



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 04:39 PM EST

PDB ID : 6BNQ
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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

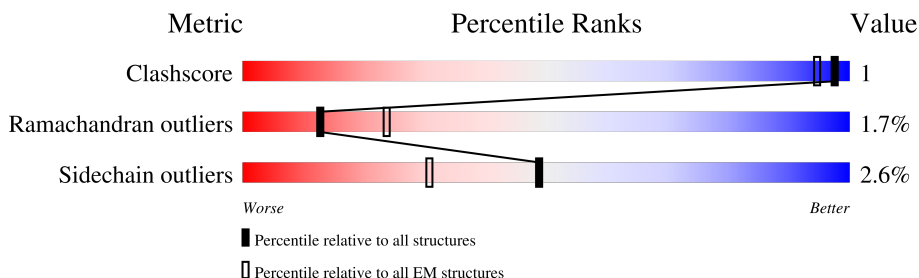
1 Overall quality at a glance

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.





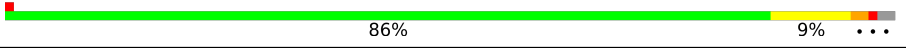



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>16%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	J	704	<div> <div>14%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	K	704	<div> <div>15%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	L	704	<div> <div>16%</div> <div>92%</div> <div>7%</div> </div>
1	M	704	<div> <div>14%</div> <div>91%</div> <div>8%</div> </div>
1	N	704	<div> <div>15%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
2	A	373	<div> <div>90%</div> <div>8%</div> <div>..</div> </div>
2	B	373	<div> <div>89%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	373	 91%7% ..
2	D	373	 89%9% ..
2	E	373	 86%9% ...
2	F	373	 88%9% ..
2	G	373	 90%7% ..
2	H	373	 87%8% ..

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		

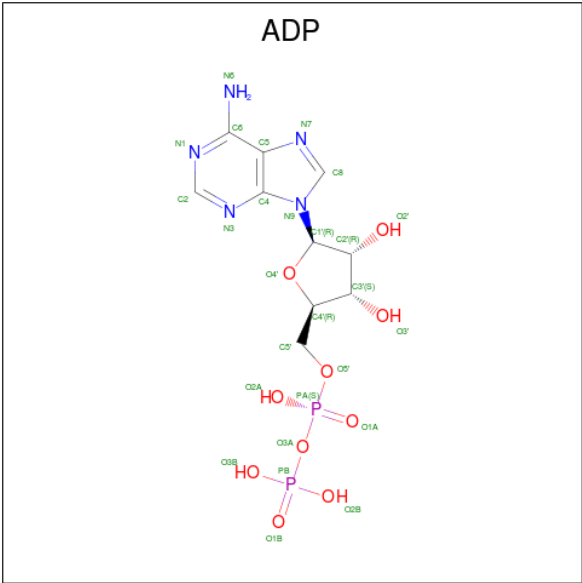
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

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 (three-letter code: 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 (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



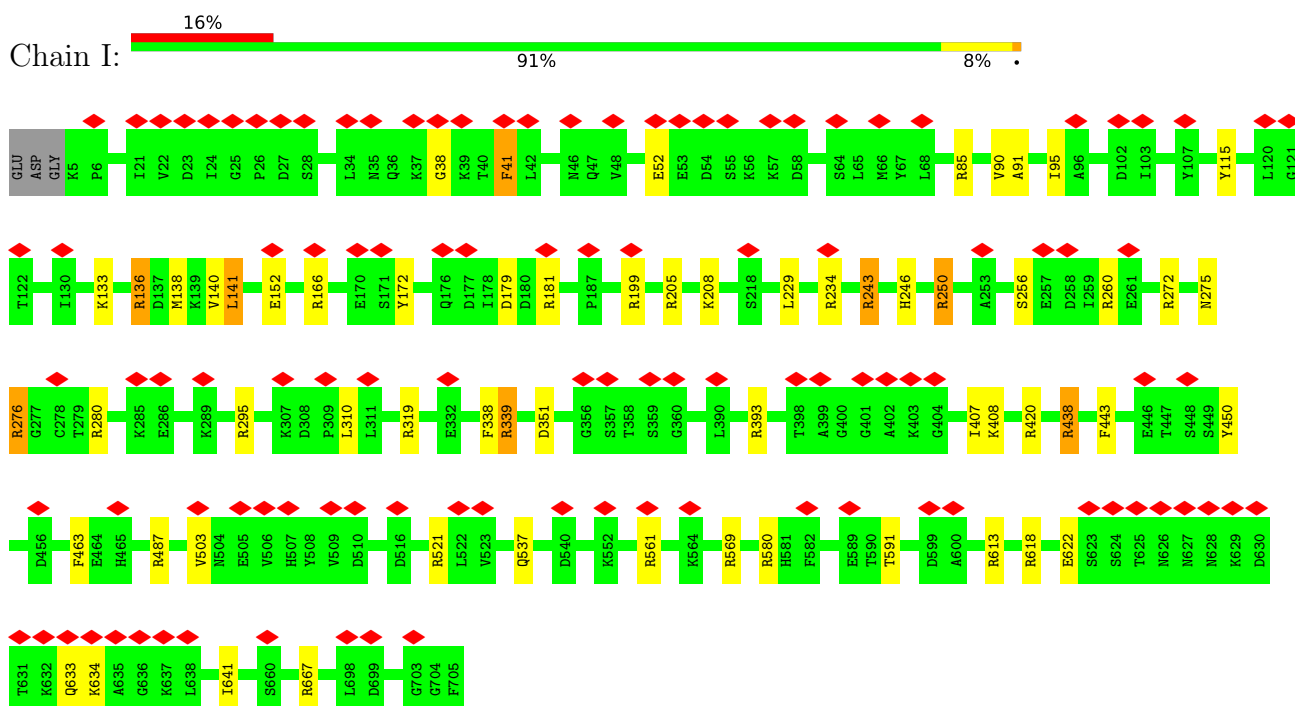
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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

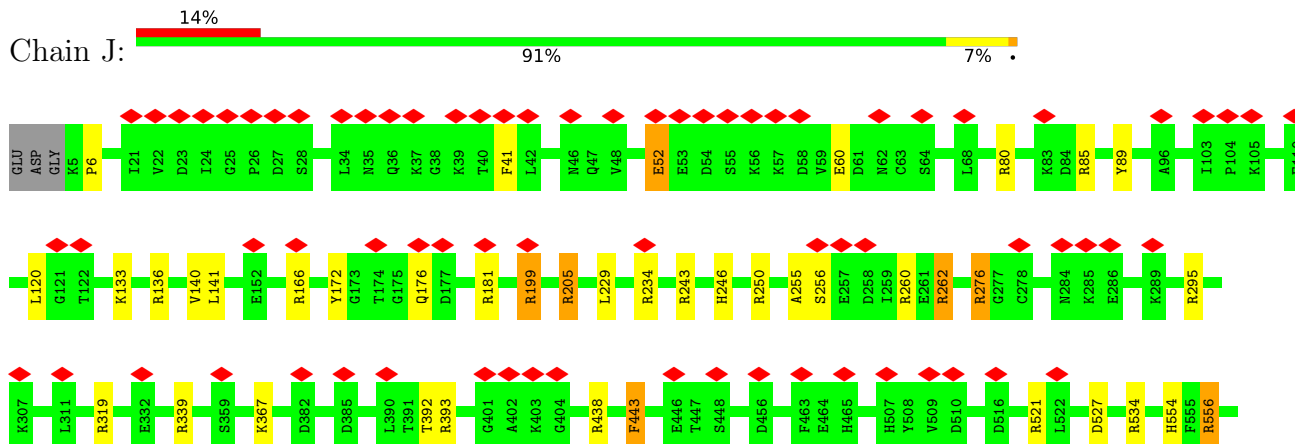
3 Residue-property plots

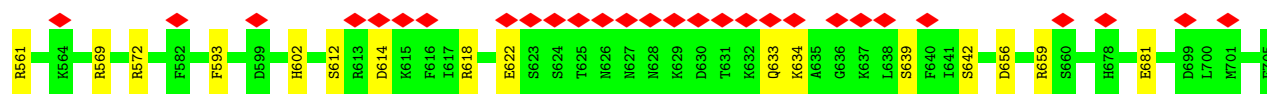
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

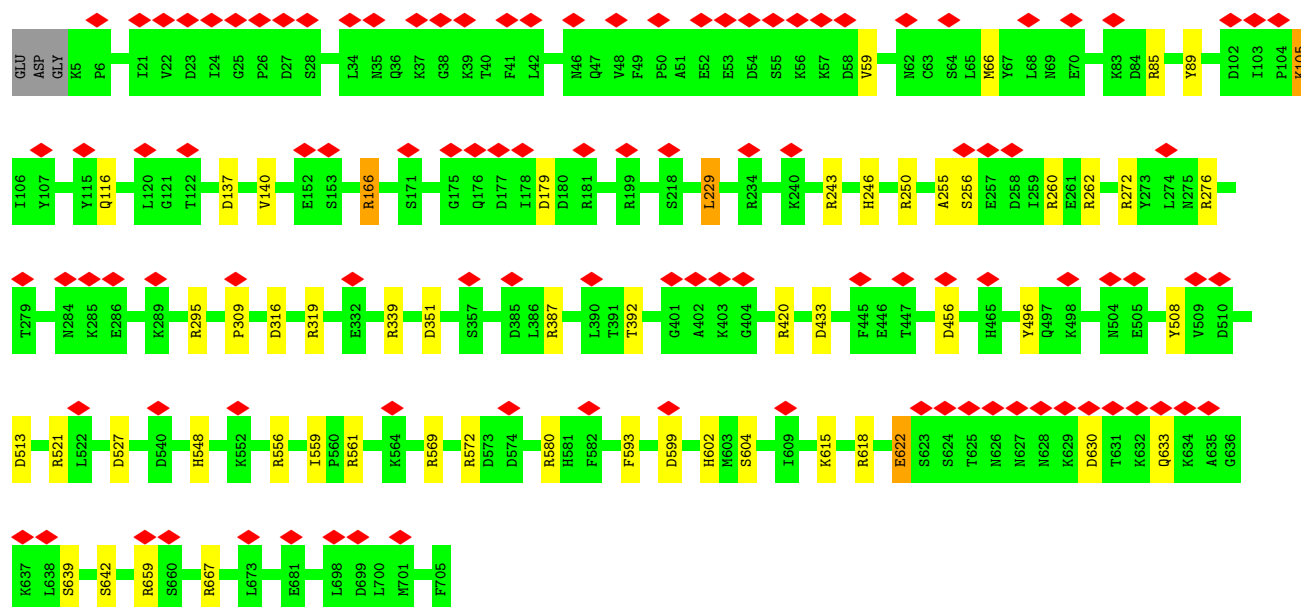


• Molecule 1: Unconventional myosin-VI

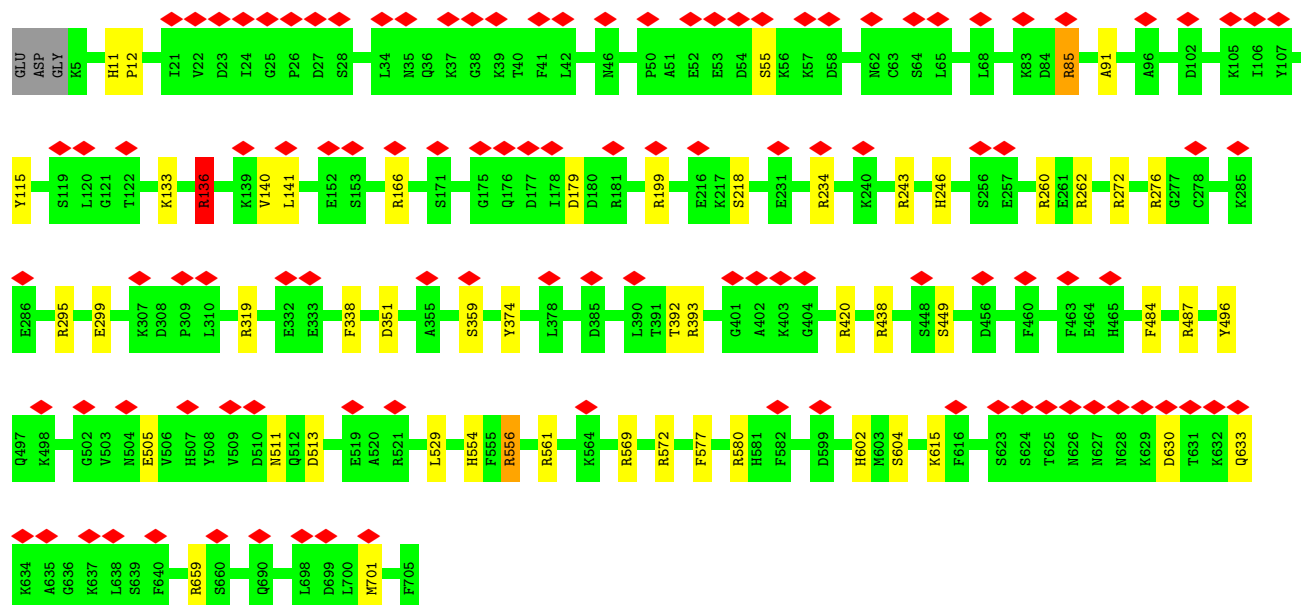
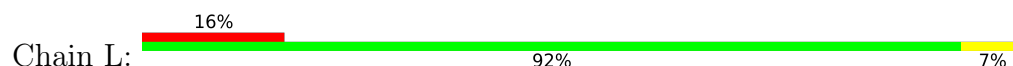




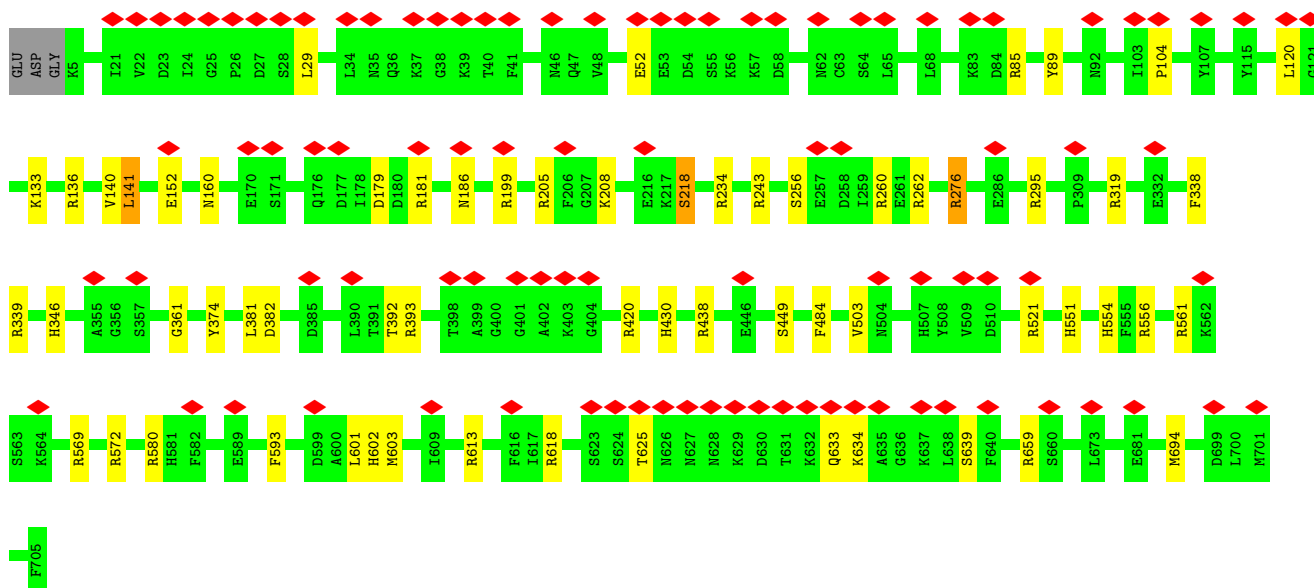
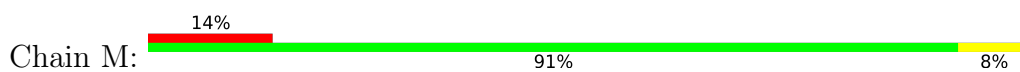
• Molecule 1: Unconventional myosin-VI



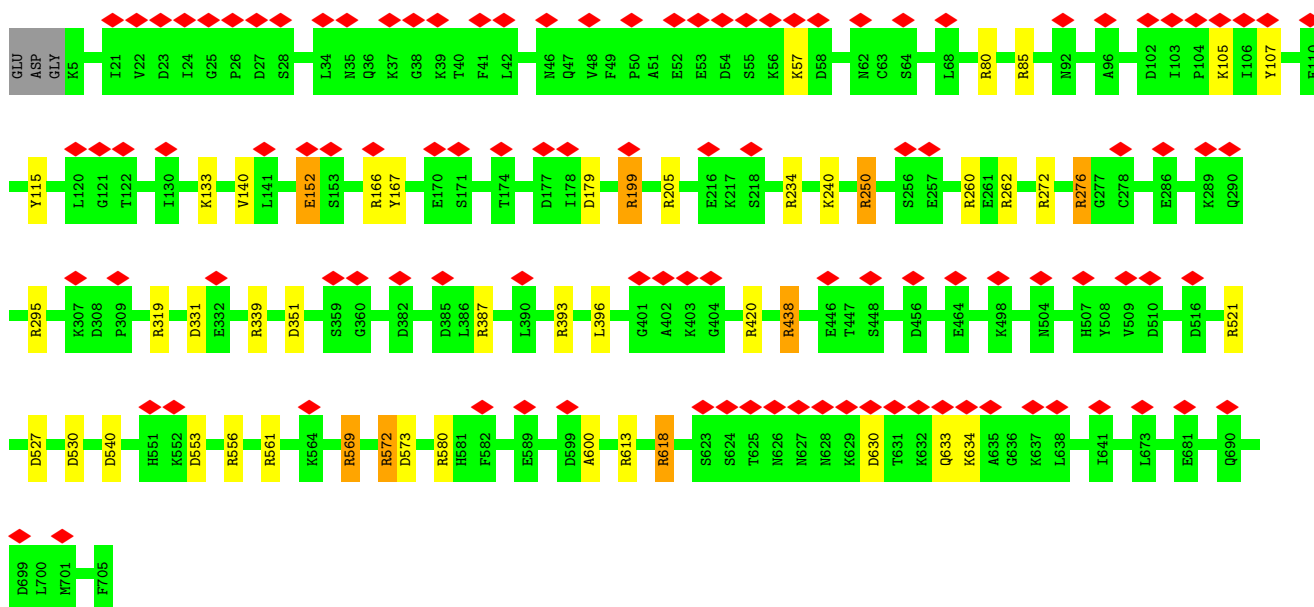
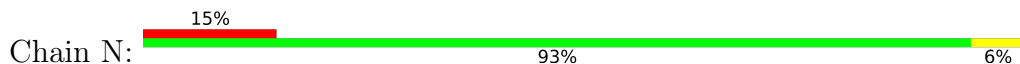
• Molecule 1: Unconventional myosin-VI



• Molecule 1: Unconventional myosin-VI



• Molecule 1: Unconventional myosin-VI



• Molecule 2: Actin, alpha skeletal muscle





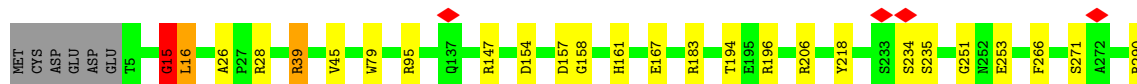
- Molecule 2: Actin, alpha skeletal muscle

Chain B: 89% 9% ..



- Molecule 2: Actin, alpha skeletal muscle

Chain C: 91% 7% ..



- Molecule 2: Actin, alpha skeletal muscle

Chain D: 89% 9% ..




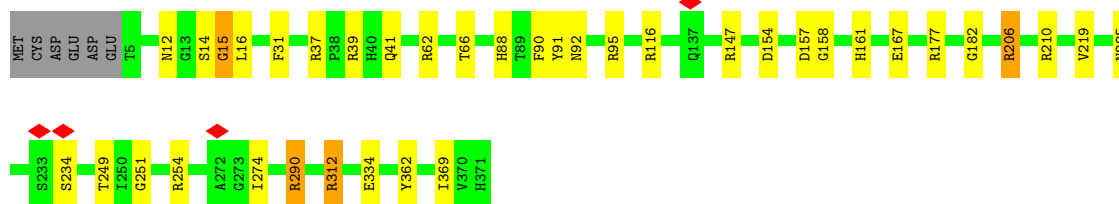
- Molecule 2: Actin, alpha skeletal muscle

Chain E: 86% 9% ...



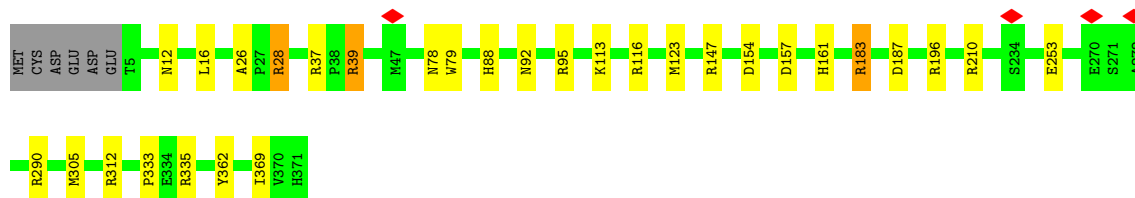
- Molecule 2: Actin, alpha skeletal muscle

Chain F:  88% 9% ..




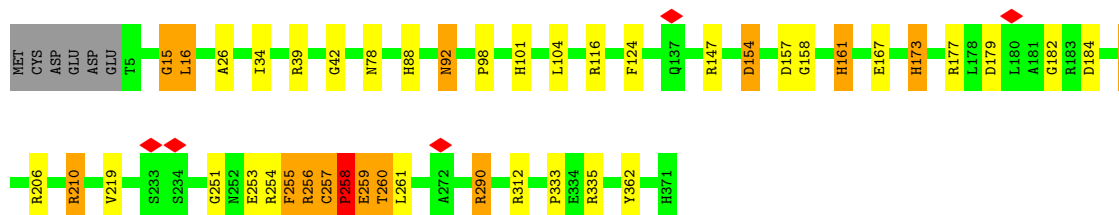
- Molecule 2: Actin, alpha skeletal muscle

Chain G:  90% 7% ..



- Molecule 2: Actin, alpha skeletal muscle

Chain H:  87% 8% ..



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: 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	0.72	0/5696	1.07	32/7677 (0.4%)
1	J	0.71	0/5696	1.07	32/7677 (0.4%)
1	K	0.72	0/5696	1.08	31/7677 (0.4%)
1	L	0.71	0/5696	1.07	32/7677 (0.4%)
1	M	0.72	0/5696	1.08	34/7677 (0.4%)
1	N	0.72	0/5696	1.06	29/7677 (0.4%)
2	A	0.75	1/2924 (0.0%)	1.18	18/3963 (0.5%)
2	B	0.72	0/2924	1.17	25/3963 (0.6%)
2	C	0.71	0/2924	1.15	15/3963 (0.4%)
2	D	0.71	0/2924	1.20	24/3963 (0.6%)
2	E	0.72	0/2924	1.20	24/3963 (0.6%)
2	F	0.72	0/2924	1.15	20/3963 (0.5%)
2	G	0.71	0/2924	1.14	14/3963 (0.4%)
2	H	1.00	20/2924 (0.7%)	1.36	40/3963 (1.0%)
All	All	0.73	21/57568 (0.0%)	1.12	370/77766 (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	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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	258	PRO	CA-C	13.08	1.79	1.52
2	H	259	GLU	N-CA	11.08	1.68	1.46
2	H	257	CYS	N-CA	10.38	1.67	1.46
2	H	259	GLU	CA-CB	9.25	1.74	1.53
2	H	258	PRO	CA-CB	9.11	1.71	1.53
2	H	260	THR	CA-C	8.87	1.76	1.52
2	H	260	THR	N-CA	8.57	1.63	1.46
2	H	260	THR	C-N	7.90	1.52	1.34
2	A	260	THR	N-CA	-7.25	1.31	1.46
2	H	261	LEU	CA-CB	6.99	1.69	1.53
2	H	257	CYS	CA-C	6.94	1.71	1.52
2	H	255	PHE	CA-CB	6.75	1.68	1.53
2	H	254	ARG	C-N	6.32	1.48	1.34
2	H	259	GLU	CA-C	5.94	1.68	1.52
2	H	256	ARG	N-CA	-5.77	1.34	1.46
2	H	261	LEU	CA-C	-5.74	1.38	1.52
2	H	261	LEU	N-CA	5.37	1.57	1.46
2	H	259	GLU	C-N	5.35	1.46	1.34
2	H	260	THR	CA-CB	5.32	1.67	1.53
2	H	259	GLU	CG-CD	-5.28	1.44	1.51
2	H	257	CYS	C-O	5.02	1.32	1.23

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	258	PRO	O-C-N	-22.14	87.28	122.70
2	H	260	THR	O-C-N	-11.84	103.75	122.70
2	H	258	PRO	CB-CA-C	-11.59	83.03	112.00
2	D	39	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	M	295	ARG	NE-CZ-NH2	-9.46	115.57	120.30
2	H	257	CYS	O-C-N	-9.40	103.24	121.10
1	J	234	ARG	NE-CZ-NH1	9.35	124.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	659	ARG	NE-CZ-NH1	9.03	124.81	120.30
2	E	210	ARG	NE-CZ-NH1	8.94	124.77	120.30
2	B	254	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	J	136	ARG	NE-CZ-NH1	8.86	124.73	120.30
2	A	312	ARG	NE-CZ-NH1	8.71	124.66	120.30
2	C	39	ARG	NE-CZ-NH1	8.65	124.62	120.30
2	F	312	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	I	319	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	D	254	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	M	85	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	J	521	ARG	NE-CZ-NH1	8.34	124.47	120.30
2	D	210	ARG	NE-CZ-NH1	8.33	124.46	120.30
2	A	183	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	K	250	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	A	260	THR	CA-CB-OG1	8.29	126.41	109.00
2	B	62	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	K	295	ARG	NE-CZ-NH1	8.17	124.38	120.30
2	H	258	PRO	CA-C-N	8.16	135.16	117.20
1	M	319	ARG	NE-CZ-NH1	8.09	124.34	120.30
2	H	258	PRO	CA-CB-CG	-8.07	88.67	104.00
2	H	312	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	L	272	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	N	339	ARG	NE-CZ-NH1	8.03	124.32	120.30
2	C	312	ARG	NE-CZ-NH1	8.02	124.31	120.30
2	G	154	ASP	CB-CG-OD2	8.01	125.51	118.30
1	K	260	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	I	521	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	M	339	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	J	618	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	A	154	ASP	CB-CG-OD2	7.86	125.38	118.30
1	K	250	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	M	234	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	G	147	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	N	250	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	J	250	ARG	NE-CZ-NH1	7.77	124.19	120.30
2	F	154	ASP	CB-CG-OD1	7.77	125.29	118.30
2	A	39	ARG	NE-CZ-NH1	7.77	124.18	120.30
2	H	154	ASP	CB-CG-OD1	7.72	125.25	118.30
2	E	154	ASP	CB-CG-OD2	7.72	125.25	118.30
2	E	62	ARG	NE-CZ-NH2	-7.69	116.45	120.30
2	D	266	PHE	CB-CG-CD1	7.62	126.14	120.80
2	F	116	ARG	NE-CZ-NH2	-7.62	116.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	I	339	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	K	339	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	D	37	ARG	NE-CZ-NH1	7.55	124.08	120.30
2	B	116	ARG	NE-CZ-NH1	7.53	124.06	120.30
2	G	39	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	K	295	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	K	556	ARG	NE-CZ-NH1	7.51	124.05	120.30
2	D	154	ASP	CB-CG-OD1	7.51	125.06	118.30
2	A	116	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	H	256	ARG	CA-CB-CG	7.49	129.88	113.40
1	M	199	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	G	39	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	J	438	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	I	199	ARG	NE-CZ-NH1	7.43	124.02	120.30
2	H	254	ARG	CB-CA-C	7.39	125.19	110.40
2	C	290	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	A	39	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	I	295	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	F	39	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	B	312	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	K	561	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	L	295	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	K	561	ARG	NE-CZ-NH1	-7.29	116.65	120.30
2	E	210	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	B	154	ASP	CB-CG-OD1	7.27	124.84	118.30
2	H	210	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	I	487	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	J	89	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	K	456	ASP	CB-CG-OD1	7.20	124.78	118.30
2	H	256	ARG	C-N-CA	-7.19	103.72	121.70
1	M	89	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	L	260	ARG	NE-CZ-NH2	-7.17	116.71	120.30
2	C	154	ASP	CB-CG-OD2	7.17	124.76	118.30
2	E	37	ARG	NE-CZ-NH1	7.17	123.89	120.30
2	G	183	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	H	261	LEU	N-CA-CB	-7.15	96.09	110.40
2	B	196	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	A	116	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	M	181	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	J	393	ARG	NE-CZ-NH1	7.10	123.85	120.30
2	E	95	ARG	NE-CZ-NH1	7.08	123.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	166	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	D	266	PHE	CB-CG-CD2	-7.08	115.85	120.80
1	K	618	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	I	136	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	L	496	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	I	166	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	A	206	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	N	276	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	B	62	ARG	NE-CZ-NH1	7.01	123.80	120.30
2	A	183	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	N	234	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	E	39	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	L	556	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	J	521	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	N	618	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	K	166	ARG	NE-CZ-NH1	6.97	123.78	120.30
2	E	154	ASP	CB-CG-OD1	6.96	124.56	118.30
1	M	295	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	C	95	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	M	262	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	N	393	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	E	154	ASP	OD1-CG-OD2	-6.91	110.16	123.30
2	H	39	ARG	NE-CZ-NH1	6.89	123.75	120.30
2	D	312	ARG	NE-CZ-NH1	6.89	123.75	120.30
2	C	266	PHE	CB-CG-CD1	6.84	125.59	120.80
2	H	258	PRO	CA-C-O	6.84	136.62	120.20
2	B	254	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	L	580	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	I	276	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	L	484	PHE	CB-CG-CD1	6.80	125.56	120.80
2	D	183	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	H	260	THR	OG1-CB-CG2	-6.80	94.36	110.00
1	I	260	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	I	420	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	G	335	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	K	272	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	D	183	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	H	258	PRO	N-CA-CB	-6.70	95.23	102.60
2	F	39	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	J	659	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	K	272	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	N	556	ARG	NE-CZ-NH1	6.63	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	181	ARG	NE-CZ-NH1	6.63	123.62	120.30
2	B	90	PHE	CB-CG-CD2	-6.63	116.16	120.80
1	L	484	PHE	CB-CG-CD2	-6.62	116.16	120.80
2	D	147	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	L	234	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	N	166	ARG	NE-CZ-NH2	-6.59	117.00	120.30
2	A	62	ARG	NE-CZ-NH1	6.59	123.59	120.30
2	C	154	ASP	CB-CG-OD1	6.58	124.22	118.30
2	D	154	ASP	OD1-CG-OD2	-6.57	110.81	123.30
2	H	258	PRO	N-CD-CG	-6.57	93.34	103.20
2	H	154	ASP	OD1-CG-OD2	-6.56	110.84	123.30
1	M	181	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	N	272	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	L	272	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	B	90	PHE	CB-CG-CD1	6.48	125.34	120.80
1	M	420	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	C	154	ASP	OD1-CG-OD2	-6.47	111.01	123.30
2	E	290	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	F	95	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	K	387	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	D	154	ASP	CB-CG-OD2	6.44	124.10	118.30
2	B	154	ASP	OD1-CG-OD2	-6.42	111.10	123.30
1	N	85	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	J	534	ARG	NE-CZ-NH1	6.41	123.51	120.30
2	B	154	ASP	CB-CG-OD2	6.39	124.05	118.30
1	L	420	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	E	91	TYR	CB-CG-CD2	6.38	124.83	121.00
2	F	154	ASP	OD1-CG-OD2	-6.38	111.19	123.30
2	F	206	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	M	393	ARG	NE-CZ-NH1	6.35	123.47	120.30
2	E	91	TYR	CB-CG-CD1	-6.35	117.19	121.00
2	C	266	PHE	CB-CG-CD2	-6.34	116.36	120.80
2	D	116	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	E	290	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	J	556	ARG	NE-CZ-NH2	-6.31	117.14	120.30
2	B	206	ARG	NE-CZ-NH2	-6.31	117.14	120.30
2	G	116	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	K	319	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	A	28	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	H	260	THR	CA-C-O	6.26	133.24	120.10
2	C	206	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	I	181	ARG	NE-CZ-NH1	6.22	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	90	PHE	CB-CG-CD1	6.22	125.16	120.80
1	I	569	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	J	166	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	H	154	ASP	CB-CG-OD2	6.22	123.89	118.30
1	L	580	ARG	NE-CZ-NH2	6.21	123.40	120.30
2	A	196	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	A	260	THR	CA-CB-CG2	6.19	121.07	112.40
1	M	374	TYR	CB-CG-CD2	-6.18	117.29	121.00
2	F	37	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	K	276	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	L	136	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	C	206	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	N	521	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	I	41	PHE	CB-CG-CD2	6.16	125.11	120.80
1	J	89	TYR	CB-CG-CD1	6.15	124.69	121.00
2	F	62	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	H	210	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	G	95	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	J	534	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	L	295	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	N	387	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	B	196	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	N	199	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	E	312	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	N	295	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	N	272	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	J	166	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	L	496	TYR	CB-CG-CD1	6.05	124.63	121.00
2	H	256	ARG	N-CA-CB	6.04	121.48	110.60
1	J	85	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	C	28	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	N	319	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	M	521	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	L	659	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	266	PHE	CB-CG-CD1	6.01	125.01	120.80
1	I	138	MET	CG-SD-CE	-6.00	90.59	100.20
2	B	39	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	B	206	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	L	338	PHE	CB-CG-CD1	5.99	124.99	120.80
1	M	374	TYR	CB-CG-CD1	5.97	124.58	121.00
1	I	338	PHE	CB-CG-CD1	5.96	124.97	120.80
1	K	580	ARG	NE-CZ-NH2	5.96	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	255	PHE	CB-CG-CD1	-5.96	116.63	120.80
1	L	393	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	M	556	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	M	618	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	B	147	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	I	618	ARG	NE-CZ-NH1	5.93	123.26	120.30
2	E	15	GLY	C-N-CA	5.92	136.51	121.70
2	B	266	PHE	CB-CG-CD2	-5.92	116.65	120.80
1	K	89	TYR	CB-CG-CD2	-5.92	117.45	121.00
2	H	257	CYS	CB-CA-C	-5.90	98.60	110.40
2	C	39	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	M	420	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	N	572	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	D	90	PHE	CB-CG-CD2	-5.86	116.69	120.80
1	L	438	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	B	177	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	I	393	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	L	569	ARG	NE-CZ-NH2	5.84	123.22	120.30
2	D	37	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	E	116	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	J	199	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	D	116	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	N	205	ARG	NE-CZ-NH1	5.81	123.21	120.30
2	F	62	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	F	154	ASP	CB-CG-OD2	5.80	123.52	118.30
1	K	496	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	I	243	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	K	569	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	K	572	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	L	199	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	H	147	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	G	37	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	L	569	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	M	338	PHE	CB-CG-CD1	5.74	124.82	120.80
2	G	196	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	M	260	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	H	196	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	L	85	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	M	260	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	M	338	PHE	CB-CG-CD2	-5.70	116.81	120.80
2	H	15	GLY	C-N-CA	5.68	135.91	121.70
2	D	39	ARG	NE-CZ-NH2	-5.67	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	89	TYR	CB-CG-CD1	5.66	124.39	121.00
2	C	15	GLY	C-N-CA	5.65	135.82	121.70
1	K	262	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	D	335	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	F	37	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	F	116	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	A	256	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	B	116	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	B	37	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	L	374	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	L	338	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	J	569	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	N	569	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	J	205	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	K	556	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	J	260	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	A	210	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	H	147	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	N	205	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	M	218	SER	N-CA-CB	5.53	118.80	110.50
2	D	154	ASP	N-CA-C	-5.53	96.06	111.00
1	J	234	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	N	260	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	I	276	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	B	147	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	J	319	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	H	206	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	J	443	PHE	CB-CG-CD1	5.49	124.64	120.80
1	N	393	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	I	250	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	M	243	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	N	438	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	M	276	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	L	262	ARG	NE-CZ-NH2	5.47	123.04	120.30
2	F	90	PHE	CB-CG-CD1	5.46	124.62	120.80
2	H	260	THR	CA-CB-OG1	-5.46	97.53	109.00
2	E	39	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	G	305	MET	CG-SD-CE	-5.45	91.48	100.20
2	E	90	PHE	CB-CG-CD2	-5.45	116.98	120.80
1	J	262	ARG	NE-CZ-NH1	-5.45	117.58	120.30
2	F	177	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	M	572	ARG	NE-CZ-NH1	5.43	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	254	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	H	256	ARG	O-C-N	5.42	131.38	122.70
1	K	387	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	F	290	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	G	312	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	H	254	ARG	O-C-N	5.40	131.34	122.70
2	H	259	GLU	C-N-CA	-5.39	108.22	121.70
1	I	338	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	J	339	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	I	41	PHE	CB-CG-CD1	-5.37	117.05	120.80
1	L	420	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	I	393	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	J	276	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	E	313	MET	CG-SD-CE	-5.35	91.65	100.20
2	B	15	GLY	C-N-CA	5.34	135.06	121.70
1	J	250	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	H	256	ARG	CA-C-O	-5.34	108.89	120.10
1	I	295	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	M	484	PHE	CB-CG-CD1	5.33	124.53	120.80
2	G	28	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	K	496	TYR	CB-CG-CD1	5.32	124.19	121.00
1	M	569	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	M	572	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	F	91	TYR	CB-CG-CD1	5.31	124.18	121.00
1	K	420	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	E	90	PHE	CB-CG-CD1	5.29	124.50	120.80
2	H	258	PRO	N-CA-C	-5.29	98.36	112.10
1	J	438	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	F	90	PHE	CB-CG-CD2	-5.26	117.11	120.80
1	M	484	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	K	569	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	N	262	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	M	613	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	K	66	MET	CG-SD-CE	-5.24	91.82	100.20
1	I	280	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	D	254	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	H	116	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	I	272	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	I	450	TYR	CB-CG-CD2	-5.21	117.87	121.00
2	C	147	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	D	62	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	E	33	SER	N-CA-CB	5.19	118.28	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	37	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	J	569	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	L	166	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	I	613	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	J	295	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	D	95	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	L	487	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	H	116	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	A	154	ASP	N-CA-CB	5.13	119.84	110.60
2	G	210	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	H	290	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	N	107	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	L	276	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	I	250	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	L	319	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	E	177	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	N	580	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	N	613	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	K	85	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	K	456	ASP	OD1-CG-OD2	-5.05	113.70	123.30
2	E	62	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	F	15	GLY	C-N-CA	5.04	134.30	121.70
1	I	580	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	I	438	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	N	260	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	L	561	ARG	NE-CZ-NH2	5.00	122.80	120.30
2	E	254	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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	3	0
1	K	5590	0	5536	3	0
1	L	5590	0	5536	4	0
1	M	5590	0	5536	5	0
1	N	5590	0	5536	0	0
2	A	2862	0	2831	1	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	5	0
2	F	2862	0	2831	2	0
2	G	2862	0	2831	2	0
2	H	2862	0	2831	20	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
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	58	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 (58) 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:259:GLU:N	2:H:259:GLU:CA	1.68	1.53
2:H:260:THR:CA	2:H:260:THR:C	1.76	1.51
2:H:258:PRO:C	2:H:258:PRO:CA	1.79	1.51
2:H:258:PRO:O	2:H:259:GLU:CA	2.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:258:PRO:C	2:H:258:PRO:CB	2.32	0.97
2:H:260:THR:C	2:H:260:THR:CB	2.62	0.69
2:H:258:PRO:C	2:H:259:GLU:CA	2.59	0.67
2:H:258:PRO:C	2:H:258:PRO:N	2.47	0.64
2:H:255:PHE:O	2:H:259:GLU:HB2	1.98	0.63
2:H:258:PRO:C	2:H:258:PRO:HB2	2.19	0.59
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
1:M:29:LEU:H	1:M:29:LEU:HD23	1.73	0.53
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:H:259:GLU:O	2:H:260:THR:C	2.51	0.49
2:C:158:GLY:HA2	2:C:183:ARG:H	1.77	0.49
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
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:H:161:HIS:CE1	2:H:177:ARG:HB2	2.50	0.46
2:E:15:GLY:HA3	2:E:16:LEU:HB2	1.97	0.46
2:B:253:GLU:H	2:B:253:GLU:CD	2.19	0.46
2:H:173:HIS:CD2	2:H:173:HIS:H	2.31	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:G:253:GLU:H	2:G:253:GLU:CD	2.20	0.44
1:L:11:HIS:CD2	1:L:12:PRO:HD2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:430:HIS:CE1	1:M:625:THR:HG21	2.55	0.42
2:D:253:GLU:H	2:D:253:GLU:CD	2.24	0.42
2:H:258:PRO:O	2:H:259:GLU:C	2.59	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:J:60:GLU:CD	1:J:80:ARG:HH12	2.24	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:K:243:ARG:HH21	1:K:246:HIS:CD2	2.39	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 ⓘ

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	699/704 (99%)	641 (92%)	49 (7%)	9 (1%)	12	47
1	J	699/704 (99%)	631 (90%)	56 (8%)	12 (2%)	9	41
1	K	699/704 (99%)	636 (91%)	53 (8%)	10 (1%)	11	45
1	L	699/704 (99%)	639 (91%)	52 (7%)	8 (1%)	14	51
1	M	699/704 (99%)	634 (91%)	56 (8%)	9 (1%)	12	47
1	N	699/704 (99%)	633 (91%)	60 (9%)	6 (1%)	17	56
2	A	365/373 (98%)	325 (89%)	33 (9%)	7 (2%)	8	38
2	B	365/373 (98%)	326 (89%)	32 (9%)	7 (2%)	8	38
2	C	365/373 (98%)	327 (90%)	27 (7%)	11 (3%)	4	28
2	D	365/373 (98%)	326 (89%)	32 (9%)	7 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	365/373 (98%)	325 (89%)	27 (7%)	13 (4%)	3	25
2	F	365/373 (98%)	319 (87%)	39 (11%)	7 (2%)	8	38
2	G	365/373 (98%)	331 (91%)	29 (8%)	5 (1%)	11	45
2	H	365/373 (98%)	325 (89%)	32 (9%)	8 (2%)	6	35
All	All	7114/7208 (99%)	6418 (90%)	577 (8%)	119 (2%)	13	41

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	603 (97%)	16 (3%)	46	67
1	J	619/621 (100%)	605 (98%)	14 (2%)	50	70
1	K	619/621 (100%)	604 (98%)	15 (2%)	49	69
1	L	619/621 (100%)	606 (98%)	13 (2%)	53	72
1	M	619/621 (100%)	603 (97%)	16 (3%)	46	67
1	N	619/621 (100%)	605 (98%)	14 (2%)	50	70
2	A	310/316 (98%)	302 (97%)	8 (3%)	46	67
2	B	310/316 (98%)	300 (97%)	10 (3%)	39	61
2	C	310/316 (98%)	304 (98%)	6 (2%)	57	75
2	D	310/316 (98%)	302 (97%)	8 (3%)	46	67
2	E	310/316 (98%)	299 (96%)	11 (4%)	36	60
2	F	310/316 (98%)	299 (96%)	11 (4%)	36	60
2	G	310/316 (98%)	302 (97%)	8 (3%)	46	67
2	H	310/316 (98%)	298 (96%)	12 (4%)	32	57
All	All	6194/6254 (99%)	6032 (97%)	162 (3%)	49	67

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	41	PHE
1	I	52	GLU
1	I	115	TYR
1	I	133	LYS

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Mol	Chain	Res	Type
1	I	136	ARG
1	I	141	LEU
1	I	152	GLU
1	I	208	LYS
1	I	229	LEU
1	I	275	ASN
1	I	276	ARG
1	I	310	LEU
1	I	351	ASP
1	I	443	PHE
1	I	463	PHE
1	I	537	GLN
1	J	41	PHE
1	J	52	GLU
1	J	133	LYS
1	J	141	LEU
1	J	176	GLN
1	J	229	LEU
1	J	276	ARG
1	J	367	LYS
1	J	443	PHE
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	137	ASP
1	K	229	LEU
1	K	316	ASP
1	K	351	ASP
1	K	433	ASP
1	K	513	ASP
1	K	527	ASP
1	K	593	PHE
1	K	599	ASP
1	K	604	SER
1	K	615	LYS
1	K	622	GLU
1	K	630	ASP
1	L	115	TYR

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Mol	Chain	Res	Type
1	L	133	LYS
1	L	136	ARG
1	L	141	LEU
1	L	299	GLU
1	L	351	ASP
1	L	505	GLU
1	L	511	ASN
1	L	513	ASP
1	L	529	LEU
1	L	577	PHE
1	L	615	LYS
1	L	701	MET
1	M	52	GLU
1	M	104	PRO
1	M	133	LYS
1	M	141	LEU
1	M	152	GLU
1	M	160	ASN
1	M	186	ASN
1	M	208	LYS
1	M	276	ARG
1	M	346	HIS
1	M	381	LEU
1	M	382	ASP
1	M	593	PHE
1	M	601	LEU
1	M	603	MET
1	M	694	MET
1	N	57	LYS
1	N	115	TYR
1	N	133	LYS
1	N	152	GLU
1	N	276	ARG
1	N	331	ASP
1	N	351	ASP
1	N	396	LEU
1	N	527	ASP
1	N	530	ASP
1	N	540	ASP
1	N	553	ASP
1	N	573	ASP
1	N	630	ASP

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Mol	Chain	Res	Type
2	A	12	ASN
2	A	16	LEU
2	A	66	THR
2	A	113	LYS
2	A	157	ASP
2	A	253	GLU
2	A	260	THR
2	A	355	MET
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	179	ASP
2	B	253	GLU
2	C	39	ARG
2	C	79	TRP
2	C	157	ASP
2	C	161	HIS
2	C	194	THR
2	C	253	GLU
2	D	12	ASN
2	D	39	ARG
2	D	92	ASN
2	D	124	PHE
2	D	149	THR
2	D	157	ASP
2	D	179	ASP
2	D	242	LEU
2	E	12	ASN
2	E	14	SER
2	E	37	ARG
2	E	44	MET
2	E	107	GLU
2	E	113	LYS
2	E	154	ASP
2	E	157	ASP
2	E	177	ARG
2	E	219	VAL

Continued on next page...

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Mol	Chain	Res	Type
2	E	253	GLU
2	F	12	ASN
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	274	ILE
2	G	12	ASN
2	G	39	ARG
2	G	79	TRP
2	G	113	LYS
2	G	123	MET
2	G	157	ASP
2	G	161	HIS
2	G	187	ASP
2	H	92	ASN
2	H	104	LEU
2	H	124	PHE
2	H	154	ASP
2	H	157	ASP
2	H	161	HIS
2	H	173	HIS
2	H	179	ASP
2	H	184	ASP
2	H	219	VAL
2	H	253	GLU
2	H	258	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	275	ASN
1	I	434	HIS
1	I	497	GLN
1	J	227	HIS
1	K	568	HIS
1	L	290	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	M	430	HIS
1	M	434	HIS
1	M	497	GLN
1	M	554	HIS
1	N	75	HIS
1	N	290	GLN
1	N	592	GLN
1	N	678	HIS
2	A	40	HIS
2	B	88	HIS
2	B	161	HIS
2	B	225	ASN
2	C	173	HIS
2	D	88	HIS
2	D	92	ASN
2	D	275	HIS
2	E	87	HIS
2	E	88	HIS
2	E	92	ASN
2	E	161	HIS
2	E	275	HIS
2	F	88	HIS
2	F	275	HIS
2	G	88	HIS
2	G	92	ASN
2	G	161	HIS
2	H	40	HIS
2	H	88	HIS
2	H	92	ASN
2	H	101	HIS
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 [i](#)

There are no monosaccharides 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	B	402	3	24,29,29	0.92	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	H	402	3	24,29,29	0.92	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	G	402	3	24,29,29	0.91	1 (4%)	29,45,45	1.51	4 (13%)
4	ADP	E	402	3	24,29,29	0.93	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	D	402	3	24,29,29	0.91	1 (4%)	29,45,45	1.51	4 (13%)
4	ADP	C	402	3	24,29,29	0.91	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	A	402	3	24,29,29	0.91	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	F	402	3	24,29,29	0.92	1 (4%)	29,45,45	1.51	4 (13%)

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	B	402	3	-	3/12/32/32	0/3/3/3
4	ADP	H	402	3	-	3/12/32/32	0/3/3/3
4	ADP	G	402	3	-	3/12/32/32	0/3/3/3
4	ADP	E	402	3	-	3/12/32/32	0/3/3/3
4	ADP	D	402	3	-	3/12/32/32	0/3/3/3
4	ADP	C	402	3	-	3/12/32/32	0/3/3/3
4	ADP	A	402	3	-	3/12/32/32	0/3/3/3
4	ADP	F	402	3	-	3/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	402	ADP	C5-C4	2.48	1.47	1.40
4	F	402	ADP	C5-C4	2.47	1.47	1.40
4	C	402	ADP	C5-C4	2.45	1.47	1.40
4	D	402	ADP	C5-C4	2.45	1.47	1.40
4	H	402	ADP	C5-C4	2.44	1.47	1.40
4	B	402	ADP	C5-C4	2.44	1.47	1.40
4	E	402	ADP	C5-C4	2.41	1.47	1.40
4	A	402	ADP	C5-C4	2.40	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	ADP	PA-O3A-PB	-3.95	119.25	132.83
4	B	402	ADP	PA-O3A-PB	-3.94	119.29	132.83
4	C	402	ADP	PA-O3A-PB	-3.94	119.31	132.83
4	E	402	ADP	PA-O3A-PB	-3.93	119.33	132.83
4	D	402	ADP	PA-O3A-PB	-3.93	119.34	132.83
4	G	402	ADP	PA-O3A-PB	-3.93	119.36	132.83
4	H	402	ADP	PA-O3A-PB	-3.92	119.36	132.83
4	F	402	ADP	PA-O3A-PB	-3.92	119.39	132.83
4	H	402	ADP	C3'-C2'-C1'	3.13	105.70	100.98
4	B	402	ADP	C4-C5-N7	-3.12	106.15	109.40
4	E	402	ADP	C3'-C2'-C1'	3.11	105.65	100.98
4	F	402	ADP	C3'-C2'-C1'	3.08	105.61	100.98
4	B	402	ADP	C3'-C2'-C1'	3.08	105.61	100.98
4	G	402	ADP	C4-C5-N7	-3.07	106.20	109.40
4	C	402	ADP	C3'-C2'-C1'	3.05	105.57	100.98
4	D	402	ADP	C4-C5-N7	-3.05	106.22	109.40
4	A	402	ADP	C3'-C2'-C1'	3.05	105.57	100.98
4	H	402	ADP	C4-C5-N7	-3.05	106.22	109.40
4	F	402	ADP	C4-C5-N7	-3.03	106.24	109.40
4	C	402	ADP	C4-C5-N7	-3.03	106.24	109.40
4	D	402	ADP	C3'-C2'-C1'	3.02	105.53	100.98
4	E	402	ADP	C4-C5-N7	-3.02	106.25	109.40
4	G	402	ADP	C3'-C2'-C1'	3.02	105.53	100.98
4	A	402	ADP	N3-C2-N1	-2.99	124.00	128.68
4	A	402	ADP	C4-C5-N7	-2.99	106.28	109.40
4	H	402	ADP	N3-C2-N1	-2.96	124.05	128.68
4	E	402	ADP	N3-C2-N1	-2.95	124.07	128.68
4	C	402	ADP	N3-C2-N1	-2.95	124.08	128.68
4	B	402	ADP	N3-C2-N1	-2.93	124.10	128.68
4	D	402	ADP	N3-C2-N1	-2.91	124.14	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	402	ADP	N3-C2-N1	-2.90	124.14	128.68
4	F	402	ADP	N3-C2-N1	-2.87	124.20	128.68

There are no chirality outliers.

All (24) torsion outliers are listed below:

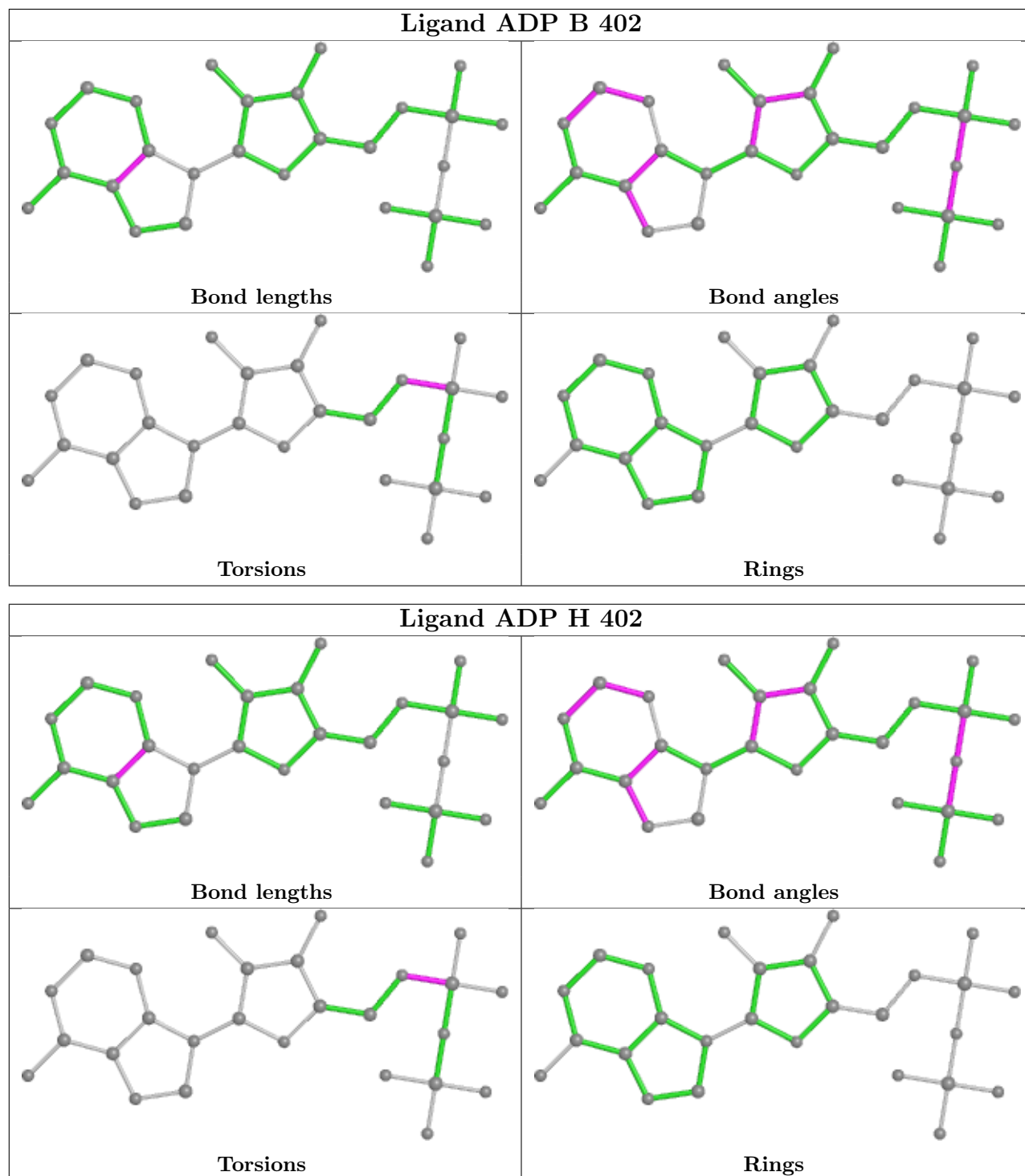
Mol	Chain	Res	Type	Atoms
4	A	402	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	C5'-O5'-PA-O2A
4	B	402	ADP	C5'-O5'-PA-O1A
4	B	402	ADP	C5'-O5'-PA-O2A
4	C	402	ADP	C5'-O5'-PA-O1A
4	C	402	ADP	C5'-O5'-PA-O2A
4	D	402	ADP	C5'-O5'-PA-O1A
4	D	402	ADP	C5'-O5'-PA-O2A
4	E	402	ADP	C5'-O5'-PA-O1A
4	E	402	ADP	C5'-O5'-PA-O2A
4	F	402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

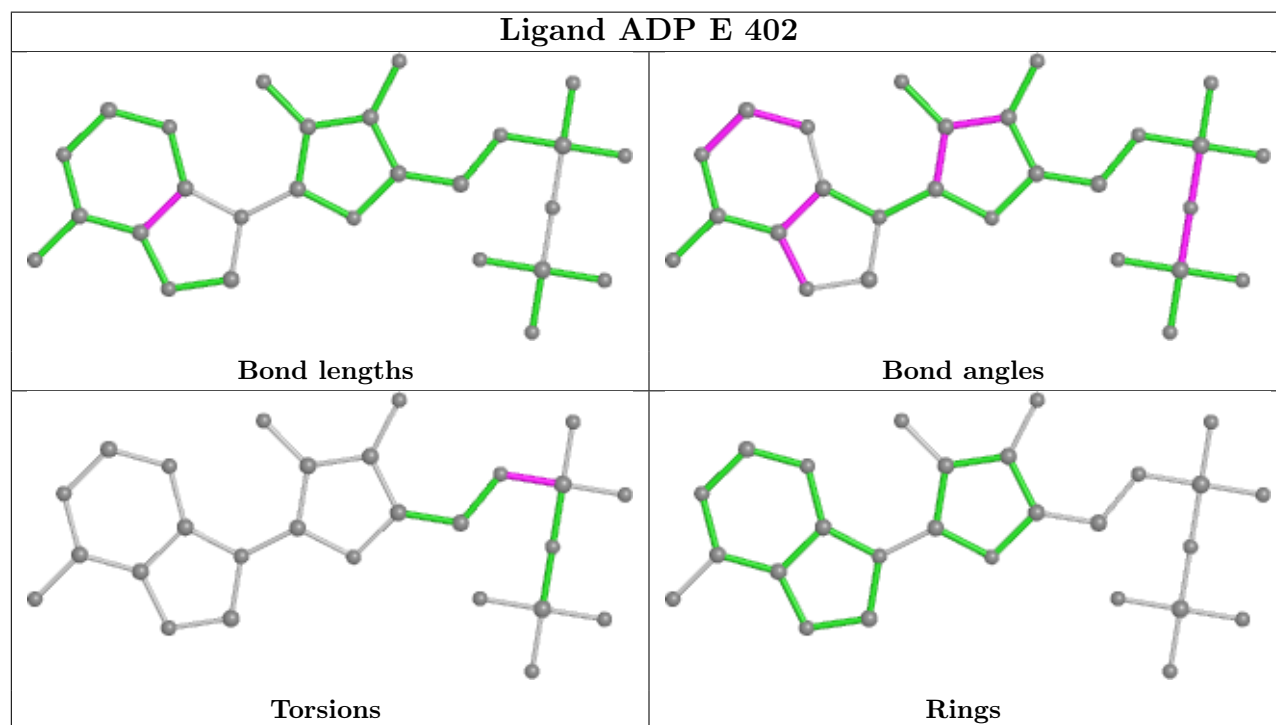
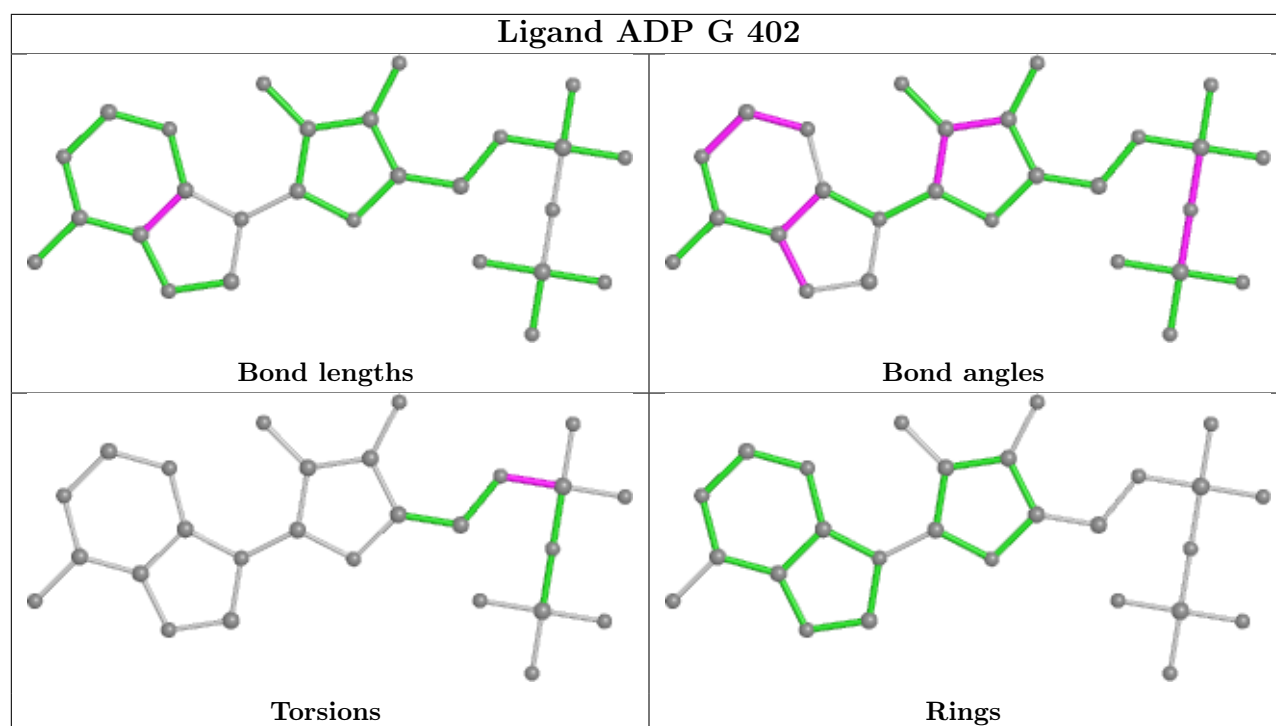
There are no ring outliers.

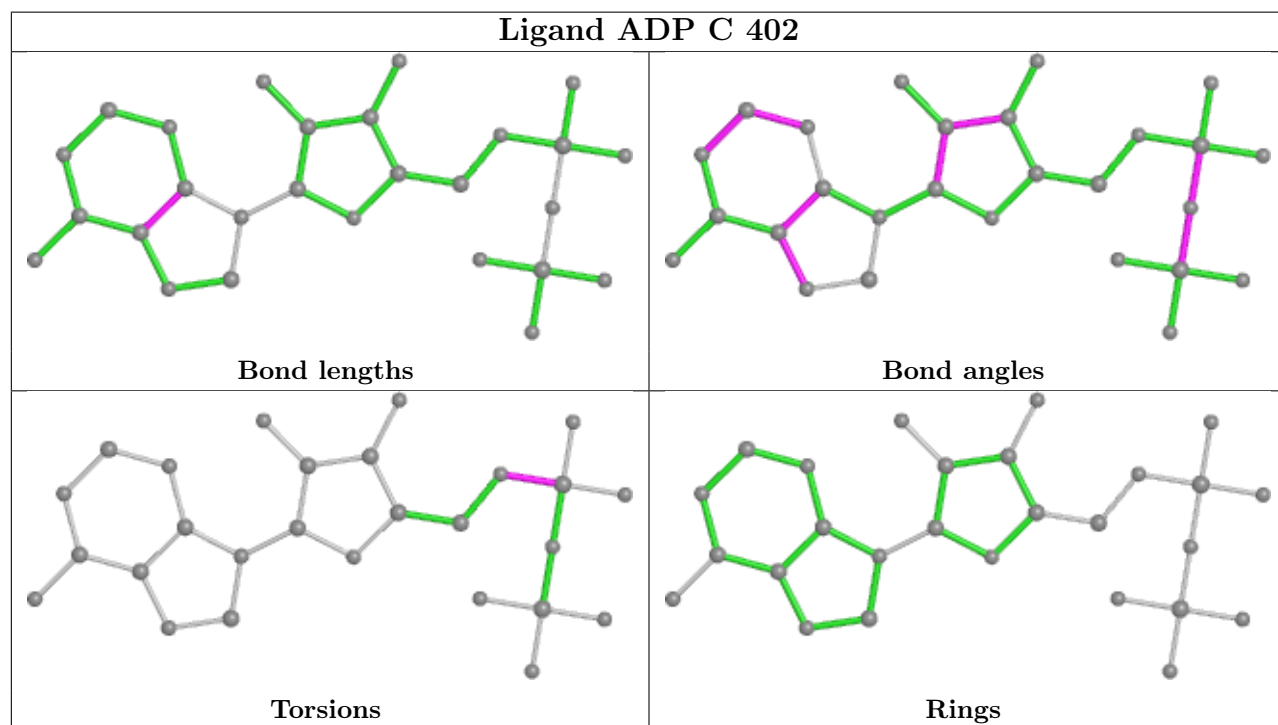
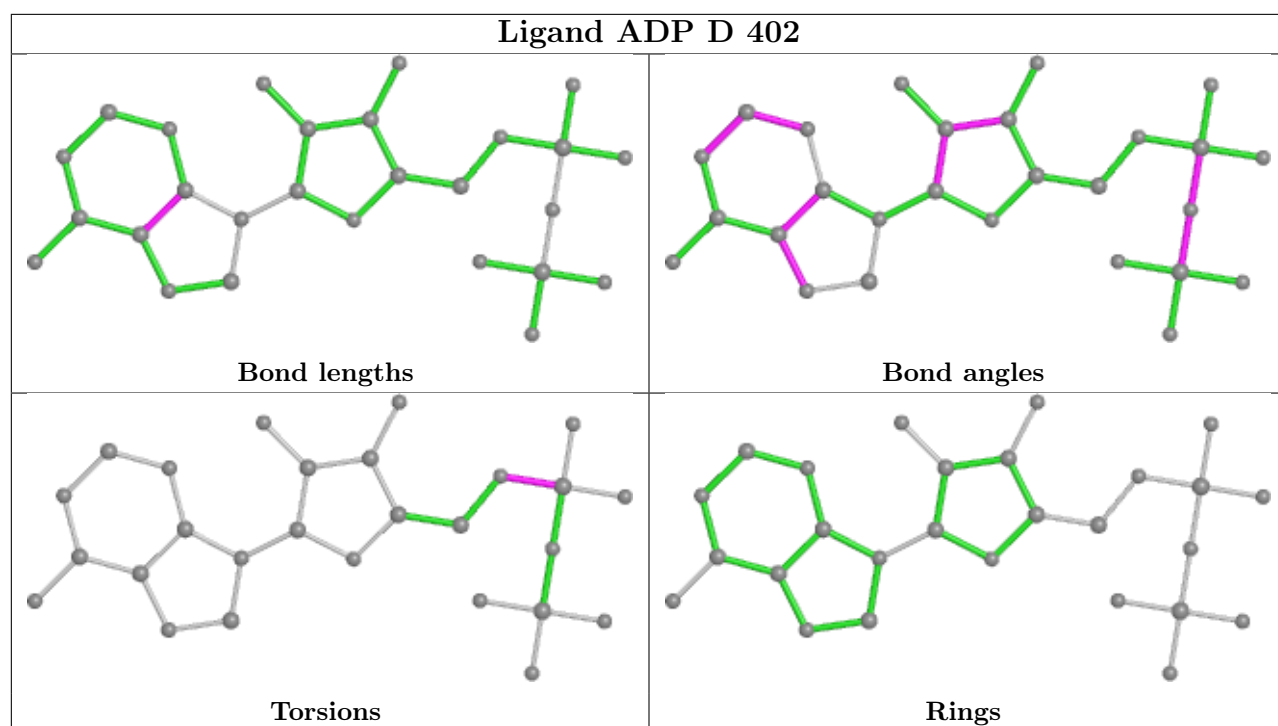
No monomer is involved in short contacts.

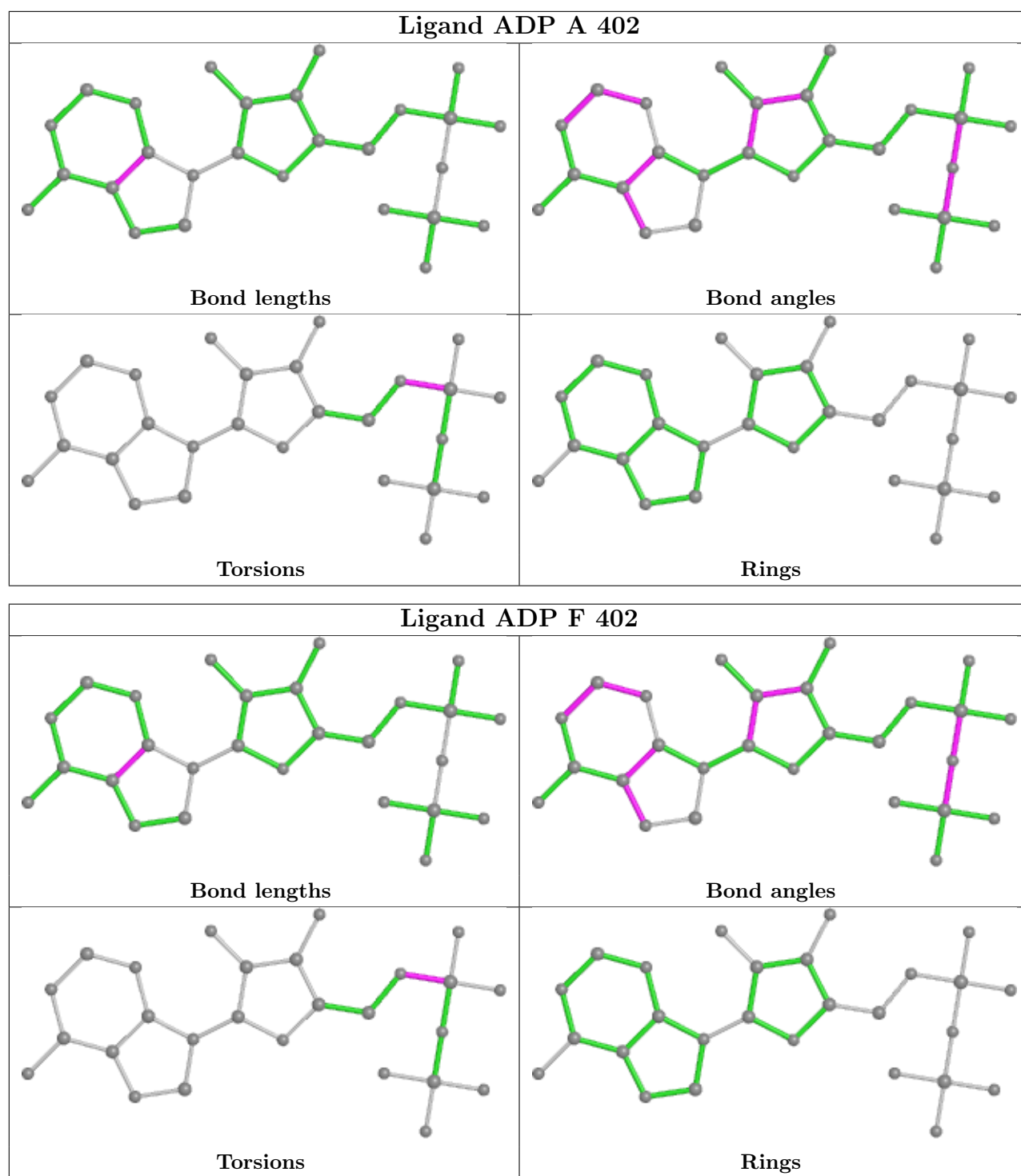
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

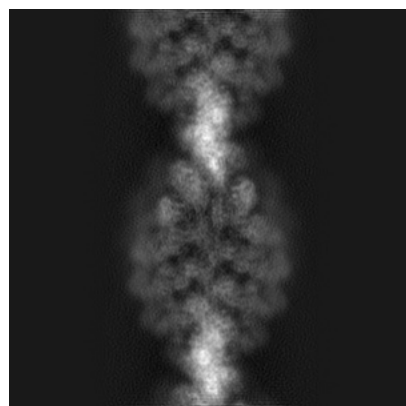
6 Map visualisation [i](#)

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.

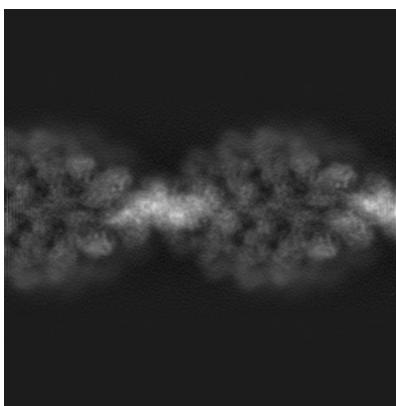
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

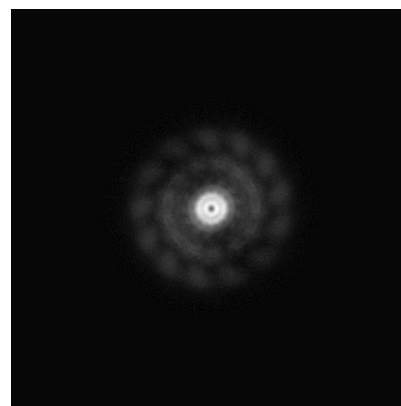
6.1.1 Primary map



X

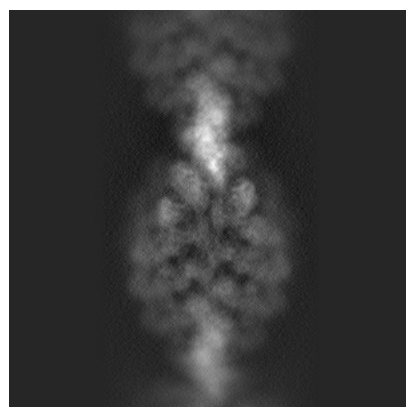


Y

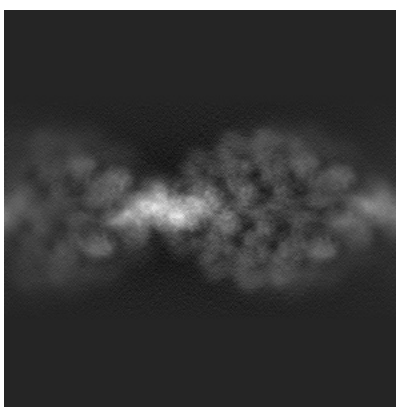


Z

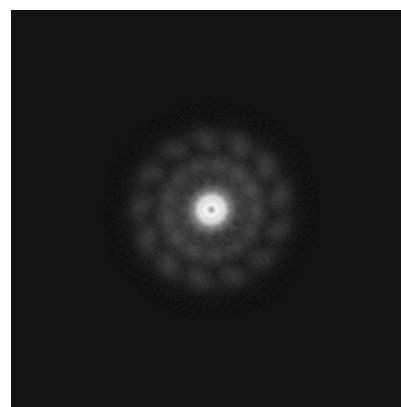
6.1.2 Raw map



X



Y

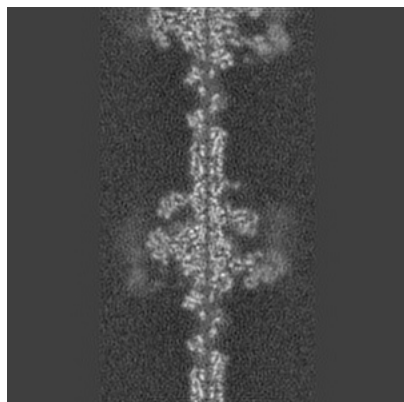


Z

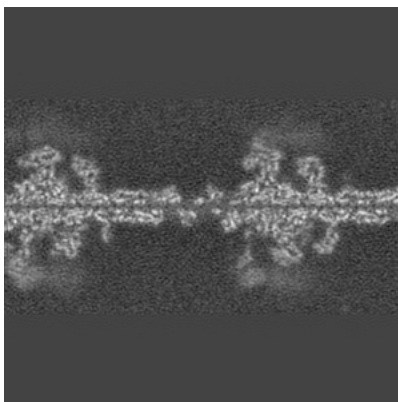
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

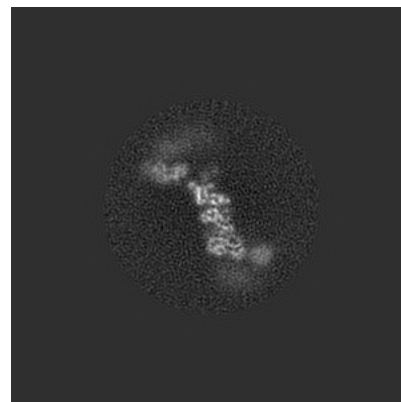
6.2.1 Primary map



X Index: 256

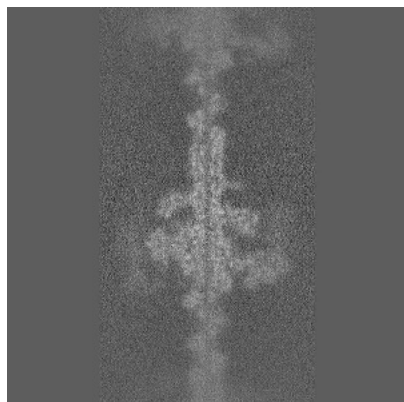


Y Index: 256

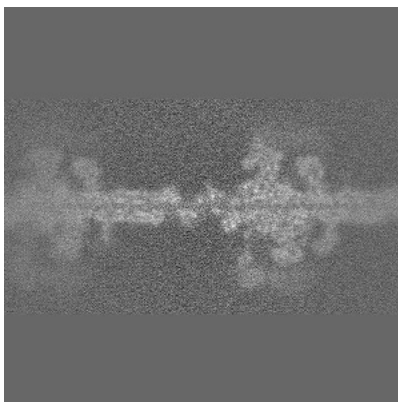


Z Index: 256

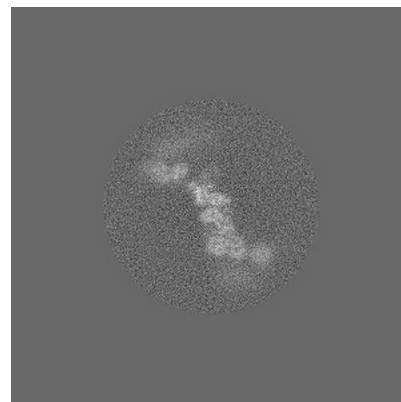
6.2.2 Raw map



X Index: 256



Y Index: 256

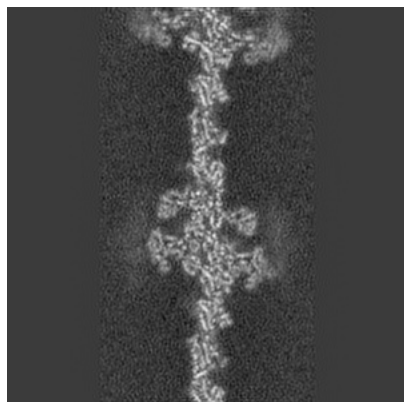


Z Index: 256

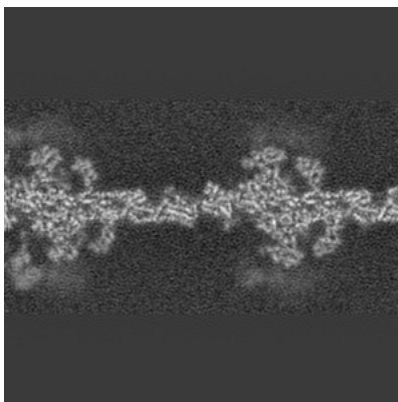
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

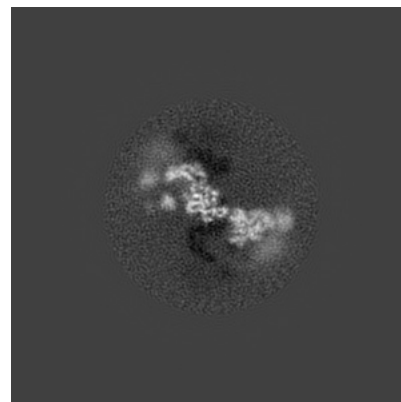
6.3.1 Primary map



X Index: 262

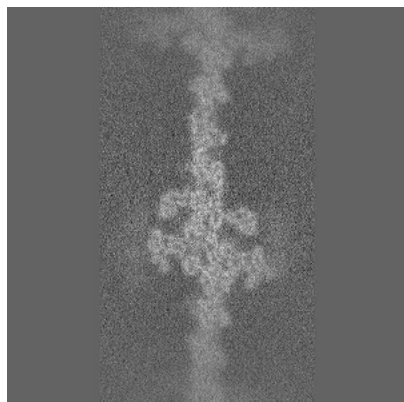


Y Index: 251

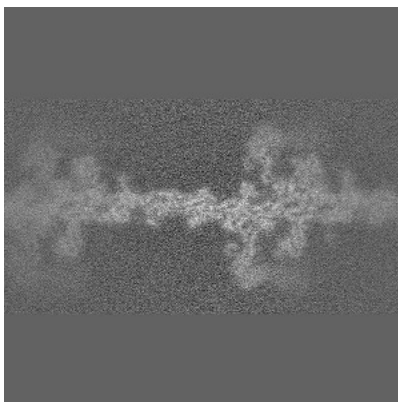


Z Index: 1

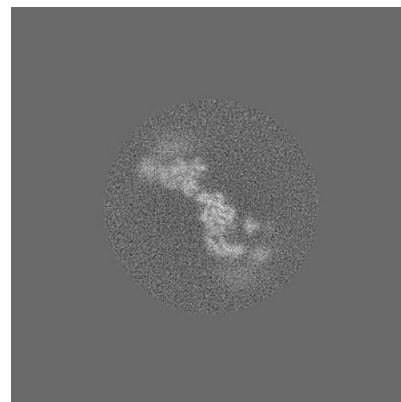
6.3.2 Raw map



X Index: 262



Y Index: 263

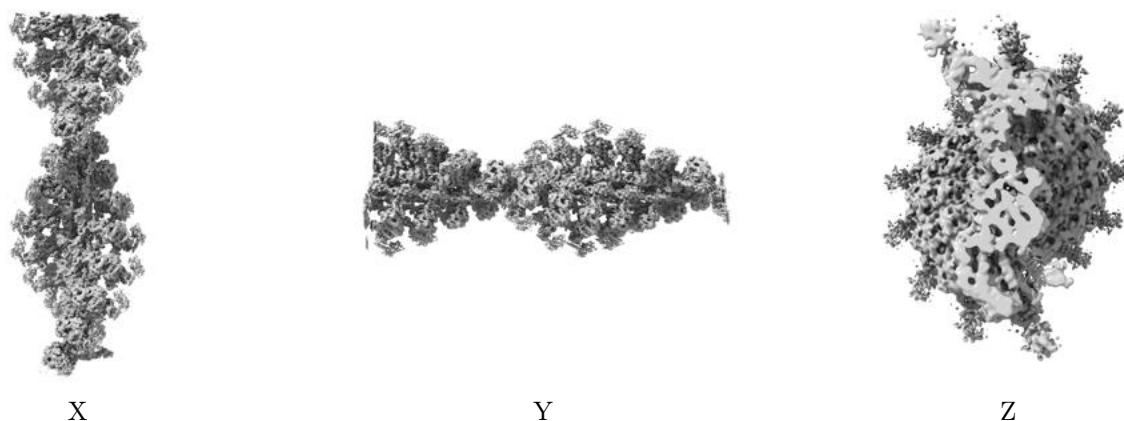


Z Index: 266

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

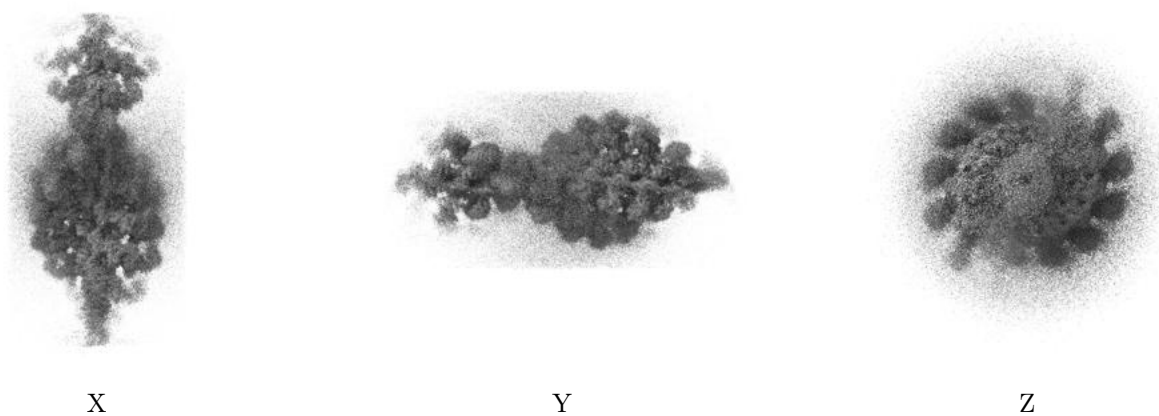
6.4 Orthogonal surface views [i](#)

6.4.1 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.

6.4.2 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.

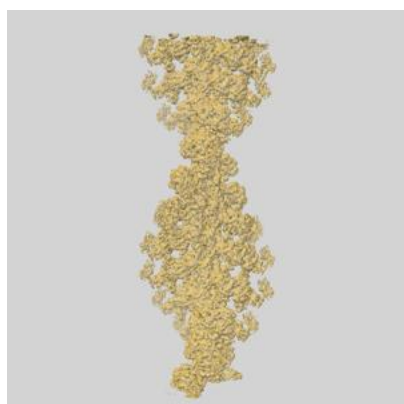
6.5 Mask visualisation [i](#)

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

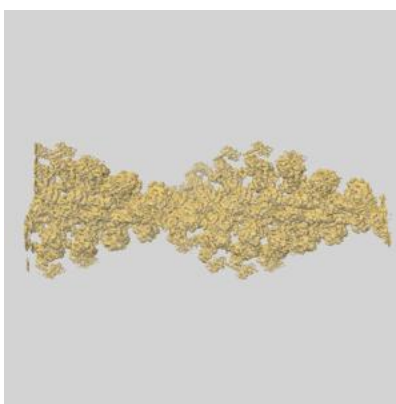
A mask typically either:

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

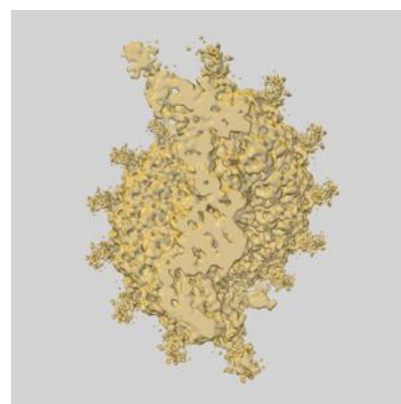
6.5.1 emd_7117_msk_2.map [i](#)



X

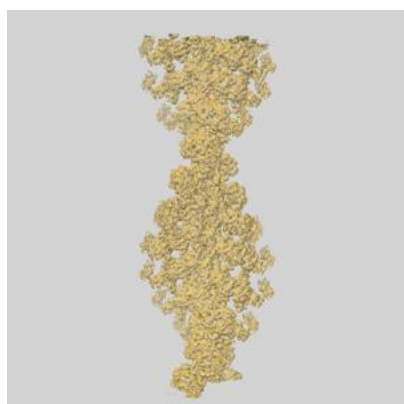


Y

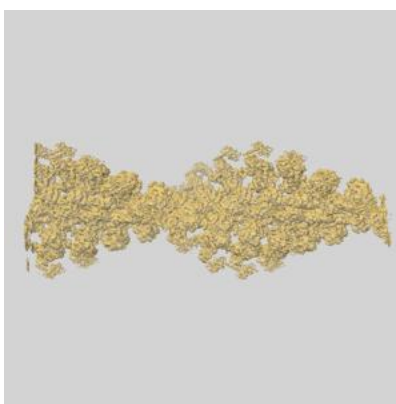


Z

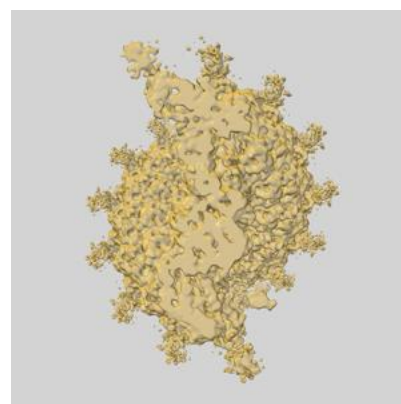
6.5.2 emd_7117_msk_1.map [i](#)



X



Y

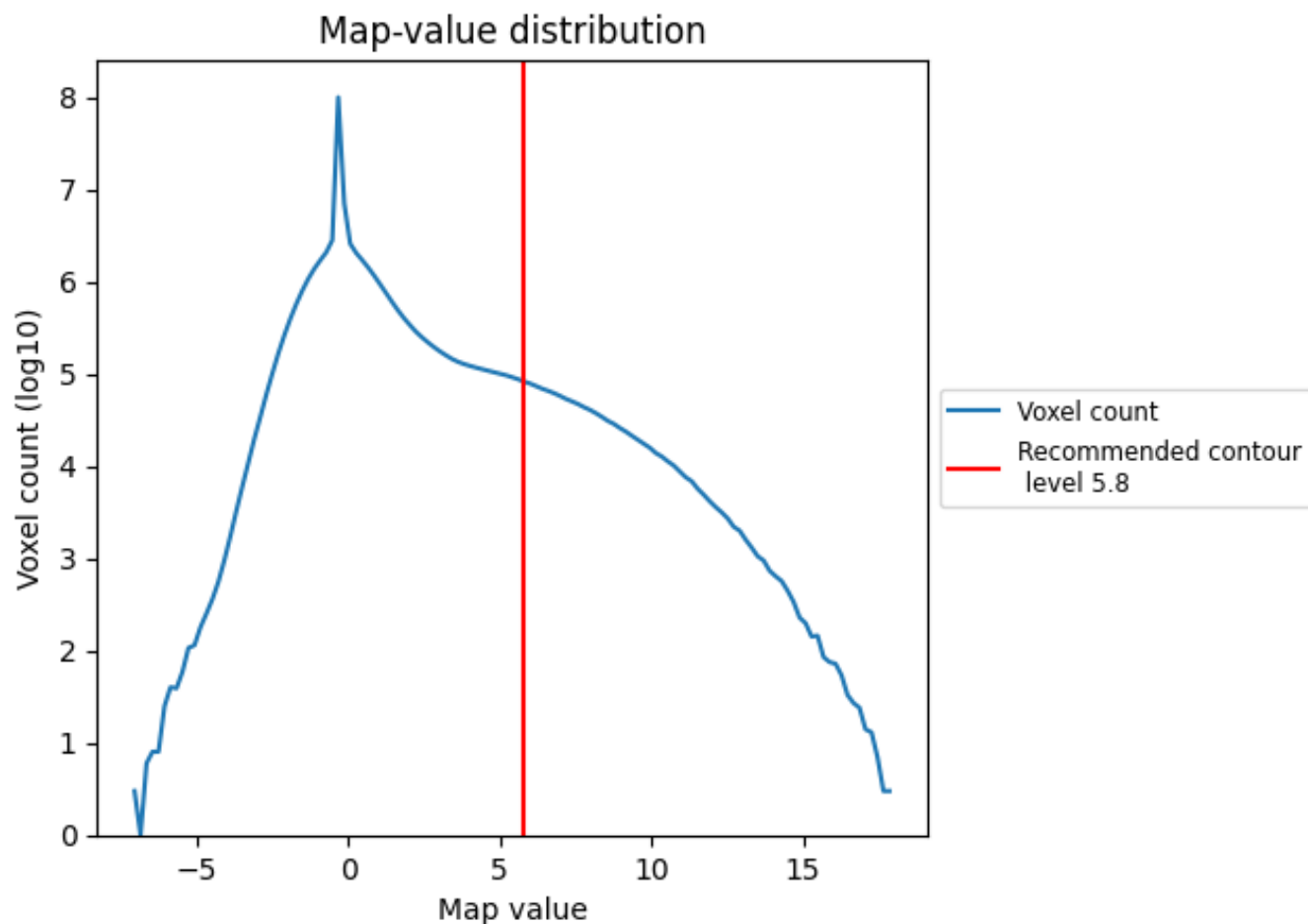


Z

7 Map analysis [i](#)

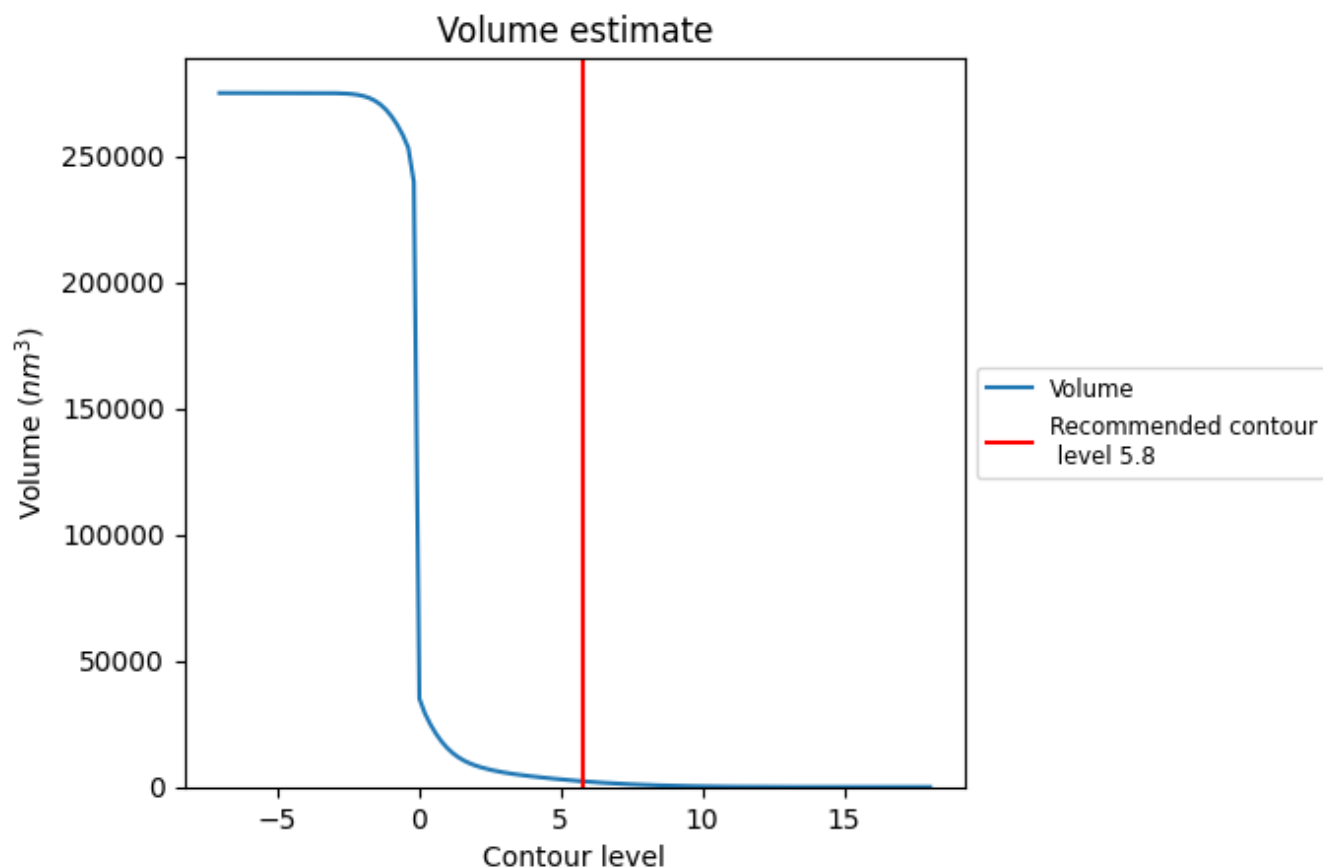
This section contains the results of statistical analysis of the map.

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.

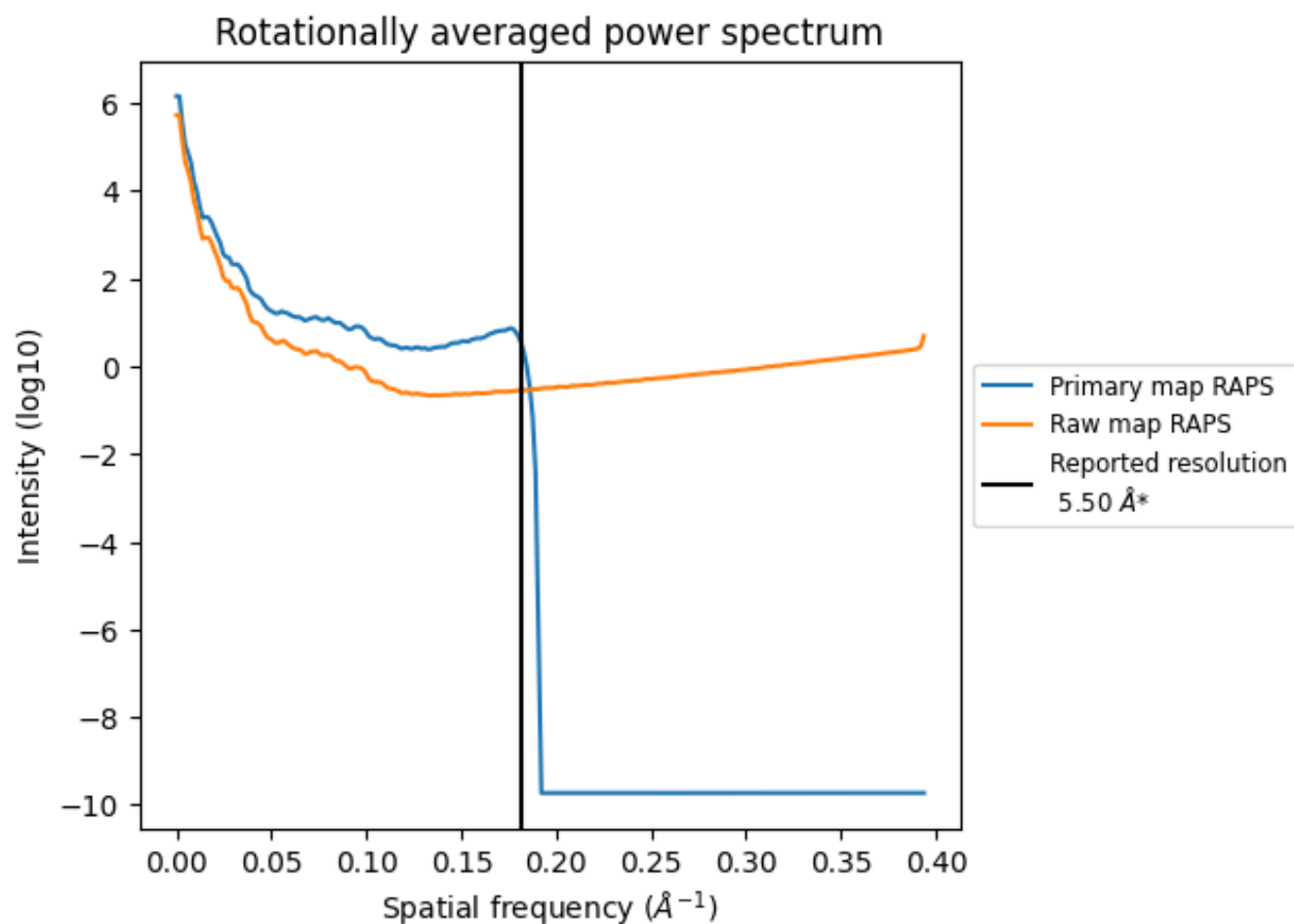
7.2 Volume estimate [i](#)



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 ⓘ

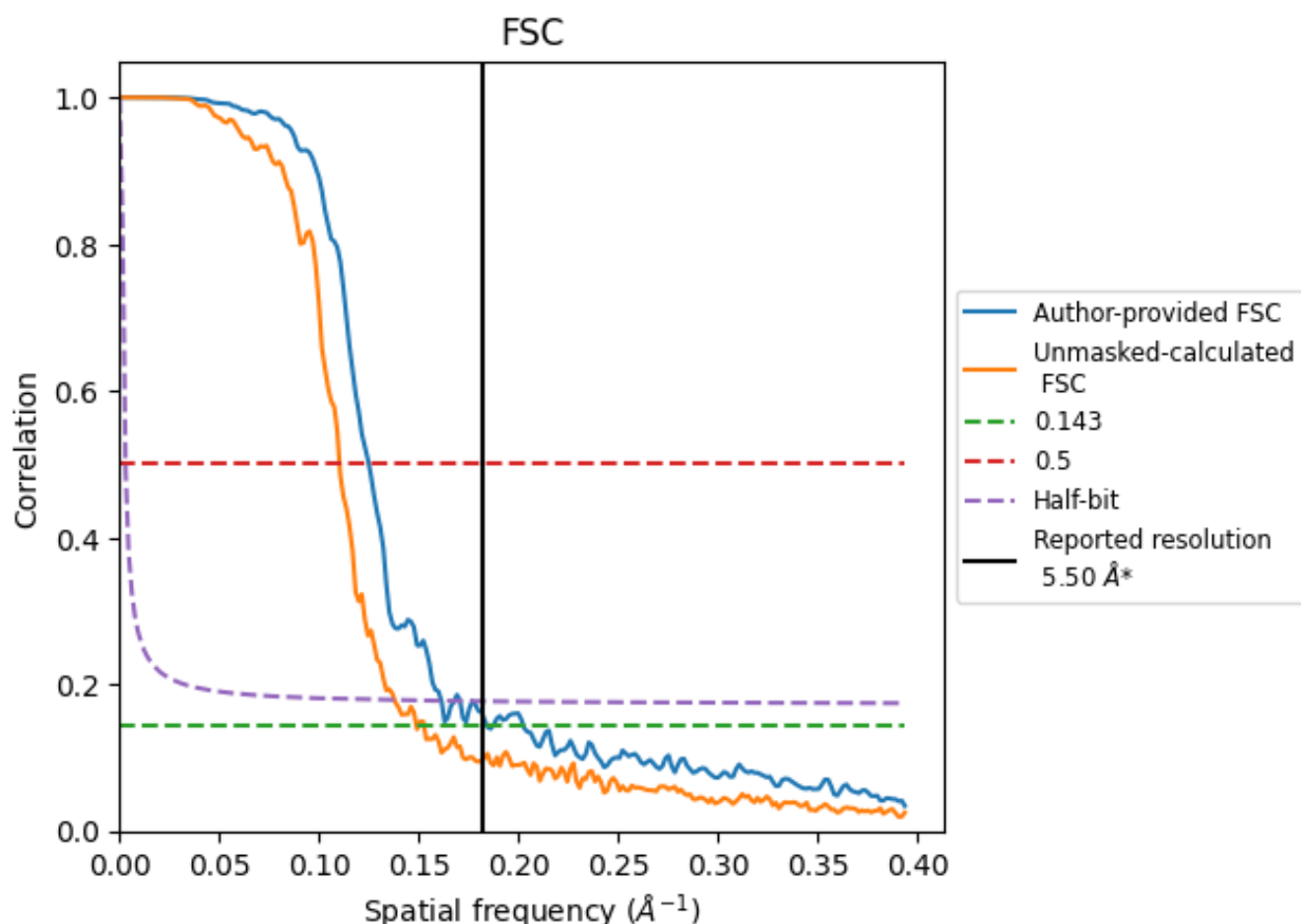


*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

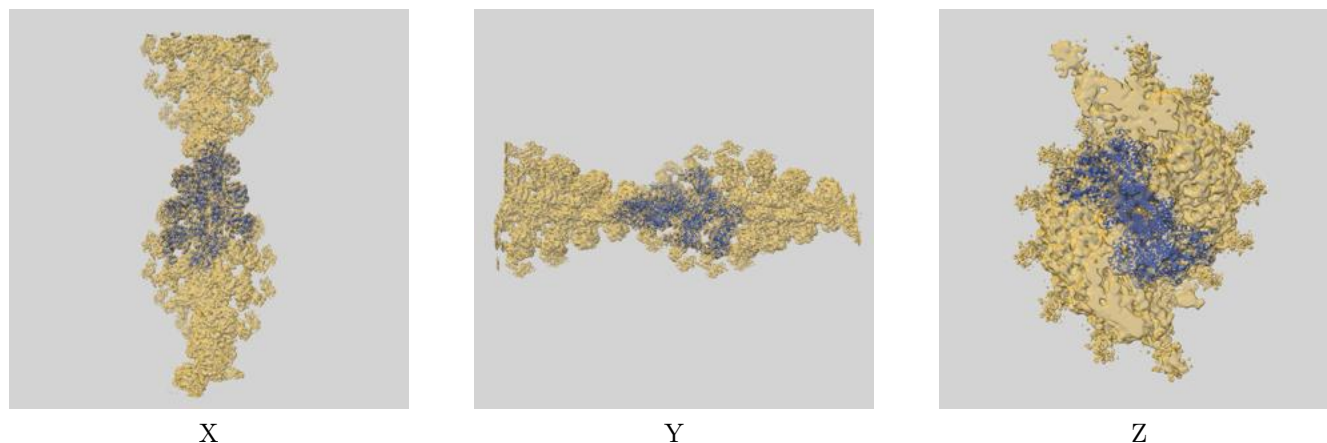
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.43	8.00	6.20
Unmasked-calculated*	6.72	9.07	7.25

*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](#)

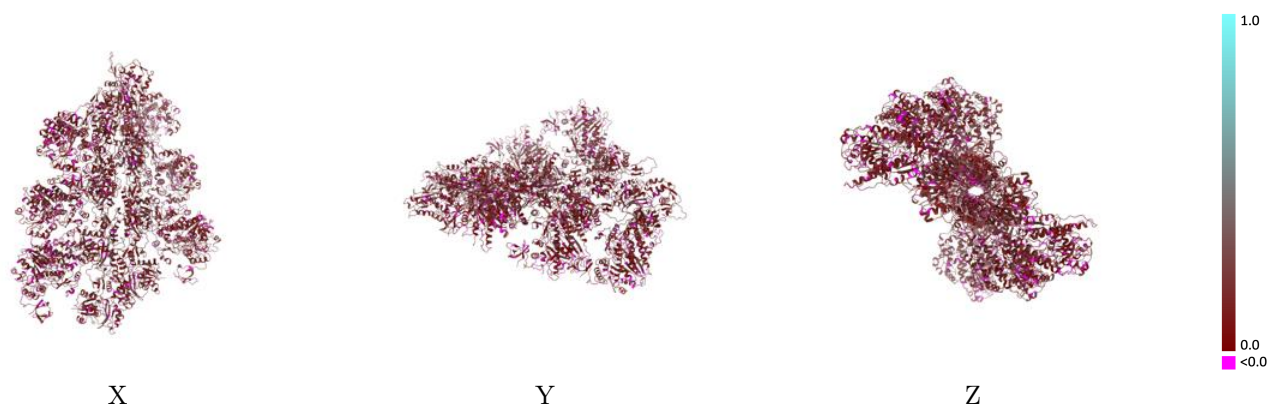
This section contains information regarding the fit between EMDB map EMD-7117 and PDB model 6BNQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



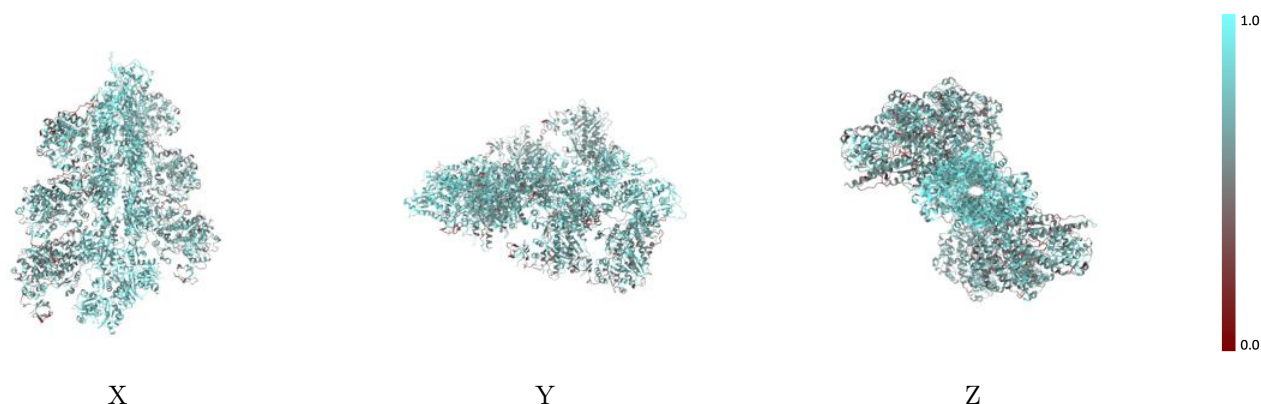
The images above show the 3D surface view of the map at the recommended contour level 5.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



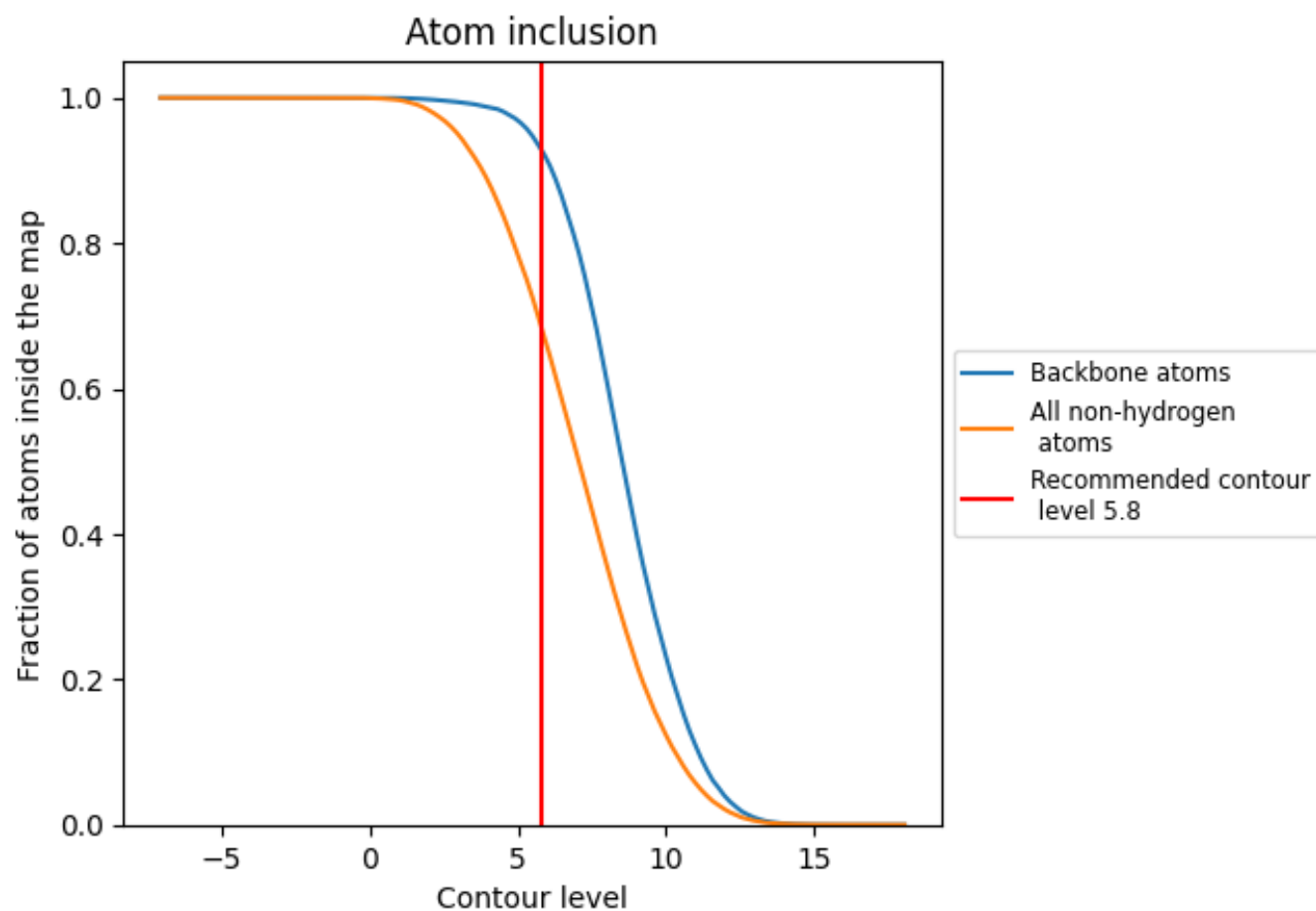
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6841	 0.1680
A	 0.7972	 0.1910
B	 0.7898	 0.1870
C	 0.7898	 0.1900
D	 0.7927	 0.1910
E	 0.7898	 0.1890
F	 0.8011	 0.1920
G	 0.7958	 0.1880
H	 0.7944	 0.1850
I	 0.6040	 0.1510
J	 0.6115	 0.1550
K	 0.6139	 0.1530
L	 0.6066	 0.1520
M	 0.6088	 0.1520
N	 0.6069	 0.1540

