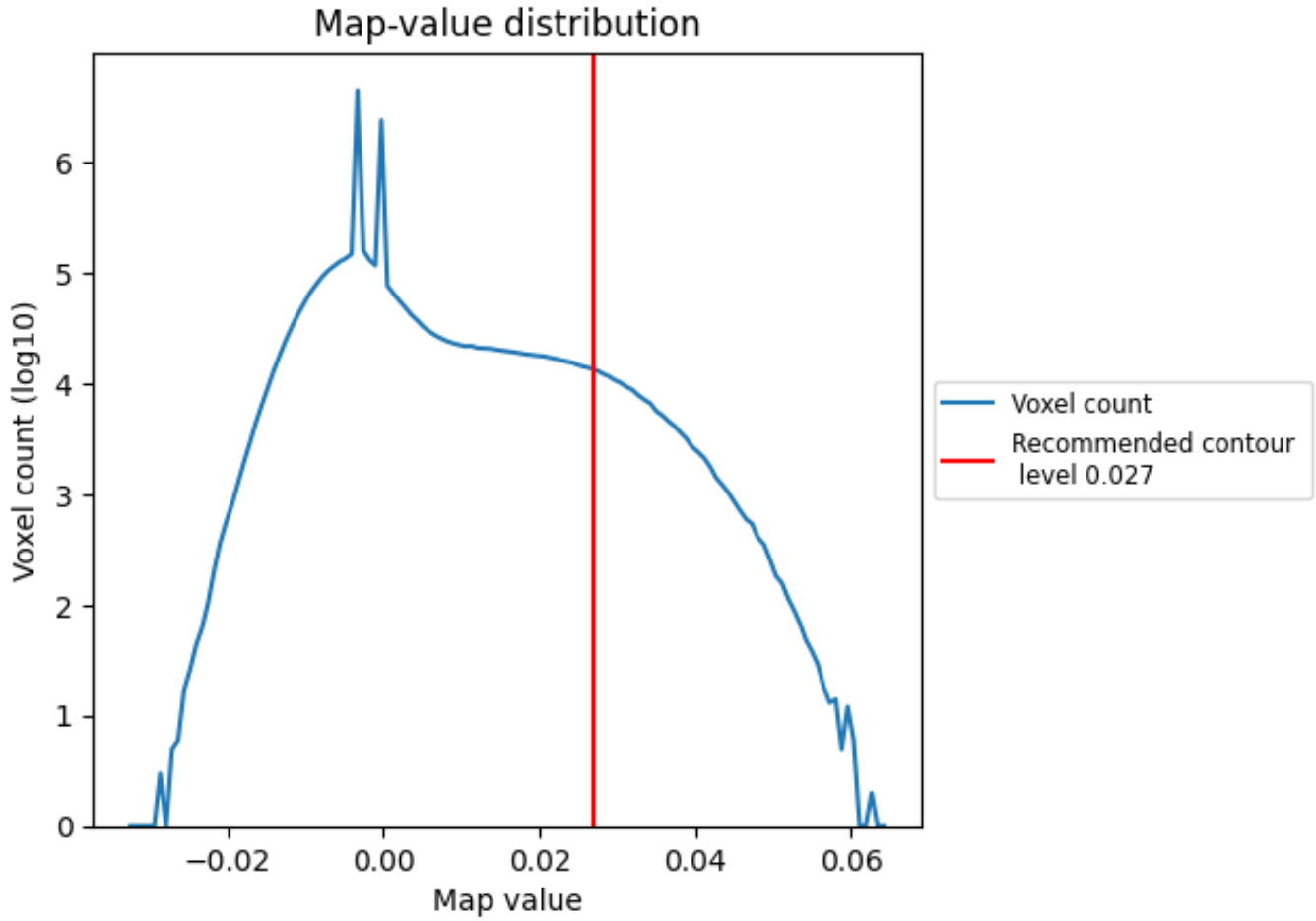
6.6 Mask visualisation (i)

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

7 Map analysis

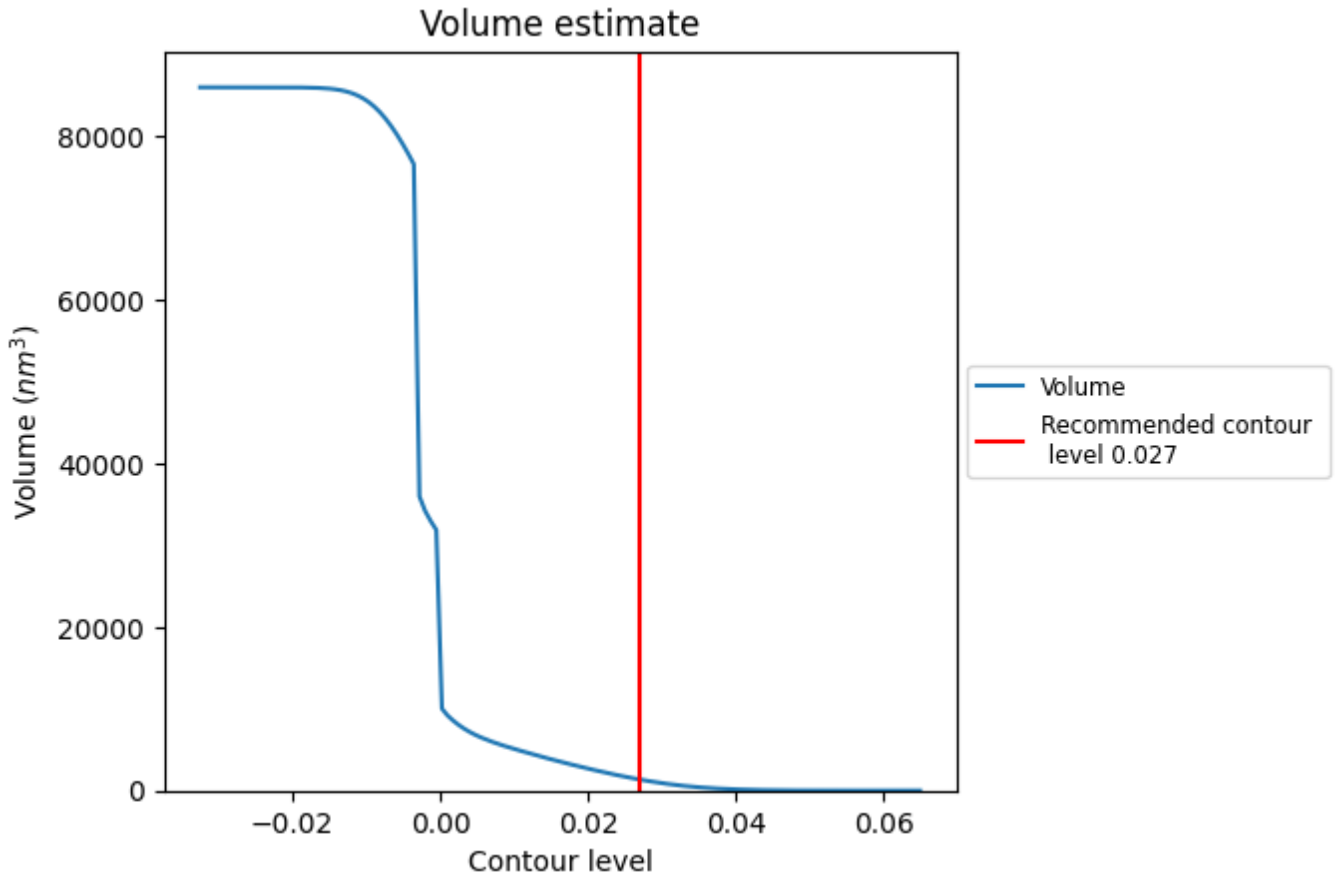
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 1350 nm^3; 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

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

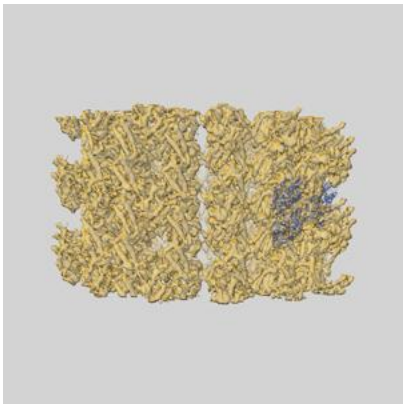
8 Fourier-Shell correlation (i)

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

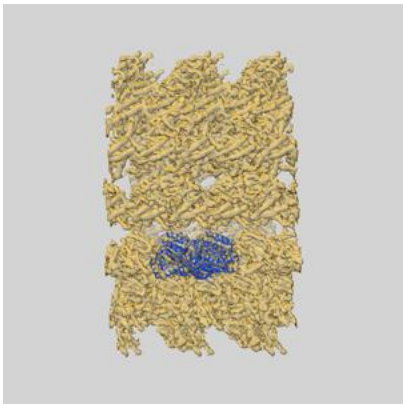
9 Map-model fit

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.

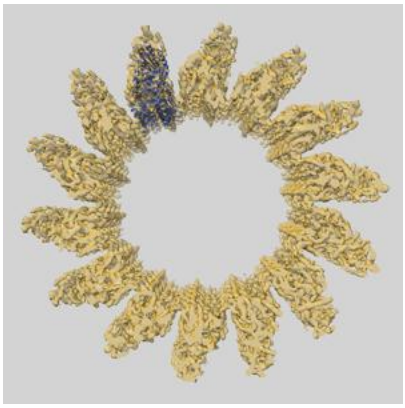
9.1 Map-model overlay



X



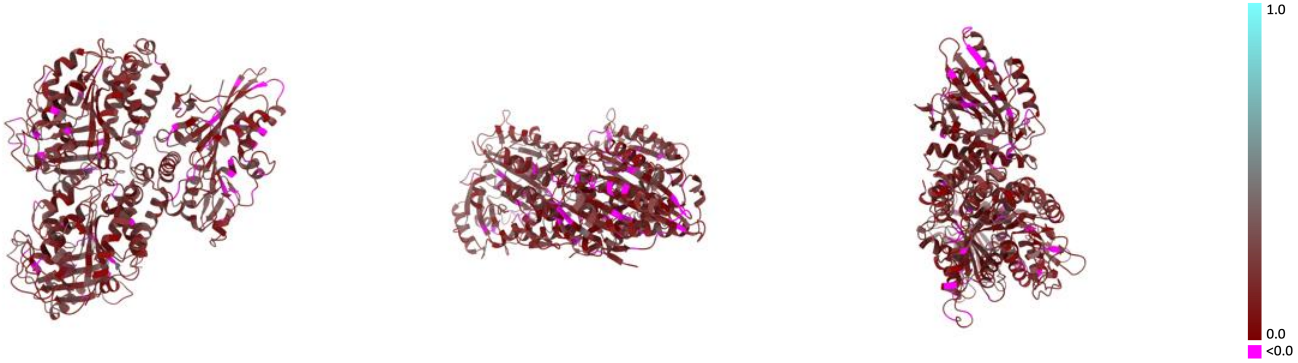
Y



Z

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.

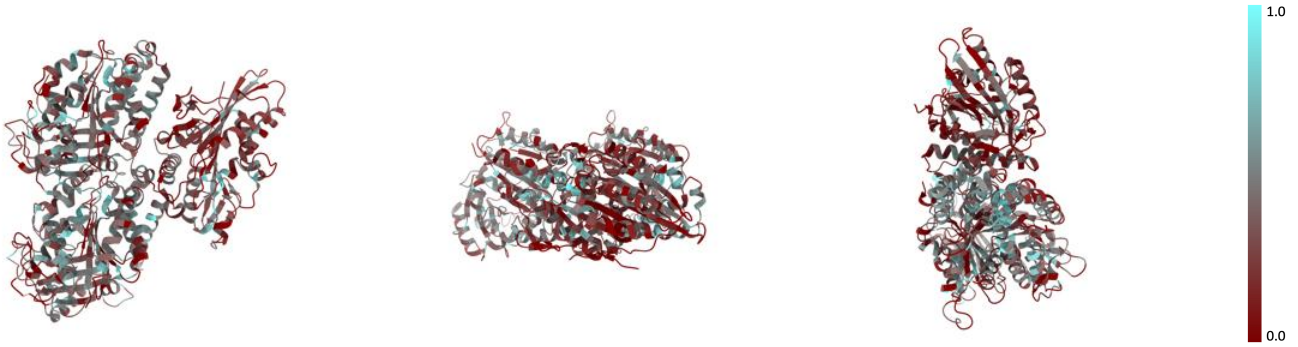
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

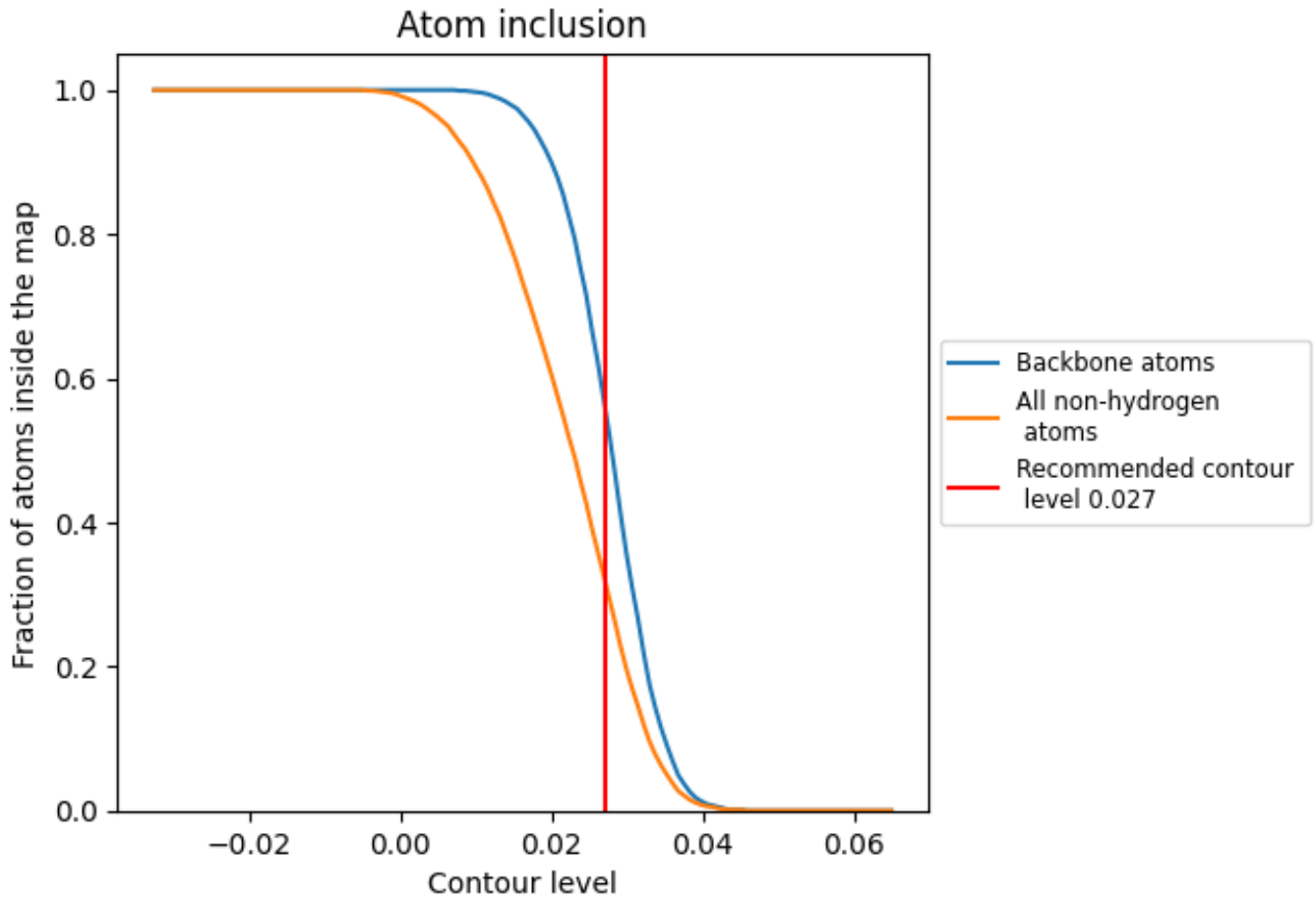
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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