Full wwPDB EM Validation Report ⓘ

Feb 13, 2024 – 11:16 PM EST

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

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

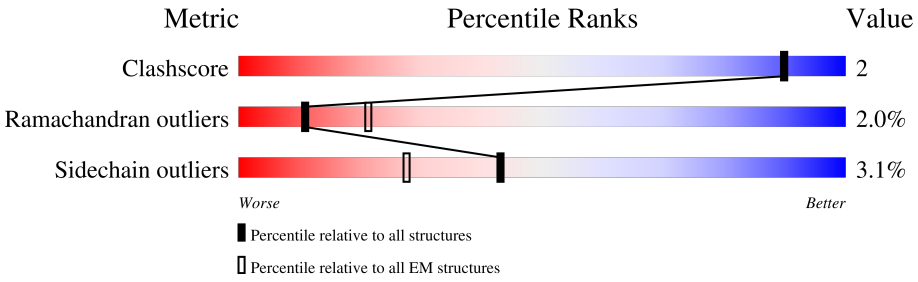
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	54% 67% 21% • 9%
2	A	451	18% 68% 23% • 5%
3	B	445	19% 67% 25% 5% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9295 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Kinesin-1 heavy chain.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

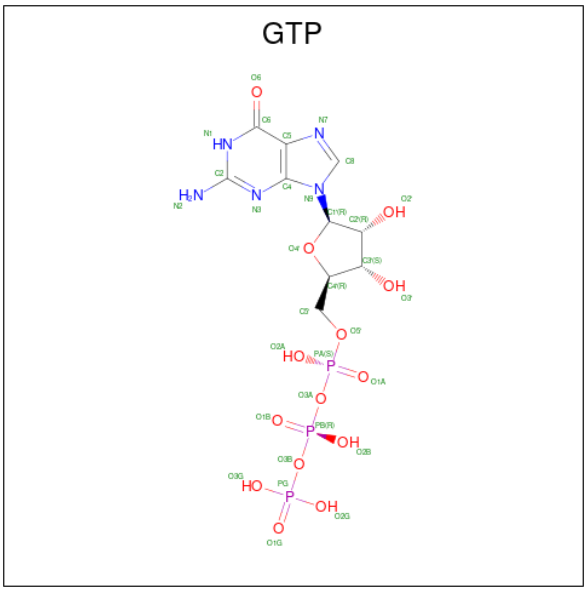
- Molecule 3 is a protein called Tubulin beta-2B chain.

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

There is a discrepancy between the modelled and reference sequences:

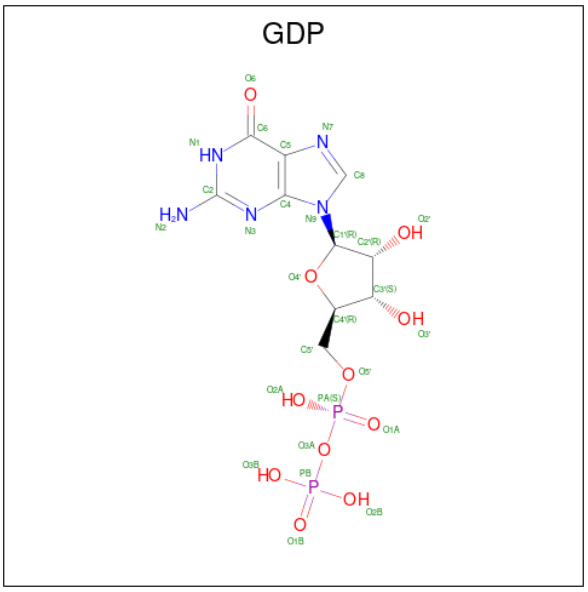
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	conflict	UNP F2Z5B2

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



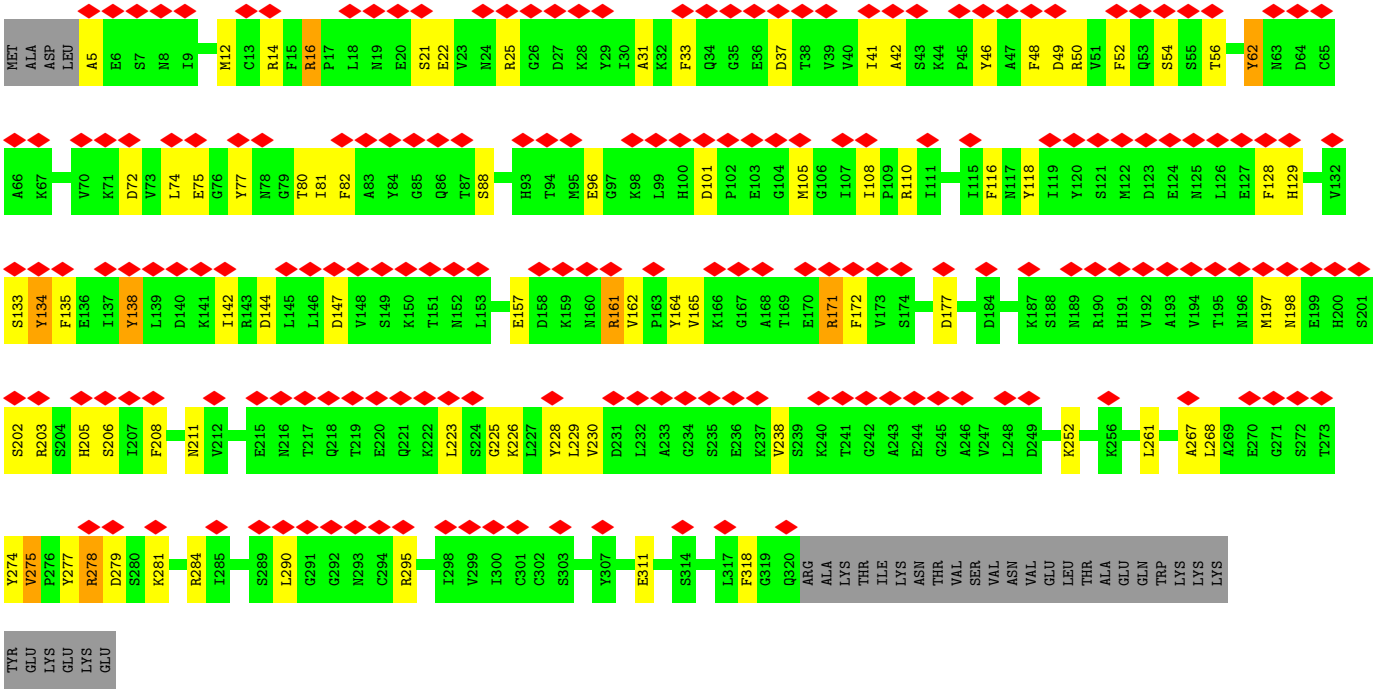
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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.

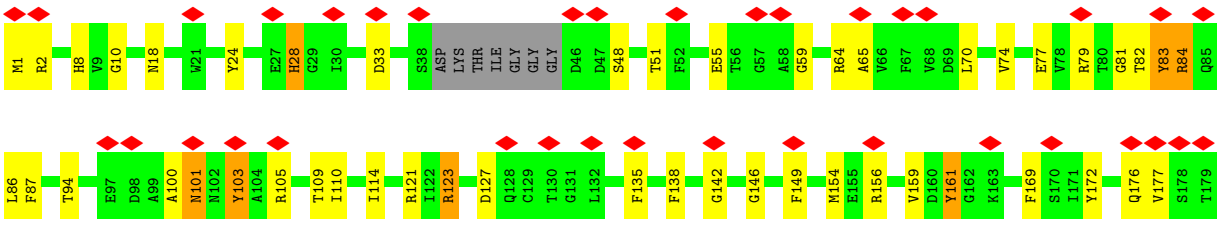
• Molecule 1: Kinesin-1 heavy chain

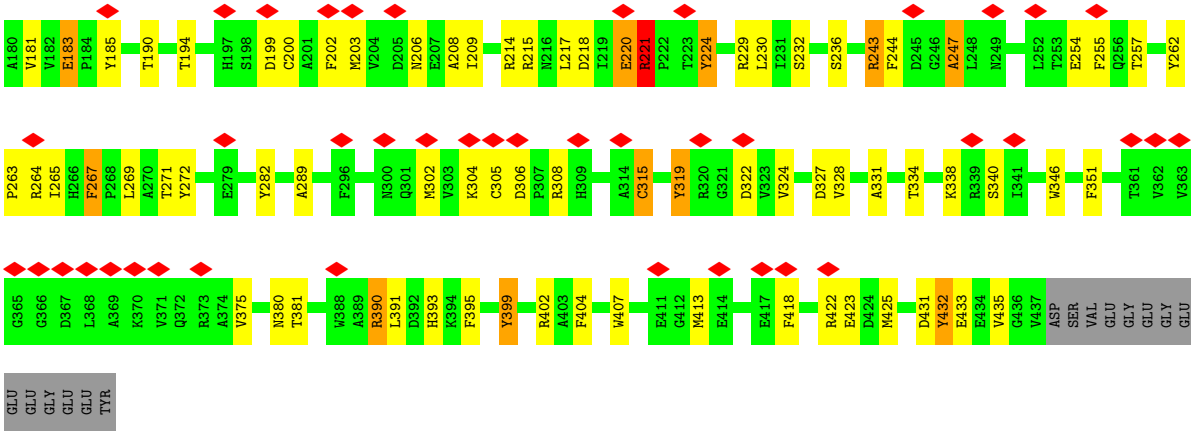
Chain K:



• Molecule 2: Tubulin alpha-1B chain

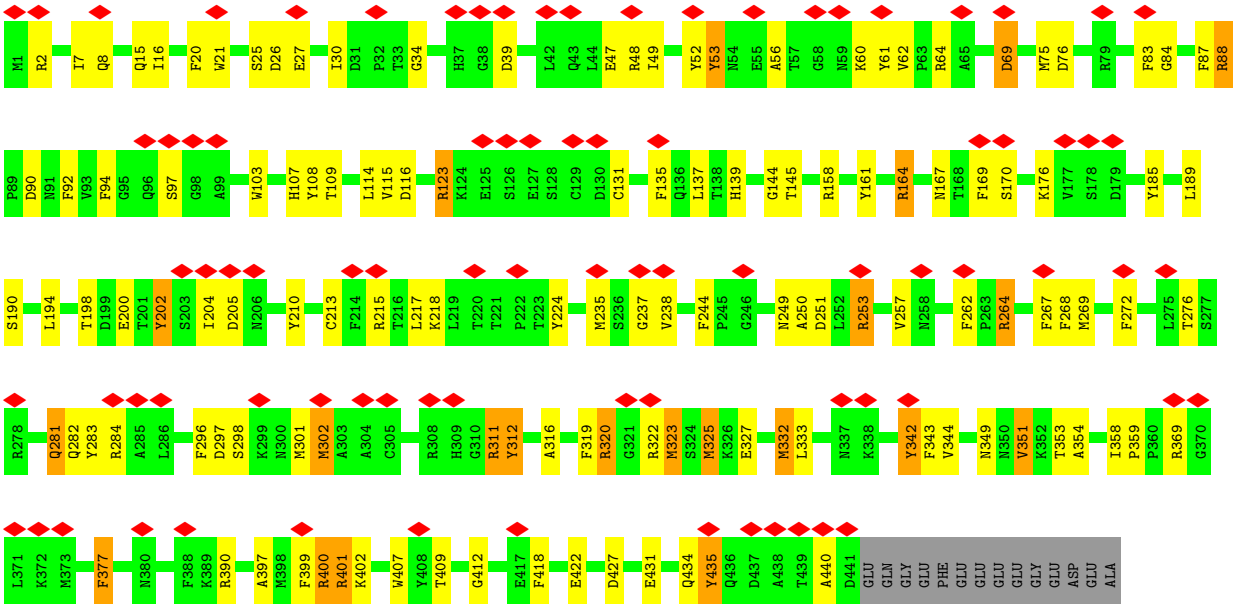
Chain A:





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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.64	15/2513 (0.6%)	1.96	67/3389 (2.0%)
2	A	1.64	21/3450 (0.6%)	2.01	92/4685 (2.0%)
3	B	1.61	16/3464 (0.5%)	2.06	119/4692 (2.5%)
All	All	1.63	52/9427 (0.6%)	2.02	278/12766 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	10
2	A	1	19
3	B	0	18
All	All	1	47

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	412	GLY	CA-C	-7.85	1.39	1.51
1	K	277	TYR	CG-CD2	7.84	1.49	1.39
2	A	282	TYR	CG-CD2	7.35	1.48	1.39
1	K	206	SER	CA-CB	7.00	1.63	1.52
2	A	305	CYS	CB-SG	6.45	1.93	1.82
3	B	213	CYS	CB-SG	6.24	1.92	1.82
2	A	10	GLY	CA-C	-6.12	1.42	1.51
1	K	5	ALA	CA-CB	6.03	1.65	1.52
2	A	346	TRP	CD2-CE3	-6.02	1.31	1.40
3	B	97	SER	CA-CB	6.00	1.61	1.52
2	A	423	GLU	CB-CG	5.96	1.63	1.52
2	A	315	CYS	CB-SG	5.96	1.92	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	272	TYR	CE1-CZ	5.96	1.46	1.38
2	A	185	TYR	CG-CD2	5.93	1.46	1.39
2	A	24	TYR	CG-CD1	5.90	1.46	1.39
3	B	237	GLY	CA-C	-5.88	1.42	1.51
3	B	190	SER	CA-CB	5.87	1.61	1.52
3	B	407	TRP	N-CA	-5.85	1.34	1.46
1	K	22	GLU	CB-CG	5.81	1.63	1.52
1	K	105	MET	CG-SD	5.59	1.95	1.81
2	A	319	TYR	CE2-CZ	5.55	1.45	1.38
2	A	267	PHE	CG-CD2	5.49	1.47	1.38
1	K	16	ARG	NE-CZ	5.46	1.40	1.33
2	A	432	TYR	CG-CD2	5.46	1.46	1.39
3	B	39	ASP	CA-CB	5.46	1.66	1.53
1	K	172	PHE	CE1-CZ	5.45	1.47	1.37
2	A	10	GLY	N-CA	5.44	1.54	1.46
3	B	21	TRP	CB-CG	5.43	1.60	1.50
1	K	134	TYR	CZ-OH	5.42	1.47	1.37
3	B	185	TYR	CB-CG	5.37	1.59	1.51
2	A	200	CYS	CB-SG	5.36	1.91	1.82
1	K	54	SER	CB-OG	5.36	1.49	1.42
2	A	169	PHE	CG-CD2	5.34	1.46	1.38
3	B	25	SER	CA-CB	5.32	1.60	1.52
2	A	77	GLU	CG-CD	-5.32	1.44	1.51
2	A	399	TYR	CE1-CZ	5.32	1.45	1.38
2	A	254	GLU	CD-OE1	5.31	1.31	1.25
3	B	20	PHE	CG-CD1	5.30	1.46	1.38
3	B	103	TRP	CE3-CZ3	5.27	1.47	1.38
1	K	46	TYR	CG-CD1	5.24	1.46	1.39
1	K	157	GLU	CG-CD	-5.24	1.44	1.51
1	K	275	VAL	CB-CG2	5.22	1.63	1.52
2	A	142	GLY	C-N	5.21	1.42	1.33
2	A	183	GLU	CD-OE2	5.17	1.31	1.25
3	B	312	TYR	CZ-OH	5.15	1.46	1.37
3	B	47	GLU	CD-OE1	-5.14	1.20	1.25
3	B	210	TYR	CG-CD1	-5.13	1.32	1.39
1	K	164	TYR	CD2-CE2	5.13	1.47	1.39
3	B	52	TYR	CE1-CZ	5.12	1.45	1.38
2	A	236	SER	CA-CB	5.11	1.60	1.52
1	K	88	SER	CB-OG	5.05	1.48	1.42
1	K	208	PHE	CB-CG	5.00	1.59	1.51

All (278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	278	ARG	NE-CZ-NH2	-17.75	111.43	120.30
2	A	272	TYR	CB-CG-CD2	-17.55	110.47	121.00
2	A	243	ARG	NE-CZ-NH1	17.17	128.88	120.30
3	B	108	TYR	CB-CG-CD1	16.12	130.68	121.00
1	K	25	ARG	NE-CZ-NH1	15.52	128.06	120.30
3	B	322	ARG	NE-CZ-NH2	15.38	127.99	120.30
2	A	255	PHE	CB-CG-CD2	-15.35	110.05	120.80
2	A	264	ARG	NE-CZ-NH1	15.21	127.91	120.30
2	A	402	ARG	NE-CZ-NH1	14.74	127.67	120.30
2	A	24	TYR	CB-CG-CD1	-13.97	112.62	121.00
3	B	202	TYR	CB-CG-CD2	-13.04	113.17	121.00
3	B	88	ARG	NE-CZ-NH1	12.96	126.78	120.30
3	B	53	TYR	CB-CG-CD1	12.88	128.73	121.00
1	K	278	ARG	NE-CZ-NH1	12.68	126.64	120.30
3	B	108	TYR	CB-CG-CD2	-12.67	113.40	121.00
3	B	53	TYR	CB-CG-CD2	-12.09	113.74	121.00
3	B	158	ARG	NE-CZ-NH1	11.43	126.01	120.30
3	B	435	TYR	CB-CG-CD2	-11.41	114.16	121.00
2	A	24	TYR	CB-CG-CD2	10.79	127.47	121.00
2	A	432	TYR	CB-CG-CD1	10.45	127.27	121.00
3	B	202	TYR	CB-CG-CD1	10.32	127.19	121.00
3	B	75	MET	CG-SD-CE	-10.25	83.79	100.20
3	B	135	PHE	CB-CG-CD2	-10.08	113.75	120.80
2	A	214	ARG	NE-CZ-NH1	9.90	125.25	120.30
3	B	210	TYR	CB-CG-CD2	-9.86	115.08	121.00
1	K	284	ARG	NE-CZ-NH2	9.52	125.06	120.30
2	A	322	ASP	CB-CG-OD2	9.49	126.84	118.30
3	B	418	PHE	CB-CG-CD1	-9.48	114.17	120.80
2	A	185	TYR	CB-CG-CD2	9.29	126.58	121.00
1	K	295	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	A	123	ARG	NE-CZ-NH1	9.05	124.82	120.30
3	B	244	PHE	CB-CG-CD1	-8.95	114.54	120.80
2	A	399	TYR	CB-CG-CD1	-8.94	115.64	121.00
2	A	255	PHE	CB-CG-CD1	8.85	127.00	120.80
3	B	158	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	K	49	ASP	CB-CG-OD2	8.81	126.22	118.30
3	B	311	ARG	NE-CZ-NH2	8.59	124.60	120.30
2	A	224	TYR	CB-CG-CD2	-8.51	115.89	121.00
1	K	72	ASP	CB-CG-OD2	-8.39	110.75	118.30
2	A	395	PHE	CB-CG-CD2	-8.39	114.92	120.80
3	B	401	ARG	NE-CZ-NH1	8.39	124.49	120.30
2	A	127	ASP	CB-CG-OD1	8.36	125.82	118.30
3	B	342	TYR	CB-CG-CD1	8.29	125.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	161	TYR	CB-CG-CD1	-8.15	116.11	121.00
3	B	342	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	K	147	ASP	CB-CG-OD2	-8.07	111.04	118.30
2	A	308	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	K	77	TYR	CB-CG-CD2	-8.04	116.18	121.00
3	B	390	ARG	NE-CZ-NH2	-8.02	116.29	120.30
3	B	92	PHE	CB-CG-CD1	-7.95	115.24	120.80
3	B	397	ALA	N-CA-CB	-7.71	99.30	110.10
1	K	134	TYR	CB-CG-CD2	-7.66	116.40	121.00
1	K	82	PHE	CB-CG-CD2	-7.65	115.44	120.80
2	A	64	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	A	105	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	K	177	ASP	CB-CG-OD1	-7.60	111.46	118.30
2	A	264	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	K	318	PHE	CB-CG-CD2	-7.57	115.50	120.80
3	B	311	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	A	306	ASP	CB-CG-OD2	7.55	125.10	118.30
3	B	272	PHE	N-CA-CB	-7.55	97.00	110.60
3	B	343	PHE	CB-CG-CD1	-7.41	115.61	120.80
3	B	268	PHE	CB-CG-CD2	7.40	125.98	120.80
2	A	1	MET	CG-SD-CE	-7.35	88.43	100.20
3	B	311	ARG	NH1-CZ-NH2	-7.35	111.31	119.40
2	A	418	PHE	CB-CG-CD1	7.33	125.93	120.80
2	A	390	ARG	NE-CZ-NH1	7.31	123.95	120.30
2	A	161	TYR	CA-CB-CG	-7.27	99.58	113.40
2	A	199	ASP	CB-CG-OD2	7.23	124.80	118.30
2	A	65	ALA	O-C-N	-7.19	111.20	122.70
3	B	400	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	A	282	TYR	CB-CG-CD2	7.14	125.28	121.00
1	K	228	TYR	CB-CG-CD1	-7.13	116.72	121.00
1	K	77	TYR	CB-CG-CD1	7.08	125.25	121.00
3	B	103	TRP	CG-CD2-CE3	-7.08	127.53	133.90
2	A	247	ALA	CB-CA-C	7.07	120.71	110.10
2	A	156	ARG	NE-CZ-NH2	-7.07	116.77	120.30
2	A	83	TYR	CB-CG-CD2	-7.06	116.76	121.00
3	B	164	ARG	NE-CZ-NH1	7.03	123.82	120.30
2	A	433	GLU	O-C-N	-7.03	111.45	122.70
1	K	277	TYR	CB-CG-CD1	7.01	125.20	121.00
3	B	170	SER	N-CA-CB	7.00	121.00	110.50
1	K	50	ARG	NE-CZ-NH1	-6.96	116.82	120.30
3	B	322	ARG	NH1-CZ-NH2	-6.93	111.77	119.40
1	K	274	TYR	CB-CG-CD1	6.93	125.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	26	ASP	CB-CG-OD1	6.91	124.52	118.30
3	B	251	ASP	CB-CG-OD1	-6.90	112.09	118.30
2	A	202	PHE	CB-CG-CD2	-6.84	116.02	120.80
3	B	319	PHE	CB-CG-CD2	-6.82	116.03	120.80
1	K	48	PHE	CB-CG-CD1	-6.78	116.06	120.80
3	B	21	TRP	CB-CG-CD1	6.77	135.80	127.00
3	B	262	PHE	CB-CG-CD1	6.77	125.54	120.80
2	A	404	PHE	CB-CG-CD2	-6.77	116.06	120.80
2	A	272	TYR	CB-CG-CD1	6.77	125.06	121.00
2	A	395	PHE	CB-CG-CD1	6.76	125.53	120.80
3	B	167	ASN	O-C-N	-6.75	111.89	122.70
2	A	404	PHE	CB-CG-CD1	6.73	125.51	120.80
1	K	42	ALA	CB-CA-C	6.71	120.16	110.10
1	K	205	HIS	N-CA-CB	6.70	122.65	110.60
1	K	161	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	K	105	MET	CG-SD-CE	6.66	110.85	100.20
3	B	296	PHE	CB-CG-CD1	6.63	125.44	120.80
3	B	161	TYR	CB-CG-CD2	6.60	124.96	121.00
1	K	21	SER	N-CA-CB	6.59	120.38	110.50
2	A	319	TYR	CB-CG-CD1	-6.56	117.06	121.00
3	B	114	LEU	O-C-N	-6.54	112.24	122.70
2	A	262	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	K	311	GLU	OE1-CD-OE2	-6.50	115.50	123.30
2	A	269	LEU	O-C-N	-6.47	112.34	122.70
1	K	52	PHE	CB-CG-CD1	-6.46	116.28	120.80
2	A	215	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	A	159	VAL	CA-CB-CG1	6.42	120.53	110.90
3	B	2	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	A	154	MET	CG-SD-CE	-6.42	89.93	100.20
3	B	123	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	K	31	ALA	N-CA-CB	-6.35	101.21	110.10
3	B	431	GLU	O-C-N	-6.31	112.61	122.70
2	A	121	ARG	NE-CZ-NH1	-6.30	117.15	120.30
3	B	61	TYR	CB-CG-CD2	-6.30	117.22	121.00
3	B	390	ARG	CB-CA-C	6.29	122.99	110.40
2	A	105	ARG	NE-CZ-NH1	6.28	123.44	120.30
3	B	397	ALA	CB-CA-C	6.26	119.48	110.10
3	B	210	TYR	CB-CG-CD1	6.25	124.75	121.00
3	B	185	TYR	CG-CD1-CE1	-6.25	116.30	121.30
2	A	87	PHE	CB-CG-CD2	-6.25	116.43	120.80
3	B	235	MET	CG-SD-CE	-6.24	90.21	100.20
1	K	171	ARG	NE-CZ-NH1	6.23	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	76	ASP	CB-CG-OD1	6.22	123.90	118.30
2	A	243	ARG	CG-CD-NE	-6.21	98.75	111.80
1	K	37	ASP	CB-CG-OD1	-6.21	112.71	118.30
3	B	103	TRP	CB-CG-CD2	6.16	134.61	126.60
3	B	320	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	K	164	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	K	25	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	K	12	MET	CG-SD-CE	-6.12	90.41	100.20
3	B	90	ASP	CB-CG-OD2	6.11	123.80	118.30
3	B	244	PHE	CB-CG-CD2	6.11	125.07	120.80
3	B	267	PHE	CB-CG-CD1	6.07	125.05	120.80
2	A	224	TYR	CB-CG-CD1	6.04	124.63	121.00
1	K	101	ASP	CB-CG-OD2	-6.04	112.86	118.30
3	B	205	ASP	CB-CG-OD2	-6.04	112.86	118.30
3	B	401	ARG	NH1-CZ-NH2	-6.03	112.76	119.40
1	K	46	TYR	CB-CG-CD2	6.03	124.62	121.00
3	B	323	MET	CG-SD-CE	-6.03	90.56	100.20
3	B	253	ARG	NE-CZ-NH1	6.01	123.31	120.30
3	B	399	PHE	CG-CD1-CE1	-6.01	114.19	120.80
2	A	169	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	K	197	MET	CG-SD-CE	-5.99	90.61	100.20
3	B	116	ASP	CB-CG-OD1	-5.97	112.93	118.30
3	B	402	LYS	N-CA-CB	5.97	121.34	110.60
3	B	354	ALA	CB-CA-C	5.96	119.04	110.10
2	A	138	PHE	CZ-CE2-CD2	5.96	127.25	120.10
3	B	224	TYR	CG-CD1-CE1	-5.91	116.57	121.30
1	K	62	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	K	144	ASP	CB-CG-OD2	-5.89	112.99	118.30
3	B	21	TRP	CB-CG-CD2	-5.87	118.97	126.60
2	A	402	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	K	202	SER	N-CA-CB	5.86	119.29	110.50
2	A	24	TYR	CZ-CE2-CD2	-5.86	114.53	119.80
3	B	316	ALA	N-CA-CB	-5.86	101.90	110.10
3	B	302	MET	CG-SD-CE	-5.81	90.90	100.20
3	B	88	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	A	181	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	K	62	TYR	CG-CD2-CE2	-5.79	116.67	121.30
3	B	320	ARG	NE-CZ-NH1	5.78	123.19	120.30
3	B	377	PHE	CB-CG-CD1	-5.76	116.77	120.80
2	A	203	MET	CG-SD-CE	-5.76	90.99	100.20
2	A	331	ALA	N-CA-CB	5.75	118.15	110.10
2	A	172	TYR	CG-CD2-CE2	-5.75	116.70	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	215	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	A	272	TYR	CD1-CG-CD2	5.74	124.22	117.90
3	B	399	PHE	CD1-CE1-CZ	5.74	126.98	120.10
1	K	72	ASP	CB-CG-OD1	5.72	123.45	118.30
3	B	369	ARG	NE-CZ-NH1	-5.72	117.44	120.30
3	B	409	THR	N-CA-CB	5.72	121.17	110.30
2	A	94	THR	CA-CB-CG2	-5.71	104.40	112.40
3	B	251	ASP	CB-CG-OD2	5.71	123.44	118.30
3	B	27	GLU	O-C-N	-5.71	113.57	122.70
1	K	128	PHE	CB-CG-CD1	-5.69	116.81	120.80
2	A	324	VAL	CA-CB-CG1	5.69	119.44	110.90
3	B	262	PHE	CB-CG-CD2	-5.68	116.82	120.80
3	B	88	ARG	CD-NE-CZ	-5.67	115.67	123.60
2	A	55	GLU	CA-CB-CG	5.66	125.85	113.40
3	B	264	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	A	243	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	K	108	ILE	CA-C-N	5.62	132.82	117.10
3	B	47	GLU	CB-CA-C	5.61	121.62	110.40
2	A	232	SER	N-CA-CB	5.61	118.91	110.50
1	K	33	PHE	CB-CG-CD1	-5.61	116.88	120.80
3	B	94	PHE	CB-CG-CD2	-5.61	116.88	120.80
2	A	334	THR	O-C-N	-5.60	113.73	122.70
3	B	301	MET	CG-SD-CE	-5.60	91.24	100.20
3	B	224	TYR	CB-CG-CD1	-5.59	117.64	121.00
2	A	64	ARG	NE-CZ-NH1	5.57	123.08	120.30
3	B	26	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	K	277	TYR	CB-CA-C	-5.53	99.33	110.40
3	B	39	ASP	CB-CG-OD2	5.53	123.28	118.30
1	K	147	ASP	CB-CG-OD1	5.53	123.28	118.30
3	B	62	VAL	CG1-CB-CG2	-5.53	102.05	110.90
3	B	296	PHE	CB-CA-C	-5.53	99.34	110.40
1	K	164	TYR	CB-CG-CD1	5.53	124.31	121.00
1	K	268	LEU	CB-CG-CD1	-5.51	101.64	111.00
2	A	172	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	B	2	ARG	NE-CZ-NH1	-5.47	117.56	120.30
3	B	435	TYR	CD1-CG-CD2	5.47	123.92	117.90
1	K	25	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
3	B	189	LEU	O-C-N	-5.46	113.96	122.70
2	A	229	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	B	94	PHE	CB-CG-CD1	5.46	124.62	120.80
3	B	276	THR	CA-CB-CG2	-5.45	104.77	112.40
3	B	351	VAL	O-C-N	-5.44	113.99	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	139	HIS	N-CA-CB	-5.44	100.81	110.60
3	B	400	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	B	281	GLN	C-N-CA	5.41	135.22	121.70
2	A	48	SER	N-CA-CB	5.39	118.58	110.50
2	A	161	TYR	CD1-CE1-CZ	-5.38	114.95	119.80
3	B	69	ASP	CB-CG-OD1	5.38	123.14	118.30
2	A	177	VAL	O-C-N	-5.36	114.12	122.70
2	A	84	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	K	134	TYR	CG-CD1-CE1	-5.36	117.01	121.30
2	A	271	THR	N-CA-CB	5.36	120.48	110.30
1	K	223	LEU	CB-CG-CD1	-5.35	101.91	111.00
2	A	79	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	A	123	ARG	CD-NE-CZ	5.31	131.03	123.60
3	B	377	PHE	CG-CD2-CE2	-5.31	114.96	120.80
1	K	21	SER	CB-CA-C	-5.30	100.02	110.10
1	K	80	THR	CA-CB-CG2	-5.29	105.00	112.40
3	B	48	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	A	103	TYR	CB-CG-CD1	-5.28	117.83	121.00
3	B	297	ASP	CB-CG-OD2	5.27	123.04	118.30
1	K	116	PHE	O-C-N	-5.26	114.28	122.70
2	A	289	ALA	N-CA-CB	-5.26	102.73	110.10
2	A	263	PRO	N-CA-CB	5.25	109.60	103.30
2	A	433	GLU	CA-C-O	5.24	131.11	120.10
3	B	217	LEU	CB-CA-C	5.24	120.16	110.20
3	B	200	GLU	N-CA-CB	5.24	120.02	110.60
2	A	431	ASP	CB-CG-OD2	5.23	123.00	118.30
1	K	228	TYR	CG-CD1-CE1	-5.23	117.12	121.30
2	A	432	TYR	CA-CB-CG	-5.22	103.47	113.40
3	B	135	PHE	CA-CB-CG	-5.22	101.38	113.90
1	K	133	SER	N-CA-CB	5.21	118.32	110.50
3	B	327	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	K	252	LYS	CD-CE-NZ	5.21	123.69	111.70
1	K	177	ASP	CB-CG-OD2	5.21	122.98	118.30
2	A	380	ASN	CB-CA-C	5.20	120.80	110.40
1	K	49	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	A	84	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	B	269	MET	N-CA-CB	-5.17	101.29	110.60
1	K	96	GLU	O-C-N	-5.16	114.43	123.20
2	A	135	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	A	221	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	K	238	VAL	O-C-N	-5.14	114.48	122.70
3	B	64	ARG	O-C-N	5.11	130.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	338	LYS	O-C-N	-5.11	114.52	122.70
3	B	107	HIS	CA-CB-CG	5.11	122.29	113.60
1	K	274	TYR	CZ-CE2-CD2	5.11	124.40	119.80
2	A	375	VAL	CA-CB-CG2	5.11	118.56	110.90
3	B	344	VAL	N-CA-CB	5.10	122.73	111.50
1	K	267	ALA	N-CA-CB	5.10	117.24	110.10
2	A	364	PRO	CA-N-CD	5.09	118.83	111.70
2	A	220	GLU	OE1-CD-OE2	-5.09	117.19	123.30
3	B	64	ARG	NE-CZ-NH1	5.09	122.84	120.30
3	B	90	ASP	CB-CG-OD1	-5.08	113.72	118.30
2	A	74	VAL	CA-CB-CG1	5.08	118.52	110.90
3	B	15	GLN	N-CA-CB	5.08	119.75	110.60
2	A	156	ARG	N-CA-CB	5.06	119.70	110.60
1	K	198	ASN	CA-CB-CG	-5.05	102.28	113.40
3	B	353	THR	CA-CB-CG2	-5.05	105.33	112.40
1	K	277	TYR	CA-CB-CG	-5.04	103.82	113.40
2	A	308	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	K	230	VAL	N-CA-CB	-5.03	100.43	111.50
3	B	16	ILE	CA-CB-CG1	5.03	120.56	111.00
3	B	135	PHE	CB-CG-CD1	5.02	124.31	120.80
3	B	427	ASP	N-CA-CB	5.02	119.63	110.60
1	K	138	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	K	16	ARG	NE-CZ-NH2	-5.01	117.79	120.30
3	B	283	TYR	CG-CD2-CE2	-5.01	117.29	121.30
2	A	257	THR	N-CA-CB	5.00	119.81	110.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	46	ASP	CA

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	100	ALA	Peptide
2	A	101	ASN	Peptide
2	A	103	TYR	Sidechain
2	A	114	ILE	Peptide
2	A	123	ARG	Sidechain
2	A	146	GLY	Peptide
2	A	149	PHE	Sidechain
2	A	161	TYR	Sidechain

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

5.2 Too-close contacts (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	2474	0	2434	6	0
2	A	3372	0	3287	16	0
3	B	3389	0	3266	13	0
4	A	32	0	12	0	0
5	B	28	0	12	0	0
All	All	9295	0	9011	31	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 (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:208:ALA:HB2	2:A:304:LYS:HB2	1.87	0.56
3:B:332:MET:HG3	3:B:351:VAL:HG11	1.87	0.56
2:A:407:TRP:CE3	3:B:257:VAL:HG22	2.41	0.55
3:B:69:ASP:HA	3:B:145:THR:HG21	1.87	0.55
3:B:30:ILE:HD11	3:B:49:ILE:HD11	1.90	0.53
2:A:407:TRP:CE2	3:B:257:VAL:HA	2.44	0.52
1:K:142:ILE:HD11	1:K:281:LYS:HE2	1.92	0.51
2:A:109:THR:HG22	2:A:110:ILE:HD13	1.92	0.51
2:A:265:ILE:HG23	2:A:432:TYR:CZ	2.47	0.49
2:A:217:LEU:HD23	2:A:217:LEU:O	2.14	0.48
3:B:320:ARG:HB3	3:B:359:PRO:HA	1.96	0.47
2:A:190:THR:O	2:A:194:THR:HG23	2.15	0.47
2:A:18:ASN:HD21	2:A:82:THR:HG21	1.81	0.46
2:A:28:HIS:CE1	2:A:244:PHE:CZ	3.04	0.46
3:B:7:ILE:HD12	3:B:137:LEU:HD12	2.00	0.44
1:K:135:PHE:CZ	1:K:165:VAL:HG21	2.51	0.44
2:A:221:ARG:HH12	3:B:325:MET:HB2	1.83	0.44
2:A:315:CYS:HB2	2:A:351:PHE:CD1	2.52	0.44
3:B:253:ARG:HG3	3:B:257:VAL:HG23	2.00	0.44
1:K:162:VAL:HG11	1:K:226:LYS:NZ	2.32	0.43
2:A:176:GLN:HG2	3:B:333:LEU:HD22	2.00	0.43
3:B:194:LEU:HD22	3:B:198:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:319:TYR:CE1	2:A:328:VAL:HG13	2.55	0.42
1:K:41:ILE:HD13	1:K:41:ILE:HA	1.87	0.41
2:A:208:ALA:HB3	2:A:302:MET:O	2.20	0.41
3:B:358:ILE:HG22	3:B:359:PRO:O	2.20	0.41
3:B:34:GLY:O	3:B:60:LYS:HA	2.21	0.41
1:K:81:ILE:HB	1:K:229:LEU:HD23	2.01	0.41
2:A:265:ILE:HG23	2:A:432:TYR:CE2	2.55	0.41
1:K:261:LEU:HD11	1:K:290:LEU:HD21	2.03	0.41
2:A:391:LEU:HD23	2:A:425:MET:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (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	314/349 (90%)	273 (87%)	39 (12%)	2 (1%)	25 65
2	A	428/451 (95%)	374 (87%)	44 (10%)	10 (2%)	6 36
3	B	429/445 (96%)	367 (86%)	51 (12%)	11 (3%)	5 34
All	All	1171/1245 (94%)	1014 (87%)	134 (11%)	23 (2%)	11 39

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	220	GLU
3	B	84	GLY
3	B	282	GLN
3	B	349	ASN
2	A	59	GLY
2	A	247	ALA
3	B	325	MET
2	A	101	ASN

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

5.3.2 Protein sidechains (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	279/311 (90%)	272 (98%)	7 (2%)	47	68
2	A	364/379 (96%)	352 (97%)	12 (3%)	38	61
3	B	372/383 (97%)	360 (97%)	12 (3%)	39	61
All	All	1015/1073 (95%)	984 (97%)	31 (3%)	43	62

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	14	ARG
1	K	56	THR
1	K	74	LEU
1	K	118	TYR
1	K	134	TYR
1	K	211	ASN
1	K	279	ASP

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Mol	Chain	Res	Type
2	A	8	HIS
2	A	33	ASP
2	A	51	THR
2	A	86	LEU
2	A	183	GLU
2	A	206	ASN
2	A	209	ILE
2	A	221	ARG
2	A	230	LEU
2	A	327	ASP
2	A	381	THR
2	A	413	MET
3	B	8	GLN
3	B	83	PHE
3	B	115	VAL
3	B	131	CYS
3	B	176	LYS
3	B	204	ILE
3	B	238	VAL
3	B	302	MET
3	B	323	MET
3	B	332	MET
3	B	422	GLU
3	B	434	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	A	600	-	26,34,34	1.81	7 (26%)	32,54,54	2.17	7 (21%)
5	GDP	B	501	-	24,30,30	1.97	5 (20%)	30,47,47	1.89	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	GTP	A	600	-	-	5/18/38/38	0/3/3/3
5	GDP	B	501	-	-	5/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	C2'-C1'	-6.68	1.43	1.53
4	A	600	GTP	C3'-C4'	4.58	1.64	1.53
5	B	501	GDP	C8-N7	-3.75	1.28	1.35
4	A	600	GTP	O4'-C4'	3.40	1.52	1.45
4	A	600	GTP	O4'-C1'	3.34	1.45	1.41
5	B	501	GDP	O2'-C2'	2.77	1.49	1.43
4	A	600	GTP	C6-N1	2.47	1.41	1.37
5	B	501	GDP	O4'-C4'	2.23	1.50	1.45
4	A	600	GTP	C8-N7	-2.19	1.31	1.35
4	A	600	GTP	PA-O2A	-2.11	1.45	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	C2'-C3'	2.09	1.59	1.53
5	B	501	GDP	C2-N2	-2.07	1.29	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	600	GTP	PA-O3A-PB	-8.40	104.01	132.83
5	B	501	GDP	PA-O3A-PB	-5.01	115.63	132.83
4	A	600	GTP	O4'-C1'-C2'	4.96	114.17	106.93
5	B	501	GDP	O4'-C4'-C3'	-3.51	98.17	105.11
5	B	501	GDP	O6-C6-C5	3.22	130.66	124.37
5	B	501	GDP	O3'-C3'-C2'	3.08	121.80	111.82
5	B	501	GDP	C2-N1-C6	2.91	130.46	125.10
4	A	600	GTP	PB-O3B-PG	-2.87	122.98	132.83
4	A	600	GTP	O2'-C2'-C3'	2.35	119.41	111.82
4	A	600	GTP	N2-C2-N3	2.34	124.29	119.74
4	A	600	GTP	N2-C2-N1	-2.29	111.83	116.71
4	A	600	GTP	O2G-PG-O3B	2.28	112.28	104.64
5	B	501	GDP	O3B-PB-O3A	2.17	111.91	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

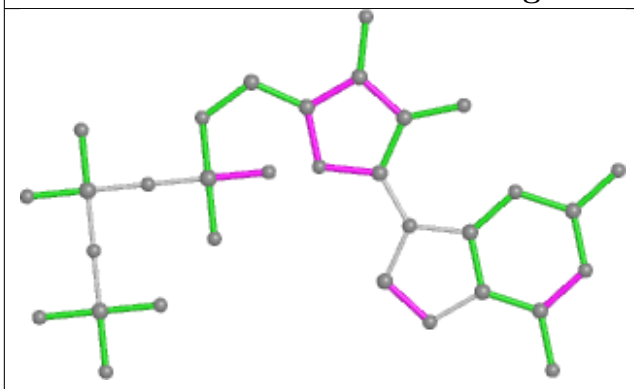
There are no ring outliers.

No monomer is involved in short contacts.

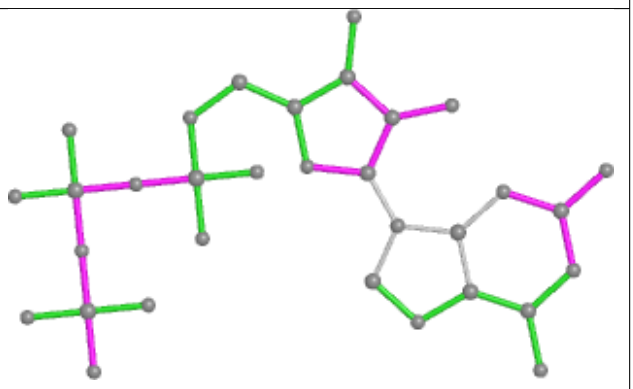
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

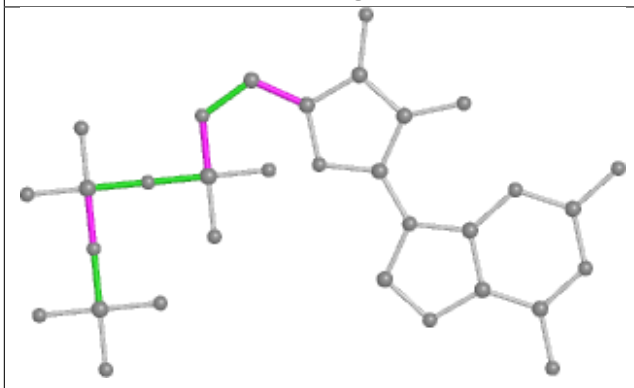
Ligand GTP A 600



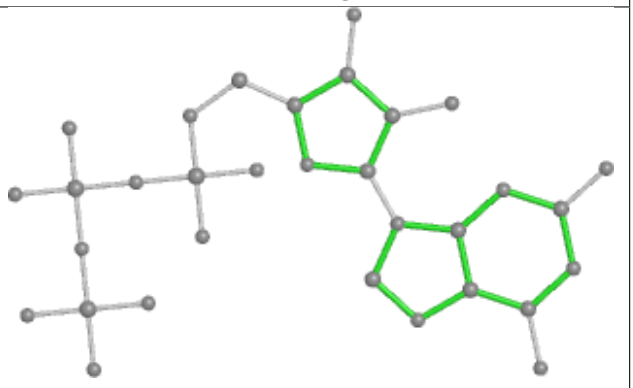
Bond lengths



Bond angles

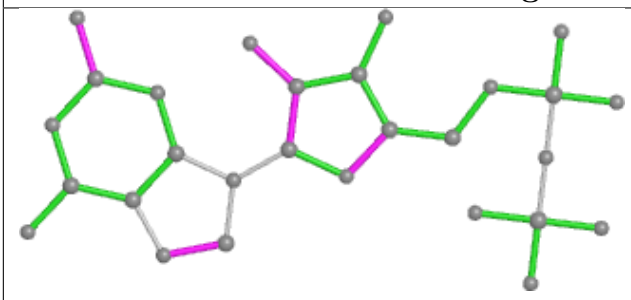


Torsions

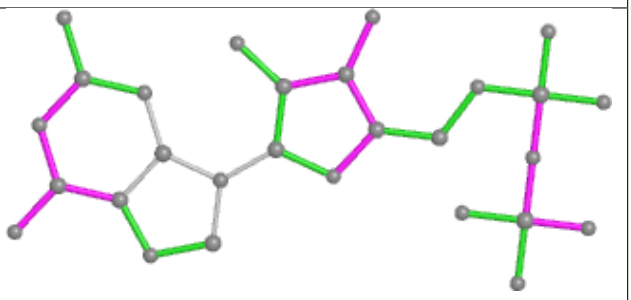


Rings

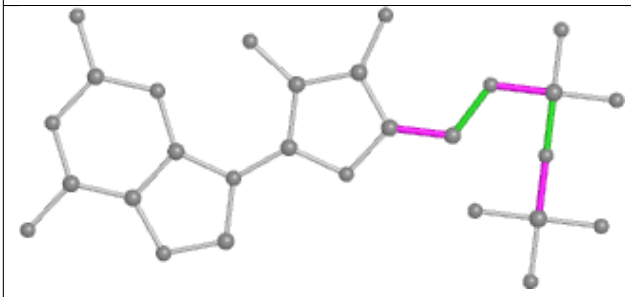
Ligand GDP B 501



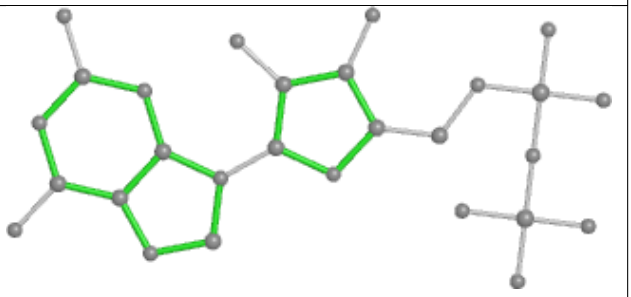
Bond lengths



Bond angles



Torsions



Rings

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.

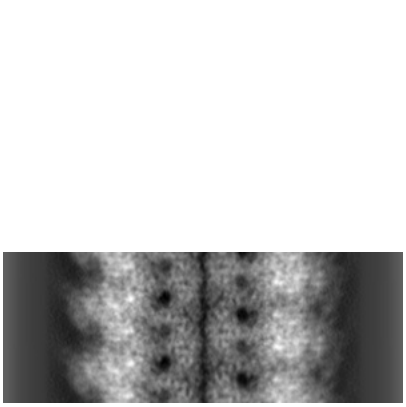
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6187. These allow visual inspection of the internal detail of the map and identification of artifacts.

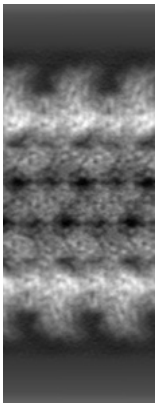
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

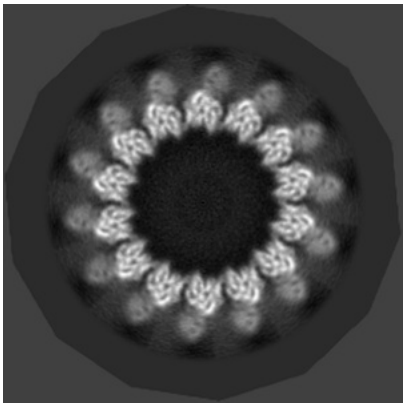
6.1.1 Primary map



X



Y

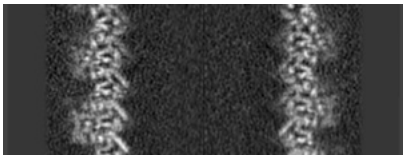


Z

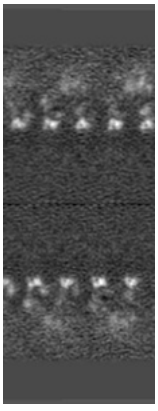
The images above show the map projected in three orthogonal directions.

6.2 Central slices

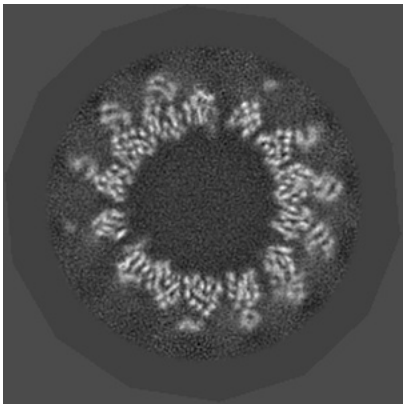
6.2.1 Primary map



X Index: 128



Y Index: 128

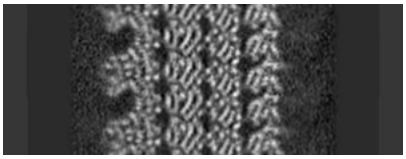


Z Index: 48

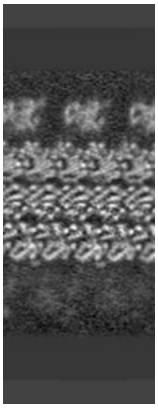
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

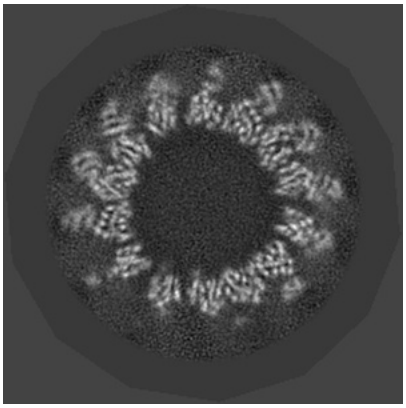
6.3.1 Primary map



X Index: 182



Y Index: 74

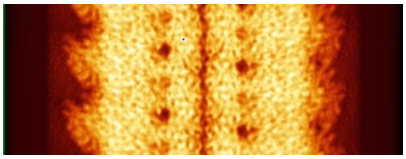


Z Index: 41

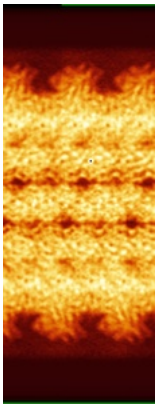
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

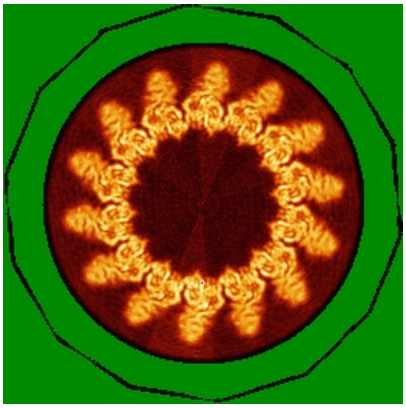
6.4.1 Primary map



X



Y

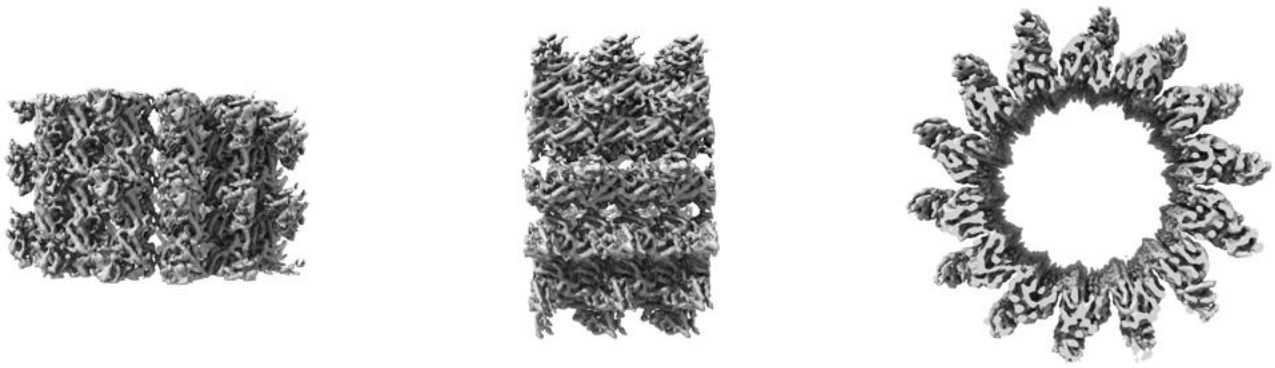


Z

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

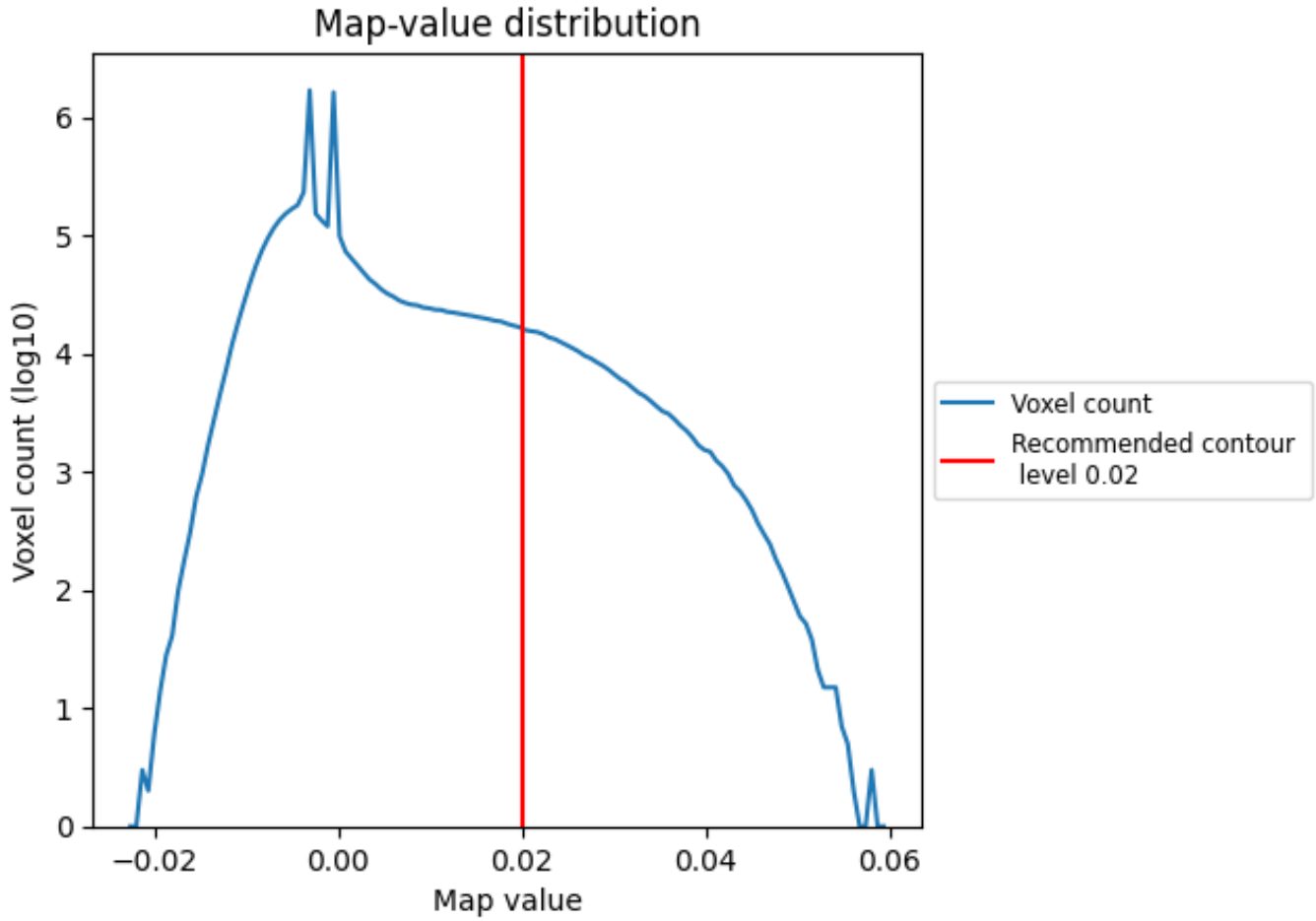
6.6 Mask visualisation (i)

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

7 Map analysis

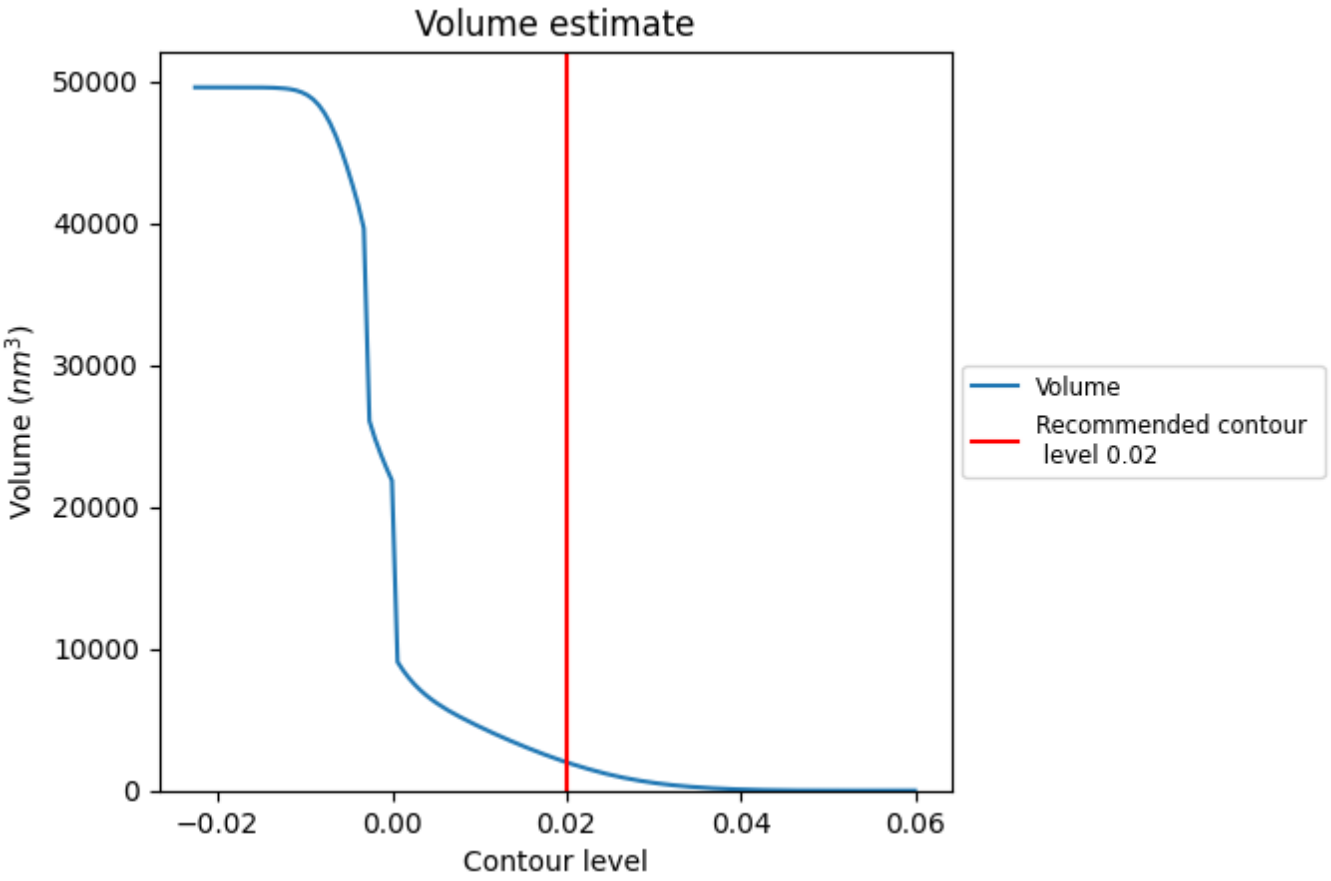
This section contains the results of statistical analysis of the map.

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 1994 nm^3; this corresponds to an approximate mass of 1801 kDa.

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

7.3 Rotationally averaged power spectrum

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

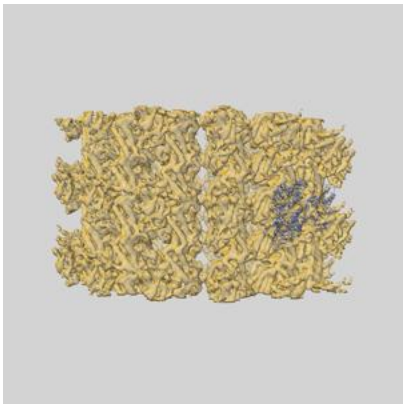
8 Fourier-Shell correlation (i)

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

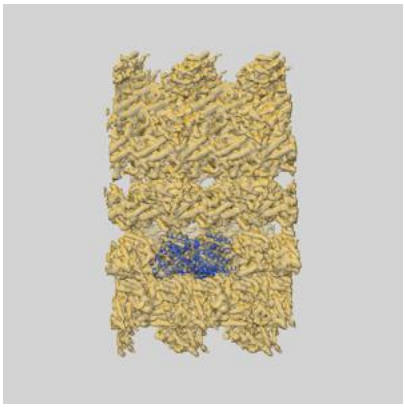
9 Map-model fit

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

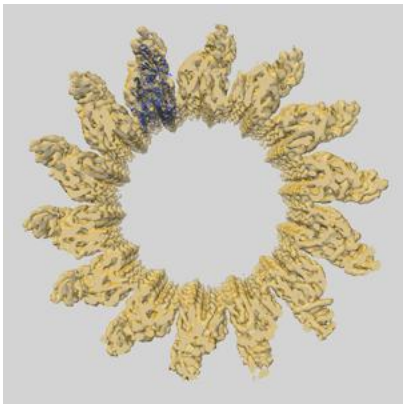
9.1 Map-model overlay



X



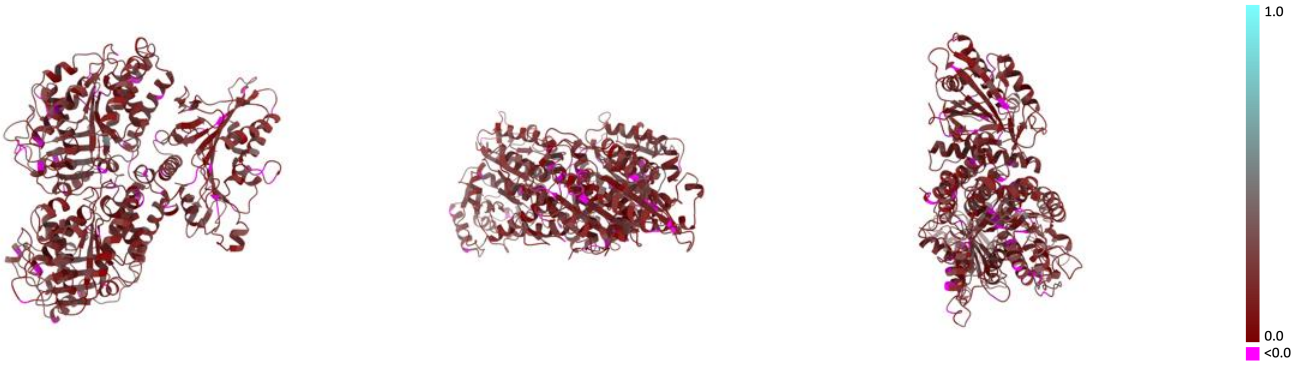
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

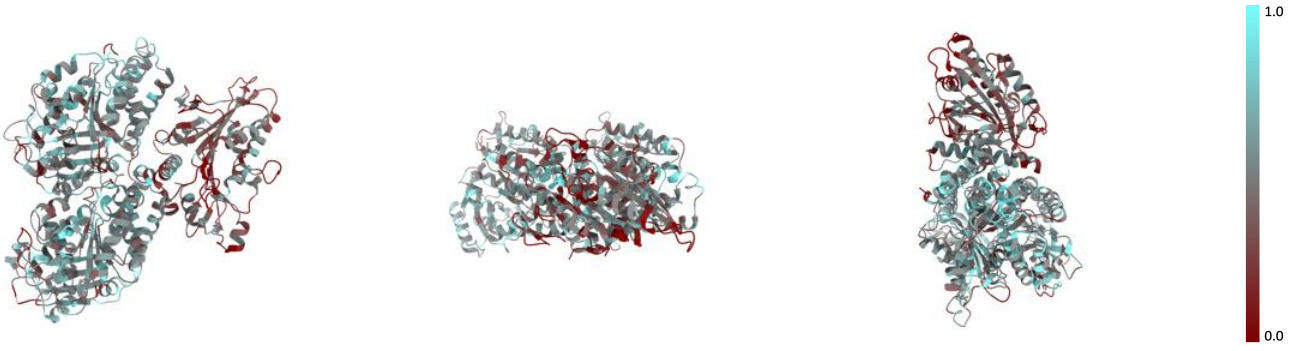
9.2 Q-score mapped to coordinate model (i)



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.

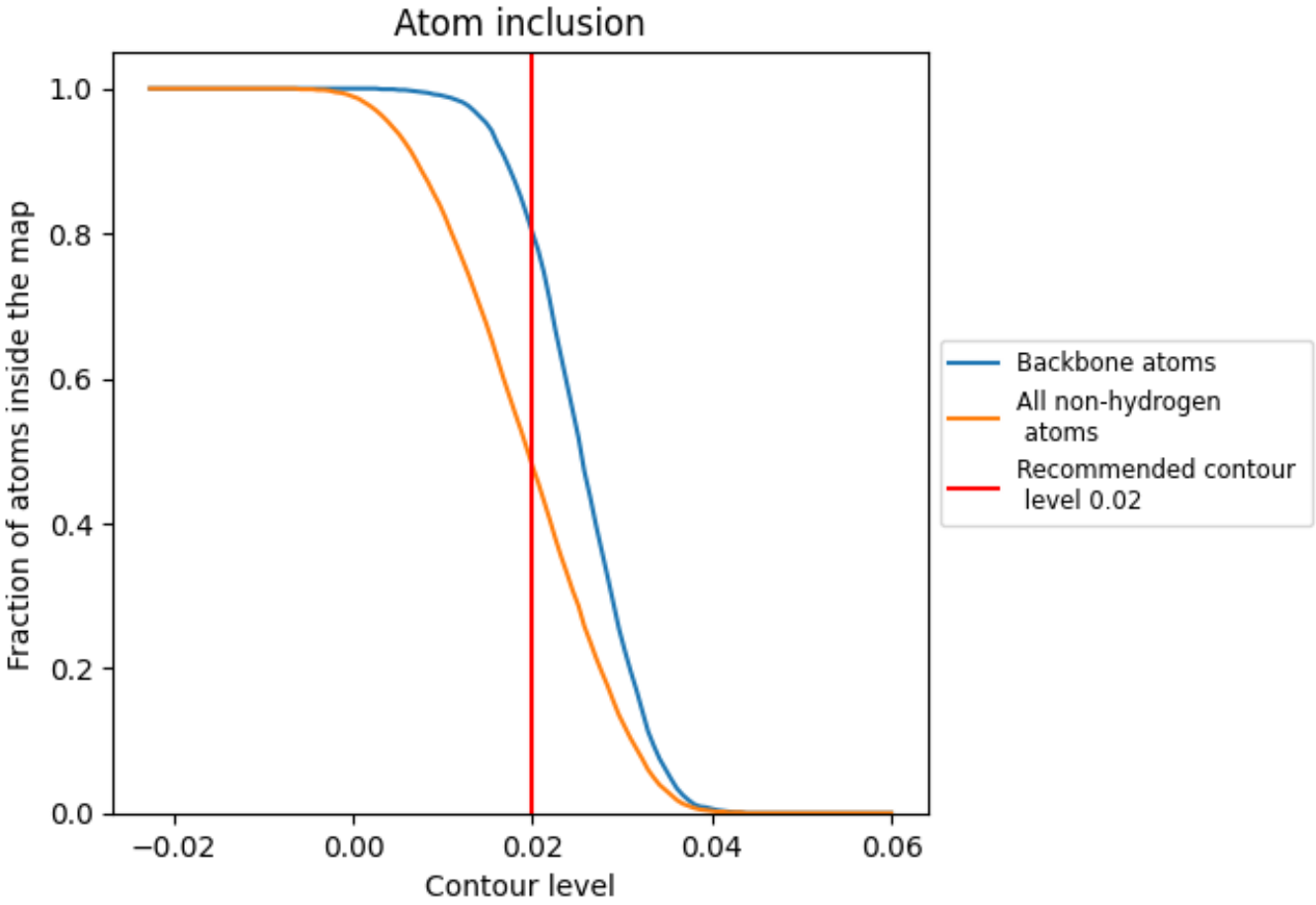
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

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