



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:59 PM UTC

PDB ID : 7PDZ / pdb_00007pdz
EMDB ID : EMD-13343
Title : Structure of capping protein bound to the barbed end of a cytoplasmic actin filament
Authors : Funk, J.; Merino, F.; Schacks, M.; Rottner, K.; Raunser, S.; Bieling, P.
Deposited on : 2021-08-09
Resolution : 3.80 Å(reported)
Based on initial model : 5ADX

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:

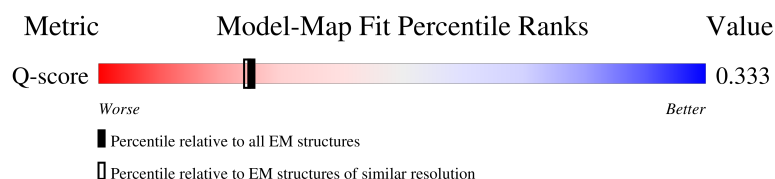
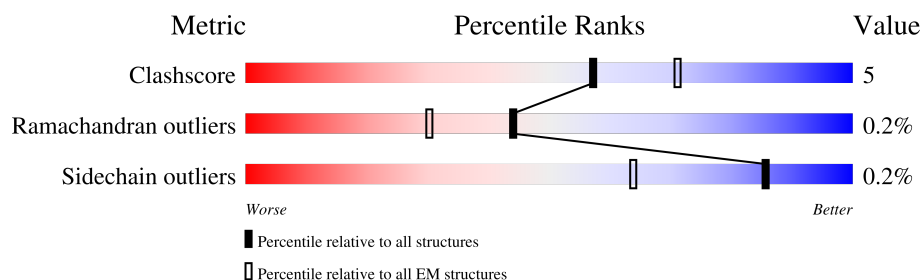
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

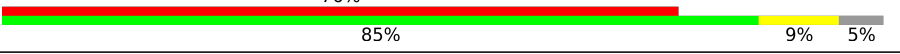
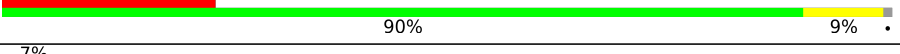
The reported resolution of this entry is 3.80 Å.

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.



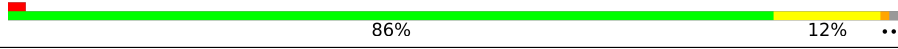
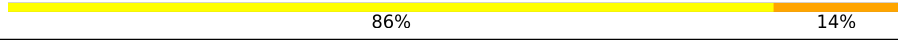
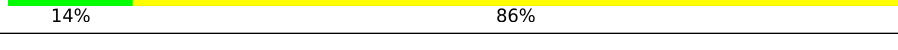
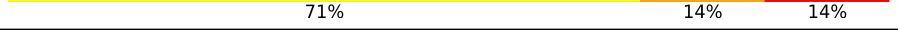
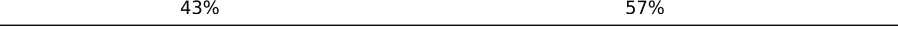
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	E	272	 82% 90% 10%
2	F	286	 76% 85% 9% 5%
3	I	375	 24% 90% 9% .
3	J	375	 7% 90% 8% ..

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Mol	Chain	Length	Quality of chain
3	K	375	
3	L	375	
3	N	375	
3	O	375	
4	P	7	
4	Q	7	
4	R	7	
4	S	7	
4	T	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTH	P	6	-	X	-	-
4	DTH	Q	6	-	X	-	-
4	EEP	R	4	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22185 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 Isoform 2 of F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	272	Total	C	N	O	S	0	0
			2146	1336	374	423	13		

- Molecule 2 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	272	Total	C	N	O	S	0	0
			2212	1396	384	427	5		

- Molecule 3 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	371	Total	C	N	O	S	0	0
			2894	1834	487	551	22		
3	J	371	Total	C	N	O	S	0	0
			2894	1834	487	551	22		
3	K	371	Total	C	N	O	S	0	0
			2894	1834	487	551	22		
3	L	371	Total	C	N	O	S	0	0
			2894	1834	487	551	22		
3	N	371	Total	C	N	O	S	0	0
			2894	1834	487	551	22		
3	O	371	Total	C	N	O	S	0	0
			2894	1834	487	551	22		

- Molecule 4 is a protein called Phalloidin.

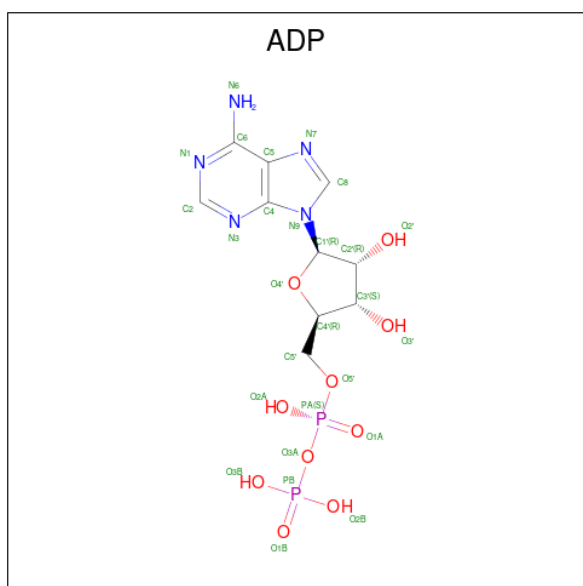
Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
4	R	7	Total	C	N	O	S	0	0
			55	35	8	11	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
4	T	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
4	P	7	Total	C	N	O	S	0	0
			55	35	8	11	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

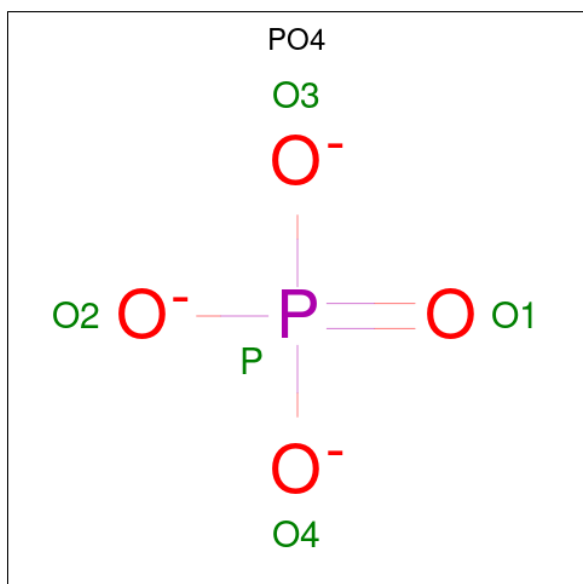


Mol	Chain	Residues	Atoms					AltConf
5	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	I	1	Total	Mg	0
			1	1	
6	J	1	Total	Mg	0
			1	1	
6	K	1	Total	Mg	0
			1	1	
6	L	1	Total	Mg	0
			1	1	
6	N	1	Total	Mg	0
			1	1	
6	O	1	Total	Mg	0
			1	1	

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

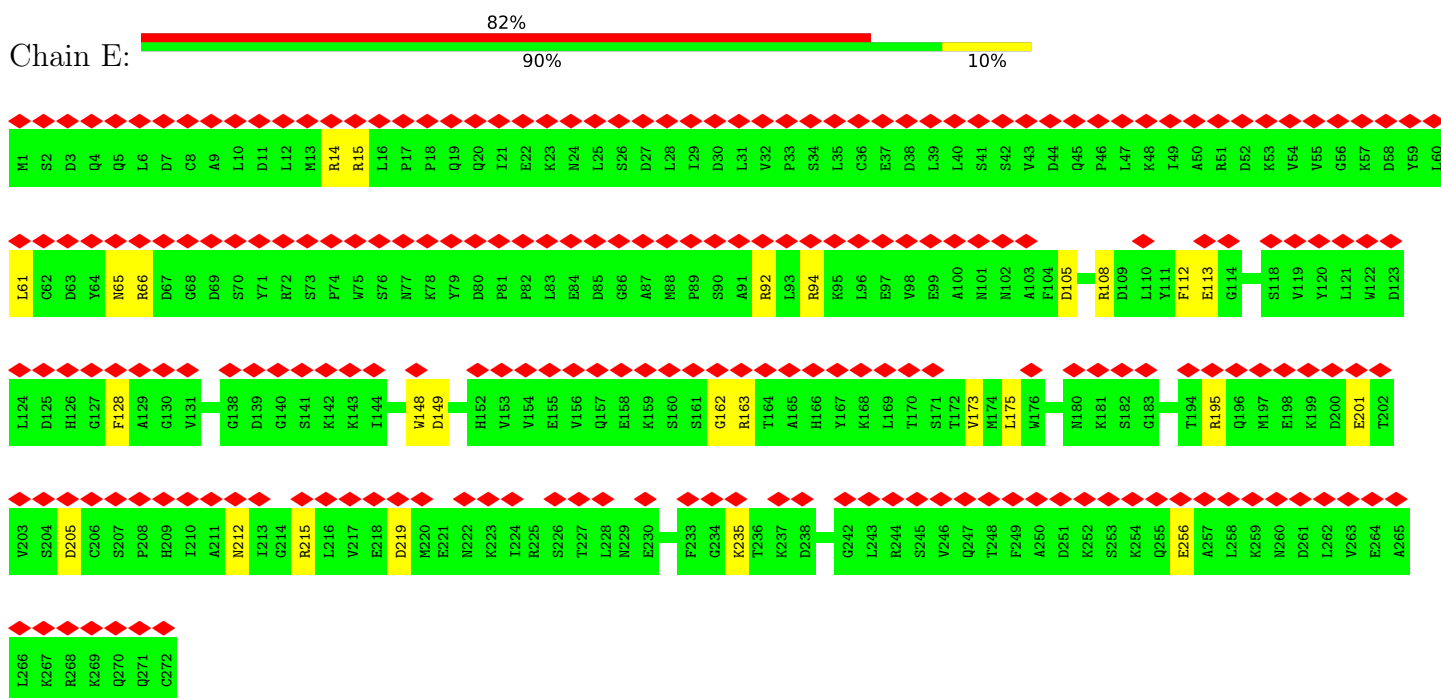


Mol	Chain	Residues	Atoms			AltConf
7	K	1	Total	O	P	0
			5	4	1	
7	L	1	Total	O	P	0
			5	4	1	
7	N	1	Total	O	P	0
			5	4	1	
7	O	1	Total	O	P	0
			5	4	1	

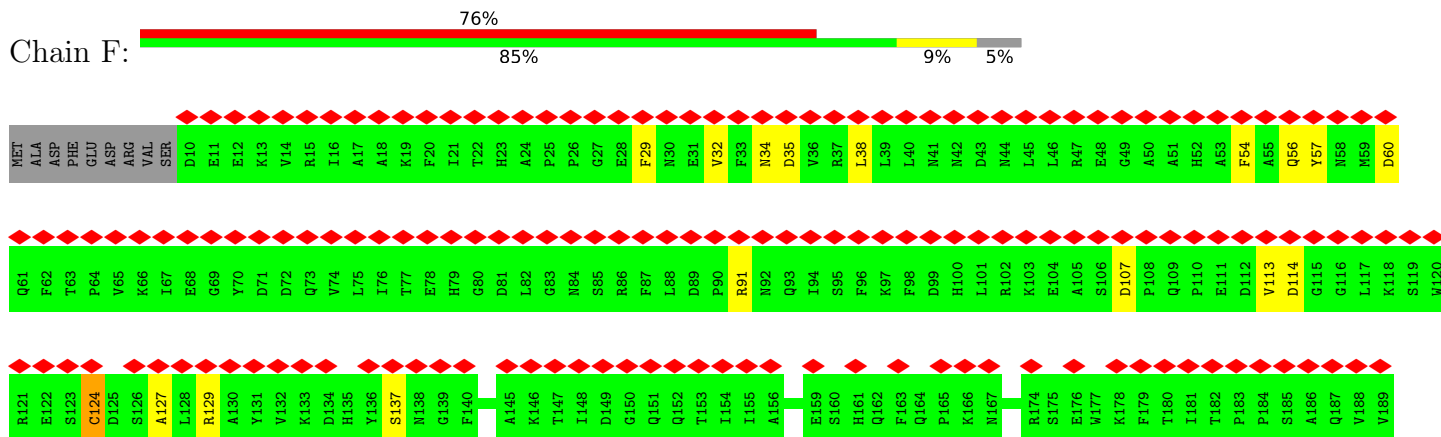
3 Residue-property plots

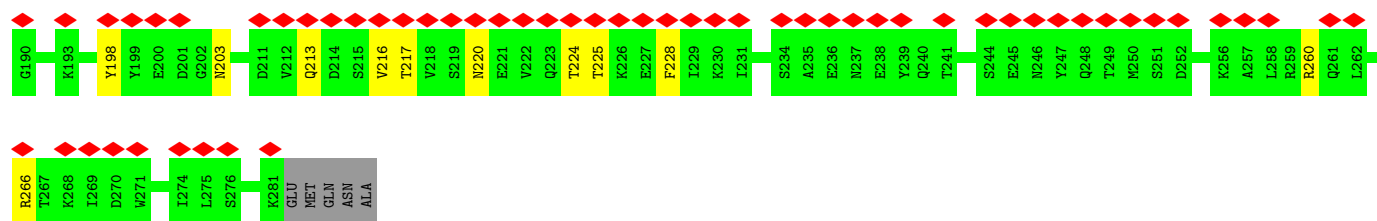
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Isoform 2 of F-actin-capping protein subunit beta

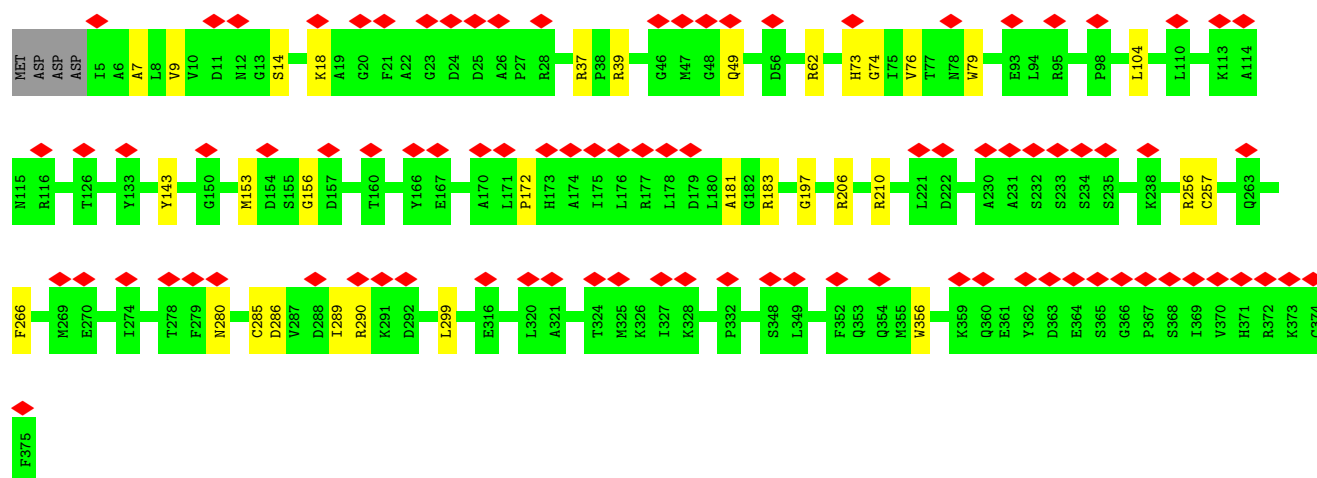
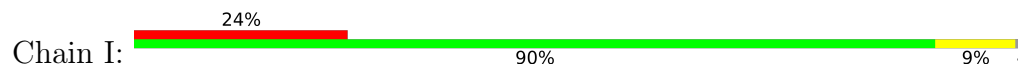


- Molecule 2: F-actin-capping protein subunit alpha-1

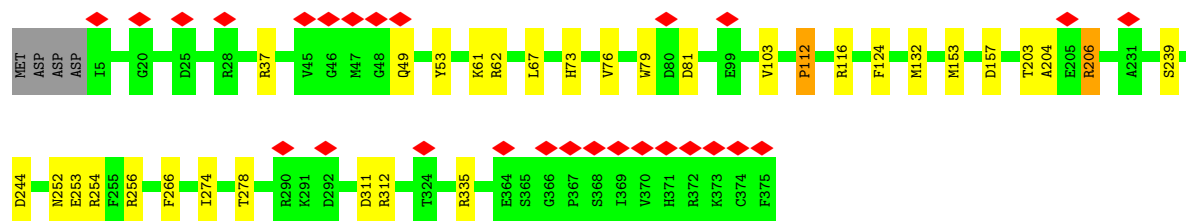
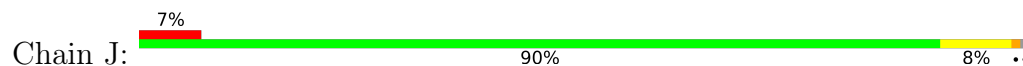




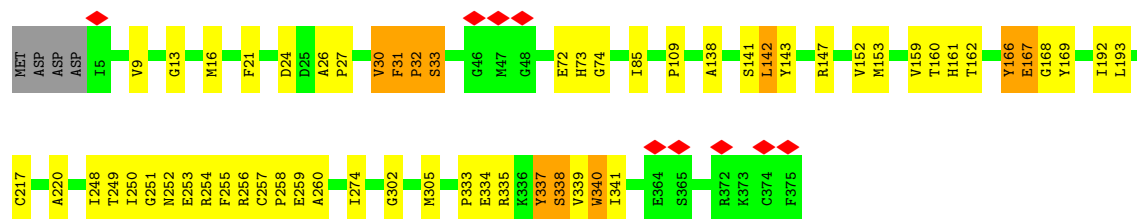
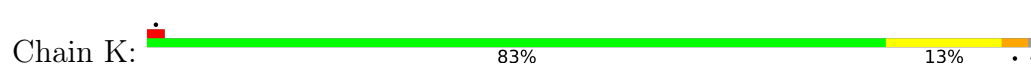
- Molecule 3: Actin, cytoplasmic 1



- Molecule 3: Actin, cytoplasmic 1



- Molecule 3: Actin, cytoplasmic 1



- Molecule 3: Actin, cytoplasmic 1

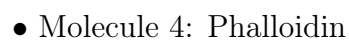
Response	Percentage
Good job	89%
Not doing a good job	9%



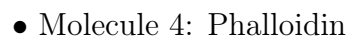
Response	Percentage
Doing a good job	86%
Not doing a good job	12%



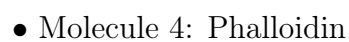
Response	Percentage
Yes	89%
No	10%



Response	Percentage
Yes, more action	43%
No, not more action	43%
Don't know	14%



Satisfaction Level	Percentage
Very satisfied	14%
Satisfied	86%

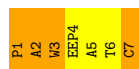


Category	Percentage
Very bad	71%
Bad	14%
Good	14%



- Molecule 4: Phalloidin

Chain T:  43% 57%



- Molecule 4: Phalloidin

Chain P:  86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.045	Depositor
Map size ($\text{\AA}$)	464.64, 464.64, 464.64	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.21, 1.21, 1.21	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HIC, ADP, EEP, MG, HYP, PO4, DTH

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	E	1.25	16/2180 (0.7%)	1.48	13/2936 (0.4%)
2	F	1.15	8/2263 (0.4%)	1.54	12/3066 (0.4%)
3	I	1.22	17/2944 (0.6%)	1.40	10/3984 (0.3%)
3	J	1.23	16/2944 (0.5%)	1.37	14/3984 (0.4%)
3	K	0.64	1/2944 (0.0%)	1.07	16/3984 (0.4%)
3	L	0.60	0/2944	1.00	8/3984 (0.2%)
3	N	0.97	13/2944 (0.4%)	1.19	6/3984 (0.2%)
3	O	0.77	4/2944 (0.1%)	1.06	3/3984 (0.1%)
4	P	4.01	7/29 (24.1%)	2.22	1/36 (2.8%)
4	Q	4.02	8/29 (27.6%)	2.38	2/36 (5.6%)
4	R	3.93	7/29 (24.1%)	2.00	1/36 (2.8%)
4	S	4.00	8/29 (27.6%)	1.84	0/36
4	T	3.92	7/29 (24.1%)	2.22	1/36 (2.8%)
All	All	1.05	112/22252 (0.5%)	1.27	87/30086 (0.3%)

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	2	ALA	CA-C	-9.88	1.32	1.52
4	P	2	ALA	CA-C	-9.67	1.32	1.52
4	T	2	ALA	CA-C	-9.53	1.32	1.52
4	Q	2	ALA	CA-C	-9.49	1.33	1.52
4	R	2	ALA	CA-C	-9.17	1.33	1.52
4	T	3	TRP	N-CA	-8.20	1.30	1.46
4	Q	3	TRP	N-CA	-8.03	1.30	1.46
4	S	3	TRP	N-CA	-8.02	1.31	1.46
4	P	3	TRP	N-CA	-8.00	1.31	1.46
2	F	260	ARG	CZ-NH2	-7.73	1.23	1.33
4	R	3	TRP	N-CA	-7.72	1.31	1.46
3	I	39	ARG	CZ-NH2	-7.59	1.23	1.33
3	I	210	ARG	CZ-NH2	-7.54	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	62	ARG	CZ-NH2	-7.48	1.23	1.33
3	I	206	ARG	CZ-NH2	-7.36	1.23	1.33
3	J	37	ARG	CZ-NH2	-7.29	1.24	1.33
1	E	92	ARG	CZ-NH2	-7.24	1.24	1.33
3	O	183	ARG	CZ-NH2	-7.24	1.24	1.33
3	I	290	ARG	CZ-NH1	-7.24	1.22	1.32
2	F	266	ARG	CZ-NH2	-7.22	1.24	1.33
1	E	163	ARG	CZ-NH2	-7.19	1.24	1.33
3	N	210	ARG	CZ-NH2	-7.18	1.24	1.33
1	E	94	ARG	CZ-NH2	-7.17	1.24	1.33
3	I	183	ARG	CZ-NH2	-7.14	1.24	1.33
1	E	108	ARG	CZ-NH1	-7.10	1.22	1.32
1	E	215	ARG	CZ-NH2	-7.09	1.24	1.33
3	J	62	ARG	CZ-NH2	-7.09	1.24	1.33
3	O	177	ARG	CZ-NH2	-7.08	1.24	1.33
3	J	256	ARG	CZ-NH2	-7.07	1.24	1.33
4	Q	3	TRP	CA-C	-7.07	1.38	1.52
3	J	254	ARG	CZ-NH2	-7.02	1.24	1.33
3	J	206	ARG	CZ-NH2	-6.98	1.24	1.33
3	N	39	ARG	CZ-NH2	-6.96	1.24	1.33
3	I	290	ARG	CZ-NH2	-6.93	1.24	1.33
1	E	108	ARG	CZ-NH2	-6.93	1.24	1.33
3	I	256	ARG	CZ-NH1	-6.93	1.23	1.32
1	E	195	ARG	CZ-NH2	-6.91	1.24	1.33
3	J	206	ARG	CZ-NH1	-6.91	1.23	1.32
3	J	256	ARG	CZ-NH1	-6.90	1.23	1.32
3	J	116	ARG	CZ-NH1	-6.88	1.23	1.32
3	N	37	ARG	CZ-NH2	-6.87	1.24	1.33
3	J	335	ARG	CZ-NH2	-6.87	1.24	1.33
3	N	312	ARG	CZ-NH2	-6.84	1.24	1.33
3	N	37	ARG	CZ-NH1	-6.83	1.23	1.32
3	I	256	ARG	CZ-NH2	-6.83	1.24	1.33
1	E	163	ARG	CZ-NH1	-6.82	1.23	1.32
3	I	183	ARG	CZ-NH1	-6.81	1.23	1.32
3	I	206	ARG	CZ-NH1	-6.79	1.23	1.32
3	N	206	ARG	CZ-NH2	-6.79	1.24	1.33
3	J	116	ARG	CZ-NH2	-6.78	1.24	1.33
3	N	312	ARG	CZ-NH1	-6.78	1.23	1.32
1	E	94	ARG	CZ-NH1	-6.77	1.23	1.32
3	J	312	ARG	CZ-NH2	-6.77	1.24	1.33
3	N	256	ARG	CZ-NH2	-6.76	1.24	1.33
3	O	183	ARG	CZ-NH1	-6.76	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	14	ARG	CZ-NH2	-6.74	1.24	1.33
1	E	195	ARG	CZ-NH1	-6.71	1.23	1.32
4	P	3	TRP	CA-C	-6.68	1.39	1.52
3	I	37	ARG	CZ-NH1	-6.67	1.23	1.32
3	J	254	ARG	CZ-NH1	-6.66	1.23	1.32
1	E	15	ARG	CZ-NH2	-6.66	1.24	1.33
3	I	62	ARG	CZ-NH1	-6.65	1.23	1.32
3	J	37	ARG	CZ-NH1	-6.63	1.23	1.32
2	F	129	ARG	CZ-NH2	-6.62	1.24	1.33
3	I	37	ARG	CZ-NH2	-6.62	1.24	1.33
3	J	312	ARG	CZ-NH1	-6.62	1.23	1.32
2	F	91	ARG	CZ-NH2	-6.62	1.24	1.33
3	N	256	ARG	CZ-NH1	-6.61	1.23	1.32
1	E	14	ARG	CZ-NH1	-6.61	1.23	1.32
1	E	215	ARG	CZ-NH1	-6.57	1.23	1.32
3	O	177	ARG	CZ-NH1	-6.57	1.23	1.32
3	J	62	ARG	CZ-NH1	-6.56	1.23	1.32
4	R	3	TRP	CA-C	-6.53	1.39	1.52
4	T	5	ALA	CA-C	-6.50	1.39	1.52
3	J	335	ARG	CZ-NH1	-6.47	1.23	1.32
2	F	260	ARG	CZ-NH1	-6.46	1.23	1.32
1	E	92	ARG	CZ-NH1	-6.45	1.23	1.32
3	I	210	ARG	CZ-NH1	-6.43	1.23	1.32
2	F	129	ARG	CZ-NH1	-6.41	1.23	1.32
4	P	5	ALA	CA-C	-6.40	1.39	1.52
3	N	206	ARG	CZ-NH1	-6.38	1.23	1.32
1	E	15	ARG	CZ-NH1	-6.38	1.23	1.32
3	N	39	ARG	CZ-NH1	-6.30	1.24	1.32
4	S	3	TRP	CA-C	-6.27	1.39	1.52
4	P	3	TRP	CA-CB	-6.26	1.41	1.53
4	Q	5	ALA	CA-C	-6.24	1.39	1.52
3	N	210	ARG	CZ-NH1	-6.22	1.24	1.32
4	S	2	ALA	N-CA	-6.22	1.34	1.46
2	F	91	ARG	CZ-NH1	-6.15	1.24	1.32
2	F	266	ARG	CZ-NH1	-6.14	1.24	1.32
4	S	5	ALA	CA-C	-6.08	1.40	1.52
4	T	3	TRP	CA-C	-6.06	1.40	1.52
4	Q	3	TRP	CA-CB	-5.99	1.41	1.53
4	R	2	ALA	N-CA	-5.97	1.34	1.46
4	R	5	ALA	CA-C	-5.93	1.40	1.52
3	I	39	ARG	CZ-NH1	-5.87	1.24	1.32
4	R	3	TRP	CA-CB	-5.86	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	3	TRP	CA-CB	-5.71	1.42	1.53
3	I	181	ALA	CA-CB	-5.67	1.46	1.53
4	S	3	TRP	CA-CB	-5.56	1.42	1.53
4	P	5	ALA	N-CA	-5.43	1.35	1.46
4	S	7	CYS	CA-C	-5.33	1.41	1.52
4	R	5	ALA	N-CA	-5.32	1.36	1.46
4	P	2	ALA	N-CA	-5.30	1.36	1.46
3	K	338	SER	CA-C	-5.27	1.45	1.52
4	S	5	ALA	N-CA	-5.26	1.36	1.46
4	Q	5	ALA	N-CA	-5.23	1.36	1.46
4	T	5	ALA	N-CA	-5.16	1.36	1.46
4	Q	2	ALA	N-CA	-5.15	1.36	1.46
4	T	2	ALA	N-CA	-5.09	1.36	1.46
3	N	340	TRP	CA-C	-5.01	1.46	1.52
4	Q	7	CYS	CA-C	-5.00	1.42	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	32	PRO	N-CA-C	-7.83	98.97	111.03
3	I	143	TYR	CA-CB-CG	7.29	127.03	113.90
2	F	54	PHE	CA-CB-CG	7.27	121.07	113.80
3	L	340	TRP	N-CA-C	-7.07	103.57	111.28
2	F	228	PHE	CA-CB-CG	6.94	120.74	113.80
3	K	166	TYR	CB-CA-C	-6.85	96.28	109.37
4	T	2	ALA	N-CA-CB	6.83	120.64	110.40
3	K	31	PHE	CB-CA-C	6.81	120.41	109.51
4	P	2	ALA	N-CA-CB	6.76	120.55	110.40
3	I	266	PHE	CA-CB-CG	6.72	120.52	113.80
4	Q	2	ALA	N-CA-CB	6.71	120.47	110.40
3	N	340	TRP	N-CA-C	-6.46	105.70	113.97
3	N	291	LYS	CB-CA-C	-6.42	100.71	110.92
3	O	37	ARG	CB-CA-C	6.42	119.60	109.27
3	K	337	TYR	N-CA-C	-6.38	105.35	112.57
3	N	266	PHE	CA-CB-CG	6.31	120.11	113.80
1	E	149	ASP	CA-CB-CG	6.09	118.69	112.60
3	K	167	GLU	N-CA-C	-6.02	105.01	112.47
3	I	356	TRP	CA-CB-CG	5.97	124.95	113.60
3	J	266	PHE	CA-CB-CG	5.96	119.76	113.80
3	I	257	CYS	N-CA-CB	5.92	116.01	110.39
1	E	162	GLY	CA-C-N	5.90	132.81	121.54
1	E	162	GLY	C-N-CA	5.90	132.81	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	27	PRO	N-CA-C	-5.87	100.97	110.55
1	E	148	TRP	CA-CB-CG	5.82	124.66	113.60
3	N	311	ASP	CA-CB-CG	5.79	118.39	112.60
2	F	124	CYS	CA-C-N	5.75	127.91	120.44
2	F	124	CYS	C-N-CA	5.75	127.91	120.44
3	L	177	ARG	CB-CA-C	-5.74	101.43	110.79
3	O	38	PRO	N-CA-C	5.73	120.22	111.34
2	F	35	ASP	CA-CB-CG	5.71	118.31	112.60
3	J	335	ARG	CA-C-N	5.71	130.26	121.19
3	J	335	ARG	C-N-CA	5.71	130.26	121.19
1	E	128	PHE	CA-CB-CG	5.68	119.48	113.80
2	F	213	GLN	CB-CG-CD	5.63	122.17	112.60
3	K	340	TRP	N-CA-C	-5.55	105.71	113.37
3	K	249	THR	CB-CA-C	-5.54	101.99	111.31
1	E	105	ASP	CA-CB-CG	5.54	118.14	112.60
3	L	289	ILE	CA-C-N	-5.49	111.06	121.54
3	L	289	ILE	C-N-CA	-5.49	111.06	121.54
3	I	62	ARG	CD-NE-CZ	5.48	132.08	124.40
3	J	112	PRO	CA-C-N	5.48	127.89	120.38
3	J	112	PRO	C-N-CA	5.48	127.89	120.38
3	I	7	ALA	CA-C-N	5.47	130.26	122.72
3	I	7	ALA	C-N-CA	5.47	130.26	122.72
3	J	81	ASP	CA-CB-CG	5.39	117.99	112.60
3	J	239	SER	CA-C-N	5.35	131.12	122.29
3	J	239	SER	C-N-CA	5.35	131.12	122.29
1	E	219	ASP	CA-CB-CG	5.29	117.89	112.60
3	L	339	VAL	CA-C-N	-5.28	113.21	120.28
3	L	339	VAL	C-N-CA	-5.28	113.21	120.28
3	I	280	ASN	CA-CB-CG	5.28	117.88	112.60
1	E	113	GLU	CA-C-N	5.28	128.19	120.91
1	E	113	GLU	C-N-CA	5.28	128.19	120.91
1	E	205	ASP	CA-CB-CG	5.26	117.86	112.60
2	F	203	ASN	CA-CB-CG	5.25	117.85	112.60
3	K	33	SER	CA-C-N	5.25	130.35	122.75
3	K	33	SER	C-N-CA	5.25	130.35	122.75
1	E	112	PHE	CA-CB-CG	5.23	119.03	113.80
3	J	124	PHE	CA-CB-CG	5.23	119.03	113.80
3	O	183	ARG	CD-NE-CZ	5.22	131.71	124.40
3	N	177	ARG	CB-CA-C	-5.17	100.19	111.71
3	K	142	LEU	CA-C-N	-5.13	113.35	120.38
3	K	142	LEU	C-N-CA	-5.13	113.35	120.38
3	J	252	ASN	CA-C-N	5.10	127.62	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	252	ASN	C-N-CA	5.10	127.62	120.28
3	L	284	LYS	CA-C-N	-5.10	113.93	123.05
3	L	284	LYS	C-N-CA	-5.10	113.93	123.05
3	K	340	TRP	CA-C-N	-5.09	113.09	121.34
3	K	340	TRP	C-N-CA	-5.09	113.09	121.34
2	F	56	GLN	CA-C-N	5.08	127.36	120.65
2	F	56	GLN	C-N-CA	5.08	127.36	120.65
1	E	256	GLU	CA-CB-CG	5.08	124.25	114.10
3	J	311	ASP	CA-CB-CG	5.06	117.66	112.60
3	J	62	ARG	CD-NE-CZ	5.05	131.48	124.40
2	F	107	ASP	CA-CB-CG	5.05	117.65	112.60
3	J	254	ARG	CD-NE-CZ	5.04	131.46	124.40
1	E	108	ARG	CD-NE-CZ	5.04	131.46	124.40
4	R	3	TRP	CB-CG-CD2	-5.04	119.74	126.80
3	I	172	PRO	CA-C-N	5.04	127.54	120.28
3	I	172	PRO	C-N-CA	5.04	127.54	120.28
3	K	30	VAL	CA-C-N	-5.04	114.14	121.20
3	K	30	VAL	C-N-CA	-5.04	114.14	121.20
2	F	137	SER	CA-C-N	5.03	130.48	122.74
2	F	137	SER	C-N-CA	5.03	130.48	122.74
3	N	256	ARG	CD-NE-CZ	5.02	131.43	124.40
4	Q	3	TRP	CB-CG-CD2	-5.01	119.79	126.80

There are no chirality outliers.

There are no planarity outliers.

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	E	2146	0	2138	6	0
2	F	2212	0	2134	13	0
3	I	2894	0	2868	11	0
3	J	2894	0	2868	14	0
3	K	2894	0	2868	67	0
3	L	2894	0	2868	41	0
3	N	2894	0	2867	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2894	0	2868	30	0
4	P	55	0	36	0	0
4	Q	55	0	35	2	0
4	R	55	0	36	0	0
4	S	55	0	35	4	0
4	T	55	0	36	3	0
5	I	27	0	12	3	0
5	J	27	0	12	1	0
5	K	27	0	12	3	0
5	L	27	0	12	0	0
5	N	27	0	12	1	0
5	O	27	0	12	2	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
7	K	5	0	0	0	0
7	L	5	0	0	0	0
7	N	5	0	0	0	0
7	O	5	0	0	0	0
All	All	22185	0	21729	212	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 5.

All (212) 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)
3:O:202:THR:HG23	3:O:205:GLU:H	1.24	1.01
3:K:31:PHE:CZ	3:K:85:ILE:HG23	1.97	0.99
1:E:201:GLU:HB3	1:E:212:ASN:HD21	1.35	0.91
3:J:244:ASP:HB2	3:L:287:VAL:HG13	1.58	0.83
3:K:340:TRP:O	3:K:340:TRP:CE3	2.33	0.82
3:K:251:GLY:C	3:K:253:GLU:H	1.86	0.81
3:I:18:LYS:NZ	5:I:401:ADP:O2B	2.14	0.79
3:K:305:MET:SD	3:K:335:ARG:HG3	2.22	0.79
3:K:193:LEU:HD22	3:K:250:ILE:HD12	1.64	0.78
3:K:31:PHE:HZ	3:K:85:ILE:HG23	1.45	0.78
3:K:251:GLY:C	3:K:253:GLU:N	2.38	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:30:VAL:HG12	3:K:30:VAL:O	1.86	0.76
3:O:36:GLY:O	3:O:65:LEU:HD22	1.86	0.75
3:K:31:PHE:CE2	3:K:85:ILE:HG23	2.23	0.74
3:L:285:CYS:HB3	3:L:289:ILE:HD11	1.70	0.73
3:K:250:ILE:HG22	3:K:253:GLU:HB2	1.72	0.70
3:N:176:LEU:HD11	3:N:277:THR:HB	1.73	0.70
3:K:340:TRP:O	3:K:340:TRP:CD2	2.45	0.70
2:F:29:PHE:O	2:F:32:VAL:HG12	1.93	0.69
3:I:153:MET:HE3	3:I:299:LEU:HD22	1.74	0.69
3:N:14:SER:HB2	3:N:157:ASP:HB3	1.75	0.68
3:L:285:CYS:O	3:L:290:ARG:NH2	2.27	0.67
3:K:166:TYR:C	3:K:168:GLY:N	2.52	0.66
3:L:288:ASP:O	3:L:290:ARG:N	2.26	0.66
3:I:49:GLN:HB2	3:K:169:TYR:OH	1.96	0.65
3:L:159:VAL:HG21	3:L:177:ARG:HH21	1.60	0.65
3:O:18:LYS:NZ	5:O:401:ADP:O2B	2.27	0.65
3:K:257:CYS:HB3	3:K:258:PRO:HD3	1.78	0.64
3:K:16:MET:HG2	3:K:32:PRO:HA	1.78	0.64
1:E:65:ASN:OD1	1:E:66:ARG:N	2.31	0.64
3:N:282:ILE:HG21	3:N:294:TYR:CE1	2.32	0.64
3:K:253:GLU:OE2	3:K:253:GLU:HA	1.99	0.63
3:L:219:VAL:HG22	3:L:258:PRO:HB2	1.80	0.62
3:J:153:MET:HE2	3:J:278:THR:HG23	1.82	0.62
3:N:285:CYS:HB3	3:N:289:ILE:HD11	1.82	0.61
4:S:3:TRP:HB2	4:S:7:CYS:H	1.63	0.61
3:J:244:ASP:OD1	3:L:290:ARG:HD2	2.01	0.61
3:K:9:VAL:HB	3:K:340:TRP:NE1	2.16	0.61
3:K:339:VAL:C	3:K:341:ILE:N	2.55	0.60
3:N:287:VAL:HG21	4:Q:6:DTH:HG21	1.83	0.60
3:K:16:MET:HA	3:K:33:SER:H	1.65	0.60
3:O:188:TYR:HB2	3:O:267:LEU:HD11	1.83	0.60
3:L:285:CYS:HB3	3:L:289:ILE:CD1	2.32	0.59
3:J:157:ASP:OD1	5:J:401:ADP:O3'	2.20	0.59
3:K:24:ASP:HB2	3:K:340:TRP:HH2	1.67	0.59
3:J:49:GLN:HB2	3:L:169:TYR:OH	2.02	0.59
3:K:220:ALA:HB2	3:K:255:PHE:HB2	1.83	0.59
3:L:253:GLU:CD	3:L:253:GLU:H	2.10	0.59
3:I:156:GLY:HA3	5:I:401:ADP:O1B	2.02	0.59
2:F:113:VAL:HG12	2:F:114:ASP:N	2.18	0.59
3:N:153:MET:HE2	3:N:299:LEU:HD22	1.85	0.59
3:O:153:MET:HE2	3:O:299:LEU:HD22	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:251:GLY:O	3:K:253:GLU:HG2	2.02	0.58
2:F:216:VAL:HG12	2:F:217:THR:N	2.18	0.58
3:L:72:GLU:C	3:L:74:GLY:H	2.10	0.57
2:F:34:ASN:O	2:F:38:LEU:HG	2.05	0.57
3:O:253:GLU:CD	3:O:253:GLU:H	2.12	0.57
3:I:9:VAL:HG13	3:I:104:LEU:HD23	1.85	0.57
3:K:153:MET:HE2	3:K:274:ILE:HB	1.87	0.57
3:K:217:CYS:HA	3:K:254:ARG:HB3	1.85	0.57
3:L:159:VAL:HG13	3:L:177:ARG:HG3	1.87	0.57
3:K:166:TYR:C	3:K:168:GLY:H	2.11	0.56
3:K:248:ILE:HG22	3:K:250:ILE:HD11	1.85	0.56
3:K:339:VAL:C	3:K:341:ILE:H	2.13	0.56
3:J:253:GLU:CD	3:J:253:GLU:H	2.14	0.56
3:K:142:LEU:HG	3:K:147:ARG:O	2.06	0.56
3:L:282:ILE:CG2	3:L:290:ARG:HG3	2.36	0.56
3:N:16:MET:HE2	5:N:401:ADP:H5'2	1.88	0.55
4:Q:3:TRP:HB2	4:Q:7:CYS:O	2.07	0.55
3:L:73:HIC:O	3:L:177:ARG:NH2	2.40	0.55
3:L:159:VAL:CG1	3:L:177:ARG:HG3	2.37	0.55
3:L:216:LEU:HD13	3:L:250:ILE:HG13	1.89	0.55
3:K:302:GLY:H	5:K:402:ADP:PA	2.30	0.54
3:L:290:ARG:O	3:L:291:LYS:C	2.48	0.54
3:K:166:TYR:O	3:K:169:TYR:N	2.36	0.54
3:N:24:ASP:HB2	3:N:340:TRP:HH2	1.73	0.54
3:O:202:THR:HG23	3:O:205:GLU:N	2.07	0.54
3:O:369:ILE:HD12	3:O:372:ARG:HH11	1.71	0.54
3:K:337:TYR:C	3:K:339:VAL:H	2.16	0.54
3:L:110:LEU:O	3:L:177:ARG:NH1	2.41	0.54
3:K:302:GLY:N	5:K:402:ADP:O1A	2.29	0.53
2:F:127:ALA:CB	2:F:225:THR:CG2	2.86	0.53
3:L:217:CYS:HB2	3:L:306:TYR:CE1	2.43	0.53
3:N:72:GLU:HB3	3:N:73:HIC:HD2	1.89	0.53
3:O:297:THR:OG1	3:O:329:ILE:HD13	2.09	0.53
3:N:288:ASP:C	3:N:290:ARG:H	2.17	0.53
3:K:138:ALA:HB2	3:K:161:HIS:HD2	1.73	0.53
3:O:43:VAL:O	3:O:43:VAL:HG23	2.09	0.53
3:O:202:THR:OG1	3:O:203:THR:N	2.41	0.52
3:O:201:THR:H	3:O:205:GLU:CD	2.17	0.52
3:K:192:ILE:CG2	3:K:256:ARG:HH21	2.22	0.52
3:K:9:VAL:HB	3:K:340:TRP:HE1	1.73	0.52
3:J:153:MET:HE3	3:J:274:ILE:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:72:GLU:C	3:K:74:GLY:H	2.17	0.51
3:I:285:CYS:HB3	3:I:289:ILE:HD11	1.93	0.51
3:O:67:LEU:HB2	3:O:203:THR:HG21	1.92	0.51
3:O:71:ILE:HG12	3:O:76:VAL:HG22	1.91	0.51
2:F:127:ALA:HB3	2:F:225:THR:CG2	2.41	0.51
3:J:112:PRO:HD3	4:S:3:TRP:CH2	2.45	0.51
3:N:340:TRP:O	3:N:340:TRP:CE3	2.63	0.51
3:N:253:GLU:H	3:N:253:GLU:CD	2.20	0.50
3:O:157:ASP:N	5:O:401:ADP:H5'2	2.27	0.50
3:K:142:LEU:HD13	3:K:152:VAL:CG2	2.42	0.50
3:K:13:GLY:HA3	5:K:402:ADP:O2B	2.12	0.50
3:O:206:ARG:O	3:O:209:VAL:N	2.45	0.49
3:J:204:ALA:HB1	3:L:288:ASP:OD2	2.11	0.49
3:K:9:VAL:HG12	3:K:340:TRP:CD1	2.46	0.49
3:L:72:GLU:C	3:L:74:GLY:N	2.70	0.49
4:S:3:TRP:HB2	4:S:7:CYS:N	2.27	0.49
3:L:153:MET:HE1	3:L:274:ILE:HD12	1.93	0.49
3:N:293:LEU:O	3:N:294:TYR:C	2.52	0.49
3:K:252:ASN:HA	3:K:255:PHE:CZ	2.48	0.49
3:L:294:TYR:O	3:L:327:ILE:HA	2.13	0.49
3:L:159:VAL:CG1	3:L:177:ARG:HE	2.25	0.49
3:L:219:VAL:HG12	3:L:219:VAL:O	2.11	0.49
3:O:297:THR:OG1	3:O:328:LYS:O	2.30	0.49
3:I:49:GLN:HB2	3:K:169:TYR:CZ	2.48	0.48
3:L:218:TYR:OH	3:L:236:LEU:HD21	2.13	0.48
3:L:217:CYS:HB2	3:L:306:TYR:HE1	1.78	0.48
3:N:140:LEU:HB2	3:N:339:VAL:HG13	1.94	0.48
3:J:203:THR:O	3:J:206:ARG:HB3	2.13	0.48
3:K:21:PHE:O	3:K:340:TRP:HZ2	1.97	0.48
3:K:250:ILE:CG2	3:K:253:GLU:HB2	2.43	0.48
3:I:14:SER:N	5:I:401:ADP:O3B	2.46	0.48
3:N:340:TRP:O	3:N:340:TRP:CD2	2.67	0.47
3:L:286:ASP:OD1	3:L:287:VAL:N	2.47	0.47
3:L:290:ARG:O	3:L:293:LEU:N	2.47	0.47
3:L:289:ILE:O	3:L:289:ILE:HG13	2.14	0.47
3:N:288:ASP:C	3:N:290:ARG:N	2.73	0.47
4:T:3:TRP:HB2	4:T:7:CYS:O	2.15	0.47
3:N:158:GLY:C	3:N:181:ALA:CB	2.88	0.47
3:N:166:TYR:CD2	3:N:289:ILE:HB	2.50	0.47
3:O:76:VAL:HB	3:O:79:TRP:CZ2	2.50	0.47
3:I:197:GLY:HA2	4:S:3:TRP:HZ3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:113:VAL:CG1	2:F:114:ASP:N	2.78	0.46
2:F:216:VAL:CG1	2:F:217:THR:N	2.78	0.46
3:K:30:VAL:O	3:K:30:VAL:CG1	2.56	0.46
3:L:219:VAL:HG23	3:L:306:TYR:HB3	1.96	0.46
3:K:141:SER:O	3:K:142:LEU:C	2.55	0.46
3:N:290:ARG:O	3:N:291:LYS:C	2.55	0.46
3:O:37:ARG:HG2	3:O:52:SER:HB3	1.98	0.46
3:N:338:SER:OG	3:N:339:VAL:N	2.49	0.46
3:L:24:ASP:HB2	3:L:340:TRP:HH2	1.81	0.46
2:F:57:TYR:HA	2:F:60:ASP:OD2	2.16	0.46
3:K:192:ILE:HG22	3:K:256:ARG:HH21	1.80	0.46
3:L:159:VAL:HG11	3:L:177:ARG:HE	1.82	0.45
3:N:199:SER:HB2	4:T:3:TRP:CD2	2.51	0.45
3:O:206:ARG:O	3:O:207:GLU:C	2.58	0.45
3:O:67:LEU:HB2	3:O:203:THR:CG2	2.46	0.45
3:K:138:ALA:HB2	3:K:161:HIS:CD2	2.52	0.45
3:N:288:ASP:O	3:N:290:ARG:N	2.50	0.45
3:N:291:LYS:O	3:N:294:TYR:N	2.50	0.45
1:E:61:LEU:HA	1:E:65:ASN:HD21	1.82	0.45
3:K:252:ASN:HA	3:K:255:PHE:CE1	2.51	0.45
3:N:188:TYR:HB2	3:N:267:LEU:HD13	1.98	0.45
3:N:361:GLU:O	3:N:365:SER:OG	2.31	0.45
3:L:171:LEU:HB3	3:L:285:CYS:SG	2.57	0.45
3:N:291:LYS:O	3:N:292:ASP:C	2.59	0.45
3:L:213:LYS:O	3:L:214:GLU:C	2.58	0.44
1:E:235:LYS:HE2	2:F:198:TYR:CE1	2.52	0.44
3:K:166:TYR:CG	3:K:167:GLU:N	2.85	0.44
3:K:337:TYR:C	3:K:339:VAL:N	2.74	0.44
3:L:140:LEU:HD12	3:L:339:VAL:HG13	1.99	0.44
3:L:286:ASP:H	3:L:289:ILE:HD11	1.82	0.44
3:K:142:LEU:O	3:K:143:TYR:C	2.58	0.44
3:O:166:TYR:CE2	3:O:289:ILE:HB	2.53	0.44
3:O:39:ARG:HB2	3:O:40:HIS:H	1.52	0.44
3:K:333:PRO:O	3:K:334:GLU:HB2	2.18	0.44
2:F:127:ALA:HB3	2:F:225:THR:HG23	2.00	0.43
3:K:109:PRO:HG3	3:K:161:HIS:CB	2.47	0.43
3:L:219:VAL:HG11	3:L:262:PHE:CE2	2.52	0.43
3:J:53:TYR:CZ	3:J:61:LYS:HE3	2.53	0.43
3:I:286:ASP:O	3:I:289:ILE:HG12	2.19	0.43
3:K:340:TRP:O	3:K:340:TRP:CG	2.71	0.43
1:E:173:VAL:HG12	1:E:175:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:258:PRO:C	3:K:260:ALA:N	2.76	0.43
3:K:72:GLU:C	3:K:74:GLY:N	2.74	0.43
3:K:337:TYR:O	3:K:339:VAL:N	2.52	0.43
3:K:152:VAL:O	3:K:162:THR:HA	2.19	0.42
3:K:159:VAL:HG12	3:K:160:THR:N	2.33	0.42
3:N:156:GLY:O	3:N:303:THR:HG23	2.19	0.42
3:J:67:LEU:HB2	3:J:203:THR:HG21	2.01	0.42
3:N:109:PRO:O	3:N:177:ARG:NH1	2.52	0.42
3:O:5:ILE:HD12	3:O:102:PRO:HD3	2.00	0.42
3:K:31:PHE:HZ	3:K:85:ILE:CG2	2.25	0.42
3:O:202:THR:N	3:O:205:GLU:HB2	2.35	0.42
3:N:76:VAL:HB	3:N:79:TRP:CZ2	2.55	0.42
3:O:12:ASN:O	3:O:71:ILE:HD13	2.20	0.42
3:O:297:THR:OG1	3:O:329:ILE:HA	2.19	0.42
3:K:251:GLY:O	3:K:253:GLU:N	2.53	0.42
3:K:254:ARG:O	3:K:258:PRO:HD3	2.20	0.42
3:K:26:ALA:C	3:K:340:TRP:CZ3	2.98	0.42
3:K:248:ILE:HG22	3:K:250:ILE:CD1	2.49	0.42
3:N:340:TRP:CE3	3:N:340:TRP:C	2.98	0.41
3:O:202:THR:H	3:O:205:GLU:HB2	1.85	0.41
3:O:372:ARG:CZ	3:O:372:ARG:HA	2.50	0.41
3:K:256:ARG:O	3:K:257:CYS:C	2.61	0.41
3:J:103:VAL:O	3:J:132:MET:HA	2.20	0.41
3:L:219:VAL:HG11	3:L:262:PHE:HE2	1.86	0.41
4:T:1:HYP:C	4:T:3:TRP:H	2.33	0.41
3:J:76:VAL:HB	3:J:79:TRP:CZ2	2.56	0.41
2:F:220:ASN:O	2:F:224:THR:HG22	2.21	0.41
3:L:339:VAL:O	3:L:340:TRP:C	2.55	0.41
3:O:202:THR:HG22	3:O:205:GLU:CG	2.51	0.41
3:N:152:VAL:O	3:N:162:THR:HA	2.21	0.41
3:K:248:ILE:CG2	3:K:250:ILE:HD11	2.51	0.40
3:N:158:GLY:C	3:N:181:ALA:HB3	2.46	0.40
1:E:173:VAL:HG12	1:E:175:LEU:HD11	2.03	0.40
3:L:219:VAL:HG22	3:L:258:PRO:CB	2.49	0.40
2:F:124:CYS:HA	2:F:225:THR:HG23	2.03	0.40
3:I:76:VAL:HG11	3:I:79:TRP:CE3	2.56	0.40
3:K:258:PRO:O	3:K:259:GLU:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	270/272 (99%)	260 (96%)	10 (4%)	0	100	100
2	F	270/286 (94%)	259 (96%)	11 (4%)	0	100	100
3	I	368/375 (98%)	345 (94%)	22 (6%)	1 (0%)	36	67
3	J	368/375 (98%)	344 (94%)	24 (6%)	0	100	100
3	K	368/375 (98%)	340 (92%)	27 (7%)	1 (0%)	36	67
3	L	368/375 (98%)	344 (94%)	24 (6%)	0	100	100
3	N	368/375 (98%)	348 (95%)	20 (5%)	0	100	100
3	O	368/375 (98%)	348 (95%)	20 (5%)	0	100	100
4	P	3/7 (43%)	2 (67%)	0	1 (33%)	0	0
4	Q	3/7 (43%)	2 (67%)	0	1 (33%)	0	0
4	R	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
4	S	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
4	T	3/7 (43%)	2 (67%)	0	1 (33%)	0	0
All	All	2763/2843 (97%)	2598 (94%)	160 (6%)	5 (0%)	44	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Q	2	ALA
4	T	2	ALA
4	P	2	ALA
3	I	74	GLY
3	K	338	SER

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	E	241/241 (100%)	241 (100%)	0	100	100
2	F	243/255 (95%)	243 (100%)	0	100	100
3	I	313/317 (99%)	313 (100%)	0	100	100
3	J	313/317 (99%)	313 (100%)	0	100	100
3	K	313/317 (99%)	313 (100%)	0	100	100
3	L	313/317 (99%)	313 (100%)	0	100	100
3	N	313/317 (99%)	313 (100%)	0	100	100
3	O	313/317 (99%)	312 (100%)	1 (0%)	86	84
4	P	2/2 (100%)	1 (50%)	1 (50%)	0	0
4	Q	2/2 (100%)	1 (50%)	1 (50%)	0	0
4	R	2/2 (100%)	2 (100%)	0	100	100
4	S	2/2 (100%)	1 (50%)	1 (50%)	0	0
4	T	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	2372/2408 (98%)	2367 (100%)	5 (0%)	85	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	39	ARG
4	Q	7	CYS
4	S	7	CYS
4	T	7	CYS
4	P	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	GLN
1	E	157	GLN
1	E	212	ASN
2	F	34	ASN
2	F	73	GLN
2	F	79	HIS

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Mol	Chain	Res	Type
2	F	138	ASN
2	F	187	GLN
2	F	203	ASN
2	F	213	GLN
2	F	220	ASN
2	F	223	GLN
2	F	272	ASN
3	I	40	HIS
3	I	87	HIS
3	I	92	ASN
3	J	49	GLN
3	J	87	HIS
3	J	92	ASN
3	K	92	ASN
3	K	263	GLN
3	L	92	ASN
3	L	354	GLN
3	N	40	HIS
3	N	92	ASN
3	N	252	ASN
3	O	87	HIS
3	O	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

21 non-standard protein/DNA/RNA residues are modelled in this entry.

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	EEP	P	4	4	7,9,10	6.80	5 (71%)	3,12,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HYP	Q	1	4	7,8,9	5.61	6 (85%)	5,10,12	1.68	1 (20%)
3	HIC	I	73	3	10,11,12	1.53	1 (10%)	9,14,16	1.28	1 (11%)
4	HYP	S	1	4	7,8,9	5.53	6 (85%)	5,10,12	1.90	2 (40%)
3	HIC	L	73	3	10,11,12	1.37	1 (10%)	9,14,16	1.24	1 (11%)
4	DTH	P	6	4	5,6,7	3.59	4 (80%)	5,7,9	1.78	1 (20%)
4	DTH	T	6	4	5,6,7	3.66	4 (80%)	5,7,9	2.22	1 (20%)
4	EEP	S	4	4	7,9,10	6.75	5 (71%)	3,12,14	0.79	0
4	DTH	S	6	4	5,6,7	3.57	4 (80%)	5,7,9	1.53	1 (20%)
3	HIC	N	73	3	10,11,12	1.42	1 (10%)	9,14,16	1.40	1 (11%)
4	EEP	Q	4	4	7,9,10	6.74	5 (71%)	3,12,14	0.90	0
4	DTH	Q	6	4	5,6,7	3.67	4 (80%)	5,7,9	1.41	1 (20%)
4	HYP	P	1	4	7,8,9	5.66	6 (85%)	5,10,12	1.66	1 (20%)
4	EEP	R	4	4	7,9,10	6.80	5 (71%)	3,12,14	0.85	0
3	HIC	K	73	3	10,11,12	1.36	1 (10%)	9,14,16	1.51	1 (11%)
4	EEP	T	4	4	7,9,10	6.72	5 (71%)	3,12,14	0.84	0
3	HIC	J	73	3	10,11,12	1.43	1 (10%)	9,14,16	1.36	1 (11%)
3	HIC	O	73	3	10,11,12	1.30	1 (10%)	9,14,16	1.43	2 (22%)
4	HYP	R	1	4	7,8,9	5.46	6 (85%)	5,10,12	1.97	2 (40%)
4	HYP	T	1	4	7,8,9	5.46	6 (85%)	5,10,12	1.77	2 (40%)
4	DTH	R	6	4	5,6,7	3.60	4 (80%)	5,7,9	1.70	1 (20%)

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	EEP	P	4	4	-	7/9/10/12	-
4	HYP	Q	1	4	-	0/0/11/13	0/1/1/1
3	HIC	I	73	3	-	2/5/6/8	0/1/1/1
4	HYP	S	1	4	-	0/0/11/13	0/1/1/1
3	HIC	L	73	3	-	1/5/6/8	0/1/1/1
4	DTH	P	6	4	-	4/5/6/8	-
4	DTH	T	6	4	-	0/5/6/8	-
4	EEP	S	4	4	-	5/9/10/12	-
4	DTH	S	6	4	-	0/5/6/8	-
3	HIC	N	73	3	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EEP	Q	4	4	-	5/9/10/12	-
4	DTH	Q	6	4	-	5/5/6/8	-
4	HYP	P	1	4	-	0/0/11/13	0/1/1/1
4	EEP	R	4	4	-	8/9/10/12	-
3	HIC	K	73	3	-	1/5/6/8	0/1/1/1
4	EEP	T	4	4	-	3/9/10/12	-
3	HIC	J	73	3	-	2/5/6/8	0/1/1/1
3	HIC	O	73	3	-	2/5/6/8	0/1/1/1
4	HYP	R	1	4	-	0/0/11/13	0/1/1/1
4	HYP	T	1	4	-	0/0/11/13	0/1/1/1
4	DTH	R	6	4	-	1/5/6/8	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	4	EEP	CD2-CG	-14.43	1.36	1.52
4	T	4	EEP	CD2-CG	-14.41	1.36	1.52
4	R	4	EEP	CD2-CG	-14.37	1.36	1.52
4	S	4	EEP	CD2-CG	-14.36	1.36	1.52
4	Q	4	EEP	CD2-CG	-14.25	1.36	1.52
4	P	1	HYP	CA-N	-9.69	1.31	1.48
4	S	1	HYP	CA-N	-9.63	1.31	1.48
4	Q	1	HYP	CA-N	-9.49	1.32	1.48
4	T	1	HYP	CA-N	-9.33	1.32	1.48
4	R	1	HYP	CA-N	-9.14	1.32	1.48
4	R	4	EEP	CB-CA	-7.65	1.44	1.54
4	S	4	EEP	CB-CA	-7.52	1.44	1.54
4	Q	4	EEP	CB-CA	-7.42	1.44	1.54
4	P	4	EEP	CB-CA	-7.37	1.44	1.54
4	T	4	EEP	CB-CA	-7.24	1.44	1.54
4	R	1	HYP	CD-CG	-6.89	1.38	1.53
4	P	1	HYP	CD-CG	-6.84	1.38	1.53
4	Q	1	HYP	CD-CG	-6.83	1.38	1.53
4	S	1	HYP	CD-CG	-6.76	1.38	1.53
4	T	1	HYP	CD-CG	-6.45	1.39	1.53
4	Q	1	HYP	CB-CA	-6.17	1.40	1.54
4	T	1	HYP	CB-CA	-6.09	1.41	1.54
4	P	1	HYP	CB-CA	-5.99	1.41	1.54
4	R	1	HYP	CB-CA	-5.86	1.41	1.54
4	S	1	HYP	CB-CA	-5.80	1.41	1.54
4	P	4	EEP	CA-N	-5.24	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	4	EEP	CA-N	-5.13	1.33	1.48
4	P	1	HYP	CB-CG	-4.98	1.43	1.52
4	R	4	EEP	CA-N	-4.98	1.34	1.48
4	T	4	EEP	CA-N	-4.81	1.34	1.48
4	Q	1	HYP	CB-CG	-4.79	1.44	1.52
4	S	4	EEP	CA-N	-4.77	1.34	1.48
4	R	1	HYP	CB-CG	-4.62	1.44	1.52
4	Q	6	DTH	CB-CA	-4.57	1.40	1.53
4	T	1	HYP	CB-CG	-4.52	1.44	1.52
4	R	6	DTH	CB-CA	-4.51	1.40	1.53
4	S	1	HYP	CB-CG	-4.51	1.44	1.52
4	T	6	DTH	CB-CA	-4.50	1.40	1.53
4	S	6	DTH	CB-CA	-4.40	1.41	1.53
4	Q	6	DTH	CA-N	-4.37	1.35	1.47
4	P	6	DTH	CA-N	-4.37	1.35	1.47
4	P	6	DTH	CB-CA	-4.32	1.41	1.53
4	T	6	DTH	CA-N	-4.24	1.35	1.47
4	R	6	DTH	CA-N	-4.20	1.35	1.47
4	T	6	DTH	OG1-CB	-4.17	1.32	1.43
4	S	6	DTH	CA-N	-4.11	1.35	1.47
4	S	6	DTH	OG1-CB	-4.07	1.32	1.43
4	Q	6	DTH	OG1-CB	-4.03	1.32	1.43
4	P	6	DTH	OG1-CB	-4.02	1.32	1.43
4	R	6	DTH	OG1-CB	-3.99	1.32	1.43
4	S	4	EEP	O1-CG	-3.97	1.38	1.44
4	R	4	EEP	O1-CG	-3.97	1.38	1.44
4	P	4	EEP	O1-CG	-3.91	1.39	1.44
4	Q	4	EEP	CD1-CG	-3.90	1.43	1.51
4	P	4	EEP	CD1-CG	-3.89	1.43	1.51
4	Q	4	EEP	O1-CG	-3.88	1.39	1.44
4	T	4	EEP	CD1-CG	-3.87	1.43	1.51
4	P	1	HYP	OD1-CG	-3.86	1.32	1.43
4	T	4	EEP	O1-CG	-3.83	1.39	1.44
4	R	4	EEP	CD1-CG	-3.81	1.43	1.51
4	Q	1	HYP	OD1-CG	-3.79	1.32	1.43
4	R	1	HYP	OD1-CG	-3.78	1.32	1.43
4	S	1	HYP	OD1-CG	-3.77	1.32	1.43
4	T	1	HYP	OD1-CG	-3.76	1.32	1.43
4	S	4	EEP	CD1-CG	-3.74	1.43	1.51
3	I	73	HIC	CD2-CG	3.12	1.41	1.36
4	T	6	DTH	CG2-CB	-2.86	1.43	1.51
3	L	73	HIC	CD2-CG	2.79	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	6	DTH	CG2-CB	-2.79	1.43	1.51
3	J	73	HIC	CD2-CG	2.77	1.41	1.36
4	R	6	DTH	CG2-CB	-2.76	1.43	1.51
4	S	6	DTH	CG2-CB	-2.73	1.44	1.51
4	P	6	DTH	CG2-CB	-2.71	1.44	1.51
3	N	73	HIC	CD2-CG	2.62	1.40	1.36
3	K	73	HIC	CD2-CG	2.50	1.40	1.36
3	O	73	HIC	CD2-CG	2.34	1.40	1.36
4	T	1	HYP	CD-N	-2.26	1.39	1.47
4	P	1	HYP	CD-N	-2.24	1.39	1.47
4	Q	1	HYP	CD-N	-2.22	1.39	1.47
4	R	1	HYP	CD-N	-2.19	1.40	1.47
4	S	1	HYP	CD-N	-2.06	1.40	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	6	DTH	O-C-CA	-4.66	112.78	124.77
4	P	6	DTH	O-C-CA	-3.62	115.47	124.77
3	K	73	HIC	NE2-CE1-ND1	-3.59	111.29	112.66
3	O	73	HIC	NE2-CE1-ND1	-3.30	111.40	112.66
3	N	73	HIC	NE2-CE1-ND1	-3.27	111.41	112.66
4	Q	1	HYP	O-C-CA	-3.25	116.42	124.77
4	P	1	HYP	O-C-CA	-3.20	116.54	124.77
3	J	73	HIC	NE2-CE1-ND1	-3.15	111.46	112.66
4	R	1	HYP	O-C-CA	-3.14	116.69	124.77
4	R	6	DTH	O-C-CA	-3.04	116.96	124.77
3	I	73	HIC	NE2-CE1-ND1	-3.02	111.51	112.66
4	S	6	DTH	O-C-CA	-2.84	117.48	124.77
4	Q	6	DTH	O-C-CA	-2.80	117.58	124.77
4	S	1	HYP	O-C-CA	-2.72	117.79	124.77
3	L	73	HIC	NE2-CE1-ND1	-2.57	111.68	112.66
4	T	1	HYP	O-C-CA	-2.35	118.73	124.77
4	R	1	HYP	CG-CB-CA	2.32	106.43	103.75
4	S	1	HYP	CG-CB-CA	2.30	106.42	103.75
4	T	1	HYP	CB-CG-CD	2.21	105.61	103.16
3	O	73	HIC	CA-CB-CG	-2.18	108.38	113.77

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	73	HIC	O-C-CA-CB
3	L	73	HIC	O-C-CA-CB
4	Q	4	EEP	CA-CB-CG-CD1
4	Q	4	EEP	N-CA-CB-CG
4	R	4	EEP	CA-CB-CG-CD1
4	R	4	EEP	O2-CD1-CG-CB
4	R	4	EEP	O2-CD1-CG-O1
4	R	4	EEP	O2-CD1-CG-CD2
4	R	4	EEP	N-CA-CB-CG
4	R	4	EEP	C-CA-CB-CG
4	S	4	EEP	O2-CD1-CG-CB
4	S	4	EEP	O2-CD1-CG-O1
4	S	4	EEP	O2-CD1-CG-CD2
4	S	4	EEP	N-CA-CB-CG
4	T	4	EEP	N-CA-CB-CG
4	T	4	EEP	C-CA-CB-CG
4	P	4	EEP	O2-CD1-CG-CB
4	P	4	EEP	O2-CD1-CG-O1
4	P	4	EEP	O2-CD1-CG-CD2
4	Q	6	DTH	N-CA-CB-OG1
4	Q	6	DTH	C-CA-CB-CG2
4	Q	6	DTH	C-CA-CB-OG1
4	P	6	DTH	N-CA-CB-CG2
4	P	6	DTH	N-CA-CB-OG1
4	P	6	DTH	C-CA-CB-CG2
4	P	6	DTH	C-CA-CB-OG1
3	O	73	HIC	CA-CB-CG-ND1
3	I	73	HIC	CA-CB-CG-ND1
3	J	73	HIC	CA-CB-CG-ND1
4	Q	4	EEP	CA-CB-CG-CD2
4	P	4	EEP	N-CA-CB-CG
3	I	73	HIC	CA-CB-CG-CD2
3	O	73	HIC	CA-CB-CG-CD2
4	Q	6	DTH	N-CA-CB-CG2
4	Q	4	EEP	CA-CB-CG-O1
4	R	4	EEP	CA-CB-CG-O1
4	P	4	EEP	CA-CB-CG-O1
4	P	4	EEP	CA-CB-CG-CD1
4	S	4	EEP	C-CA-CB-CG
4	R	4	EEP	CA-CB-CG-CD2
4	P	4	EEP	CA-CB-CG-CD2
3	J	73	HIC	CA-CB-CG-CD2
4	T	4	EEP	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
4	Q	6	DTH	O-C-CA-CB
4	R	6	DTH	O-C-CA-CB
4	Q	4	EEP	O2-CD1-CG-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	73	HIC	1	0
3	N	73	HIC	1	0
4	Q	6	DTH	1	0
4	T	1	HYP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\# Z > 2$
5	ADP	O	401	6	28,29,29	1.37	5 (17%)	43,45,45	1.83	10 (23%)
5	ADP	L	401	6	28,29,29	1.36	5 (17%)	43,45,45	1.96	11 (25%)
7	PO4	L	403	6	4,4,4	1.09	0	6,6,6	0.47	0
7	PO4	N	403	6	4,4,4	1.02	0	6,6,6	0.46	0
5	ADP	J	401	6	28,29,29	1.37	6 (21%)	43,45,45	1.83	9 (20%)
5	ADP	N	401	6	28,29,29	1.32	5 (17%)	43,45,45	1.87	12 (27%)
5	ADP	I	401	6	28,29,29	1.37	5 (17%)	43,45,45	1.84	13 (30%)
7	PO4	O	403	6	4,4,4	1.03	0	6,6,6	0.43	0
7	PO4	K	401	6	4,4,4	0.99	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	K	402	6	28,29,29	1.37	5 (17%)	43,45,45	1.89	11 (25%)

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
5	ADP	O	401	6	-	0/16/32/32	0/3/3/3
5	ADP	L	401	6	-	6/16/32/32	0/3/3/3
5	ADP	J	401	6	-	6/16/32/32	0/3/3/3
5	ADP	N	401	6	-	6/16/32/32	0/3/3/3
5	ADP	I	401	6	-	6/16/32/32	0/3/3/3
5	ADP	K	402	6	-	0/16/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	401	ADP	C5-C4	4.30	1.46	1.39
5	O	401	ADP	C5-C4	4.26	1.46	1.39
5	L	401	ADP	C5-C4	4.23	1.46	1.39
5	K	402	ADP	C5-C4	4.14	1.46	1.39
5	J	401	ADP	C5-C4	4.04	1.46	1.39
5	N	401	ADP	C5-C4	3.94	1.46	1.39
5	O	401	ADP	C5-C6	2.69	1.48	1.41
5	K	402	ADP	C5-N7	-2.65	1.34	1.39
5	K	402	ADP	C5-C6	2.59	1.48	1.41
5	L	401	ADP	C5-C6	2.58	1.48	1.41
5	J	401	ADP	C5-N7	-2.57	1.34	1.39
5	I	401	ADP	C5-C6	2.55	1.48	1.41
5	N	401	ADP	C5-N7	-2.47	1.34	1.39
5	J	401	ADP	C5-C6	2.47	1.47	1.41
5	L	401	ADP	C5-N7	-2.46	1.34	1.39
5	N	401	ADP	C5-C6	2.46	1.47	1.41
5	I	401	ADP	C5-N7	-2.45	1.34	1.39
5	L	401	ADP	C4-N9	-2.43	1.32	1.37
5	J	401	ADP	C4-N9	-2.37	1.32	1.37
5	I	401	ADP	C4-N9	-2.35	1.32	1.37
5	O	401	ADP	C5-N7	-2.29	1.34	1.39
5	O	401	ADP	C4-N9	-2.24	1.33	1.37
5	I	401	ADP	C8-N7	2.21	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	401	ADP	C8-N7	2.20	1.35	1.31
5	J	401	ADP	C8-N9	-2.19	1.33	1.37
5	N	401	ADP	C4-N9	-2.19	1.33	1.37
5	N	401	ADP	C8-N7	2.16	1.35	1.31
5	L	401	ADP	C8-N7	2.10	1.35	1.31
5	K	402	ADP	C4-N9	-2.10	1.33	1.37
5	K	402	ADP	C8-N7	2.08	1.35	1.31
5	J	401	ADP	C8-N7	2.03	1.35	1.31

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	402	ADP	C5-C4-N3	-5.98	118.49	126.72
5	I	401	ADP	C5-C4-N3	-5.82	118.70	126.72
5	J	401	ADP	C5-C4-N3	-5.81	118.72	126.72
5	L	401	ADP	C5-C4-N3	-5.79	118.74	126.72
5	N	401	ADP	C5-C4-N3	-5.64	118.94	126.72
5	O	401	ADP	C5-C4-N3	-5.33	119.38	126.72
5	L	401	ADP	N3-C4-N9	4.67	135.11	127.17
5	K	402	ADP	N3-C4-N9	4.56	134.92	127.17
5	J	401	ADP	N3-C4-N9	4.52	134.85	127.17
5	I	401	ADP	N3-C4-N9	4.43	134.71	127.17
5	N	401	ADP	N3-C4-N9	4.40	134.64	127.17
5	O	401	ADP	N3-C4-N9	4.30	134.48	127.17
5	L	401	ADP	C2'-C1'-N9	-3.83	103.80	113.30
5	L	401	ADP	C2-N3-C4	3.71	120.90	111.83
5	K	402	ADP	C2-N3-C4	3.71	120.88	111.83
5	N	401	ADP	C2-N3-C4	3.70	120.87	111.83
5	J	401	ADP	C2-N3-C4	3.65	120.75	111.83
5	J	401	ADP	C4-C5-N7	-3.65	106.41	110.58
5	O	401	ADP	C2-N3-C4	3.64	120.73	111.83
5	I	401	ADP	C2-N3-C4	3.64	120.71	111.83
5	K	402	ADP	C4-C5-N7	-3.54	106.53	110.58
5	I	401	ADP	C4-C5-N7	-3.53	106.54	110.58
5	N	401	ADP	C4-C5-N7	-3.51	106.57	110.58
5	O	401	ADP	C4-C5-N7	-3.36	106.74	110.58
5	L	401	ADP	C4-C5-N7	-3.35	106.76	110.58
5	O	401	ADP	N3-C2-N1	-3.32	123.56	128.58
5	N	401	ADP	N3-C2-N1	-3.30	123.59	128.58
5	L	401	ADP	N3-C2-N1	-3.23	123.69	128.58
5	J	401	ADP	N3-C2-N1	-3.15	123.81	128.58
5	O	401	ADP	C4-N9-C8	3.15	109.04	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	401	ADP	C4-N9-C8	3.10	108.99	105.74
5	K	402	ADP	N3-C2-N1	-3.07	123.93	128.58
5	I	401	ADP	N3-C2-N1	-3.06	123.95	128.58
5	N	401	ADP	C4-N9-C8	2.95	108.84	105.74
5	L	401	ADP	O4'-C1'-N9	2.92	113.70	108.09
5	J	401	ADP	C4-N9-C8	2.92	108.81	105.74
5	K	402	ADP	C2'-C1'-N9	-2.81	106.32	113.30
5	N	401	ADP	O4'-C1'-N9	2.75	113.37	108.09
5	I	401	ADP	C4-N9-C8	2.65	108.52	105.74
5	N	401	ADP	C5-N7-C8	2.64	107.60	103.45
5	K	402	ADP	C3'-C2'-C1'	2.62	106.42	101.46
5	J	401	ADP	C5-N7-C8	2.57	107.50	103.45
5	K	402	ADP	C5-N7-C8	2.52	107.40	103.45
5	O	401	ADP	C3'-C2'-C1'	2.49	106.17	101.46
5	O	401	ADP	C5-N7-C8	2.47	107.33	103.45
5	I	401	ADP	C5-N7-C8	2.43	107.27	103.45
5	K	402	ADP	O4'-C1'-N9	2.41	112.72	108.09
5	L	401	ADP	C5-N7-C8	2.38	107.20	103.45
5	K	402	ADP	C4-N9-C8	2.37	108.23	105.74
5	N	401	ADP	N9-C8-N7	-2.36	110.59	113.94
5	O	401	ADP	C6-C5-N7	2.36	136.63	132.09
5	L	401	ADP	C3'-C2'-C1'	2.34	105.89	101.46
5	N	401	ADP	C2'-C1'-N9	-2.26	107.69	113.30
5	O	401	ADP	N9-C8-N7	-2.25	110.74	113.94
5	N	401	ADP	O3B-PB-O2B	2.25	116.22	107.80
5	I	401	ADP	C2'-C1'-N9	-2.23	107.77	113.30
5	I	401	ADP	O3B-PB-O2B	2.21	116.08	107.80
5	J	401	ADP	N9-C8-N7	-2.17	110.86	113.94
5	N	401	ADP	C6-C5-N7	2.16	136.25	132.09
5	L	401	ADP	N9-C8-N7	-2.15	110.89	113.94
5	I	401	ADP	O4'-C1'-N9	2.11	112.14	108.09
5	J	401	ADP	C6-C5-N7	2.09	136.12	132.09
5	I	401	ADP	C3'-C2'-C1'	2.06	105.36	101.46
5	I	401	ADP	N9-C8-N7	-2.02	111.07	113.94
5	I	401	ADP	C6-C5-N7	2.02	135.98	132.09
5	K	402	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	401	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	I	401	ADP	C5'-O5'-PA-O2A
5	J	401	ADP	C5'-O5'-PA-O1A
5	J	401	ADP	C5'-O5'-PA-O2A
5	J	401	ADP	C5'-O5'-PA-O3A
5	L	401	ADP	C5'-O5'-PA-O1A
5	L	401	ADP	C5'-O5'-PA-O2A
5	N	401	ADP	C5'-O5'-PA-O2A
5	I	401	ADP	O4'-C4'-C5'-O5'
5	I	401	ADP	C3'-C4'-C5'-O5'
5	L	401	ADP	O4'-C4'-C5'-O5'
5	L	401	ADP	C3'-C4'-C5'-O5'
5	N	401	ADP	O4'-C4'-C5'-O5'
5	N	401	ADP	C3'-C4'-C5'-O5'
5	J	401	ADP	O4'-C4'-C5'-O5'
5	J	401	ADP	C3'-C4'-C5'-O5'
5	N	401	ADP	PA-O3A-PB-O2B
5	I	401	ADP	PB-O3A-PA-O1A
5	I	401	ADP	C5'-O5'-PA-O3A
5	L	401	ADP	C5'-O5'-PA-O3A
5	N	401	ADP	C5'-O5'-PA-O1A
5	N	401	ADP	C5'-O5'-PA-O3A
5	J	401	ADP	PB-O3A-PA-O2A
5	L	401	ADP	PB-O3A-PA-O2A

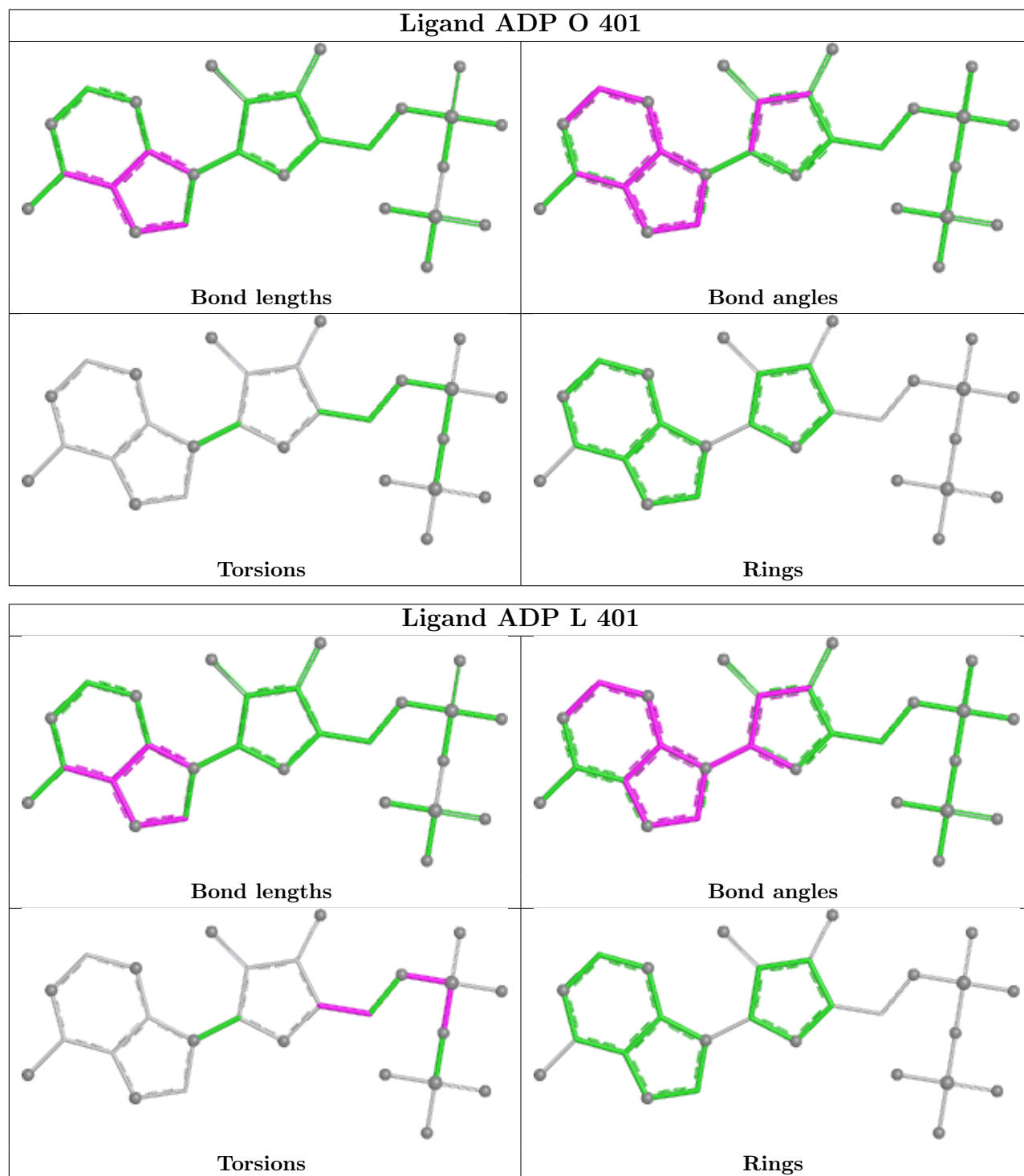
There are no ring outliers.

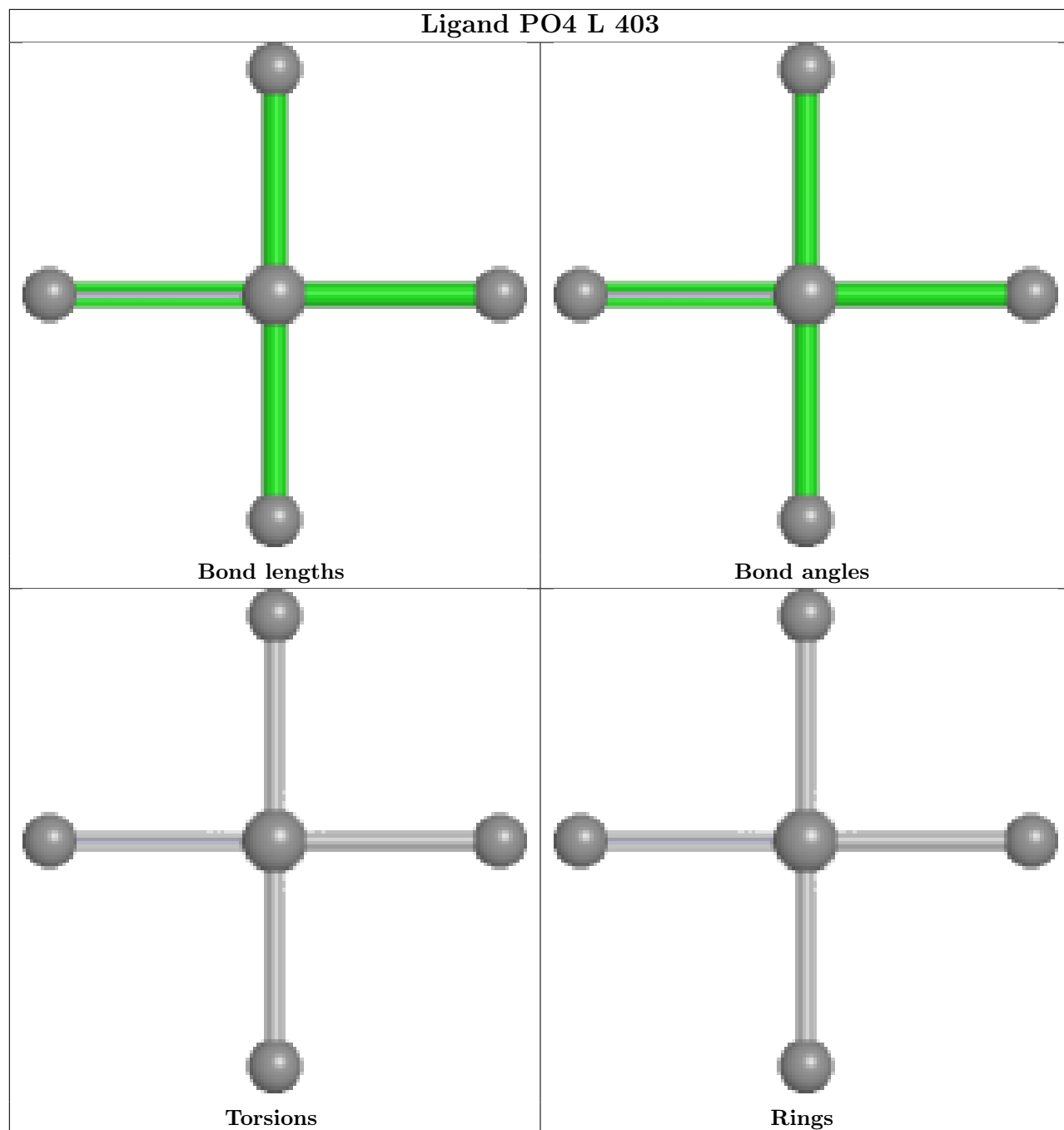
5 monomers are involved in 10 short contacts:

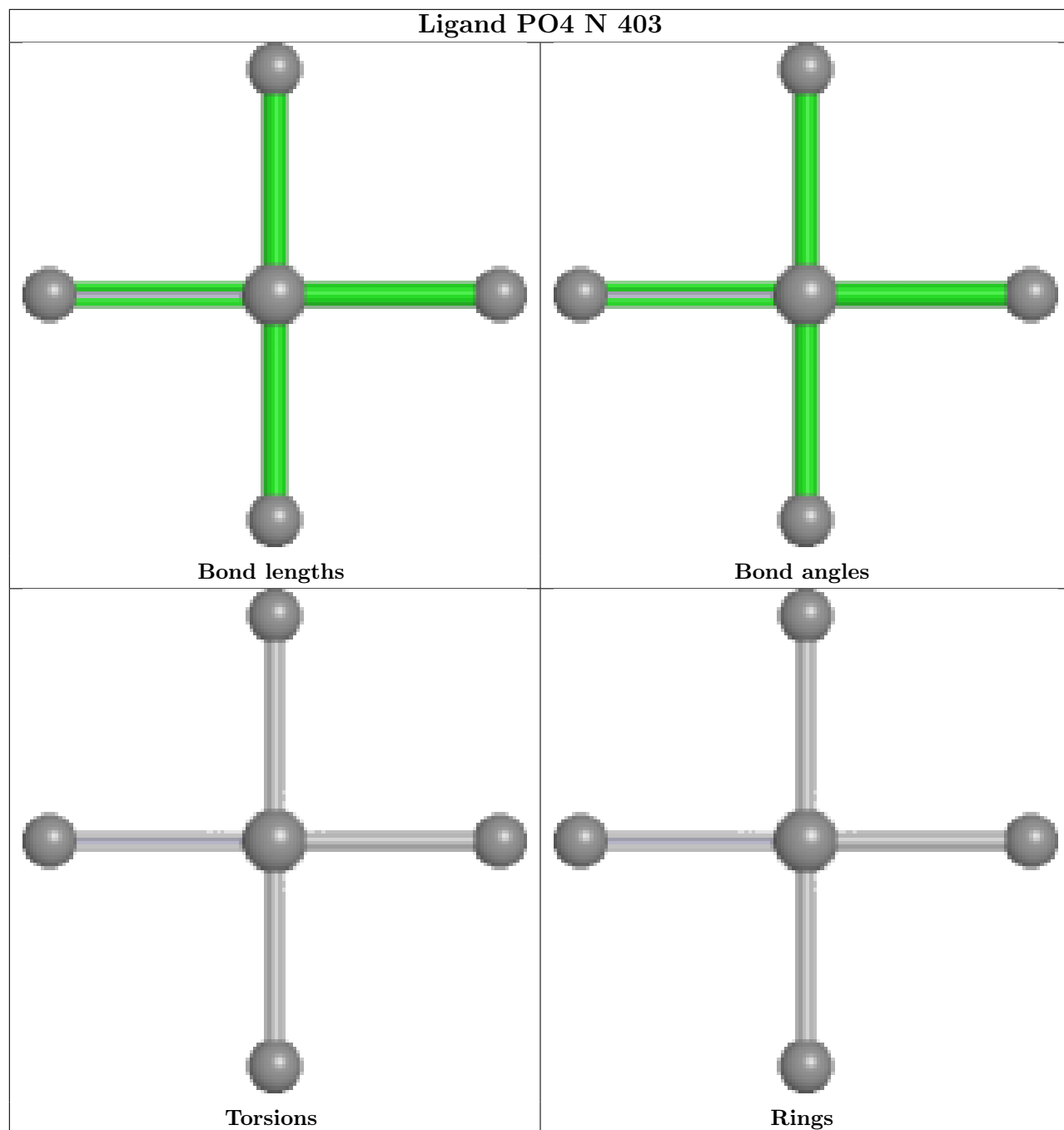
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	401	ADP	2	0
5	J	401	ADP	1	0
5	N	401	ADP	1	0
5	I	401	ADP	3	0
5	K	402	ADP	3	0

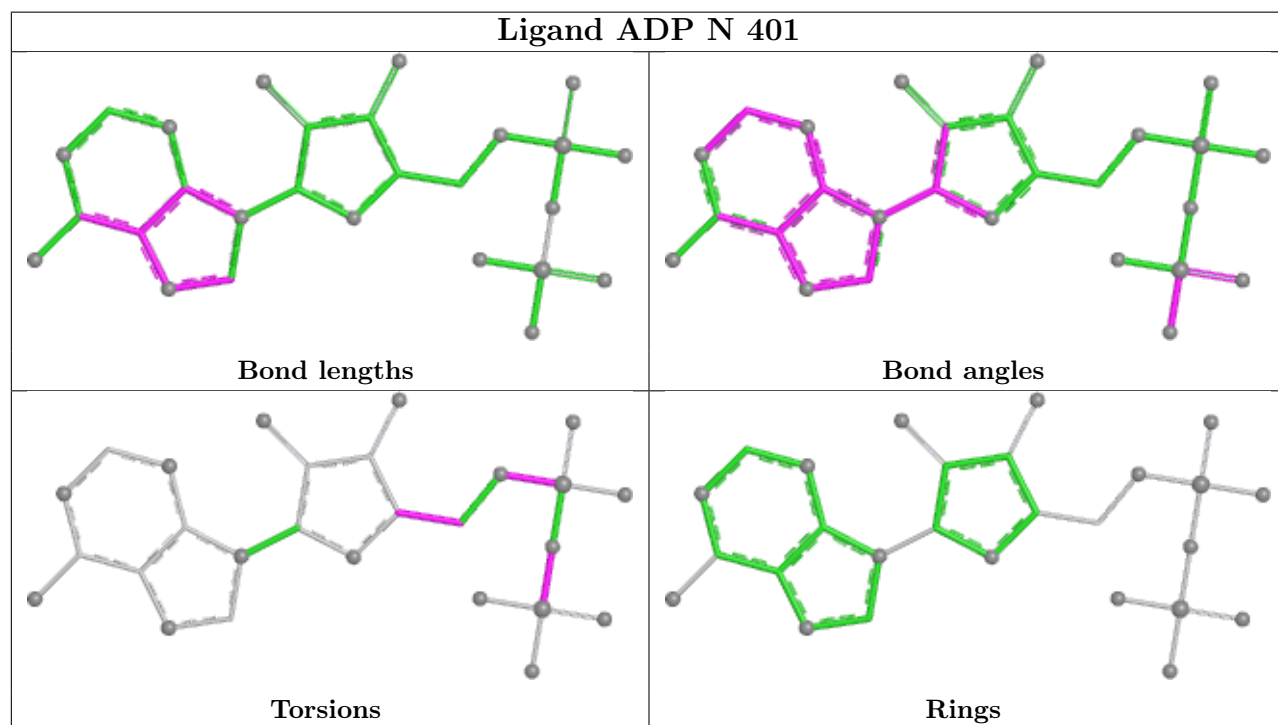
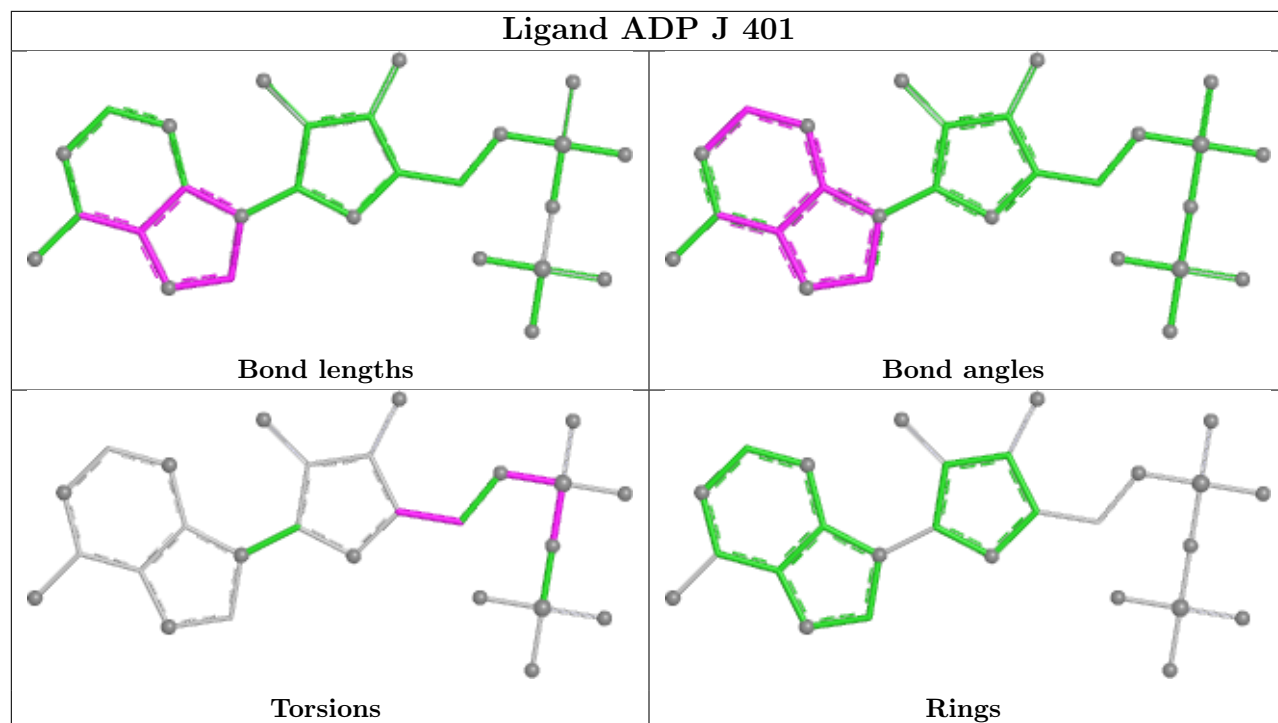
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

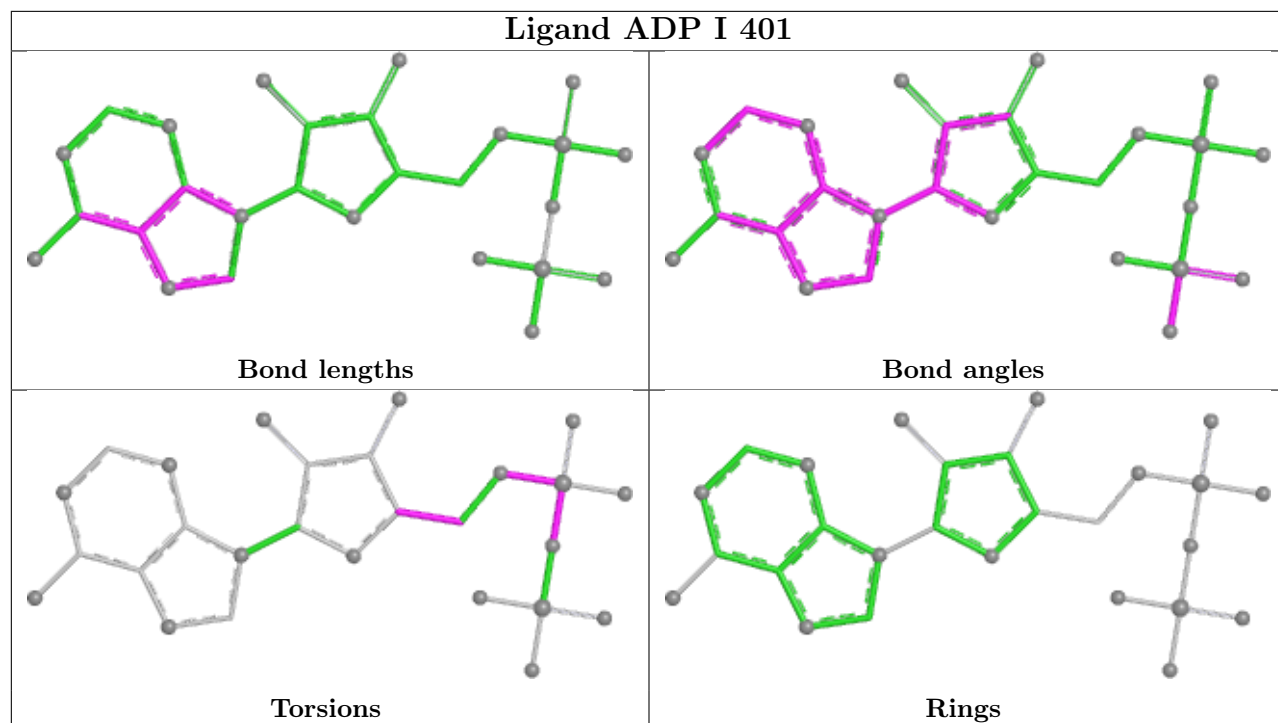
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

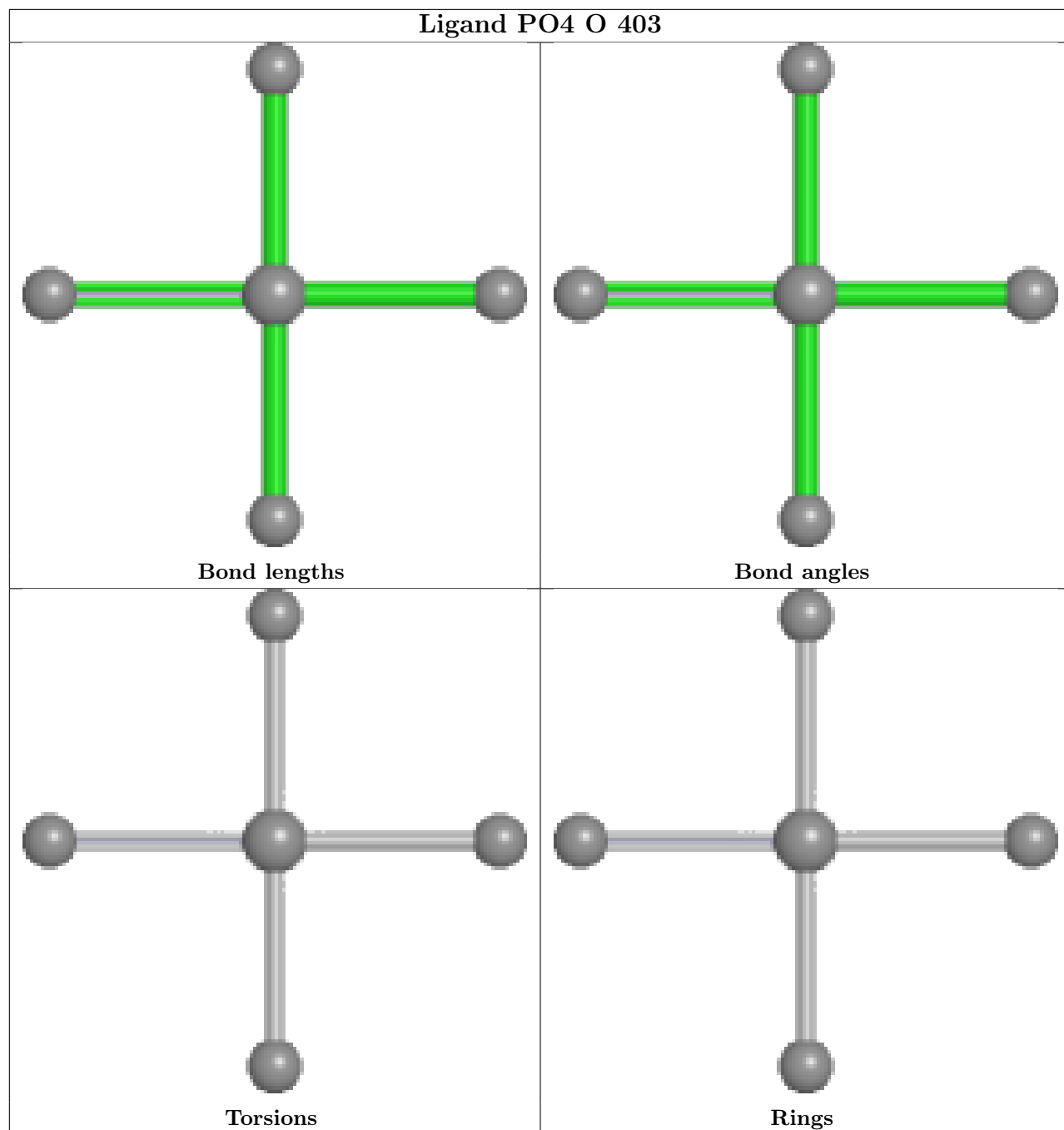


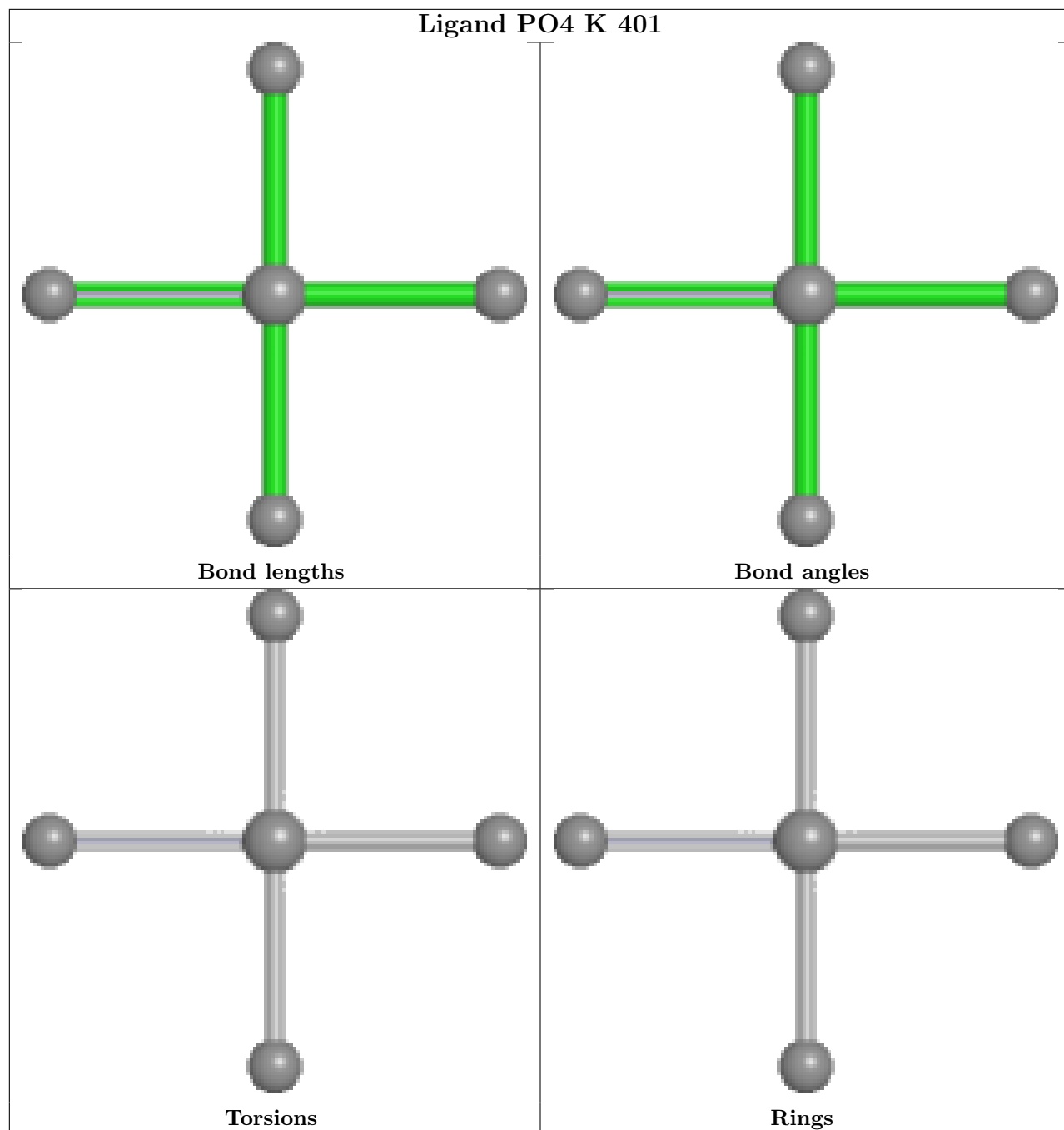


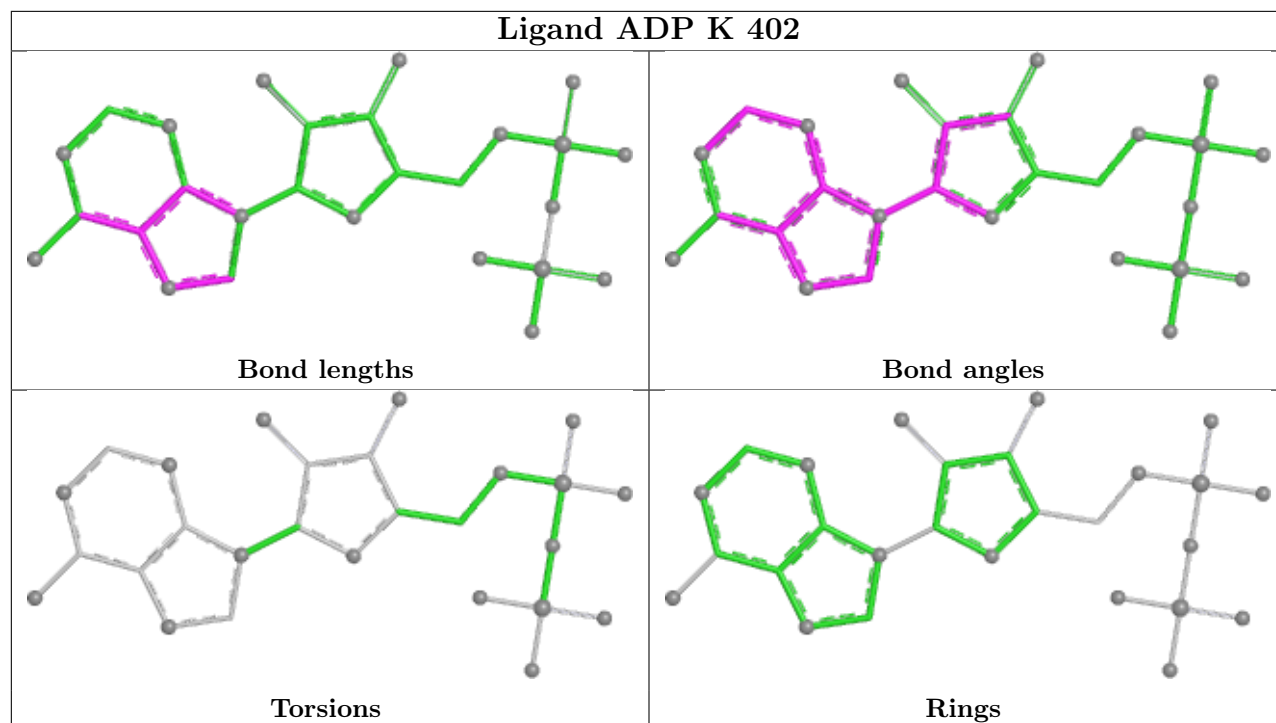












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

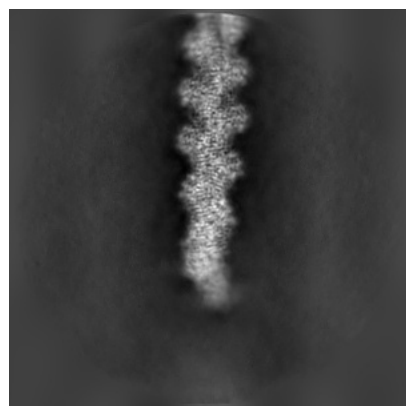
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13343. These allow visual inspection of the internal detail of the map and identification of artifacts.

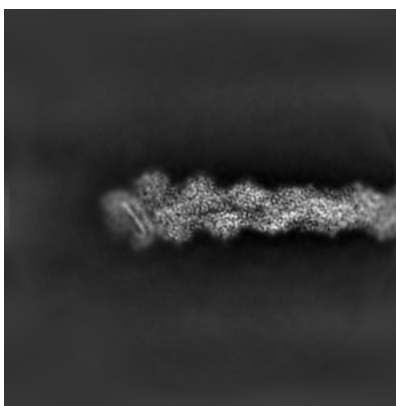
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

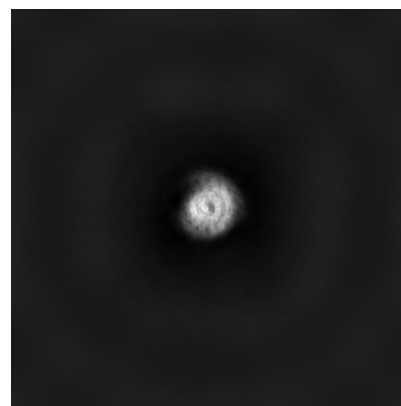
6.1.1 Primary map



X

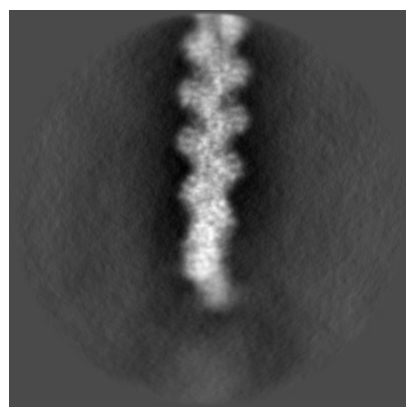


Y

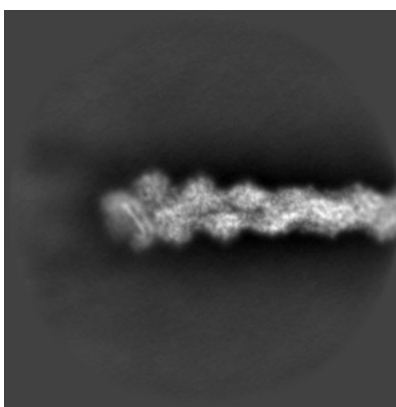


Z

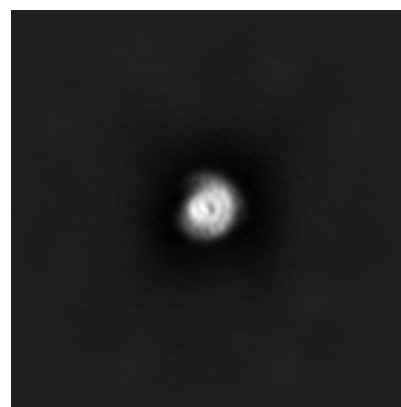
6.1.2 Raw map



X



Y

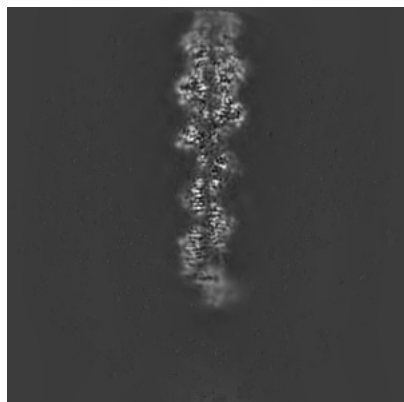


Z

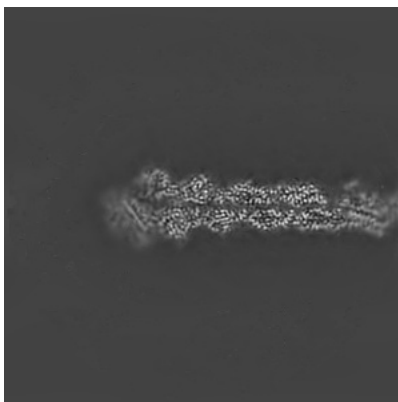
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

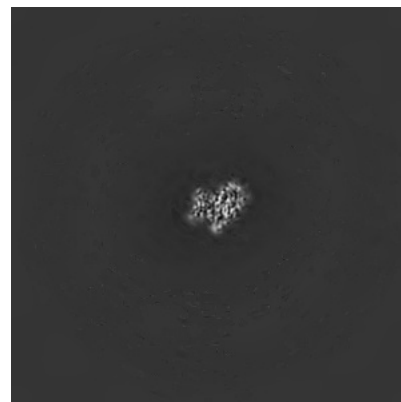
6.2.1 Primary map



X Index: 192

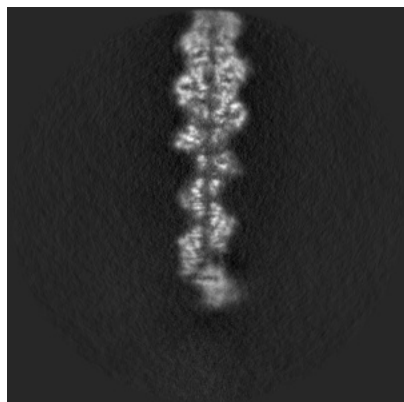


Y Index: 192

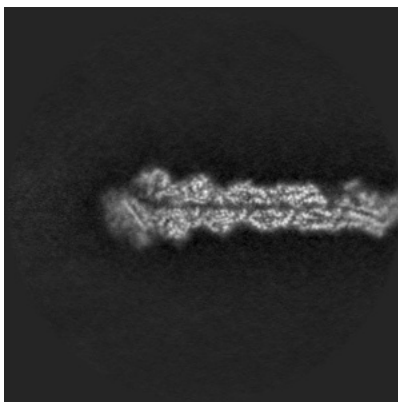


Z Index: 192

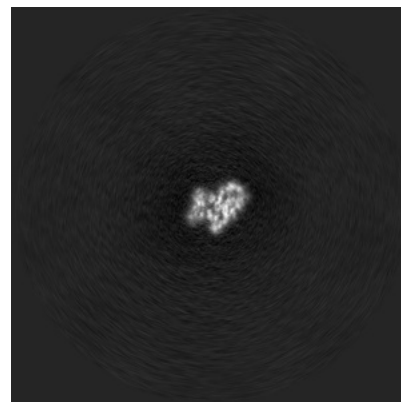
6.2.2 Raw map



X Index: 192



Y Index: 192

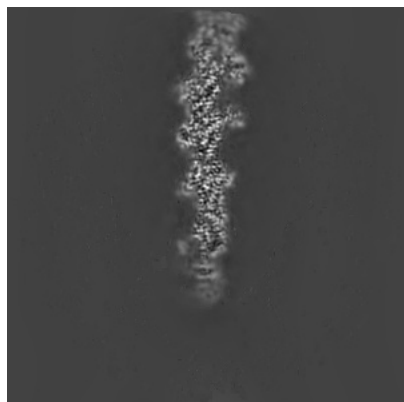


Z Index: 192

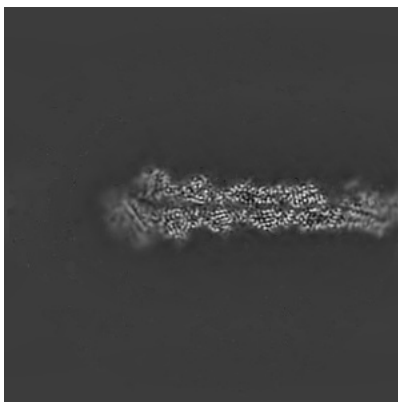
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

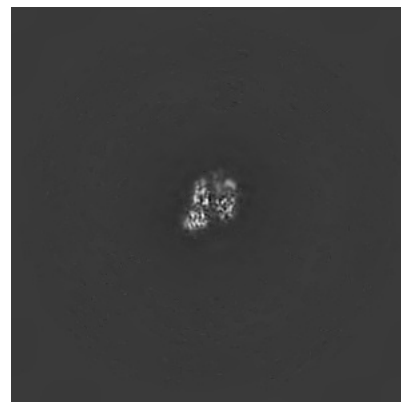
6.3.1 Primary map



X Index: 184

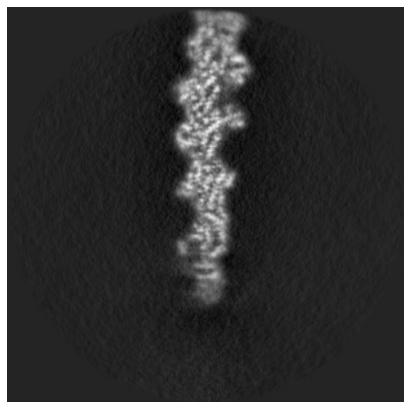


Y Index: 191

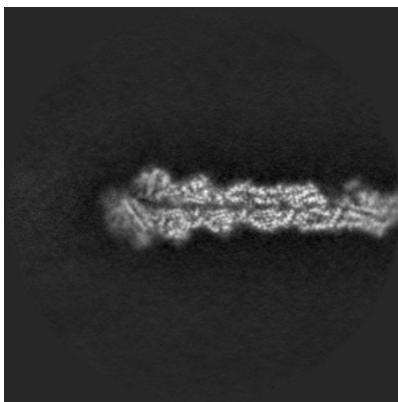


Z Index: 222

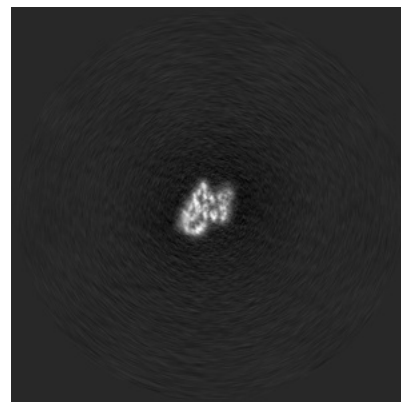
6.3.2 Raw map



X Index: 184



Y Index: 191

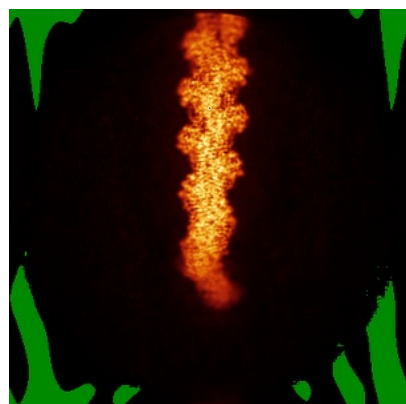


Z Index: 214

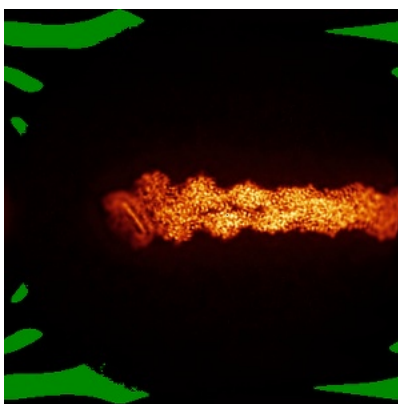
The images above show the largest variance slices of the map in three orthogonal directions.

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

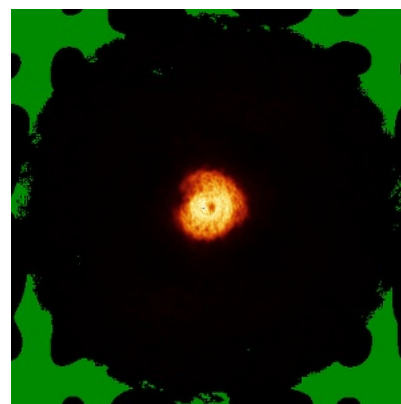
6.4.1 Primary map



X

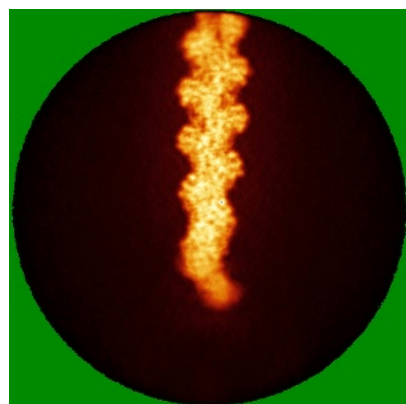


Y



Z

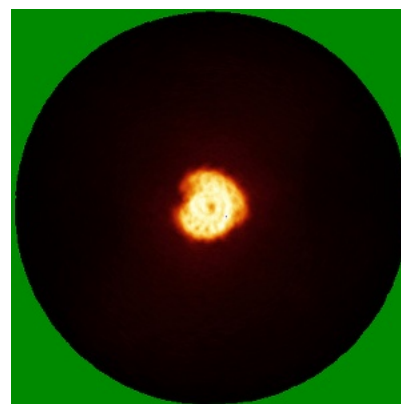
6.4.2 Raw map



X



Y

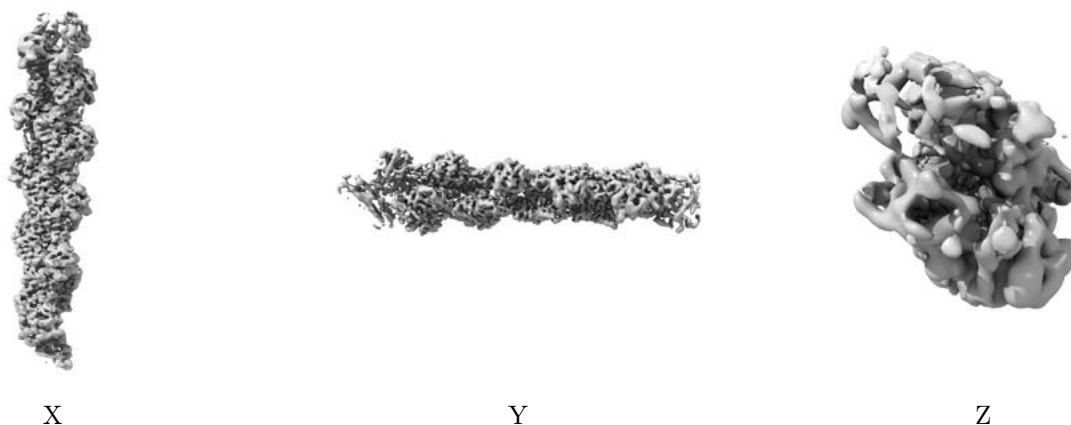


Z

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.

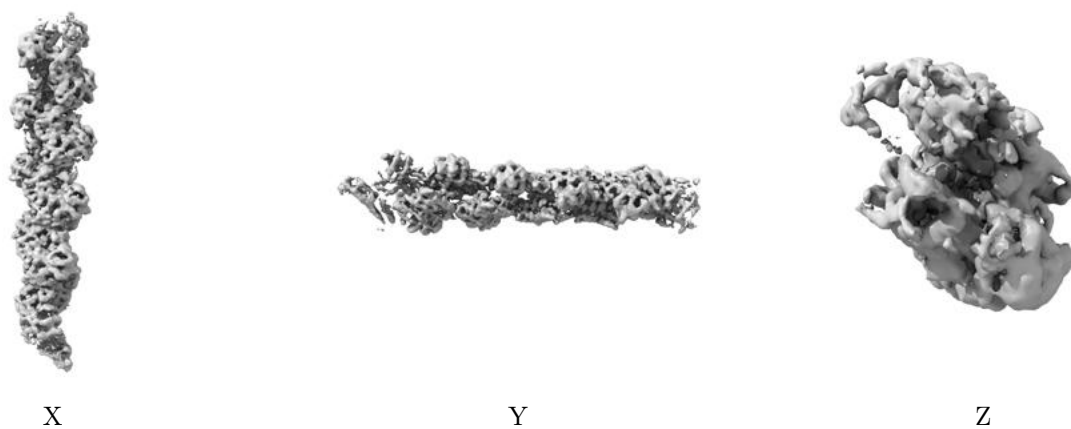
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

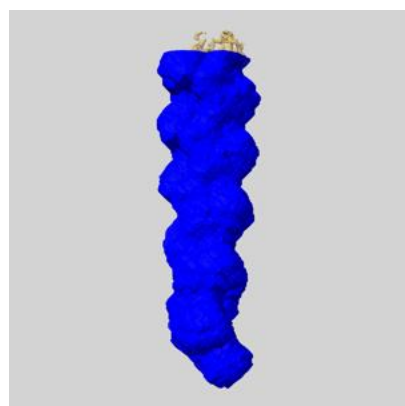
6.6 Mask visualisation [i](#)

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

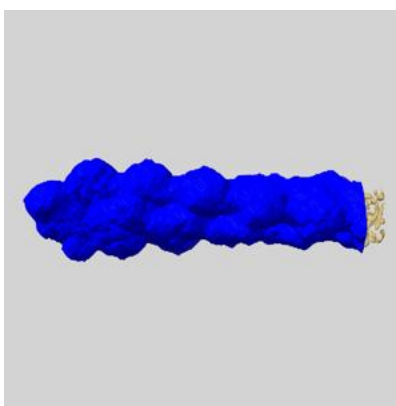
A mask typically either:

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

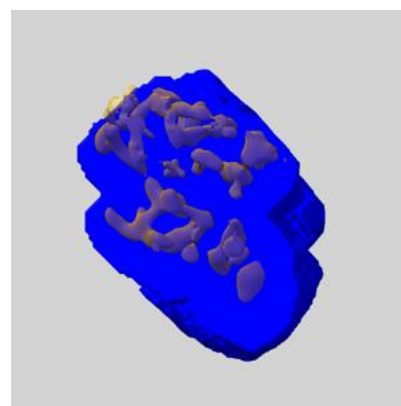
6.6.1 emd_13343_msk_1.map [i](#)



X



Y

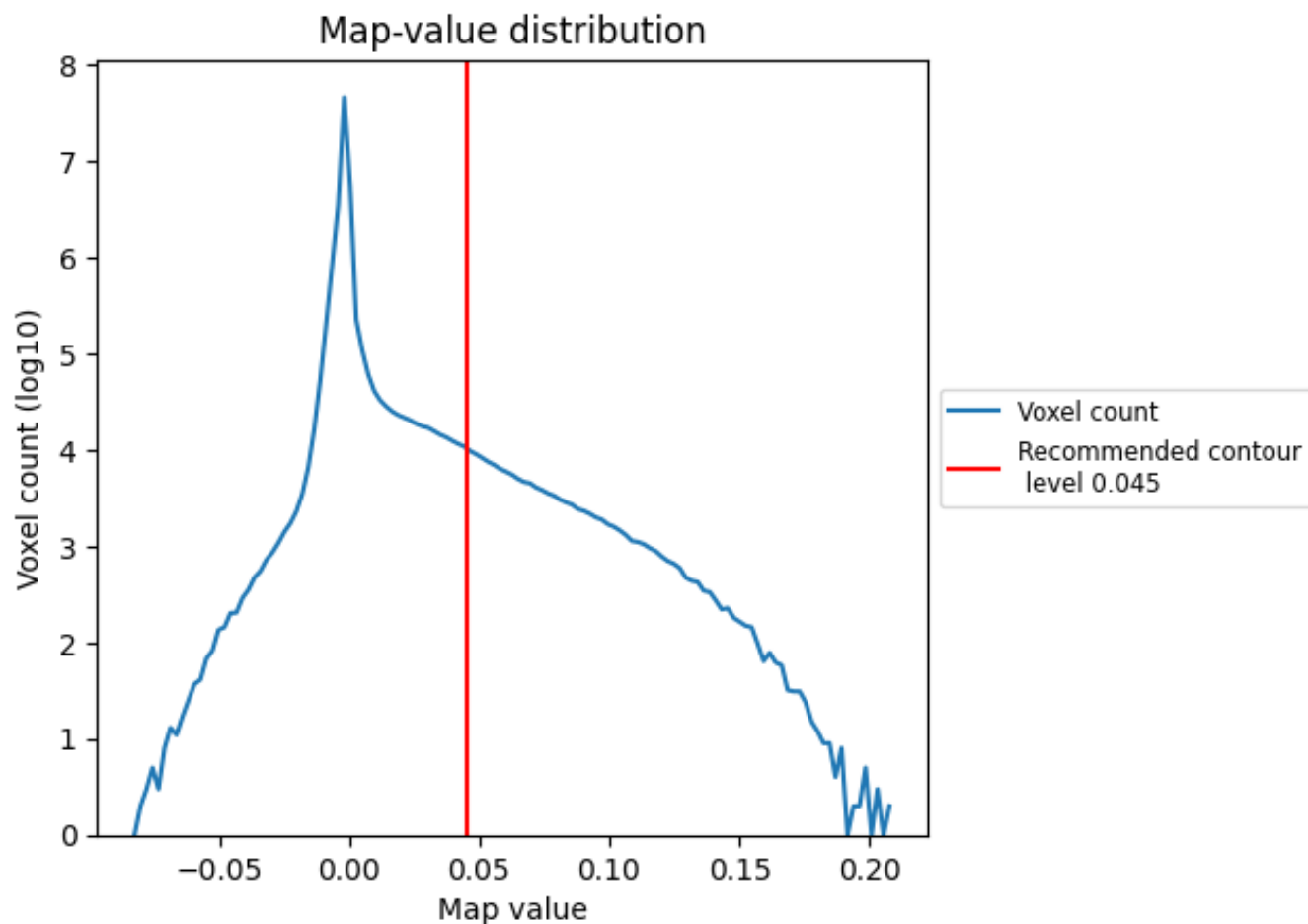


Z

7 Map analysis [i](#)

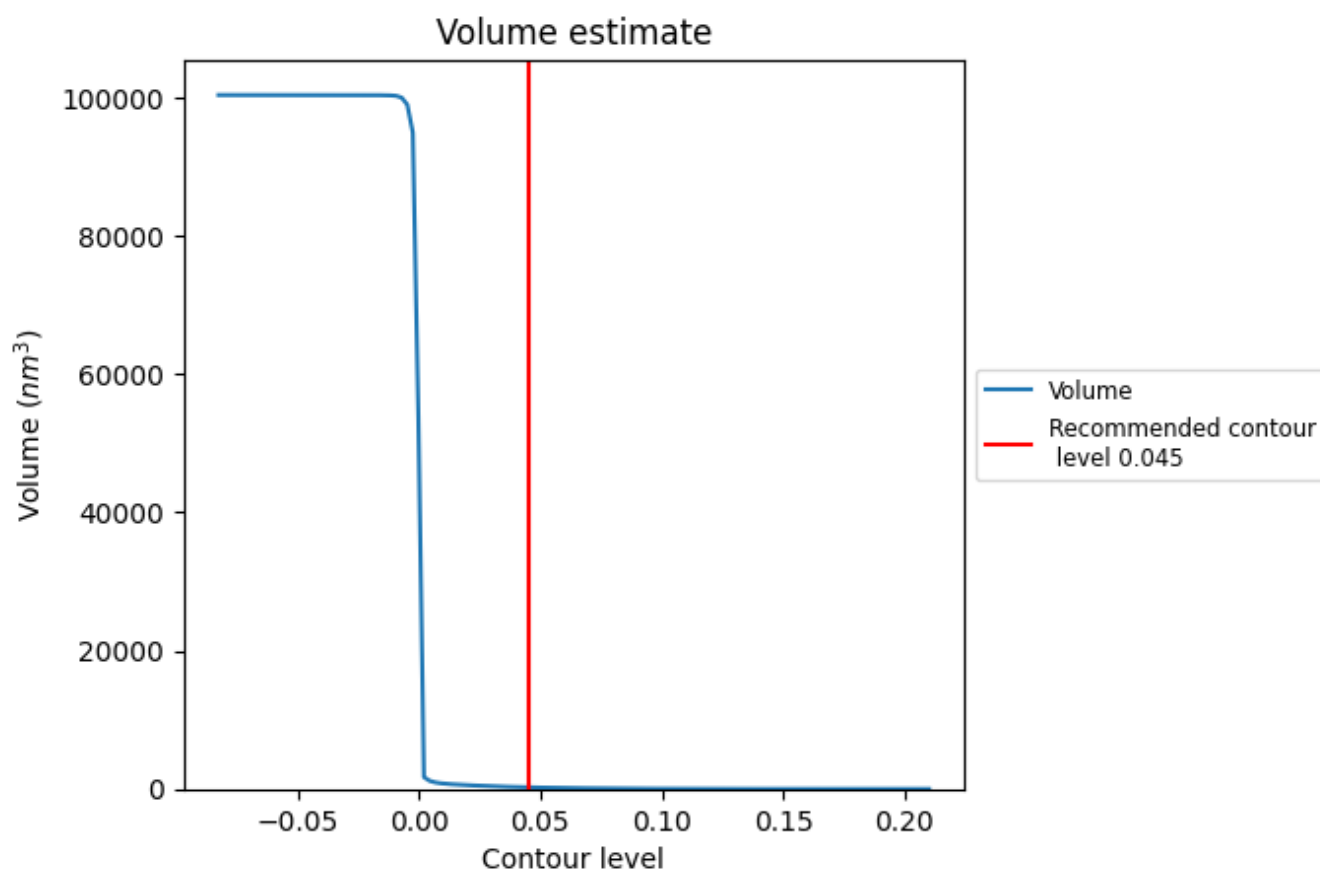
This section contains the results of statistical analysis of the map.

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.

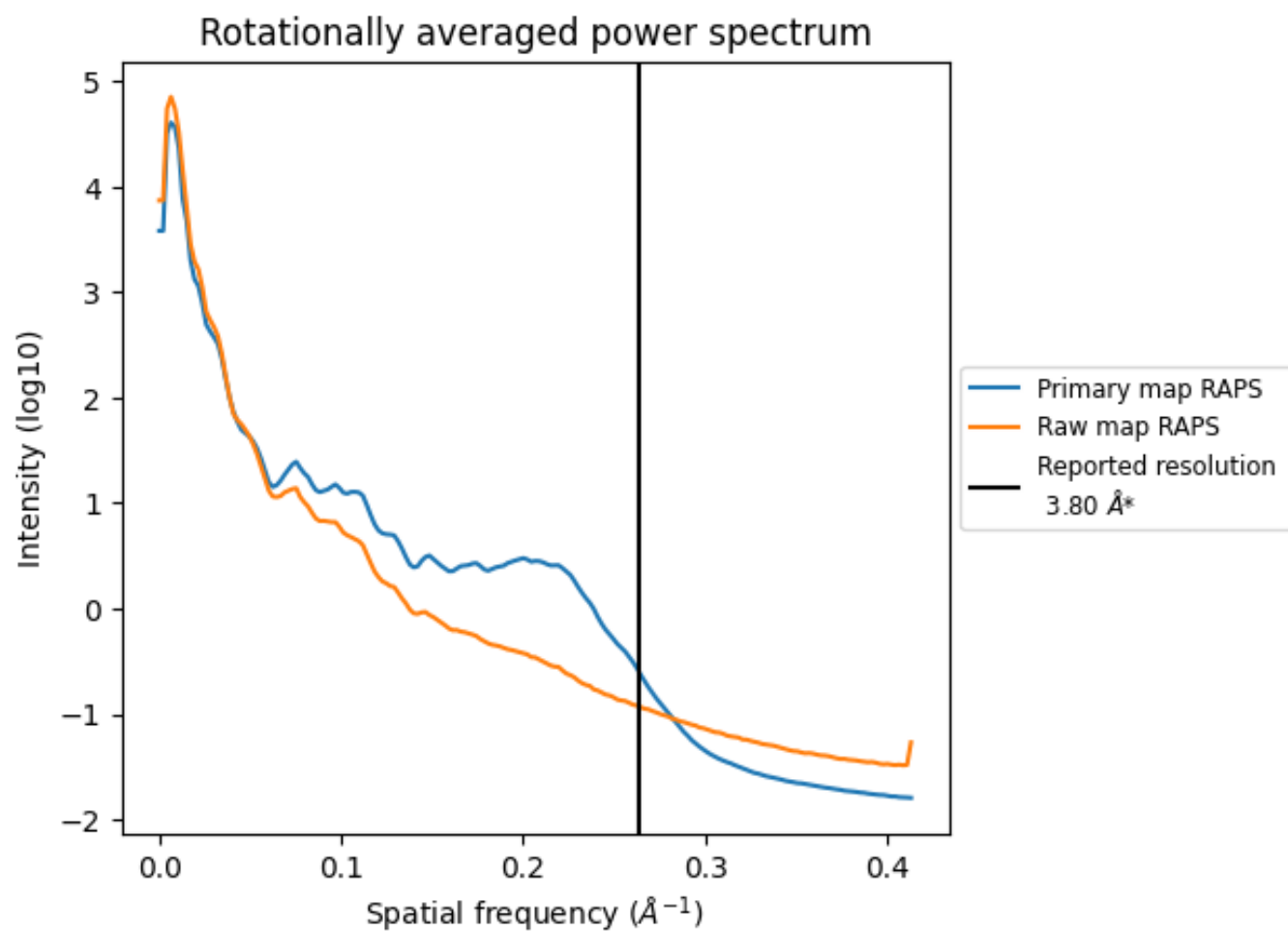
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm³; this corresponds to an approximate mass of 212 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 ⓘ

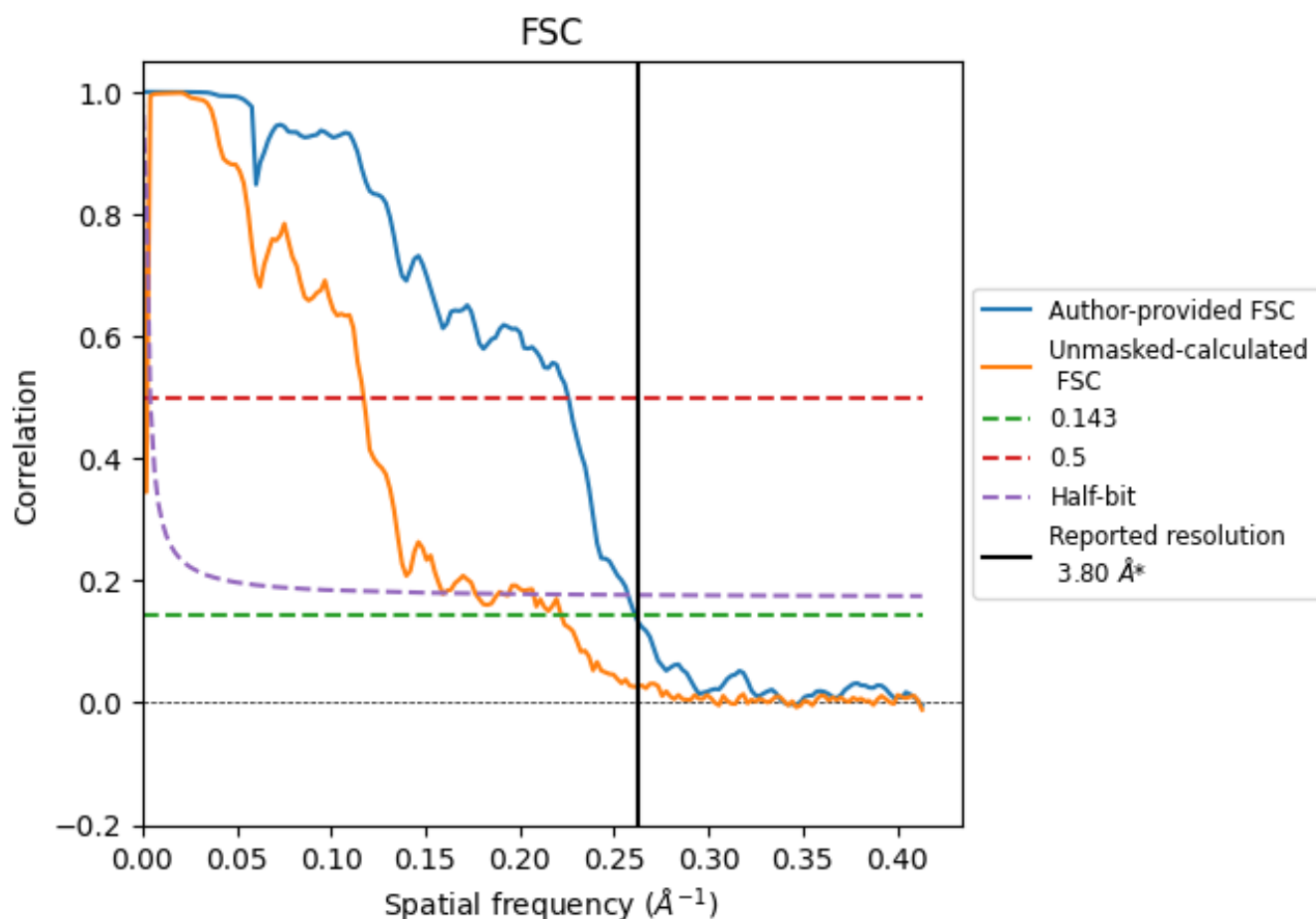


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

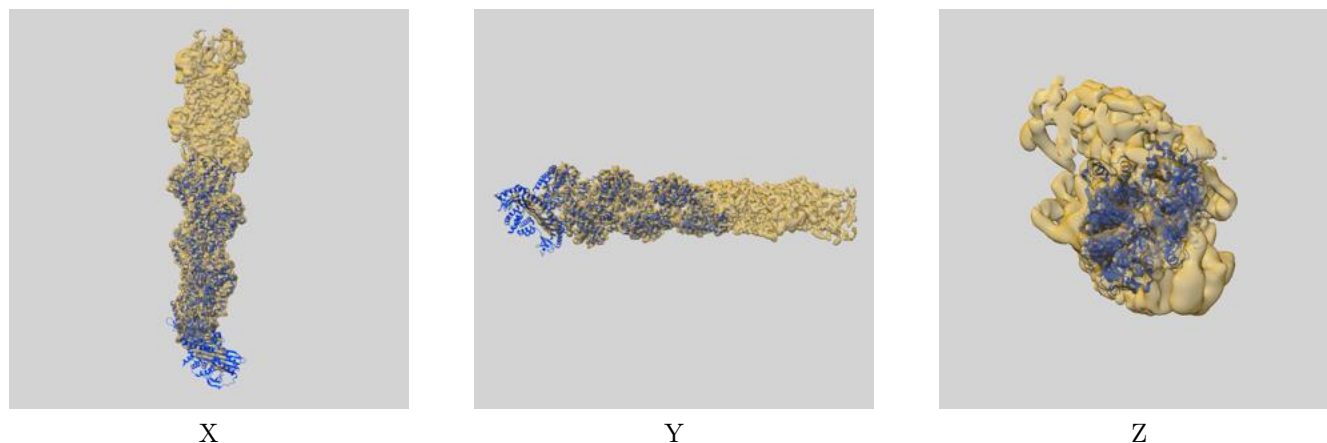
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.43	3.89
Unmasked-calculated*	4.50	370.37	312.50

*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 4.50 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

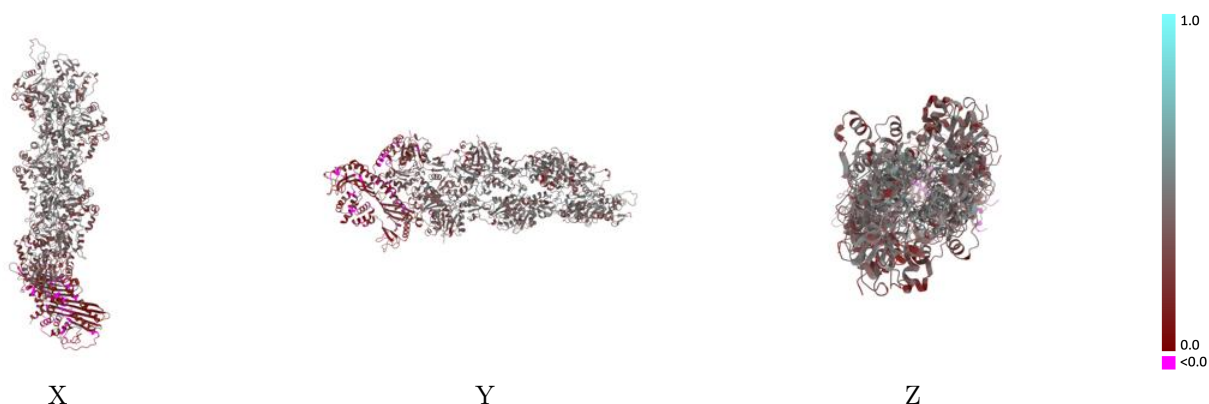
This section contains information regarding the fit between EMDB map EMD-13343 and PDB model 7PDZ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



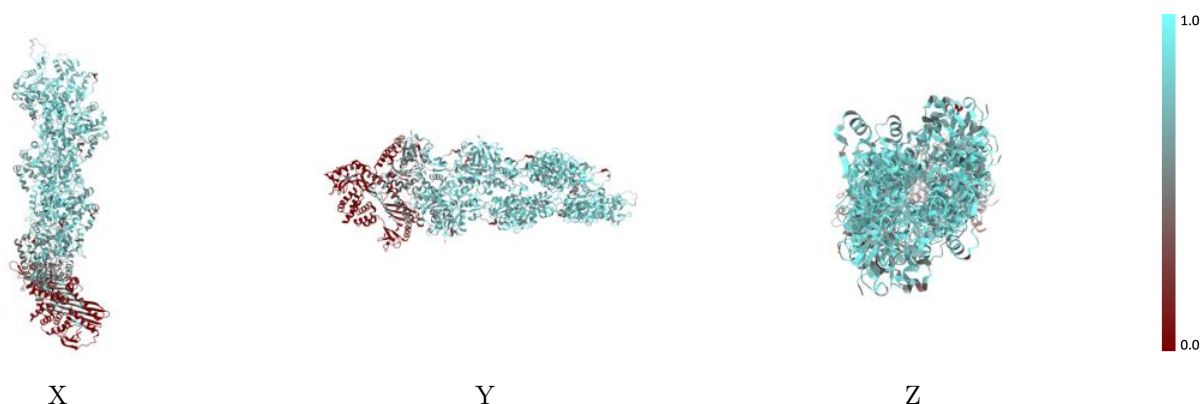
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



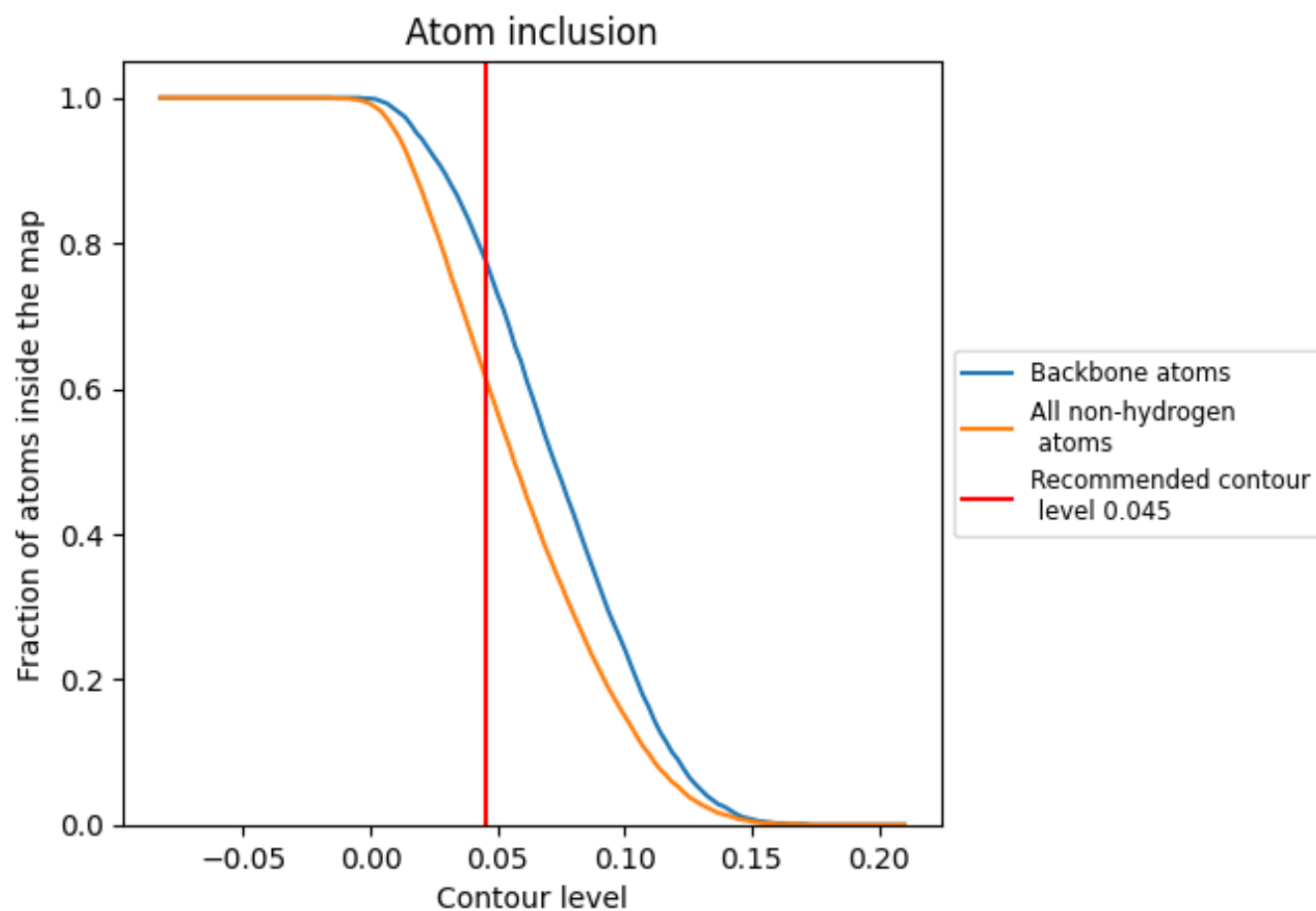
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 62% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6180	 0.3330
E	 0.1400	 0.1410
F	 0.1570	 0.1210
I	 0.5540	 0.3030
J	 0.7230	 0.3690
K	 0.7770	 0.4040
L	 0.7730	 0.4040
N	 0.7820	 0.4060
O	 0.7700	 0.3990
P	 0.9630	 0.5060
Q	 0.9070	 0.5310
R	 0.8700	 0.5160
S	 0.9260	 0.4990
T	 0.9440	 0.4760

