



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:06 AM UTC

PDB ID : 6BNO / pdb_00006bno
EMDB ID : EMD-7115
Title : Structure of bare actin filament
Authors : Gurel, P.S.; Alushin, G.A.
Deposited on : 2017-11-17
Resolution : 5.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

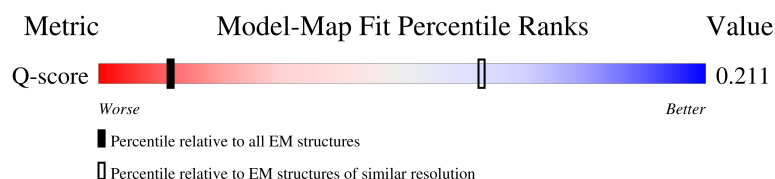
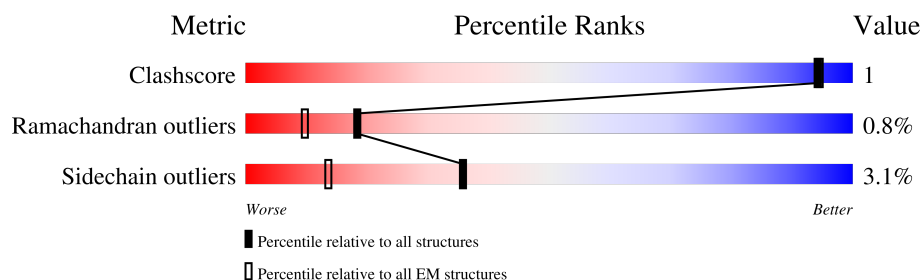
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.50 Å.

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



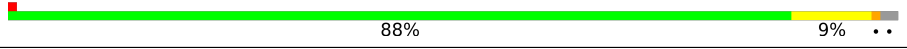
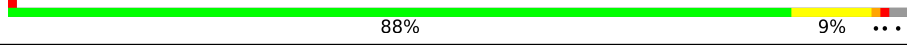
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	520 (5.00 - 6.00)

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

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	
1	D	373	

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Mol	Chain	Length	Quality of chain
1	E	373	 87%10%...
1	F	373	 88%9%..
1	G	373	 88%9%..
1	H	373	 88%9%...

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23120 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 Actin, alpha skeletal muscle.

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

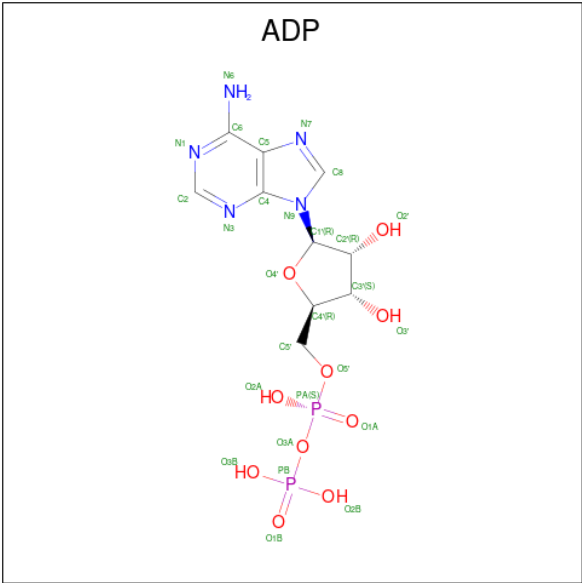
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	
2	B	1	Total	Mg	0
			1	1	
2	C	1	Total	Mg	0
			1	1	
2	D	1	Total	Mg	0
			1	1	
2	E	1	Total	Mg	0
			1	1	
2	F	1	Total	Mg	0
			1	1	
2	G	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
2	H	1	Total	Mg	0
			1	1	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

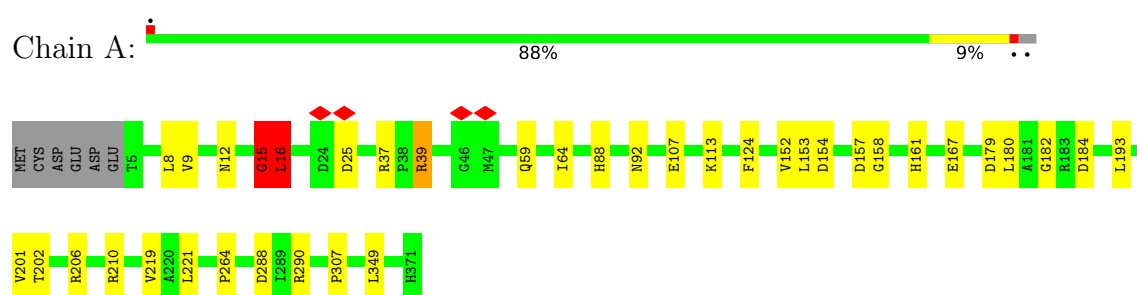


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10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

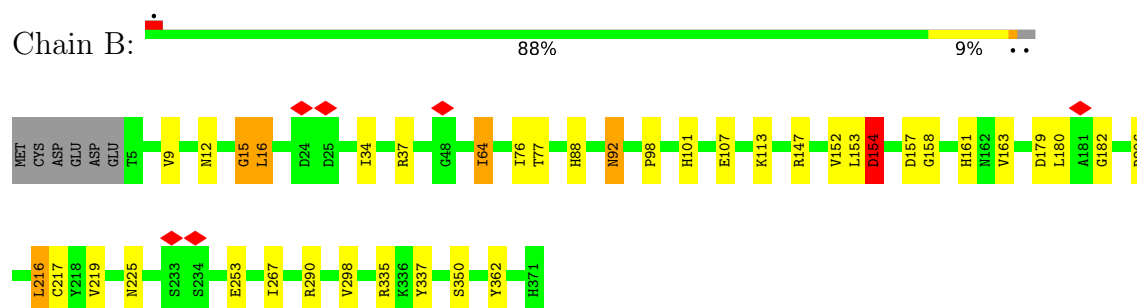
3 Residue-property plots [i](#)

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

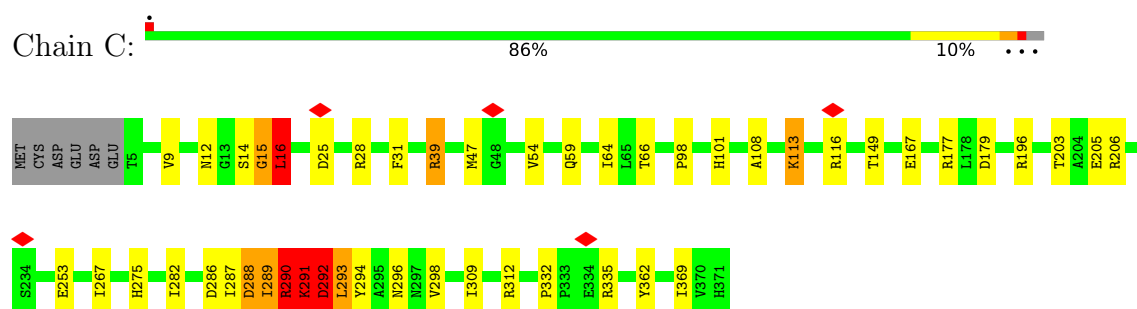
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

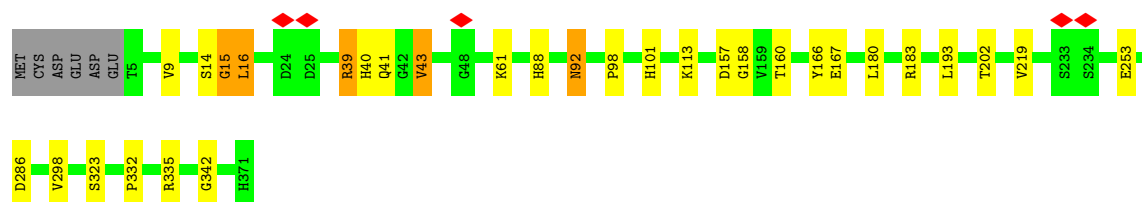


- Molecule 1: Actin, alpha skeletal muscle



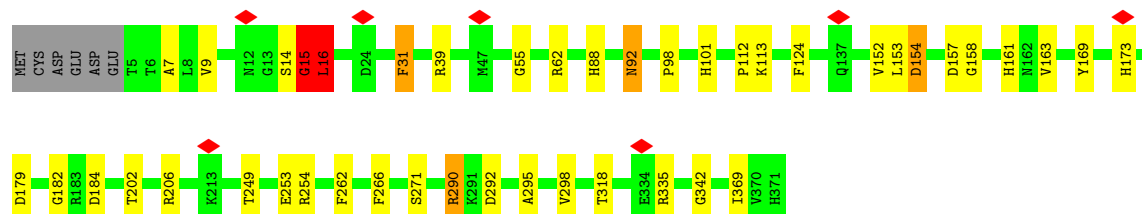
- Molecule 1: Actin, alpha skeletal muscle





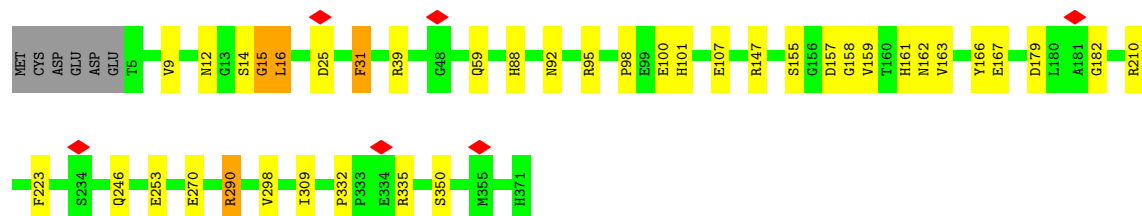
- Molecule 1: Actin, alpha skeletal muscle

Chain E: 87% 10% ...



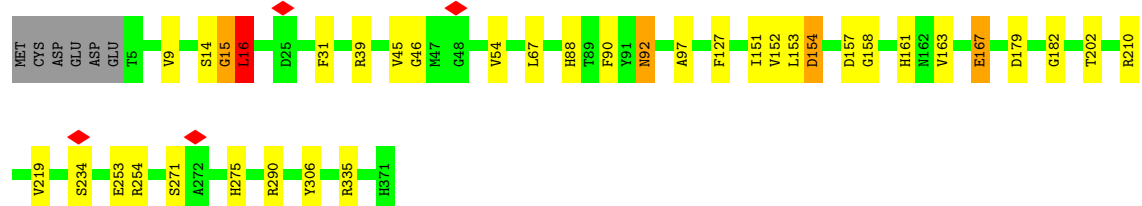
- Molecule 1: Actin, alpha skeletal muscle

Chain F: 88% 9% ..



- Molecule 1: Actin, alpha skeletal muscle

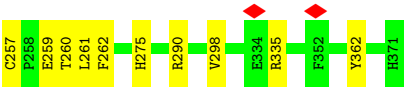
Chain G: 88% 9% ..



- Molecule 1: Actin, alpha skeletal muscle

Chain H: 88% 9% ...





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.6°, rise=28.11 Å, axial sym=C1	Depositor
Number of segments used	63139	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	35.019	Depositor
Minimum map value	-14.238	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	12	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	A	0.87	1/2924 (0.0%)	1.52	29/3963 (0.7%)
1	B	0.88	1/2924 (0.0%)	1.52	22/3963 (0.6%)
1	C	1.32	17/2924 (0.6%)	1.86	51/3963 (1.3%)
1	D	0.86	0/2924	1.52	16/3963 (0.4%)
1	E	0.89	1/2924 (0.0%)	1.54	29/3963 (0.7%)
1	F	0.87	1/2924 (0.0%)	1.54	27/3963 (0.7%)
1	G	0.88	1/2924 (0.0%)	1.53	23/3963 (0.6%)
1	H	0.91	2/2924 (0.1%)	1.59	36/3963 (0.9%)
All	All	0.95	24/23392 (0.1%)	1.58	233/31704 (0.7%)

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	A	0	6
1	B	0	7
1	C	0	17
1	D	0	3
1	E	0	5
1	F	0	6
1	G	0	5
1	H	0	5
All	All	0	54

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	291	LYS	CA-C	25.45	1.87	1.52
1	C	292	ASP	CA-C	20.50	1.89	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	ARG	C-N	17.44	1.58	1.34
1	C	293	LEU	CA-C	13.21	1.70	1.52
1	C	293	LEU	N-CA	12.57	1.62	1.46
1	C	290	ARG	CA-C	12.45	1.70	1.52
1	C	291	LYS	N-CA	11.75	1.61	1.46
1	C	293	LEU	CA-CB	11.14	1.71	1.53
1	C	289	ILE	N-CA	10.82	1.60	1.46
1	C	292	ASP	C-O	-10.43	1.08	1.24
1	C	290	ARG	N-CA	7.69	1.56	1.46
1	C	294	TYR	CA-C	-7.00	1.43	1.52
1	C	290	ARG	CA-CB	-6.89	1.40	1.53
1	E	154	ASP	CA-CB	6.88	1.62	1.53
1	H	154	ASP	CA-CB	6.83	1.62	1.53
1	C	291	LYS	CD-CE	6.80	1.72	1.52
1	B	154	ASP	CA-CB	6.78	1.61	1.53
1	C	292	ASP	CB-CG	-6.76	1.35	1.52
1	A	154	ASP	CA-CB	6.75	1.61	1.53
1	G	154	ASP	CA-CB	6.71	1.61	1.53
1	H	259	GLU	CA-C	6.70	1.62	1.52
1	C	288	ASP	CA-C	5.66	1.60	1.52
1	C	291	LYS	CA-CB	5.55	1.62	1.53
1	F	161	HIS	CB-CG	5.39	1.57	1.50

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	ILE	CA-C-O	-27.16	91.14	120.47
1	C	292	ASP	O-C-N	-17.98	93.47	122.42
1	C	291	LYS	CA-C-O	-17.03	100.39	119.97
1	C	290	ARG	N-CA-C	17.01	133.29	112.87
1	C	292	ASP	CA-CB-CG	-16.90	95.70	112.60
1	C	293	LEU	CA-C-O	-14.58	102.59	119.79
1	C	290	ARG	CA-C-O	-14.21	101.20	119.10
1	C	292	ASP	CB-CA-C	-13.94	84.57	110.36
1	C	289	ILE	CA-C-N	-12.66	97.44	120.99
1	C	289	ILE	C-N-CA	-12.66	97.44	120.99
1	C	288	ASP	O-C-N	-12.40	109.30	122.07
1	H	260	THR	CA-CB-OG1	11.85	127.37	109.60
1	C	292	ASP	N-CA-CB	11.18	127.68	110.46
1	C	291	LYS	O-C-N	10.96	135.75	122.27
1	C	291	LYS	CA-C-N	10.58	143.47	122.31
1	C	291	LYS	C-N-CA	10.58	143.47	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	154	ASP	CA-CB-CG	10.10	122.70	112.60
1	C	289	ILE	N-CA-C	10.03	123.63	111.09
1	E	154	ASP	CA-CB-CG	9.91	122.52	112.60
1	C	290	ARG	NE-CZ-NH1	9.87	131.37	121.50
1	H	259	GLU	CA-C-N	9.49	134.23	120.38
1	H	259	GLU	C-N-CA	9.49	134.23	120.38
1	B	154	ASP	CA-CB-CG	9.48	122.08	112.60
1	G	154	ASP	CA-CB-CG	9.07	121.67	112.60
1	C	15	GLY	CA-C-N	8.75	137.45	121.70
1	C	15	GLY	C-N-CA	8.75	137.45	121.70
1	C	291	LYS	CB-CA-C	-8.73	93.91	110.67
1	H	15	GLY	CA-C-N	8.63	137.24	121.70
1	H	15	GLY	C-N-CA	8.63	137.24	121.70
1	E	15	GLY	CA-C-N	8.26	136.57	121.70
1	E	15	GLY	C-N-CA	8.26	136.57	121.70
1	A	154	ASP	CA-CB-CG	8.24	120.84	112.60
1	G	15	GLY	CA-C-N	8.21	136.48	121.70
1	G	15	GLY	C-N-CA	8.21	136.48	121.70
1	C	288	ASP	CA-C-O	8.16	129.38	120.82
1	C	290	ARG	O-C-N	7.97	133.03	122.43
1	F	15	GLY	CA-C-N	7.91	135.94	121.70
1	F	15	GLY	C-N-CA	7.91	135.94	121.70
1	D	15	GLY	CA-C-N	7.89	135.90	121.70
1	D	15	GLY	C-N-CA	7.89	135.90	121.70
1	G	153	LEU	N-CA-C	7.74	122.14	107.75
1	A	15	GLY	CA-C-N	7.69	135.54	121.70
1	A	15	GLY	C-N-CA	7.69	135.54	121.70
1	C	293	LEU	CB-CA-C	-7.62	94.84	110.38
1	C	291	LYS	N-CA-C	7.56	120.59	111.82
1	C	290	ARG	CB-CG-CD	7.47	128.48	111.30
1	B	15	GLY	CA-C-N	7.44	135.08	121.70
1	B	15	GLY	C-N-CA	7.44	135.08	121.70
1	H	180	LEU	N-CA-C	7.40	119.35	111.28
1	C	290	ARG	N-CA-CB	-7.40	96.86	110.32
1	C	289	ILE	CB-CA-C	-7.16	100.66	112.26
1	F	161	HIS	CA-CB-CG	7.14	120.94	113.80
1	C	286	ASP	N-CA-C	7.01	120.39	110.23
1	E	153	LEU	N-CA-C	6.92	120.61	107.75
1	F	163	VAL	N-CA-C	6.86	115.55	107.73
1	B	153	LEU	N-CA-C	6.78	120.36	107.75
1	A	153	LEU	N-CA-C	6.75	120.31	107.75
1	C	291	LYS	N-CA-CB	-6.72	99.86	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	179	ASP	CA-C-N	6.63	129.17	120.28
1	H	179	ASP	C-N-CA	6.63	129.17	120.28
1	C	179	ASP	CA-C-N	6.62	129.15	120.28
1	C	179	ASP	C-N-CA	6.62	129.15	120.28
1	H	25	ASP	N-CA-C	6.61	118.56	111.36
1	C	14	SER	N-CA-C	-6.50	105.18	113.23
1	C	293	LEU	CA-CB-CG	-6.49	93.60	116.30
1	C	275	HIS	CA-CB-CG	6.43	120.23	113.80
1	F	270	GLU	N-CA-C	6.42	118.36	111.36
1	E	298	VAL	N-CA-C	6.37	117.04	107.80
1	C	298	VAL	N-CA-C	6.28	116.91	107.80
1	H	153	LEU	N-CA-C	6.24	119.36	107.75
1	F	161	HIS	CE1-NE2-CD2	-6.19	102.81	109.00
1	H	257	CYS	CA-C-N	6.17	125.72	119.19
1	H	257	CYS	C-N-CA	6.17	125.72	119.19
1	B	180	LEU	N-CA-C	6.11	117.94	111.28
1	A	180	LEU	N-CA-C	6.10	117.60	111.07
1	C	15	GLY	O-C-N	-6.10	114.77	122.70
1	F	59	GLN	N-CA-C	-6.07	105.83	113.72
1	C	290	ARG	CG-CD-NE	6.05	125.32	112.00
1	C	25	ASP	N-CA-C	6.02	117.65	111.14
1	H	275	HIS	CA-CB-CG	5.96	119.76	113.80
1	D	298	VAL	N-CA-C	5.94	116.41	107.80
1	C	296	ASN	N-CA-C	-5.91	103.35	110.44
1	H	152	VAL	N-CA-C	5.91	116.80	108.36
1	E	179	ASP	CA-C-N	5.90	128.19	120.28
1	E	179	ASP	C-N-CA	5.90	128.19	120.28
1	C	291	LYS	CA-CB-CG	5.87	125.85	114.10
1	B	216	LEU	N-CA-C	5.87	118.91	111.69
1	H	260	THR	N-CA-CB	-5.86	100.89	110.14
1	F	14	SER	N-CA-C	-5.78	106.36	113.41
1	D	202	THR	CA-C-N	5.76	127.93	120.44
1	D	202	THR	C-N-CA	5.76	127.93	120.44
1	F	25	ASP	N-CA-C	5.76	117.37	111.14
1	H	298	VAL	N-CA-C	5.76	115.90	107.37
1	C	59	GLN	N-CA-C	-5.76	106.23	113.72
1	H	154	ASP	N-CA-C	-5.76	98.36	108.20
1	H	260	THR	CA-CB-CG2	-5.74	100.73	110.50
1	H	14	SER	N-CA-C	-5.74	105.38	112.90
1	E	262	PHE	CA-CB-CG	-5.73	108.07	113.80
1	C	31	PHE	N-CA-C	5.73	113.38	108.22
1	D	15	GLY	O-C-N	-5.73	115.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	179	ASP	CA-C-N	5.69	127.90	120.28
1	G	179	ASP	C-N-CA	5.69	127.90	120.28
1	A	25	ASP	N-CA-C	5.68	117.28	111.14
1	B	298	VAL	N-CA-C	5.68	115.77	107.37
1	G	127	PHE	CA-CB-CG	-5.65	108.15	113.80
1	H	152	VAL	CA-C-N	5.63	130.68	122.85
1	H	152	VAL	C-N-CA	5.63	130.68	122.85
1	F	290	ARG	CA-C-N	5.59	128.04	120.38
1	F	290	ARG	C-N-CA	5.59	128.04	120.38
1	C	291	LYS	CG-CD-CE	-5.59	98.45	111.30
1	E	154	ASP	OD1-CG-OD2	-5.58	109.50	122.90
1	G	152	VAL	CA-C-N	5.57	130.59	122.85
1	G	152	VAL	C-N-CA	5.57	130.59	122.85
1	A	184	ASP	CA-CB-CG	-5.56	107.04	112.60
1	B	154	ASP	OD1-CG-OD2	-5.54	109.59	122.90
1	G	154	ASP	OD1-CG-OD2	-5.54	109.60	122.90
1	F	332	PRO	CA-C-O	-5.53	116.92	120.90
1	A	113	LYS	CA-C-N	5.53	131.65	121.70
1	A	113	LYS	C-N-CA	5.53	131.65	121.70
1	H	59	GLN	N-CA-C	-5.52	106.54	113.72
1	E	254	ARG	N-CA-C	5.52	117.30	111.28
1	H	154	ASP	OD1-CG-OD2	-5.51	109.67	122.90
1	A	179	ASP	CA-C-N	5.48	127.57	120.44
1	A	179	ASP	C-N-CA	5.48	127.57	120.44
1	F	155	SER	N-CA-C	5.48	117.62	108.02
1	C	290	ARG	NH1-CZ-NH2	-5.47	112.19	119.30
1	B	179	ASP	CA-C-N	5.47	127.61	120.28
1	B	179	ASP	C-N-CA	5.47	127.61	120.28
1	B	15	GLY	O-C-N	-5.46	115.61	122.70
1	G	152	VAL	N-CA-C	5.43	116.13	108.36
1	D	113	LYS	CA-C-N	5.42	131.46	121.70
1	D	113	LYS	C-N-CA	5.42	131.46	121.70
1	G	90	PHE	CA-CB-CG	5.41	119.21	113.80
1	F	162	ASN	CA-CB-CG	5.41	118.01	112.60
1	E	31	PHE	CA-CB-CG	5.40	119.20	113.80
1	C	203	THR	N-CA-C	5.40	116.85	111.07
1	F	157	ASP	CA-C-N	5.38	131.39	121.70
1	F	157	ASP	C-N-CA	5.38	131.39	121.70
1	B	113	LYS	O-C-N	-5.37	116.91	123.19
1	B	154	ASP	N-CA-C	-5.37	99.03	108.20
1	C	108	ALA	CA-C-N	5.36	125.43	119.32
1	C	108	ALA	C-N-CA	5.36	125.43	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	LYS	O-C-N	-5.36	116.94	123.10
1	D	180	LEU	N-CA-C	5.36	116.81	111.07
1	E	202	THR	CA-C-N	5.36	127.41	120.44
1	E	202	THR	C-N-CA	5.36	127.41	120.44
1	A	152	VAL	CA-C-N	5.36	130.30	122.85
1	A	152	VAL	C-N-CA	5.36	130.30	122.85
1	H	253	GLU	CA-C-N	5.36	127.46	120.28
1	H	253	GLU	C-N-CA	5.36	127.46	120.28
1	B	163	VAL	N-CA-C	5.35	113.82	107.73
1	B	64	ILE	N-CA-C	-5.34	106.65	113.22
1	A	307	PRO	N-CA-C	5.34	123.47	112.47
1	A	264	PRO	CA-C-N	5.33	128.16	120.38
1	A	264	PRO	C-N-CA	5.33	128.16	120.38
1	G	163	VAL	N-CA-C	5.33	113.81	107.73
1	A	221	LEU	N-CA-C	-5.33	106.83	113.55
1	G	167	GLU	CA-C-N	5.33	131.29	121.70
1	G	167	GLU	C-N-CA	5.33	131.29	121.70
1	E	113	LYS	CA-C-N	5.31	131.25	121.70
1	E	113	LYS	C-N-CA	5.31	131.25	121.70
1	E	16	LEU	N-CA-CB	5.30	119.50	110.50
1	D	286	ASP	N-CA-C	5.29	117.12	110.24
1	E	173	HIS	CA-CB-CG	5.28	119.08	113.80
1	H	261	LEU	N-CA-C	5.28	118.82	112.38
1	H	260	THR	N-CA-C	-5.27	105.00	111.75
1	F	100	GLU	N-CA-C	5.27	117.02	111.28
1	A	157	ASP	CA-C-N	5.27	131.18	121.70
1	A	157	ASP	C-N-CA	5.27	131.18	121.70
1	H	262	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	16	LEU	N-CA-CB	5.25	119.43	110.50
1	A	201	VAL	N-CA-C	5.25	116.02	110.72
1	A	202	THR	CA-C-N	5.25	127.26	120.44
1	A	202	THR	C-N-CA	5.25	127.26	120.44
1	E	184	ASP	CA-CB-CG	-5.24	107.36	112.60
1	F	179	ASP	CA-C-N	5.23	127.29	120.28
1	F	179	ASP	C-N-CA	5.23	127.29	120.28
1	G	15	GLY	O-C-N	-5.23	115.91	122.70
1	D	41	GLN	N-CA-C	5.21	117.59	110.24
1	A	59	GLN	N-CA-C	-5.20	106.96	113.72
1	E	163	VAL	N-CA-C	5.19	113.65	107.73
1	C	332	PRO	CA-C-O	-5.19	117.16	120.90
1	H	16	LEU	N-CA-CB	5.19	119.32	110.50
1	E	266	PHE	CA-CB-CG	-5.18	108.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ASN	CA-CB-CG	-5.17	107.42	112.60
1	H	23	GLY	O-C-N	-5.17	117.22	122.70
1	A	154	ASP	OD1-CG-OD2	-5.15	110.54	122.90
1	H	119	MET	CA-C-N	5.15	127.43	120.38
1	H	119	MET	C-N-CA	5.15	127.43	120.38
1	C	16	LEU	N-CA-CB	5.14	119.25	110.50
1	B	34	ILE	N-CA-C	5.14	116.31	109.37
1	D	332	PRO	CA-C-O	-5.14	117.20	120.90
1	E	290	ARG	CA-C-N	5.14	127.42	120.38
1	E	290	ARG	C-N-CA	5.14	127.42	120.38
1	D	43	VAL	N-CA-C	5.13	120.02	109.34
1	H	113	LYS	O-C-N	-5.12	117.32	123.06
1	E	55	GLY	CA-C-N	5.12	130.92	121.70
1	E	55	GLY	C-N-CA	5.12	130.92	121.70
1	F	15	GLY	O-C-N	-5.12	116.04	122.70
1	C	113	LYS	O-C-N	-5.12	116.71	123.21
1	H	15	GLY	O-C-N	-5.11	116.05	122.70
1	G	275	HIS	CA-CB-CG	5.10	118.90	113.80
1	C	309	ILE	N-CA-C	-5.10	101.14	108.53
1	B	217	CYS	N-CA-C	5.08	117.27	110.35
1	G	16	LEU	N-CA-CB	5.08	119.14	110.50
1	E	152	VAL	N-CA-C	5.08	115.63	108.36
1	D	342	GLY	CA-C-N	5.08	125.72	120.03
1	D	342	GLY	C-N-CA	5.08	125.72	120.03
1	F	350	SER	O-C-N	-5.08	116.87	122.86
1	F	298	VAL	N-CA-C	5.07	114.87	107.37
1	G	202	THR	CA-C-N	5.07	127.03	120.44
1	G	202	THR	C-N-CA	5.07	127.03	120.44
1	E	342	GLY	CA-C-N	5.06	125.70	120.03
1	E	342	GLY	C-N-CA	5.06	125.70	120.03
1	F	31	PHE	N-CA-C	5.06	112.77	108.22
1	E	7	ALA	N-CA-C	5.06	117.05	110.43
1	B	152	VAL	N-CA-C	5.05	115.59	108.36
1	H	154	ASP	N-CA-CB	5.05	118.70	110.37
1	A	64	ILE	N-CA-C	-5.05	108.06	112.90
1	G	97	ALA	CA-C-N	5.04	125.07	119.32
1	G	97	ALA	C-N-CA	5.04	125.07	119.32
1	A	154	ASP	N-CA-C	-5.04	99.58	108.20
1	F	223	PHE	CA-C-N	5.02	127.26	120.38
1	F	223	PHE	C-N-CA	5.02	127.26	120.38
1	B	350	SER	O-C-N	-5.02	116.88	122.75
1	A	167	GLU	CA-C-N	5.01	130.73	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	GLU	C-N-CA	5.01	130.73	121.70
1	F	309	ILE	CA-C-N	5.01	130.72	121.70
1	F	309	ILE	C-N-CA	5.01	130.72	121.70
1	G	46	GLY	N-CA-C	5.01	118.55	112.49
1	E	113	LYS	O-C-N	-5.00	116.78	122.89
1	B	152	VAL	CA-C-N	5.00	129.80	122.85
1	B	152	VAL	C-N-CA	5.00	129.80	122.85

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ARG	Sidechain
1	A	210	ARG	Sidechain
1	A	290	ARG	Sidechain
1	A	349	LEU	Peptide
1	A	37	ARG	Sidechain
1	A	39	ARG	Sidechain
1	B	147	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	290	ARG	Sidechain
1	B	335	ARG	Sidechain
1	B	337	TYR	Sidechain
1	B	362	TYR	Sidechain
1	B	37	ARG	Sidechain
1	C	116	ARG	Sidechain
1	C	177	ARG	Sidechain
1	C	196	ARG	Sidechain
1	C	206	ARG	Sidechain
1	C	28	ARG	Sidechain
1	C	288	ASP	Mainchain
1	C	289	ILE	Mainchain,Peptide
1	C	290	ARG	Sidechain
1	C	291	LYS	Mainchain,Peptide
1	C	292	ASP	Mainchain,Peptide
1	C	312	ARG	Sidechain
1	C	335	ARG	Sidechain
1	C	362	TYR	Sidechain
1	C	39	ARG	Sidechain
1	D	166	TYR	Sidechain
1	D	183	ARG	Sidechain
1	D	335	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	206	ARG	Sidechain
1	E	290	ARG	Sidechain
1	E	335	ARG	Sidechain
1	E	39	ARG	Sidechain
1	E	62	ARG	Sidechain
1	F	147	ARG	Sidechain
1	F	166	TYR	Sidechain
1	F	210	ARG	Sidechain
1	F	290	ARG	Sidechain
1	F	335	ARG	Sidechain
1	F	95	ARG	Sidechain
1	G	210	ARG	Sidechain
1	G	254	ARG	Sidechain
1	G	290	ARG	Sidechain
1	G	306	TYR	Sidechain
1	G	335	ARG	Sidechain
1	H	183	ARG	Sidechain
1	H	290	ARG	Sidechain
1	H	335	ARG	Sidechain
1	H	362	TYR	Sidechain
1	H	39	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	A	2862	0	2831	3	0
1	B	2862	0	2831	7	0
1	C	2862	0	2831	15	0
1	D	2862	0	2831	7	0
1	E	2862	0	2831	8	0
1	F	2862	0	2831	5	0
1	G	2862	0	2831	5	0
1	H	2862	0	2831	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
All	All	23120	0	22744	56	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 (56) 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)
1:C:291:LYS:CA	1:C:291:LYS:C	1.87	1.46
1:C:292:ASP:CA	1:C:292:ASP:C	1.89	1.46
1:C:292:ASP:C	1:C:292:ASP:CB	2.32	1.02
1:C:291:LYS:C	1:C:291:LYS:CB	2.55	0.79
1:C:291:LYS:CA	1:C:291:LYS:O	2.39	0.65
1:C:292:ASP:C	1:C:292:ASP:HB3	2.21	0.63
1:C:282:ILE:HG23	1:C:290:ARG:HB3	1.87	0.56
1:A:158:GLY:HA2	1:A:182:GLY:H	1.72	0.55
1:B:253:GLU:H	1:B:253:GLU:CD	2.16	0.54
1:C:253:GLU:H	1:C:253:GLU:CD	2.17	0.53
1:D:88:HIS:CE1	1:D:92:ASN:HD21	2.26	0.53
1:C:291:LYS:CA	1:C:292:ASP:N	2.65	0.52
1:B:98:PRO:HA	1:B:101:HIS:CE1	2.45	0.51
1:H:154:ASP:HB3	1:H:161:HIS:CE1	2.45	0.51
1:F:158:GLY:HA2	1:F:182:GLY:H	1.76	0.50
1:A:88:HIS:CE1	1:A:92:ASN:HD21	2.30	0.50
1:F:253:GLU:H	1:F:253:GLU:CD	2.19	0.50
1:B:158:GLY:HA2	1:B:182:GLY:H	1.77	0.50
1:A:15:GLY:HA3	1:A:16:LEU:HB2	1.95	0.49
1:D:39:ARG:HH11	1:D:40:HIS:CE1	2.30	0.49
1:E:154:ASP:HB3	1:E:161:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ILE:H	1:C:287:ILE:HD12	1.77	0.48
1:C:64:ILE:HD11	1:E:169:TYR:HB2	1.94	0.48
1:D:253:GLU:H	1:D:253:GLU:CD	2.22	0.48
1:E:98:PRO:HA	1:E:101:HIS:CE1	2.49	0.47
1:H:15:GLY:HA3	1:H:16:LEU:HB2	1.96	0.47
1:G:154:ASP:HB3	1:G:161:HIS:CE1	2.50	0.47
1:G:158:GLY:HA2	1:G:182:GLY:H	1.79	0.47
1:E:15:GLY:HA3	1:E:16:LEU:HB2	1.98	0.46
1:E:88:HIS:CE1	1:E:92:ASN:HD21	2.34	0.46
1:F:15:GLY:HA3	1:F:16:LEU:HB2	1.97	0.46
1:G:15:GLY:HA3	1:G:16:LEU:HB2	1.98	0.46
1:E:88:HIS:CD2	1:E:92:ASN:HD21	2.34	0.45
1:E:158:GLY:HA2	1:E:182:GLY:H	1.80	0.45
1:B:154:ASP:HB3	1:B:161:HIS:CE1	2.51	0.45
1:B:15:GLY:HA3	1:B:16:LEU:HB2	1.99	0.45
1:C:98:PRO:HA	1:C:101:HIS:CE1	2.52	0.45
1:H:253:GLU:H	1:H:253:GLU:CD	2.25	0.45
1:D:15:GLY:HA3	1:D:16:LEU:HB2	1.99	0.45
1:H:157:ASP:HA	1:H:182:GLY:H	1.81	0.45
1:D:98:PRO:HA	1:D:101:HIS:CE1	2.52	0.44
1:B:88:HIS:CE1	1:B:92:ASN:HD21	2.35	0.44
1:H:98:PRO:HA	1:H:101:HIS:CE1	2.51	0.44
1:D:157:ASP:HB2	3:D:402:ADP:H4'	2.00	0.44
1:F:88:HIS:CE1	1:F:92:ASN:HD21	2.36	0.43
1:G:88:HIS:CE1	1:G:92:ASN:HD21	2.36	0.43
1:H:158:GLY:HA2	1:H:182:GLY:H	1.83	0.43
1:F:98:PRO:HA	1:F:101:HIS:CE1	2.53	0.43
1:C:15:GLY:HA3	1:C:16:LEU:HB2	2.00	0.43
1:E:253:GLU:H	1:E:253:GLU:CD	2.26	0.42
1:D:157:ASP:HA	1:D:158:GLY:HA2	1.90	0.42
1:H:76:ILE:HD13	1:H:76:ILE:H	1.84	0.42
1:C:290:ARG:HA	1:C:293:LEU:HG	2.01	0.41
1:C:287:ILE:H	1:C:287:ILE:CD1	2.33	0.41
1:G:253:GLU:H	1:G:253:GLU:CD	2.28	0.41
1:B:76:ILE:HD12	1:B:76:ILE:H	1.85	0.41

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	A	365/373 (98%)	332 (91%)	31 (8%)	2 (0%)	24	64
1	B	365/373 (98%)	335 (92%)	29 (8%)	1 (0%)	36	72
1	C	365/373 (98%)	328 (90%)	34 (9%)	3 (1%)	16	54
1	D	365/373 (98%)	330 (90%)	32 (9%)	3 (1%)	16	54
1	E	365/373 (98%)	330 (90%)	30 (8%)	5 (1%)	9	39
1	F	365/373 (98%)	332 (91%)	31 (8%)	2 (0%)	24	64
1	G	365/373 (98%)	334 (92%)	27 (7%)	4 (1%)	11	45
1	H	365/373 (98%)	333 (91%)	30 (8%)	2 (0%)	24	64
All	All	2920/2984 (98%)	2654 (91%)	244 (8%)	22 (1%)	18	54

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	167	GLU
1	H	16	LEU
1	A	16	LEU
1	C	16	LEU
1	C	167	GLU
1	D	16	LEU
1	D	43	VAL
1	E	16	LEU
1	E	271	SER
1	F	16	LEU
1	G	16	LEU
1	G	167	GLU
1	G	234	SER
1	G	271	SER
1	B	16	LEU
1	F	167	GLU
1	A	15	GLY

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Mol	Chain	Res	Type
1	H	45	VAL
1	E	295	ALA
1	E	369	ILE
1	E	15	GLY
1	C	369	ILE

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	A	310/316 (98%)	300 (97%)	10 (3%)	34	55
1	B	310/316 (98%)	299 (96%)	11 (4%)	32	53
1	C	310/316 (98%)	299 (96%)	11 (4%)	32	53
1	D	310/316 (98%)	301 (97%)	9 (3%)	37	57
1	E	310/316 (98%)	300 (97%)	10 (3%)	34	55
1	F	310/316 (98%)	303 (98%)	7 (2%)	44	63
1	G	310/316 (98%)	299 (96%)	11 (4%)	32	53
1	H	310/316 (98%)	303 (98%)	7 (2%)	44	63
All	All	2480/2528 (98%)	2404 (97%)	76 (3%)	36	56

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	VAL
1	A	12	ASN
1	A	39	ARG
1	A	107	GLU
1	A	124	PHE
1	A	161	HIS
1	A	193	LEU
1	A	219	VAL
1	A	288	ASP

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Mol	Chain	Res	Type
1	B	9	VAL
1	B	12	ASN
1	B	64	ILE
1	B	77	THR
1	B	92	ASN
1	B	107	GLU
1	B	154	ASP
1	B	157	ASP
1	B	216	LEU
1	B	219	VAL
1	B	267	ILE
1	C	9	VAL
1	C	12	ASN
1	C	39	ARG
1	C	47	MET
1	C	54	VAL
1	C	66	THR
1	C	113	LYS
1	C	149	THR
1	C	205	GLU
1	C	267	ILE
1	C	290	ARG
1	D	9	VAL
1	D	14	SER
1	D	39	ARG
1	D	61	LYS
1	D	92	ASN
1	D	160	THR
1	D	193	LEU
1	D	219	VAL
1	D	323	SER
1	E	9	VAL
1	E	14	SER
1	E	31	PHE
1	E	92	ASN
1	E	112	PRO
1	E	124	PHE
1	E	157	ASP
1	E	249	THR
1	E	292	ASP
1	E	318	THR
1	F	9	VAL

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Mol	Chain	Res	Type
1	F	12	ASN
1	F	31	PHE
1	F	39	ARG
1	F	107	GLU
1	F	159	VAL
1	F	246	GLN
1	G	9	VAL
1	G	14	SER
1	G	31	PHE
1	G	39	ARG
1	G	45	VAL
1	G	54	VAL
1	G	67	LEU
1	G	92	ASN
1	G	151	ILE
1	G	157	ASP
1	G	219	VAL
1	H	9	VAL
1	H	12	ASN
1	H	31	PHE
1	H	76	ILE
1	H	98	PRO
1	H	154	ASP
1	H	249	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	88	HIS
1	A	92	ASN
1	A	275	HIS
1	A	280	ASN
1	A	297	ASN
1	B	12	ASN
1	B	88	HIS
1	B	92	ASN
1	B	101	HIS
1	B	161	HIS
1	B	275	HIS
1	B	280	ASN
1	B	296	ASN

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Mol	Chain	Res	Type
1	C	12	ASN
1	C	41	GLN
1	C	88	HIS
1	C	92	ASN
1	C	275	HIS
1	C	296	ASN
1	D	88	HIS
1	D	92	ASN
1	D	275	HIS
1	E	12	ASN
1	E	41	GLN
1	E	88	HIS
1	E	92	ASN
1	E	101	HIS
1	E	161	HIS
1	E	280	ASN
1	E	296	ASN
1	E	371	HIS
1	F	12	ASN
1	F	41	GLN
1	F	49	GLN
1	F	73	HIS
1	F	88	HIS
1	F	92	ASN
1	F	101	HIS
1	F	173	HIS
1	F	275	HIS
1	F	297	ASN
1	G	78	ASN
1	G	87	HIS
1	G	88	HIS
1	G	92	ASN
1	G	161	HIS
1	G	263	GLN
1	G	280	ASN
1	G	354	GLN
1	H	40	HIS
1	H	73	HIS
1	H	88	HIS
1	H	92	ASN
1	H	101	HIS
1	H	161	HIS

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Mol	Chain	Res	Type
1	H	246	GLN
1	H	275	HIS
1	H	280	ASN
1	H	371	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	402	2	28,29,29	1.38	4 (14%)	43,45,45	1.82	10 (23%)
3	ADP	F	402	2	28,29,29	1.39	4 (14%)	43,45,45	1.81	10 (23%)
3	ADP	H	402	2	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)
3	ADP	G	402	2	28,29,29	1.38	4 (14%)	43,45,45	1.82	10 (23%)
3	ADP	B	402	2	28,29,29	1.40	4 (14%)	43,45,45	1.83	10 (23%)
3	ADP	D	402	2	28,29,29	1.39	4 (14%)	43,45,45	1.81	10 (23%)
3	ADP	C	402	2	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)
3	ADP	E	402	2	28,29,29	1.40	4 (14%)	43,45,45	1.83	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	402	2	-	3/16/32/32	0/3/3/3
3	ADP	F	402	2	-	3/16/32/32	0/3/3/3
3	ADP	H	402	2	-	3/16/32/32	0/3/3/3
3	ADP	G	402	2	-	3/16/32/32	0/3/3/3
3	ADP	B	402	2	-	3/16/32/32	0/3/3/3
3	ADP	D	402	2	-	3/16/32/32	0/3/3/3
3	ADP	C	402	2	-	3/16/32/32	0/3/3/3
3	ADP	E	402	2	-	3/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	ADP	C5-C4	4.69	1.47	1.39
3	B	402	ADP	C5-C4	4.68	1.47	1.39
3	C	402	ADP	C5-C4	4.67	1.47	1.39
3	H	402	ADP	C5-C4	4.66	1.47	1.39
3	D	402	ADP	C5-C4	4.64	1.47	1.39
3	G	402	ADP	C5-C4	4.62	1.47	1.39
3	F	402	ADP	C5-C4	4.62	1.47	1.39
3	A	402	ADP	C5-C4	4.62	1.47	1.39
3	D	402	ADP	C5-C6	2.84	1.48	1.41
3	B	402	ADP	C5-C6	2.84	1.48	1.41
3	H	402	ADP	C5-C6	2.83	1.48	1.41
3	G	402	ADP	C5-C6	2.83	1.48	1.41
3	C	402	ADP	C5-C6	2.83	1.48	1.41
3	F	402	ADP	C5-C6	2.82	1.48	1.41
3	A	402	ADP	C5-C6	2.81	1.48	1.41
3	E	402	ADP	C5-C6	2.79	1.48	1.41
3	A	402	ADP	C8-N7	2.46	1.36	1.31
3	E	402	ADP	C8-N7	2.43	1.36	1.31
3	F	402	ADP	C8-N7	2.42	1.36	1.31
3	B	402	ADP	C8-N7	2.40	1.36	1.31
3	G	402	ADP	C8-N7	2.40	1.36	1.31
3	C	402	ADP	C8-N7	2.38	1.36	1.31
3	D	402	ADP	C8-N7	2.38	1.36	1.31
3	H	402	ADP	C8-N7	2.34	1.36	1.31
3	B	402	ADP	C5-N7	-2.24	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	ADP	C5-N7	-2.20	1.35	1.39
3	H	402	ADP	C5-N7	-2.20	1.35	1.39
3	C	402	ADP	C5-N7	-2.19	1.35	1.39
3	G	402	ADP	C5-N7	-2.18	1.35	1.39
3	E	402	ADP	C5-N7	-2.16	1.35	1.39
3	F	402	ADP	C5-N7	-2.16	1.35	1.39
3	A	402	ADP	C5-N7	-2.11	1.35	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ADP	C5-C4-N3	-5.72	118.84	126.72
3	C	402	ADP	C5-C4-N3	-5.70	118.87	126.72
3	H	402	ADP	C5-C4-N3	-5.69	118.88	126.72
3	E	402	ADP	C5-C4-N3	-5.68	118.89	126.72
3	G	402	ADP	C5-C4-N3	-5.68	118.89	126.72
3	B	402	ADP	C5-C4-N3	-5.66	118.92	126.72
3	F	402	ADP	C5-C4-N3	-5.65	118.93	126.72
3	D	402	ADP	C5-C4-N3	-5.64	118.96	126.72
3	B	402	ADP	N3-C4-N9	4.38	134.61	127.17
3	C	402	ADP	N3-C4-N9	4.36	134.59	127.17
3	G	402	ADP	N3-C4-N9	4.36	134.59	127.17
3	F	402	ADP	N3-C4-N9	4.36	134.58	127.17
3	E	402	ADP	N3-C4-N9	4.35	134.56	127.17
3	H	402	ADP	N3-C4-N9	4.33	134.54	127.17
3	D	402	ADP	N3-C4-N9	4.33	134.54	127.17
3	A	402	ADP	N3-C4-N9	4.32	134.51	127.17
3	A	402	ADP	C4-C5-N7	-3.86	106.17	110.58
3	E	402	ADP	C4-C5-N7	-3.86	106.17	110.58
3	H	402	ADP	C4-C5-N7	-3.84	106.19	110.58
3	C	402	ADP	C4-C5-N7	-3.83	106.20	110.58
3	G	402	ADP	C4-C5-N7	-3.78	106.26	110.58
3	D	402	ADP	C4-C5-N7	-3.76	106.28	110.58
3	B	402	ADP	C4-C5-N7	-3.76	106.29	110.58
3	F	402	ADP	C4-C5-N7	-3.72	106.33	110.58
3	B	402	ADP	C2-N3-C4	3.60	120.63	111.83
3	G	402	ADP	C2-N3-C4	3.60	120.61	111.83
3	F	402	ADP	C2-N3-C4	3.58	120.57	111.83
3	A	402	ADP	C2-N3-C4	3.57	120.55	111.83
3	H	402	ADP	C2-N3-C4	3.56	120.53	111.83
3	D	402	ADP	C2-N3-C4	3.56	120.52	111.83
3	E	402	ADP	C2-N3-C4	3.55	120.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	ADP	C2-N3-C4	3.53	120.46	111.83
3	B	402	ADP	N3-C2-N1	-3.05	123.96	128.58
3	G	402	ADP	N3-C2-N1	-3.05	123.97	128.58
3	F	402	ADP	N3-C2-N1	-3.02	124.02	128.58
3	D	402	ADP	N3-C2-N1	-2.99	124.06	128.58
3	A	402	ADP	N3-C2-N1	-2.97	124.08	128.58
3	E	402	ADP	N3-C2-N1	-2.97	124.09	128.58
3	H	402	ADP	N3-C2-N1	-2.95	124.12	128.58
3	H	402	ADP	C5-N7-C8	2.88	107.97	103.45
3	C	402	ADP	N3-C2-N1	-2.87	124.24	128.58
3	E	402	ADP	C5-N7-C8	2.85	107.94	103.45
3	C	402	ADP	C5-N7-C8	2.84	107.92	103.45
3	B	402	ADP	C5-N7-C8	2.84	107.91	103.45
3	G	402	ADP	C5-N7-C8	2.83	107.90	103.45
3	D	402	ADP	C5-N7-C8	2.81	107.87	103.45
3	A	402	ADP	C5-N7-C8	2.80	107.86	103.45
3	E	402	ADP	C4-N9-C8	2.80	108.68	105.74
3	B	402	ADP	C4-N9-C8	2.79	108.67	105.74
3	F	402	ADP	C5-N7-C8	2.76	107.79	103.45
3	G	402	ADP	C4-N9-C8	2.75	108.63	105.74
3	C	402	ADP	C4-N9-C8	2.74	108.61	105.74
3	F	402	ADP	C4-N9-C8	2.73	108.61	105.74
3	A	402	ADP	C4-N9-C8	2.72	108.59	105.74
3	D	402	ADP	C4-N9-C8	2.71	108.59	105.74
3	H	402	ADP	C4-N9-C8	2.70	108.58	105.74
3	E	402	ADP	C6-C5-N7	2.31	136.54	132.09
3	E	402	ADP	N9-C8-N7	-2.30	110.67	113.94
3	B	402	ADP	N9-C8-N7	-2.30	110.67	113.94
3	H	402	ADP	N9-C8-N7	-2.29	110.69	113.94
3	H	402	ADP	C6-C5-N7	2.29	136.50	132.09
3	G	402	ADP	N9-C8-N7	-2.28	110.70	113.94
3	C	402	ADP	C6-C5-N7	2.27	136.47	132.09
3	A	402	ADP	N9-C8-N7	-2.26	110.73	113.94
3	B	402	ADP	C6-C5-N7	2.26	136.44	132.09
3	C	402	ADP	N9-C8-N7	-2.26	110.74	113.94
3	D	402	ADP	C6-C5-N7	2.24	136.41	132.09
3	D	402	ADP	N9-C8-N7	-2.24	110.76	113.94
3	A	402	ADP	C6-C5-N7	2.22	136.37	132.09
3	F	402	ADP	N9-C8-N7	-2.22	110.79	113.94
3	G	402	ADP	C6-C5-N7	2.21	136.35	132.09
3	F	402	ADP	C6-C5-N7	2.20	136.34	132.09
3	G	402	ADP	C3'-C2'-C1'	2.20	105.62	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	ADP	C3'-C2'-C1'	2.19	105.60	101.46
3	A	402	ADP	C3'-C2'-C1'	2.17	105.58	101.46
3	D	402	ADP	C3'-C2'-C1'	2.16	105.56	101.46
3	B	402	ADP	C3'-C2'-C1'	2.16	105.55	101.46
3	C	402	ADP	C3'-C2'-C1'	2.16	105.55	101.46
3	F	402	ADP	C3'-C2'-C1'	2.15	105.53	101.46
3	H	402	ADP	C3'-C2'-C1'	2.15	105.53	101.46

There are no chirality outliers.

All (24) torsion outliers are listed below:

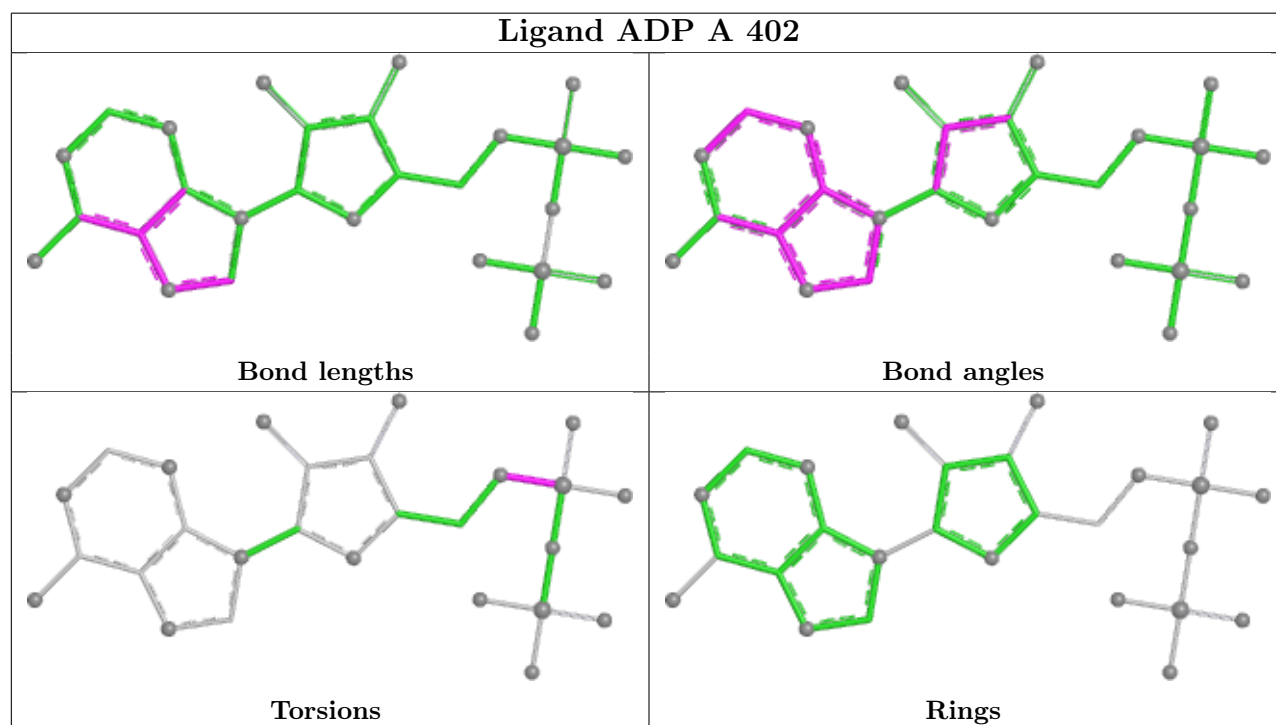
Mol	Chain	Res	Type	Atoms
3	A	402	ADP	C5'-O5'-PA-O1A
3	A	402	ADP	C5'-O5'-PA-O2A
3	A	402	ADP	C5'-O5'-PA-O3A
3	B	402	ADP	C5'-O5'-PA-O1A
3	B	402	ADP	C5'-O5'-PA-O2A
3	B	402	ADP	C5'-O5'-PA-O3A
3	C	402	ADP	C5'-O5'-PA-O1A
3	C	402	ADP	C5'-O5'-PA-O2A
3	C	402	ADP	C5'-O5'-PA-O3A
3	D	402	ADP	C5'-O5'-PA-O1A
3	D	402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

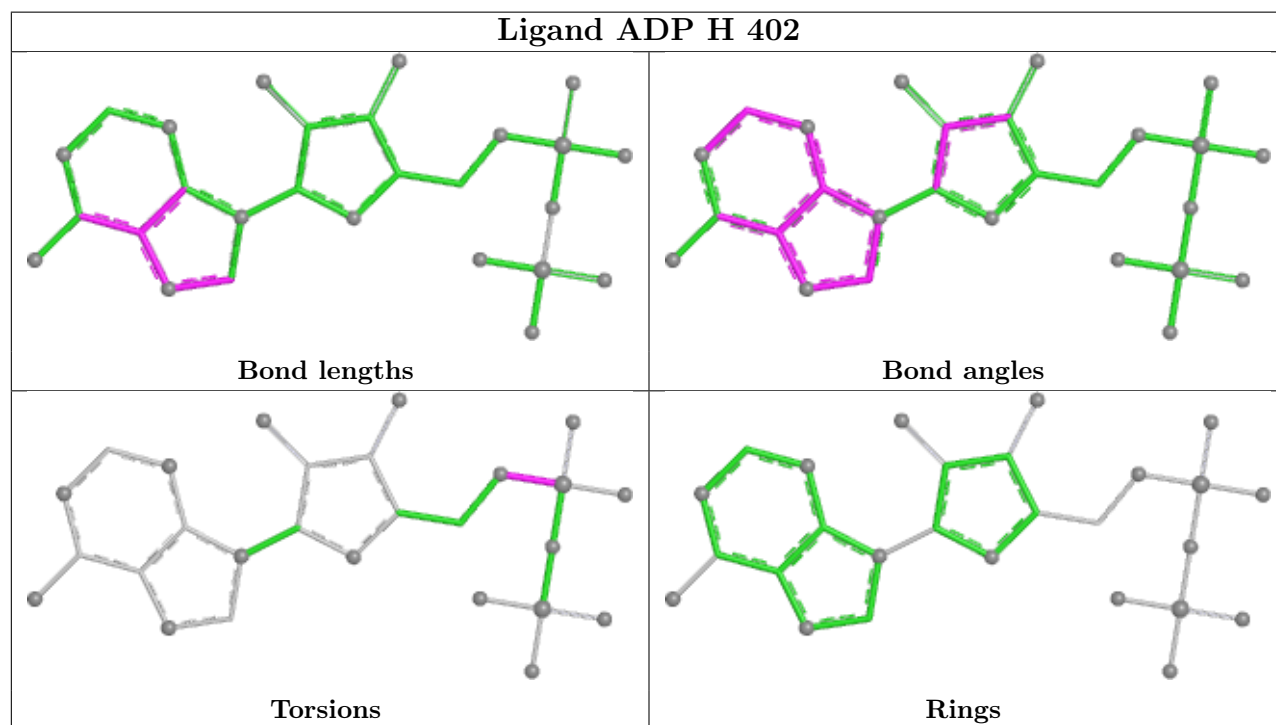
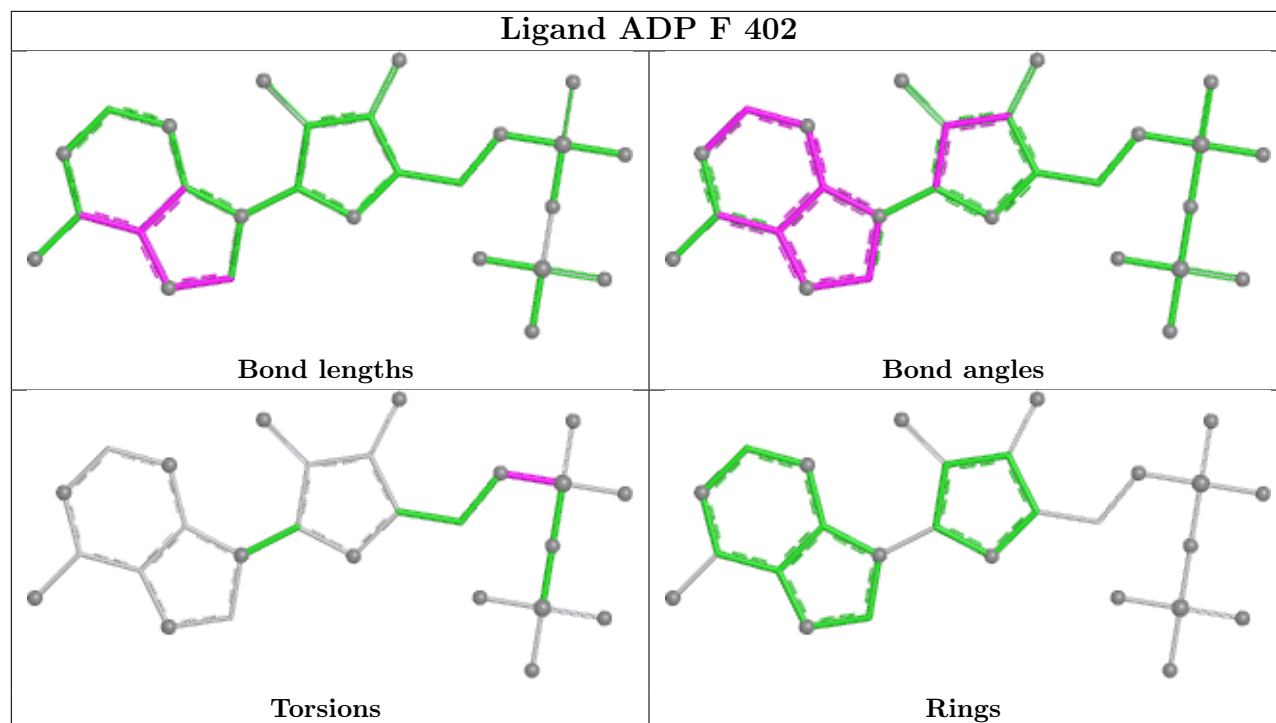
There are no ring outliers.

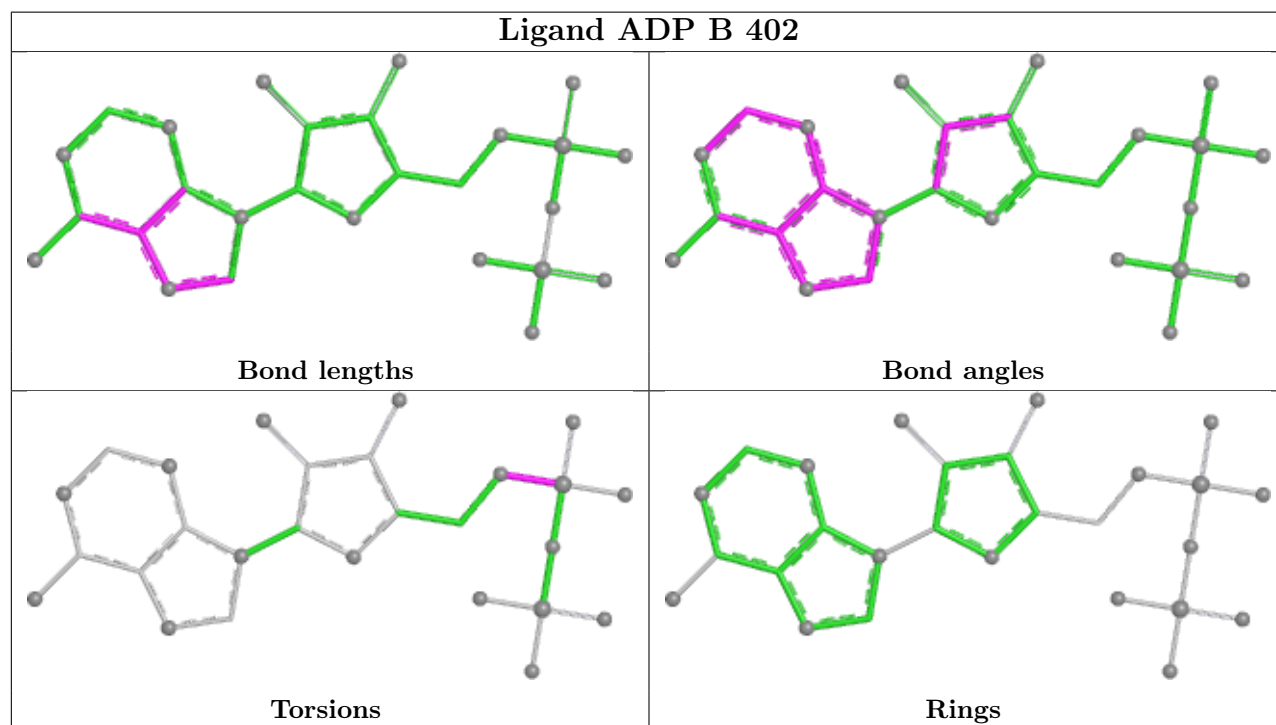
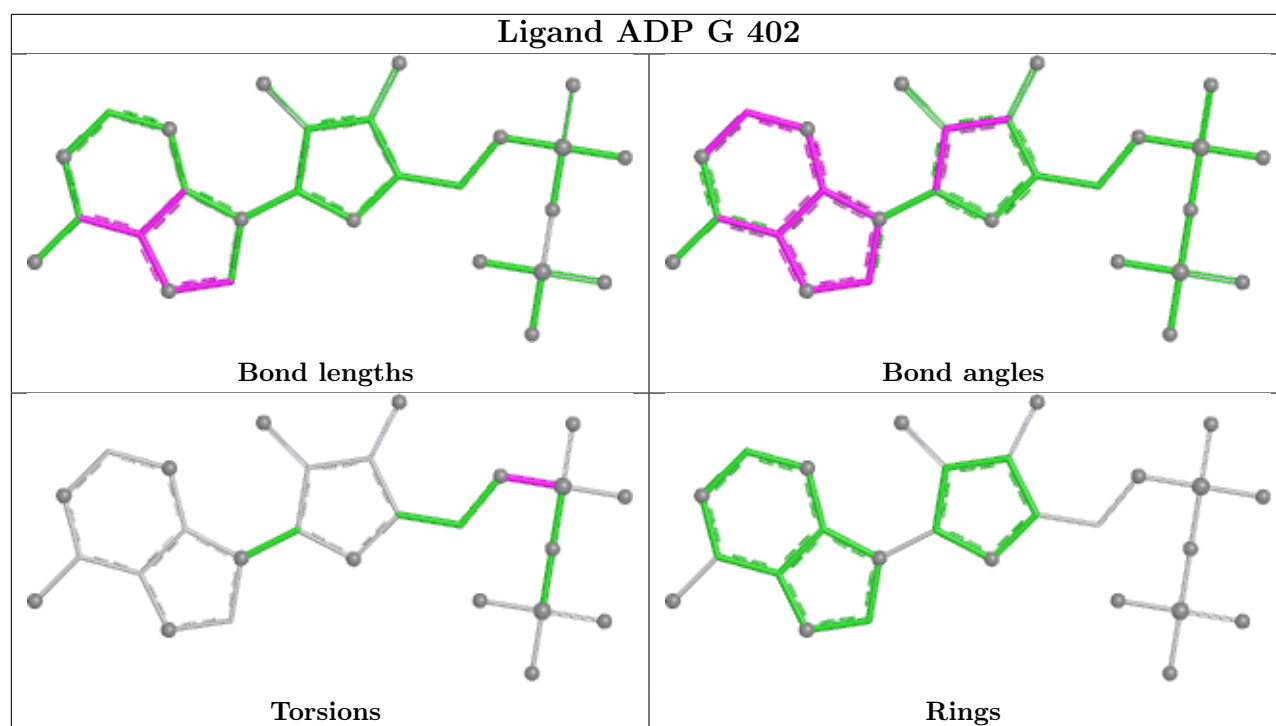
1 monomer is involved in 1 short contact:

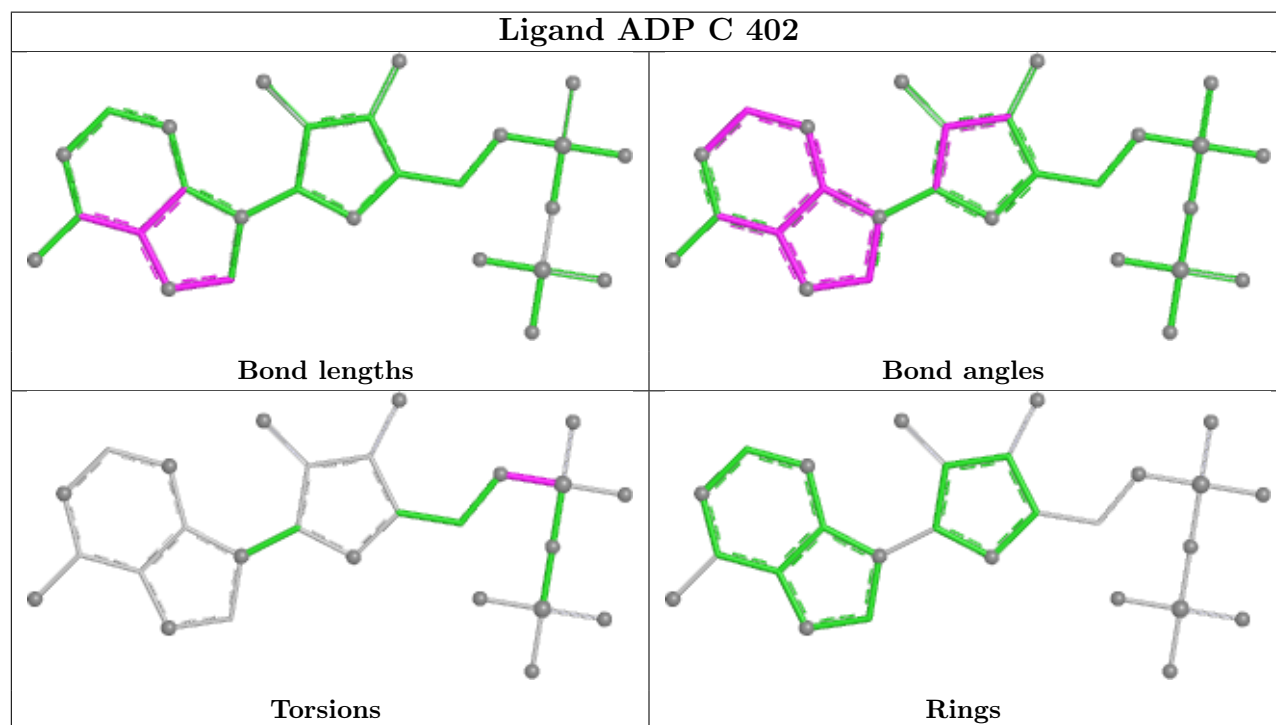
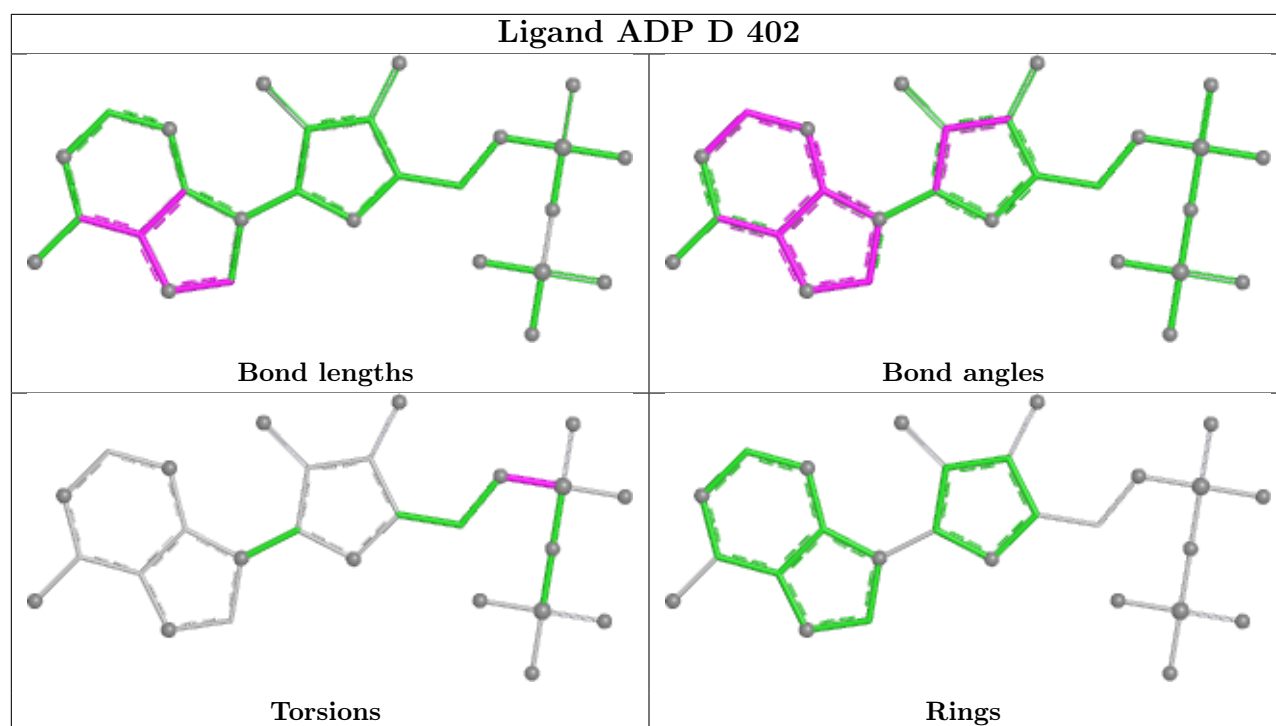
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	ADP	1	0

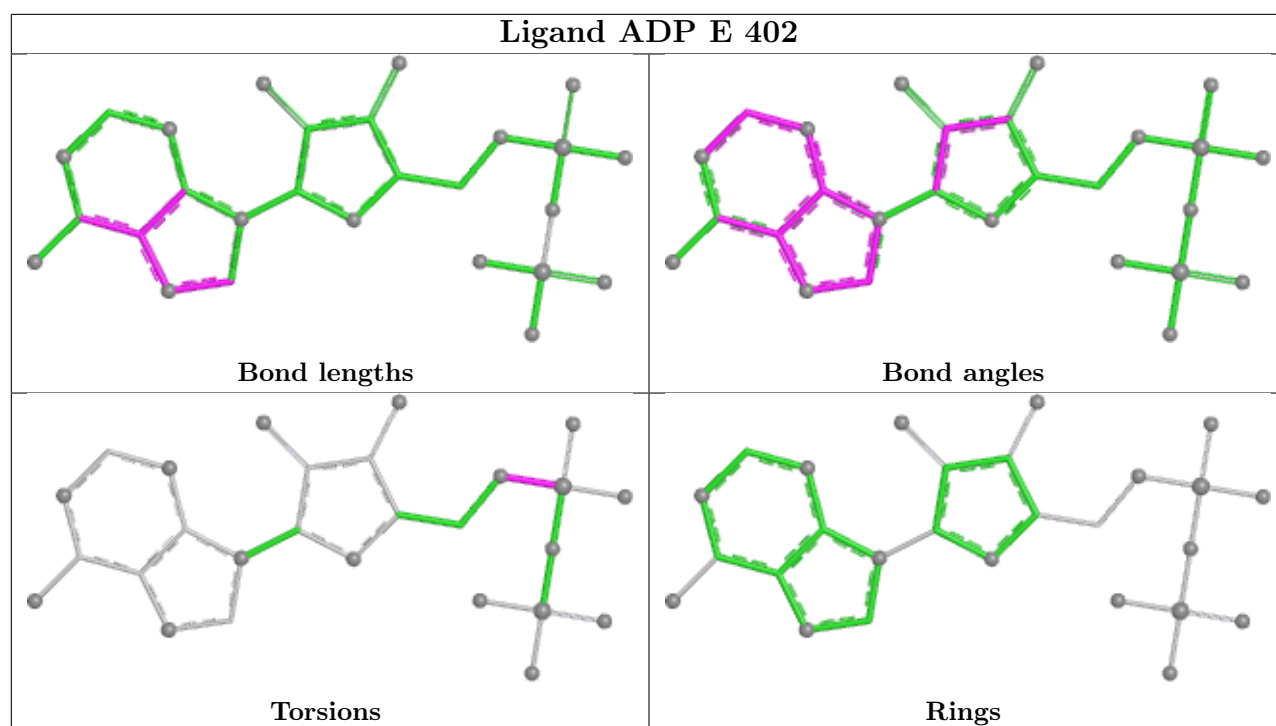
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

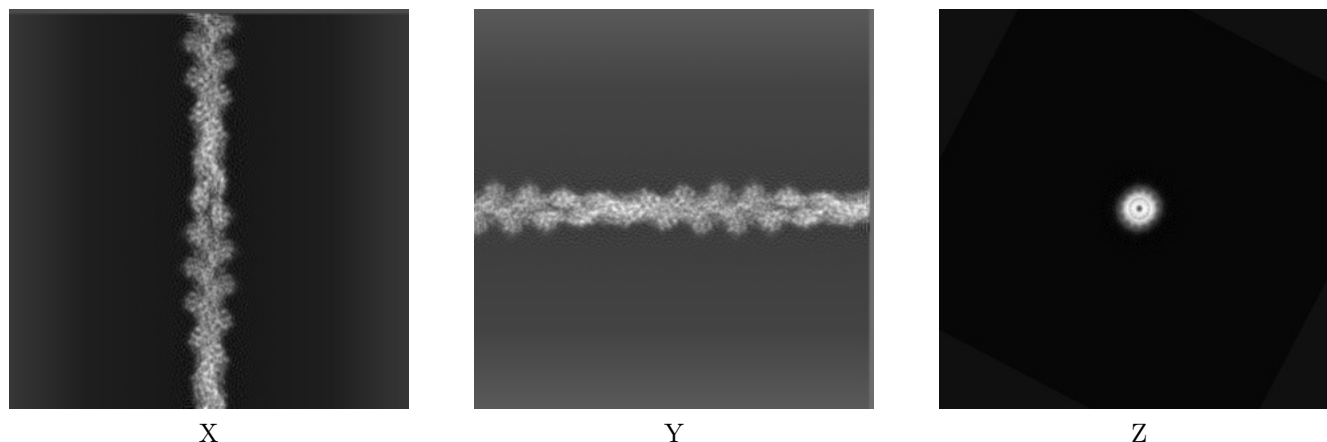
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7115. These allow visual inspection of the internal detail of the map and identification of artifacts.

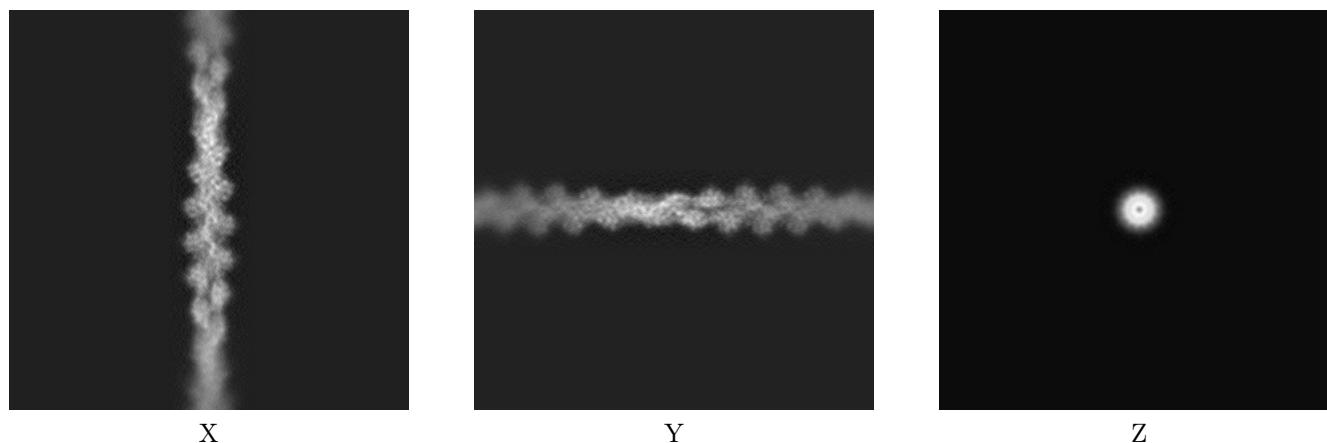
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



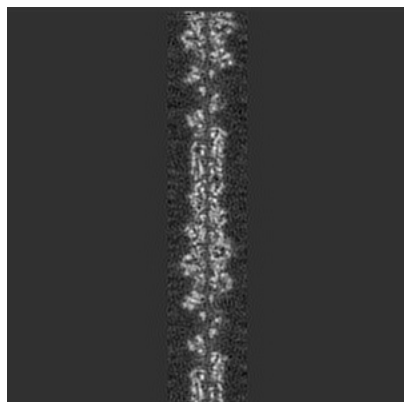
6.1.2 Raw map



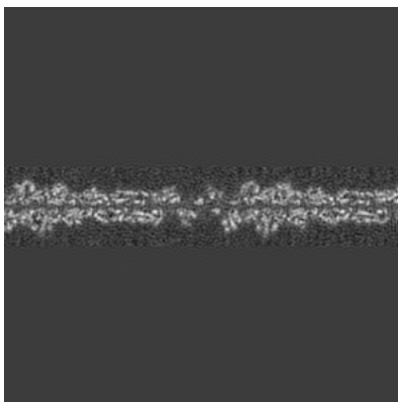
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

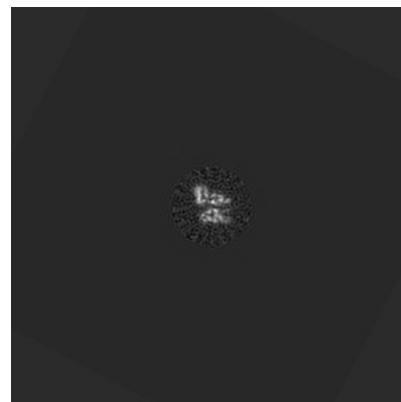
6.2.1 Primary map



X Index: 256

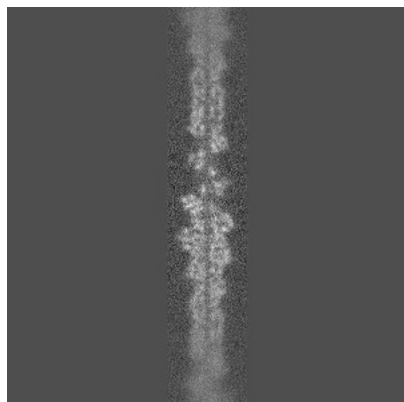


Y Index: 256

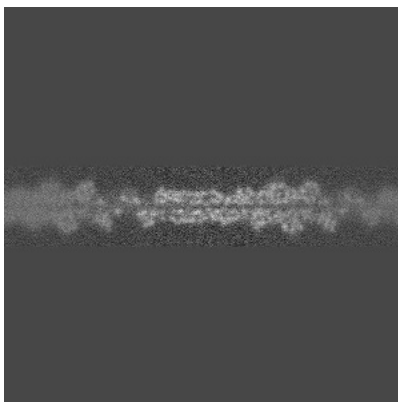


Z Index: 256

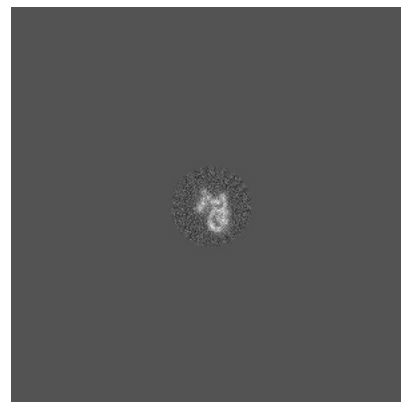
6.2.2 Raw map



X Index: 256



Y Index: 256

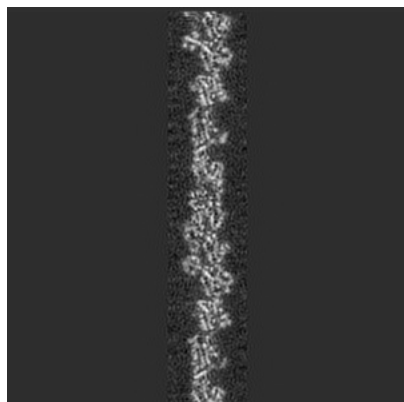


Z Index: 256

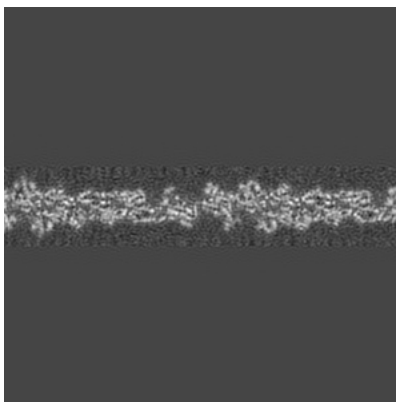
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

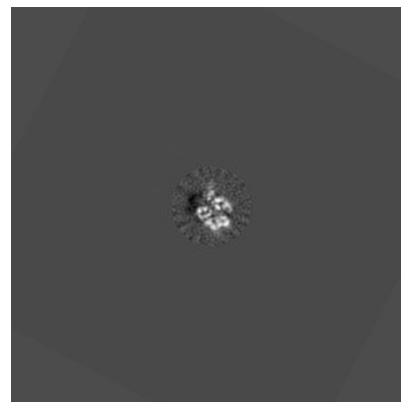
6.3.1 Primary map



X Index: 262

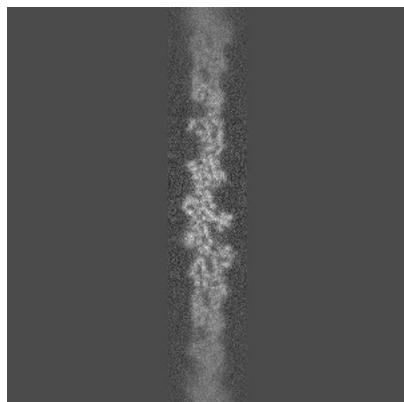


Y Index: 252

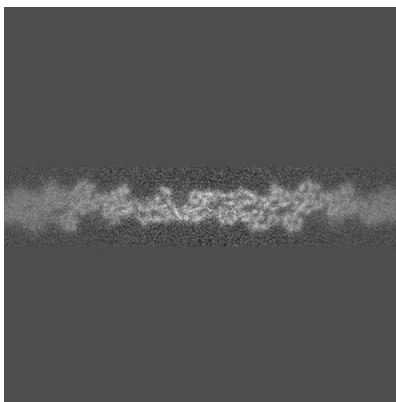


Z Index: 505

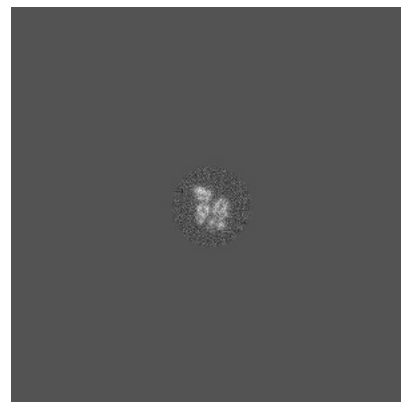
6.3.2 Raw map



X Index: 263



Y Index: 262

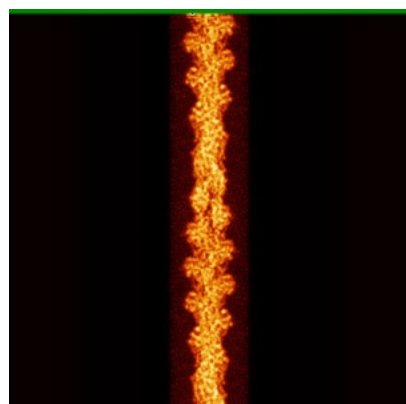


Z Index: 270

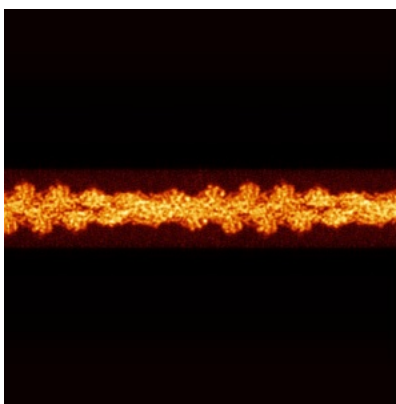
The images above show the largest variance slices of the map in three orthogonal directions.

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

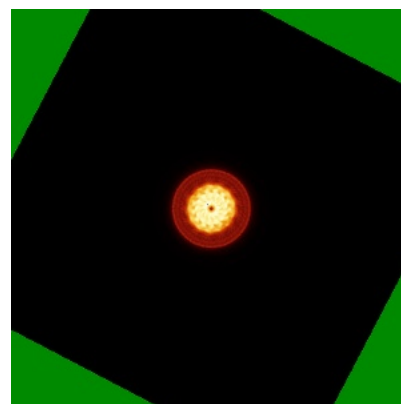
6.4.1 Primary map



X

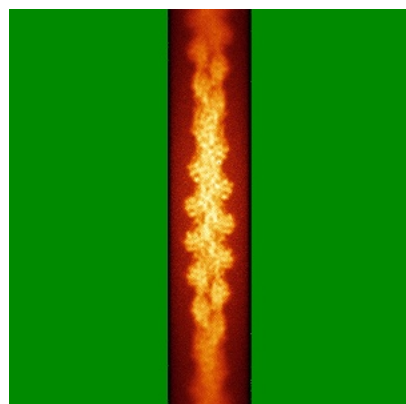


Y

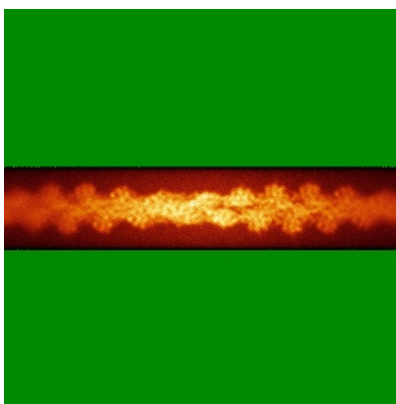


Z

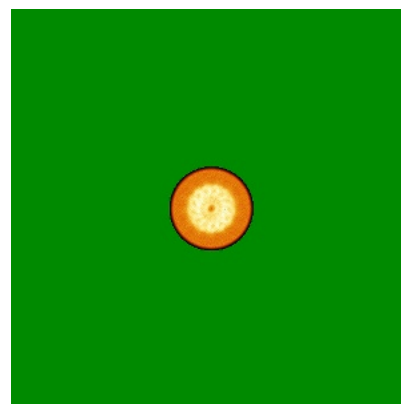
6.4.2 Raw map



X



Y

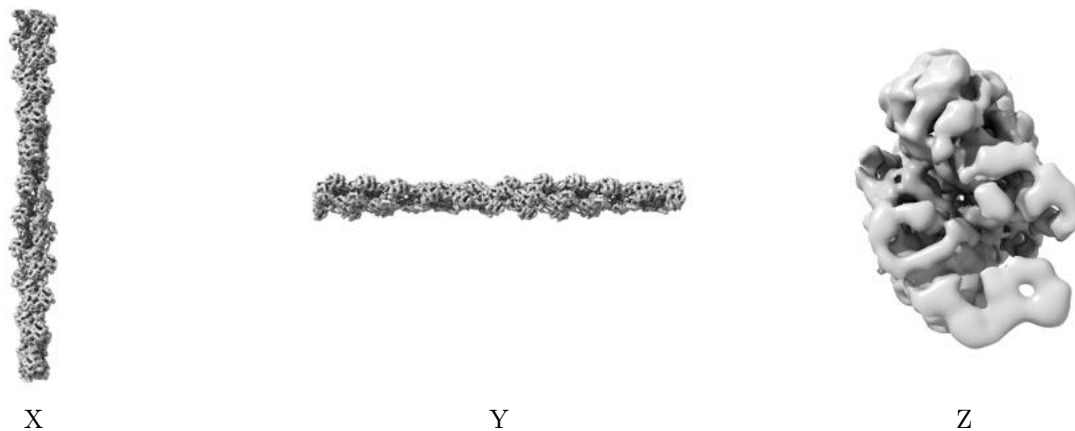


Z

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

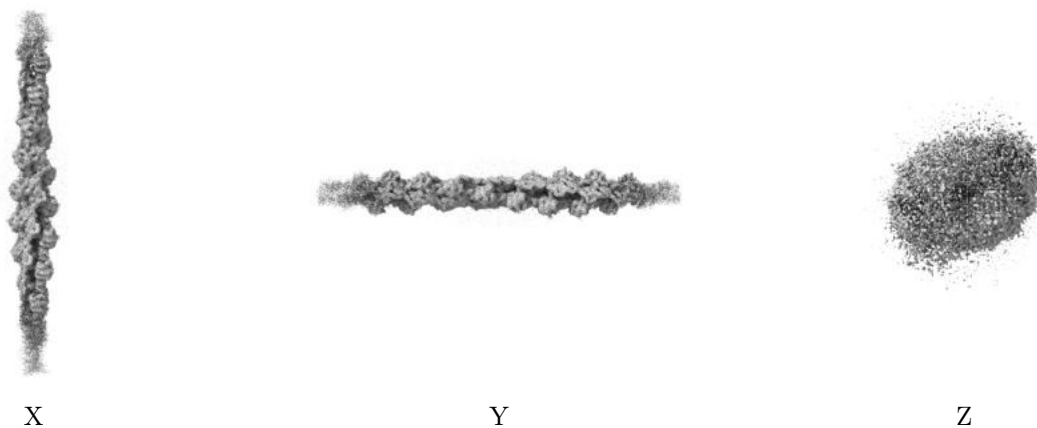
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 12.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

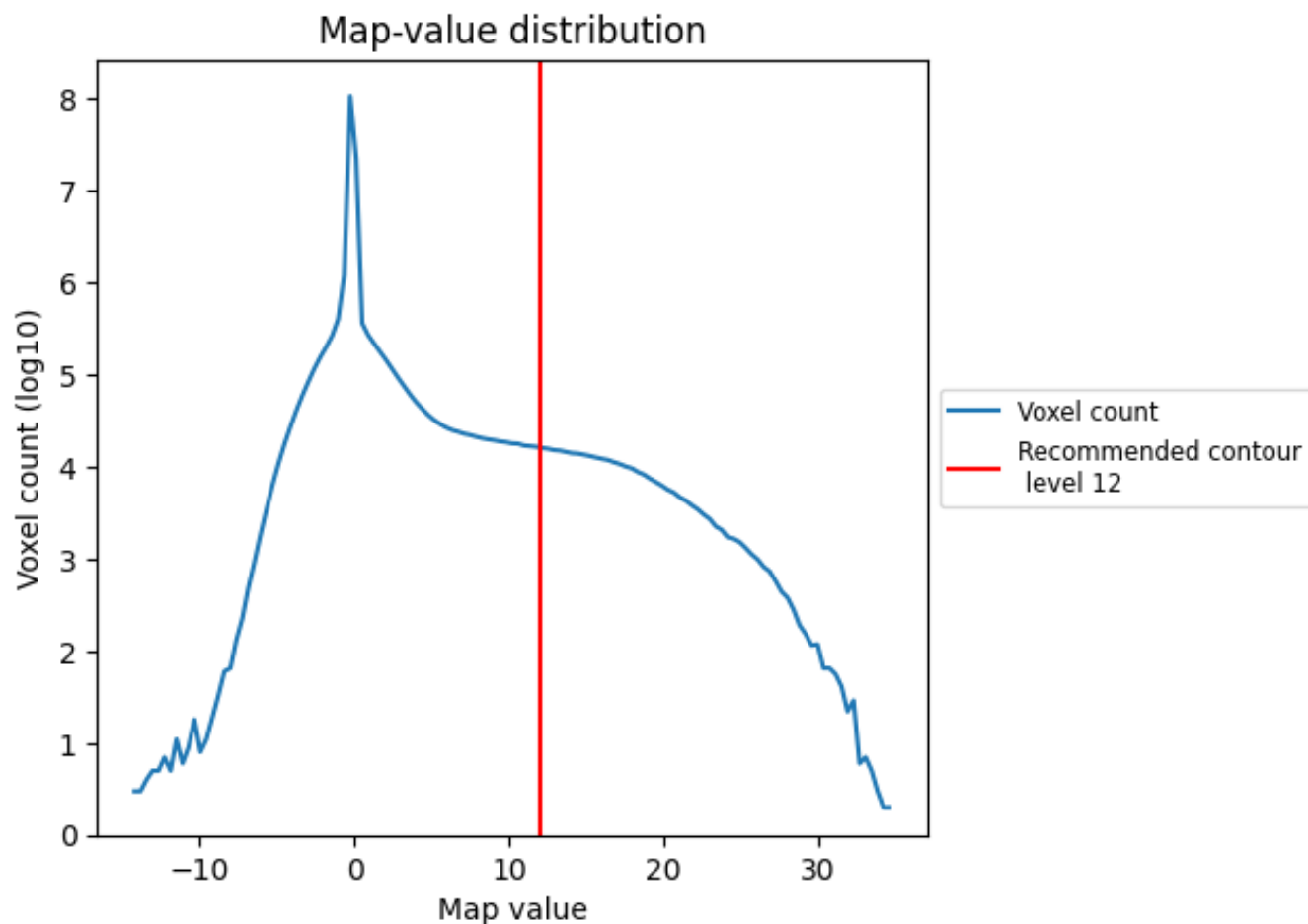
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

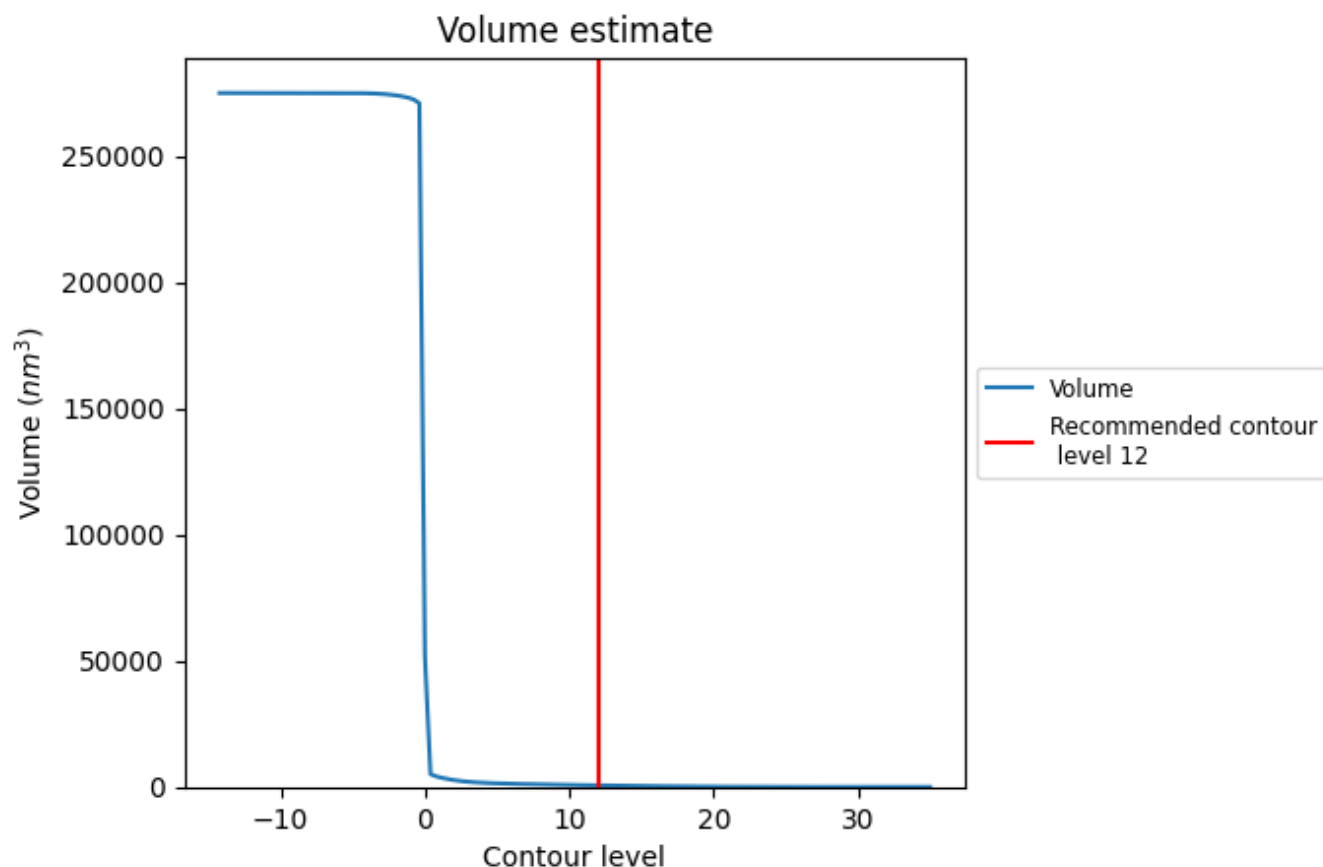
This section contains the results of statistical analysis of the map.

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.

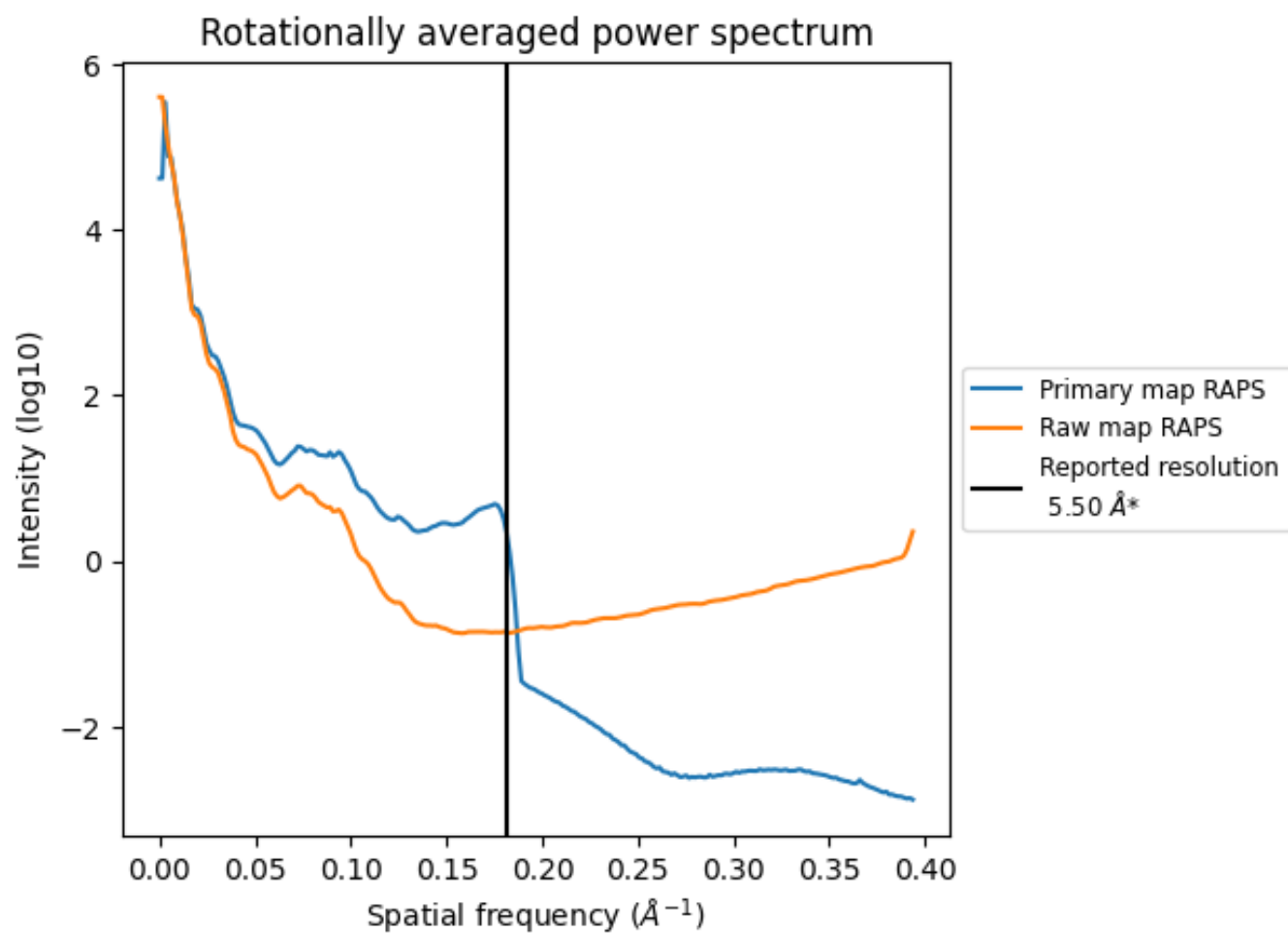
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 620 nm^3 ; this corresponds to an approximate mass of 560 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 [i](#)

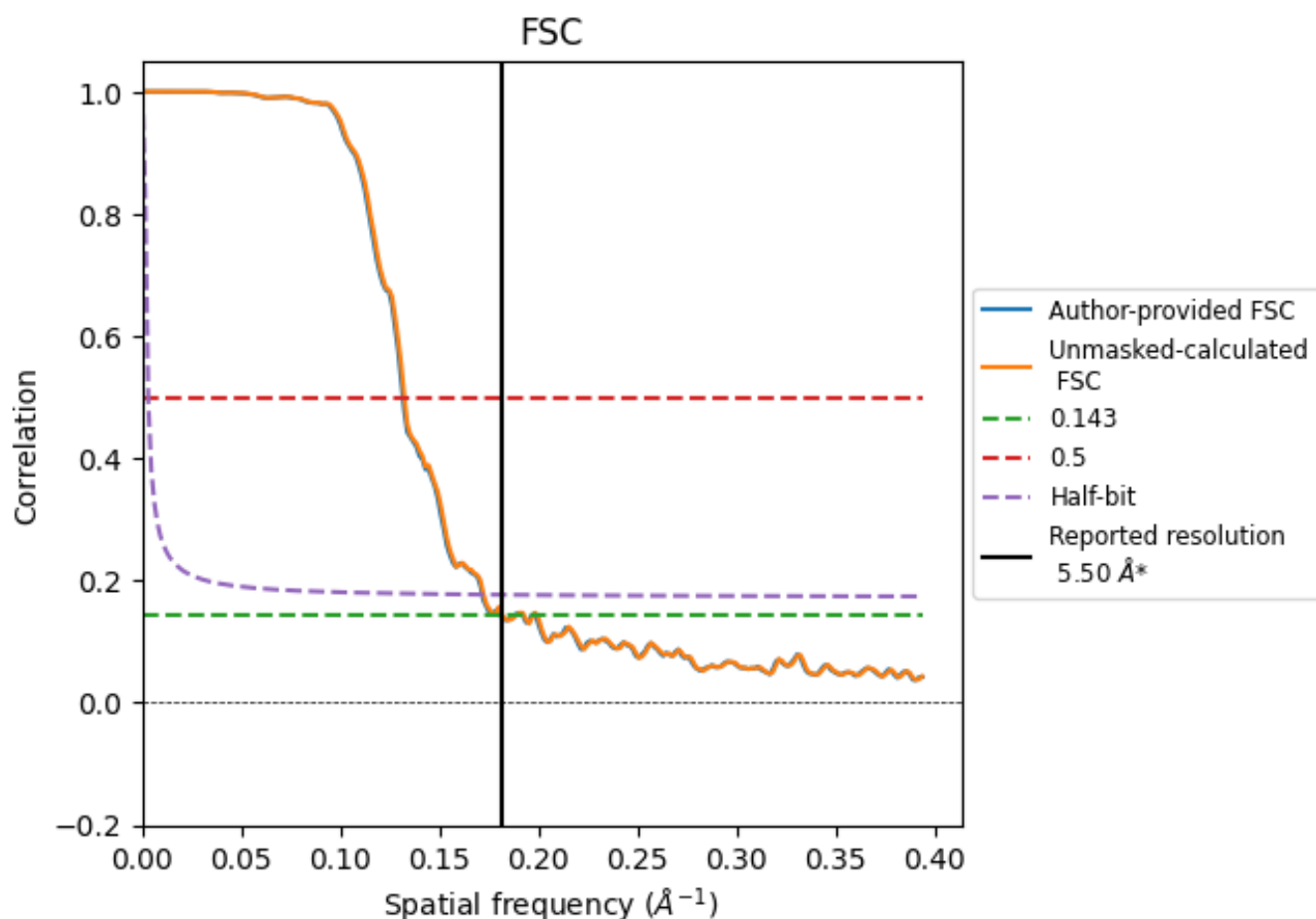


*Reported resolution corresponds to spatial frequency of $0.182 \text{ \AA}^{-1}$

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](#)

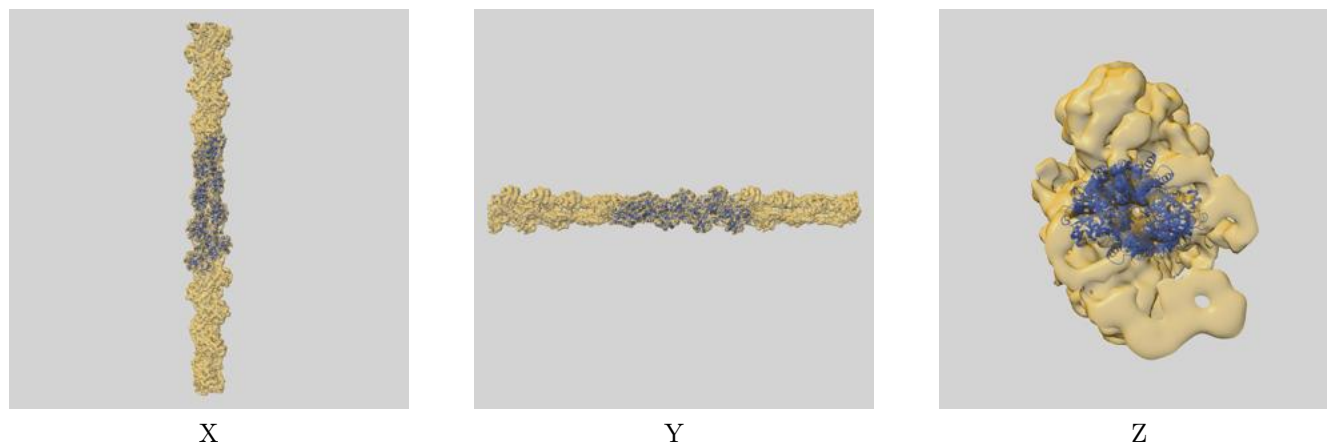
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.52	7.60	5.82
Unmasked-calculated*	5.50	7.56	5.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

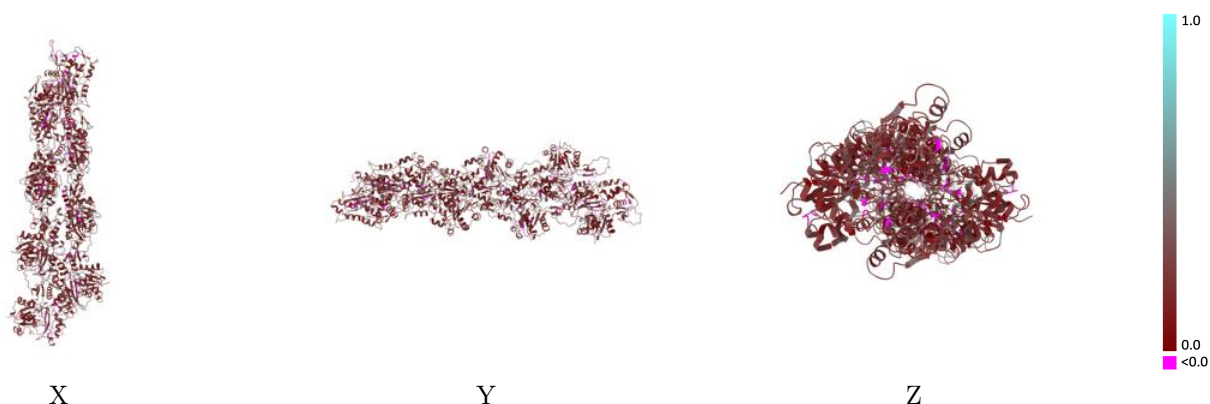
This section contains information regarding the fit between EMDB map EMD-7115 and PDB model 6BNO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



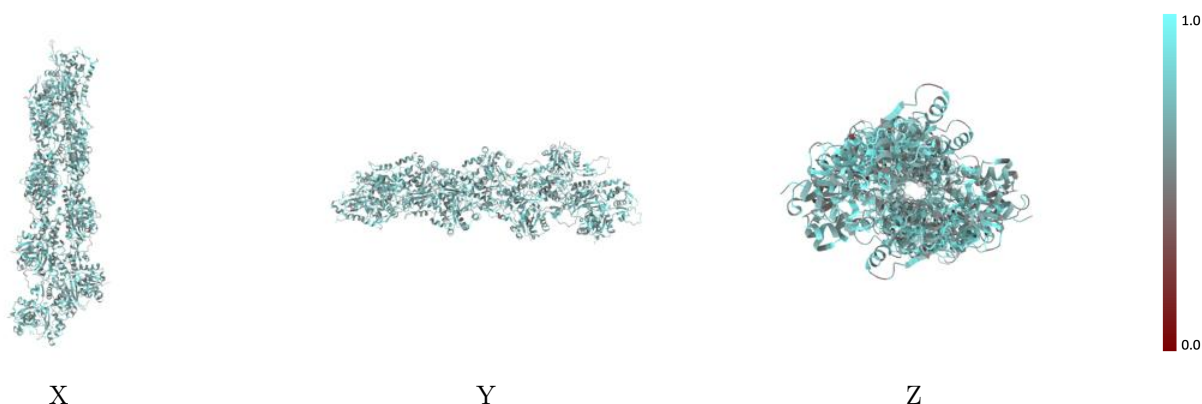
The images above show the 3D surface view of the map at the recommended contour level 12.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



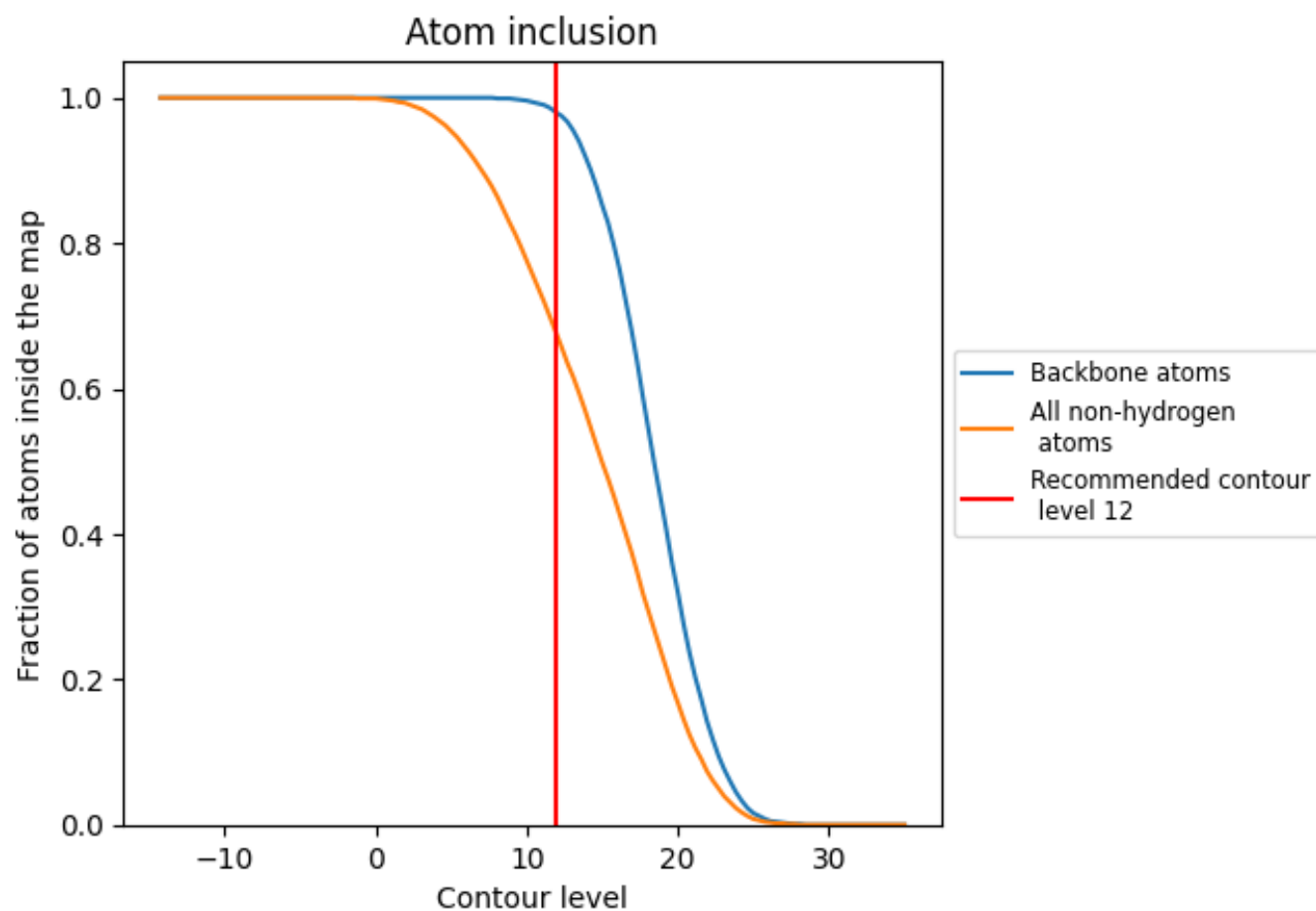
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 67% 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 (12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6740	0.2110
A	0.6730	0.2070
B	0.6660	0.2070
C	0.6720	0.2120
D	0.6800	0.2180
E	0.6740	0.2110
F	0.6740	0.2100
G	0.6760	0.2090
H	0.6770	0.2100

1.0

0.0

<0.0