



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 08:58 PM UTC

PDB ID : 6BNP / pdb_00006bnp
EMDB ID : EMD-7116
Title : CryoEM structure of MyosinVI-actin complex in the rigor (nucleotide-free) state
Authors : Gurel, P.S.; Alushin, G.A.
Deposited on : 2017-11-17
Resolution : 4.60 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:

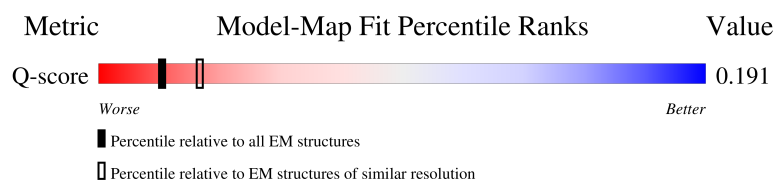
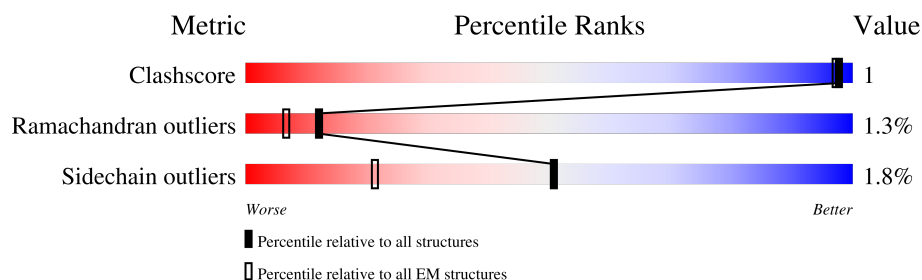
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

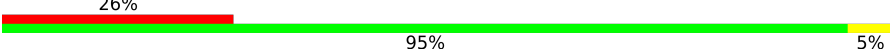
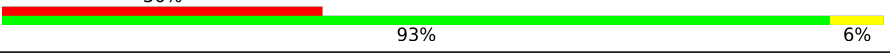
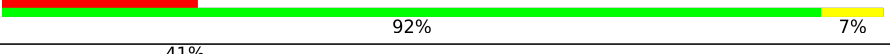
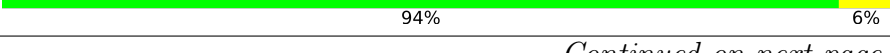
The reported resolution of this entry is 4.60 Å.

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	2407 (4.10 - 5.10)

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	
1	J	704	
1	K	704	
1	L	704	

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Mol	Chain	Length	Quality of chain
1	M	704	
1	N	704	
2	A	373	
2	B	373	
2	C	373	
2	D	373	
2	E	373	
2	F	373	
2	G	373	
2	H	373	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 56792 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	704	Total	C	N	O	S	0	0
			5612	3541	975	1071	25		
1	J	704	Total	C	N	O	S	0	0
			5612	3541	975	1071	25		
1	K	704	Total	C	N	O	S	0	0
			5612	3541	975	1071	25		
1	L	704	Total	C	N	O	S	0	0
			5612	3541	975	1071	25		
1	M	704	Total	C	N	O	S	0	0
			5612	3541	975	1071	25		
1	N	704	Total	C	N	O	S	0	0
			5612	3541	975	1071	25		

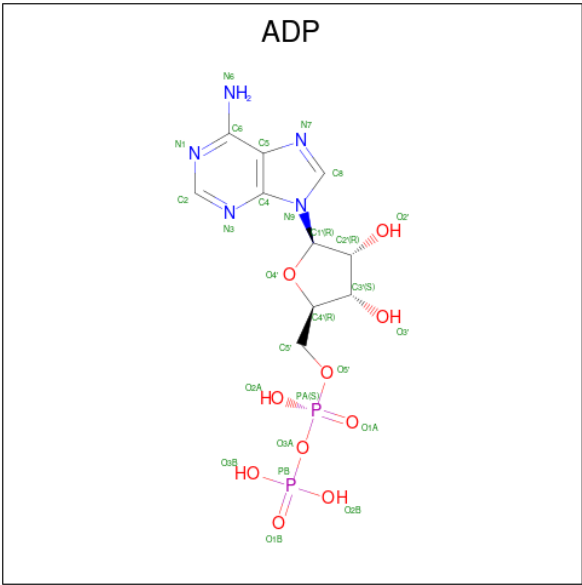
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

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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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	

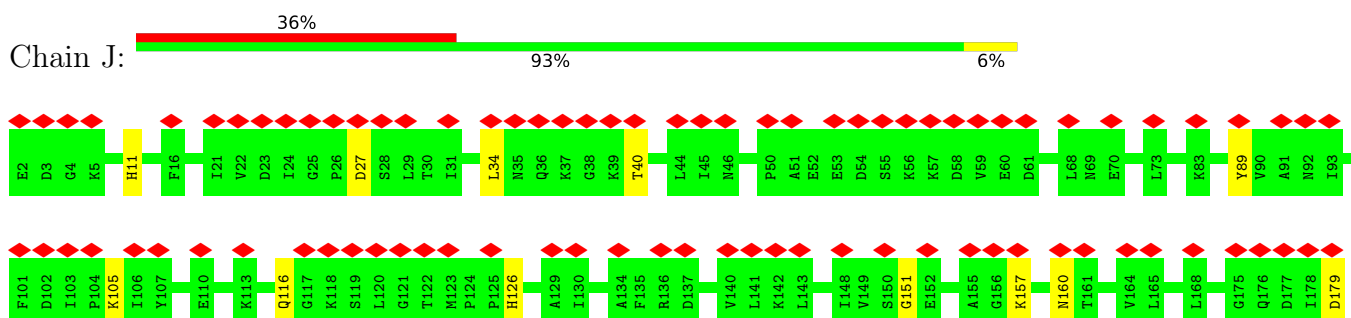
3 Residue-property plots

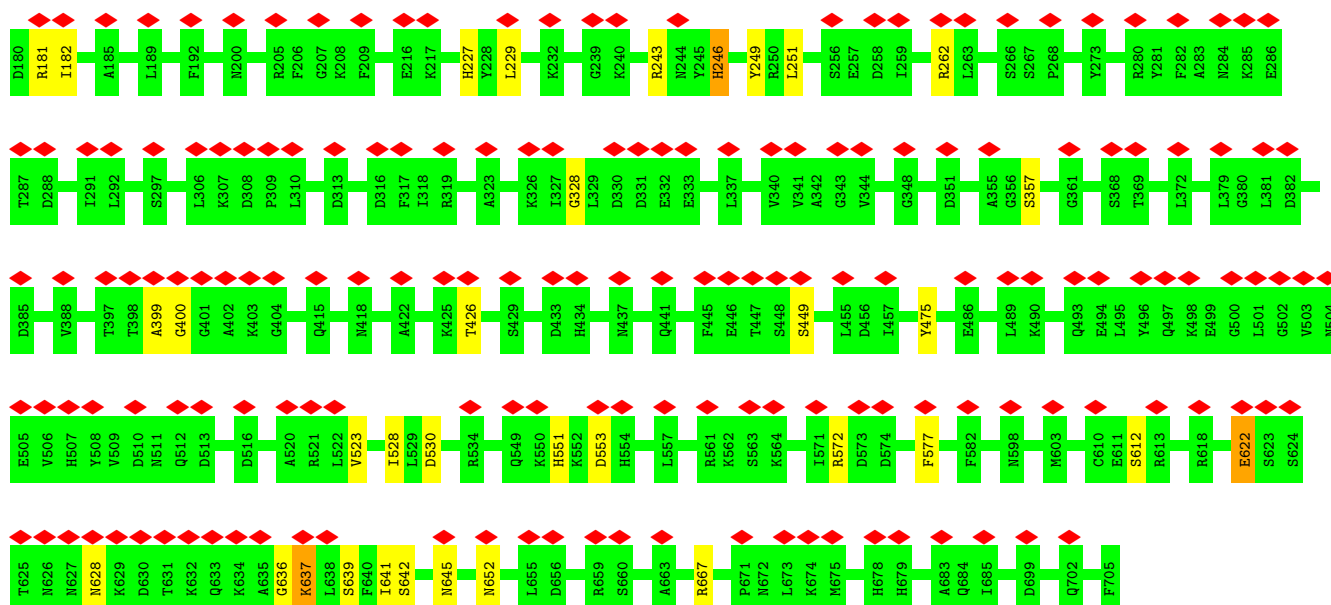
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

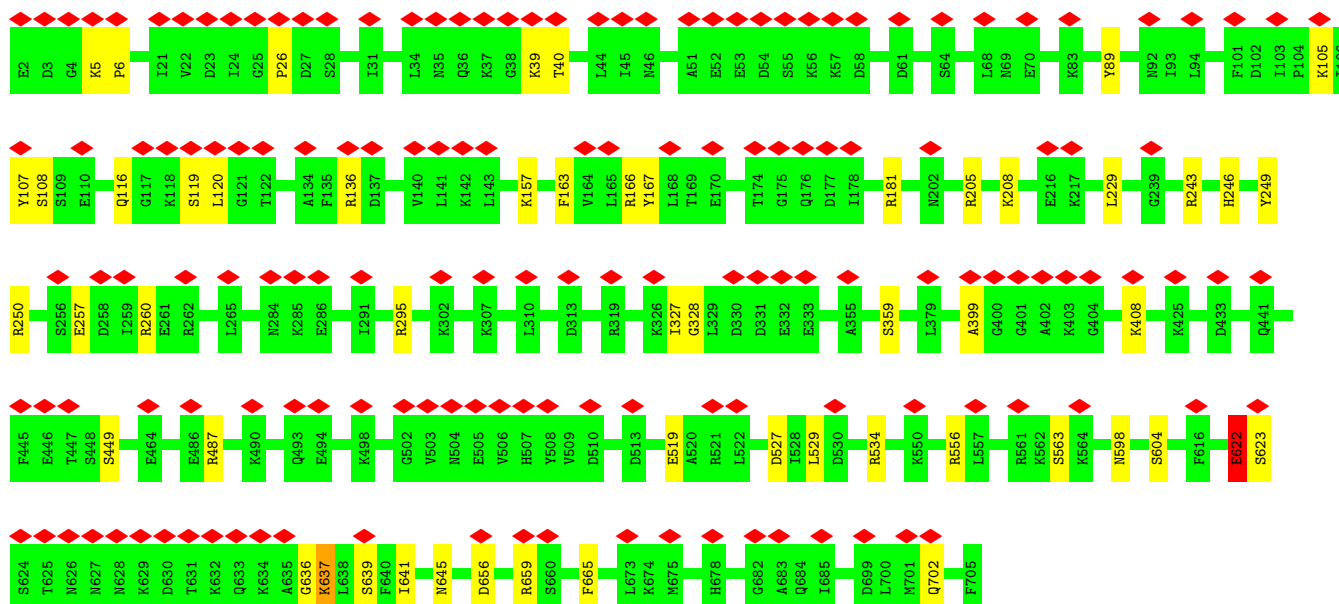
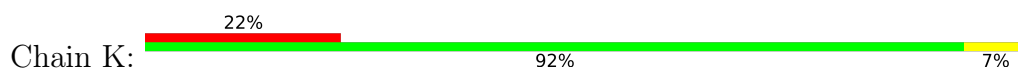


• Molecule 1: Unconventional myosin-VI

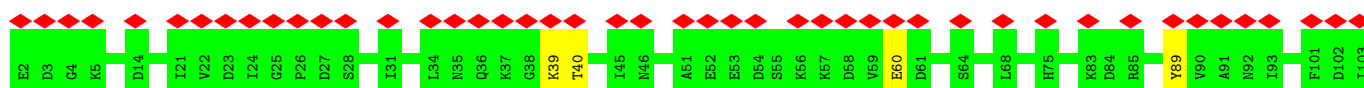


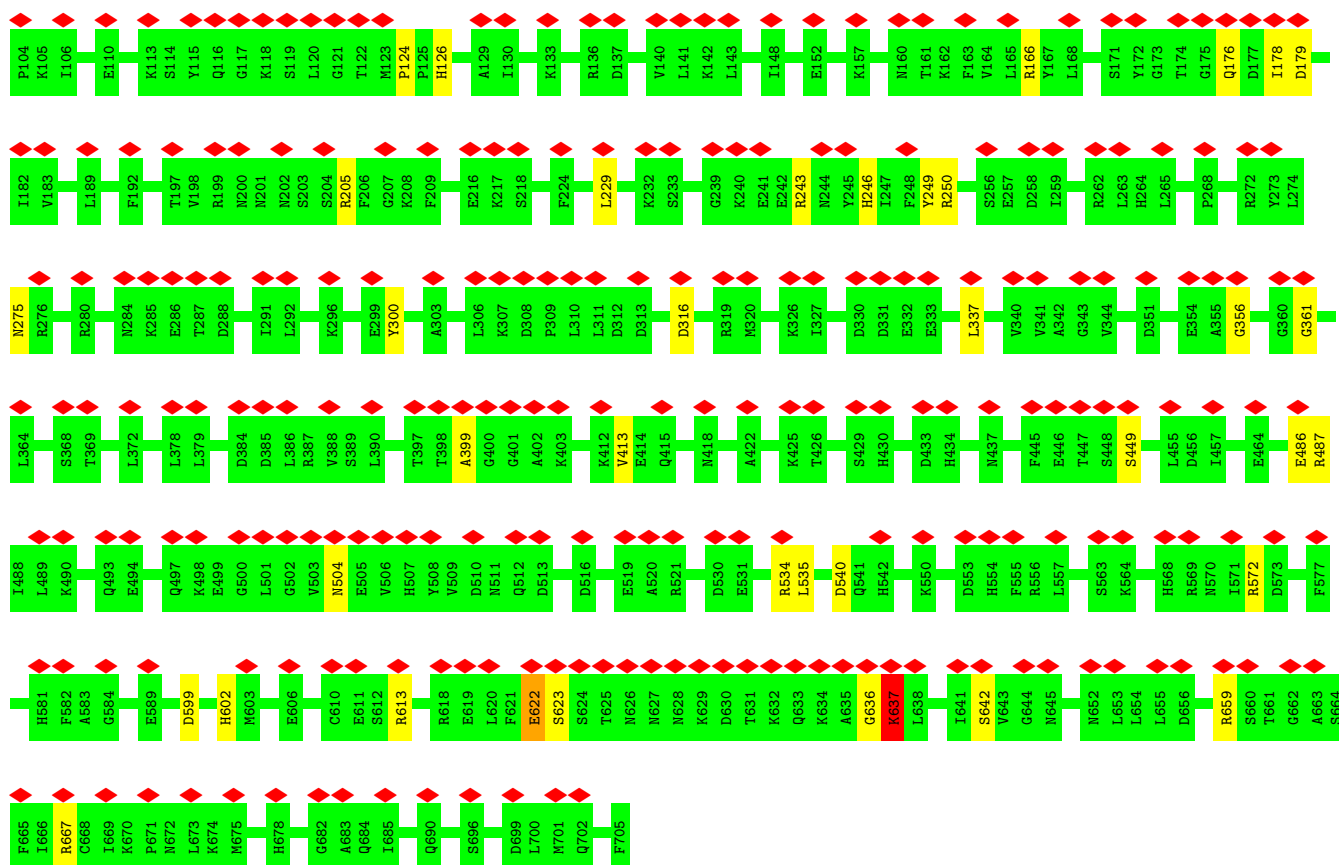


• Molecule 1: Unconventional myosin-VI

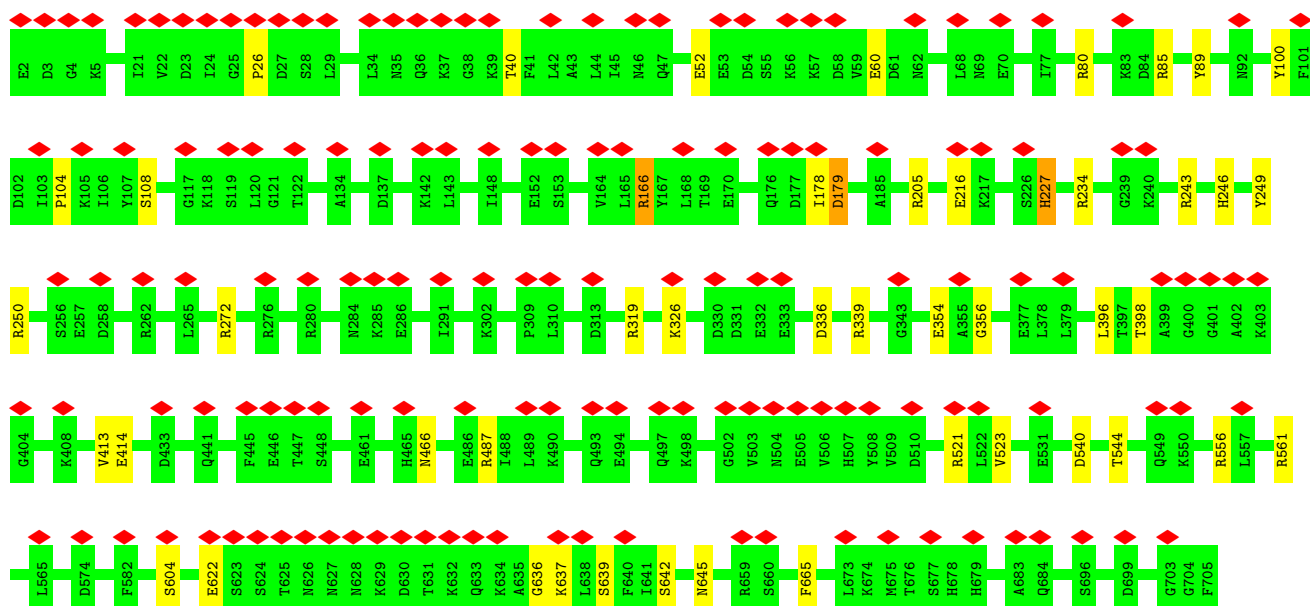


• Molecule 1: Unconventional myosin-VI

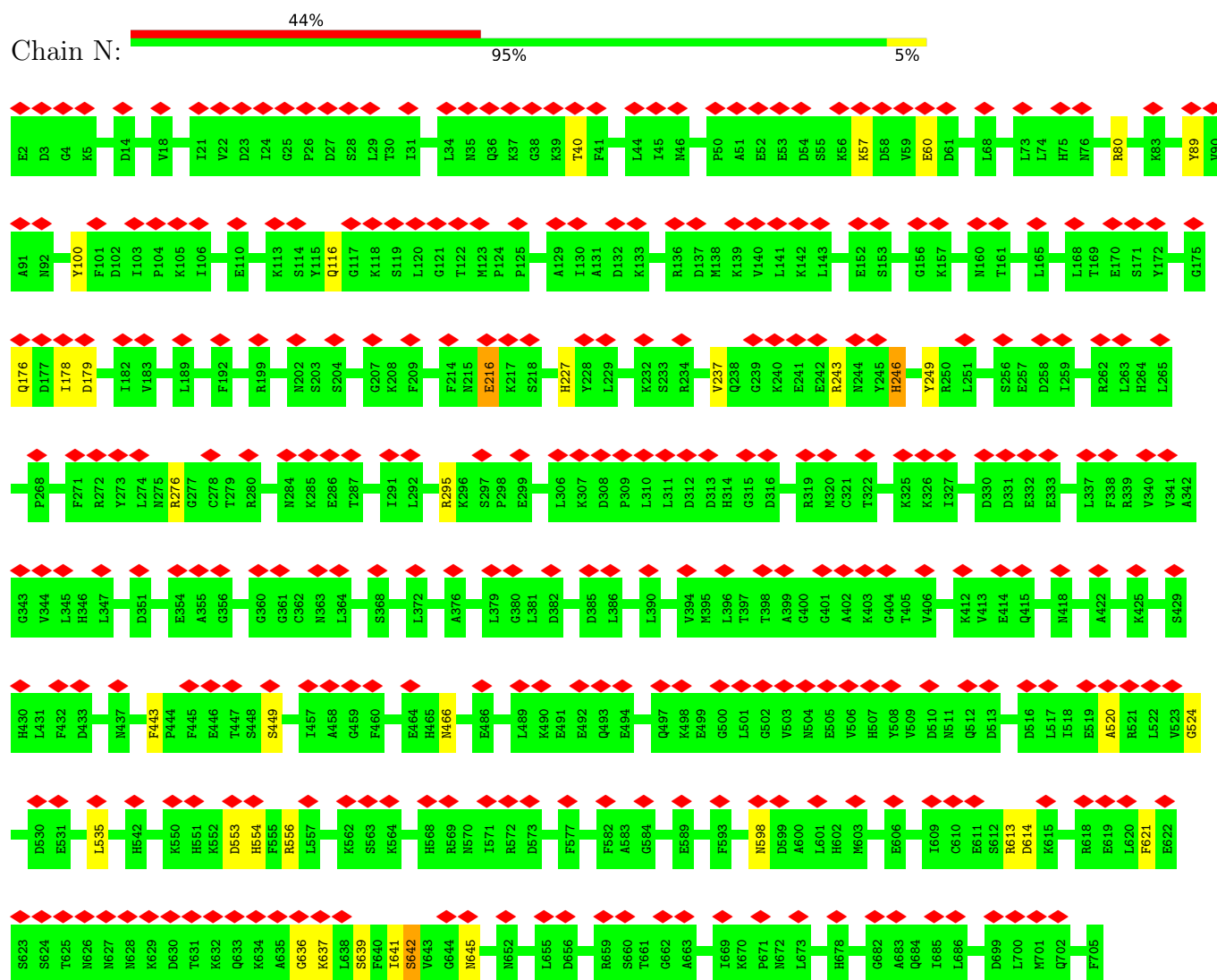




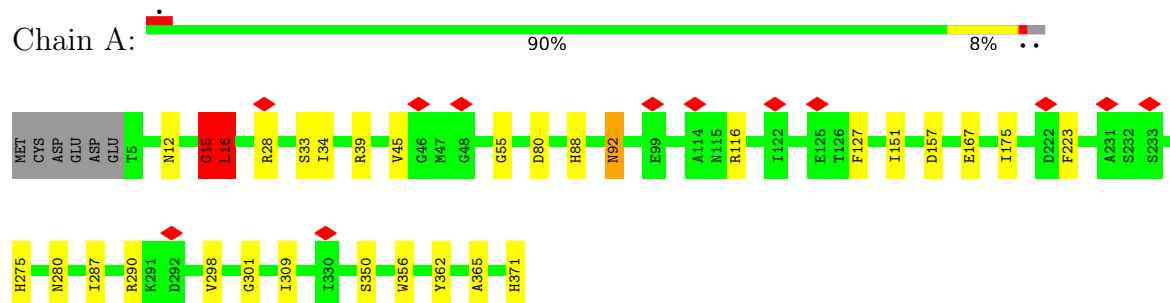
• Molecule 1: Unconventional myosin-VI



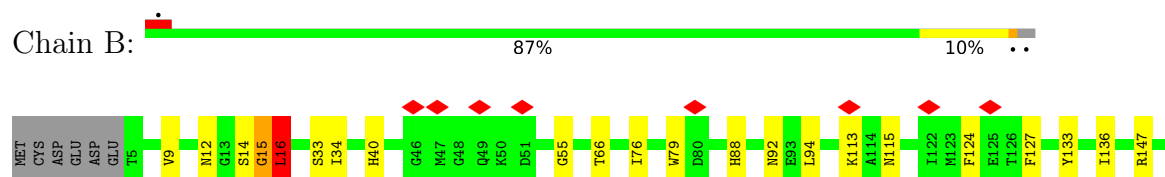
• Molecule 1: Unconventional myosin-VI

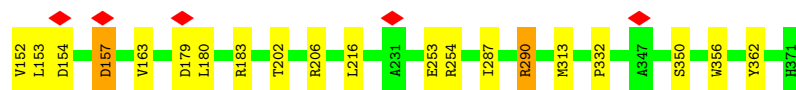


• Molecule 2: Actin, alpha skeletal muscle



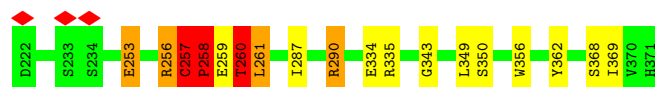
• Molecule 2: Actin, alpha skeletal muscle





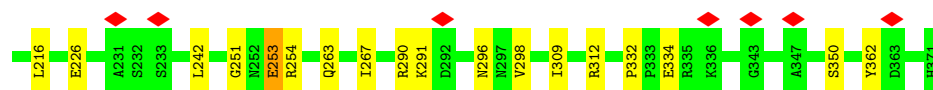
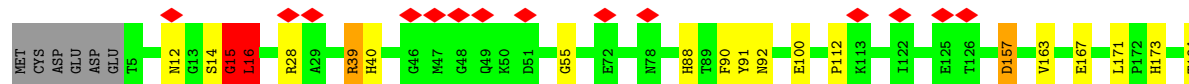
- Molecule 2: Actin, alpha skeletal muscle

Chain C: 87% 10% ..



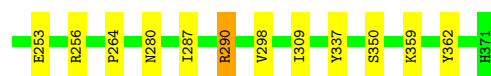
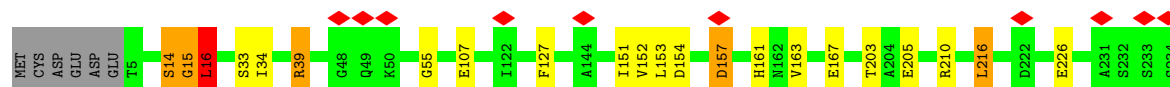
- Molecule 2: Actin, alpha skeletal muscle

Chain D: 6% 88% 9% ..



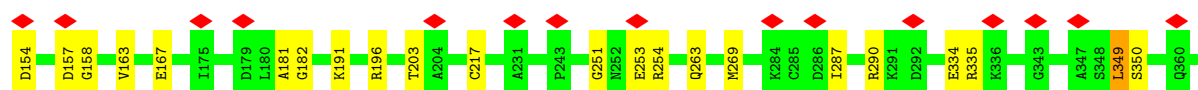
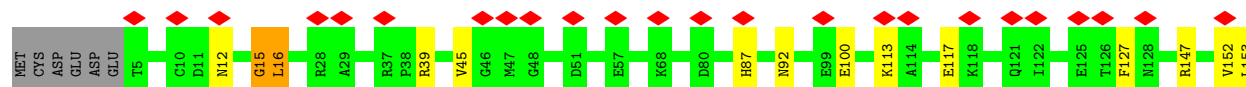
- Molecule 2: Actin, alpha skeletal muscle

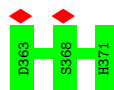
Chain E: 89% 7% ..



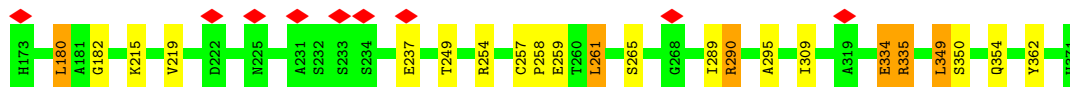
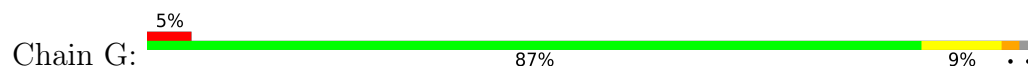
- Molecule 2: Actin, alpha skeletal muscle

Chain F: 11% 89% 9% ..

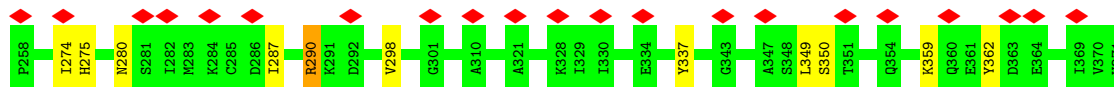
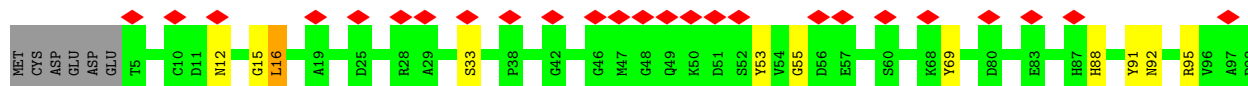
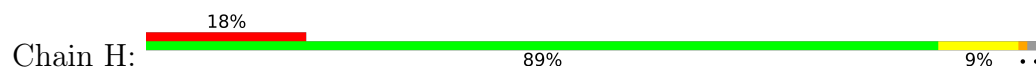




- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.73°, rise=28.06 Å, axial sym=C1	Depositor
Number of segments used	56116	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 ($e^-/\text{\AA}^2$)	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	20.608	Depositor
Minimum map value	-9.432	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	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: ADP, MG

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	0/5718	1.38	15/7705 (0.2%)
1	J	0.87	0/5718	1.40	24/7705 (0.3%)
1	K	0.87	0/5718	1.38	23/7705 (0.3%)
1	L	0.87	0/5718	1.41	26/7705 (0.3%)
1	M	0.87	0/5718	1.39	16/7705 (0.2%)
1	N	0.87	0/5718	1.38	16/7705 (0.2%)
2	A	0.85	0/2924	1.54	20/3963 (0.5%)
2	B	0.86	1/2924 (0.0%)	1.59	30/3963 (0.8%)
2	C	1.18	15/2924 (0.5%)	1.82	49/3963 (1.2%)
2	D	0.85	0/2924	1.55	30/3963 (0.8%)
2	E	0.88	1/2924 (0.0%)	1.59	33/3963 (0.8%)
2	F	0.87	1/2924 (0.0%)	1.56	27/3963 (0.7%)
2	G	0.96	4/2924 (0.1%)	1.59	32/3963 (0.8%)
2	H	0.87	1/2924 (0.0%)	1.56	31/3963 (0.8%)
All	All	0.89	23/57700 (0.0%)	1.48	372/77934 (0.5%)

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	7
1	J	0	6
1	K	0	12
1	L	0	8
1	M	0	13
1	N	0	6
2	A	0	5
2	B	0	6
2	C	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	5
2	E	0	6
2	F	0	4
2	G	0	5
2	H	0	8
All	All	0	101

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	260	THR	CA-C	22.08	1.82	1.52
2	G	258	PRO	C-O	19.16	1.46	1.24
2	C	259	GLU	C-N	18.48	1.59	1.33
2	C	257	CYS	CA-C	14.02	1.69	1.52
2	C	260	THR	C-N	11.12	1.49	1.33
2	C	257	CYS	CA-CB	10.27	1.66	1.53
2	C	261	LEU	CA-CB	9.68	1.69	1.53
2	G	258	PRO	N-CA	8.89	1.59	1.47
2	C	261	LEU	C-O	-8.84	1.12	1.24
2	C	261	LEU	CA-C	-8.43	1.41	1.52
2	E	154	ASP	CA-CB	7.62	1.63	1.53
2	C	260	THR	CA-CB	7.29	1.65	1.53
2	F	154	ASP	CA-CB	6.81	1.62	1.53
2	H	154	ASP	CA-CB	6.76	1.61	1.53
2	C	154	ASP	CA-CB	6.59	1.61	1.53
2	B	154	ASP	CA-CB	6.28	1.61	1.53
2	G	154	ASP	CA-CB	6.09	1.61	1.53
2	C	260	THR	N-CA	6.00	1.53	1.46
2	G	257	CYS	CA-C	5.98	1.59	1.52
2	C	260	THR	CB-OG1	-5.97	1.34	1.43
2	C	258	PRO	N-CA	5.76	1.54	1.47
2	C	256	ARG	C-N	5.42	1.41	1.33
2	C	260	THR	C-O	5.32	1.30	1.24

All (372) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	259	GLU	O-C-N	18.57	141.80	122.12
2	C	260	THR	CA-C-N	18.34	156.58	121.54
2	C	260	THR	C-N-CA	18.34	156.58	121.54
2	C	260	THR	CB-CA-C	-17.43	75.73	110.42
2	C	259	GLU	CA-C-N	-16.75	89.54	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	259	GLU	C-N-CA	-16.75	89.54	121.54
2	C	260	THR	N-CA-CB	15.51	136.71	110.49
2	C	260	THR	CA-CB-CG2	14.14	134.55	110.50
2	C	260	THR	N-CA-C	13.73	140.05	110.80
2	C	259	GLU	N-CA-C	-11.97	98.23	111.28
2	C	260	THR	O-C-N	-10.82	108.20	122.59
2	G	154	ASP	CA-CB-CG	10.55	123.15	112.60
2	E	154	ASP	CA-CB-CG	8.75	121.35	112.60
2	G	15	GLY	CA-C-N	8.75	137.46	121.70
2	G	15	GLY	C-N-CA	8.75	137.46	121.70
2	B	15	GLY	CA-C-N	8.48	136.96	121.70
2	B	15	GLY	C-N-CA	8.48	136.96	121.70
2	C	259	GLU	CA-C-O	-8.46	111.58	120.55
2	F	154	ASP	CA-CB-CG	8.39	120.99	112.60
2	C	256	ARG	CA-C-N	-8.32	108.65	120.97
2	C	256	ARG	C-N-CA	-8.32	108.65	120.97
2	H	127	PHE	CA-CB-CG	-8.29	105.50	113.80
2	F	153	LEU	N-CA-C	8.22	123.04	107.75
2	E	15	GLY	CA-C-N	8.18	136.42	121.70
2	E	15	GLY	C-N-CA	8.18	136.42	121.70
2	G	258	PRO	N-CA-CB	-8.15	94.88	103.52
2	C	260	THR	CA-CB-OG1	-8.11	97.43	109.60
2	F	15	GLY	CA-C-N	7.97	136.04	121.70
2	F	15	GLY	C-N-CA	7.97	136.04	121.70
2	B	154	ASP	CA-CB-CG	7.92	120.52	112.60
2	E	153	LEU	N-CA-C	7.89	122.43	107.75
2	H	153	LEU	N-CA-C	7.88	122.40	107.75
2	C	154	ASP	CA-CB-CG	7.72	120.33	112.60
2	G	100	GLU	N-CA-C	7.72	119.69	111.28
2	B	153	LEU	N-CA-C	7.61	121.90	107.75
2	E	152	VAL	N-CA-C	7.60	119.23	108.36
2	C	15	GLY	CA-C-N	7.58	135.34	121.70
2	C	15	GLY	C-N-CA	7.58	135.34	121.70
2	G	257	CYS	O-C-N	-7.57	113.74	120.48
2	C	153	LEU	N-CA-C	7.55	121.80	107.75
2	H	15	GLY	CA-C-N	7.45	135.12	121.70
2	H	15	GLY	C-N-CA	7.45	135.12	121.70
2	C	258	PRO	N-CA-C	-7.43	97.16	112.47
2	H	154	ASP	CA-CB-CG	7.42	120.02	112.60
2	E	280	ASN	CA-CB-CG	7.40	120.00	112.60
2	C	257	CYS	O-C-N	-7.40	113.52	120.55
2	C	258	PRO	CB-CA-C	-7.38	99.39	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	350	SER	O-C-N	-7.23	114.84	122.94
1	M	622	GLU	CA-C-N	7.23	134.71	121.70
1	M	622	GLU	C-N-CA	7.23	134.71	121.70
2	G	127	PHE	CA-CB-CG	-7.13	106.67	113.80
2	C	55	GLY	CA-C-N	7.12	134.52	121.70
2	C	55	GLY	C-N-CA	7.12	134.52	121.70
2	C	261	LEU	CA-C-O	-7.11	110.34	120.51
1	L	504	ASN	N-CA-C	7.06	119.96	110.35
1	L	622	GLU	CA-C-N	6.85	134.03	121.70
1	L	622	GLU	C-N-CA	6.85	134.03	121.70
2	C	287	ILE	N-CA-C	6.84	116.98	110.42
2	F	163	VAL	N-CA-C	6.83	115.52	107.73
1	I	622	GLU	CA-C-N	6.76	133.86	121.70
1	I	622	GLU	C-N-CA	6.76	133.86	121.70
2	C	349	LEU	N-CA-C	6.75	119.54	110.35
2	G	258	PRO	N-CA-C	6.72	122.37	113.57
2	F	152	VAL	N-CA-C	6.71	117.96	108.36
2	H	152	VAL	CA-C-N	6.71	132.17	122.85
2	H	152	VAL	C-N-CA	6.71	132.17	122.85
1	M	178	ILE	N-CA-C	6.63	117.39	110.62
1	L	89	TYR	CB-CA-C	-6.59	99.76	110.77
2	D	15	GLY	CA-C-N	6.59	133.57	121.70
2	D	15	GLY	C-N-CA	6.59	133.57	121.70
2	H	152	VAL	N-CA-C	6.57	117.75	108.36
2	D	350	SER	CA-C-N	6.56	133.50	121.70
2	D	350	SER	C-N-CA	6.56	133.50	121.70
2	B	163	VAL	N-CA-C	6.55	115.20	107.73
2	A	157	ASP	O-C-N	-6.55	114.98	122.97
2	H	350	SER	O-C-N	-6.47	115.81	123.06
2	B	127	PHE	CA-CB-CG	-6.46	107.34	113.80
1	K	327	ILE	N-CA-C	6.46	116.62	110.42
1	L	540	ASP	N-CA-C	-6.45	105.71	113.97
1	I	637	LYS	CA-C-N	6.45	133.31	121.70
1	I	637	LYS	C-N-CA	6.45	133.31	121.70
2	H	275	HIS	CA-CB-CG	6.39	120.19	113.80
2	B	287	ILE	N-CA-C	6.35	117.09	110.62
2	D	91	TYR	N-CA-C	6.32	119.11	111.40
2	D	55	GLY	CA-C-N	6.26	132.97	121.70
2	D	55	GLY	C-N-CA	6.26	132.97	121.70
2	E	264	PRO	CA-C-N	6.26	129.52	120.38
2	E	264	PRO	C-N-CA	6.26	129.52	120.38
1	I	39	LYS	CA-C-N	6.23	133.45	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	39	LYS	C-N-CA	6.23	133.45	121.54
2	F	152	VAL	CA-C-N	6.23	131.51	122.85
2	F	152	VAL	C-N-CA	6.23	131.51	122.85
2	E	154	ASP	N-CA-CB	6.21	120.62	110.37
2	H	55	GLY	CA-C-N	6.21	132.88	121.70
2	H	55	GLY	C-N-CA	6.21	132.88	121.70
2	A	127	PHE	CA-CB-CG	-6.21	107.59	113.80
1	L	637	LYS	CA-C-N	6.19	132.85	121.70
1	L	637	LYS	C-N-CA	6.19	132.85	121.70
2	H	287	ILE	N-CA-C	6.14	116.32	110.42
2	E	127	PHE	CA-CB-CG	-6.13	107.67	113.80
2	C	343	GLY	CA-C-N	6.12	128.40	120.44
2	C	343	GLY	C-N-CA	6.12	128.40	120.44
2	G	335	ARG	N-CA-C	6.12	119.58	111.75
2	C	152	VAL	CA-C-N	6.10	131.32	122.85
2	C	152	VAL	C-N-CA	6.10	131.32	122.85
2	C	258	PRO	CA-C-N	6.09	128.44	120.28
2	C	258	PRO	C-N-CA	6.09	128.44	120.28
2	C	152	VAL	N-CA-C	6.09	117.07	108.36
1	N	178	ILE	N-CA-C	6.09	116.83	110.62
1	L	179	ASP	N-CA-C	6.08	118.71	111.71
1	I	527	ASP	CA-CB-CG	-6.08	106.52	112.60
2	A	34	ILE	N-CA-C	6.07	117.41	109.58
2	B	152	VAL	CA-C-N	6.05	131.26	122.85
2	B	152	VAL	C-N-CA	6.05	131.26	122.85
1	L	316	ASP	CA-CB-CG	-6.05	106.55	112.60
2	H	173	HIS	CA-CB-CG	6.04	119.84	113.80
2	H	350	SER	CA-C-N	6.02	132.53	121.70
2	H	350	SER	C-N-CA	6.02	132.53	121.70
1	M	179	ASP	N-CA-C	6.01	117.83	111.28
2	B	15	GLY	O-C-N	-5.98	114.93	122.70
1	J	229	LEU	N-CA-C	5.98	119.64	111.39
1	N	641	ILE	CA-C-N	5.96	132.93	121.54
1	N	641	ILE	C-N-CA	5.96	132.93	121.54
1	J	179	ASP	N-CA-C	5.95	117.44	111.07
2	E	152	VAL	CA-C-N	5.94	131.11	122.85
2	E	152	VAL	C-N-CA	5.94	131.11	122.85
2	E	287	ILE	N-CA-C	5.92	116.10	110.42
2	F	335	ARG	N-CA-C	5.92	119.32	111.75
2	G	15	GLY	O-C-N	-5.91	115.01	122.70
2	C	258	PRO	O-C-N	-5.91	114.66	122.64
1	N	227	HIS	CA-CB-CG	5.91	119.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	258	PRO	CA-C-O	5.91	128.03	119.34
2	E	216	LEU	N-CA-C	5.90	120.48	113.28
2	G	349	LEU	N-CA-C	5.89	118.36	110.35
1	J	249	TYR	N-CA-C	-5.84	105.42	113.18
1	K	105	LYS	N-CA-C	5.82	119.58	111.90
2	F	100	GLU	N-CA-C	5.81	117.61	111.28
2	F	113	LYS	O-C-N	-5.80	116.61	123.22
2	E	309	ILE	N-CA-C	-5.80	99.42	108.81
1	J	645	ASN	N-CA-C	-5.79	106.76	113.88
1	M	540	ASP	CA-CB-CG	5.78	118.38	112.60
2	F	350	SER	O-C-N	-5.78	116.47	122.94
1	I	31	ILE	N-CA-C	5.77	117.06	108.23
1	K	702	GLN	CA-C-N	5.76	126.50	119.99
1	K	702	GLN	C-N-CA	5.76	126.50	119.99
2	D	100	GLU	N-CA-C	5.75	117.63	111.36
2	B	34	ILE	N-CA-C	5.74	117.72	109.51
1	K	656	ASP	CA-CB-CG	-5.74	106.86	112.60
1	J	160	ASN	CA-CB-CG	-5.73	106.87	112.60
1	L	599	ASP	CA-CB-CG	5.73	118.33	112.60
2	F	87	HIS	CA-CB-CG	5.73	119.53	113.80
2	H	91	TYR	N-CA-C	5.72	118.38	111.40
1	K	39	LYS	CA-C-N	5.72	132.46	121.54
1	K	39	LYS	C-N-CA	5.72	132.46	121.54
2	B	16	LEU	N-CA-CB	5.72	120.22	110.50
1	K	622	GLU	O-C-N	-5.71	114.99	122.59
2	B	115	ASN	CA-CB-CG	-5.71	106.89	112.60
1	L	361	GLY	N-CA-C	5.71	118.03	111.36
2	G	153	LEU	N-CA-C	5.70	118.35	107.75
2	G	16	LEU	N-CA-CB	5.70	120.19	110.50
1	J	426	THR	N-CA-C	-5.70	105.43	112.72
2	E	55	GLY	CA-C-N	5.69	131.94	121.70
2	E	55	GLY	C-N-CA	5.69	131.94	121.70
2	G	237	GLU	N-CA-C	5.67	118.45	110.23
1	L	275	ASN	N-CA-C	5.66	117.45	111.28
2	A	350	SER	O-C-N	-5.66	115.85	122.81
2	E	359	LYS	N-CA-C	5.65	117.11	111.07
2	G	167	GLU	CA-C-N	5.64	131.85	121.70
2	G	167	GLU	C-N-CA	5.64	131.85	121.70
2	B	154	ASP	N-CA-CB	5.63	119.66	110.37
1	M	249	TYR	N-CA-C	-5.63	105.69	113.18
2	D	298	VAL	N-CA-C	5.63	115.70	107.37
2	D	15	GLY	O-C-N	-5.62	115.39	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	89	TYR	CB-CA-C	-5.62	101.55	110.81
2	C	167	GLU	CA-C-N	5.61	131.81	121.70
2	C	167	GLU	C-N-CA	5.61	131.81	121.70
2	G	152	VAL	N-CA-C	5.61	116.38	108.36
2	C	87	HIS	CA-CB-CG	5.61	119.41	113.80
2	C	290	ARG	CA-C-N	5.61	128.06	120.38
2	C	290	ARG	C-N-CA	5.61	128.06	120.38
1	K	598	ASN	N-CA-C	5.60	118.78	108.58
1	L	637	LYS	O-C-N	-5.60	115.14	122.59
2	E	154	ASP	OD1-CG-OD2	-5.60	109.47	122.90
1	M	645	ASN	N-CA-C	-5.59	107.01	113.88
2	D	157	ASP	CA-C-N	5.58	131.75	121.70
2	D	157	ASP	C-N-CA	5.58	131.75	121.70
2	D	157	ASP	O-C-N	-5.57	116.04	122.95
2	A	157	ASP	CA-C-N	5.57	131.72	121.70
2	A	157	ASP	C-N-CA	5.57	131.72	121.70
2	E	157	ASP	O-C-N	-5.57	115.19	122.59
1	K	163	PHE	CA-CB-CG	-5.57	108.23	113.80
1	J	628	ASN	N-CA-C	5.56	118.08	110.24
2	H	154	ASP	OD1-CG-OD2	-5.54	109.59	122.90
2	E	15	GLY	O-C-N	-5.53	115.51	122.70
1	K	5	LYS	CA-C-N	5.52	126.75	119.84
1	K	5	LYS	C-N-CA	5.52	126.75	119.84
2	C	15	GLY	O-C-N	-5.52	115.52	122.70
2	B	350	SER	CA-C-N	5.51	131.62	121.70
2	B	350	SER	C-N-CA	5.51	131.62	121.70
1	N	246	HIS	CA-CB-CG	-5.51	108.29	113.80
2	H	154	ASP	N-CA-CB	5.51	119.46	110.37
2	F	350	SER	CA-C-N	5.49	131.59	121.70
2	F	350	SER	C-N-CA	5.49	131.59	121.70
2	H	15	GLY	O-C-N	-5.49	115.56	122.70
2	A	309	ILE	CA-C-N	5.49	131.57	121.70
2	A	309	ILE	C-N-CA	5.49	131.57	121.70
1	K	637	LYS	CA-C-N	5.48	131.57	121.70
1	K	637	LYS	C-N-CA	5.48	131.57	121.70
2	A	15	GLY	CA-C-N	5.48	131.56	121.70
2	A	15	GLY	C-N-CA	5.48	131.56	121.70
2	H	359	LYS	N-CA-C	5.47	117.25	111.28
1	I	637	LYS	O-C-N	-5.47	115.32	122.59
2	E	34	ILE	N-CA-C	5.47	117.33	109.51
1	I	622	GLU	O-C-N	-5.46	115.33	122.59
2	B	179	ASP	CA-CB-CG	-5.46	107.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	GLY	O-C-N	-5.46	115.60	122.70
2	C	147	ARG	N-CA-C	5.45	117.33	110.24
2	B	157	ASP	O-C-N	-5.45	115.34	122.59
2	D	16	LEU	N-CA-CB	5.45	119.77	110.50
2	E	163	VAL	N-CA-C	5.45	113.94	107.73
1	L	39	LYS	CA-C-N	5.44	131.94	121.54
1	L	39	LYS	C-N-CA	5.44	131.94	121.54
2	A	365	ALA	N-CA-C	5.44	117.02	111.14
2	H	349	LEU	N-CA-C	5.44	118.79	110.20
1	N	249	TYR	N-CA-C	-5.43	105.95	113.18
1	M	108	SER	N-CA-C	5.43	117.55	110.43
1	N	524	GLY	N-CA-C	5.42	119.51	112.25
1	L	356	GLY	CA-C-N	5.41	131.88	121.54
1	L	356	GLY	C-N-CA	5.41	131.88	121.54
2	F	287	ILE	N-CA-C	5.41	115.61	110.42
1	L	622	GLU	O-C-N	-5.41	115.40	122.59
2	F	349	LEU	N-CA-C	5.40	118.27	110.28
1	N	621	PHE	CA-CB-CG	-5.40	108.40	113.80
2	C	335	ARG	N-CA-C	5.39	118.65	111.75
2	D	254	ARG	N-CA-C	5.38	117.85	111.33
1	I	563	SER	N-CA-C	5.38	117.23	110.24
2	C	91	TYR	N-CA-C	5.37	117.95	111.40
2	B	332	PRO	CA-C-O	-5.37	117.04	120.90
1	N	179	ASP	N-CA-C	5.37	117.55	111.11
2	F	181	ALA	CA-C-N	5.37	131.36	121.70
2	F	181	ALA	C-N-CA	5.37	131.36	121.70
2	B	152	VAL	N-CA-C	5.36	116.03	108.36
2	G	91	TYR	N-CA-C	5.36	117.94	111.40
1	L	535	LEU	CA-C-N	5.35	124.80	119.24
1	L	535	LEU	C-N-CA	5.35	124.80	119.24
1	N	535	LEU	CA-C-N	5.35	124.80	119.24
1	N	535	LEU	C-N-CA	5.35	124.80	119.24
2	G	309	ILE	CA-C-N	5.35	131.33	121.70
2	G	309	ILE	C-N-CA	5.35	131.33	121.70
2	D	90	PHE	CB-CA-C	-5.35	102.49	110.88
2	G	290	ARG	CA-C-N	5.34	127.70	120.38
2	G	290	ARG	C-N-CA	5.34	127.70	120.38
2	C	350	SER	O-C-N	-5.34	117.00	123.03
1	L	249	TYR	N-CA-C	-5.34	106.08	113.18
2	D	334	GLU	CA-C-N	5.34	128.18	120.38
2	D	334	GLU	C-N-CA	5.34	128.18	120.38
2	H	254	ARG	N-CA-C	5.34	117.10	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	287	ILE	N-CA-C	5.34	116.06	110.62
2	G	261	LEU	CA-C-N	-5.34	113.33	121.66
2	G	261	LEU	C-N-CA	-5.34	113.33	121.66
2	A	298	VAL	N-CA-C	5.33	115.53	107.80
1	K	665	PHE	N-CA-C	5.32	116.81	109.15
2	D	112	PRO	N-CA-C	5.32	119.93	111.26
2	D	332	PRO	CA-C-O	-5.32	116.53	120.73
1	L	60	GLU	CA-C-N	5.31	129.47	122.30
1	L	60	GLU	C-N-CA	5.31	129.47	122.30
1	J	622	GLU	CA-C-N	5.30	131.25	121.70
1	J	622	GLU	C-N-CA	5.30	131.25	121.70
2	E	253	GLU	CA-C-N	5.30	127.64	120.38
2	E	253	GLU	C-N-CA	5.30	127.64	120.38
2	H	290	ARG	CA-C-N	5.30	127.64	120.38
2	H	290	ARG	C-N-CA	5.30	127.64	120.38
1	L	413	VAL	N-CA-C	5.29	115.92	110.36
1	K	645	ASN	N-CA-C	-5.29	107.37	113.88
2	D	226	GLU	CA-C-N	5.28	127.79	120.29
2	D	226	GLU	C-N-CA	5.28	127.79	120.29
1	M	665	PHE	N-CA-C	5.28	116.75	109.15
1	N	466	ASN	CA-CB-CG	-5.28	107.32	112.60
2	A	223	PHE	CA-C-N	5.27	127.60	120.38
2	A	223	PHE	C-N-CA	5.27	127.60	120.38
2	B	254	ARG	N-CA-C	5.27	117.02	111.28
2	B	113	LYS	O-C-N	-5.25	116.90	123.04
2	B	350	SER	O-C-N	-5.24	116.36	122.81
2	F	16	LEU	N-CA-CB	5.24	119.41	110.50
2	A	55	GLY	CA-C-N	5.24	131.13	121.70
2	A	55	GLY	C-N-CA	5.24	131.13	121.70
2	C	350	SER	CA-C-N	5.24	131.13	121.70
2	C	350	SER	C-N-CA	5.24	131.13	121.70
1	I	540	ASP	CA-CB-CG	5.23	117.83	112.60
1	J	637	LYS	CA-C-N	5.22	131.10	121.70
1	J	637	LYS	C-N-CA	5.22	131.10	121.70
2	G	157	ASP	CA-C-N	5.22	131.10	121.70
2	G	157	ASP	C-N-CA	5.22	131.10	121.70
1	M	89	TYR	CB-CA-C	-5.21	102.07	110.77
2	D	309	ILE	CA-C-N	5.21	131.07	121.70
2	D	309	ILE	C-N-CA	5.21	131.07	121.70
2	H	167	GLU	CA-C-N	5.21	131.07	121.70
2	H	167	GLU	C-N-CA	5.21	131.07	121.70
2	G	334	GLU	N-CA-CB	5.20	119.28	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	246	HIS	CA-CB-CG	-5.19	108.61	113.80
1	J	105	LYS	N-CA-C	5.19	118.40	111.24
2	E	39	ARG	N-CA-C	5.19	119.59	113.16
1	L	124	PRO	N-CA-C	5.18	117.02	110.70
1	K	622	GLU	CA-C-N	5.18	131.03	121.70
1	K	622	GLU	C-N-CA	5.18	131.03	121.70
2	H	274	ILE	N-CA-C	5.18	116.52	110.62
1	J	246	HIS	CA-CB-CG	-5.17	108.63	113.80
1	K	249	TYR	N-CA-C	-5.16	106.31	113.18
2	A	275	HIS	CA-CB-CG	5.16	118.96	113.80
1	K	529	LEU	N-CA-C	5.16	116.90	111.28
2	D	163	VAL	N-CA-C	5.15	113.60	107.73
2	D	267	ILE	CA-C-O	5.15	124.76	119.35
2	B	313	MET	CA-C-N	5.15	127.45	120.65
2	B	313	MET	C-N-CA	5.15	127.45	120.65
2	A	15	GLY	O-C-N	-5.14	116.01	122.70
2	F	127	PHE	CA-CB-CG	-5.14	108.66	113.80
2	F	217	CYS	N-CA-C	5.14	117.75	110.50
2	G	254	ARG	N-CA-C	5.14	116.88	111.28
1	M	227	HIS	CA-CB-CG	5.14	118.94	113.80
2	F	154	ASP	N-CA-CB	5.13	118.84	110.37
2	C	157	ASP	O-C-N	-5.13	115.77	122.59
2	F	254	ARG	N-CA-C	5.12	116.86	111.28
2	H	163	VAL	N-CA-C	5.12	113.57	107.73
1	J	637	LYS	O-C-N	-5.12	115.78	122.59
1	M	104	PRO	N-CA-C	5.12	119.24	110.95
2	F	154	ASP	OD1-CG-OD2	-5.12	110.61	122.90
1	L	229	LEU	N-CA-C	5.12	118.19	111.28
2	E	157	ASP	CA-C-N	5.11	130.90	121.70
2	E	157	ASP	C-N-CA	5.11	130.90	121.70
1	K	519	GLU	N-CA-C	5.11	120.14	112.94
2	B	290	ARG	CA-C-N	5.11	127.38	120.38
2	B	290	ARG	C-N-CA	5.11	127.38	120.38
2	H	154	ASP	N-CA-C	-5.11	99.47	108.20
1	M	413	VAL	N-CA-C	5.10	115.32	110.42
1	N	553	ASP	CA-C-N	5.10	131.29	121.54
1	N	553	ASP	C-N-CA	5.10	131.29	121.54
1	M	356	GLY	CA-C-N	5.09	131.27	121.54
1	M	356	GLY	C-N-CA	5.09	131.27	121.54
2	E	350	SER	CA-C-N	5.09	130.87	121.70
2	E	350	SER	C-N-CA	5.09	130.87	121.70
2	B	94	LEU	N-CA-C	5.09	117.56	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	298	VAL	N-CA-C	5.08	114.89	107.37
2	A	16	LEU	N-CA-CB	5.08	119.14	110.50
2	D	253	GLU	CA-C-N	5.08	127.34	120.38
2	D	253	GLU	C-N-CA	5.08	127.34	120.38
1	K	107	TYR	CA-C-N	5.07	131.23	121.54
1	K	107	TYR	C-N-CA	5.07	131.23	121.54
2	F	154	ASP	N-CA-C	-5.07	99.54	108.20
2	C	154	ASP	OD1-CG-OD2	-5.06	110.75	122.90
1	J	641	ILE	CA-C-N	5.06	131.20	121.54
1	J	641	ILE	C-N-CA	5.06	131.20	121.54
1	I	92	ASN	CA-CB-CG	5.06	117.66	112.60
1	M	466	ASN	CA-CB-CG	-5.05	107.55	112.60
1	J	11	HIS	CA-C-N	5.05	124.49	119.24
1	J	11	HIS	C-N-CA	5.05	124.49	119.24
2	E	290	ARG	CA-C-N	5.05	127.30	120.38
2	E	290	ARG	C-N-CA	5.05	127.30	120.38
2	G	215	LYS	N-CA-C	5.05	116.59	111.14
2	G	113	LYS	O-C-N	-5.05	117.47	123.22
1	I	612	SER	N-CA-C	5.04	116.79	110.24
1	J	151	GLY	N-CA-C	5.04	119.20	112.65
1	N	645	ASN	N-CA-C	-5.04	107.69	113.88
2	E	14	SER	N-CA-C	-5.03	105.89	112.23
1	J	528	ILE	CA-C-N	5.03	127.02	120.28
1	J	528	ILE	C-N-CA	5.03	127.02	120.28
2	D	296	ASN	N-CA-C	-5.02	105.47	112.30
2	B	55	GLY	CA-C-N	5.02	130.74	121.70
2	B	55	GLY	C-N-CA	5.02	130.74	121.70
1	N	642	SER	N-CA-CB	5.02	118.97	110.49
2	G	350	SER	O-C-N	-5.01	117.33	123.10
1	J	182	ILE	CA-C-N	5.00	127.32	120.46
1	J	182	ILE	C-N-CA	5.00	127.32	120.46

There are no chirality outliers.

All (101) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	116	ARG	Sidechain
2	A	28	ARG	Sidechain
2	A	290	ARG	Sidechain
2	A	362	TYR	Sidechain
2	A	39	ARG	Sidechain
2	B	133	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	147	ARG	Sidechain
2	B	183	ARG	Sidechain
2	B	206	ARG	Sidechain
2	B	290	ARG	Sidechain
2	B	362	TYR	Sidechain
2	C	116	ARG	Sidechain
2	C	196	ARG	Sidechain
2	C	210	ARG	Sidechain
2	C	257	CYS	Mainchain
2	C	260	THR	Peptide,Mainchain
2	C	28	ARG	Sidechain
2	C	290	ARG	Sidechain
2	C	362	TYR	Sidechain
2	C	39	ARG	Sidechain
2	D	28	ARG	Sidechain
2	D	290	ARG	Sidechain
2	D	312	ARG	Sidechain
2	D	362	TYR	Sidechain
2	D	39	ARG	Sidechain
2	E	210	ARG	Sidechain
2	E	256	ARG	Sidechain
2	E	290	ARG	Sidechain
2	E	337	TYR	Sidechain
2	E	362	TYR	Sidechain
2	E	39	ARG	Sidechain
2	F	147	ARG	Sidechain
2	F	196	ARG	Sidechain
2	F	290	ARG	Sidechain
2	F	39	ARG	Sidechain
2	G	290	ARG	Sidechain
2	G	335	ARG	Sidechain
2	G	349	LEU	Peptide
2	G	362	TYR	Sidechain
2	G	39	ARG	Sidechain
2	H	116	ARG	Sidechain
2	H	196	ARG	Sidechain
2	H	290	ARG	Sidechain
2	H	337	TYR	Sidechain
2	H	362	TYR	Sidechain
2	H	53	TYR	Sidechain
2	H	69	TYR	Sidechain
2	H	95	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	100	TYR	Sidechain
1	I	166	ARG	Sidechain
1	I	250	ARG	Sidechain
1	I	262	ARG	Sidechain
1	I	613	ARG	Sidechain
1	I	636	GLY	Peptide
1	I	85	ARG	Sidechain
1	J	181	ARG	Sidechain
1	J	262	ARG	Sidechain
1	J	475	TYR	Sidechain
1	J	572	ARG	Sidechain
1	J	636	GLY	Peptide
1	J	667	ARG	Sidechain
1	K	136	ARG	Sidechain
1	K	166	ARG	Sidechain
1	K	167	TYR	Sidechain
1	K	181	ARG	Sidechain
1	K	205	ARG	Sidechain
1	K	250	ARG	Sidechain
1	K	295	ARG	Sidechain
1	K	487	ARG	Sidechain
1	K	534	ARG	Sidechain
1	K	556	ARG	Sidechain
1	K	636	GLY	Peptide
1	K	89	TYR	Sidechain
1	L	166	ARG	Sidechain
1	L	205	ARG	Sidechain
1	L	250	ARG	Sidechain
1	L	300	TYR	Sidechain
1	L	487	ARG	Sidechain
1	L	613	ARG	Sidechain
1	L	636	GLY	Peptide
1	L	667	ARG	Sidechain
1	M	100	TYR	Sidechain
1	M	166	ARG	Sidechain
1	M	205	ARG	Sidechain
1	M	234	ARG	Sidechain
1	M	250	ARG	Sidechain
1	M	272	ARG	Sidechain
1	M	319	ARG	Sidechain
1	M	487	ARG	Sidechain
1	M	521	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	556	ARG	Sidechain
1	M	561	ARG	Sidechain
1	M	636	GLY	Peptide
1	M	85	ARG	Sidechain
1	N	100	TYR	Sidechain
1	N	276	ARG	Sidechain
1	N	295	ARG	Sidechain
1	N	556	ARG	Sidechain
1	N	613	ARG	Sidechain
1	N	636	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	5612	0	5549	3	0
1	J	5612	0	5549	1	0
1	K	5612	0	5549	3	0
1	L	5612	0	5549	5	0
1	M	5612	0	5549	5	0
1	N	5612	0	5549	3	0
2	A	2862	0	2831	2	0
2	B	2862	0	2831	4	0
2	C	2862	0	2831	11	0
2	D	2862	0	2831	6	0
2	E	2862	0	2831	1	0
2	F	2862	0	2831	3	0
2	G	2862	0	2831	14	0
2	H	2862	0	2831	2	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
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	56792	0	56038	61	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 (61) 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:C:260:THR:CA	2:C:260:THR:C	1.82	1.53
2:C:260:THR:C	2:C:260:THR:CB	2.14	1.20
2:C:260:THR:C	2:C:260:THR:HB	1.97	0.89
2:G:219:VAL:HG13	2:G:259:GLU:HG2	1.57	0.86
2:G:180:LEU:HD21	2:G:261:LEU:HD12	1.73	0.70
2:G:180:LEU:CD2	2:G:261:LEU:HD12	2.27	0.64
2:C:257:CYS:C	2:C:260:THR:H	2.07	0.62
2:G:180:LEU:CD2	2:G:261:LEU:CD1	2.77	0.62
2:C:260:THR:C	2:C:260:THR:CG2	2.73	0.61
2:C:256:ARG:O	2:C:260:THR:N	2.35	0.59
2:H:253:GLU:H	2:H:253:GLU:CD	2.11	0.59
2:F:253:GLU:H	2:F:253:GLU:CD	2.12	0.58
1:I:243:ARG:HH21	1:I:246:HIS:CD2	2.23	0.57
1:J:243:ARG:HH21	1:J:246:HIS:CD2	2.24	0.56
2:C:88:HIS:CD2	2:C:92:ASN:HD21	2.27	0.52
2:D:253:GLU:H	2:D:253:GLU:CD	2.18	0.52
1:K:243:ARG:HH21	1:K:246:HIS:CD2	2.28	0.51
1:N:243:ARG:HH21	1:N:246:HIS:CD2	2.27	0.51
2:D:88:HIS:CE1	2:D:92:ASN:HD21	2.29	0.51
1:M:243:ARG:HH21	1:M:246:HIS:CD2	2.30	0.49
1:N:60:GLU:CD	1:N:80:ARG:HH12	2.19	0.49
2:C:257:CYS:HB3	2:C:258:PRO:HD3	1.95	0.48
2:G:180:LEU:HD23	2:G:261:LEU:HD11	1.96	0.48
2:A:15:GLY:HA3	2:A:16:LEU:HB2	1.95	0.48
2:D:15:GLY:HA3	2:D:16:LEU:HB2	1.95	0.48
1:L:243:ARG:HH21	1:L:246:HIS:CD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:88:HIS:CE1	2:A:92:ASN:HD21	2.32	0.48
2:B:15:GLY:HA3	2:B:16:LEU:HB2	1.96	0.47
2:G:180:LEU:CD2	2:G:261:LEU:HD11	2.44	0.47
2:G:15:GLY:HA3	2:G:16:LEU:HB2	1.97	0.47
2:H:88:HIS:CE1	2:H:92:ASN:HD21	2.32	0.47
2:C:260:THR:C	2:C:260:THR:HG22	2.41	0.46
1:M:166:ARG:HH12	1:M:179:ASP:CG	2.24	0.46
2:C:98:PRO:HA	2:C:101:HIS:CE1	2.51	0.45
2:B:40:HIS:CE1	2:D:173:HIS:HE1	2.35	0.45
2:G:157:ASP:HA	2:G:182:GLY:H	1.81	0.45
1:L:602:HIS:CD2	1:L:602:HIS:H	2.34	0.45
2:G:180:LEU:HD23	2:G:261:LEU:CD1	2.47	0.44
1:M:60:GLU:CD	1:M:80:ARG:HH12	2.26	0.44
1:K:257:GLU:CD	1:K:260:ARG:HH21	2.25	0.43
2:B:88:HIS:CE1	2:B:92:ASN:HD21	2.36	0.43
1:L:486:GLU:CD	1:L:659:ARG:HH21	2.27	0.43
2:C:253:GLU:H	2:C:253:GLU:CD	2.26	0.43
2:B:76:ILE:HD11	2:B:79:TRP:CE2	2.54	0.42
2:F:158:GLY:HA2	2:F:182:GLY:H	1.83	0.42
2:G:166:TYR:CD1	2:G:289:ILE:HG23	2.54	0.42
1:K:622:GLU:HB3	1:K:623:SER:HA	2.01	0.42
2:G:219:VAL:HG13	2:G:259:GLU:CG	2.38	0.42
1:I:622:GLU:HB3	1:I:623:SER:HA	2.02	0.41
1:L:534:ARG:HB2	2:F:349:LEU:HD21	2.02	0.41
2:D:171:LEU:H	2:D:171:LEU:HD22	1.84	0.41
1:N:216:GLU:H	1:N:216:GLU:CD	2.28	0.41
2:G:19:ALA:HB1	2:G:94:LEU:HD11	2.03	0.41
1:L:622:GLU:HB3	1:L:623:SER:HA	2.02	0.41
1:M:396:LEU:HD23	1:M:396:LEU:H	1.86	0.41
2:D:39:ARG:HH11	2:D:40:HIS:HE2	1.68	0.41
2:E:15:GLY:HA3	2:E:16:LEU:HB2	2.03	0.41
2:G:88:HIS:CD2	2:G:92:ASN:HD21	2.38	0.40
2:G:88:HIS:CE1	2:G:92:ASN:HD21	2.38	0.40
1:I:257:GLU:CD	1:I:260:ARG:HH21	2.29	0.40
1:M:336:ASP:CG	1:M:339:ARG:HH21	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	702/704 (100%)	636 (91%)	58 (8%)	8 (1%)	11	45
1	J	702/704 (100%)	644 (92%)	46 (7%)	12 (2%)	7	35
1	K	702/704 (100%)	644 (92%)	42 (6%)	16 (2%)	5	28
1	L	702/704 (100%)	641 (91%)	54 (8%)	7 (1%)	12	47
1	M	702/704 (100%)	640 (91%)	55 (8%)	7 (1%)	12	47
1	N	702/704 (100%)	637 (91%)	55 (8%)	10 (1%)	9	39
2	A	365/373 (98%)	331 (91%)	30 (8%)	4 (1%)	11	45
2	B	365/373 (98%)	330 (90%)	32 (9%)	3 (1%)	16	53
2	C	365/373 (98%)	320 (88%)	39 (11%)	6 (2%)	7	37
2	D	365/373 (98%)	325 (89%)	35 (10%)	5 (1%)	9	39
2	E	365/373 (98%)	327 (90%)	35 (10%)	3 (1%)	16	53
2	F	365/373 (98%)	320 (88%)	39 (11%)	6 (2%)	7	37
2	G	365/373 (98%)	325 (89%)	35 (10%)	5 (1%)	9	39
2	H	365/373 (98%)	323 (88%)	39 (11%)	3 (1%)	16	53
All	All	7132/7208 (99%)	6443 (90%)	594 (8%)	95 (1%)	12	41

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	40	THR
1	J	637	LYS
1	J	642	SER
1	M	637	LYS
1	N	449	SER
1	N	554	HIS
1	N	637	LYS
1	N	642	SER
2	B	16	LEU

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Mol	Chain	Res	Type
2	C	261	LEU
2	E	16	LEU
2	G	16	LEU
2	G	334	GLU
1	I	229	LEU
1	I	637	LYS
1	I	642	SER
1	J	40	THR
1	J	449	SER
1	J	639	SER
1	K	40	THR
1	K	449	SER
1	K	641	ILE
1	L	449	SER
1	M	639	SER
1	M	642	SER
1	N	40	THR
1	N	520	ALA
1	N	598	ASN
2	A	33	SER
2	A	167	GLU
2	C	16	LEU
2	C	368	SER
2	D	167	GLU
2	E	167	GLU
2	F	16	LEU
2	H	16	LEU
1	I	520	ALA
1	J	116	GLN
1	J	357	SER
1	J	612	SER
1	J	622	GLU
1	K	6	PRO
1	K	108	SER
1	K	119	SER
1	K	229	LEU
1	K	639	SER
1	L	40	THR
1	L	178	ILE
1	L	637	LYS
1	L	642	SER
1	M	26	PRO

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Mol	Chain	Res	Type
1	N	116	GLN
2	D	16	LEU
2	F	167	GLU
2	G	180	LEU
2	G	265	SER
1	K	26	PRO
1	K	120	LEU
1	K	328	GLY
1	K	563	SER
1	K	637	LYS
1	L	399	ALA
1	M	40	THR
1	M	354	GLU
1	N	176	GLN
1	N	639	SER
2	B	33	SER
2	D	263	GLN
2	E	33	SER
2	F	263	GLN
2	F	334	GLU
2	G	295	ALA
2	H	33	SER
1	I	504	ASN
1	J	399	ALA
1	K	116	GLN
1	K	622	GLU
1	L	176	GLN
2	B	180	LEU
2	C	334	GLU
1	K	399	ALA
2	C	369	ILE
1	I	641	ILE
1	J	400	GLY
2	F	251	GLY
2	C	45	VAL
2	F	15	GLY
1	J	328	GLY
2	A	15	GLY
2	D	251	GLY
2	H	251	GLY
1	I	10	PRO
1	M	523	VAL

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Mol	Chain	Res	Type
2	D	15	GLY
2	A	301	GLY

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	621/621 (100%)	614 (99%)	7 (1%)	65	74
1	J	621/621 (100%)	609 (98%)	12 (2%)	50	66
1	K	621/621 (100%)	614 (99%)	7 (1%)	65	74
1	L	621/621 (100%)	617 (99%)	4 (1%)	78	80
1	M	621/621 (100%)	613 (99%)	8 (1%)	61	72
1	N	621/621 (100%)	615 (99%)	6 (1%)	68	76
2	A	310/316 (98%)	300 (97%)	10 (3%)	34	55
2	B	310/316 (98%)	299 (96%)	11 (4%)	32	53
2	C	310/316 (98%)	303 (98%)	7 (2%)	44	63
2	D	310/316 (98%)	303 (98%)	7 (2%)	44	63
2	E	310/316 (98%)	299 (96%)	11 (4%)	32	53
2	F	310/316 (98%)	302 (97%)	8 (3%)	40	60
2	G	310/316 (98%)	302 (97%)	8 (3%)	40	60
2	H	310/316 (98%)	305 (98%)	5 (2%)	55	69
All	All	6206/6254 (99%)	6095 (98%)	111 (2%)	51	67

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	34	LEU
1	I	89	TYR
1	I	216	GLU
1	I	226	SER
1	I	383	GLN

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Mol	Chain	Res	Type
1	I	395	MET
1	I	697	VAL
1	J	27	ASP
1	J	34	LEU
1	J	126	HIS
1	J	157	LYS
1	J	227	HIS
1	J	251	LEU
1	J	523	VAL
1	J	530	ASP
1	J	551	HIS
1	J	553	ASP
1	J	577	PHE
1	J	652	ASN
1	K	157	LYS
1	K	208	LYS
1	K	359	SER
1	K	408	LYS
1	K	527	ASP
1	K	604	SER
1	K	659	ARG
1	L	126	HIS
1	L	337	LEU
1	L	572	ARG
1	L	637	LYS
1	M	52	GLU
1	M	216	GLU
1	M	227	HIS
1	M	326	LYS
1	M	398	THR
1	M	414	GLU
1	M	544	THR
1	M	604	SER
1	N	57	LYS
1	N	89	TYR
1	N	216	GLU
1	N	237	VAL
1	N	443	PHE
1	N	614	ASP
2	A	12	ASN
2	A	16	LEU
2	A	45	VAL

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Mol	Chain	Res	Type
2	A	80	ASP
2	A	92	ASN
2	A	151	ILE
2	A	175	ILE
2	A	280	ASN
2	A	356	TRP
2	A	371	HIS
2	B	9	VAL
2	B	12	ASN
2	B	14	SER
2	B	66	THR
2	B	124	PHE
2	B	136	ILE
2	B	157	ASP
2	B	202	THR
2	B	216	LEU
2	B	253	GLU
2	B	356	TRP
2	C	9	VAL
2	C	12	ASN
2	C	124	PHE
2	C	206	ARG
2	C	253	GLU
2	C	258	PRO
2	C	356	TRP
2	D	12	ASN
2	D	14	SER
2	D	157	ASP
2	D	194	THR
2	D	216	LEU
2	D	242	LEU
2	D	291	LYS
2	E	14	SER
2	E	16	LEU
2	E	107	GLU
2	E	151	ILE
2	E	157	ASP
2	E	161	HIS
2	E	203	THR
2	E	205	GLU
2	E	216	LEU
2	E	226	GLU

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Mol	Chain	Res	Type
2	E	298	VAL
2	F	12	ASN
2	F	45	VAL
2	F	92	ASN
2	F	117	GLU
2	F	157	ASP
2	F	191	LYS
2	F	203	THR
2	F	269	MET
2	G	9	VAL
2	G	12	ASN
2	G	56	ASP
2	G	115	ASN
2	G	124	PHE
2	G	154	ASP
2	G	249	THR
2	G	354	GLN
2	H	12	ASN
2	H	16	LEU
2	H	124	PHE
2	H	201	VAL
2	H	280	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	126	HIS
1	I	284	ASN
1	I	383	GLN
1	I	481	GLN
1	I	533	ASN
1	J	75	HIS
1	J	294	ASN
1	J	383	GLN
1	J	470	GLN
1	J	533	ASN
1	J	551	HIS
1	J	554	HIS
1	J	570	ASN
1	J	684	GLN
1	K	20	ASN
1	K	349	ASN

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Mol	Chain	Res	Type
1	K	434	HIS
1	K	481	GLN
1	K	485	ASN
1	K	533	ASN
1	K	554	HIS
1	K	568	HIS
1	L	145	GLN
1	L	194	ASN
1	L	213	HIS
1	L	270	ASN
1	L	284	ASN
1	L	418	ASN
1	L	548	HIS
1	L	551	HIS
1	L	645	ASN
1	M	194	ASN
1	M	200	ASN
1	M	293	GLN
1	M	533	ASN
1	M	551	HIS
1	M	602	HIS
1	N	11	HIS
1	N	160	ASN
1	N	264	HIS
1	N	270	ASN
1	N	284	ASN
1	N	293	GLN
1	N	314	HIS
1	N	434	HIS
1	N	533	ASN
1	N	541	GLN
1	N	549	GLN
1	N	568	HIS
1	N	602	HIS
2	A	12	ASN
2	A	49	GLN
2	A	88	HIS
2	A	92	ASN
2	A	101	HIS
2	A	161	HIS
2	A	162	ASN
2	B	12	ASN

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Mol	Chain	Res	Type
2	B	88	HIS
2	B	101	HIS
2	B	115	ASN
2	B	275	HIS
2	C	12	ASN
2	C	88	HIS
2	C	92	ASN
2	C	275	HIS
2	C	296	ASN
2	C	297	ASN
2	C	371	HIS
2	D	78	ASN
2	D	88	HIS
2	D	92	ASN
2	D	173	HIS
2	D	280	ASN
2	E	12	ASN
2	E	161	HIS
2	E	275	HIS
2	F	12	ASN
2	F	73	HIS
2	F	87	HIS
2	F	280	ASN
2	F	314	GLN
2	G	87	HIS
2	G	88	HIS
2	G	92	ASN
2	G	297	ASN
2	G	354	GLN
2	H	12	ASN
2	H	88	HIS
2	H	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	D	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	F	402	3	28,29,29	1.39	4 (14%)	43,45,45	1.81	10 (23%)
4	ADP	G	402	3	28,29,29	1.39	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	E	402	3	28,29,29	1.37	4 (14%)	43,45,45	1.82	10 (23%)
4	ADP	B	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.82	10 (23%)
4	ADP	C	402	3	28,29,29	1.38	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	H	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.82	10 (23%)
4	ADP	A	402	3	28,29,29	1.38	4 (14%)	43,45,45	1.81	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	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	G	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	B	402	3	-	3/16/32/32	0/3/3/3
4	ADP	C	402	3	-	3/16/32/32	0/3/3/3
4	ADP	H	402	3	-	3/16/32/32	0/3/3/3
4	ADP	A	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	B	402	ADP	C5-C4	4.71	1.47	1.39
4	D	402	ADP	C5-C4	4.70	1.47	1.39
4	C	402	ADP	C5-C4	4.68	1.47	1.39
4	F	402	ADP	C5-C4	4.66	1.47	1.39
4	G	402	ADP	C5-C4	4.65	1.47	1.39
4	E	402	ADP	C5-C4	4.62	1.47	1.39
4	A	402	ADP	C5-C4	4.60	1.47	1.39
4	H	402	ADP	C5-C4	4.57	1.47	1.39
4	B	402	ADP	C5-C6	2.84	1.48	1.41
4	H	402	ADP	C5-C6	2.83	1.48	1.41
4	C	402	ADP	C5-C6	2.82	1.48	1.41
4	G	402	ADP	C5-C6	2.82	1.48	1.41
4	D	402	ADP	C5-C6	2.82	1.48	1.41
4	A	402	ADP	C5-C6	2.82	1.48	1.41
4	F	402	ADP	C5-C6	2.78	1.48	1.41
4	E	402	ADP	C5-C6	2.77	1.48	1.41
4	H	402	ADP	C8-N7	2.46	1.36	1.31
4	F	402	ADP	C8-N7	2.45	1.36	1.31
4	D	402	ADP	C8-N7	2.43	1.36	1.31
4	G	402	ADP	C8-N7	2.42	1.36	1.31
4	B	402	ADP	C8-N7	2.39	1.36	1.31
4	A	402	ADP	C8-N7	2.38	1.36	1.31
4	C	402	ADP	C8-N7	2.37	1.36	1.31
4	E	402	ADP	C8-N7	2.37	1.36	1.31
4	B	402	ADP	C5-N7	-2.23	1.35	1.39
4	A	402	ADP	C5-N7	-2.23	1.35	1.39
4	G	402	ADP	C5-N7	-2.19	1.35	1.39
4	D	402	ADP	C5-N7	-2.18	1.35	1.39
4	H	402	ADP	C5-N7	-2.17	1.35	1.39
4	F	402	ADP	C5-N7	-2.16	1.35	1.39
4	C	402	ADP	C5-N7	-2.14	1.35	1.39
4	E	402	ADP	C5-N7	-2.10	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	-5.73	118.83	126.72
4	D	402	ADP	C5-C4-N3	-5.72	118.84	126.72
4	C	402	ADP	C5-C4-N3	-5.70	118.87	126.72
4	H	402	ADP	C5-C4-N3	-5.69	118.88	126.72
4	E	402	ADP	C5-C4-N3	-5.69	118.89	126.72
4	F	402	ADP	C5-C4-N3	-5.67	118.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	ADP	C5-C4-N3	-5.64	118.95	126.72
4	A	402	ADP	C5-C4-N3	-5.63	118.97	126.72
4	C	402	ADP	N3-C4-N9	4.39	134.63	127.17
4	D	402	ADP	N3-C4-N9	4.38	134.61	127.17
4	A	402	ADP	N3-C4-N9	4.33	134.53	127.17
4	H	402	ADP	N3-C4-N9	4.32	134.52	127.17
4	F	402	ADP	N3-C4-N9	4.32	134.51	127.17
4	G	402	ADP	N3-C4-N9	4.32	134.51	127.17
4	B	402	ADP	N3-C4-N9	4.31	134.49	127.17
4	E	402	ADP	N3-C4-N9	4.30	134.48	127.17
4	G	402	ADP	C4-C5-N7	-3.90	106.12	110.58
4	E	402	ADP	C4-C5-N7	-3.85	106.18	110.58
4	B	402	ADP	C4-C5-N7	-3.85	106.18	110.58
4	D	402	ADP	C4-C5-N7	-3.82	106.22	110.58
4	F	402	ADP	C4-C5-N7	-3.82	106.22	110.58
4	C	402	ADP	C4-C5-N7	-3.81	106.22	110.58
4	H	402	ADP	C4-C5-N7	-3.78	106.26	110.58
4	A	402	ADP	C4-C5-N7	-3.74	106.31	110.58
4	C	402	ADP	C2-N3-C4	3.61	120.64	111.83
4	E	402	ADP	C2-N3-C4	3.59	120.59	111.83
4	D	402	ADP	C2-N3-C4	3.58	120.58	111.83
4	A	402	ADP	C2-N3-C4	3.58	120.57	111.83
4	G	402	ADP	C2-N3-C4	3.55	120.51	111.83
4	H	402	ADP	C2-N3-C4	3.55	120.51	111.83
4	F	402	ADP	C2-N3-C4	3.53	120.46	111.83
4	B	402	ADP	C2-N3-C4	3.53	120.45	111.83
4	E	402	ADP	N3-C2-N1	-3.04	123.98	128.58
4	C	402	ADP	N3-C2-N1	-3.02	124.00	128.58
4	A	402	ADP	N3-C2-N1	-2.98	124.07	128.58
4	H	402	ADP	N3-C2-N1	-2.98	124.08	128.58
4	D	402	ADP	N3-C2-N1	-2.97	124.08	128.58
4	F	402	ADP	N3-C2-N1	-2.96	124.10	128.58
4	G	402	ADP	N3-C2-N1	-2.94	124.13	128.58
4	B	402	ADP	C5-N7-C8	2.90	108.01	103.45
4	B	402	ADP	N3-C2-N1	-2.90	124.19	128.58
4	G	402	ADP	C5-N7-C8	2.88	107.98	103.45
4	E	402	ADP	C5-N7-C8	2.86	107.94	103.45
4	C	402	ADP	C5-N7-C8	2.84	107.91	103.45
4	A	402	ADP	C5-N7-C8	2.83	107.89	103.45
4	D	402	ADP	C5-N7-C8	2.79	107.84	103.45
4	H	402	ADP	C4-N9-C8	2.79	108.67	105.74
4	D	402	ADP	C4-N9-C8	2.79	108.67	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	402	ADP	C5-N7-C8	2.78	107.82	103.45
4	H	402	ADP	C5-N7-C8	2.78	107.82	103.45
4	B	402	ADP	C4-N9-C8	2.77	108.65	105.74
4	C	402	ADP	C4-N9-C8	2.77	108.65	105.74
4	G	402	ADP	C4-N9-C8	2.72	108.60	105.74
4	F	402	ADP	C4-N9-C8	2.72	108.59	105.74
4	A	402	ADP	C4-N9-C8	2.70	108.58	105.74
4	E	402	ADP	C4-N9-C8	2.68	108.56	105.74
4	B	402	ADP	N9-C8-N7	-2.34	110.61	113.94
4	H	402	ADP	N9-C8-N7	-2.31	110.65	113.94
4	G	402	ADP	N9-C8-N7	-2.31	110.66	113.94
4	B	402	ADP	C6-C5-N7	2.31	136.54	132.09
4	E	402	ADP	N9-C8-N7	-2.28	110.70	113.94
4	F	402	ADP	C6-C5-N7	2.28	136.48	132.09
4	C	402	ADP	C6-C5-N7	2.27	136.47	132.09
4	A	402	ADP	N9-C8-N7	-2.27	110.72	113.94
4	A	402	ADP	C6-C5-N7	2.26	136.46	132.09
4	C	402	ADP	N9-C8-N7	-2.26	110.73	113.94
4	D	402	ADP	N9-C8-N7	-2.26	110.73	113.94
4	D	402	ADP	C6-C5-N7	2.26	136.45	132.09
4	G	402	ADP	C6-C5-N7	2.25	136.44	132.09
4	E	402	ADP	C6-C5-N7	2.25	136.43	132.09
4	F	402	ADP	N9-C8-N7	-2.21	110.80	113.94
4	H	402	ADP	C3'-C2'-C1'	2.19	105.61	101.46
4	H	402	ADP	C6-C5-N7	2.19	136.32	132.09
4	D	402	ADP	C3'-C2'-C1'	2.19	105.60	101.46
4	F	402	ADP	C3'-C2'-C1'	2.18	105.58	101.46
4	E	402	ADP	C3'-C2'-C1'	2.16	105.56	101.46
4	B	402	ADP	C3'-C2'-C1'	2.16	105.55	101.46
4	G	402	ADP	C3'-C2'-C1'	2.16	105.54	101.46
4	C	402	ADP	C3'-C2'-C1'	2.15	105.53	101.46
4	A	402	ADP	C3'-C2'-C1'	2.12	105.48	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

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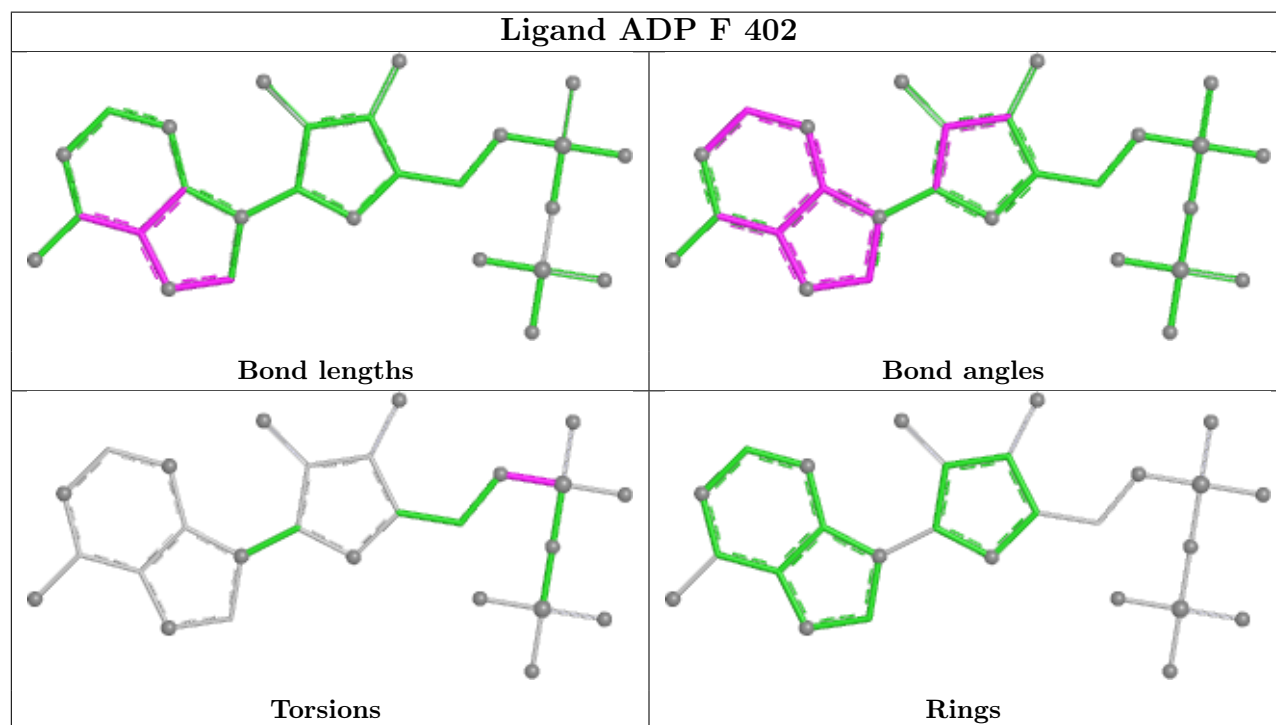
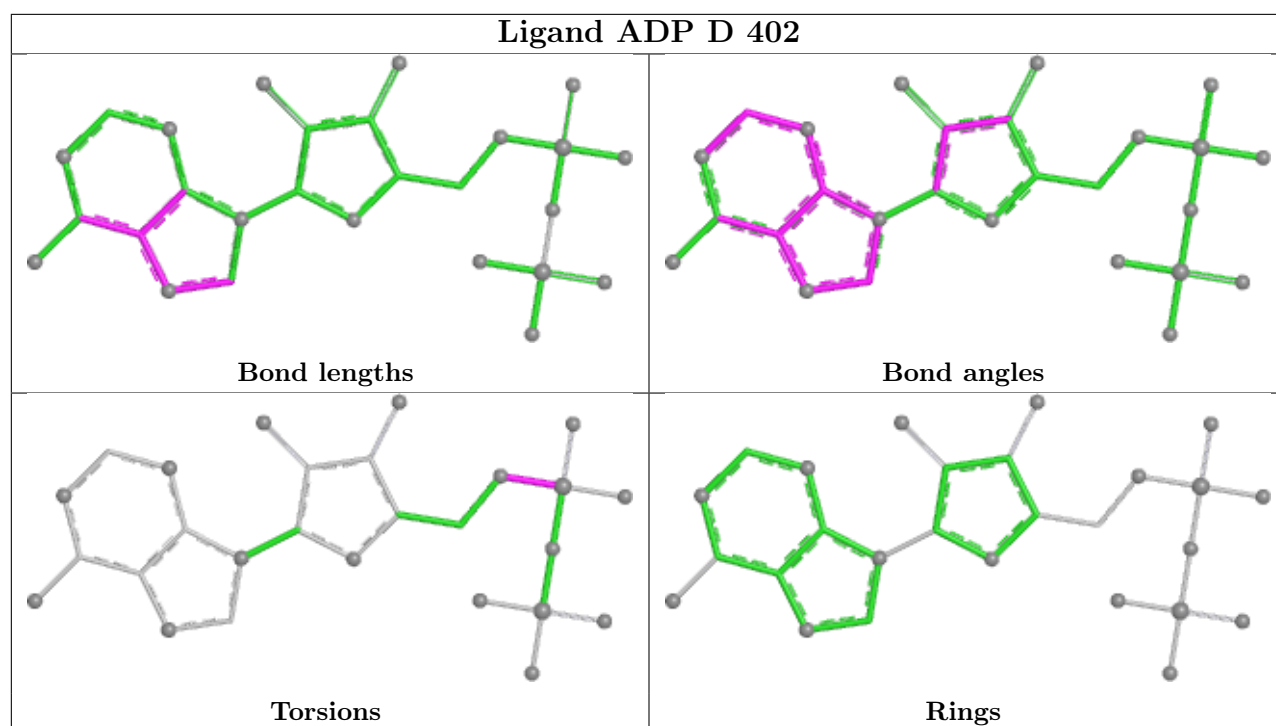
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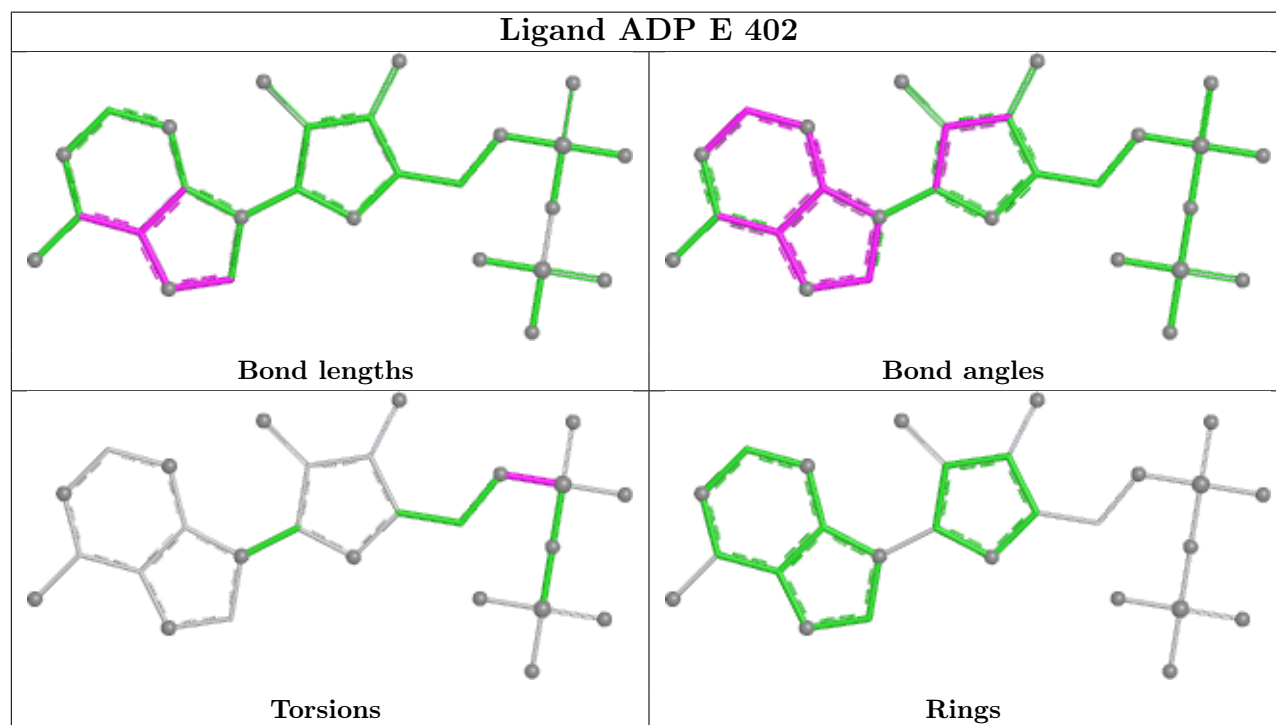
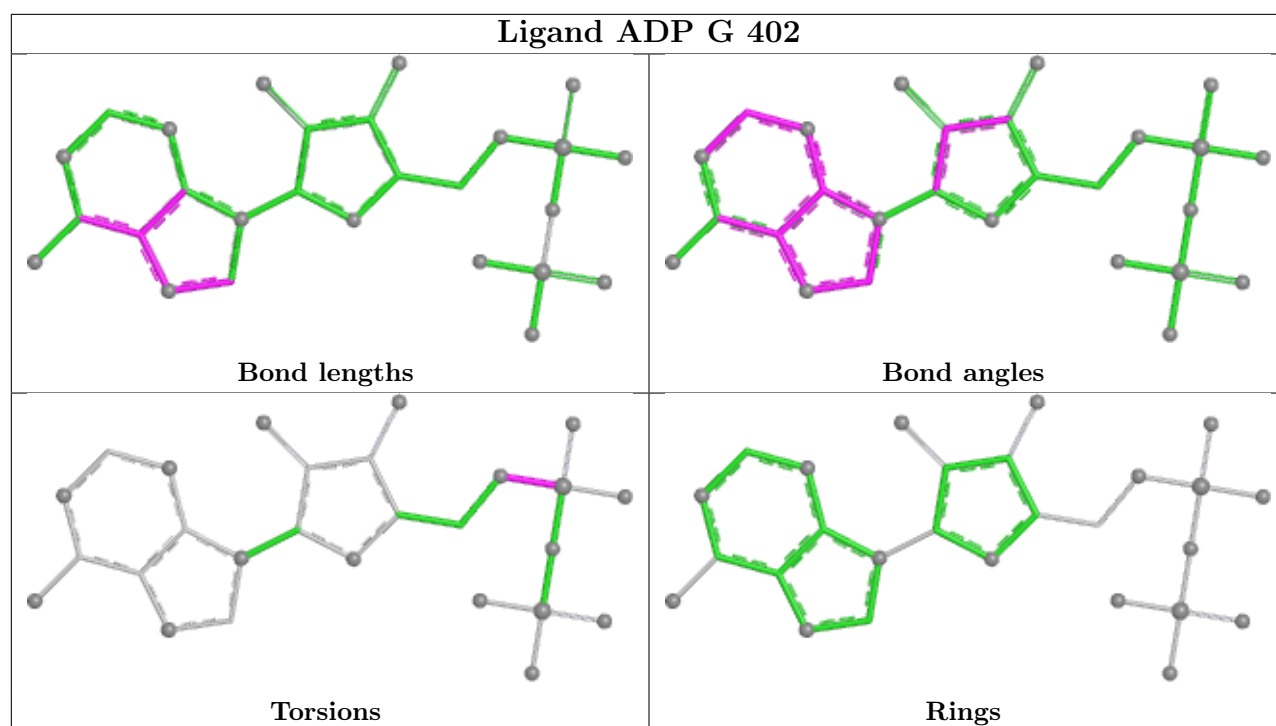
Mol	Chain	Res	Type	Atoms
4	B	402	ADP	C5'-O5'-PA-O3A
4	C	402	ADP	C5'-O5'-PA-O1A
4	C	402	ADP	C5'-O5'-PA-O2A
4	C	402	ADP	C5'-O5'-PA-O3A
4	D	402	ADP	C5'-O5'-PA-O1A
4	D	402	ADP	C5'-O5'-PA-O2A
4	D	402	ADP	C5'-O5'-PA-O3A
4	E	402	ADP	C5'-O5'-PA-O1A
4	E	402	ADP	C5'-O5'-PA-O2A
4	E	402	ADP	C5'-O5'-PA-O3A
4	F	402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

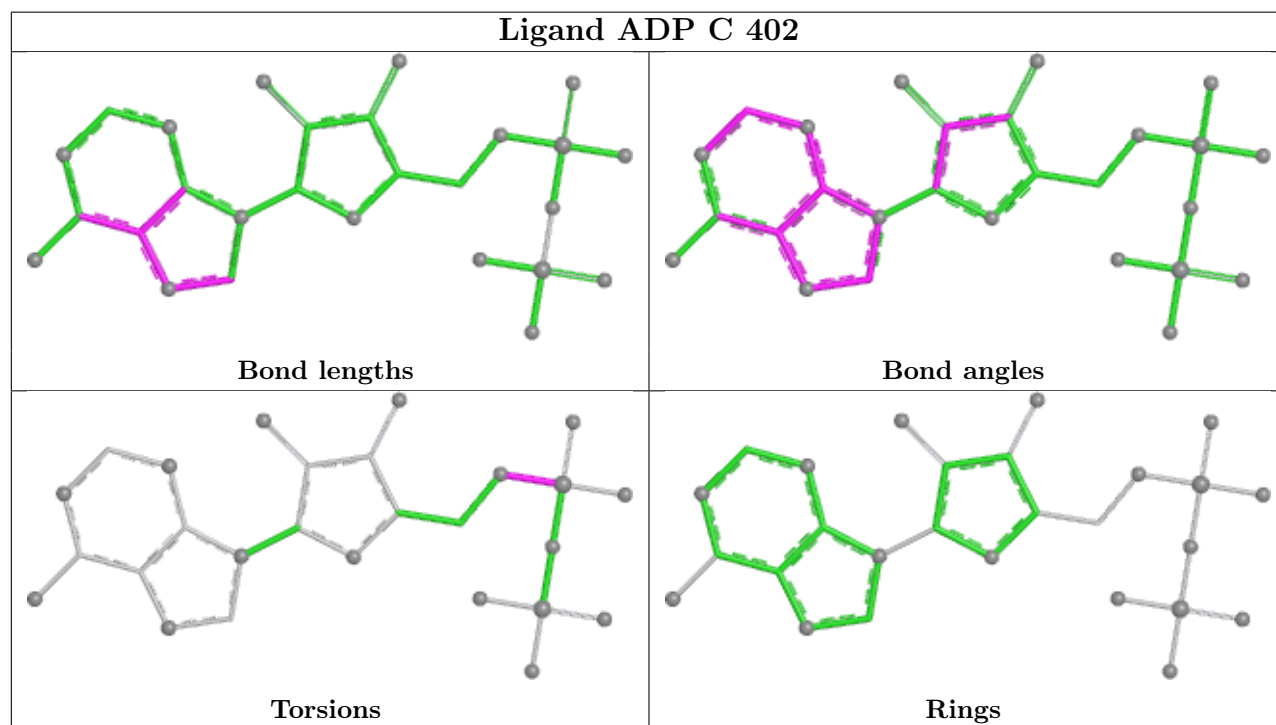
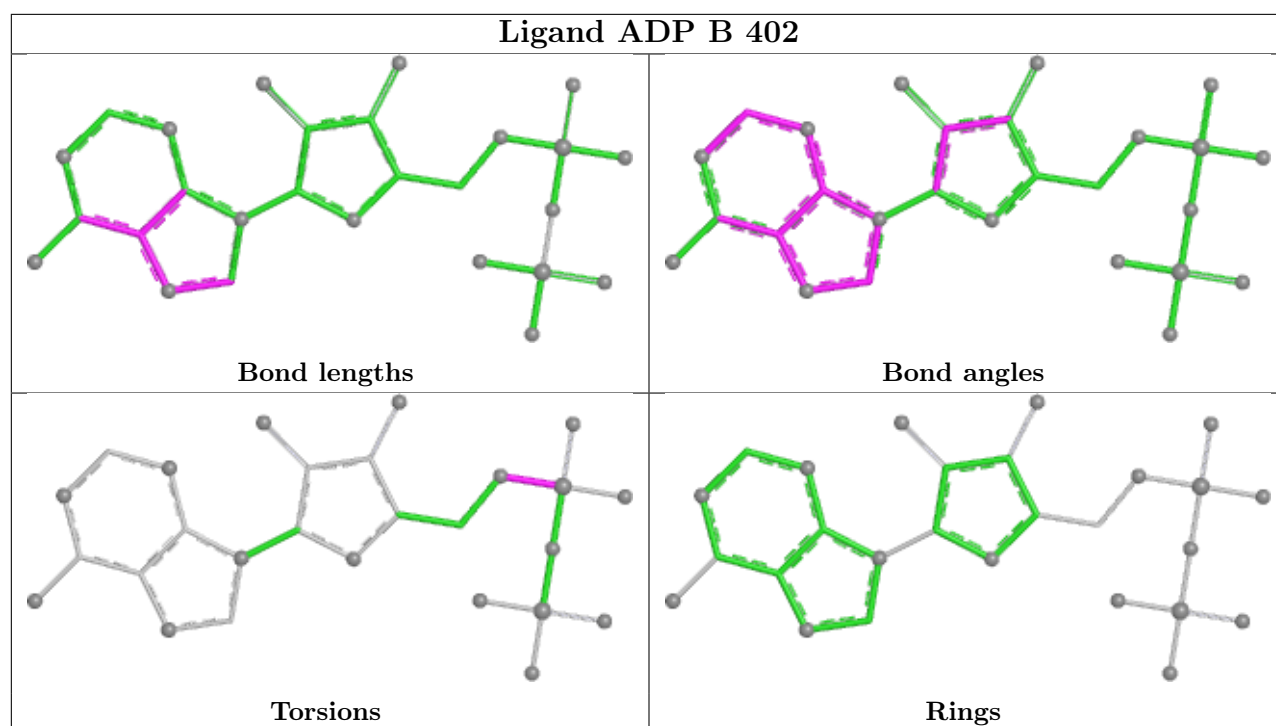
There are no ring outliers.

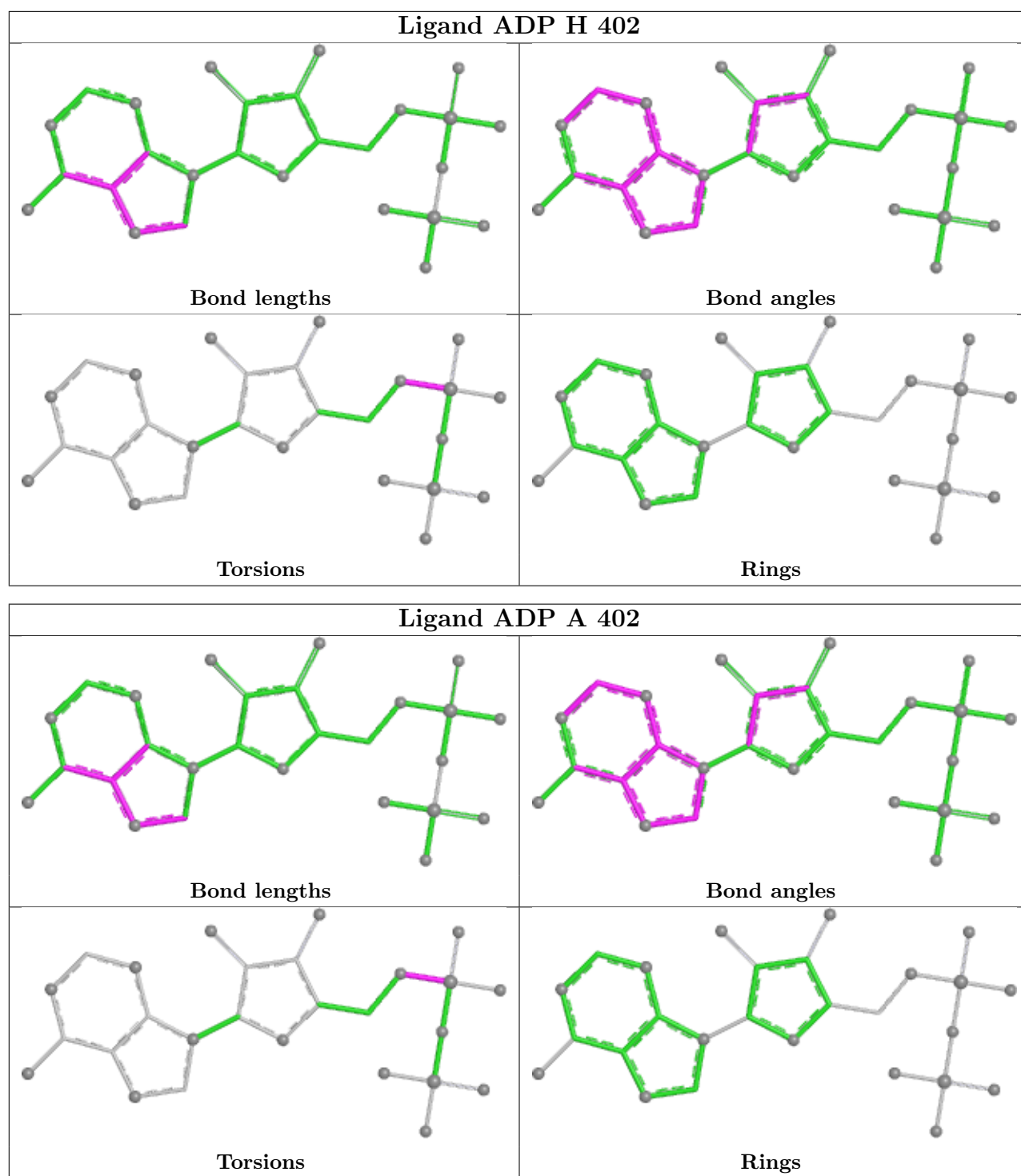
No monomer is involved in short contacts.

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.

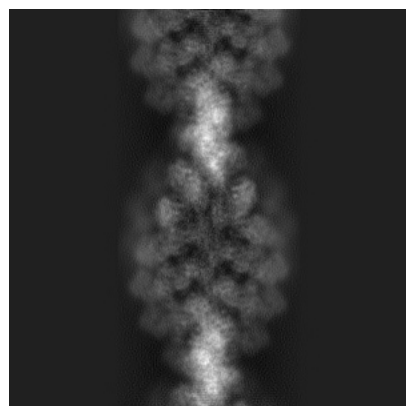
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7116. These allow visual inspection of the internal detail of the map and identification of artifacts.

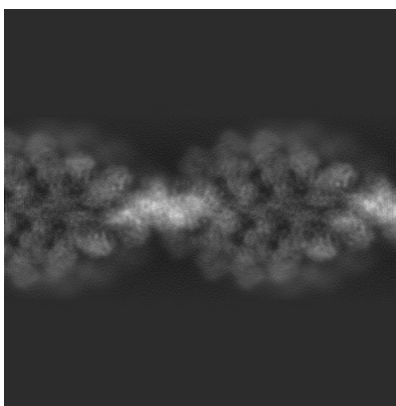
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

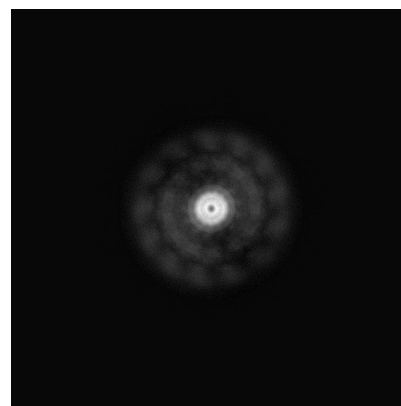
6.1.1 Primary map



X

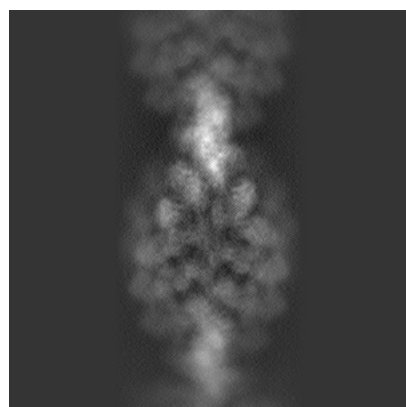


Y

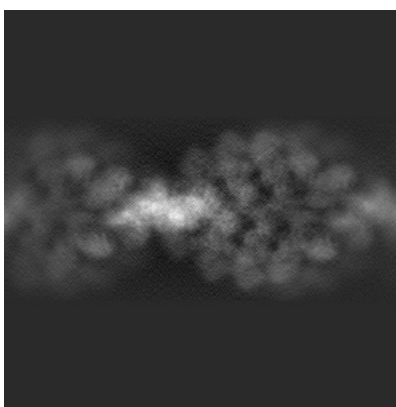


Z

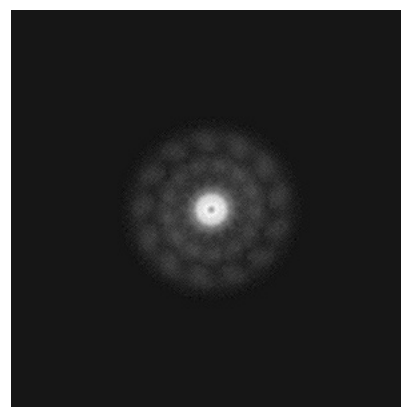
6.1.2 Raw map



X



Y

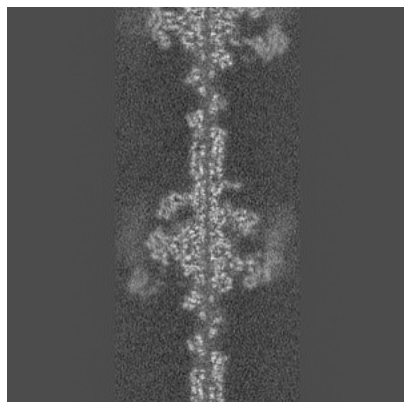


Z

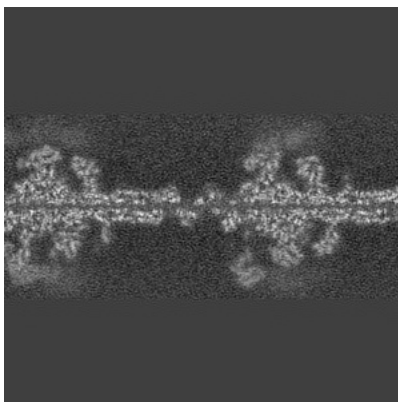
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

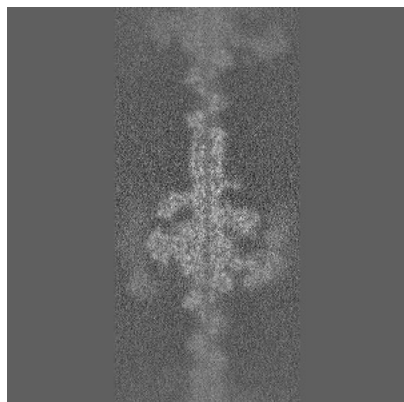


Y Index: 256

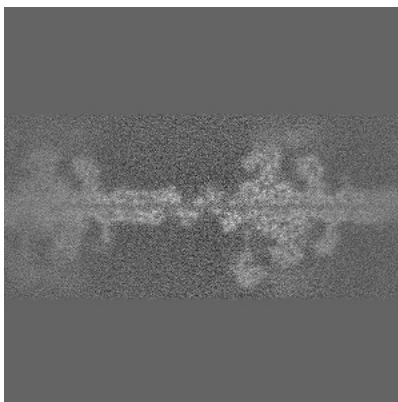


Z Index: 256

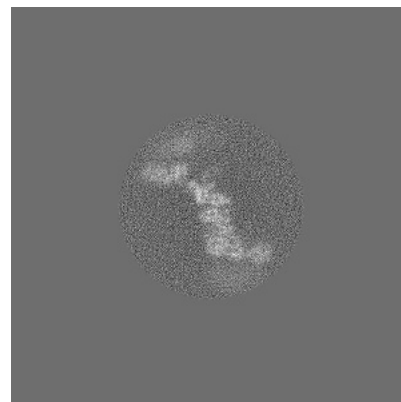
6.2.2 Raw map



X Index: 256



Y Index: 256

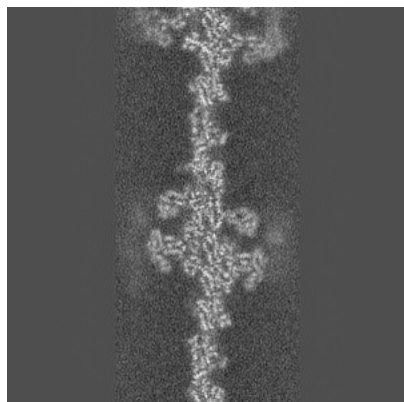


Z Index: 256

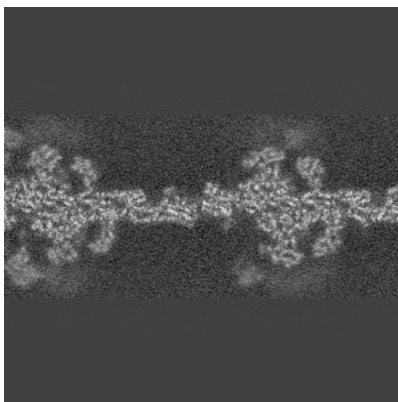
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

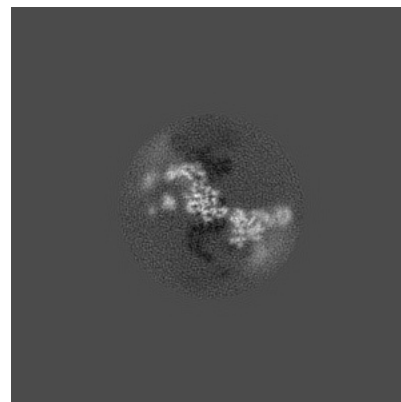
6.3.1 Primary map



X Index: 262

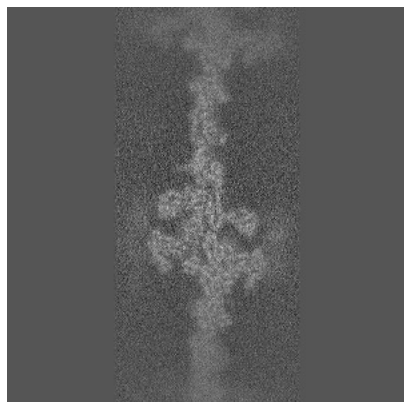


Y Index: 251

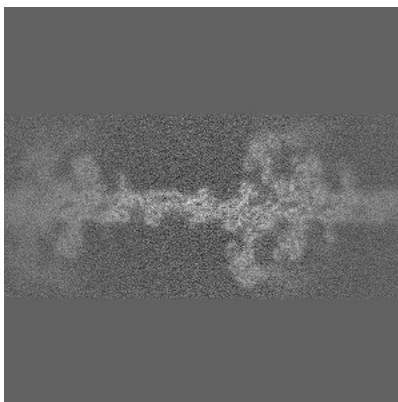


Z Index: 1

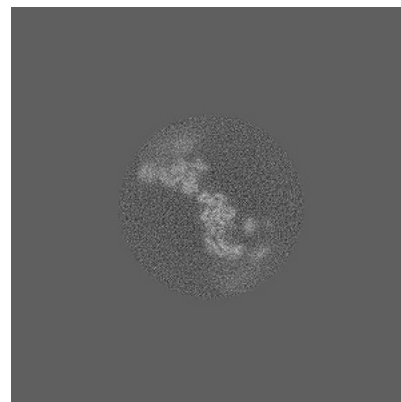
6.3.2 Raw map



X Index: 263



Y Index: 262

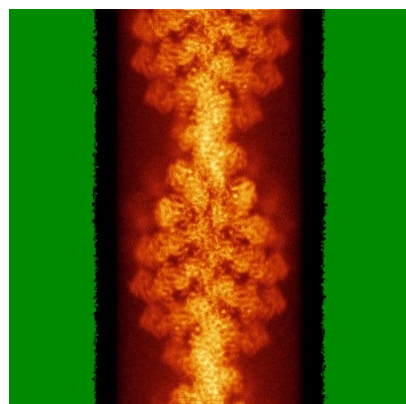


Z Index: 265

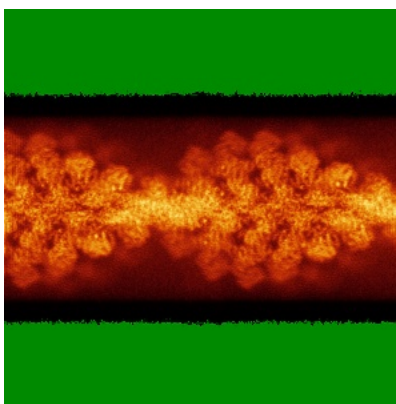
The images above show the largest variance slices of the map in three orthogonal directions.

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

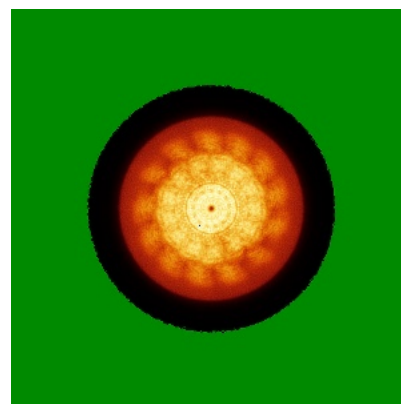
6.4.1 Primary map



X

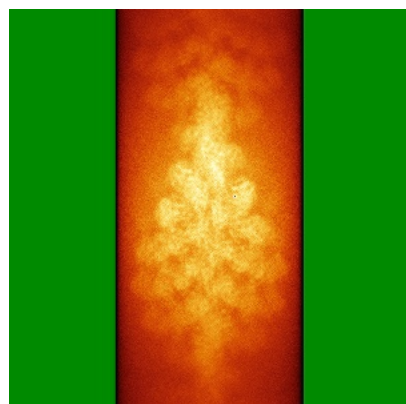


Y

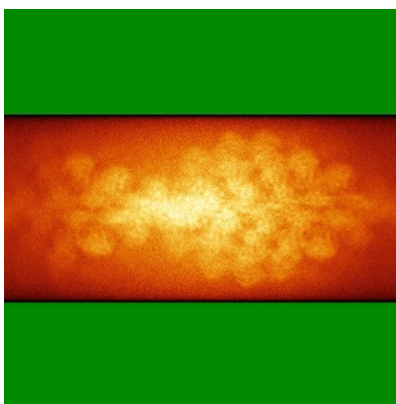


Z

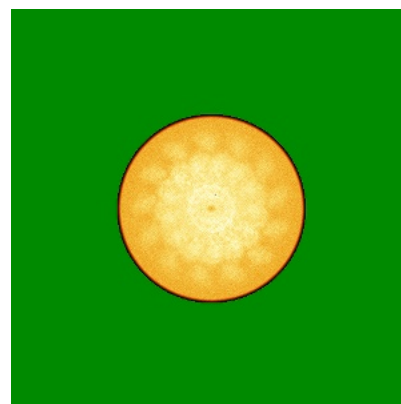
6.4.2 Raw map



X



Y

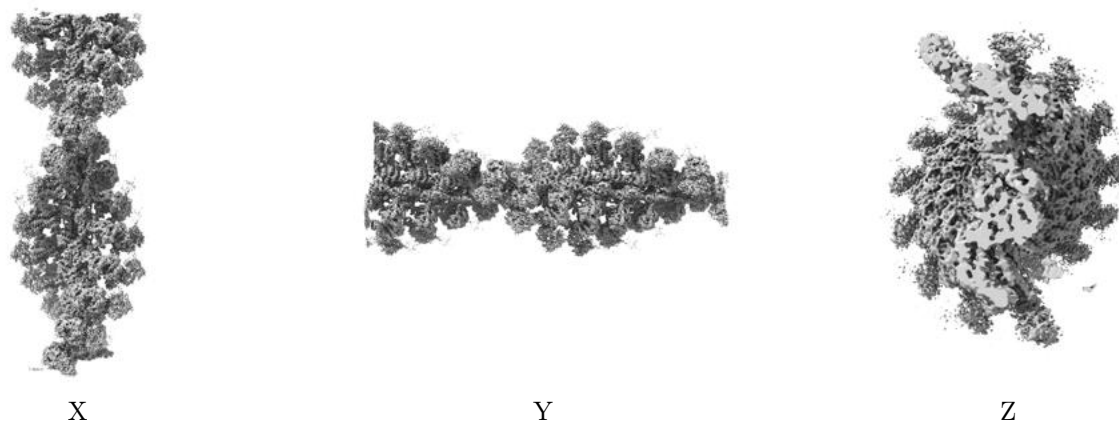


Z

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.

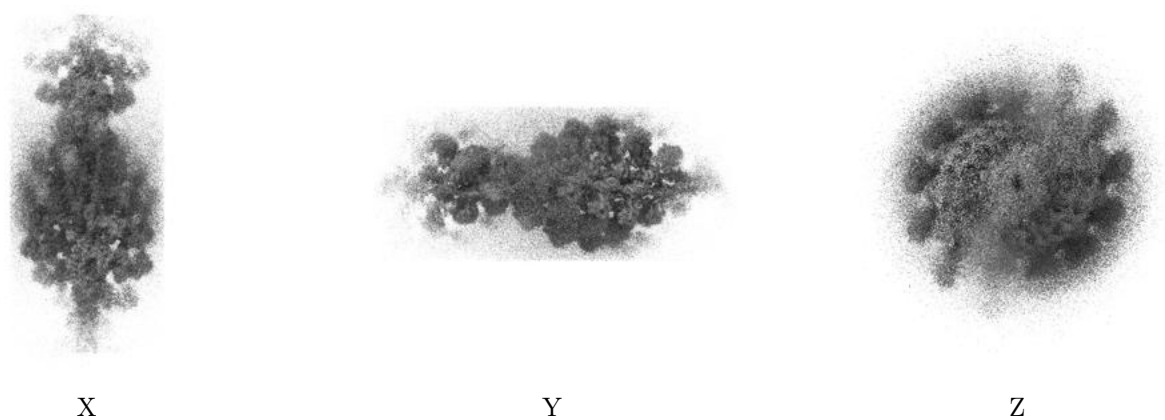
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. 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

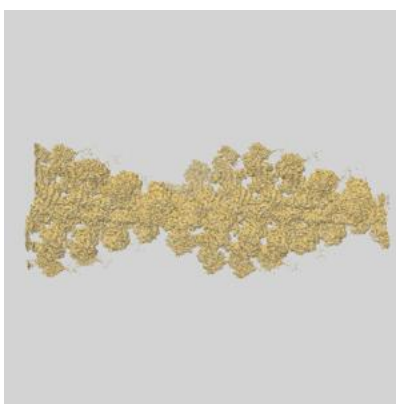
A mask typically either:

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

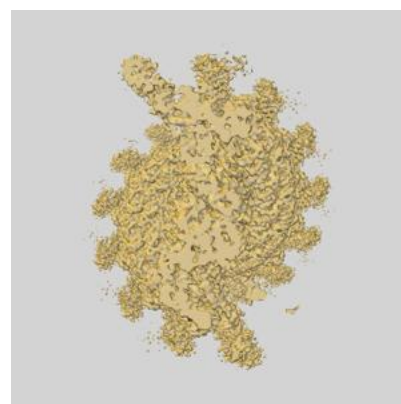
6.6.1 emd_7116_msk_2.map [i](#)



X



Y

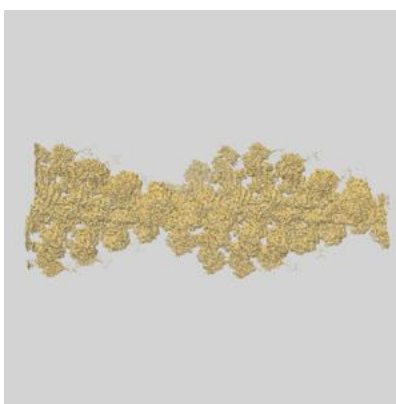


Z

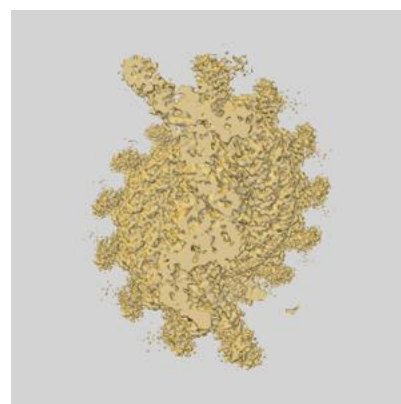
6.6.2 emd_7116_msk_1.map [i](#)



X



Y

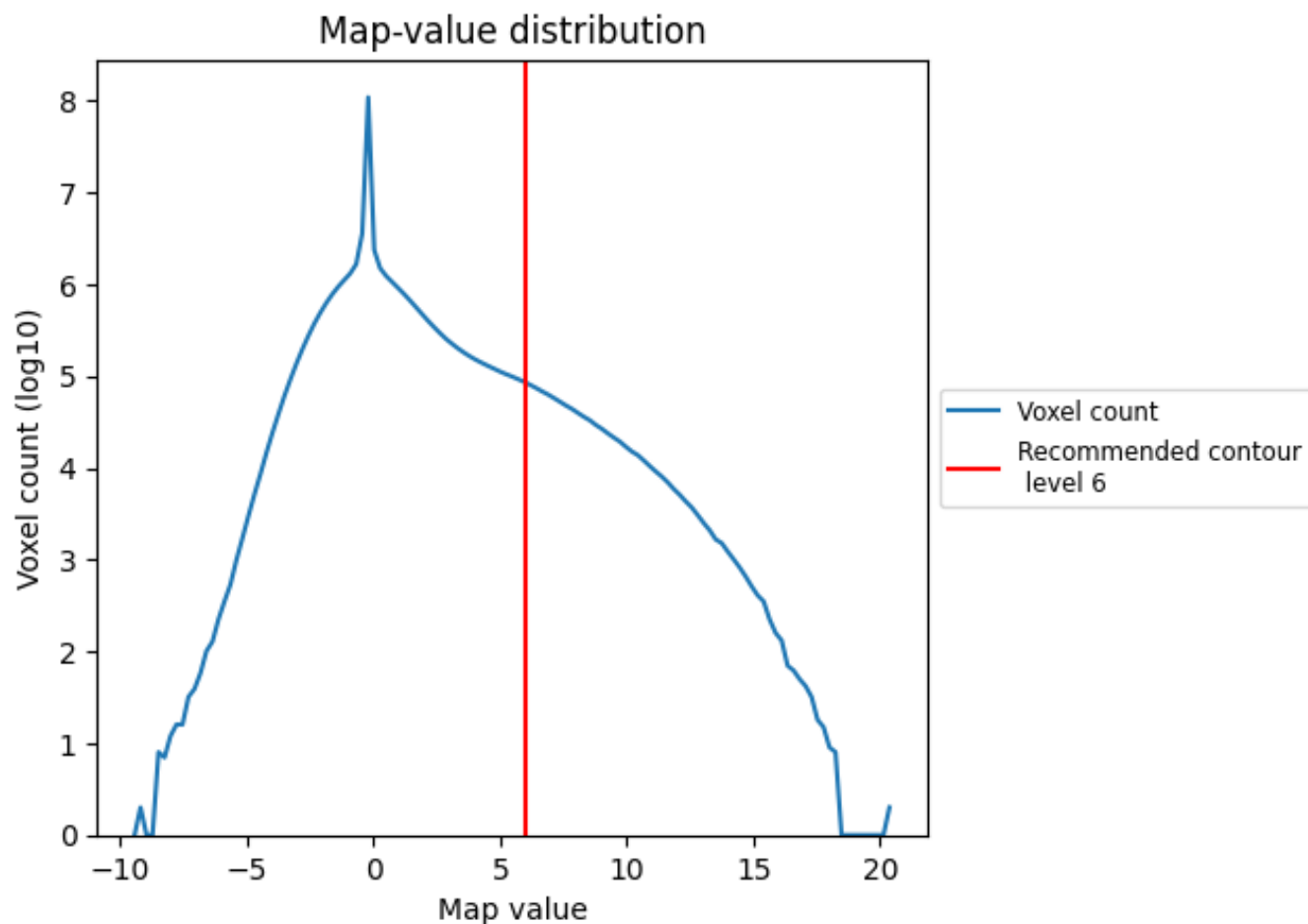


Z

7 Map analysis [i](#)

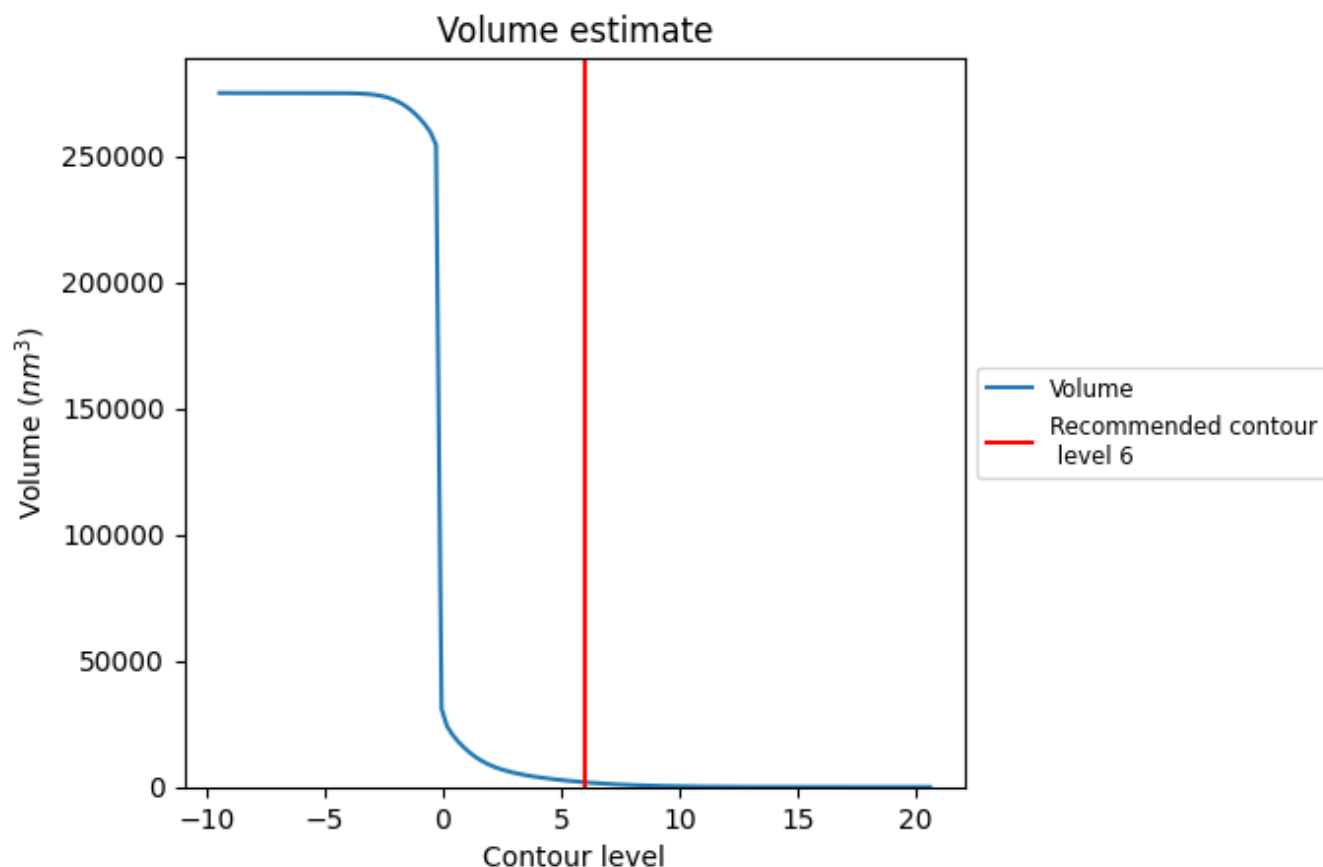
This section contains the results of statistical analysis of the map.

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.

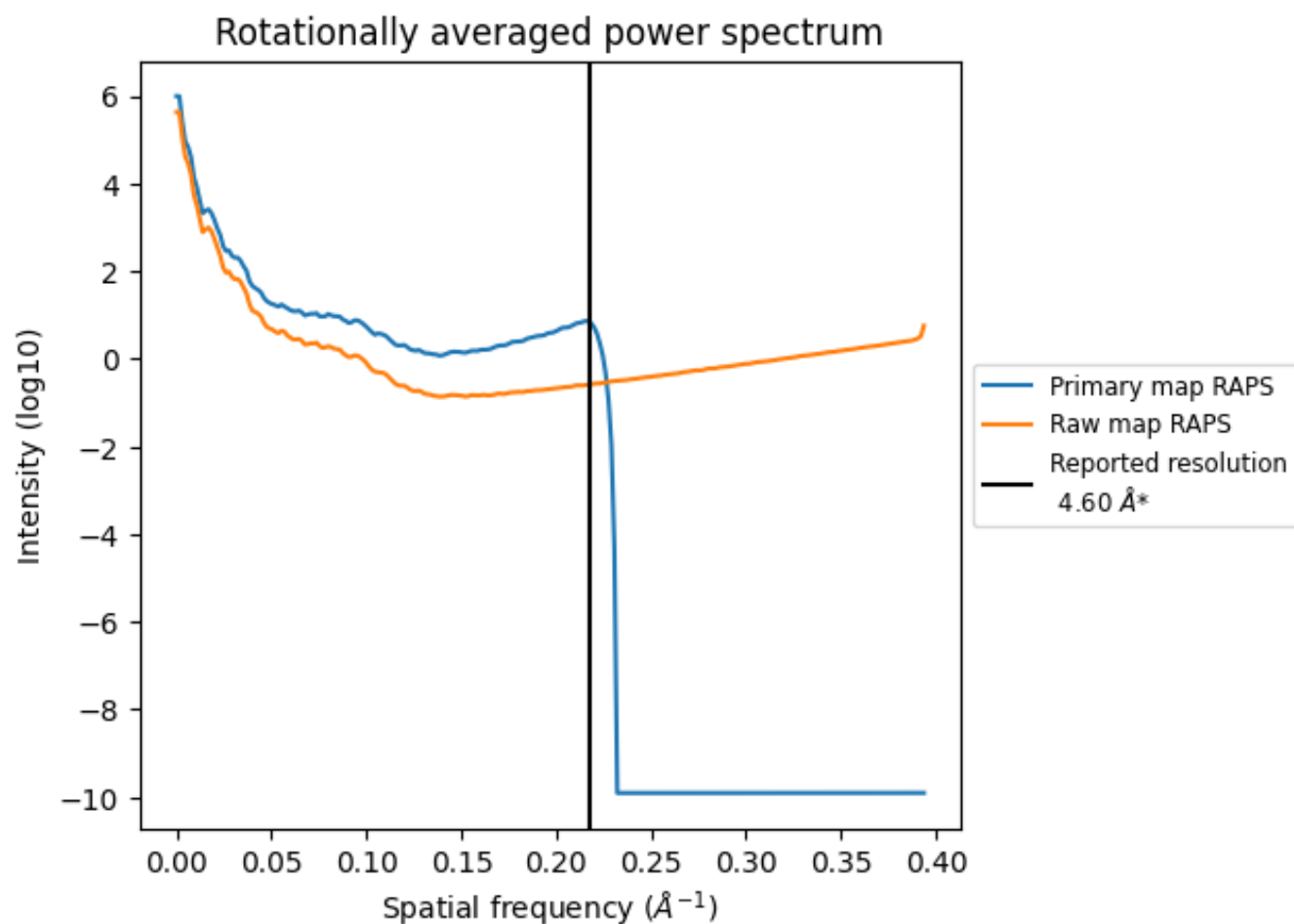
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1866 nm³; this corresponds to an approximate mass of 1686 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 ⓘ

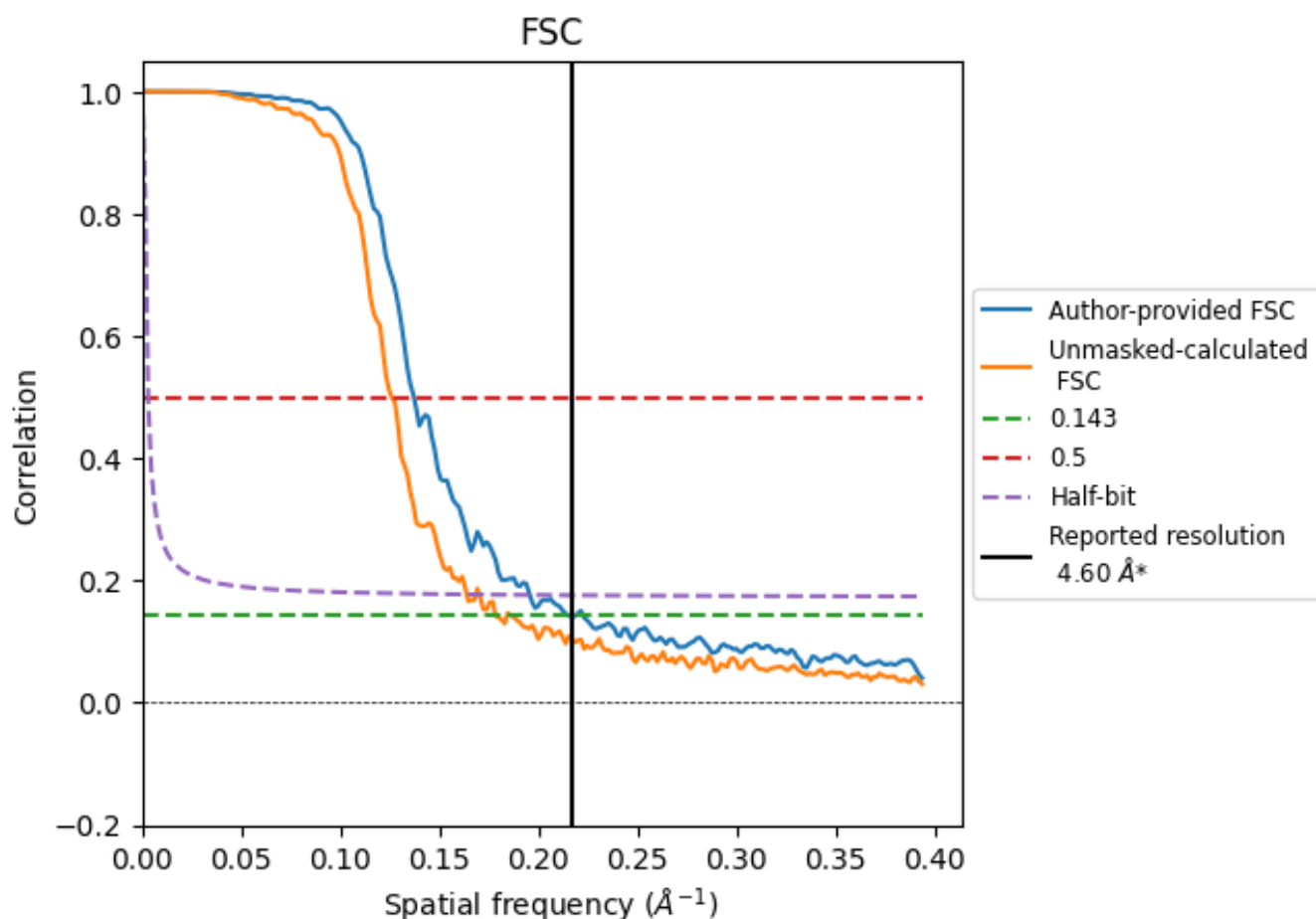


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 $0.217 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

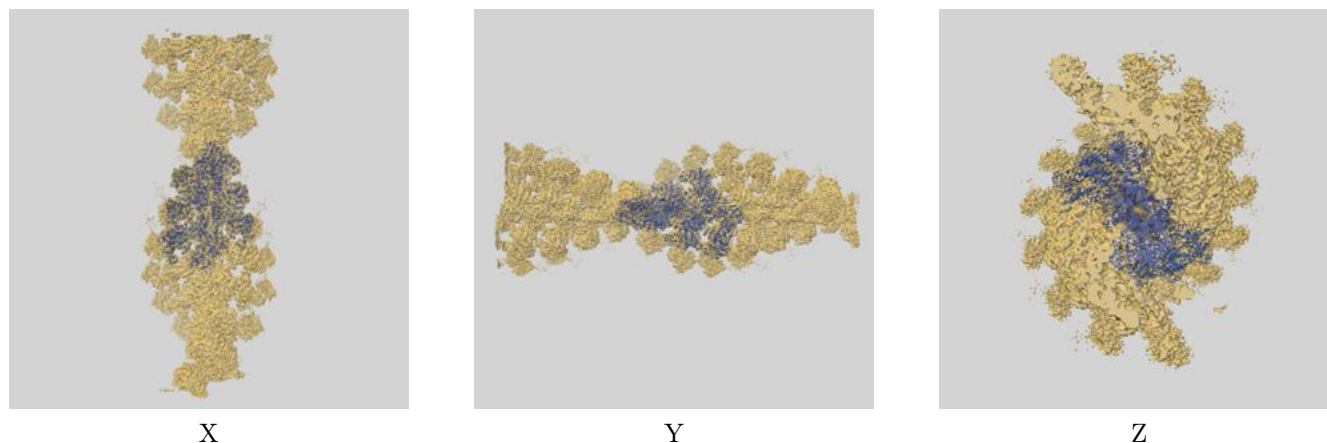
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.66	7.29	5.11
Unmasked-calculated*	5.61	7.94	6.11

*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 5.61 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

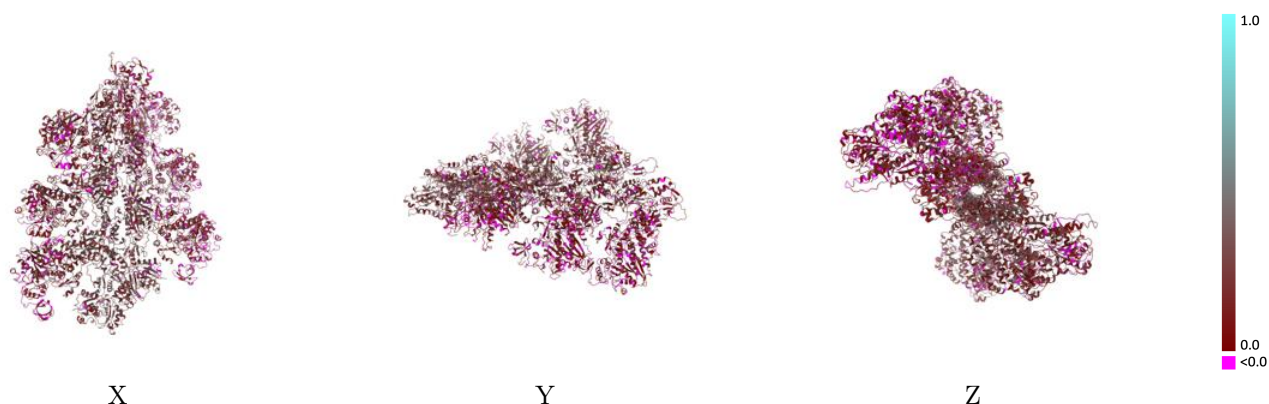
This section contains information regarding the fit between EMDB map EMD-7116 and PDB model 6BNP. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



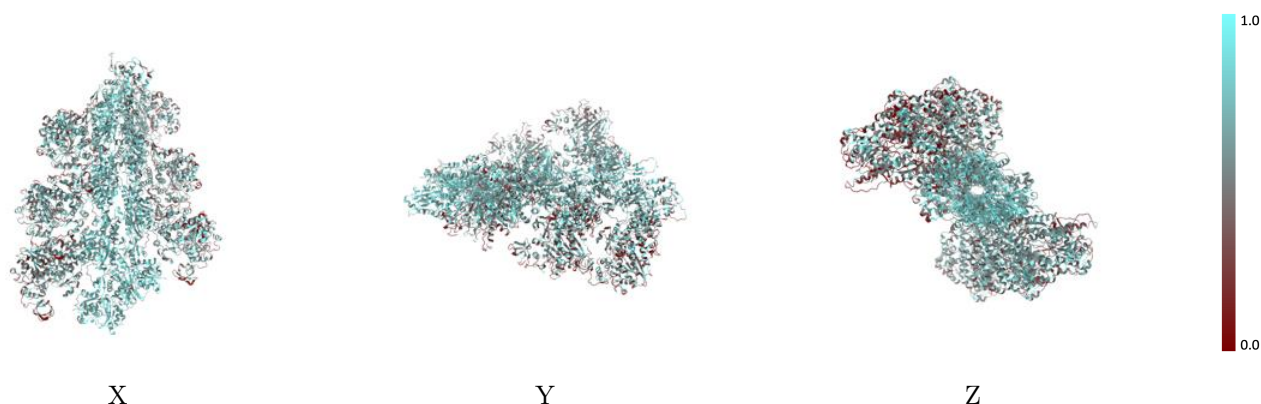
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



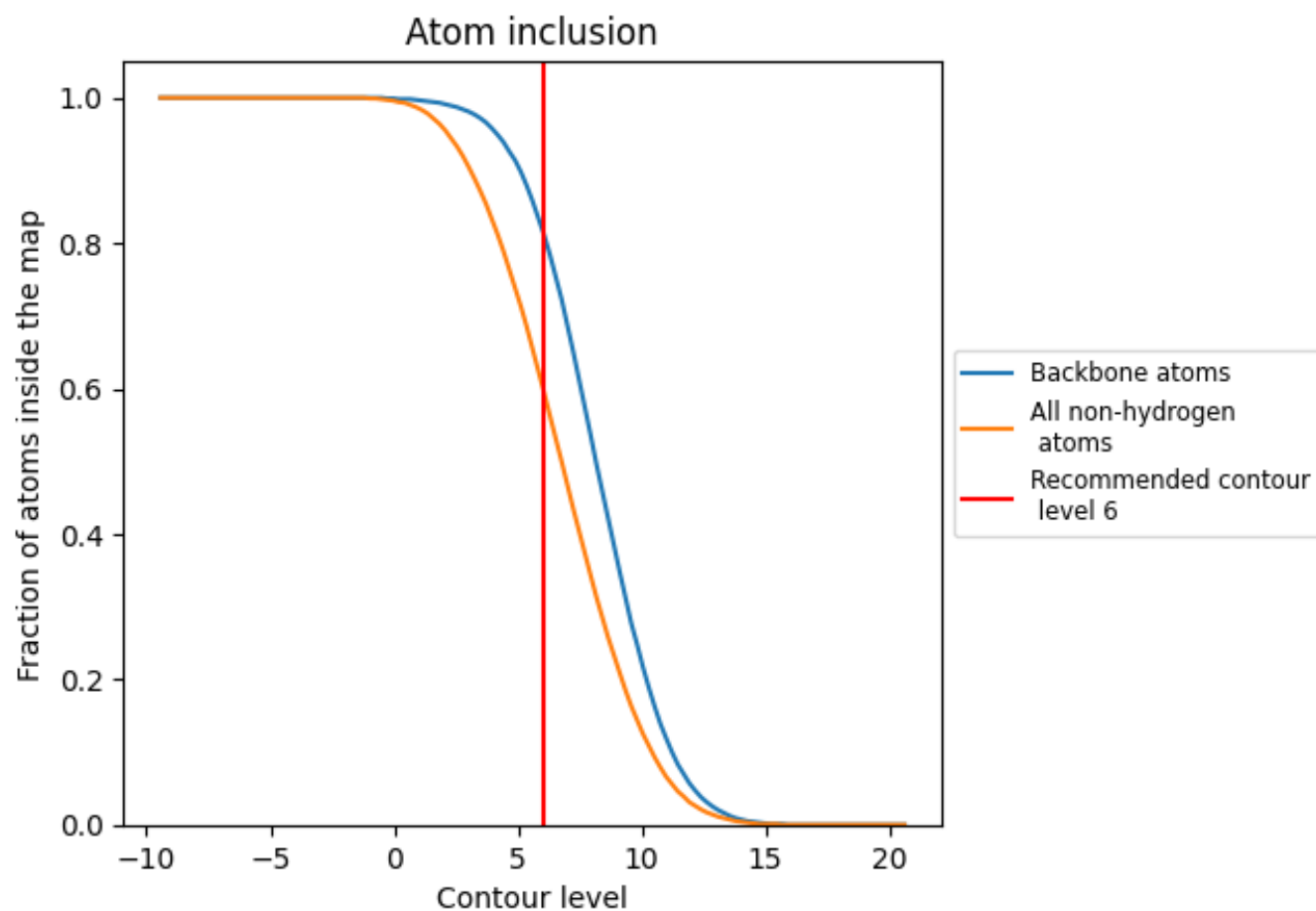
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 60% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6020	 0.1910
A	 0.7500	 0.2880
B	 0.7410	 0.2700
C	 0.7650	 0.2940
D	 0.7270	 0.2500
E	 0.7630	 0.2810
F	 0.6800	 0.2030
G	 0.7300	 0.2510
H	 0.6460	 0.1610
I	 0.5400	 0.1740
J	 0.5010	 0.1350
K	 0.5670	 0.1900
L	 0.4780	 0.1160
M	 0.5570	 0.1900
N	 0.4570	 0.1010

