



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 07:46 AM UTC

PDB ID : 6BNQ / pdb_00006bnq
EMDB ID : EMD-7117
Title : CryoEM structure of Myosin VI-Actin complex in the ADP state
Authors : Gurel, P.G.; Alushin, G.M.
Deposited on : 2017-11-17
Resolution : 5.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

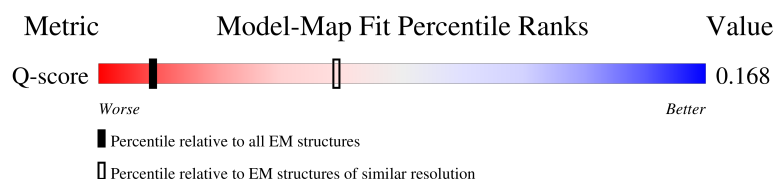
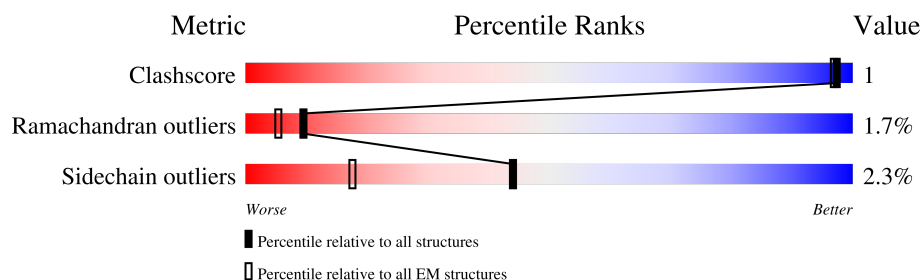
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	520 (5.00 - 6.00)

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

Mol	Chain	Length	Quality of chain
1	I	704	16% 92% 7%
1	J	704	14% 93% 7%
1	K	704	15% 93% 6%
1	L	704	16% 94% 5%

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Mol	Chain	Length	Quality of chain
1	M	704	14% 92% 7%
1	N	704	15% 94% 6%
2	A	373	90% 8% ..
2	B	373	90% 7% ..
2	C	373	90% 8% ..
2	D	373	88% 10% ..
2	E	373	86% 10% ...
2	F	373	87% 11% ..
2	G	373	89% 9% .
2	H	373	85% 10% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 56660 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 Unconventional myosin-VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	701	Total	C	N	O	S	0	0
			5590	3530	972	1063	25		
1	J	701	Total	C	N	O	S	0	0
			5590	3530	972	1063	25		
1	K	701	Total	C	N	O	S	0	0
			5590	3530	972	1063	25		
1	L	701	Total	C	N	O	S	0	0
			5590	3530	972	1063	25		
1	M	701	Total	C	N	O	S	0	0
			5590	3530	972	1063	25		
1	N	701	Total	C	N	O	S	0	0
			5590	3530	972	1063	25		

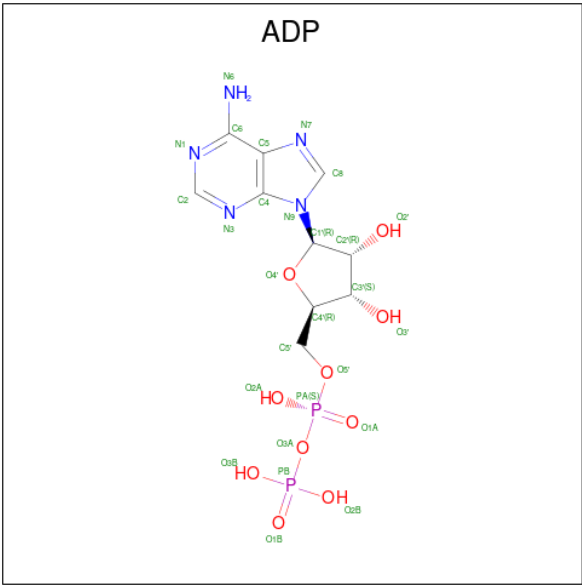
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		
2	B	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		
2	C	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		
2	D	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		
2	E	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		
2	F	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		
2	G	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		
2	H	367	Total	C	N	O	S	0	0
			2862	1812	481	549	20		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	
3	G	1	Total	Mg	0
			1	1	
3	H	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

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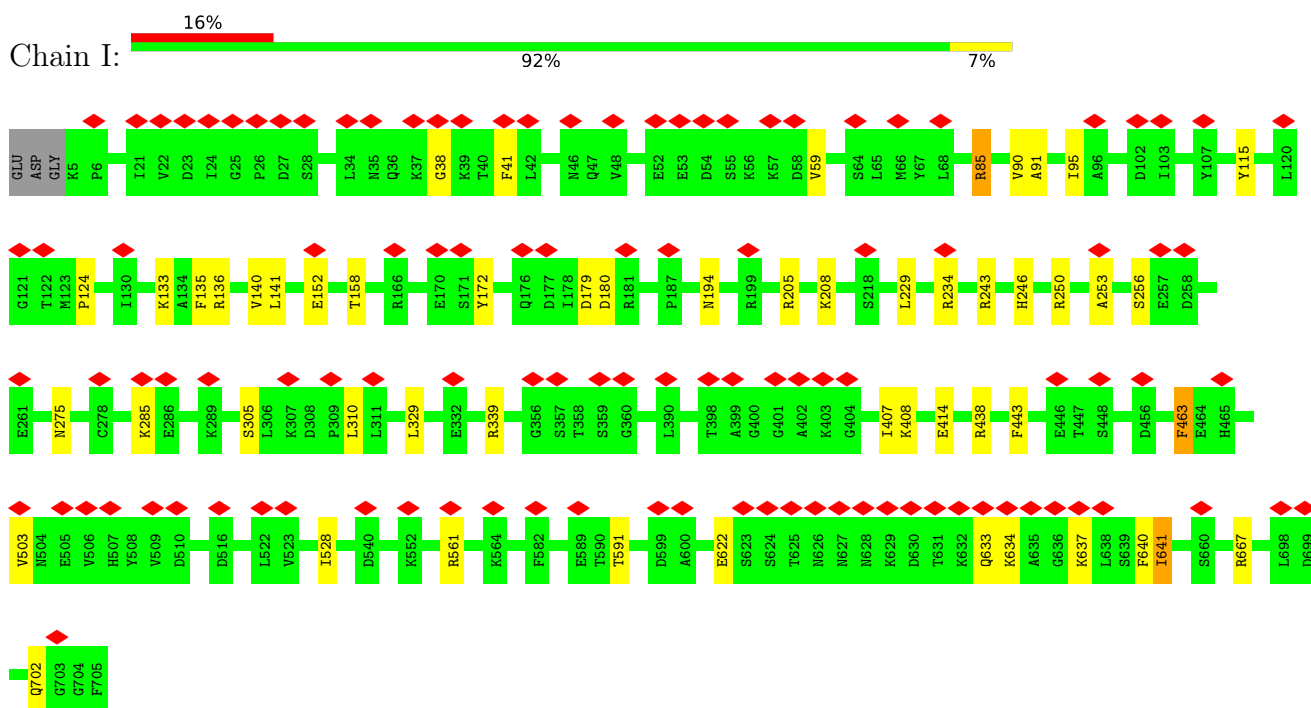
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Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

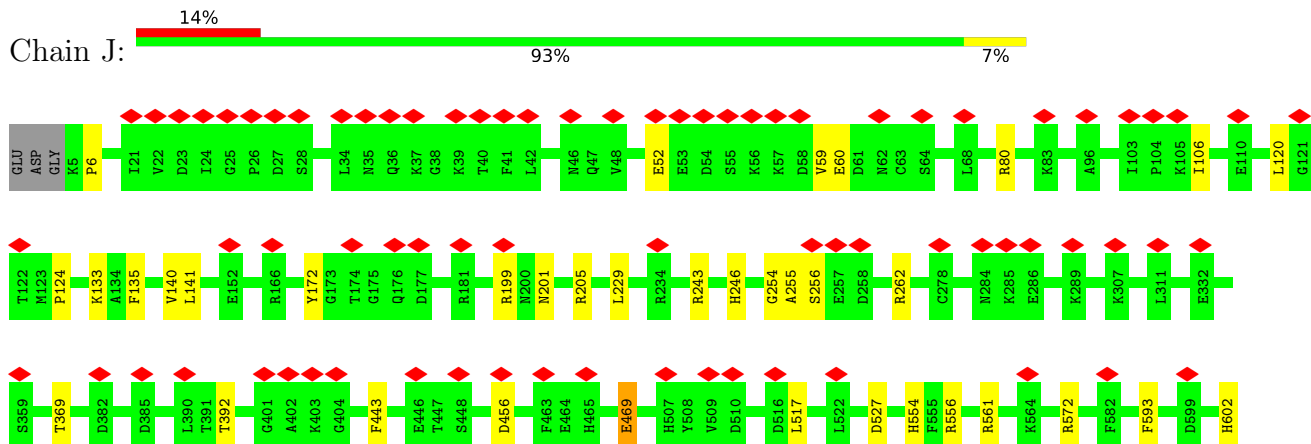
3 Residue-property plots

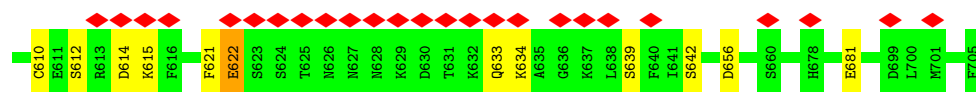
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Unconventional myosin-VI

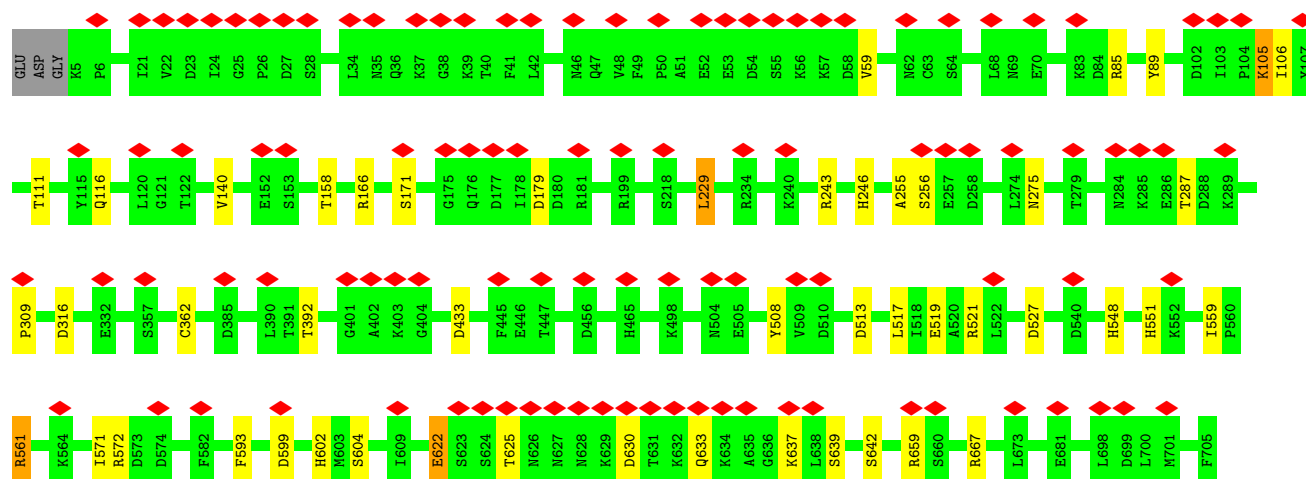
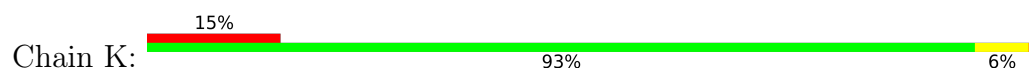


- Molecule 1: Unconventional myosin-VI

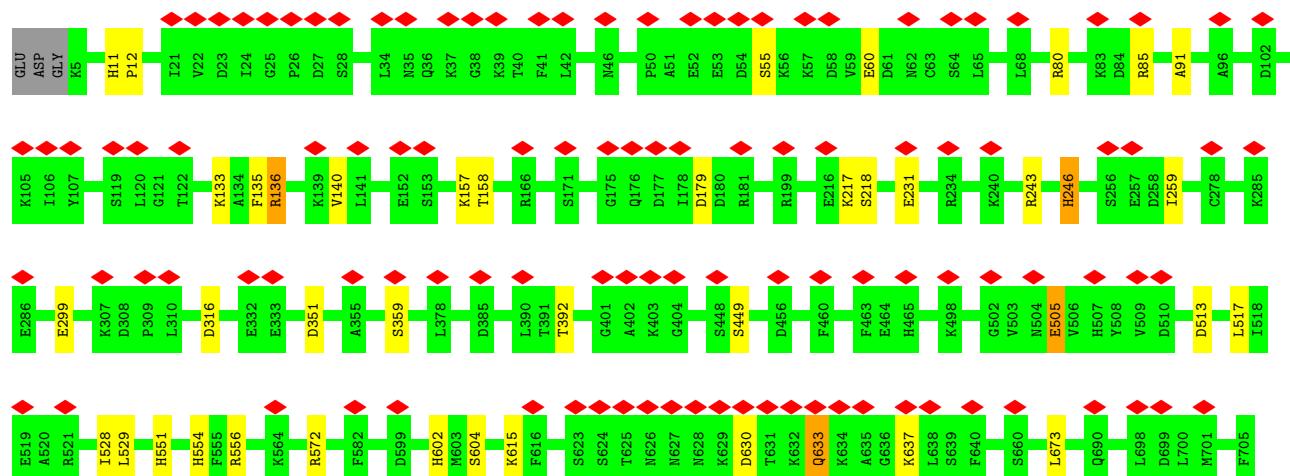
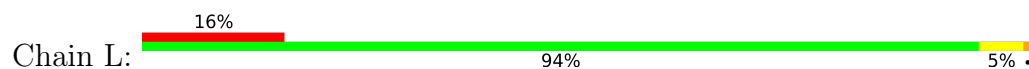




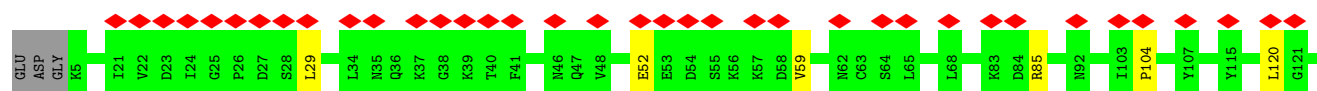
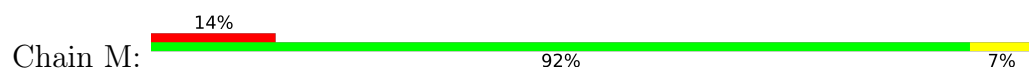
• Molecule 1: Unconventional myosin-VI

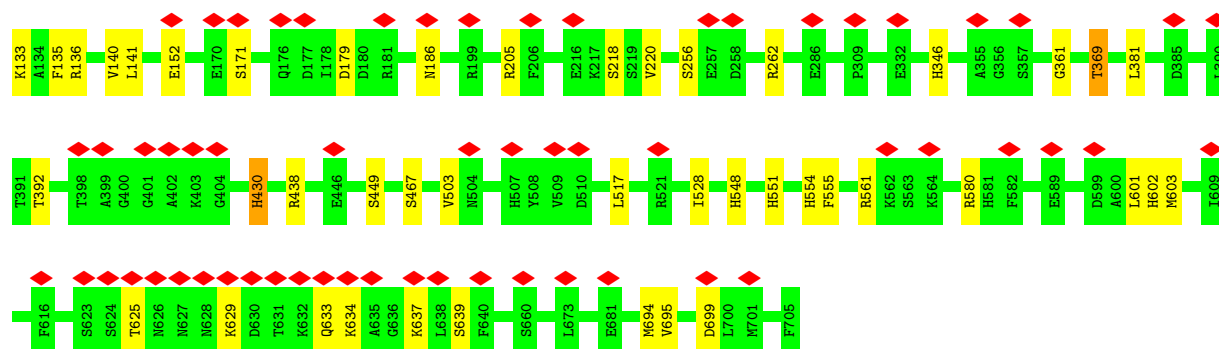


• Molecule 1: Unconventional myosin-VI

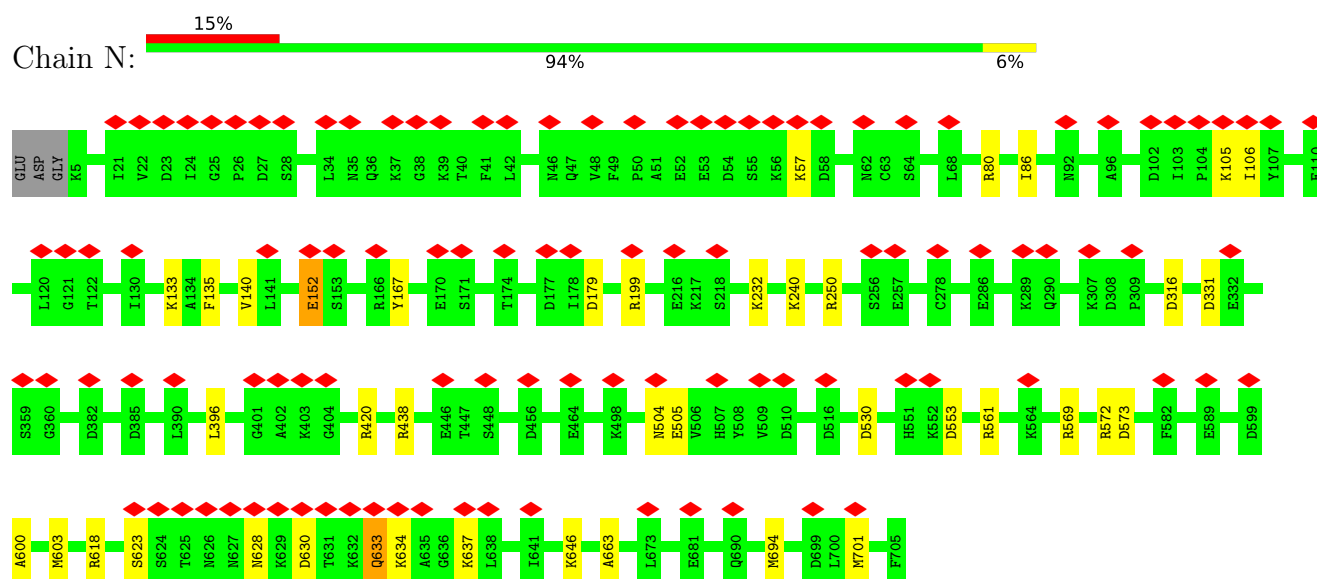


• Molecule 1: Unconventional myosin-VI

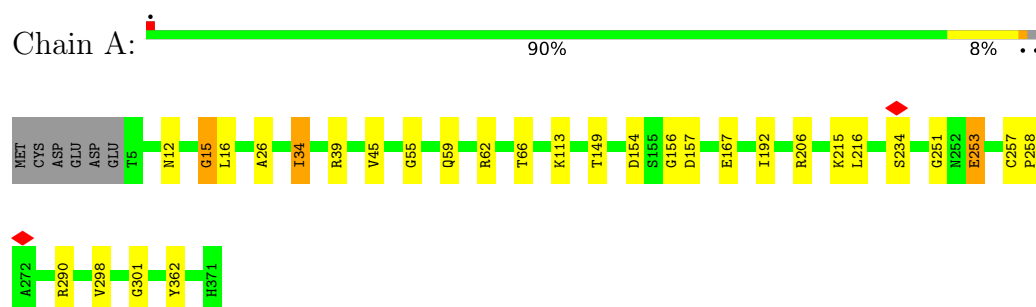




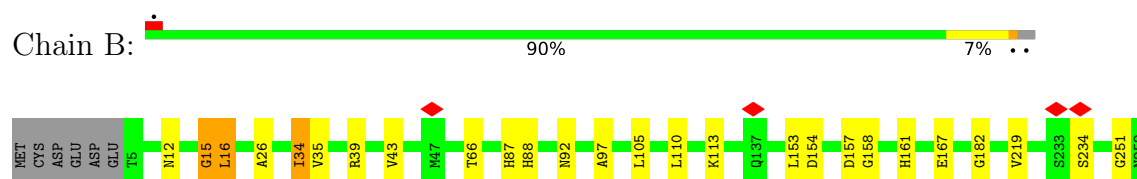
• Molecule 1: Unconventional myosin-VI

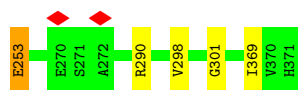


• Molecule 2: Actin, alpha skeletal muscle

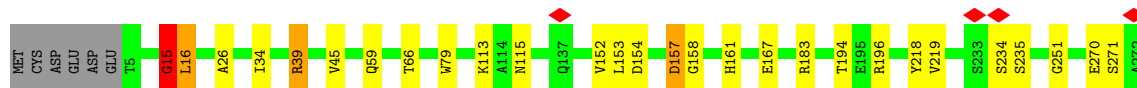
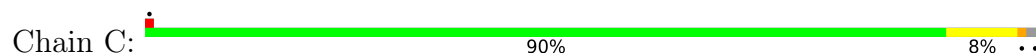


• Molecule 2: Actin, alpha skeletal muscle

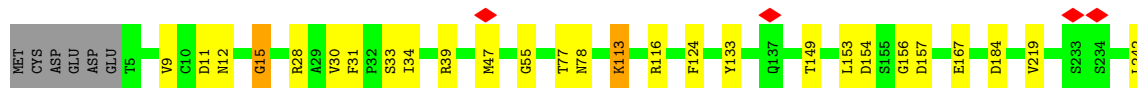
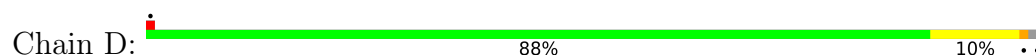




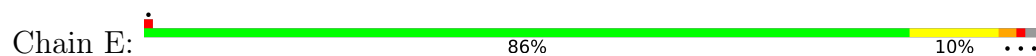
- Molecule 2: Actin, alpha skeletal muscle



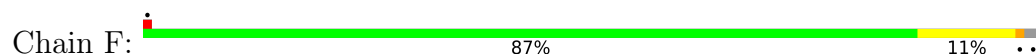
- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle

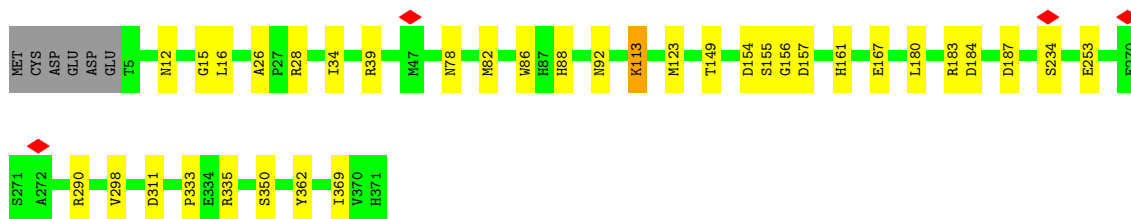


- Molecule 2: Actin, alpha skeletal muscle



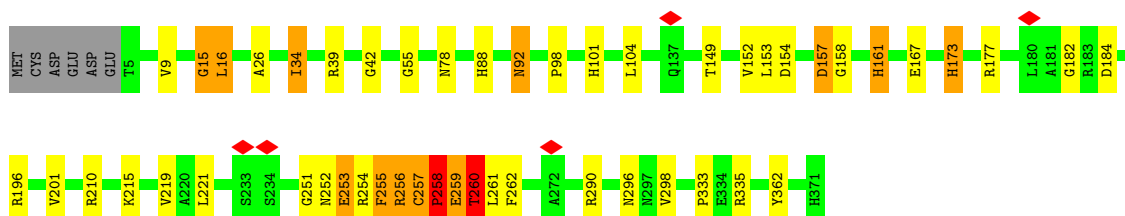
- Molecule 2: Actin, alpha skeletal muscle

Chain G:  89% 9% .



- Molecule 2: Actin, alpha skeletal muscle

Chain H:  85% 10% . . .



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.69°, rise=28.06 Å, axial sym=C1	Depositor
Number of segments used	36114	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	1.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.043	Depositor
Minimum map value	-7.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.8	Depositor
Map size (Å)	650.24, 650.24, 650.24	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	I	0.87	0/5696	1.40	22/7677 (0.3%)
1	J	0.86	0/5696	1.39	18/7677 (0.2%)
1	K	0.87	0/5696	1.40	20/7677 (0.3%)
1	L	0.86	0/5696	1.41	18/7677 (0.2%)
1	M	0.86	0/5696	1.42	19/7677 (0.2%)
1	N	0.87	0/5696	1.38	19/7677 (0.2%)
2	A	0.93	5/2924 (0.2%)	1.58	23/3963 (0.6%)
2	B	0.88	1/2924 (0.0%)	1.55	16/3963 (0.4%)
2	C	0.89	1/2924 (0.0%)	1.54	20/3963 (0.5%)
2	D	0.89	2/2924 (0.1%)	1.58	28/3963 (0.7%)
2	E	0.89	1/2924 (0.0%)	1.59	28/3963 (0.7%)
2	F	0.88	1/2924 (0.0%)	1.54	20/3963 (0.5%)
2	G	0.87	2/2924 (0.1%)	1.54	20/3963 (0.5%)
2	H	1.45	26/2924 (0.9%)	1.86	59/3963 (1.5%)
All	All	0.91	39/57568 (0.1%)	1.48	330/77766 (0.4%)

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	I	0	11
1	J	0	8
1	K	0	7
1	L	0	6
1	M	0	7
1	N	0	12
2	A	0	4
2	B	0	1
2	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	4
2	E	0	7
2	F	0	7
2	G	0	4
2	H	0	6
All	All	0	87

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	257	CYS	N-CA	26.56	1.67	1.46
2	H	260	THR	CA-C	16.81	1.76	1.52
2	H	257	CYS	CA-C	16.59	1.71	1.52
2	H	259	GLU	N-CA	16.55	1.68	1.46
2	H	258	PRO	CA-C	15.82	1.79	1.52
2	H	260	THR	N-CA	13.54	1.63	1.46
2	H	260	THR	C-N	13.54	1.52	1.33
2	H	258	PRO	CA-CB	12.06	1.71	1.53
2	H	259	GLU	CA-CB	11.74	1.74	1.53
2	H	259	GLU	CA-C	11.39	1.68	1.52
2	A	260	THR	N-CA	-11.36	1.31	1.46
2	H	261	LEU	CA-C	-10.38	1.38	1.52
2	H	254	ARG	C-N	10.35	1.48	1.33
2	H	256	ARG	N-CA	-9.63	1.34	1.46
2	H	255	PHE	CA-CB	9.49	1.68	1.53
2	H	259	GLU	C-N	9.38	1.46	1.34
2	H	256	ARG	CA-C	-9.29	1.41	1.52
2	H	261	LEU	CA-CB	9.24	1.69	1.53
2	H	257	CYS	C-O	8.59	1.32	1.24
2	H	261	LEU	N-CA	8.36	1.57	1.46
2	H	260	THR	CA-CB	8.15	1.67	1.53
2	H	256	ARG	C-O	-6.85	1.16	1.24
2	H	260	THR	C-O	6.72	1.32	1.24
2	D	156	GLY	CA-C	-6.39	1.46	1.52
2	D	154	ASP	CA-CB	6.35	1.61	1.53
2	H	154	ASP	CA-CB	6.32	1.61	1.53
2	C	154	ASP	CA-CB	6.17	1.61	1.53
2	A	259	GLU	C-O	6.02	1.31	1.24
2	A	154	ASP	CA-CB	5.90	1.60	1.53
2	A	156	GLY	CA-C	-5.81	1.47	1.52
2	H	255	PHE	C-O	5.80	1.31	1.24
2	B	154	ASP	CA-CB	5.72	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	154	ASP	CA-CB	5.67	1.60	1.53
2	E	154	ASP	CA-CB	5.60	1.60	1.53
2	F	154	ASP	CA-CB	5.57	1.60	1.53
2	A	259	GLU	C-N	-5.39	1.26	1.34
2	G	156	GLY	CA-C	-5.17	1.47	1.52
2	H	252	ASN	C-O	-5.15	1.18	1.24
2	H	253	GLU	CA-CB	5.12	1.62	1.53

All (330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	258	PRO	O-C-N	-25.75	87.28	122.30
2	H	257	CYS	O-C-N	-21.70	103.24	120.38
2	H	258	PRO	CB-CA-C	-19.62	83.03	111.68
2	H	260	THR	O-C-N	-16.18	103.75	122.20
2	H	256	ARG	CA-C-N	-12.87	103.72	120.44
2	H	256	ARG	C-N-CA	-12.87	103.72	120.44
2	H	258	PRO	CA-C-O	12.59	136.62	119.00
2	H	258	PRO	N-CA-C	-12.40	98.36	113.86
2	H	260	THR	CA-C-O	11.64	133.24	120.20
2	H	256	ARG	CA-C-O	-11.46	108.89	120.70
2	A	260	THR	CA-CB-OG1	11.21	126.41	109.60
2	H	255	PHE	CA-CB-CG	-9.14	104.66	113.80
1	I	528	ILE	N-CA-C	-8.92	104.04	112.96
2	H	254	ARG	O-C-N	8.69	131.34	122.12
1	L	528	ILE	N-CA-C	-8.67	104.84	112.12
2	H	258	PRO	N-CA-CB	-8.63	95.23	103.51
2	H	256	ARG	O-C-N	8.60	131.38	122.09
2	H	254	ARG	CB-CA-C	8.53	125.19	110.68
1	L	259	ILE	N-CA-C	-8.53	104.95	112.12
2	H	261	LEU	N-CA-CB	-8.37	96.09	110.32
2	A	260	THR	N-CA-C	8.36	122.45	111.75
2	H	258	PRO	CA-CB-CG	-8.33	88.67	104.50
2	H	259	GLU	CA-C-N	-8.33	108.22	120.38
2	H	259	GLU	C-N-CA	-8.33	108.22	120.38
2	E	15	GLY	CA-C-N	8.23	136.51	121.70
2	E	15	GLY	C-N-CA	8.23	136.51	121.70
2	H	257	CYS	CB-CA-C	-8.18	98.60	113.49
1	I	253	ALA	N-CA-C	8.09	119.73	111.07
1	M	528	ILE	N-CA-C	-8.07	104.89	112.96
2	H	260	THR	CA-CB-OG1	-8.04	97.53	109.60
2	H	15	GLY	CA-C-N	7.89	135.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	15	GLY	C-N-CA	7.89	135.91	121.70
2	H	256	ARG	CA-CB-CG	7.89	129.88	114.10
2	H	256	ARG	N-CA-CB	7.87	121.48	110.07
2	C	15	GLY	CA-C-N	7.85	135.82	121.70
2	C	15	GLY	C-N-CA	7.85	135.82	121.70
2	H	261	LEU	N-CA-C	7.70	121.77	112.38
1	M	699	ASP	N-CA-C	-7.67	105.88	114.62
2	H	255	PHE	CA-C-O	7.66	127.57	119.14
2	H	260	THR	OG1-CB-CG2	-7.47	94.36	109.30
2	B	15	GLY	CA-C-N	7.42	135.06	121.70
2	B	15	GLY	C-N-CA	7.42	135.06	121.70
2	G	298	VAL	N-CA-C	7.32	118.42	107.80
2	D	154	ASP	N-CA-C	-7.10	96.06	108.20
2	F	15	GLY	CA-C-N	7.00	134.30	121.70
2	F	15	GLY	C-N-CA	7.00	134.30	121.70
2	H	252	ASN	O-C-N	-6.96	114.90	122.07
2	B	298	VAL	N-CA-C	6.96	117.89	107.80
1	N	694	MET	N-CA-C	6.89	118.79	111.28
2	A	259	GLU	CA-C-N	6.85	130.38	120.38
2	A	259	GLU	C-N-CA	6.85	130.38	120.38
2	E	298	VAL	N-CA-C	6.75	117.58	107.80
2	H	298	VAL	N-CA-C	6.74	117.57	107.80
1	N	505	GLU	N-CA-C	6.72	119.76	110.35
2	D	154	ASP	CA-CB-CG	6.70	119.30	112.60
2	H	255	PHE	CA-C-N	6.69	129.54	120.44
2	H	255	PHE	C-N-CA	6.69	129.54	120.44
2	D	298	VAL	N-CA-C	6.65	117.45	107.80
2	H	154	ASP	CA-CB-CG	6.65	119.25	112.60
1	J	621	PHE	CA-C-N	6.62	134.19	121.54
1	J	621	PHE	C-N-CA	6.62	134.19	121.54
2	E	153	LEU	N-CA-C	6.62	120.06	107.75
2	G	15	GLY	CA-C-N	6.61	133.60	121.70
2	G	15	GLY	C-N-CA	6.61	133.60	121.70
2	H	39	ARG	N-CA-C	6.61	118.14	111.07
2	H	258	PRO	N-CD-CG	-6.57	93.34	103.20
1	J	369	THR	N-CA-C	-6.51	104.99	113.12
2	F	298	VAL	N-CA-C	6.49	117.20	107.80
2	E	154	ASP	CA-CB-CG	6.47	119.07	112.60
2	B	153	LEU	N-CA-C	6.42	119.70	107.75
1	J	456	ASP	CA-CB-CG	6.42	119.02	112.60
1	N	633	GLN	N-CA-C	6.41	118.34	111.36
2	H	259	GLU	CA-C-O	6.36	127.32	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	517	LEU	N-CA-C	-6.34	104.74	113.18
1	M	517	LEU	N-CA-C	-6.33	104.77	113.18
1	L	135	PHE	N-CA-C	-6.26	106.86	114.75
1	M	135	PHE	N-CA-C	-6.24	107.50	114.62
1	M	555	PHE	N-CA-C	6.24	120.45	112.34
2	C	154	ASP	CA-CB-CG	6.24	118.84	112.60
2	C	298	VAL	N-CA-C	6.24	116.84	107.80
2	A	260	THR	CA-CB-CG2	6.22	121.07	110.50
2	A	154	ASP	N-CA-C	-6.20	97.59	108.20
1	J	106	ILE	N-CA-C	6.14	116.89	110.62
2	H	221	LEU	N-CA-C	-6.14	105.92	113.41
2	H	254	ARG	N-CA-C	6.11	118.72	111.33
2	C	153	LEU	N-CA-C	6.09	119.08	107.75
2	H	215	LYS	N-CA-C	6.08	118.81	111.40
2	G	184	ASP	CA-CB-CG	-6.07	106.53	112.60
2	E	350	SER	O-C-N	-6.05	116.15	123.10
1	I	702	GLN	N-CA-C	6.04	117.66	111.14
1	N	135	PHE	CA-CB-CG	-6.02	107.78	113.80
2	H	257	CYS	CA-C-O	6.02	124.80	119.08
2	F	262	PHE	CA-CB-CG	-6.00	107.80	113.80
2	H	154	ASP	N-CA-C	-5.95	98.03	108.20
2	C	113	LYS	CA-C-N	5.93	132.38	121.70
2	C	113	LYS	C-N-CA	5.93	132.38	121.70
1	J	621	PHE	CA-CB-CG	-5.93	107.87	113.80
2	E	335	ARG	N-CA-C	5.91	119.31	111.75
2	D	31	PHE	N-CA-C	5.90	113.53	108.22
2	D	153	LEU	N-CA-C	5.90	118.72	107.75
2	C	154	ASP	N-CA-C	-5.90	98.11	108.20
2	G	180	LEU	N-CA-C	5.90	117.71	111.28
2	A	215	LYS	N-CA-C	5.88	118.58	111.40
1	K	551	HIS	CA-CB-CG	-5.87	107.93	113.80
1	I	85	ARG	CA-C-N	5.84	128.46	120.46
1	I	85	ARG	C-N-CA	5.84	128.46	120.46
2	D	350	SER	O-C-N	-5.84	116.52	123.06
2	A	15	GLY	CA-C-N	5.83	132.20	121.70
2	A	15	GLY	C-N-CA	5.83	132.20	121.70
2	C	270	GLU	N-CA-C	5.83	117.72	111.36
2	H	153	LEU	N-CA-C	5.81	118.55	107.75
2	E	113	LYS	O-C-N	-5.80	116.40	122.96
1	L	637	LYS	O-C-N	-5.80	116.64	123.25
2	D	55	GLY	CA-C-N	5.78	132.11	121.70
2	D	55	GLY	C-N-CA	5.78	132.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	637	LYS	CA-C-N	5.78	132.10	121.70
1	L	637	LYS	C-N-CA	5.78	132.10	121.70
2	E	43	VAL	N-CA-C	5.78	116.51	110.62
2	F	154	ASP	CA-CB-CG	5.77	118.37	112.60
1	K	158	THR	N-CA-C	-5.75	105.94	113.12
2	A	154	ASP	N-CA-CB	5.74	119.84	110.37
2	D	301	GLY	CA-C-N	5.74	127.51	120.22
2	D	301	GLY	C-N-CA	5.74	127.51	120.22
2	G	311	ASP	CA-CB-CG	5.72	118.32	112.60
2	D	184	ASP	CA-CB-CG	-5.70	106.90	112.60
1	I	135	PHE	N-CA-C	-5.69	107.58	114.75
1	I	158	THR	N-CA-C	-5.68	106.02	113.12
2	E	350	SER	CA-C-N	5.68	131.92	121.70
2	E	350	SER	C-N-CA	5.68	131.92	121.70
1	I	59	VAL	CA-C-N	5.67	127.88	120.28
1	I	59	VAL	C-N-CA	5.67	127.88	120.28
1	I	637	LYS	CA-C-N	5.67	131.90	121.70
1	I	637	LYS	C-N-CA	5.67	131.90	121.70
1	J	615	LYS	N-CA-C	5.65	118.17	111.33
1	K	106	ILE	N-CA-C	5.64	116.42	110.72
1	N	86	ILE	N-CA-C	5.64	116.38	110.62
2	E	152	VAL	N-CA-C	5.63	116.41	108.36
1	I	285	LYS	N-CA-C	5.62	117.41	111.28
1	M	430	HIS	CA-CB-CG	-5.62	108.18	113.80
2	H	259	GLU	N-CA-C	-5.62	106.27	113.01
2	H	152	VAL	N-CA-C	5.61	116.39	108.36
1	N	106	ILE	N-CA-C	5.60	116.38	110.72
1	L	517	LEU	N-CA-C	-5.59	108.24	114.62
2	H	260	THR	CB-CA-C	-5.59	99.61	110.46
1	N	663	ALA	N-CA-C	5.58	118.33	110.23
2	G	167	GLU	CA-C-N	5.58	131.75	121.70
2	G	167	GLU	C-N-CA	5.58	131.75	121.70
2	A	259	GLU	N-CA-C	5.57	119.58	112.34
2	F	180	LEU	N-CA-C	5.57	117.43	111.36
2	H	55	GLY	CA-C-N	5.57	131.72	121.70
2	H	55	GLY	C-N-CA	5.57	131.72	121.70
1	K	517	LEU	N-CA-C	-5.56	106.39	114.12
1	L	231	GLU	CA-C-N	5.56	128.28	120.28
1	L	231	GLU	C-N-CA	5.56	128.28	120.28
2	G	154	ASP	N-CA-C	-5.56	98.70	108.20
2	E	333	PRO	CA-C-N	5.55	132.15	121.54
2	E	333	PRO	C-N-CA	5.55	132.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	215	LYS	N-CA-C	5.55	118.18	111.40
2	F	335	ARG	N-CA-C	5.54	118.84	111.75
2	H	262	PHE	N-CA-CB	-5.53	102.45	110.47
2	C	113	LYS	O-C-N	-5.53	116.49	123.01
2	F	153	LEU	N-CA-C	5.52	118.03	107.75
2	A	262	PHE	CA-CB-CG	-5.52	108.28	113.80
2	E	157	ASP	O-C-N	-5.52	115.25	122.59
2	H	15	GLY	O-C-N	-5.51	115.53	122.70
2	F	301	GLY	CA-C-N	5.50	127.27	120.34
2	F	301	GLY	C-N-CA	5.50	127.27	120.34
2	D	11	ASP	CA-CB-CG	5.50	118.10	112.60
2	G	167	GLU	O-C-N	-5.50	115.28	122.59
1	J	201	ASN	CA-CB-CG	-5.49	107.11	112.60
2	A	55	GLY	CA-C-N	5.48	131.57	121.70
2	A	55	GLY	C-N-CA	5.48	131.57	121.70
1	N	316	ASP	CA-CB-CG	-5.48	107.12	112.60
2	B	167	GLU	O-C-N	-5.47	116.98	123.11
1	L	158	THR	N-CA-C	-5.46	106.30	113.12
2	C	39	ARG	N-CA-C	5.46	119.04	112.93
2	C	115	ASN	N-CA-C	5.46	117.98	111.71
1	N	603	MET	N-CA-C	5.44	117.97	111.71
1	I	641	ILE	CA-C-N	5.44	131.93	121.54
1	I	641	ILE	C-N-CA	5.44	131.93	121.54
2	H	260	THR	N-CA-C	-5.44	104.78	111.75
2	D	77	THR	CA-C-N	5.43	131.91	121.54
2	D	77	THR	C-N-CA	5.43	131.91	121.54
2	C	157	ASP	CA-C-N	5.42	131.46	121.70
2	C	157	ASP	C-N-CA	5.42	131.46	121.70
2	G	157	ASP	CA-C-N	5.42	131.46	121.70
2	G	157	ASP	C-N-CA	5.42	131.46	121.70
2	H	253	GLU	CA-C-O	-5.42	112.28	119.10
1	K	519	GLU	N-CA-C	5.40	117.25	111.36
1	M	369	THR	N-CA-C	-5.40	106.36	113.12
2	C	59	GLN	N-CA-C	-5.40	106.70	113.72
2	E	157	ASP	CA-C-N	5.40	131.41	121.70
2	E	157	ASP	C-N-CA	5.40	131.41	121.70
1	J	622	GLU	N-CA-C	5.39	122.29	110.80
2	D	15	GLY	CA-C-N	5.39	131.41	121.70
2	D	15	GLY	C-N-CA	5.39	131.41	121.70
2	E	25	ASP	N-CA-C	5.39	116.88	110.19
1	K	625	THR	N-CA-C	5.39	116.96	111.14
2	B	154	ASP	N-CA-C	-5.39	98.99	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	215	LYS	N-CA-C	5.39	117.97	111.40
1	K	571	ILE	N-CA-C	5.38	115.99	108.89
2	E	365	ALA	N-CA-C	5.38	117.22	111.36
1	M	637	LYS	CA-C-N	5.37	131.37	121.70
1	M	637	LYS	C-N-CA	5.37	131.37	121.70
2	F	95	ARG	CA-C-N	5.36	128.58	120.75
2	F	95	ARG	C-N-CA	5.36	128.58	120.75
1	K	362	CYS	N-CA-C	5.36	118.05	110.50
2	E	59	GLN	N-CA-C	-5.35	106.76	113.72
2	H	154	ASP	N-CA-CB	5.34	119.18	110.37
2	D	157	ASP	O-C-N	-5.33	116.31	122.87
2	B	43	VAL	N-CA-C	5.32	116.10	110.72
2	A	258	PRO	CB-CA-C	5.32	120.51	112.21
1	M	171	SER	N-CA-C	5.31	117.06	111.28
2	E	154	ASP	OD1-CG-OD2	-5.31	110.16	122.90
2	E	154	ASP	N-CA-CB	5.30	119.12	110.37
1	K	561	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	A	298	VAL	N-CA-C	5.30	115.48	107.80
2	B	34	ILE	N-CA-C	5.30	120.36	109.34
2	H	201	VAL	N-CA-C	5.29	117.71	111.09
2	A	157	ASP	CA-C-N	5.28	131.21	121.70
2	A	157	ASP	C-N-CA	5.28	131.21	121.70
2	A	301	GLY	CA-C-N	5.28	126.92	120.22
2	A	301	GLY	C-N-CA	5.28	126.92	120.22
2	A	59	GLN	N-CA-C	-5.28	106.86	113.72
2	H	157	ASP	O-C-N	-5.27	115.58	122.59
1	I	640	PHE	N-CA-C	5.27	116.70	111.07
2	A	157	ASP	O-C-N	-5.26	116.39	122.87
2	A	34	ILE	N-CA-C	5.26	120.28	109.34
2	C	152	VAL	N-CA-C	5.26	115.88	108.36
2	C	301	GLY	CA-C-N	5.26	126.90	120.22
2	C	301	GLY	C-N-CA	5.26	126.90	120.22
2	B	301	GLY	CA-C-N	5.25	126.71	120.14
2	B	301	GLY	C-N-CA	5.25	126.71	120.14
1	K	89	TYR	CB-CA-C	-5.24	102.70	110.67
1	K	287	THR	CA-C-N	5.24	127.30	120.28
1	K	287	THR	C-N-CA	5.24	127.30	120.28
1	N	623	SER	CA-C-N	5.24	131.12	121.70
1	N	623	SER	C-N-CA	5.24	131.12	121.70
2	D	33	SER	CA-C-N	5.24	127.63	120.35
2	D	33	SER	C-N-CA	5.24	127.63	120.35
2	G	234	SER	N-CA-C	5.23	116.67	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	548	HIS	CA-CB-CG	-5.23	108.57	113.80
2	G	157	ASP	O-C-N	-5.23	116.43	122.87
2	D	113	LYS	CA-C-N	5.23	131.12	121.70
2	D	113	LYS	C-N-CA	5.23	131.12	121.70
2	E	15	GLY	O-C-N	-5.23	115.90	122.70
1	K	572	ARG	CA-C-N	5.22	128.66	120.82
1	K	572	ARG	C-N-CA	5.22	128.66	120.82
2	F	201	VAL	N-CA-C	5.22	115.95	110.62
2	D	30	VAL	N-CA-C	-5.22	100.60	108.12
1	J	254	GLY	CA-C-N	5.22	131.51	121.54
1	J	254	GLY	C-N-CA	5.22	131.51	121.54
1	K	171	SER	N-CA-C	5.22	116.97	111.28
1	J	59	VAL	N-CA-C	5.21	116.23	108.46
1	K	85	ARG	CA-C-N	5.21	129.17	120.62
1	K	85	ARG	C-N-CA	5.21	129.17	120.62
1	J	135	PHE	N-CA-C	-5.21	106.87	113.43
1	M	695	VAL	N-CA-C	5.20	115.41	110.42
1	J	610	CYS	CA-C-N	5.20	127.76	120.28
1	J	610	CYS	C-N-CA	5.20	127.76	120.28
2	E	167	GLU	CA-C-N	5.20	131.05	121.70
2	E	167	GLU	C-N-CA	5.20	131.05	121.70
1	M	59	VAL	CA-C-N	5.19	127.23	120.28
1	M	59	VAL	C-N-CA	5.19	127.23	120.28
1	L	633	GLN	N-CA-C	5.18	116.78	111.03
2	F	179	ASP	CA-C-N	5.17	127.64	120.29
2	F	179	ASP	C-N-CA	5.17	127.64	120.29
2	B	97	ALA	CA-C-N	5.17	124.61	119.24
2	B	97	ALA	C-N-CA	5.17	124.61	119.24
2	G	34	ILE	N-CA-C	5.17	116.90	109.51
1	I	194	ASN	N-CA-CB	5.16	117.60	110.17
1	N	628	ASN	CA-C-N	5.15	128.03	120.71
1	N	628	ASN	C-N-CA	5.15	128.03	120.71
1	I	305	SER	N-CA-C	5.15	117.35	110.35
1	N	232	LYS	CA-C-N	5.15	127.69	120.28
1	N	232	LYS	C-N-CA	5.15	127.69	120.28
1	K	637	LYS	CA-C-N	5.14	130.96	121.70
1	K	637	LYS	C-N-CA	5.14	130.96	121.70
2	H	34	ILE	N-CA-C	5.14	120.03	109.34
2	B	154	ASP	N-CA-CB	5.13	118.84	110.37
2	B	154	ASP	CA-CB-CG	5.13	117.73	112.60
2	D	34	ILE	N-CA-C	5.13	117.89	109.78
1	N	637	LYS	CA-C-N	5.13	130.93	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	637	LYS	C-N-CA	5.13	130.93	121.70
2	F	349	LEU	N-CA-C	5.13	117.65	109.96
1	J	124	PRO	CA-C-N	5.12	125.41	119.93
1	J	124	PRO	C-N-CA	5.12	125.41	119.93
1	K	275	ASN	CA-CB-CG	5.11	117.71	112.60
2	C	15	GLY	O-C-N	-5.11	116.06	122.70
2	H	157	ASP	CA-C-N	5.11	130.89	121.70
2	H	157	ASP	C-N-CA	5.11	130.89	121.70
1	M	467	SER	CA-C-N	5.11	127.54	120.29
1	M	467	SER	C-N-CA	5.11	127.54	120.29
1	I	180	ASP	CA-C-N	5.10	127.11	120.28
1	I	180	ASP	C-N-CA	5.10	127.11	120.28
2	F	350	SER	O-C-N	-5.10	116.67	122.89
2	B	15	GLY	O-C-N	-5.09	116.08	122.70
2	E	113	LYS	CA-C-N	5.09	130.87	121.70
2	E	113	LYS	C-N-CA	5.09	130.87	121.70
2	B	87	HIS	CA-CB-CG	5.08	118.88	113.80
1	L	217	LYS	CA-C-N	5.08	131.24	121.54
1	L	217	LYS	C-N-CA	5.08	131.24	121.54
1	M	85	ARG	CA-C-N	5.08	128.95	120.62
1	M	85	ARG	C-N-CA	5.08	128.95	120.62
1	M	262	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	F	13	GLY	CA-C-N	5.07	127.49	120.29
2	F	13	GLY	C-N-CA	5.07	127.49	120.29
1	I	463	PHE	CA-C-N	5.07	127.07	120.28
1	I	463	PHE	C-N-CA	5.07	127.07	120.28
1	L	551	HIS	CA-CB-CG	-5.06	108.74	113.80
2	G	155	SER	CA-C-N	5.06	125.93	121.58
2	G	155	SER	C-N-CA	5.06	125.93	121.58
2	D	157	ASP	CA-C-N	5.05	130.79	121.70
2	D	157	ASP	C-N-CA	5.05	130.79	121.70
2	G	113	LYS	O-C-N	-5.05	116.90	122.86
2	D	286	ASP	CA-C-N	5.05	127.11	120.60
2	D	286	ASP	C-N-CA	5.05	127.11	120.60
1	N	504	ASN	N-CA-C	5.04	117.21	110.35
1	I	124	PRO	N-CA-C	5.04	116.85	110.70
1	L	316	ASP	CA-CB-CG	-5.04	107.56	112.60
2	G	335	ARG	N-CA-C	5.04	118.20	111.75
2	D	154	ASP	OD1-CG-OD2	-5.04	110.81	122.90
1	N	623	SER	O-C-N	-5.04	116.92	122.86
1	L	673	LEU	CA-C-N	5.03	127.01	120.28
1	L	673	LEU	C-N-CA	5.03	127.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	154	ASP	OD1-CG-OD2	-5.03	110.84	122.90
2	C	113	LYS	N-CA-C	-5.02	102.27	110.20
2	G	350	SER	O-C-N	-5.02	117.29	122.96
2	H	296	ASN	CA-CB-CG	-5.02	107.58	112.60
1	L	246	HIS	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (87) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	206	ARG	Sidechain
2	A	290	ARG	Sidechain
2	A	362	TYR	Sidechain
2	A	62	ARG	Sidechain
2	B	290	ARG	Sidechain
2	C	196	ARG	Sidechain
2	C	218	TYR	Sidechain
2	C	312	ARG	Sidechain
2	D	133	TYR	Sidechain
2	D	28	ARG	Sidechain
2	D	290	ARG	Sidechain
2	D	362	TYR	Sidechain
2	E	169	TYR	Sidechain
2	E	183	ARG	Sidechain
2	E	196	ARG	Sidechain
2	E	210	ARG	Sidechain
2	E	28	ARG	Sidechain
2	E	290	ARG	Sidechain
2	E	362	TYR	Sidechain
2	F	147	ARG	Sidechain
2	F	206	ARG	Sidechain
2	F	210	ARG	Sidechain
2	F	254	ARG	Sidechain
2	F	290	ARG	Sidechain
2	F	312	ARG	Sidechain
2	F	362	TYR	Sidechain
2	G	183	ARG	Sidechain
2	G	28	ARG	Sidechain
2	G	290	ARG	Sidechain
2	G	362	TYR	Sidechain
2	H	196	ARG	Sidechain
2	H	210	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	H	256	ARG	Sidechain
2	H	290	ARG	Sidechain
2	H	335	ARG	Sidechain
2	H	362	TYR	Sidechain
1	I	172	TYR	Sidechain
1	I	179	ASP	Peptide
1	I	205	ARG	Sidechain
1	I	234	ARG	Sidechain
1	I	250	ARG	Sidechain
1	I	339	ARG	Sidechain
1	I	438	ARG	Sidechain
1	I	561	ARG	Sidechain
1	I	633	GLN	Peptide
1	I	667	ARG	Sidechain
1	I	85	ARG	Sidechain
1	J	172	TYR	Sidechain
1	J	199	ARG	Sidechain
1	J	205	ARG	Sidechain
1	J	262	ARG	Sidechain
1	J	556	ARG	Sidechain
1	J	561	ARG	Sidechain
1	J	572	ARG	Sidechain
1	J	633	GLN	Peptide
1	K	166	ARG	Sidechain
1	K	179	ASP	Peptide
1	K	508	TYR	Sidechain
1	K	521	ARG	Sidechain
1	K	633	GLN	Peptide
1	K	659	ARG	Sidechain
1	K	667	ARG	Sidechain
1	L	136	ARG	Sidechain
1	L	179	ASP	Peptide
1	L	556	ARG	Sidechain
1	L	572	ARG	Sidechain
1	L	633	GLN	Peptide
1	L	85	ARG	Sidechain
1	M	136	ARG	Sidechain
1	M	179	ASP	Peptide
1	M	205	ARG	Sidechain
1	M	438	ARG	Sidechain
1	M	561	ARG	Sidechain
1	M	580	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	633	GLN	Peptide
1	N	167	TYR	Sidechain
1	N	179	ASP	Peptide
1	N	199	ARG	Sidechain
1	N	250	ARG	Sidechain
1	N	420	ARG	Sidechain
1	N	438	ARG	Sidechain
1	N	561	ARG	Sidechain
1	N	569	ARG	Sidechain
1	N	572	ARG	Sidechain
1	N	618	ARG	Sidechain
1	N	633	GLN	Peptide
1	N	80	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	5590	0	5536	4	0
1	J	5590	0	5536	4	0
1	K	5590	0	5536	3	0
1	L	5590	0	5536	6	0
1	M	5590	0	5536	5	0
1	N	5590	0	5536	1	0
2	A	2862	0	2831	2	0
2	B	2862	0	2831	4	0
2	C	2862	0	2831	2	0
2	D	2862	0	2831	3	0
2	E	2862	0	2831	6	0
2	F	2862	0	2831	4	0
2	G	2862	0	2831	3	0
2	H	2862	0	2831	22	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
4	G	27	0	12	0	0
4	H	27	0	12	0	0
All	All	56660	0	55960	69	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 1.

All (69) 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:H:258:PRO:C	2:H:258:PRO:CA	1.79	1.55
2:H:260:THR:CA	2:H:260:THR:C	1.76	1.55
2:H:259:GLU:N	2:H:259:GLU:CA	1.68	1.53
2:H:258:PRO:C	2:H:258:PRO:CB	2.32	1.02
2:H:258:PRO:O	2:H:259:GLU:CA	2.11	0.97
2:H:260:THR:C	2:H:260:THR:CB	2.62	0.73
2:H:258:PRO:C	2:H:259:GLU:CA	2.59	0.72
2:H:258:PRO:C	2:H:258:PRO:N	2.47	0.69
2:H:258:PRO:C	2:H:258:PRO:HB2	2.19	0.67
2:H:255:PHE:O	2:H:259:GLU:HB2	1.98	0.63
2:B:88:HIS:CD2	2:B:92:ASN:HD21	2.22	0.58
2:H:259:GLU:N	2:H:259:GLU:CB	2.68	0.56
2:F:158:GLY:HA2	2:F:182:GLY:H	1.70	0.55
2:H:158:GLY:HA2	2:H:182:GLY:H	1.72	0.55
2:B:158:GLY:HA2	2:B:182:GLY:H	1.72	0.54
2:H:259:GLU:O	2:H:260:THR:C	2.51	0.53
1:M:29:LEU:H	1:M:29:LEU:HD23	1.73	0.53
2:B:253:GLU:H	2:B:253:GLU:CD	2.19	0.51
2:E:88:HIS:CD2	2:E:92:ASN:HD21	2.28	0.51
1:L:243:ARG:HH21	1:L:246:HIS:CD2	2.29	0.50
1:I:243:ARG:HH21	1:I:246:HIS:CD2	2.30	0.49
2:G:253:GLU:H	2:G:253:GLU:CD	2.20	0.49
2:C:158:GLY:HA2	2:C:183:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:88:HIS:CD2	2:G:92:ASN:HD21	2.32	0.48
2:E:154:ASP:HB3	2:E:161:HIS:CE1	2.48	0.48
2:H:260:THR:C	2:H:260:THR:N	2.68	0.48
1:M:392:THR:O	1:M:602:HIS:CE1	2.67	0.47
1:I:407:ILE:HG22	1:I:408:LYS:H	1.79	0.47
2:A:192:ILE:HD11	2:A:257:CYS:HB2	1.97	0.47
2:D:253:GLU:H	2:D:253:GLU:CD	2.24	0.46
2:H:161:HIS:CE1	2:H:177:ARG:HB2	2.50	0.46
2:H:258:PRO:O	2:H:259:GLU:C	2.59	0.46
2:H:259:GLU:N	2:H:259:GLU:C	2.69	0.46
2:E:15:GLY:HA3	2:E:16:LEU:HB2	1.97	0.46
2:H:173:HIS:CD2	2:H:173:HIS:H	2.31	0.46
1:J:60:GLU:CD	1:J:80:ARG:HH12	2.24	0.46
2:H:15:GLY:HA3	2:H:16:LEU:HB2	1.98	0.46
2:D:116:ARG:HB3	2:D:371:HIS:CE1	2.51	0.45
2:F:88:HIS:CD2	2:F:92:ASN:HD21	2.34	0.45
2:E:253:GLU:CD	2:E:253:GLU:H	2.26	0.44
2:A:253:GLU:H	2:A:253:GLU:CD	2.25	0.44
2:F:253:GLU:H	2:F:253:GLU:CD	2.26	0.43
1:L:11:HIS:CD2	1:L:12:PRO:HD2	2.53	0.43
1:L:60:GLU:CD	1:L:80:ARG:HH12	2.26	0.43
1:J:469:GLU:H	1:J:469:GLU:CD	2.25	0.43
2:H:88:HIS:CE1	2:H:92:ASN:HD21	2.37	0.43
1:L:392:THR:O	1:L:602:HIS:CE1	2.72	0.43
1:J:243:ARG:HH21	1:J:246:HIS:CD2	2.36	0.43
1:I:90:VAL:HG21	1:I:95:ILE:HD12	2.00	0.42
1:I:141:LEU:H	1:I:141:LEU:HD23	1.83	0.42
1:J:392:THR:O	1:J:602:HIS:CE1	2.72	0.42
1:M:141:LEU:H	1:M:141:LEU:HD23	1.84	0.42
2:H:257:CYS:HB3	2:H:258:PRO:HD3	1.99	0.42
1:K:392:THR:O	1:K:602:HIS:CE1	2.73	0.42
1:L:602:HIS:CE1	1:L:604:SER:HB3	2.55	0.42
1:M:430:HIS:CE1	1:M:625:THR:HG21	2.55	0.42
2:E:219:VAL:HG23	2:E:308:GLY:H	1.86	0.41
2:B:110:LEU:H	2:B:161:HIS:CE1	2.38	0.41
2:E:158:GLY:HA2	2:E:182:GLY:H	1.85	0.41
1:K:548:HIS:CE1	1:K:559:ILE:HG22	2.56	0.41
2:D:113:LYS:HG3	2:D:371:HIS:CD2	2.56	0.41
1:M:551:HIS:CE1	1:M:554:HIS:H	2.39	0.41
2:H:98:PRO:HA	2:H:101:HIS:CE1	2.56	0.41
1:L:505:GLU:H	1:L:505:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:GLN:CD	2:F:41:GLN:H	2.29	0.41
1:K:243:ARG:HH21	1:K:246:HIS:CD2	2.39	0.40
2:G:82:MET:HE2	2:G:86:TRP:HE1	1.85	0.40
1:N:701:MET:HA	1:N:701:MET:HE2	2.04	0.40
2:C:15:GLY:HA3	2:C:16:LEU:HB2	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	I	699/704 (99%)	641 (92%)	49 (7%)	9 (1%)	9	41
1	J	699/704 (99%)	631 (90%)	56 (8%)	12 (2%)	7	35
1	K	699/704 (99%)	636 (91%)	53 (8%)	10 (1%)	9	39
1	L	699/704 (99%)	639 (91%)	52 (7%)	8 (1%)	11	45
1	M	699/704 (99%)	634 (91%)	56 (8%)	9 (1%)	9	41
1	N	699/704 (99%)	633 (91%)	60 (9%)	6 (1%)	14	50
2	A	365/373 (98%)	325 (89%)	33 (9%)	7 (2%)	6	31
2	B	365/373 (98%)	326 (89%)	32 (9%)	7 (2%)	6	31
2	C	365/373 (98%)	327 (90%)	27 (7%)	11 (3%)	3	22
2	D	365/373 (98%)	326 (89%)	32 (9%)	7 (2%)	6	31
2	E	365/373 (98%)	325 (89%)	27 (7%)	13 (4%)	2	20
2	F	365/373 (98%)	319 (87%)	39 (11%)	7 (2%)	6	31
2	G	365/373 (98%)	331 (91%)	29 (8%)	5 (1%)	9	39
2	H	365/373 (98%)	325 (89%)	32 (9%)	8 (2%)	5	28
All	All	7114/7208 (99%)	6418 (90%)	577 (8%)	119 (2%)	9	35

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	634	LYS
1	J	255	ALA
1	J	256	SER
1	J	622	GLU
1	J	634	LYS
1	K	105	LYS
1	L	218	SER
1	M	218	SER
1	N	152	GLU
1	N	600	ALA
2	A	45	VAL
2	B	26	ALA
2	C	271	SER
2	D	271	SER
2	E	334	GLU
2	F	334	GLU
1	I	503	VAL
1	J	120	LEU
1	J	554	HIS
1	K	255	ALA
1	K	256	SER
1	L	554	HIS
1	L	630	ASP
1	M	449	SER
1	N	105	LYS
1	N	634	LYS
2	A	234	SER
2	C	167	GLU
2	D	333	PRO
2	D	369	ILE
2	E	16	LEU
2	E	33	SER
2	E	167	GLU
2	E	234	SER
2	E	251	GLY
2	F	15	GLY
2	F	16	LEU
2	F	167	GLU
2	F	234	SER
2	G	78	ASN
2	H	16	LEU
2	H	167	GLU

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Mol	Chain	Res	Type
1	I	256	SER
1	I	622	GLU
1	J	6	PRO
1	J	642	SER
1	M	256	SER
2	A	15	GLY
2	A	167	GLU
2	B	15	GLY
2	B	234	SER
2	C	16	LEU
2	C	45	VAL
2	D	15	GLY
2	D	78	ASN
2	D	167	GLU
2	E	15	GLY
2	E	44	MET
2	F	369	ILE
2	H	42	GLY
2	H	78	ASN
2	H	333	PRO
1	I	91	ALA
1	I	591	THR
1	J	612	SER
1	J	639	SER
1	K	116	GLN
1	K	229	LEU
1	K	639	SER
1	K	642	SER
1	L	55	SER
1	L	91	ALA
1	L	449	SER
1	M	120	LEU
1	N	240	LYS
2	A	34	ILE
2	C	234	SER
2	C	235	SER
2	C	295	ALA
2	E	26	ALA
2	E	295	ALA
2	G	16	LEU
2	G	369	ILE
1	I	641	ILE

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Mol	Chain	Res	Type
1	J	52	GLU
1	K	622	GLU
1	L	359	SER
1	M	503	VAL
1	M	634	LYS
1	N	140	VAL
2	A	26	ALA
2	A	251	GLY
2	B	16	LEU
2	B	34	ILE
2	C	26	ALA
2	C	369	ILE
2	D	47	MET
2	E	367	PRO
2	H	26	ALA
2	H	34	ILE
1	I	140	VAL
1	J	140	VAL
1	K	140	VAL
1	L	140	VAL
1	M	140	VAL
1	M	361	GLY
1	M	639	SER
2	B	251	GLY
2	B	369	ILE
2	F	251	GLY
1	K	309	PRO
2	C	15	GLY
2	E	34	ILE
2	H	251	GLY
2	C	251	GLY
2	E	369	ILE
2	G	333	PRO
1	I	38	GLY
2	G	26	ALA

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	619/621 (100%)	606 (98%)	13 (2%)	47	65
1	J	619/621 (100%)	609 (98%)	10 (2%)	55	69
1	K	619/621 (100%)	605 (98%)	14 (2%)	44	63
1	L	619/621 (100%)	610 (98%)	9 (2%)	57	71
1	M	619/621 (100%)	606 (98%)	13 (2%)	47	65
1	N	619/621 (100%)	609 (98%)	10 (2%)	55	69
2	A	310/316 (98%)	301 (97%)	9 (3%)	37	57
2	B	310/316 (98%)	300 (97%)	10 (3%)	34	55
2	C	310/316 (98%)	302 (97%)	8 (3%)	40	61
2	D	310/316 (98%)	303 (98%)	7 (2%)	44	63
2	E	310/316 (98%)	301 (97%)	9 (3%)	37	57
2	F	310/316 (98%)	299 (96%)	11 (4%)	32	53
2	G	310/316 (98%)	303 (98%)	7 (2%)	44	63
2	H	310/316 (98%)	298 (96%)	12 (4%)	28	49
All	All	6194/6254 (99%)	6052 (98%)	142 (2%)	44	63

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	41	PHE
1	I	115	TYR
1	I	133	LYS
1	I	136	ARG
1	I	152	GLU
1	I	208	LYS
1	I	229	LEU
1	I	275	ASN
1	I	310	LEU
1	I	329	LEU
1	I	414	GLU
1	I	443	PHE
1	I	463	PHE
1	J	133	LYS
1	J	141	LEU
1	J	229	LEU
1	J	443	PHE

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Mol	Chain	Res	Type
1	J	469	GLU
1	J	527	ASP
1	J	593	PHE
1	J	614	ASP
1	J	656	ASP
1	J	681	GLU
1	K	59	VAL
1	K	105	LYS
1	K	111	THR
1	K	229	LEU
1	K	316	ASP
1	K	433	ASP
1	K	513	ASP
1	K	527	ASP
1	K	561	ARG
1	K	593	PHE
1	K	599	ASP
1	K	604	SER
1	K	622	GLU
1	K	630	ASP
1	L	133	LYS
1	L	136	ARG
1	L	157	LYS
1	L	299	GLU
1	L	351	ASP
1	L	505	GLU
1	L	513	ASP
1	L	529	LEU
1	L	615	LYS
1	M	52	GLU
1	M	104	PRO
1	M	133	LYS
1	M	152	GLU
1	M	186	ASN
1	M	220	VAL
1	M	346	HIS
1	M	369	THR
1	M	381	LEU
1	M	601	LEU
1	M	603	MET
1	M	629	LYS
1	M	694	MET

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Mol	Chain	Res	Type
1	N	57	LYS
1	N	133	LYS
1	N	152	GLU
1	N	331	ASP
1	N	396	LEU
1	N	530	ASP
1	N	553	ASP
1	N	573	ASP
1	N	630	ASP
1	N	646	LYS
2	A	12	ASN
2	A	16	LEU
2	A	39	ARG
2	A	66	THR
2	A	113	LYS
2	A	149	THR
2	A	216	LEU
2	A	253	GLU
2	A	260	THR
2	B	12	ASN
2	B	16	LEU
2	B	35	VAL
2	B	39	ARG
2	B	66	THR
2	B	105	LEU
2	B	113	LYS
2	B	157	ASP
2	B	219	VAL
2	B	253	GLU
2	C	34	ILE
2	C	39	ARG
2	C	66	THR
2	C	79	TRP
2	C	157	ASP
2	C	161	HIS
2	C	194	THR
2	C	219	VAL
2	D	9	VAL
2	D	12	ASN
2	D	39	ARG
2	D	124	PHE
2	D	149	THR

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Mol	Chain	Res	Type
2	D	219	VAL
2	D	242	LEU
2	E	12	ASN
2	E	14	SER
2	E	44	MET
2	E	107	GLU
2	E	113	LYS
2	E	154	ASP
2	E	157	ASP
2	E	219	VAL
2	E	253	GLU
2	F	14	SER
2	F	31	PHE
2	F	41	GLN
2	F	66	THR
2	F	157	ASP
2	F	161	HIS
2	F	219	VAL
2	F	225	ASN
2	F	249	THR
2	F	270	GLU
2	F	274	ILE
2	G	12	ASN
2	G	39	ARG
2	G	113	LYS
2	G	123	MET
2	G	149	THR
2	G	161	HIS
2	G	187	ASP
2	H	9	VAL
2	H	92	ASN
2	H	104	LEU
2	H	149	THR
2	H	157	ASP
2	H	161	HIS
2	H	173	HIS
2	H	184	ASP
2	H	219	VAL
2	H	253	GLU
2	H	258	PRO
2	H	260	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111)

such sidechains are listed below:

Mol	Chain	Res	Type
1	I	17	GLN
1	I	36	GLN
1	I	47	GLN
1	I	75	HIS
1	I	264	HIS
1	I	434	HIS
1	I	497	GLN
1	I	511	ASN
1	I	537	GLN
1	J	11	HIS
1	J	126	HIS
1	J	238	GLN
1	J	294	ASN
1	J	346	HIS
1	J	417	ASN
1	J	481	GLN
1	J	497	GLN
1	J	504	ASN
1	J	533	ASN
1	J	549	GLN
1	J	602	HIS
1	J	627	ASN
1	K	17	GLN
1	K	36	GLN
1	K	213	HIS
1	K	346	HIS
1	K	482	GLN
1	K	512	GLN
1	K	548	HIS
1	K	549	GLN
1	K	568	HIS
1	K	592	GLN
1	K	597	ASN
1	K	684	GLN
1	L	47	GLN
1	L	227	HIS
1	L	481	GLN
1	L	485	ASN
1	L	504	ASN
1	M	20	ASN
1	M	75	HIS
1	M	264	HIS

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Mol	Chain	Res	Type
1	M	314	HIS
1	M	346	HIS
1	M	370	GLN
1	M	430	HIS
1	M	434	HIS
1	M	485	ASN
1	M	554	HIS
1	M	592	GLN
1	M	602	HIS
1	M	678	HIS
1	N	17	GLN
1	N	20	ASN
1	N	36	GLN
1	N	75	HIS
1	N	126	HIS
1	N	145	GLN
1	N	201	ASN
1	N	238	GLN
1	N	290	GLN
1	N	434	HIS
1	N	481	GLN
1	N	493	GLN
1	N	678	HIS
2	A	40	HIS
2	A	88	HIS
2	A	92	ASN
2	A	128	ASN
2	A	246	GLN
2	B	88	HIS
2	B	92	ASN
2	B	161	HIS
2	B	225	ASN
2	B	275	HIS
2	B	296	ASN
2	C	78	ASN
2	C	101	HIS
2	C	161	HIS
2	C	173	HIS
2	C	225	ASN
2	C	246	GLN
2	D	12	ASN
2	D	88	HIS

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Mol	Chain	Res	Type
2	D	92	ASN
2	D	275	HIS
2	D	371	HIS
2	E	88	HIS
2	E	92	ASN
2	E	161	HIS
2	E	275	HIS
2	E	280	ASN
2	F	12	ASN
2	F	87	HIS
2	F	88	HIS
2	F	92	ASN
2	F	275	HIS
2	F	297	ASN
2	F	360	GLN
2	G	92	ASN
2	G	111	ASN
2	G	115	ASN
2	G	161	HIS
2	G	173	HIS
2	G	225	ASN
2	H	59	GLN
2	H	88	HIS
2	H	92	ASN
2	H	101	HIS
2	H	115	ASN
2	H	161	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	ADP	H	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)
4	ADP	E	402	3	28,29,29	1.38	4 (14%)	43,45,45	1.82	10 (23%)
4	ADP	A	402	3	28,29,29	1.38	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	G	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	B	402	3	28,29,29	1.38	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	D	402	3	28,29,29	1.39	4 (14%)	43,45,45	1.81	10 (23%)
4	ADP	F	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.82	10 (23%)
4	ADP	C	402	3	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)

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	ADP	H	402	3	-	3/16/32/32	0/3/3/3
4	ADP	E	402	3	-	3/16/32/32	0/3/3/3
4	ADP	A	402	3	-	3/16/32/32	0/3/3/3
4	ADP	G	402	3	-	3/16/32/32	0/3/3/3
4	ADP	B	402	3	-	3/16/32/32	0/3/3/3
4	ADP	D	402	3	-	3/16/32/32	0/3/3/3
4	ADP	F	402	3	-	3/16/32/32	0/3/3/3
4	ADP	C	402	3	-	3/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	402	ADP	C5-C4	4.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	402	ADP	C5-C4	4.69	1.47	1.39
4	C	402	ADP	C5-C4	4.67	1.47	1.39
4	D	402	ADP	C5-C4	4.67	1.47	1.39
4	H	402	ADP	C5-C4	4.66	1.47	1.39
4	B	402	ADP	C5-C4	4.65	1.47	1.39
4	E	402	ADP	C5-C4	4.61	1.47	1.39
4	A	402	ADP	C5-C4	4.60	1.47	1.39
4	E	402	ADP	C5-C6	2.86	1.49	1.41
4	A	402	ADP	C5-C6	2.84	1.48	1.41
4	C	402	ADP	C5-C6	2.83	1.48	1.41
4	H	402	ADP	C5-C6	2.83	1.48	1.41
4	B	402	ADP	C5-C6	2.82	1.48	1.41
4	G	402	ADP	C5-C6	2.82	1.48	1.41
4	F	402	ADP	C5-C6	2.82	1.48	1.41
4	D	402	ADP	C5-C6	2.80	1.48	1.41
4	F	402	ADP	C8-N7	2.46	1.36	1.31
4	G	402	ADP	C8-N7	2.46	1.36	1.31
4	A	402	ADP	C8-N7	2.45	1.36	1.31
4	H	402	ADP	C8-N7	2.44	1.36	1.31
4	B	402	ADP	C8-N7	2.41	1.36	1.31
4	D	402	ADP	C8-N7	2.40	1.36	1.31
4	E	402	ADP	C8-N7	2.37	1.36	1.31
4	C	402	ADP	C8-N7	2.34	1.36	1.31
4	H	402	ADP	C5-N7	-2.24	1.35	1.39
4	G	402	ADP	C5-N7	-2.22	1.35	1.39
4	F	402	ADP	C5-N7	-2.20	1.35	1.39
4	C	402	ADP	C5-N7	-2.19	1.35	1.39
4	D	402	ADP	C5-N7	-2.19	1.35	1.39
4	E	402	ADP	C5-N7	-2.16	1.35	1.39
4	A	402	ADP	C5-N7	-2.15	1.35	1.39
4	B	402	ADP	C5-N7	-2.15	1.35	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	402	ADP	C5-C4-N3	-5.77	118.77	126.72
4	H	402	ADP	C5-C4-N3	-5.73	118.82	126.72
4	B	402	ADP	C5-C4-N3	-5.70	118.86	126.72
4	D	402	ADP	C5-C4-N3	-5.70	118.87	126.72
4	A	402	ADP	C5-C4-N3	-5.68	118.89	126.72
4	F	402	ADP	C5-C4-N3	-5.67	118.91	126.72
4	E	402	ADP	C5-C4-N3	-5.62	118.97	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	ADP	C5-C4-N3	-5.62	118.97	126.72
4	H	402	ADP	N3-C4-N9	4.41	134.67	127.17
4	G	402	ADP	N3-C4-N9	4.39	134.64	127.17
4	F	402	ADP	N3-C4-N9	4.37	134.60	127.17
4	C	402	ADP	N3-C4-N9	4.37	134.59	127.17
4	A	402	ADP	N3-C4-N9	4.35	134.56	127.17
4	D	402	ADP	N3-C4-N9	4.34	134.54	127.17
4	B	402	ADP	N3-C4-N9	4.33	134.54	127.17
4	E	402	ADP	N3-C4-N9	4.31	134.50	127.17
4	B	402	ADP	C4-C5-N7	-3.88	106.15	110.58
4	G	402	ADP	C4-C5-N7	-3.83	106.20	110.58
4	D	402	ADP	C4-C5-N7	-3.82	106.22	110.58
4	H	402	ADP	C4-C5-N7	-3.81	106.22	110.58
4	F	402	ADP	C4-C5-N7	-3.80	106.24	110.58
4	C	402	ADP	C4-C5-N7	-3.80	106.24	110.58
4	E	402	ADP	C4-C5-N7	-3.79	106.25	110.58
4	A	402	ADP	C4-C5-N7	-3.76	106.28	110.58
4	G	402	ADP	C2-N3-C4	3.61	120.64	111.83
4	H	402	ADP	C2-N3-C4	3.60	120.62	111.83
4	A	402	ADP	C2-N3-C4	3.59	120.60	111.83
4	D	402	ADP	C2-N3-C4	3.57	120.54	111.83
4	F	402	ADP	C2-N3-C4	3.56	120.53	111.83
4	E	402	ADP	C2-N3-C4	3.56	120.52	111.83
4	C	402	ADP	C2-N3-C4	3.55	120.51	111.83
4	B	402	ADP	C2-N3-C4	3.55	120.49	111.83
4	A	402	ADP	N3-C2-N1	-3.03	124.00	128.58
4	H	402	ADP	N3-C2-N1	-2.99	124.05	128.58
4	E	402	ADP	N3-C2-N1	-2.98	124.07	128.58
4	C	402	ADP	N3-C2-N1	-2.98	124.08	128.58
4	B	402	ADP	N3-C2-N1	-2.96	124.10	128.58
4	D	402	ADP	N3-C2-N1	-2.94	124.14	128.58
4	G	402	ADP	N3-C2-N1	-2.93	124.14	128.58
4	F	402	ADP	N3-C2-N1	-2.90	124.20	128.58
4	B	402	ADP	C5-N7-C8	2.89	107.99	103.45
4	C	402	ADP	C5-N7-C8	2.88	107.98	103.45
4	H	402	ADP	C5-N7-C8	2.88	107.97	103.45
4	E	402	ADP	C5-N7-C8	2.85	107.93	103.45
4	G	402	ADP	C5-N7-C8	2.85	107.93	103.45
4	A	402	ADP	C5-N7-C8	2.84	107.91	103.45
4	C	402	ADP	C4-N9-C8	2.83	108.71	105.74
4	D	402	ADP	C5-N7-C8	2.83	107.90	103.45
4	F	402	ADP	C5-N7-C8	2.82	107.88	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	402	ADP	C4-N9-C8	2.82	108.69	105.74
4	F	402	ADP	C4-N9-C8	2.81	108.68	105.74
4	E	402	ADP	C4-N9-C8	2.79	108.66	105.74
4	A	402	ADP	C4-N9-C8	2.78	108.66	105.74
4	B	402	ADP	C4-N9-C8	2.75	108.63	105.74
4	G	402	ADP	C4-N9-C8	2.74	108.62	105.74
4	D	402	ADP	C4-N9-C8	2.69	108.56	105.74
4	A	402	ADP	N9-C8-N7	-2.35	110.61	113.94
4	H	402	ADP	N9-C8-N7	-2.34	110.61	113.94
4	B	402	ADP	N9-C8-N7	-2.32	110.64	113.94
4	E	402	ADP	N9-C8-N7	-2.32	110.64	113.94
4	C	402	ADP	N9-C8-N7	-2.32	110.64	113.94
4	G	402	ADP	N9-C8-N7	-2.30	110.67	113.94
4	B	402	ADP	C6-C5-N7	2.28	136.48	132.09
4	F	402	ADP	N9-C8-N7	-2.28	110.70	113.94
4	C	402	ADP	C6-C5-N7	2.27	136.47	132.09
4	H	402	ADP	C6-C5-N7	2.27	136.46	132.09
4	D	402	ADP	N9-C8-N7	-2.25	110.74	113.94
4	E	402	ADP	C6-C5-N7	2.24	136.42	132.09
4	G	402	ADP	C6-C5-N7	2.24	136.41	132.09
4	H	402	ADP	C3'-C2'-C1'	2.24	105.70	101.46
4	F	402	ADP	C6-C5-N7	2.24	136.40	132.09
4	D	402	ADP	C6-C5-N7	2.23	136.40	132.09
4	A	402	ADP	C6-C5-N7	2.23	136.38	132.09
4	E	402	ADP	C3'-C2'-C1'	2.22	105.65	101.46
4	F	402	ADP	C3'-C2'-C1'	2.19	105.61	101.46
4	B	402	ADP	C3'-C2'-C1'	2.19	105.61	101.46
4	C	402	ADP	C3'-C2'-C1'	2.17	105.57	101.46
4	A	402	ADP	C3'-C2'-C1'	2.17	105.57	101.46
4	D	402	ADP	C3'-C2'-C1'	2.15	105.53	101.46
4	G	402	ADP	C3'-C2'-C1'	2.15	105.53	101.46

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	C5'-O5'-PA-O2A
4	A	402	ADP	C5'-O5'-PA-O3A
4	B	402	ADP	C5'-O5'-PA-O1A
4	B	402	ADP	C5'-O5'-PA-O2A
4	B	402	ADP	C5'-O5'-PA-O3A

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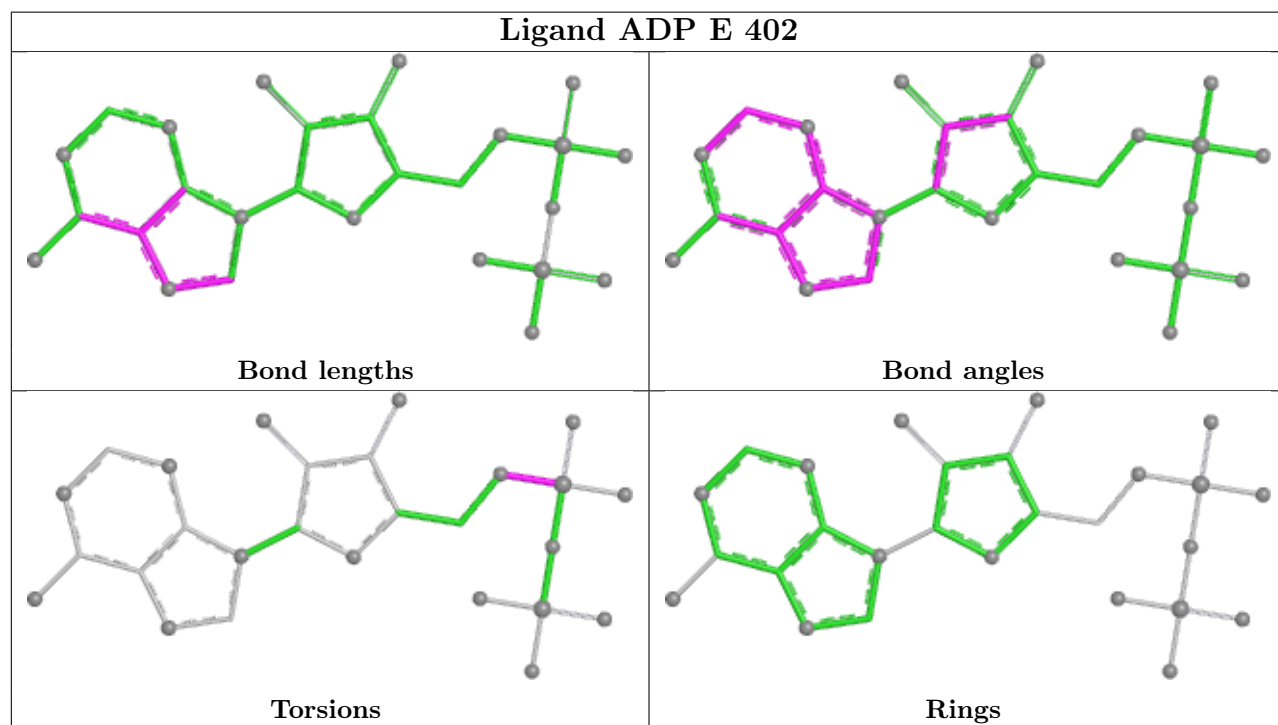
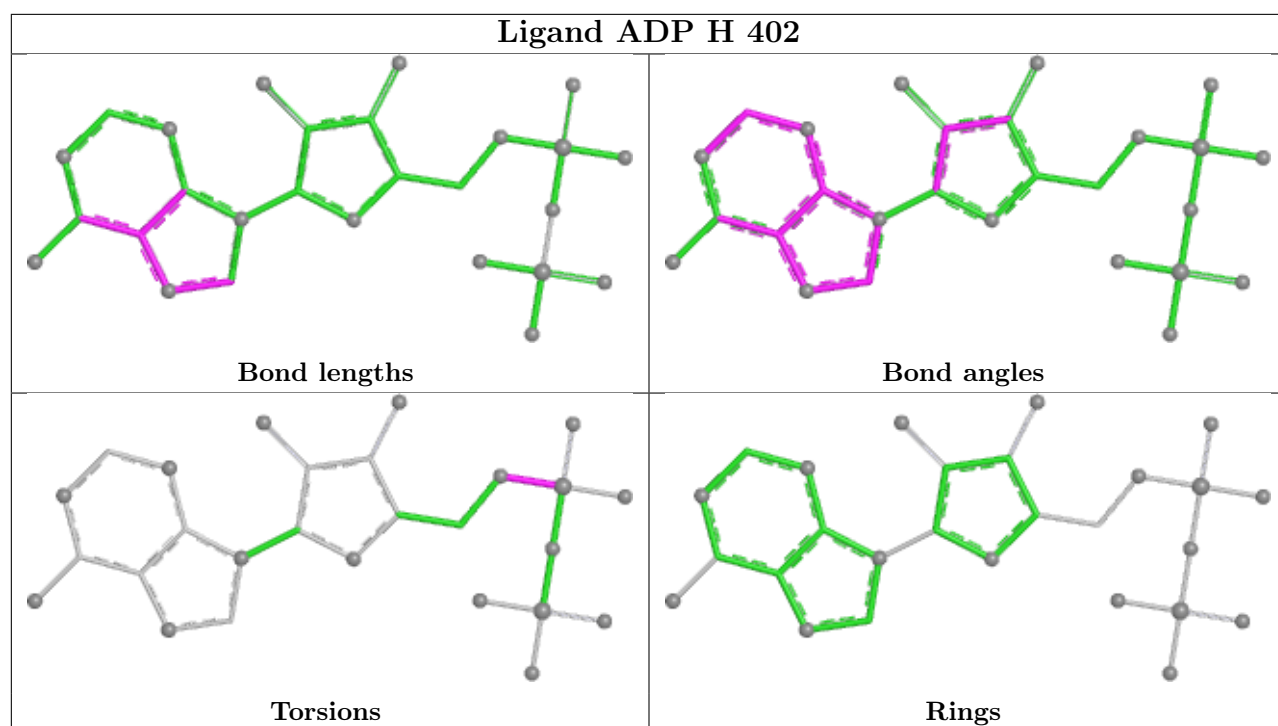
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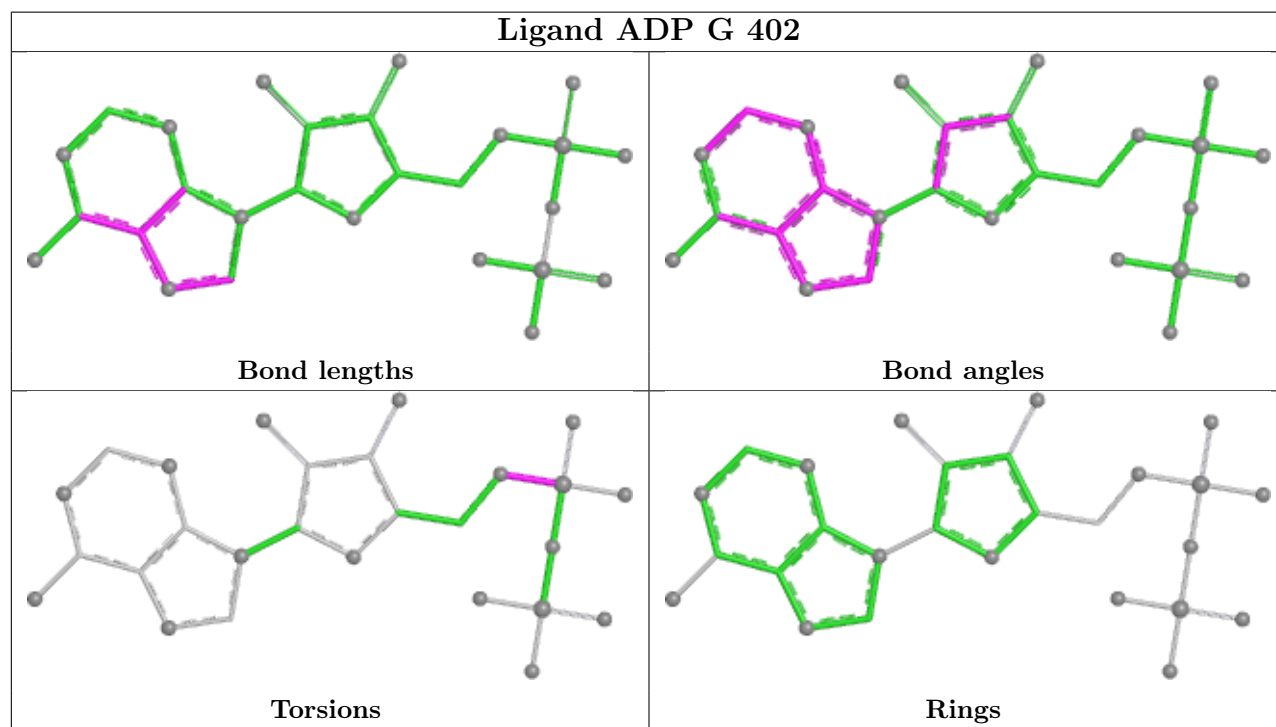
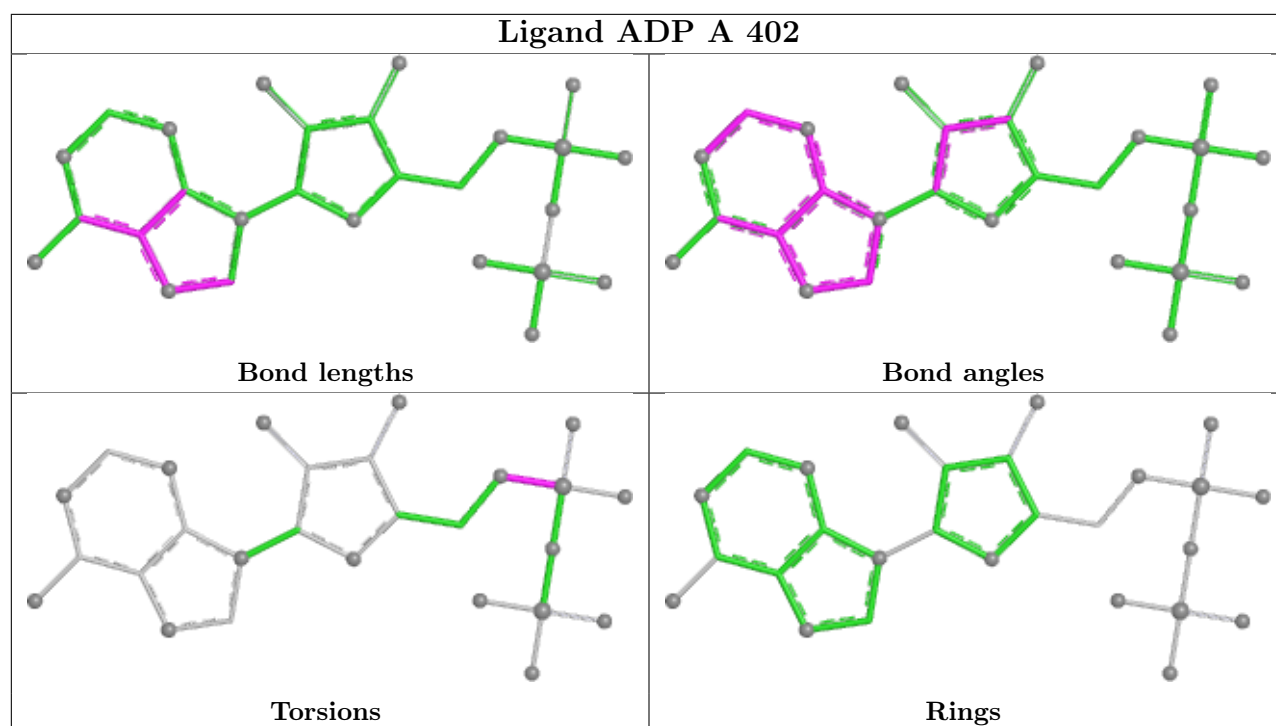
Mol	Chain	Res	Type	Atoms
4	C	402	ADP	C5'-O5'-PA-O1A
4	C	402	ADP	C5'-O5'-PA-O2A
4	C	402	ADP	C5'-O5'-PA-O3A
4	D	402	ADP	C5'-O5'-PA-O1A
4	D	402	ADP	C5'-O5'-PA-O2A
4	D	402	ADP	C5'-O5'-PA-O3A
4	E	402	ADP	C5'-O5'-PA-O1A
4	E	402	ADP	C5'-O5'-PA-O2A
4	E	402	ADP	C5'-O5'-PA-O3A
4	F	402	ADP	C5'-O5'-PA-O1A
4	F	402	ADP	C5'-O5'-PA-O2A
4	F	402	ADP	C5'-O5'-PA-O3A
4	G	402	ADP	C5'-O5'-PA-O1A
4	G	402	ADP	C5'-O5'-PA-O2A
4	G	402	ADP	C5'-O5'-PA-O3A
4	H	402	ADP	C5'-O5'-PA-O1A
4	H	402	ADP	C5'-O5'-PA-O2A
4	H	402	ADP	C5'-O5'-PA-O3A

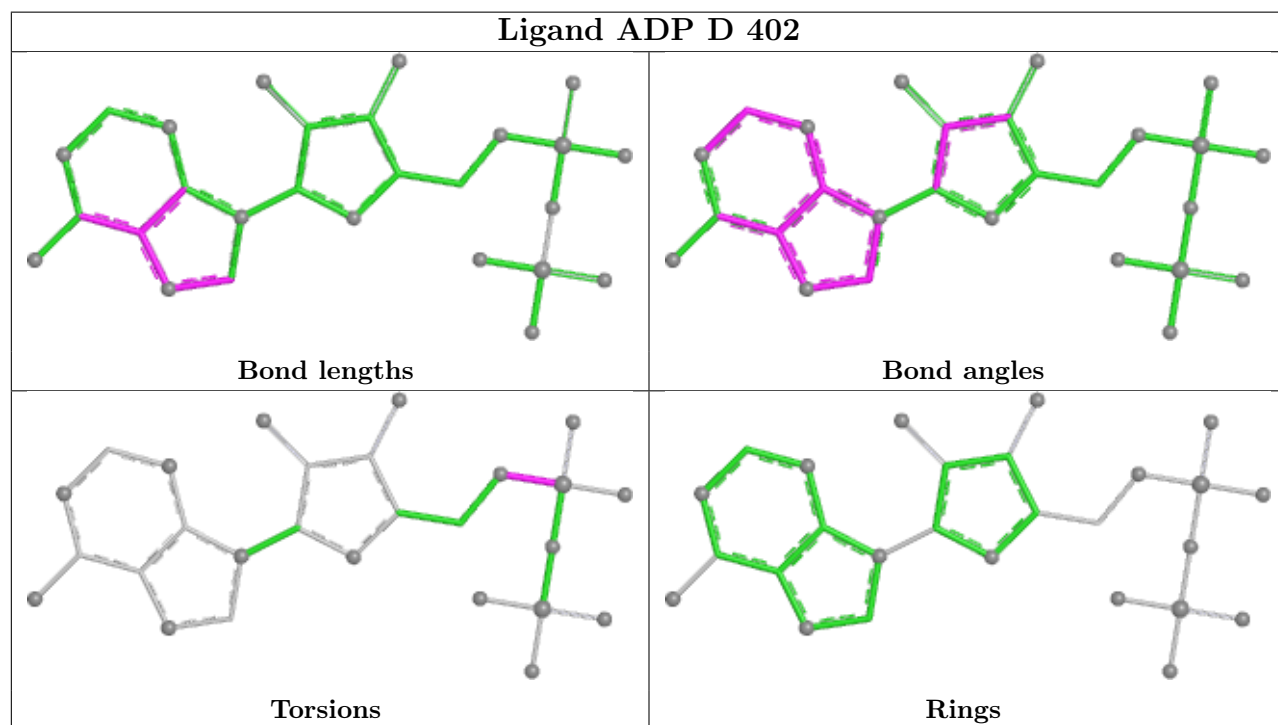
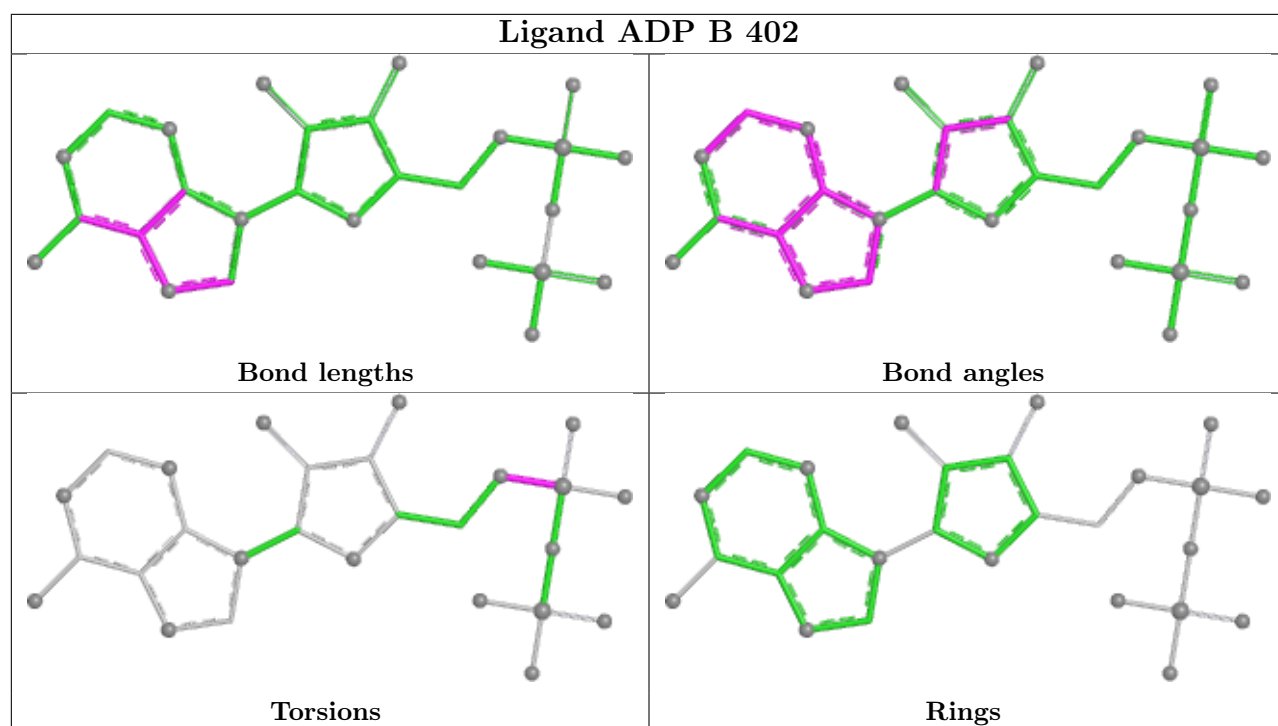
There are no ring outliers.

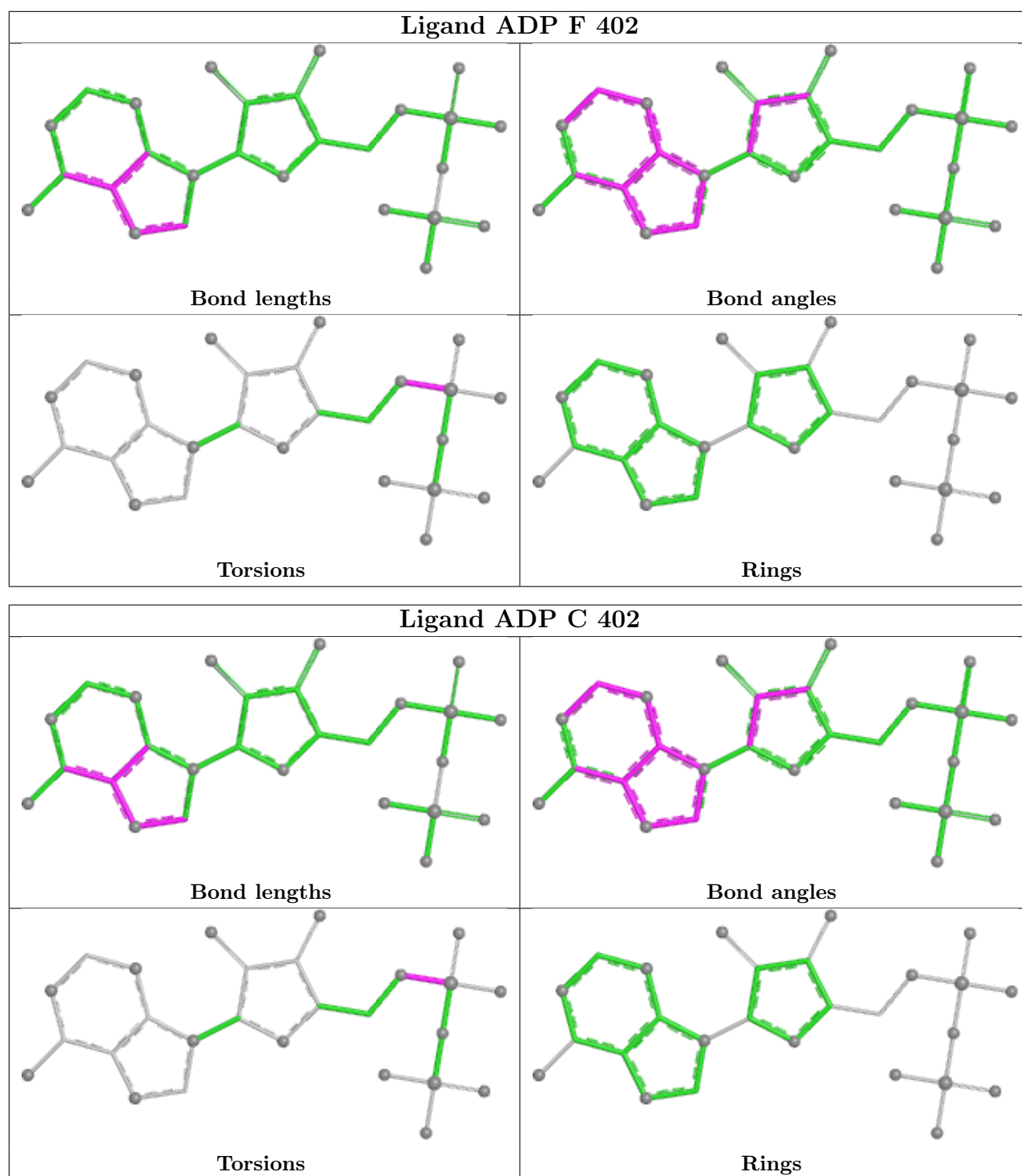
No monomer is involved in short contacts.

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

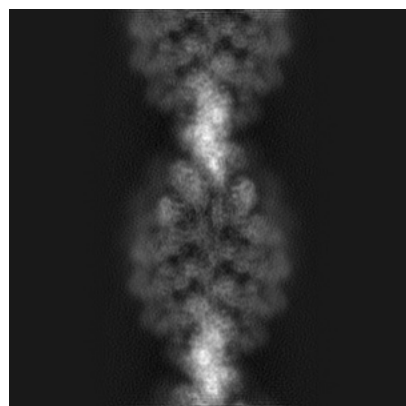
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7117. These allow visual inspection of the internal detail of the map and identification of artifacts.

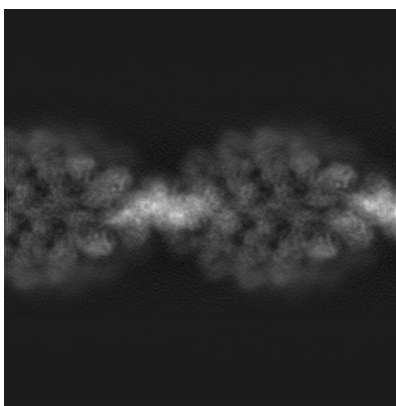
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

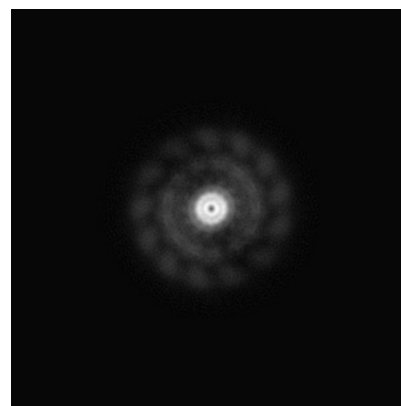
6.1.1 Primary map



X

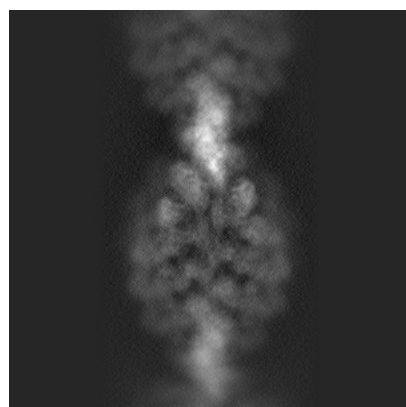


Y

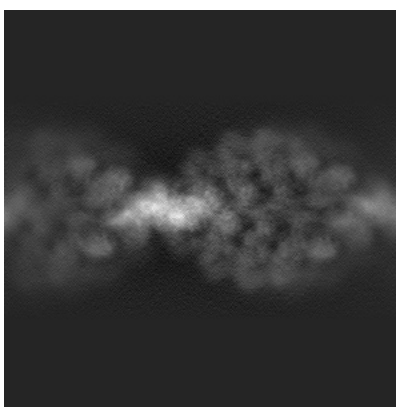


Z

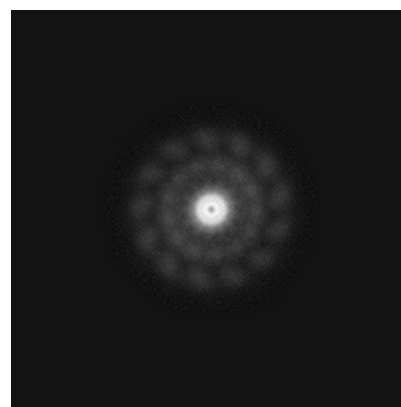
6.1.2 Raw map



X



Y

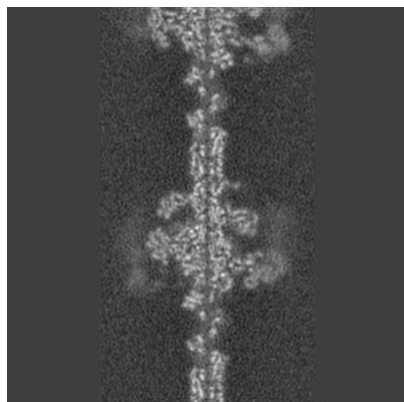


Z

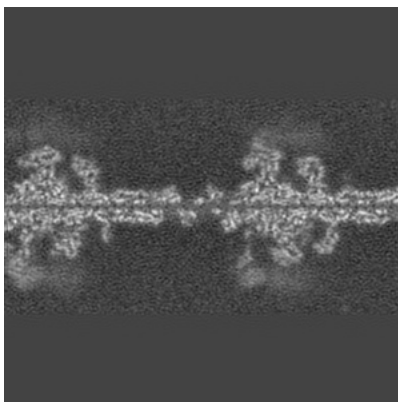
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

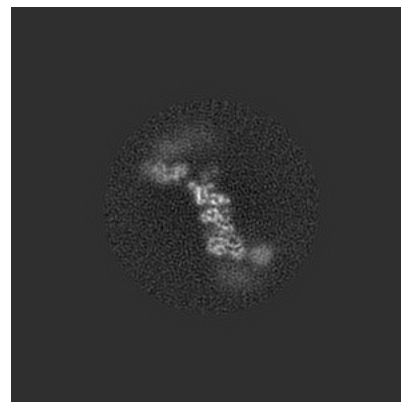
6.2.1 Primary map



X Index: 256

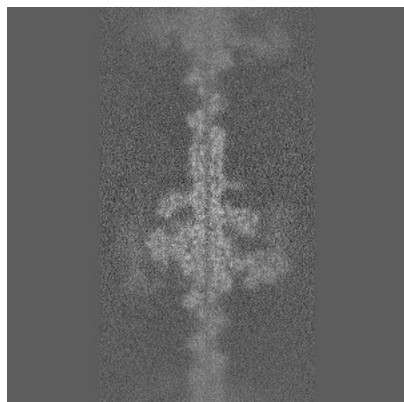


Y Index: 256

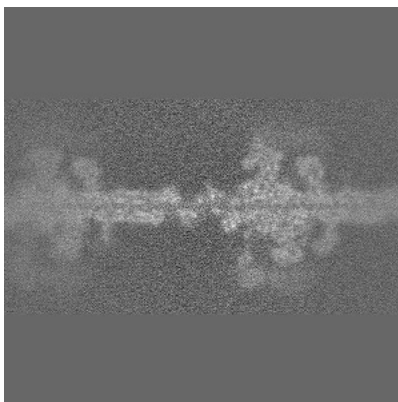


Z Index: 256

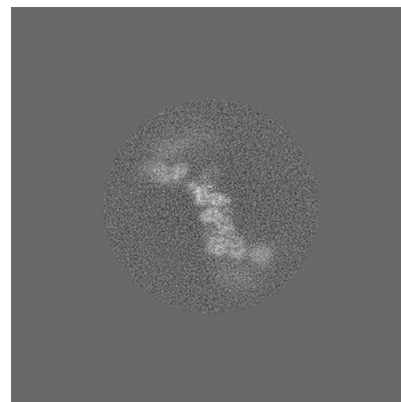
6.2.2 Raw map



X Index: 256



Y Index: 256

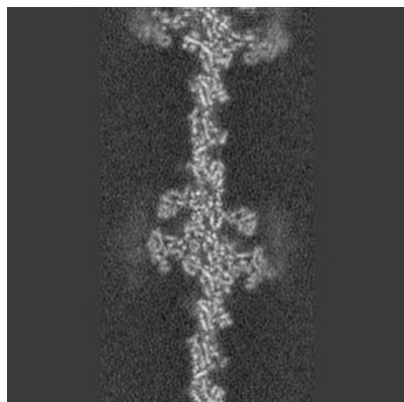


Z Index: 256

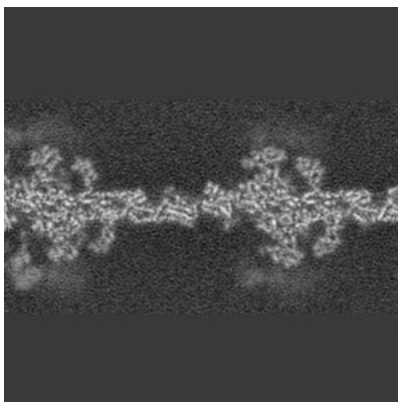
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

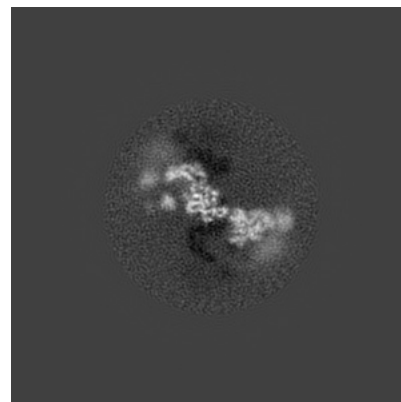
6.3.1 Primary map



X Index: 262

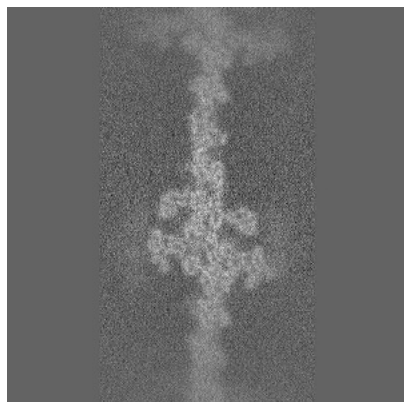


Y Index: 251

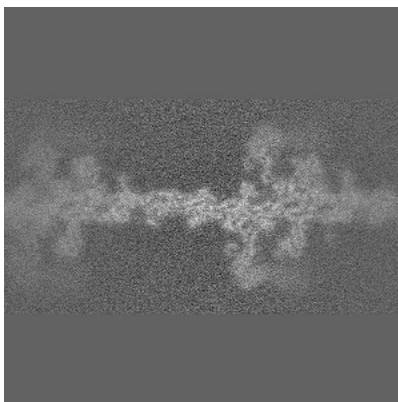


Z Index: 1

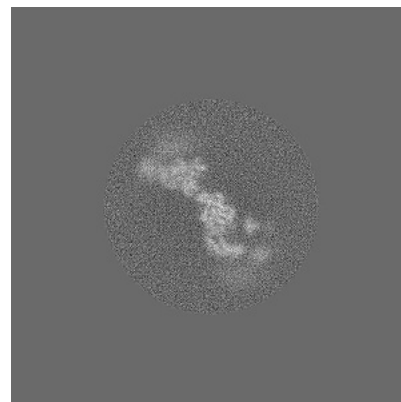
6.3.2 Raw map



X Index: 262



Y Index: 263

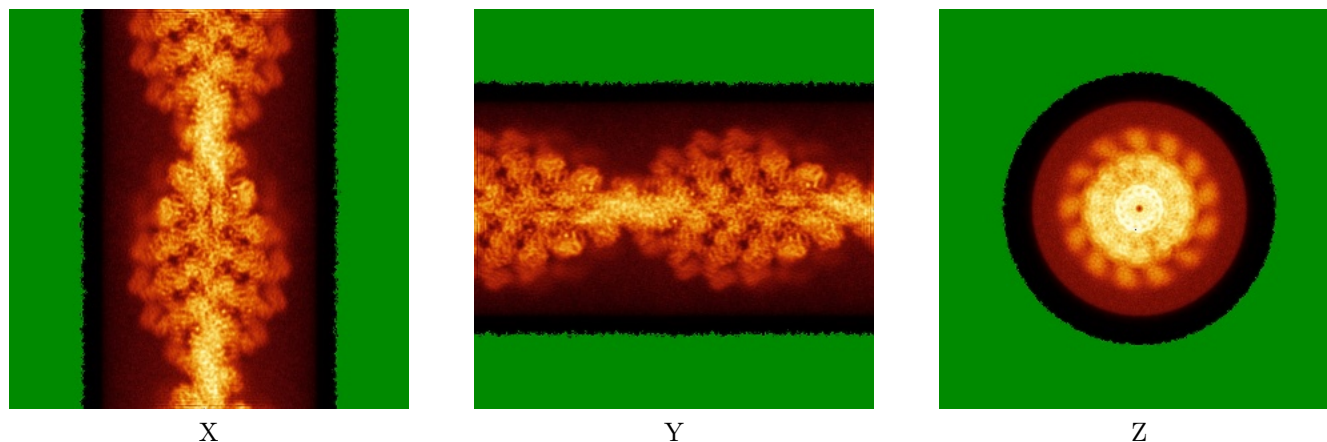


Z Index: 266

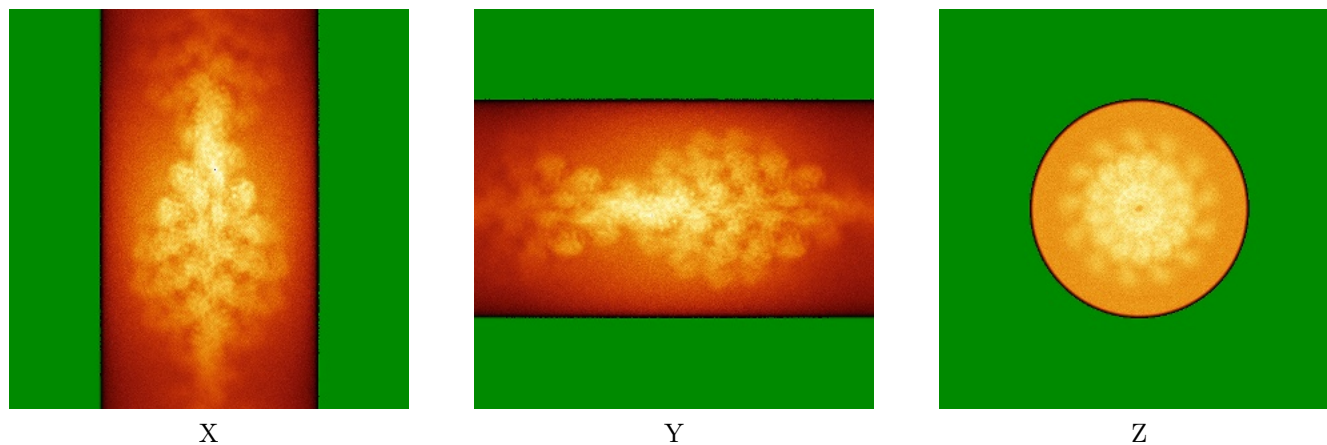
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



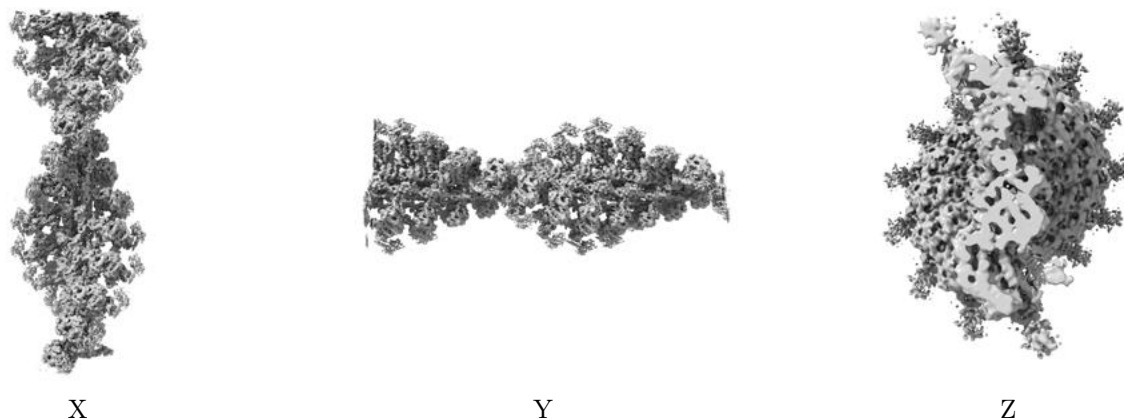
6.4.2 Raw map



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

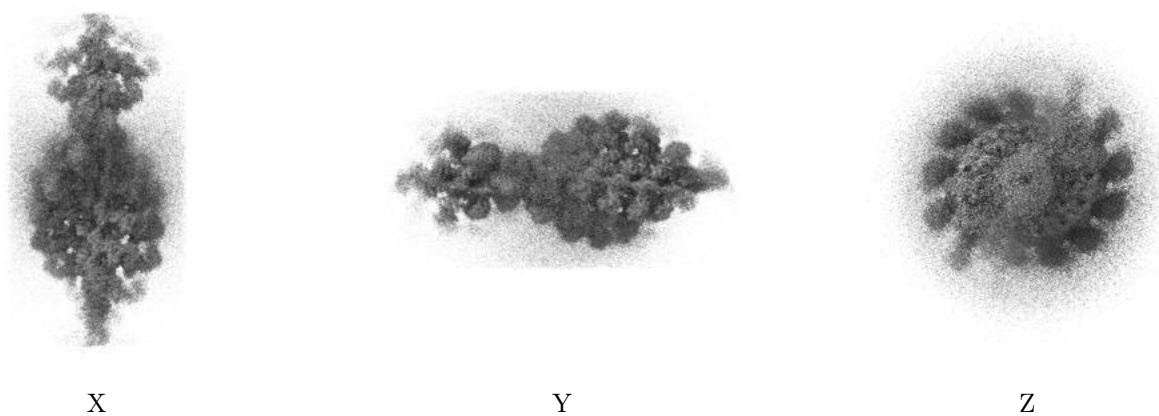
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

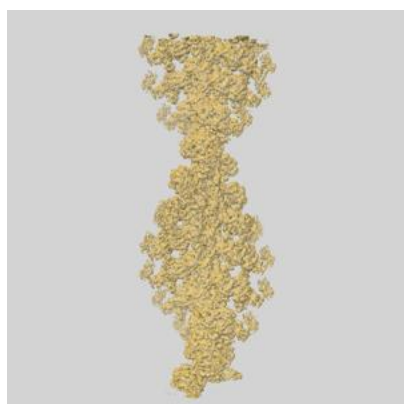
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

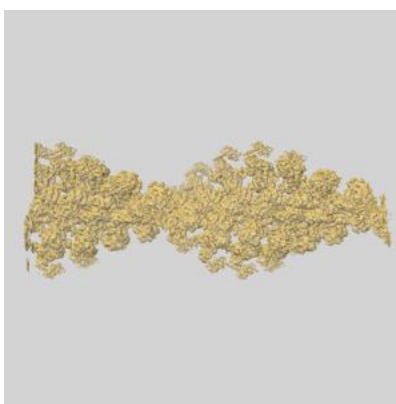
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

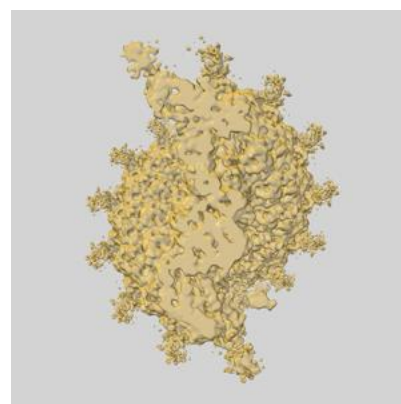
6.6.1 emd_7117_msk_2.map [i](#)



X

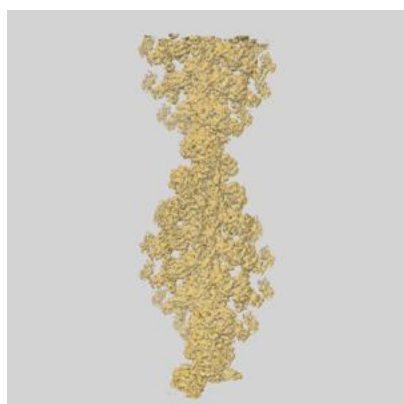


Y

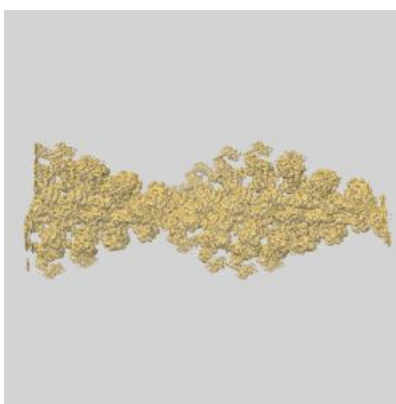


Z

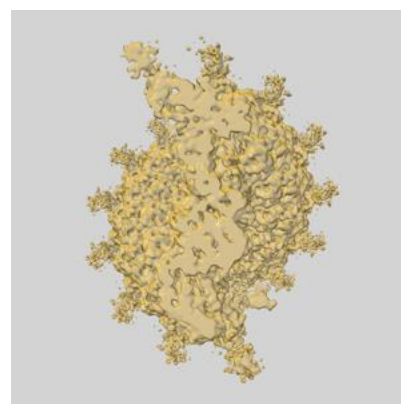
6.6.2 emd_7117_msk_1.map [i](#)



X



Y

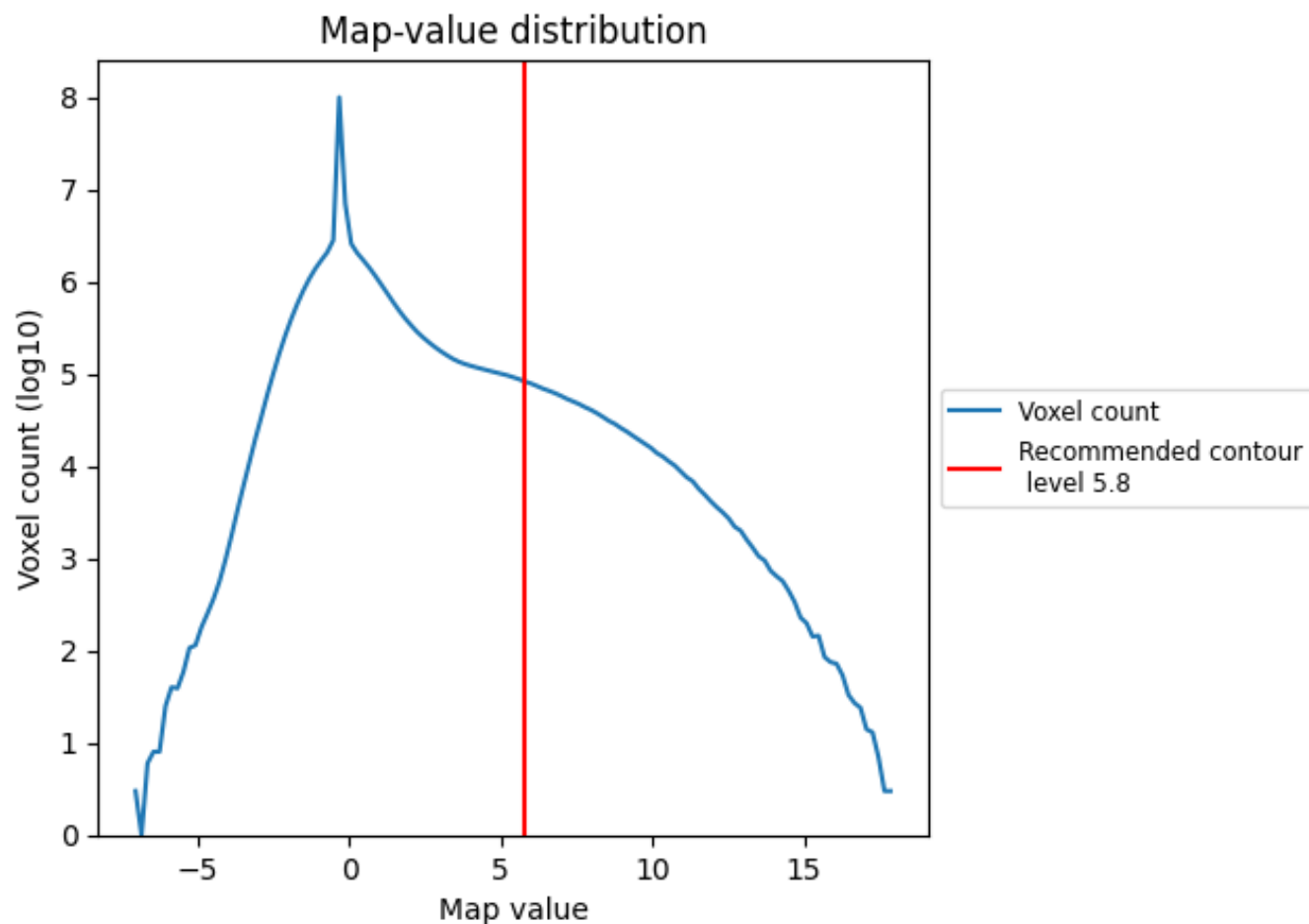


Z

7 Map analysis [i](#)

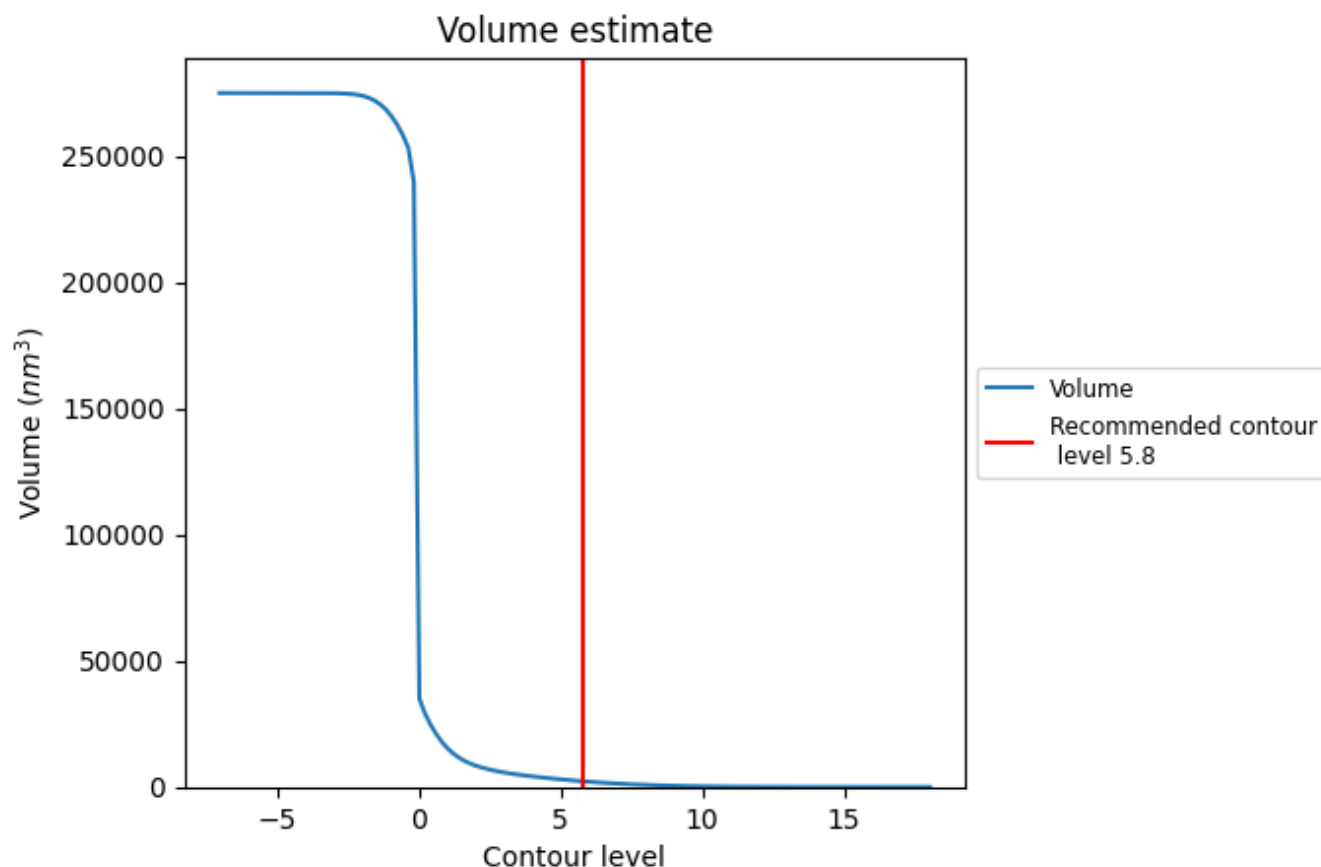
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

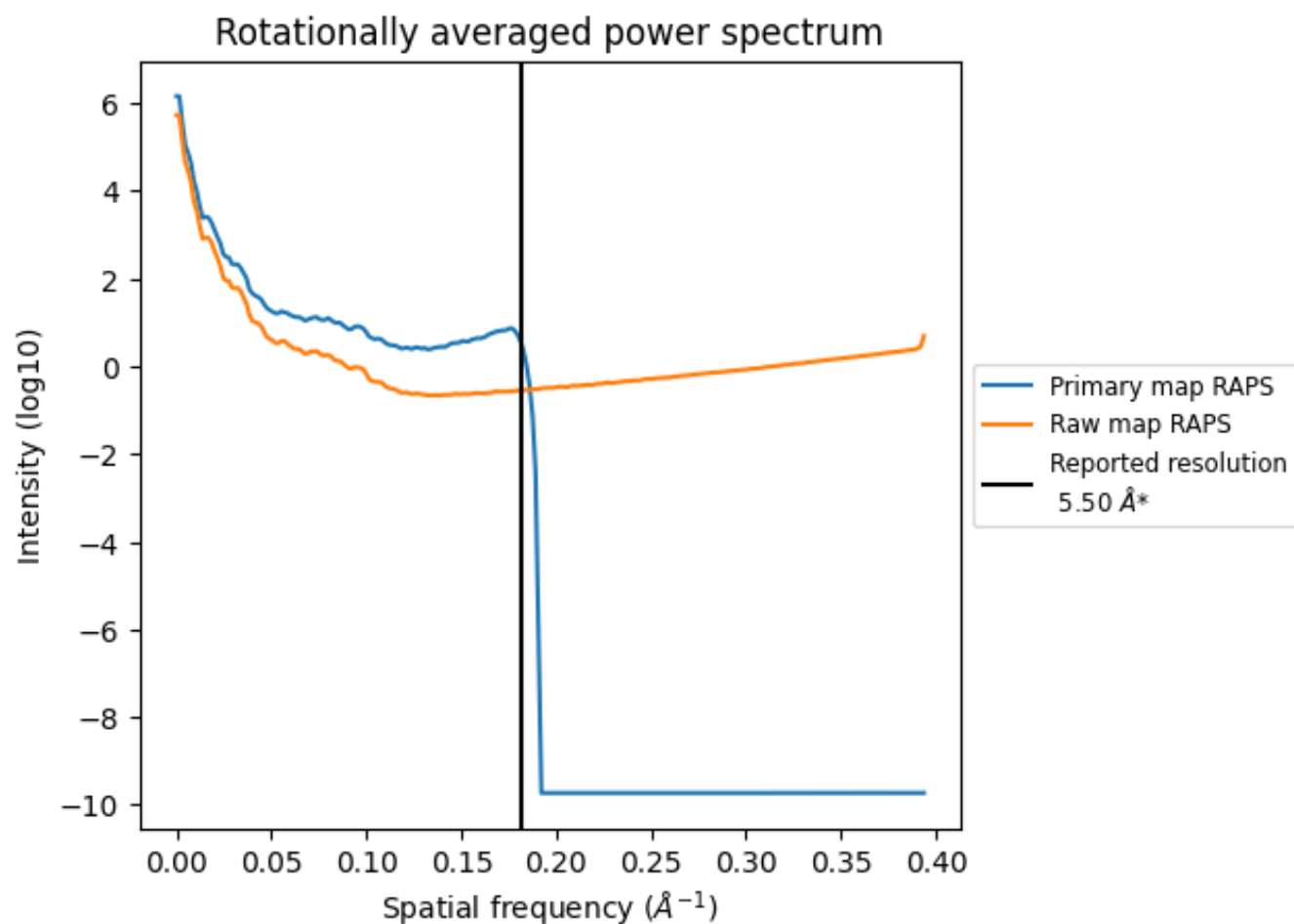
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2222 nm³; this corresponds to an approximate mass of 2007 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 ⓘ

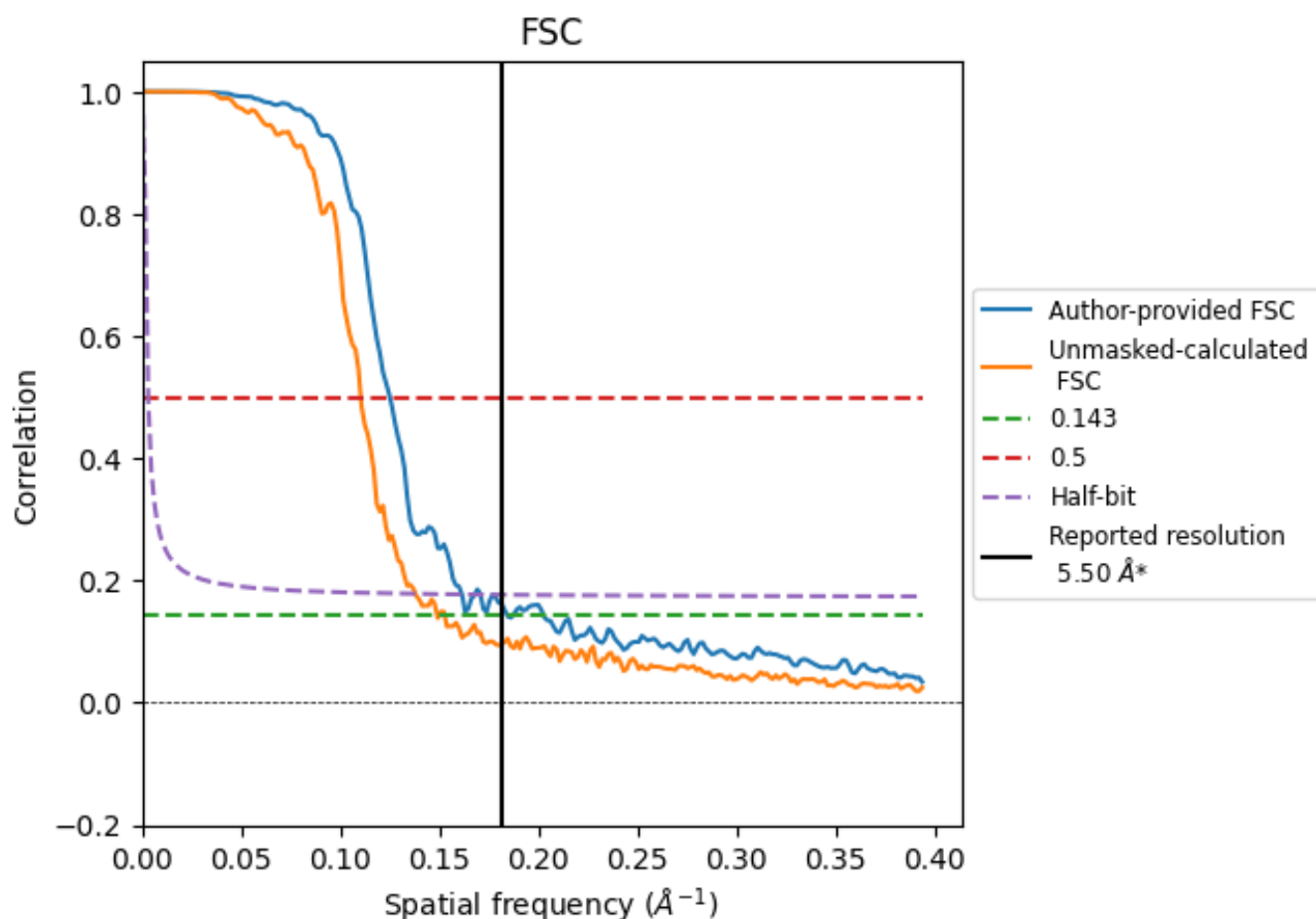


*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.182 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

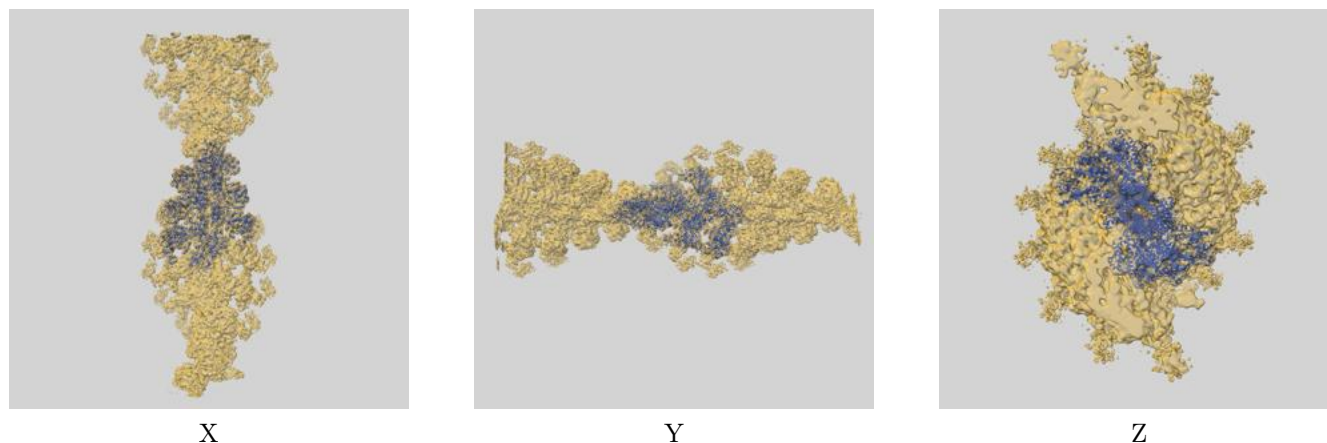
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.43	8.00	6.20
Unmasked-calculated*	6.72	9.07	7.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 5.5 by more than 10 %

9 Map-model fit [i](#)

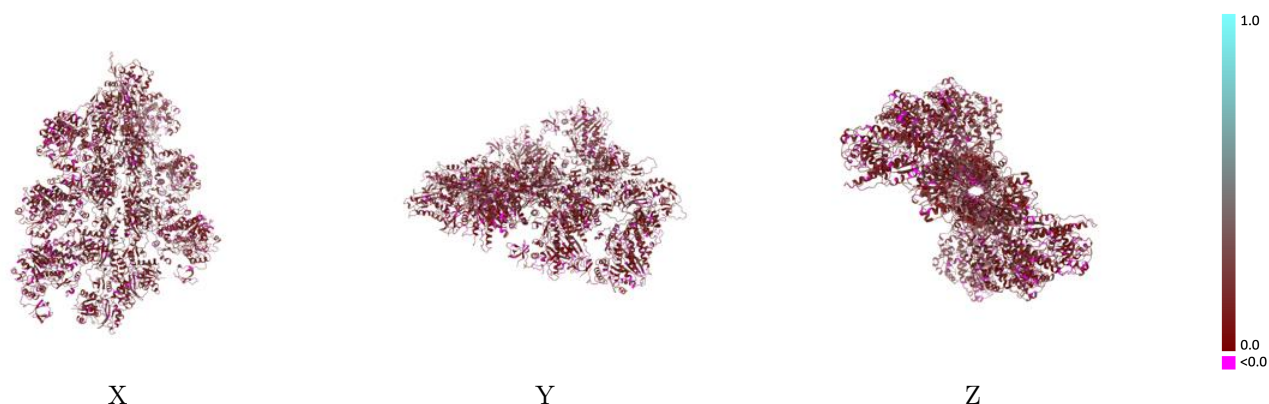
This section contains information regarding the fit between EMDB map EMD-7117 and PDB model 6BNQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



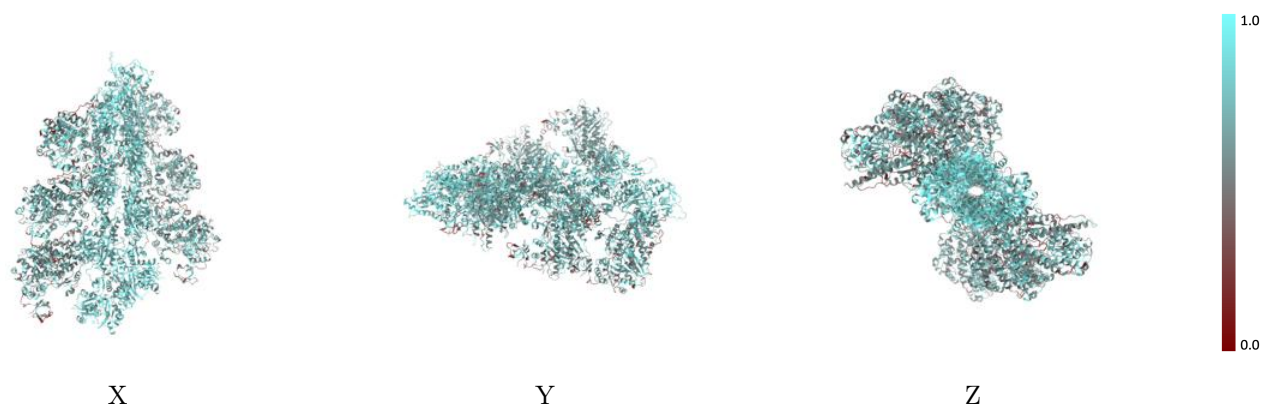
The images above show the 3D surface view of the map at the recommended contour level 5.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



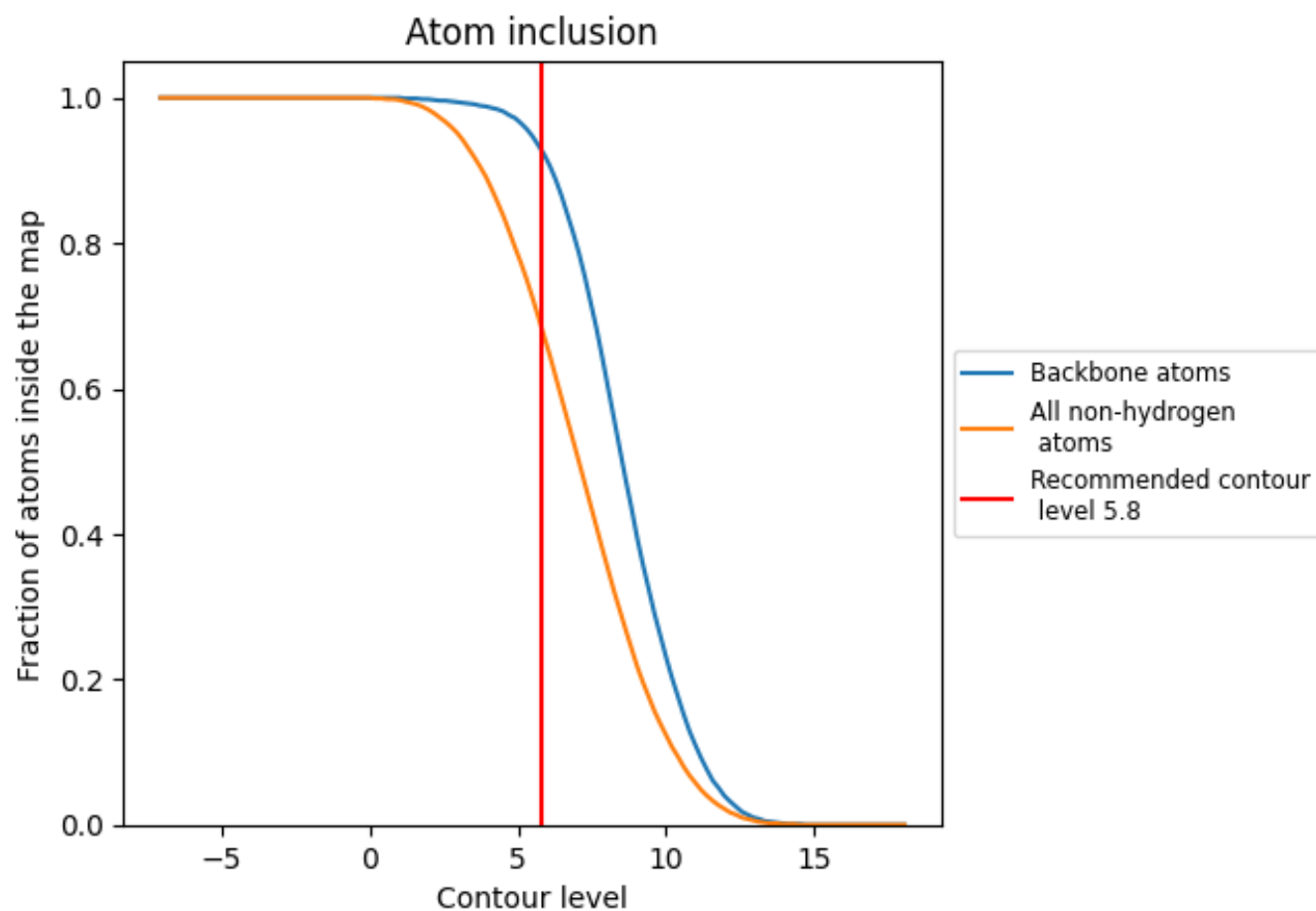
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 68% 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 (5.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6840	0.1680
A	0.7970	0.1910
B	0.7900	0.1870
C	0.7900	0.1900
D	0.7930	0.1910
E	0.7900	0.1890
F	0.8010	0.1920
G	0.7960	0.1880
H	0.7940	0.1850
I	0.6040	0.1510
J	0.6120	0.1550
K	0.6140	0.1530
L	0.6070	0.1520
M	0.6090	0.1520
N	0.6070	0.1540

