



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 02:35 PM EST

PDB ID : 6BNP
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.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

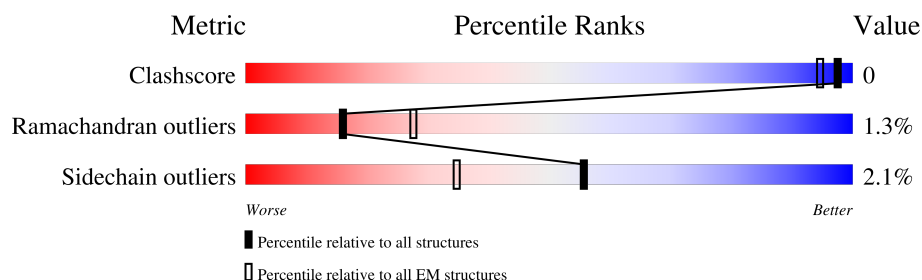
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
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>26%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	J	704	<div> <div>36%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	K	704	<div> <div>22%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	L	704	<div> <div>41%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	M	704	<div> <div>21%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	N	704	<div> <div>44%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
2	A	373	<div> <div>.</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
2	B	373	<div> <div>.</div> <div>89%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	373	<div><div></div><div>88%</div><div>8% ...</div></div>
2	D	373	<div><div>6%</div><div>89%</div><div>8% ..</div></div>
2	E	373	<div><div></div><div>90%</div><div>8% ..</div></div>
2	F	373	<div><div>11%</div><div>91%</div><div>7% ..</div></div>
2	G	373	<div><div>5%</div><div>87%</div><div>10% ..</div></div>
2	H	373	<div><div>18%</div><div>90%</div><div>8% ..</div></div>

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		

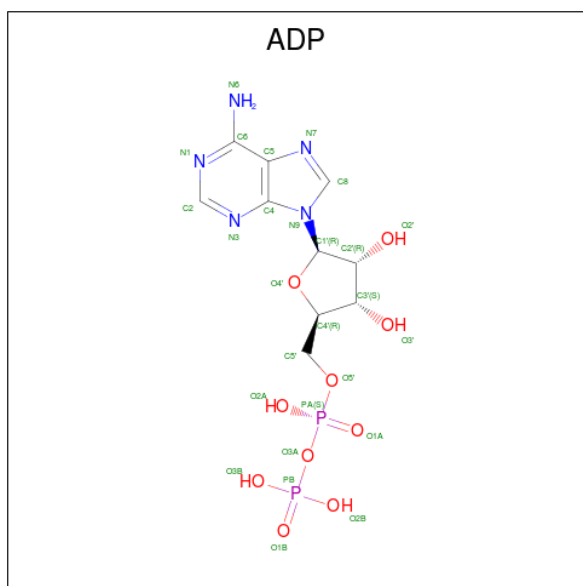
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

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 (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: $C_{10}H_{15}N_5O_{10}P_2$).



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

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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	

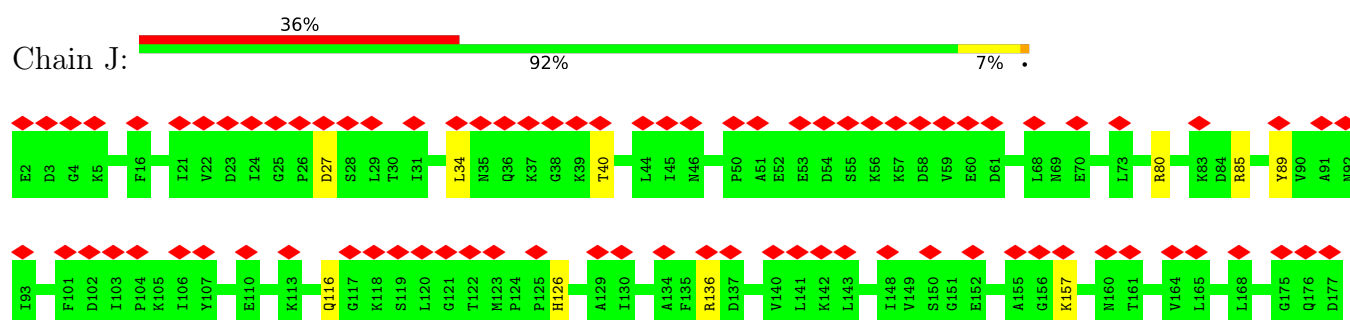
3 Residue-property plots

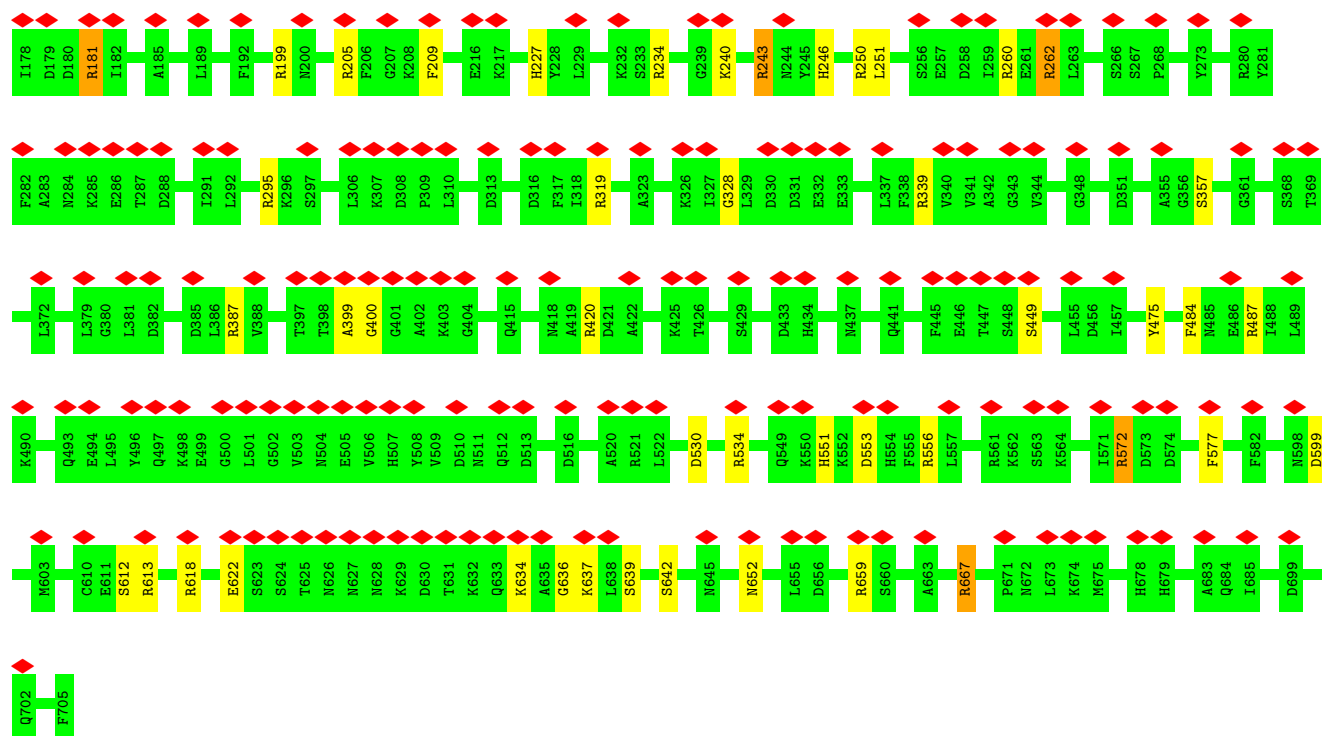
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

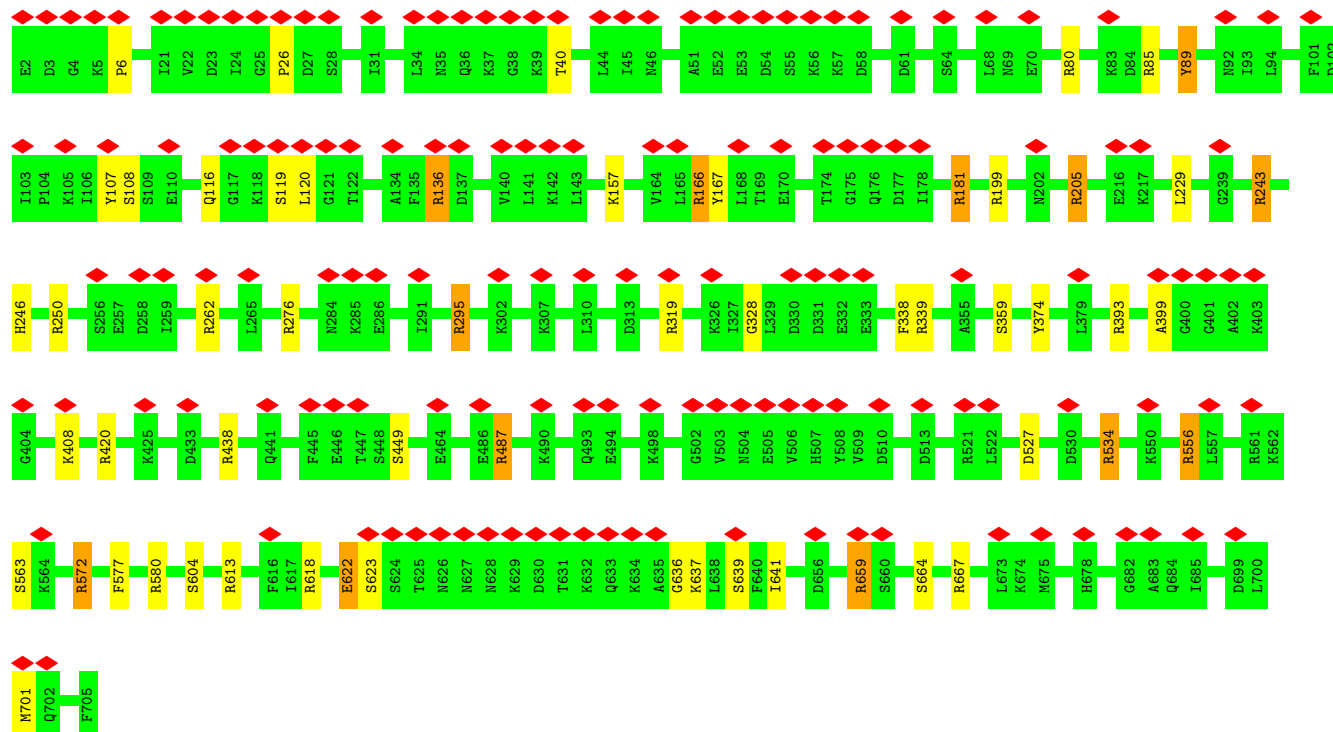
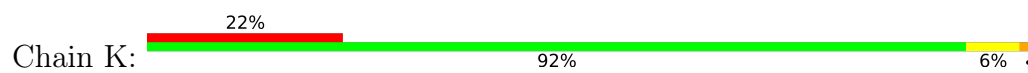


• Molecule 1: Unconventional myosin-VI

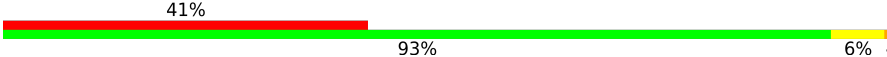


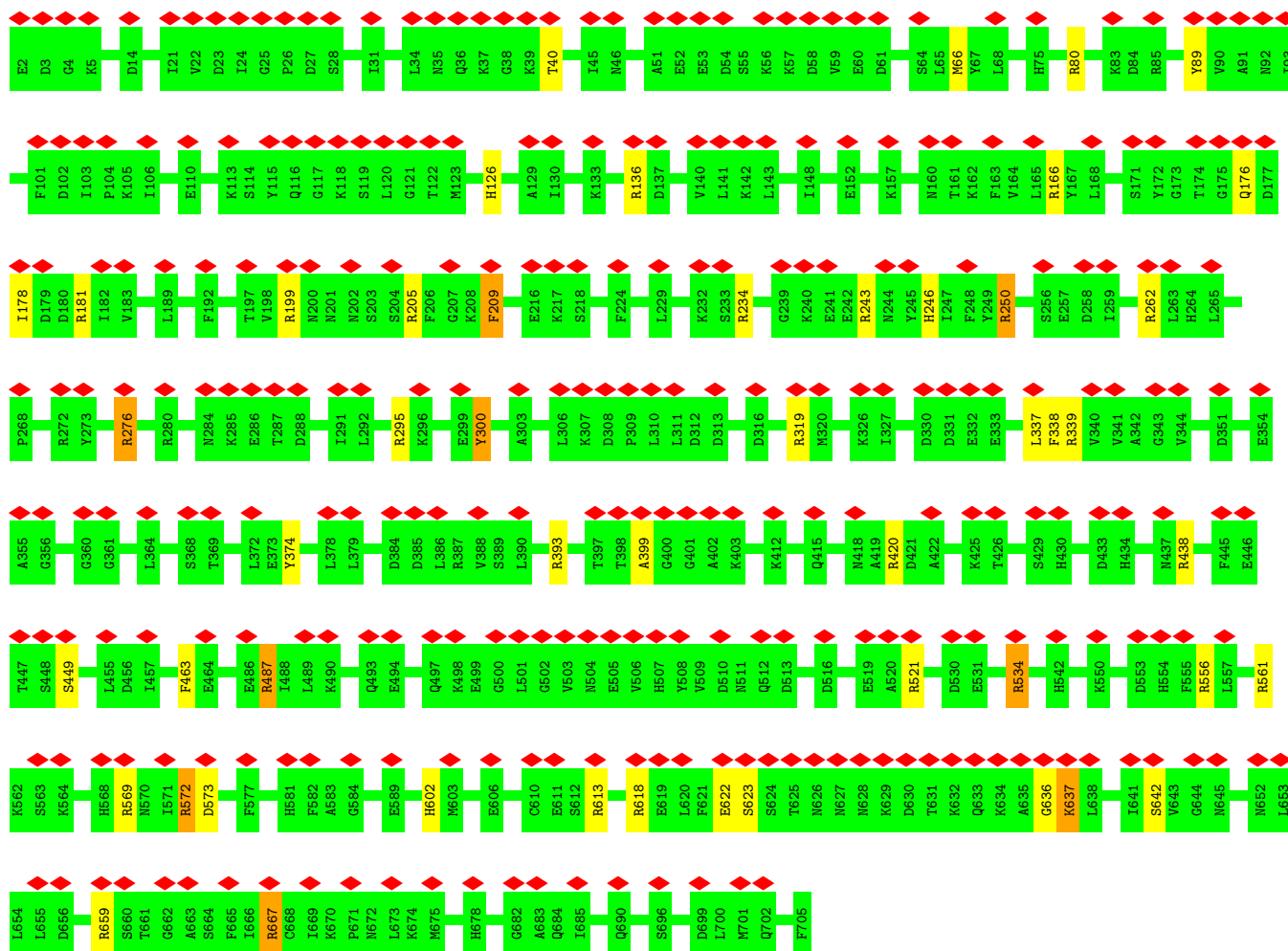


- Molecule 1: Unconventional myosin-VI



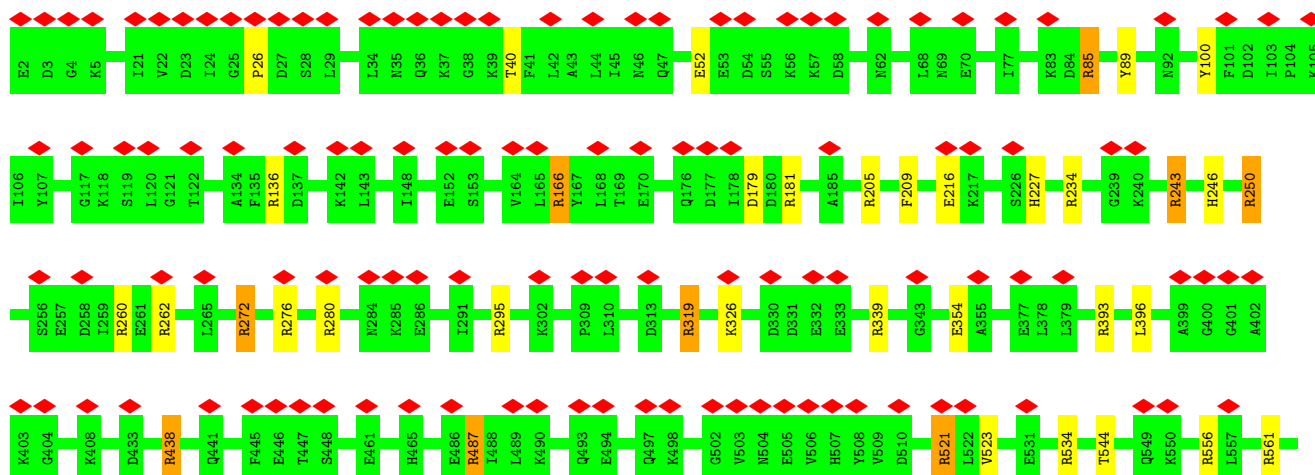
- Molecule 1: Unconventional myosin-VI

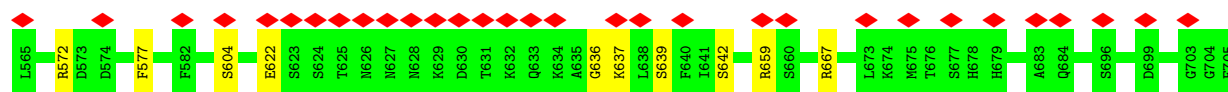
Chain L: 



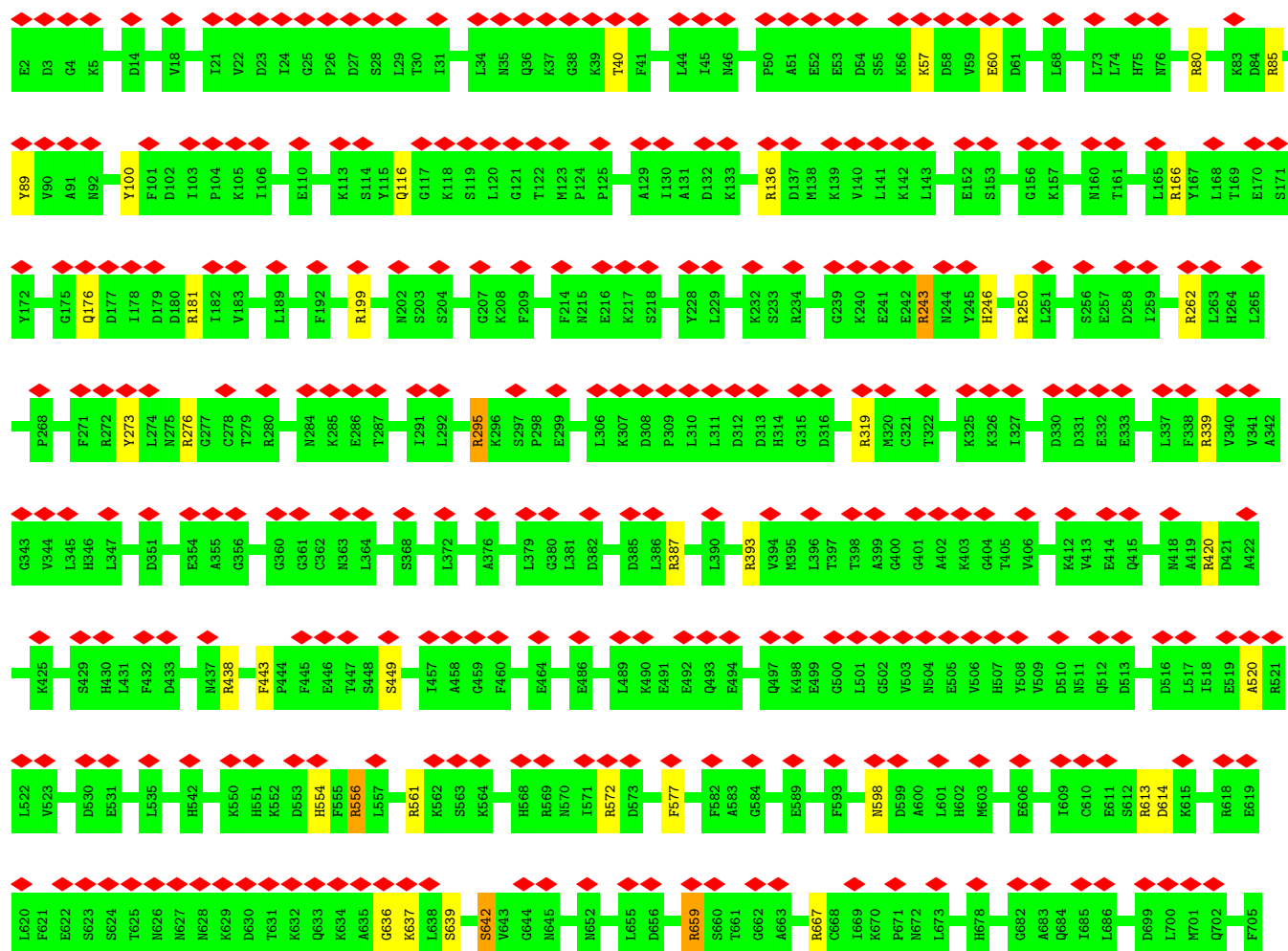
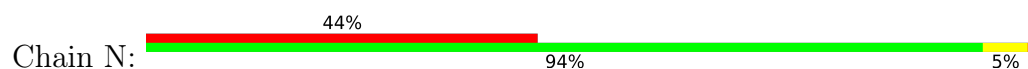
• Molecule 1: Unconventional myosin-VI

Chain M: 

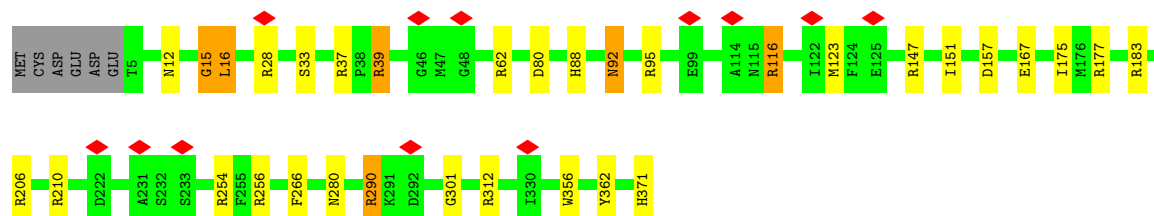
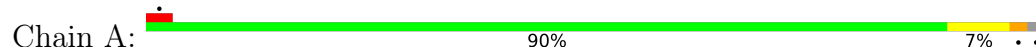





• Molecule 1: Unconventional myosin-VI

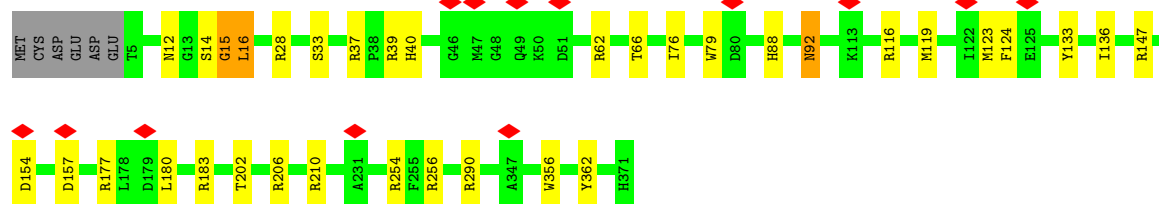


• Molecule 2: Actin, alpha skeletal muscle




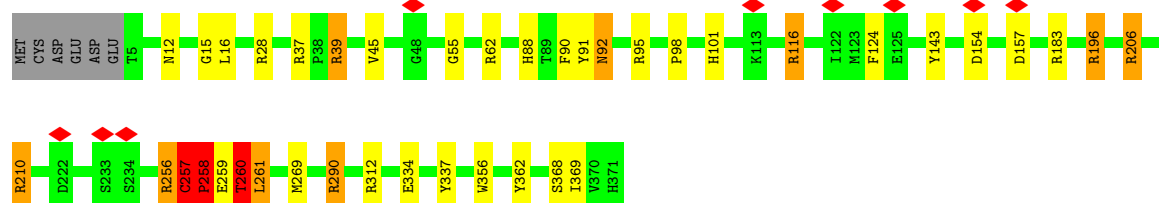
• Molecule 2: Actin, alpha skeletal muscle

Chain B:  89% 9% ..




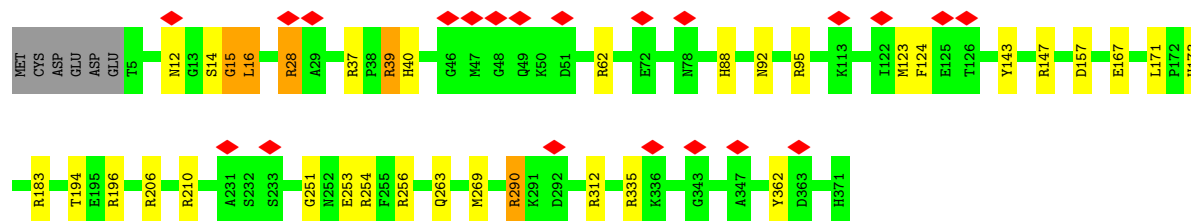
- Molecule 2: Actin, alpha skeletal muscle

Chain C:  88% 8% ...




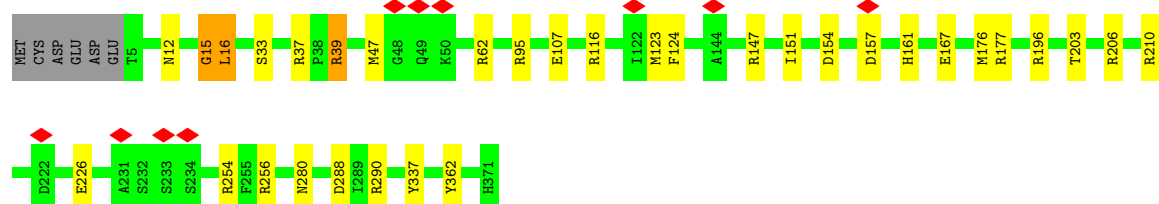
- Molecule 2: Actin, alpha skeletal muscle

Chain D:  89% 8% ..

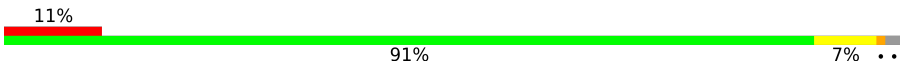


- Molecule 2: Actin, alpha skeletal muscle

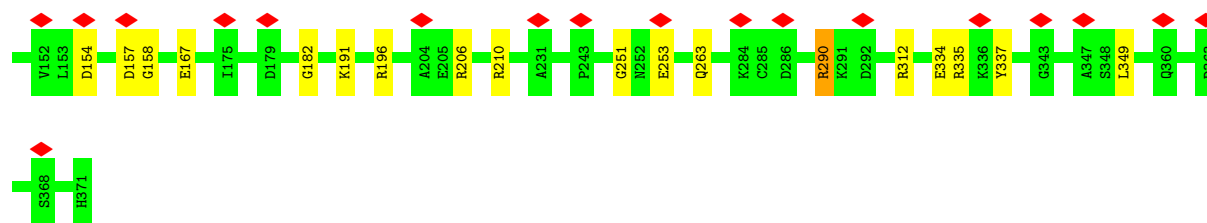
Chain E:  90% 8% ..



- Molecule 2: Actin, alpha skeletal muscle

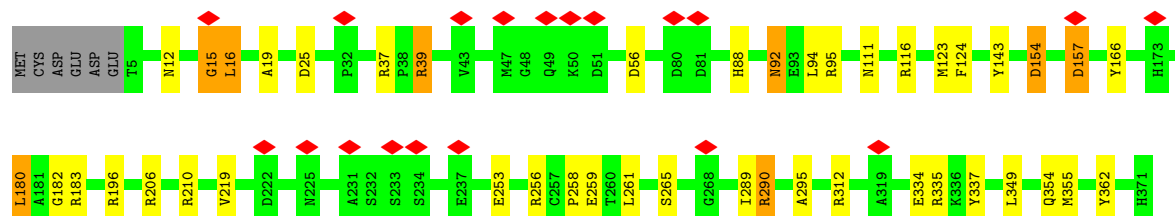
Chain F:  91% 7% ..





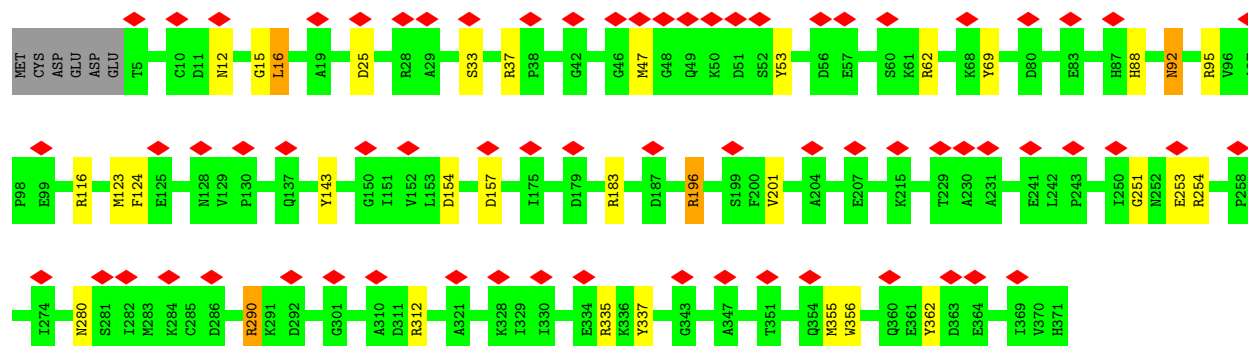
- Molecule 2: Actin, alpha skeletal muscle

Chain G: 5% 87% 10% ..



- Molecule 2: Actin, alpha skeletal muscle

Chain H: 18% 90% 8% ..



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 ($e^-/\text{Å}^2$)	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	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	6.0	Depositor
Map size (Å)	650.24, 650.24, 650.24	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	I	0.72	0/5718	1.09	39/7705 (0.5%)
1	J	0.72	0/5718	1.10	35/7705 (0.5%)
1	K	0.72	0/5718	1.08	39/7705 (0.5%)
1	L	0.72	0/5718	1.09	42/7705 (0.5%)
1	M	0.73	0/5718	1.08	32/7705 (0.4%)
1	N	0.72	0/5718	1.08	31/7705 (0.4%)
2	A	0.69	0/2924	1.18	23/3963 (0.6%)
2	B	0.69	0/2924	1.17	15/3963 (0.4%)
2	C	0.85	7/2924 (0.2%)	1.38	46/3963 (1.2%)
2	D	0.69	0/2924	1.17	21/3963 (0.5%)
2	E	0.70	0/2924	1.18	19/3963 (0.5%)
2	F	0.70	0/2924	1.17	20/3963 (0.5%)
2	G	0.75	2/2924 (0.1%)	1.20	23/3963 (0.6%)
2	H	0.69	0/2924	1.14	17/3963 (0.4%)
All	All	0.72	9/57700 (0.0%)	1.14	402/77934 (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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	258	PRO	C-O	11.57	1.46	1.23
2	C	260	THR	CA-C	11.31	1.82	1.52
2	C	259	GLU	C-N	11.09	1.59	1.34
2	G	258	PRO	N-CA	7.08	1.59	1.47
2	C	261	LEU	CA-CB	6.99	1.69	1.53
2	C	260	THR	C-N	6.61	1.49	1.34
2	C	257	CYS	CA-C	6.17	1.69	1.52
2	C	261	LEU	C-O	-5.53	1.12	1.23
2	C	257	CYS	CA-CB	5.47	1.66	1.53

All (402) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	260	THR	CA-CB-CG2	15.82	134.55	112.40
2	C	260	THR	C-N-CA	13.95	156.58	121.70
2	C	260	THR	N-CA-CB	13.90	136.71	110.30
2	C	260	THR	CB-CA-C	-13.29	75.73	111.60
2	C	259	GLU	C-N-CA	-12.86	89.54	121.70
2	C	259	GLU	O-C-N	11.94	141.80	122.70
2	C	260	THR	N-CA-C	10.76	140.05	111.00
2	A	206	ARG	NE-CZ-NH1	10.41	125.50	120.30
2	A	312	ARG	NE-CZ-NH1	10.29	125.45	120.30
2	B	154	ASP	CB-CG-OD1	9.41	126.77	118.30
1	I	89	TYR	CB-CG-CD2	-9.29	115.43	121.00
2	G	154	ASP	CB-CG-OD1	9.27	126.64	118.30
2	D	143	TYR	CB-CG-CD1	-9.25	115.45	121.00
1	N	339	ARG	NE-CZ-NH1	9.09	124.85	120.30
2	C	260	THR	O-C-N	-9.06	108.20	122.70
1	N	181	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	N	166	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	J	250	ARG	NE-CZ-NH2	-8.78	115.91	120.30
2	F	154	ASP	CB-CG-OD1	8.78	126.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	295	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	J	339	ARG	NE-CZ-NH1	8.71	124.66	120.30
2	G	312	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	I	89	TYR	CB-CG-CD1	8.60	126.16	121.00
1	L	295	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	N	319	ARG	NE-CZ-NH1	8.49	124.55	120.30
2	D	143	TYR	CB-CG-CD2	8.48	126.09	121.00
2	C	116	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	J	295	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	C	154	ASP	CB-CG-OD1	8.42	125.88	118.30
2	F	312	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	M	438	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	M	295	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	M	393	ARG	NE-CZ-NH1	8.23	124.41	120.30
2	G	183	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	I	393	ARG	NE-CZ-NH1	8.17	124.38	120.30
2	F	206	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	L	521	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	I	250	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	K	572	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	I	136	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	G	256	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	E	154	ASP	CB-CG-OD1	8.03	125.52	118.30
1	N	420	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	J	420	ARG	NE-CZ-NH2	-7.91	116.35	120.30
2	E	39	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	K	136	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	K	438	ARG	NE-CZ-NH1	7.87	124.23	120.30
2	B	177	ARG	NE-CZ-NH1	7.85	124.23	120.30
2	F	210	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	M	136	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	M	438	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	C	62	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	I	243	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	I	136	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	J	89	TYR	CB-CG-CD2	-7.73	116.36	121.00
2	G	337	TYR	CB-CG-CD2	-7.70	116.38	121.00
2	H	154	ASP	CB-CG-OD1	7.70	125.23	118.30
1	M	572	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	J	659	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	E	37	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	K	199	ARG	NE-CZ-NH1	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	210	ARG	NE-CZ-NH1	7.65	124.13	120.30
2	D	183	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	B	210	ARG	NE-CZ-NH1	7.62	124.11	120.30
2	G	116	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	K	136	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	H	154	ASP	CB-CG-OD2	7.55	125.09	118.30
1	K	85	ARG	NE-CZ-NH1	7.55	124.07	120.30
2	H	290	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	H	62	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	I	295	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	I	420	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	I	339	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	M	85	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	K	534	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	N	181	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	N	136	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	K	339	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	J	420	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	L	339	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	L	250	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	J	387	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	L	393	ARG	NE-CZ-NH1	7.35	123.97	120.30
2	G	206	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	N	556	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	L	521	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	J	339	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	N	339	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	L	556	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	D	210	ARG	NE-CZ-NH2	-7.30	116.65	120.30
2	E	154	ASP	OD1-CG-OD2	-7.28	109.47	123.30
2	G	206	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	E	154	ASP	CB-CG-OD2	7.25	124.83	118.30
2	G	143	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	N	438	ARG	NE-CZ-NH2	-7.23	116.68	120.30
2	C	206	ARG	NE-CZ-NH1	7.23	123.92	120.30
2	F	210	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	J	262	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	H	154	ASP	OD1-CG-OD2	-7.21	109.59	123.30
1	N	85	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	C	261	LEU	CA-C-N	7.19	133.01	117.20
1	K	420	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	D	62	ARG	NE-CZ-NH2	-7.18	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	487	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	D	196	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	D	210	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	K	438	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	C	143	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	L	659	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	N	561	ARG	NE-CZ-NH1	7.07	123.84	120.30
2	H	143	TYR	CB-CG-CD1	-7.07	116.76	121.00
1	J	243	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	F	62	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	M	136	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	G	258	PRO	N-CA-CB	-7.02	94.88	103.30
1	I	85	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	J	260	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	L	276	ARG	NE-CZ-NH1	6.97	123.79	120.30
2	D	147	ARG	NE-CZ-NH1	6.97	123.78	120.30
2	F	337	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	M	572	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	A	62	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	J	136	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	J	136	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	I	250	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	N	556	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	G	37	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	L	80	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	K	243	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	N	250	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	I	569	ARG	NE-CZ-NH1	6.89	123.74	120.30
2	C	337	TYR	CB-CG-CD2	-6.88	116.87	121.00
2	B	116	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	L	136	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	N	438	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	L	181	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	E	116	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	G	337	TYR	CB-CG-CD1	6.77	125.06	121.00
1	L	250	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	N	319	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	I	659	ARG	NE-CZ-NH1	6.73	123.67	120.30
2	C	206	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	M	319	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	L	262	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	M	521	ARG	NE-CZ-NH1	6.69	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	659	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	F	154	ASP	OD1-CG-OD2	-6.68	110.61	123.30
1	J	618	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	K	393	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	J	667	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	F	290	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	M	276	ARG	NE-CZ-NH1	6.61	123.61	120.30
2	C	154	ASP	OD1-CG-OD2	-6.61	110.75	123.30
1	M	243	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	28	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	F	62	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	L	667	ARG	NE-CZ-NH2	-6.53	117.04	120.30
2	C	39	ARG	NE-CZ-NH2	-6.53	117.04	120.30
2	C	290	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	J	667	ARG	NE-CZ-NH2	-6.51	117.04	120.30
2	B	37	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	B	39	ARG	NE-CZ-NH1	6.49	123.55	120.30
2	B	154	ASP	OD1-CG-OD2	-6.47	111.00	123.30
1	J	234	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	M	89	TYR	CB-CG-CD2	-6.46	117.13	121.00
2	A	62	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	D	37	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	J	199	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	E	62	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	K	319	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	L	199	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	J	181	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	J	534	ARG	NE-CZ-NH1	6.39	123.49	120.30
2	C	91	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	I	496	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	M	667	ARG	NE-CZ-NH1	6.37	123.48	120.30
2	A	266	PHE	CB-CG-CD1	6.37	125.26	120.80
2	A	266	PHE	CB-CG-CD2	-6.37	116.34	120.80
2	E	196	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	L	463	PHE	CB-CG-CD1	6.36	125.25	120.80
1	J	80	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	L	420	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	I	521	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	M	262	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	A	290	ARG	NE-CZ-NH1	6.31	123.45	120.30
2	G	15	GLY	C-N-CA	6.30	137.46	121.70
2	C	183	ARG	NE-CZ-NH2	-6.29	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	209	PHE	CB-CG-CD2	6.28	125.19	120.80
2	E	254	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	I	487	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	I	487	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	C	95	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	C	210	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	K	338	PHE	CB-CG-CD1	6.23	125.16	120.80
1	J	484	PHE	CB-CG-CD1	6.22	125.16	120.80
2	C	116	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	G	290	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	C	37	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	C	312	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	E	196	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	C	143	TYR	CB-CG-CD1	6.16	124.70	121.00
2	B	62	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	J	262	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	K	667	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	I	273	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	I	613	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	K	374	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	K	339	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	B	15	GLY	C-N-CA	6.10	136.96	121.70
1	L	463	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	N	387	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	N	295	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	G	290	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	L	374	TYR	CB-CG-CD1	-6.03	117.39	121.00
2	F	337	TYR	CB-CG-CD1	6.02	124.61	121.00
2	G	143	TYR	CB-CG-CD1	6.02	124.61	121.00
1	J	250	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	N	420	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	C	91	TYR	CB-CG-CD1	6.00	124.60	121.00
1	M	339	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	K	262	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	N	659	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	L	618	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	H	37	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	A	39	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	D	37	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	A	147	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	E	95	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	I	272	ARG	NE-CZ-NH1	5.89	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	62	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	E	15	GLY	C-N-CA	5.89	136.42	121.70
1	I	580	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	D	183	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	J	319	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	I	338	PHE	CB-CG-CD2	-5.87	116.69	120.80
2	F	206	ARG	NE-CZ-NH2	-5.87	117.37	120.30
2	F	290	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	C	337	TYR	CB-CG-CD1	5.86	124.51	121.00
1	J	181	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	C	196	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	D	28	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	I	338	PHE	CB-CG-CD1	5.85	124.89	120.80
1	L	338	PHE	CB-CG-CD1	5.85	124.89	120.80
1	N	136	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	F	147	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	L	667	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	N	572	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	L	300	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	H	37	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	H	312	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	A	256	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	H	196	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	K	420	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	A	256	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	I	262	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	J	613	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	B	210	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	A	177	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	N	295	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	K	181	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	K	89	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	K	701	MET	CG-SD-CE	-5.75	91.00	100.20
2	C	258	PRO	N-CA-C	-5.75	97.16	112.10
1	I	166	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	M	262	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	K	374	TYR	CB-CG-CD1	5.74	124.44	121.00
2	F	15	GLY	C-N-CA	5.74	136.04	121.70
2	A	183	ARG	NE-CZ-NH2	-5.73	117.43	120.30
2	B	123	MET	CG-SD-CE	-5.73	91.03	100.20
1	N	262	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	G	95	ARG	NE-CZ-NH2	-5.73	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	37	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	K	338	PHE	CB-CG-CD2	-5.72	116.79	120.80
1	K	487	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	K	276	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	C	62	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	K	166	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	E	123	MET	CG-SD-CE	-5.69	91.09	100.20
1	N	199	ARG	NE-CZ-NH1	5.69	123.14	120.30
2	E	37	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	E	116	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	J	556	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	I	438	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	N	250	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	G	210	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	L	374	TYR	CB-CG-CD2	5.66	124.40	121.00
2	H	183	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	J	85	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	N	642	SER	N-CA-CB	5.65	118.97	110.50
2	D	196	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	I	209	PHE	CB-CG-CD1	5.64	124.75	120.80
1	L	209	PHE	CB-CG-CD1	-5.64	116.86	120.80
2	D	95	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	N	393	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	M	260	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	F	335	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	E	176	MET	CG-SD-CE	-5.62	91.21	100.20
1	L	338	PHE	CB-CG-CD2	-5.62	116.87	120.80
2	A	183	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	C	154	ASP	CB-CG-OD2	5.61	123.34	118.30
1	M	250	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	L	89	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	K	556	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	M	85	ARG	NE-CZ-NH2	-5.59	117.50	120.30
2	F	116	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	E	154	ASP	N-CA-CB	5.57	120.62	110.60
2	E	147	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	M	276	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	A	210	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	D	256	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	J	484	PHE	CB-CG-CD2	-5.53	116.93	120.80
2	C	260	THR	CA-CB-OG1	-5.51	97.43	109.00
1	N	243	ARG	NE-CZ-NH1	5.51	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	66	MET	CG-SD-CE	-5.50	91.40	100.20
1	L	319	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	H	62	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	L	569	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	L	234	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	L	561	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	H	143	TYR	CB-CG-CD2	5.46	124.28	121.00
1	J	234	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	K	262	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	C	15	GLY	C-N-CA	5.46	135.34	121.70
1	J	572	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	A	123	MET	CG-SD-CE	-5.45	91.48	100.20
1	N	667	ARG	NE-CZ-NH2	-5.41	117.60	120.30
2	F	91	TYR	CB-CG-CD2	-5.41	117.76	121.00
2	D	256	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	H	15	GLY	C-N-CA	5.37	135.12	121.70
1	L	136	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	C	261	LEU	CA-CB-CG	-5.36	102.97	115.30
2	C	183	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	K	618	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	F	154	ASP	CB-CG-OD2	5.35	123.12	118.30
2	A	95	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	K	205	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	A	254	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	H	196	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	I	339	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	L	420	ARG	NE-CZ-NH2	-5.33	117.63	120.30
2	D	123	MET	CG-SD-CE	-5.33	91.67	100.20
1	J	487	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	B	256	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	M	181	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	L	89	TYR	CB-CA-C	-5.32	99.76	110.40
2	G	196	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	M	534	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	K	580	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	M	250	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	I	209	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	M	319	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	I	556	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	H	335	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	I	273	TYR	CB-CG-CD1	5.28	124.17	121.00
2	F	91	TYR	CB-CG-CD1	5.27	124.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	667	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	I	496	TYR	CB-CG-CD1	5.23	124.14	121.00
2	A	206	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	C	256	ARG	C-N-CA	-5.22	108.65	121.70
1	I	387	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	G	210	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	K	319	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	E	177	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	M	622	GLU	C-N-CA	5.20	134.71	121.70
1	I	556	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	M	487	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	K	107	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	M	272	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	L	534	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	G	39	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	C	258	PRO	CA-C-N	5.13	128.49	117.20
2	C	55	GLY	C-N-CA	5.13	134.52	121.70
2	C	210	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	C	259	GLU	CA-C-N	-5.13	105.92	117.20
1	L	572	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	I	280	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	G	123	MET	CG-SD-CE	-5.12	92.01	100.20
1	K	85	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	K	659	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	A	157	ASP	CB-CG-OD2	5.11	122.90	118.30
2	A	116	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	D	254	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	K	613	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	D	335	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	G	95	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	K	80	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	I	521	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	J	205	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	D	290	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	C	258	PRO	CB-CA-C	-5.04	99.39	112.00
2	B	154	ASP	N-CA-CB	5.04	119.66	110.60
2	C	39	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	C	90	PHE	CB-CG-CD2	-5.04	117.28	120.80
1	I	420	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	M	280	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	C	258	PRO	O-C-N	-5.03	114.66	122.70
1	L	659	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	250	ARG	CG-CD-NE	-5.01	101.28	111.80
1	N	273	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	I	561	ARG	NE-CZ-NH1	5.00	122.80	120.30
2	B	254	ARG	NE-CZ-NH2	-5.00	117.80	120.30
2	H	254	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	5612	0	5549	2	0
1	J	5612	0	5549	1	0
1	K	5612	0	5549	2	0
1	L	5612	0	5549	4	0
1	M	5612	0	5549	3	0
1	N	5612	0	5549	2	0
2	A	2862	0	2831	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2862	0	2831	4	0
2	C	2862	0	2831	10	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
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	54	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 0.

All (54) 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	1.48
2:C:260:THR:C	2:C:260:THR:CB	2.14	1.15
2:G:219:VAL:HG13	2:G:259:GLU:HG2	1.57	0.86
2:C:260:THR:C	2:C:260:THR:HB	1.97	0.84
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:G:180:LEU:CD2	2:G:261:LEU:CD1	2.77	0.62
2:C:256:ARG:O	2:C:260:THR:N	2.35	0.59
2:C:257:CYS:C	2:C:260:THR:H	2.07	0.58
1:I:243:ARG:HH21	1:I:246:HIS:CD2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:THR:C	2:C:260:THR:CG2	2.73	0.56
1:J:243:ARG:HH21	1:J:246:HIS:CD2	2.24	0.56
2:H:253:GLU:H	2:H:253:GLU:CD	2.11	0.54
2:F:253:GLU:H	2:F:253:GLU:CD	2.12	0.53
2:C:88:HIS:CD2	2:C:92:ASN:HD21	2.27	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
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
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:D:253:GLU:H	2:D:253:GLU:CD	2.18	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: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
1:N:60:GLU:CD	1:N:80:ARG:HH12	2.19	0.44
2:G:180:LEU:HD23	2:G:261:LEU:CD1	2.47	0.44
2:B:88:HIS:CE1	2:B:92:ASN:HD21	2.36	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:C:260:THR:C	2:C:260:THR:HG22	2.41	0.41
2:D:171:LEU:H	2:D:171:LEU:HD22	1.84	0.41
1:M:166:ARG:HH12	1:M:179:ASP:CG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	702/704 (100%)	636 (91%)	58 (8%)	8 (1%)	14	52
1	J	702/704 (100%)	644 (92%)	46 (7%)	12 (2%)	9	43
1	K	702/704 (100%)	644 (92%)	42 (6%)	16 (2%)	6	37
1	L	702/704 (100%)	641 (91%)	54 (8%)	7 (1%)	15	54
1	M	702/704 (100%)	640 (91%)	55 (8%)	7 (1%)	15	54
1	N	702/704 (100%)	637 (91%)	55 (8%)	10 (1%)	11	47
2	A	365/373 (98%)	331 (91%)	30 (8%)	4 (1%)	14	52
2	B	365/373 (98%)	330 (90%)	32 (9%)	3 (1%)	19	60
2	C	365/373 (98%)	320 (88%)	39 (11%)	6 (2%)	9	45
2	D	365/373 (98%)	325 (89%)	35 (10%)	5 (1%)	11	47
2	E	365/373 (98%)	327 (90%)	35 (10%)	3 (1%)	19	60
2	F	365/373 (98%)	320 (88%)	39 (11%)	6 (2%)	9	45
2	G	365/373 (98%)	325 (89%)	35 (10%)	5 (1%)	11	47
2	H	365/373 (98%)	323 (88%)	39 (11%)	3 (1%)	19	60
All	All	7132/7208 (99%)	6443 (90%)	594 (8%)	95 (1%)	16	48

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	610 (98%)	11 (2%)	59	77
1	J	621/621 (100%)	606 (98%)	15 (2%)	49	69
1	K	621/621 (100%)	612 (99%)	9 (1%)	67	81
1	L	621/621 (100%)	613 (99%)	8 (1%)	69	82
1	M	621/621 (100%)	612 (99%)	9 (1%)	67	81
1	N	621/621 (100%)	615 (99%)	6 (1%)	76	86
2	A	310/316 (98%)	301 (97%)	9 (3%)	42	64
2	B	310/316 (98%)	300 (97%)	10 (3%)	39	62
2	C	310/316 (98%)	302 (97%)	8 (3%)	46	67
2	D	310/316 (98%)	303 (98%)	7 (2%)	50	70
2	E	310/316 (98%)	298 (96%)	12 (4%)	32	57
2	F	310/316 (98%)	305 (98%)	5 (2%)	62	79
2	G	310/316 (98%)	299 (96%)	11 (4%)	36	60
2	H	310/316 (98%)	298 (96%)	12 (4%)	32	57
All	All	6206/6254 (99%)	6074 (98%)	132 (2%)	56	72

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	34	LEU
1	I	89	TYR
1	I	209	PHE
1	I	216	GLU
1	I	226	SER
1	I	383	GLN
1	I	395	MET
1	I	443	PHE
1	I	577	PHE
1	I	656	ASP
1	I	697	VAL
1	J	27	ASP
1	J	34	LEU
1	J	126	HIS
1	J	157	LYS
1	J	209	PHE
1	J	227	HIS
1	J	240	LYS
1	J	251	LEU
1	J	530	ASP
1	J	551	HIS
1	J	553	ASP
1	J	577	PHE
1	J	599	ASP
1	J	634	LYS
1	J	652	ASN
1	K	157	LYS
1	K	359	SER
1	K	408	LYS
1	K	527	ASP
1	K	572	ARG
1	K	577	PHE
1	K	604	SER
1	K	659	ARG
1	K	664	SER
1	L	126	HIS
1	L	209	PHE
1	L	276	ARG
1	L	337	LEU
1	L	438	ARG
1	L	572	ARG
1	L	573	ASP

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Mol	Chain	Res	Type
1	L	637	LYS
1	M	52	GLU
1	M	209	PHE
1	M	216	GLU
1	M	227	HIS
1	M	326	LYS
1	M	438	ARG
1	M	544	THR
1	M	577	PHE
1	M	604	SER
1	N	57	LYS
1	N	89	TYR
1	N	443	PHE
1	N	577	PHE
1	N	614	ASP
1	N	659	ARG
2	A	12	ASN
2	A	16	LEU
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	12	ASN
2	B	14	SER
2	B	66	THR
2	B	92	ASN
2	B	119	MET
2	B	124	PHE
2	B	136	ILE
2	B	157	ASP
2	B	202	THR
2	B	356	TRP
2	C	12	ASN
2	C	92	ASN
2	C	124	PHE
2	C	157	ASP
2	C	206	ARG
2	C	258	PRO
2	C	269	MET

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Mol	Chain	Res	Type
2	C	356	TRP
2	D	12	ASN
2	D	14	SER
2	D	124	PHE
2	D	157	ASP
2	D	194	THR
2	D	206	ARG
2	D	269	MET
2	E	12	ASN
2	E	47	MET
2	E	107	GLU
2	E	124	PHE
2	E	151	ILE
2	E	157	ASP
2	E	161	HIS
2	E	203	THR
2	E	206	ARG
2	E	226	GLU
2	E	280	ASN
2	E	288	ASP
2	F	12	ASN
2	F	92	ASN
2	F	124	PHE
2	F	157	ASP
2	F	191	LYS
2	G	12	ASN
2	G	25	ASP
2	G	56	ASP
2	G	92	ASN
2	G	111	ASN
2	G	124	PHE
2	G	154	ASP
2	G	157	ASP
2	G	253	GLU
2	G	354	GLN
2	G	355	MET
2	H	12	ASN
2	H	16	LEU
2	H	25	ASP
2	H	47	MET
2	H	92	ASN
2	H	123	MET

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Mol	Chain	Res	Type
2	H	124	PHE
2	H	157	ASP
2	H	201	VAL
2	H	280	ASN
2	H	355	MET
2	H	356	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	314	HIS
1	I	383	GLN
1	I	554	HIS
1	J	551	HIS
1	J	554	HIS
1	K	474	ASN
1	K	551	HIS
1	K	581	HIS
1	L	548	HIS
1	L	551	HIS
1	M	314	HIS
1	M	551	HIS
1	N	290	GLN
1	N	314	HIS
1	N	602	HIS
2	A	88	HIS
2	A	92	ASN
2	A	161	HIS
2	B	88	HIS
2	B	92	ASN
2	B	115	ASN
2	B	275	HIS
2	C	88	HIS
2	C	92	ASN
2	C	101	HIS
2	C	275	HIS
2	D	88	HIS
2	D	92	ASN
2	D	173	HIS
2	D	275	HIS
2	E	275	HIS
2	G	88	HIS

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Mol	Chain	Res	Type
2	G	92	ASN
2	H	88	HIS
2	H	92	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	E	402	3	24,29,29	0.91	1 (4%)	29,45,45	1.53	4 (13%)
4	ADP	B	402	3	24,29,29	0.92	1 (4%)	29,45,45	1.51	4 (13%)
4	ADP	A	402	3	24,29,29	0.90	1 (4%)	29,45,45	1.50	4 (13%)
4	ADP	G	402	3	24,29,29	0.91	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	D	402	3	24,29,29	0.92	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	F	402	3	24,29,29	0.93	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%)

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	E	402	3	-	3/12/32/32	0/3/3/3
4	ADP	B	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	G	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	D	402	3	-	3/12/32/32	0/3/3/3
4	ADP	F	402	3	-	3/12/32/32	0/3/3/3
4	ADP	C	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	B	402	ADP	C5-C4	2.48	1.47	1.40
4	D	402	ADP	C5-C4	2.47	1.47	1.40
4	C	402	ADP	C5-C4	2.46	1.47	1.40
4	F	402	ADP	C5-C4	2.45	1.47	1.40
4	G	402	ADP	C5-C4	2.44	1.47	1.40
4	E	402	ADP	C5-C4	2.42	1.47	1.40
4	A	402	ADP	C5-C4	2.40	1.47	1.40
4	H	402	ADP	C5-C4	2.38	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	ADP	PA-O3A-PB	-3.96	119.25	132.83
4	E	402	ADP	PA-O3A-PB	-3.95	119.28	132.83
4	F	402	ADP	PA-O3A-PB	-3.93	119.34	132.83
4	G	402	ADP	PA-O3A-PB	-3.93	119.34	132.83
4	B	402	ADP	PA-O3A-PB	-3.93	119.34	132.83
4	A	402	ADP	PA-O3A-PB	-3.93	119.35	132.83
4	H	402	ADP	PA-O3A-PB	-3.93	119.35	132.83
4	C	402	ADP	PA-O3A-PB	-3.91	119.41	132.83
4	G	402	ADP	C4-C5-N7	-3.15	106.12	109.40
4	E	402	ADP	C4-C5-N7	-3.09	106.18	109.40
4	B	402	ADP	C4-C5-N7	-3.09	106.18	109.40
4	H	402	ADP	C3'-C2'-C1'	3.08	105.61	100.98
4	D	402	ADP	C3'-C2'-C1'	3.07	105.60	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	402	ADP	C3'-C2'-C1'	3.06	105.58	100.98
4	D	402	ADP	C4-C5-N7	-3.05	106.22	109.40
4	F	402	ADP	C4-C5-N7	-3.05	106.22	109.40
4	C	402	ADP	C4-C5-N7	-3.05	106.22	109.40
4	E	402	ADP	C3'-C2'-C1'	3.04	105.56	100.98
4	B	402	ADP	C3'-C2'-C1'	3.04	105.55	100.98
4	G	402	ADP	C3'-C2'-C1'	3.03	105.54	100.98
4	C	402	ADP	C3'-C2'-C1'	3.02	105.53	100.98
4	H	402	ADP	C4-C5-N7	-3.01	106.26	109.40
4	E	402	ADP	N3-C2-N1	-3.00	123.98	128.68
4	C	402	ADP	N3-C2-N1	-2.99	124.00	128.68
4	A	402	ADP	C3'-C2'-C1'	2.99	105.48	100.98
4	A	402	ADP	C4-C5-N7	-2.96	106.31	109.40
4	A	402	ADP	N3-C2-N1	-2.95	124.07	128.68
4	H	402	ADP	N3-C2-N1	-2.94	124.08	128.68
4	D	402	ADP	N3-C2-N1	-2.94	124.08	128.68
4	F	402	ADP	N3-C2-N1	-2.93	124.10	128.68
4	G	402	ADP	N3-C2-N1	-2.91	124.13	128.68
4	B	402	ADP	N3-C2-N1	-2.87	124.19	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

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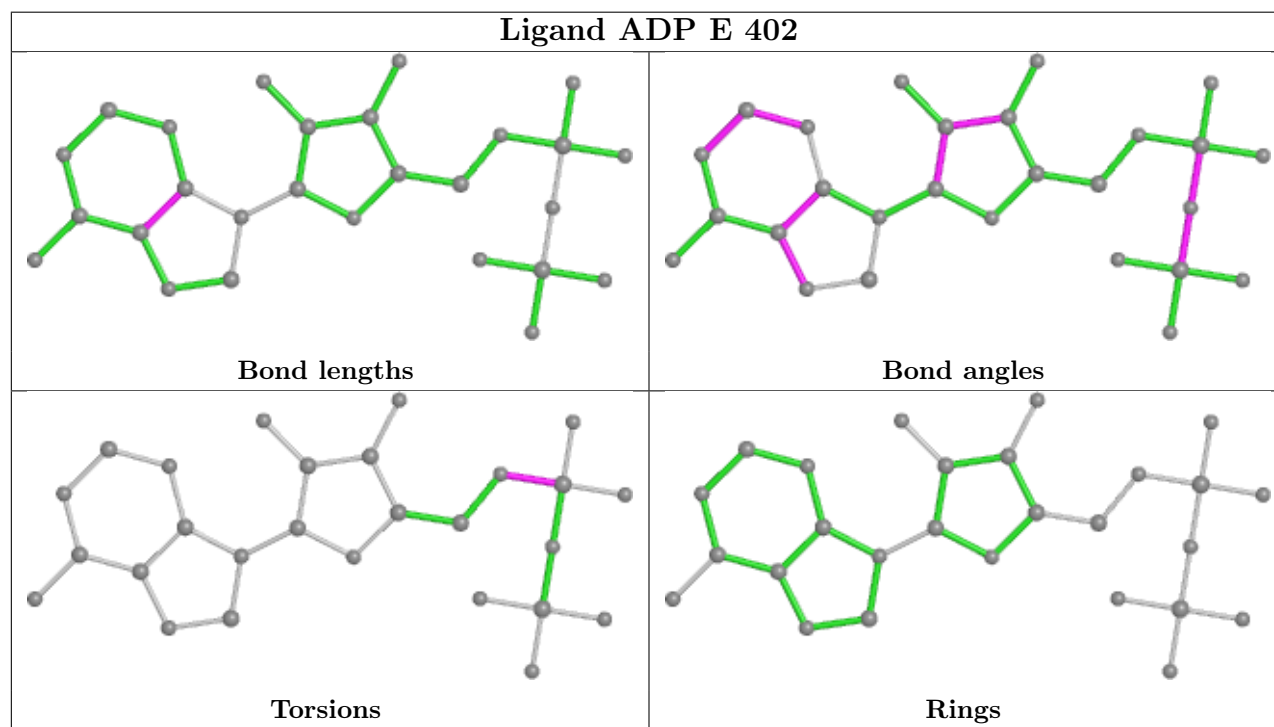
Continued from previous page...

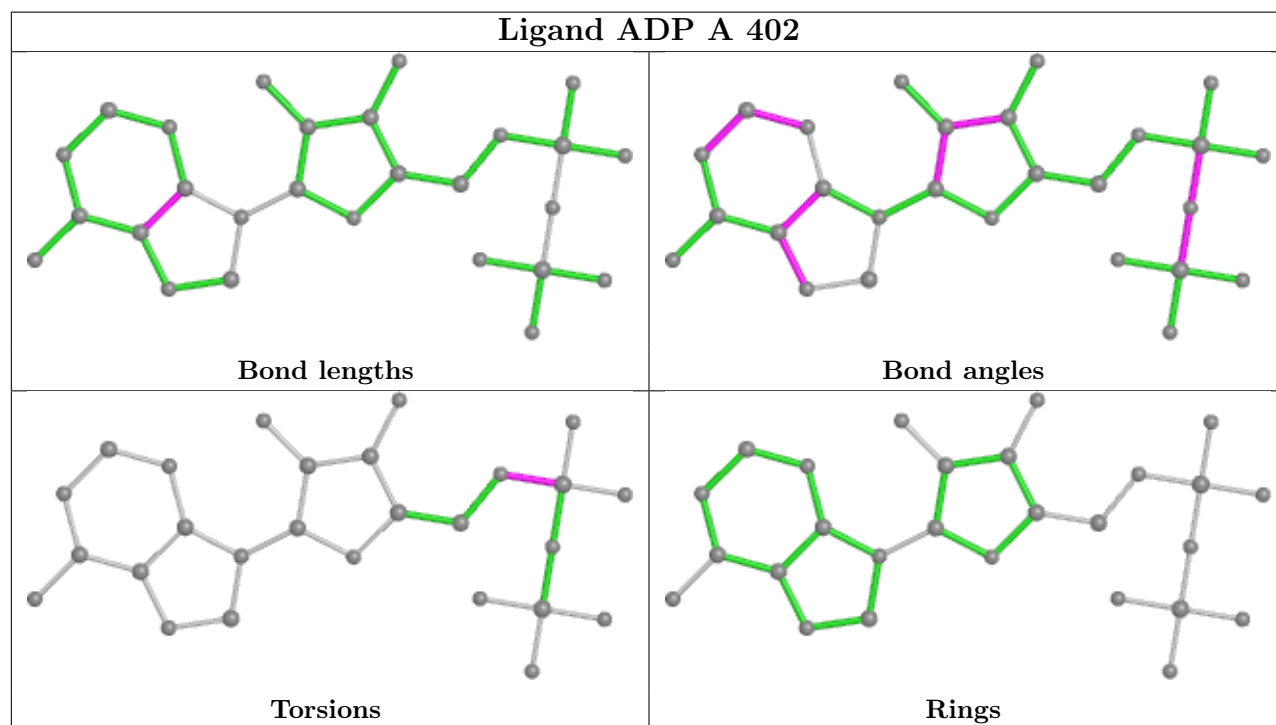
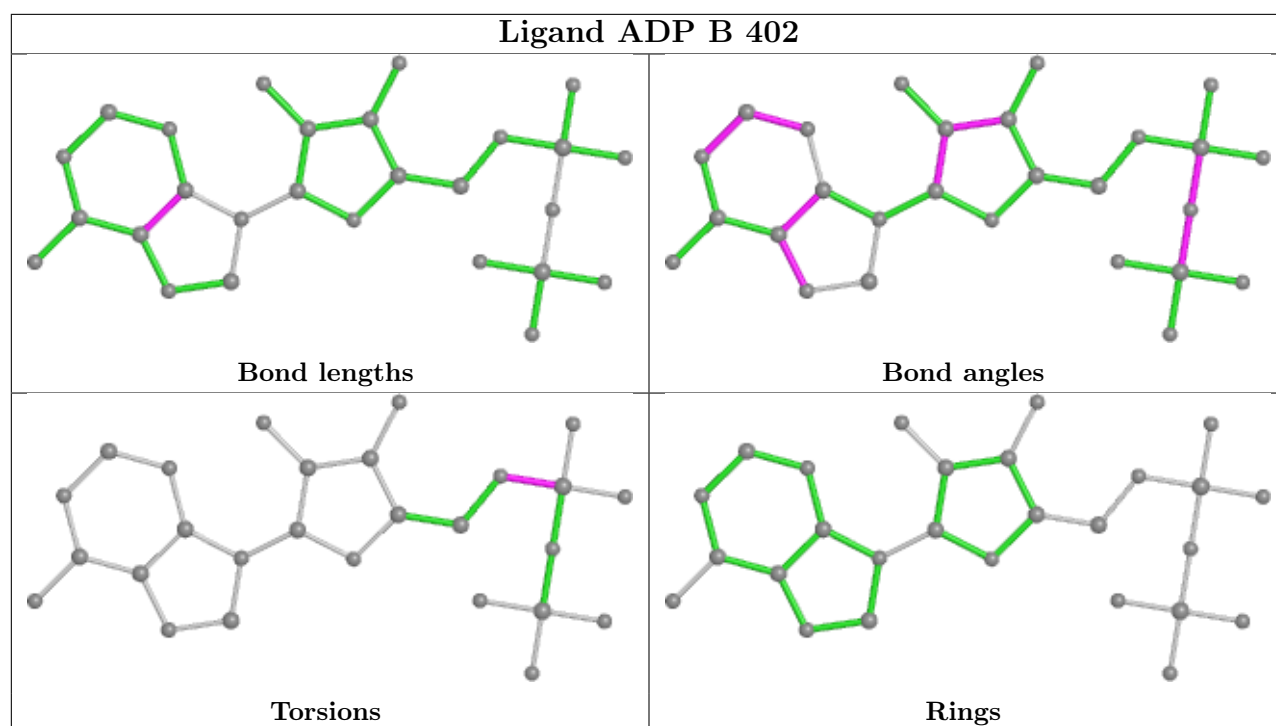
Mol	Chain	Res	Type	Atoms
4	C	402	ADP	C5'-O5'-PA-O3A
4	D	402	ADP	C5'-O5'-PA-O3A
4	E	402	ADP	C5'-O5'-PA-O3A
4	F	402	ADP	C5'-O5'-PA-O3A
4	G	402	ADP	C5'-O5'-PA-O3A
4	H	402	ADP	C5'-O5'-PA-O3A

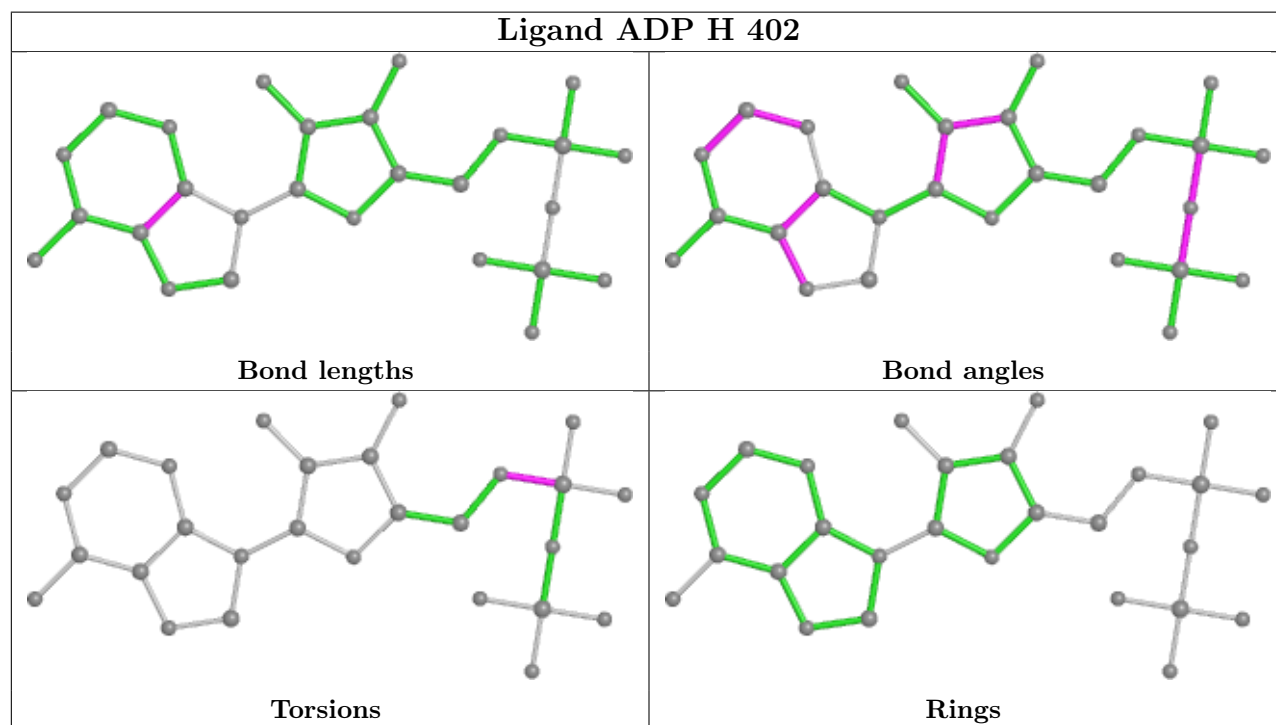
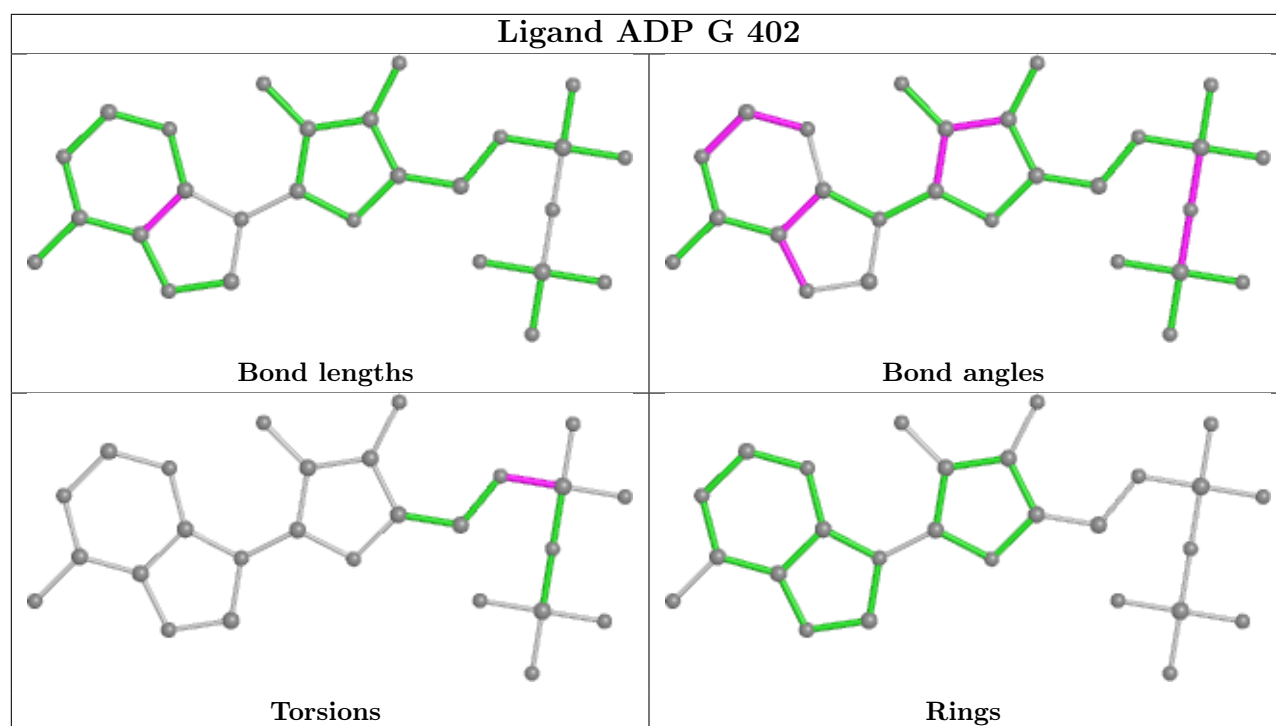
There are no ring outliers.

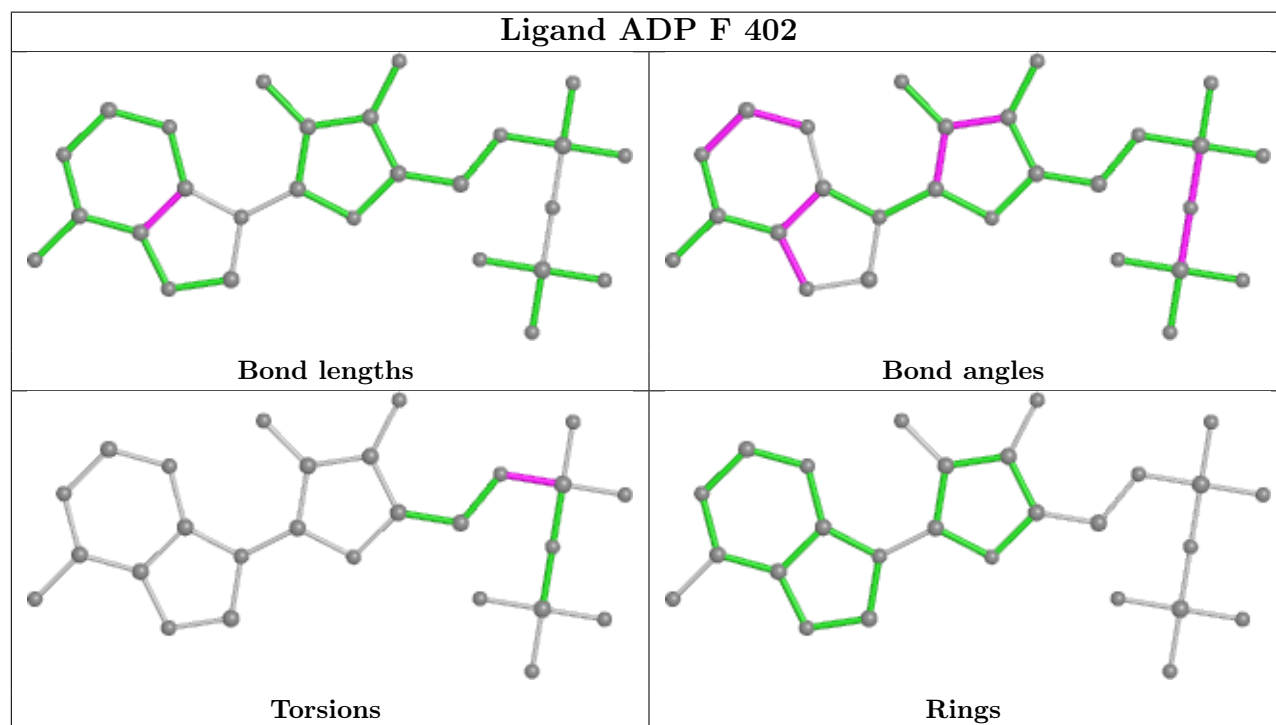
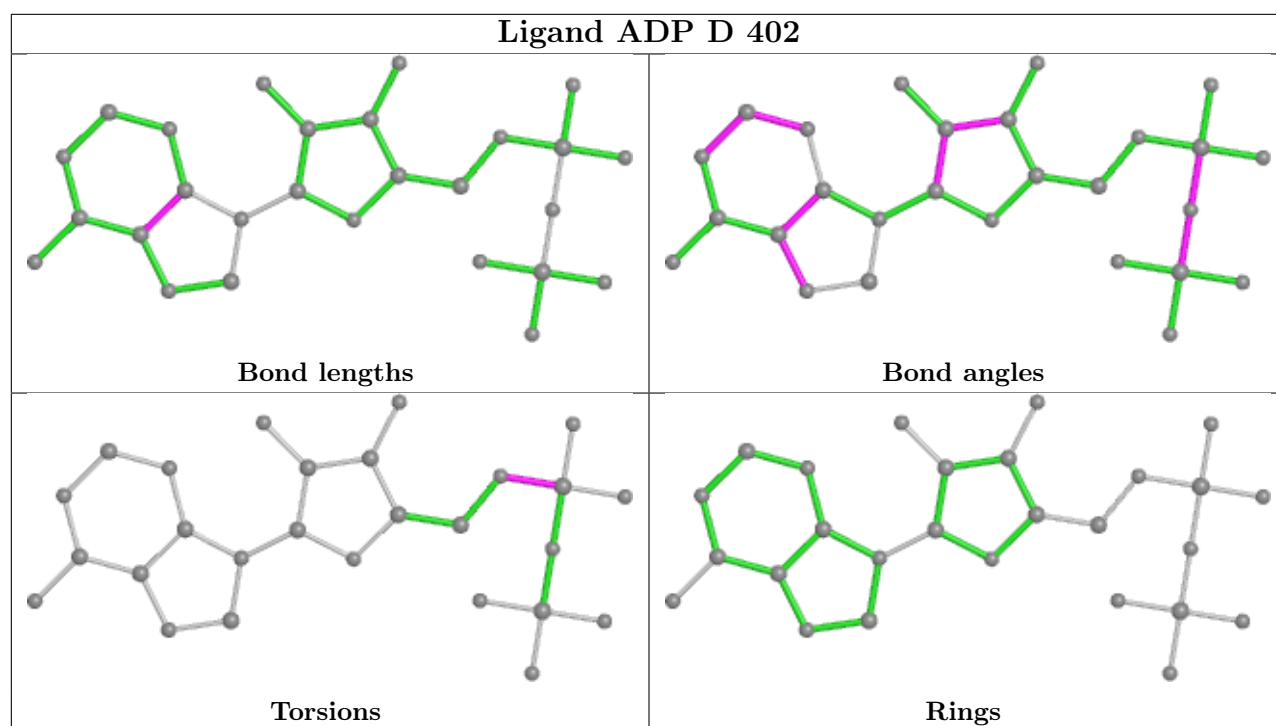
No monomer is involved in short contacts.

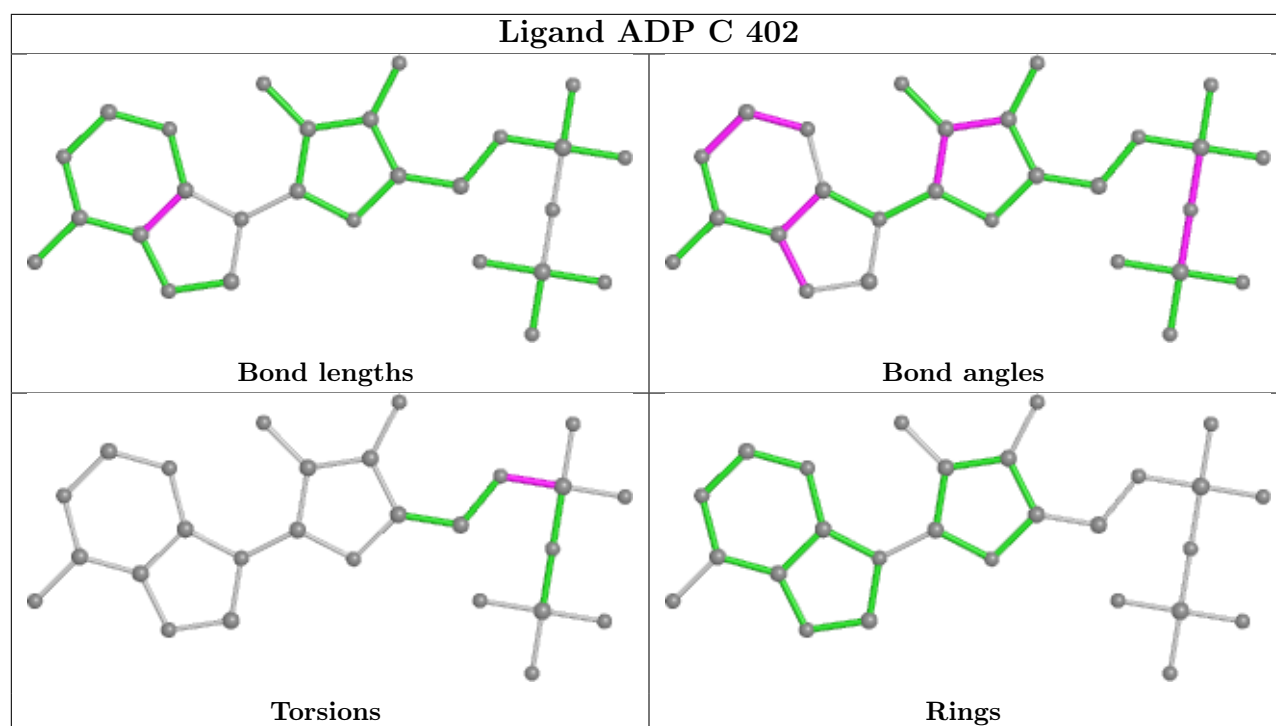
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

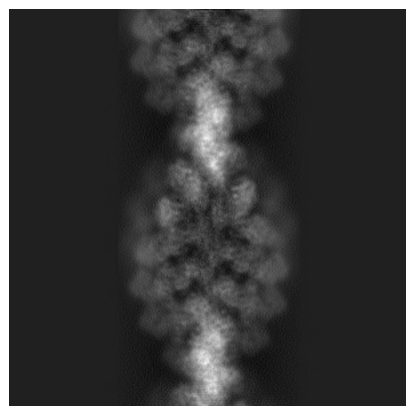
6 Map visualisation [i](#)

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.

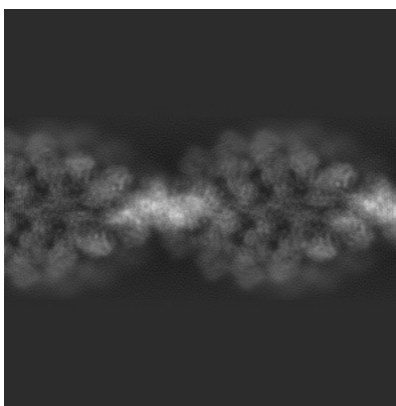
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

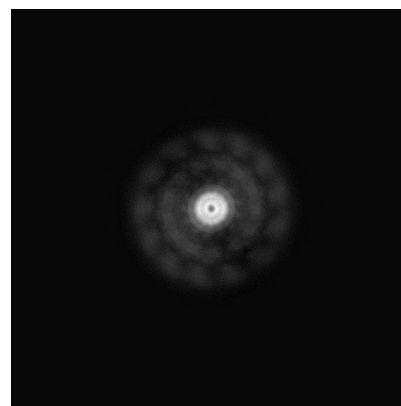
6.1.1 Primary map



X

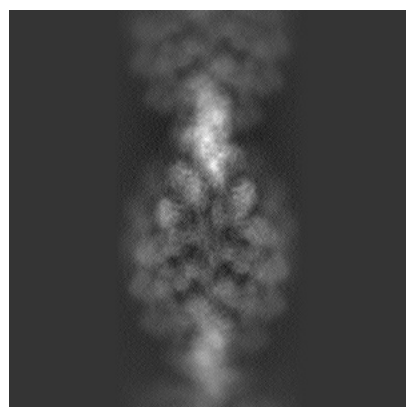


Y

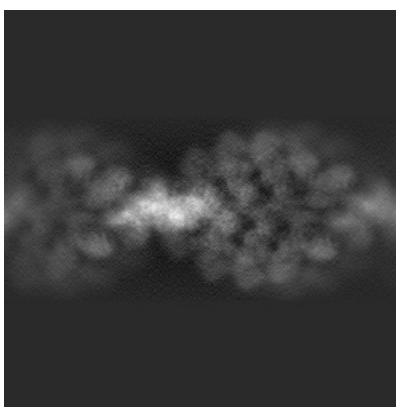


Z

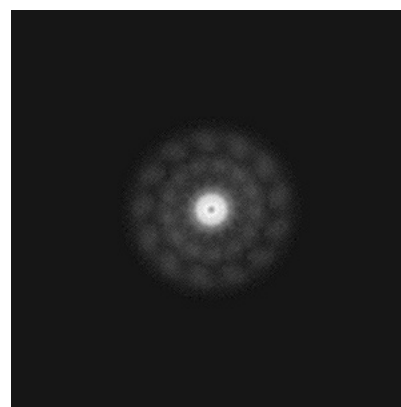
6.1.2 Raw map



X



Y

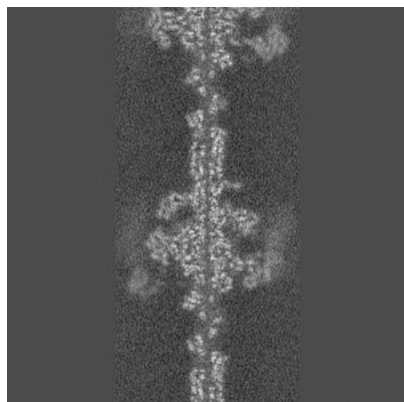


Z

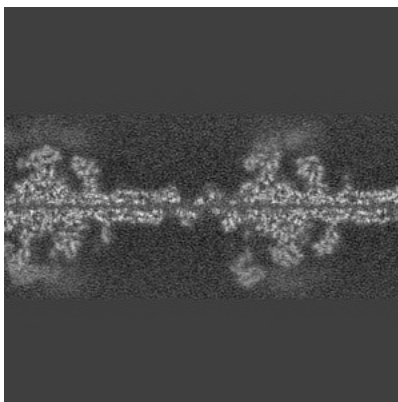
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

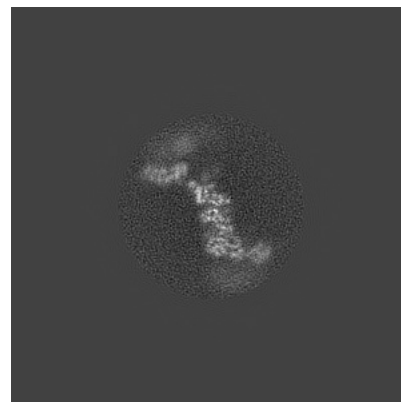
6.2.1 Primary map



X Index: 256

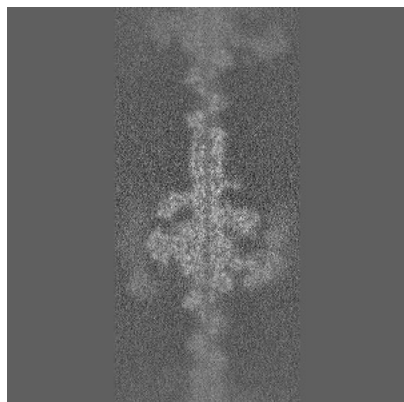


Y Index: 256

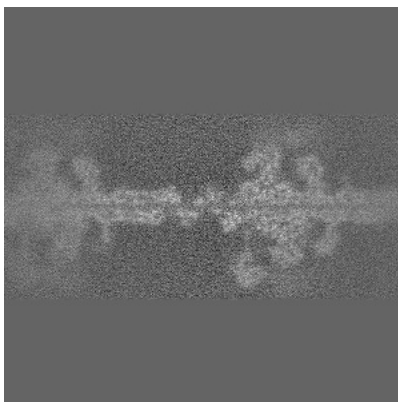


Z Index: 256

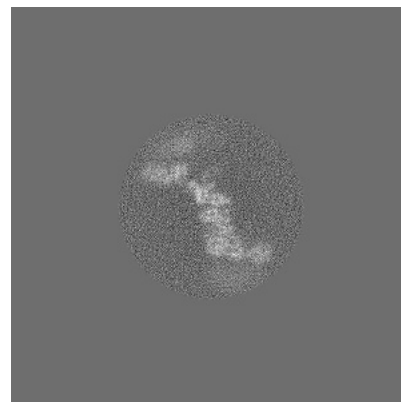
6.2.2 Raw map



X Index: 256



Y Index: 256

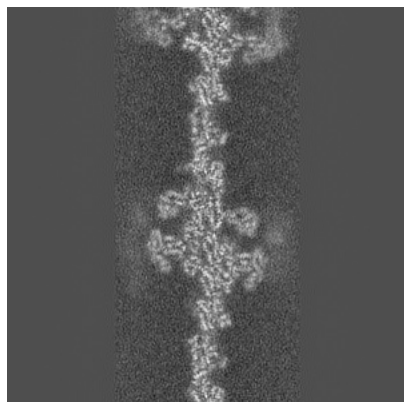


Z Index: 256

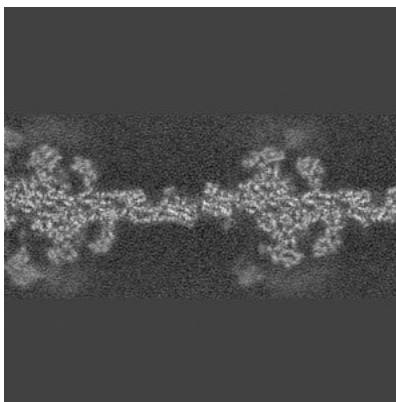
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

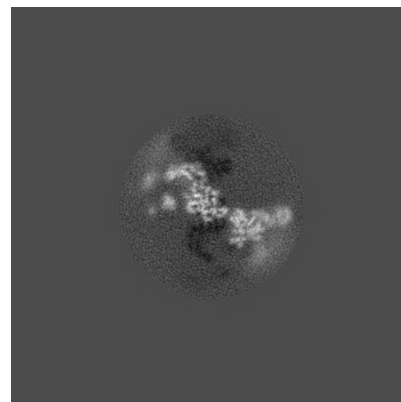
6.3.1 Primary map



X Index: 262

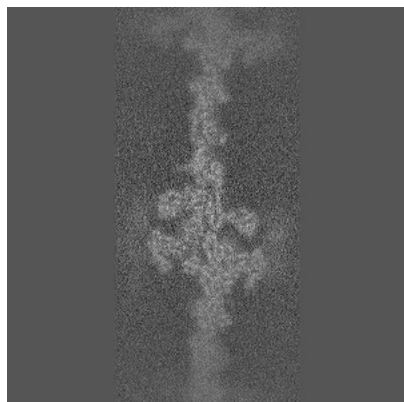


Y Index: 251

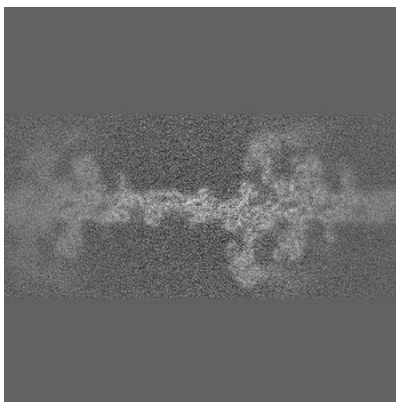


Z Index: 1

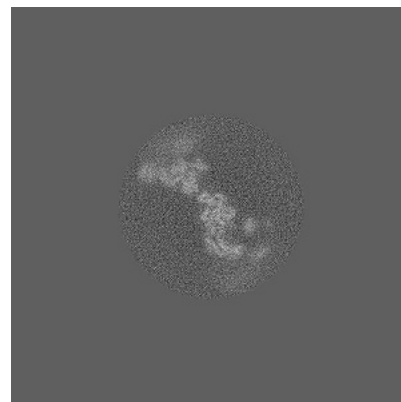
6.3.2 Raw map



X Index: 263



Y Index: 262

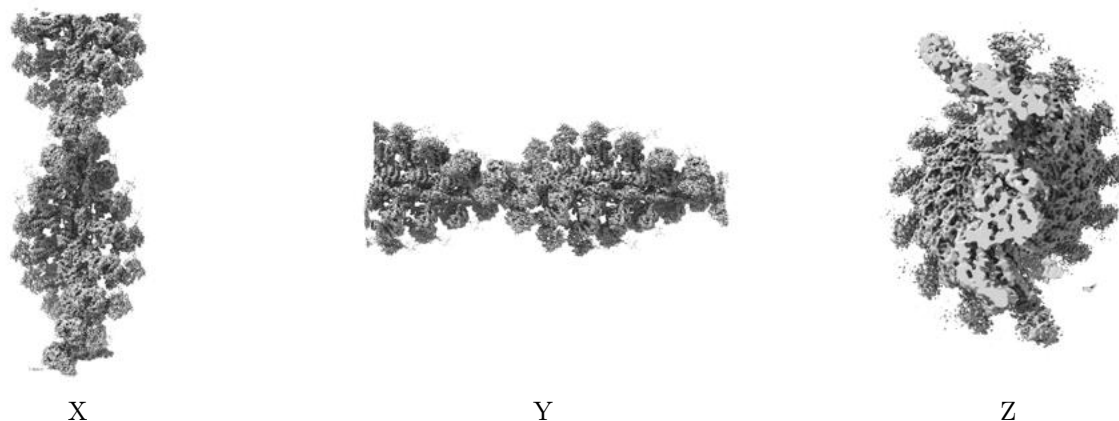


Z Index: 265

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

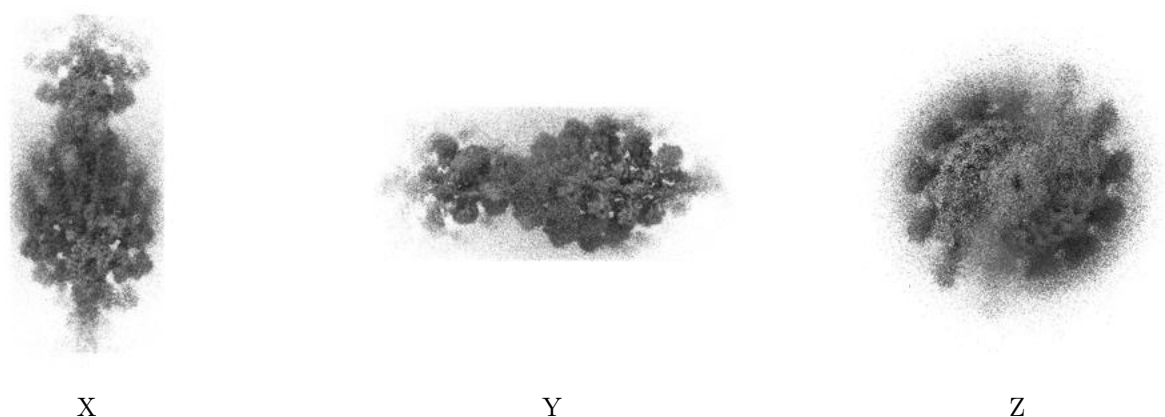
6.4 Orthogonal surface views [i](#)

6.4.1 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.

6.4.2 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

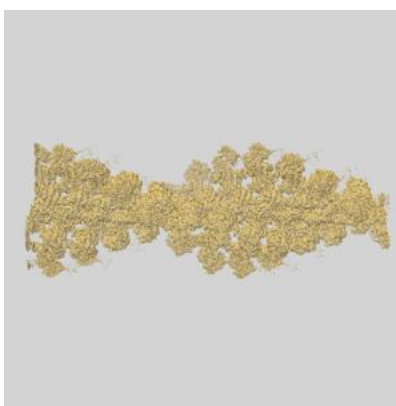
A mask typically either:

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

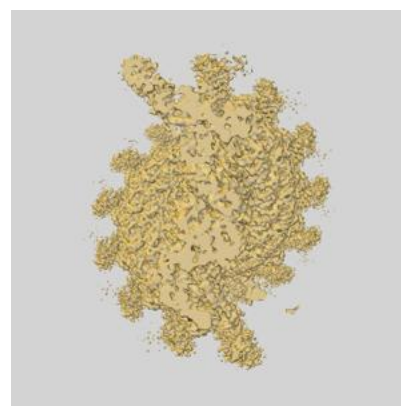
6.5.1 emd_7116_msk_2.map [i](#)



X



Y

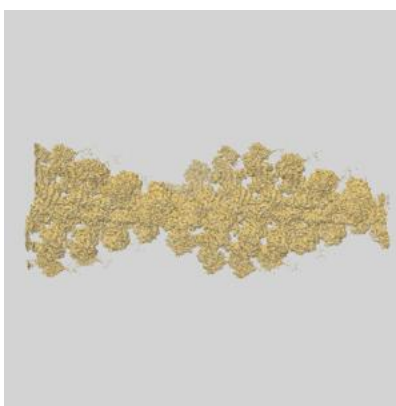


Z

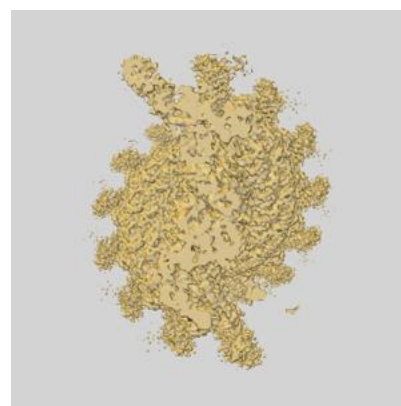
6.5.2 emd_7116_msk_1.map [i](#)



X



Y

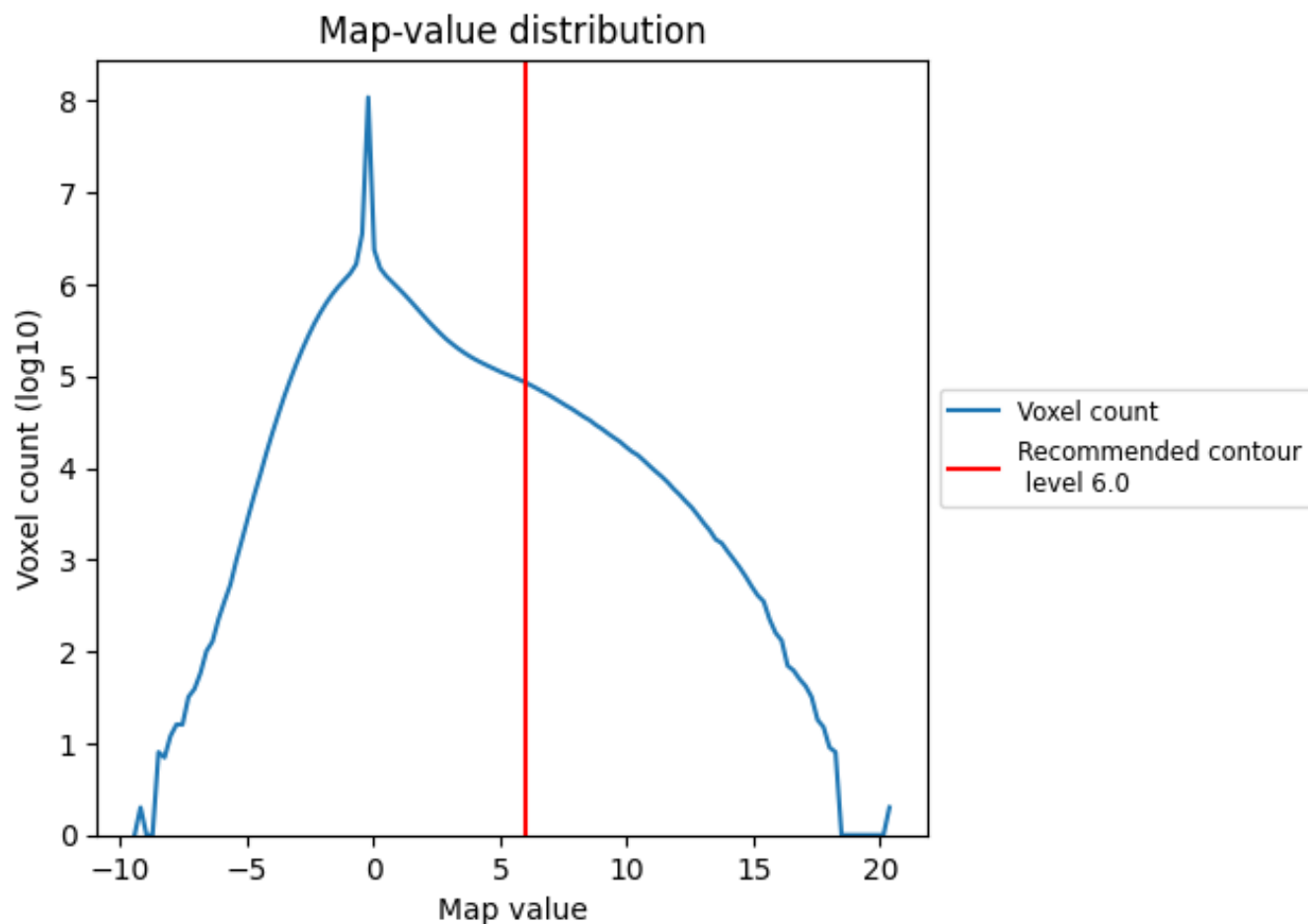


Z

7 Map analysis [i](#)

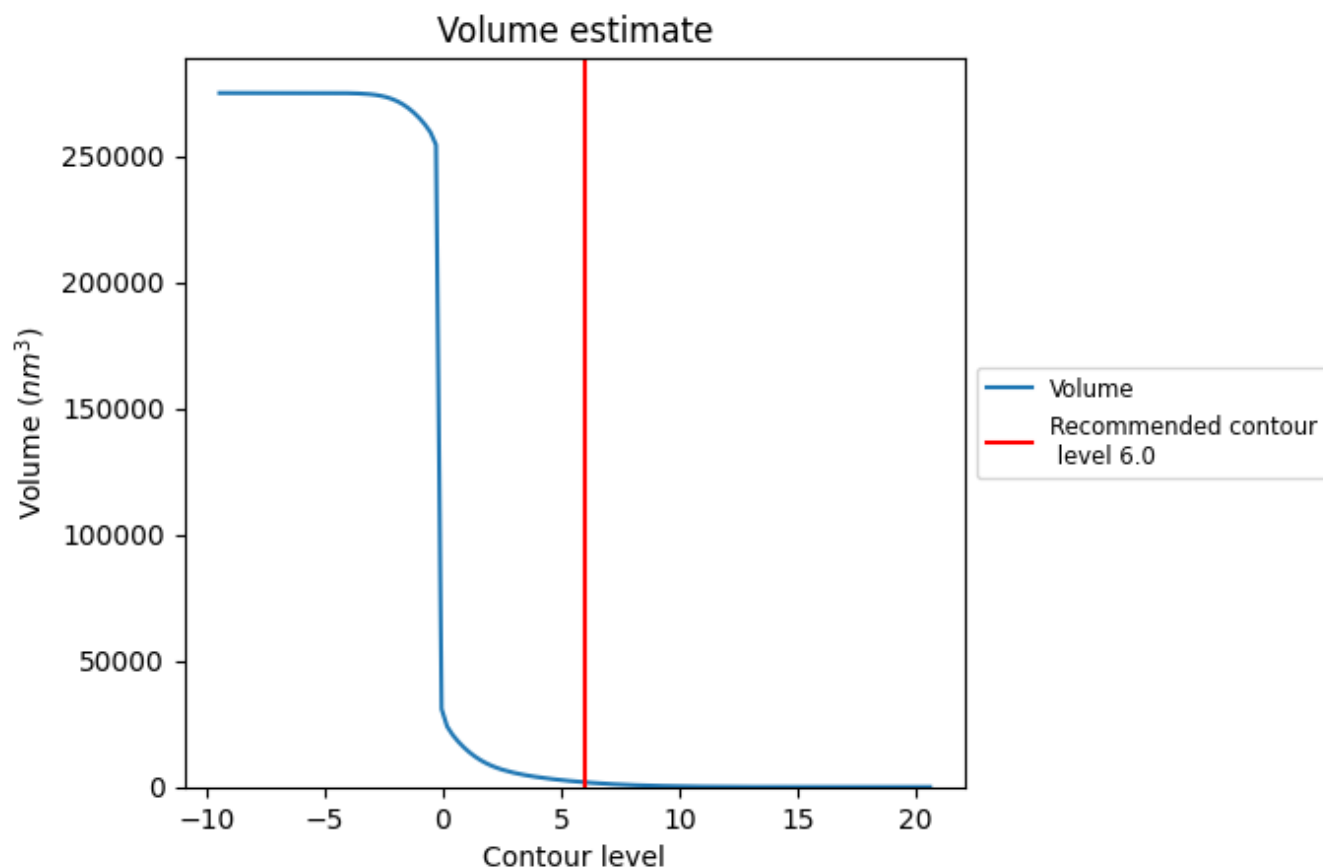
This section contains the results of statistical analysis of the map.

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.

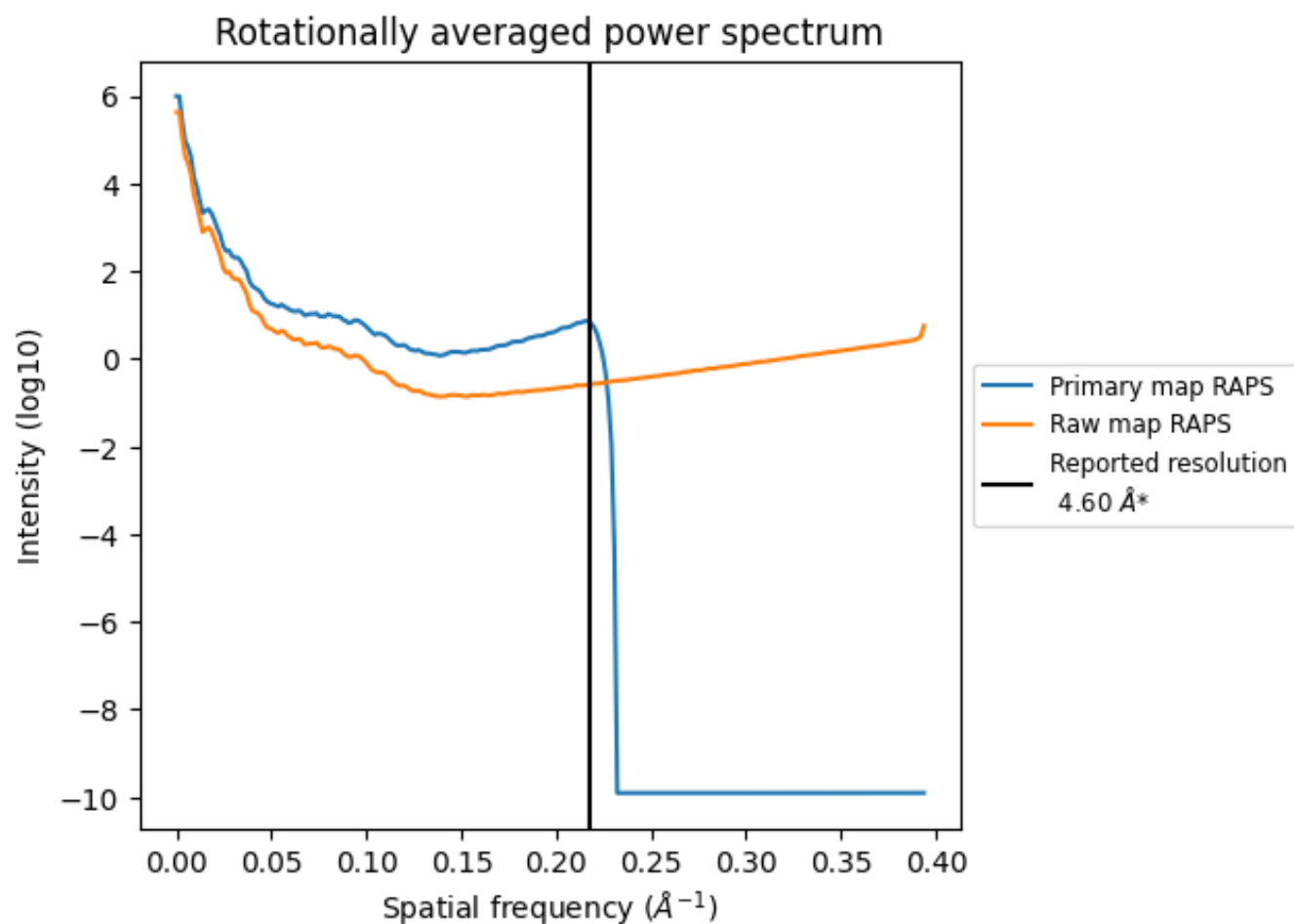
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1866 nm^3 ; 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 ⓘ

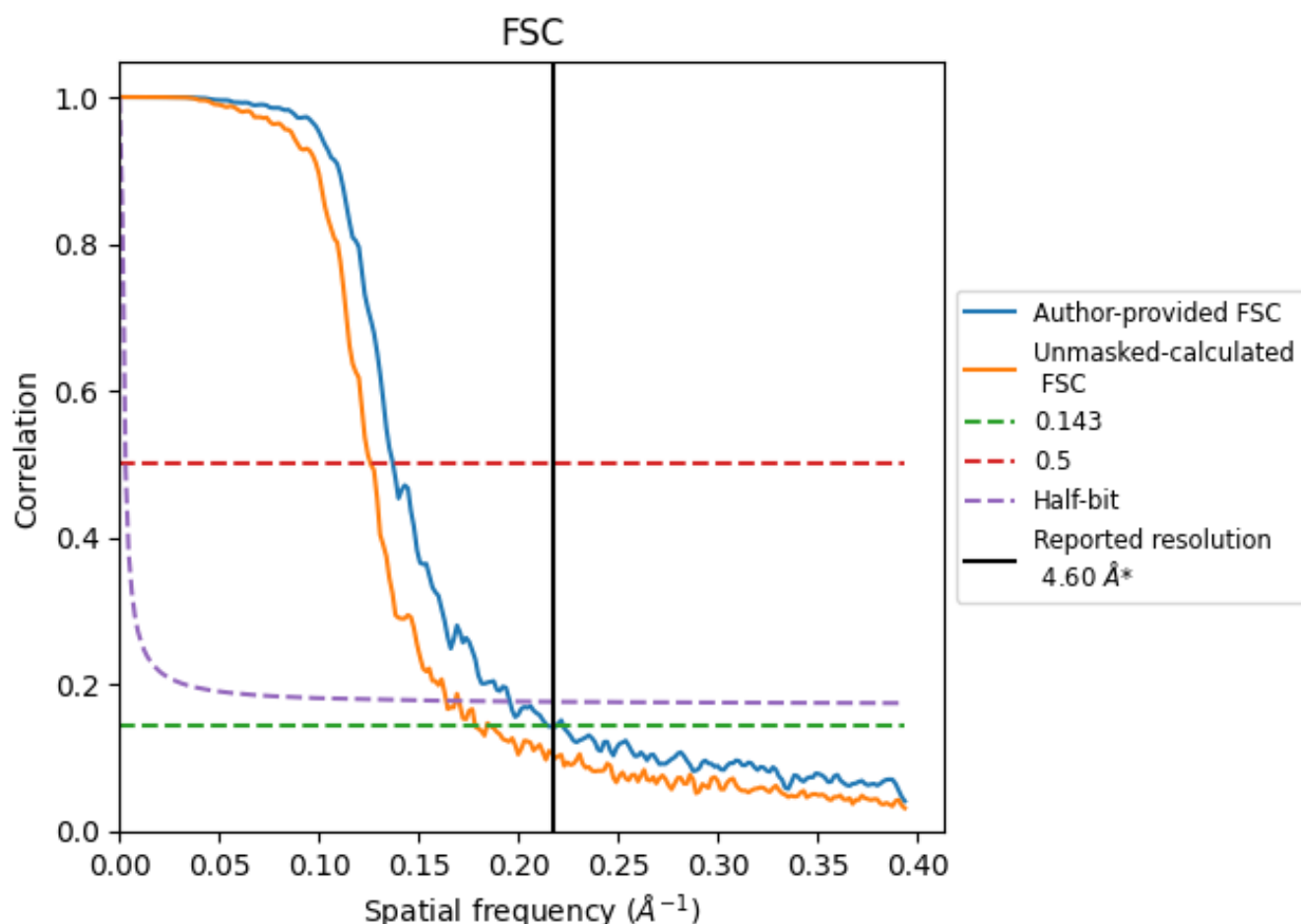


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

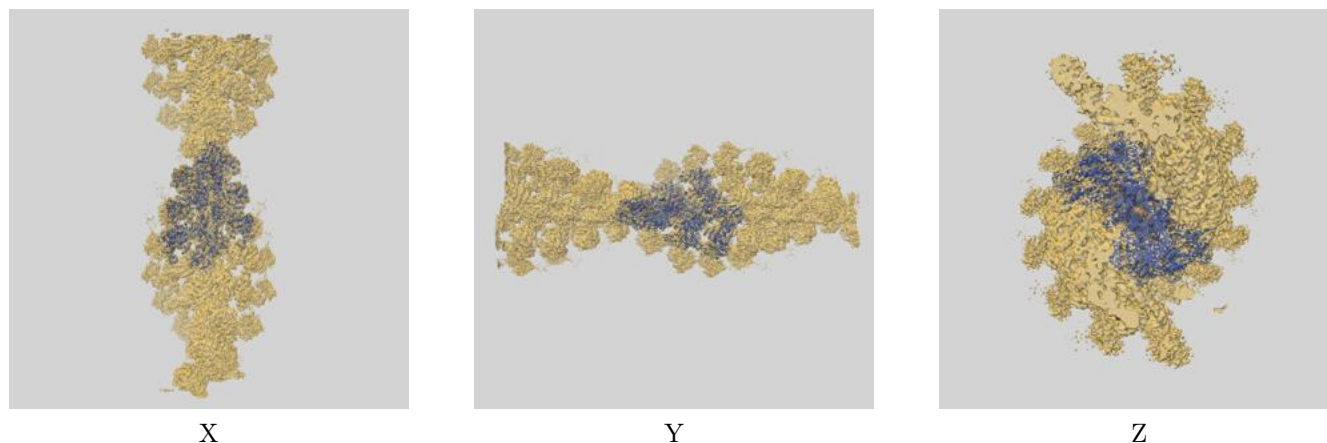
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.66	7.29	5.11
Unmasked-calculated*	5.61	7.94	6.11

*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](#)

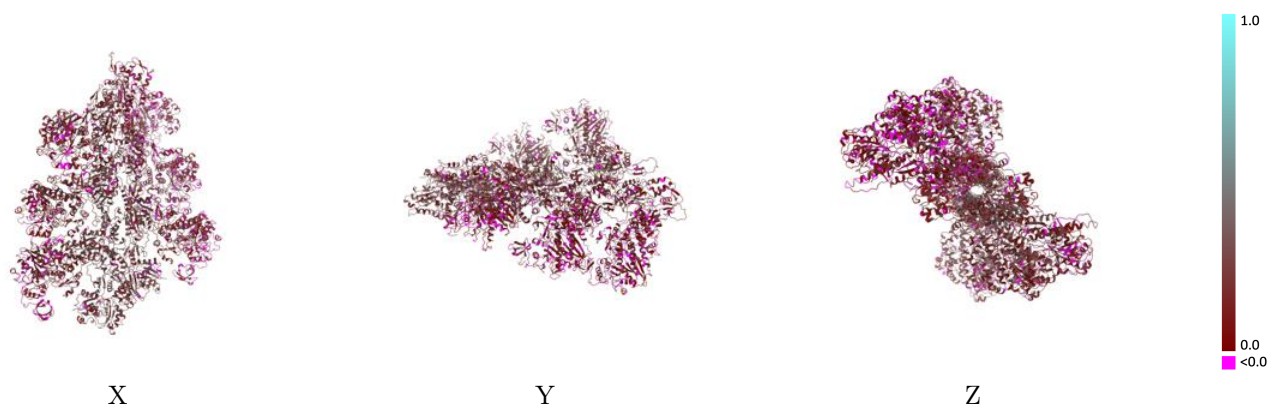
This section contains information regarding the fit between EMDB map EMD-7116 and PDB model 6BNP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



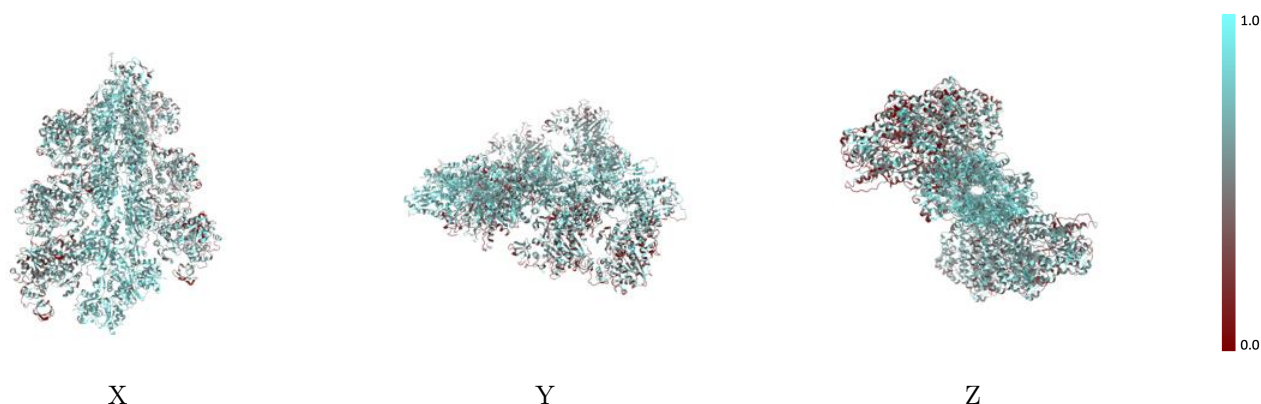
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



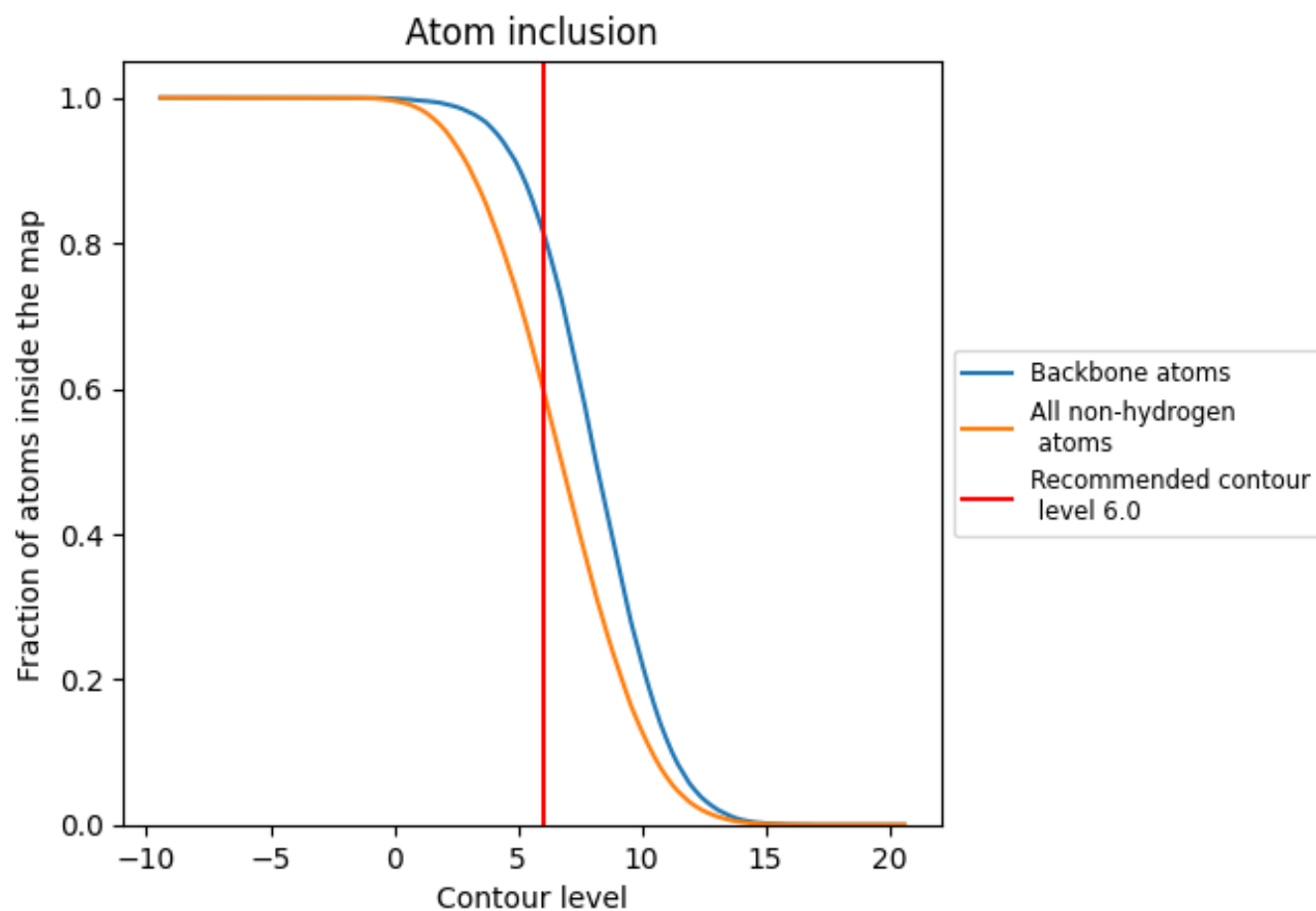
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.0).































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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6016	 0.1910
A	 0.7504	 0.2880
B	 0.7412	 0.2700
C	 0.7655	 0.2940
D	 0.7267	 0.2500
E	 0.7634	 0.2810
F	 0.6805	 0.2030
G	 0.7299	 0.2510
H	 0.6456	 0.1610
I	 0.5399	 0.1740
J	 0.5007	 0.1350
K	 0.5674	 0.1900
L	 0.4781	 0.1160
M	 0.5574	 0.1900
N	 0.4571	 0.1010

