



## Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 05:20 PM EDT

PDB ID : 9B85 / pdb\_00009b85  
EMDB ID : EMD-44333  
Title : Cryo-EM structure of human dynactin complex bound to Chlamydia effector Dre1  
Authors : Pawar, K.I.; Verba, K.A.  
Deposited on : 2024-03-28  
Resolution : 3.47 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](mailto: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>.

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

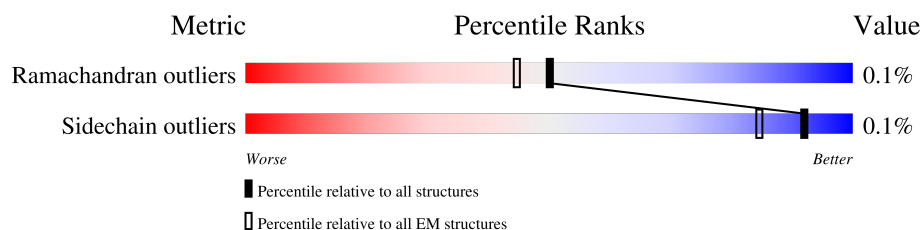
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 3.47 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.





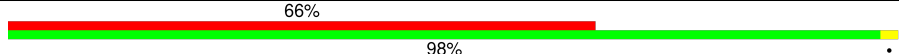
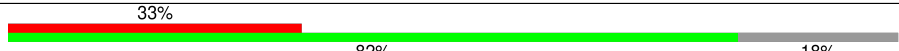

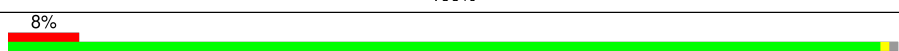
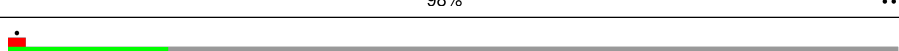
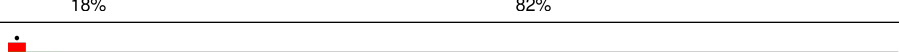
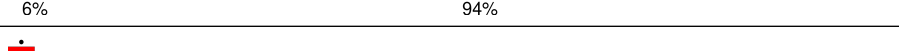
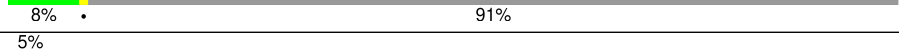
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	376	96% ..
1	B	376	97% ..
1	C	376	98% .
1	D	376	97% ..
1	E	376	97% ..
1	F	376	96% ..
1	G	376	96% ..
1	I	376	97% ..
2	H	375	98% ..

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Mol	Chain	Length	Quality of chain
3	J	417	
4	K	460	
5	L	182	
6	M	190	
7	N	286	
8	O	272	
9	P	401	
9	Q	401	
9	p	401	
9	q	401	

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 82296 atoms, of which 41052 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 Alpha-centractin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	B	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	C	375	Total	C	H	N	O	S	0	0
			5982	1918	2984	514	556	10		
1	D	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	E	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	F	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	G	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	I	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	370	Total	C	H	N	O	S	0	0
			5742	1827	2857	486	550	22		

- Molecule 3 is a protein called Actin-related protein 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	J	387	Total	C	H	N	O	S	0	0
			6140	1944	3113	514	552	17		

- Molecule 4 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	K	361	Total	C	H	N	O	S	0	0
			5895	1848	2982	517	525	23		

- Molecule 5 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	182	Total	C	H	N	O	S	0	0
			2846	897	1438	241	257	13		

- Molecule 6 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	M	156	Total	C	H	N	O	S	0	0
			2408	753	1217	206	222	10		

- Molecule 7 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	N	286	Total	C	H	N	O	S	0	0
			4559	1462	2235	404	451	7		

- Molecule 8 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	O	269	Total	C	H	N	O	S	0	0
			4236	1323	2114	370	418	11		

- Molecule 9 is a protein called Dynactin subunit 2.

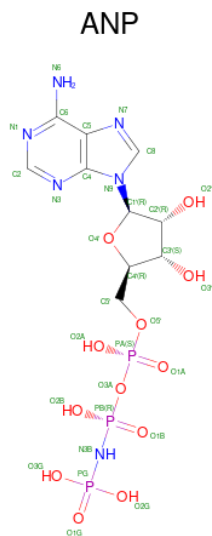
Mol	Chain	Residues	Atoms						AltConf	Trace
9	P	74	Total	C	H	N	O		0	0
			1141	361	560	98	122			
9	Q	24	Total	C	H	N	O		0	0
			361	118	173	29	41			
9	p	37	Total	C	H	N	O	S	0	0
			543	179	257	42	63	2		
9	q	48	Total	C	H	N	O		0	0
			733	238	354	59	82			

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
10	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
10	C	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
10	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
10	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
10	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
10	G	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
10	I	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						AltConf
11	H	1	Total	C	H	N	O	P	0
			46	10	15	6	12	3	

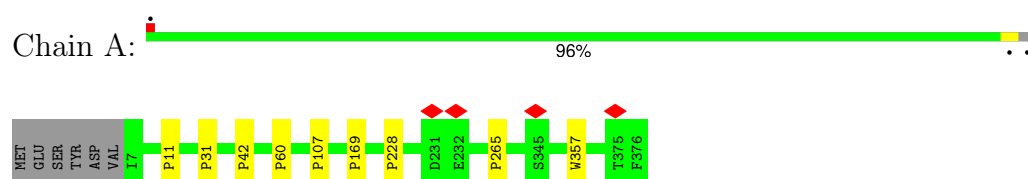
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms	AltConf
12	K	3	Total Zn 3 3	0

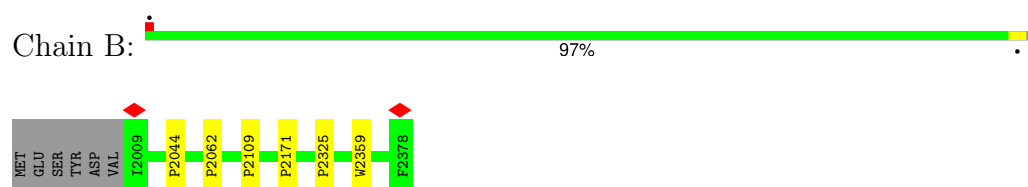
### 3 Residue-property plots [i](#)

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.

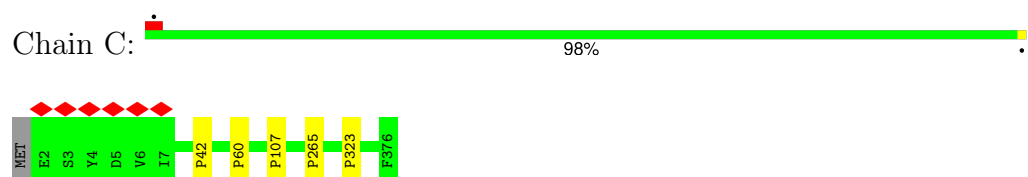
- Molecule 1: Alpha-centractin



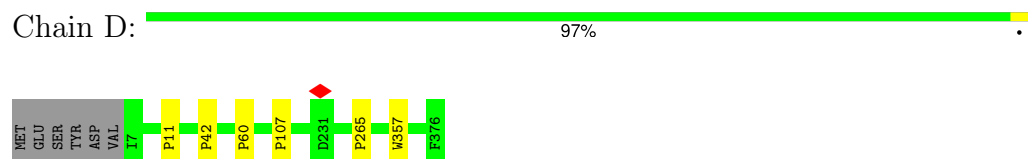
- Molecule 1: Alpha-centractin



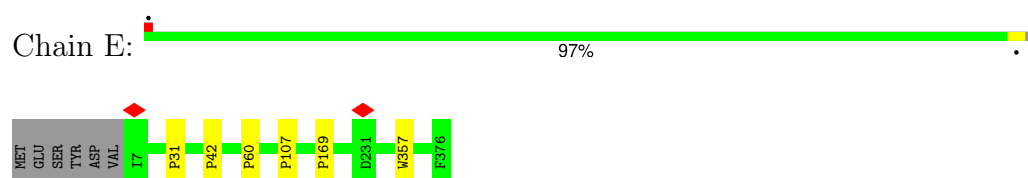
- Molecule 1: Alpha-centractin



- Molecule 1: Alpha-centractin



- Molecule 1: Alpha-centractin





- Molecule 1: Alpha-centractin

Chain F:  96%



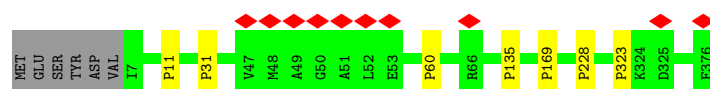
- Molecule 1: Alpha-centractin

Chain G:  96%



- Molecule 1: Alpha-centractin

Chain I:  97%



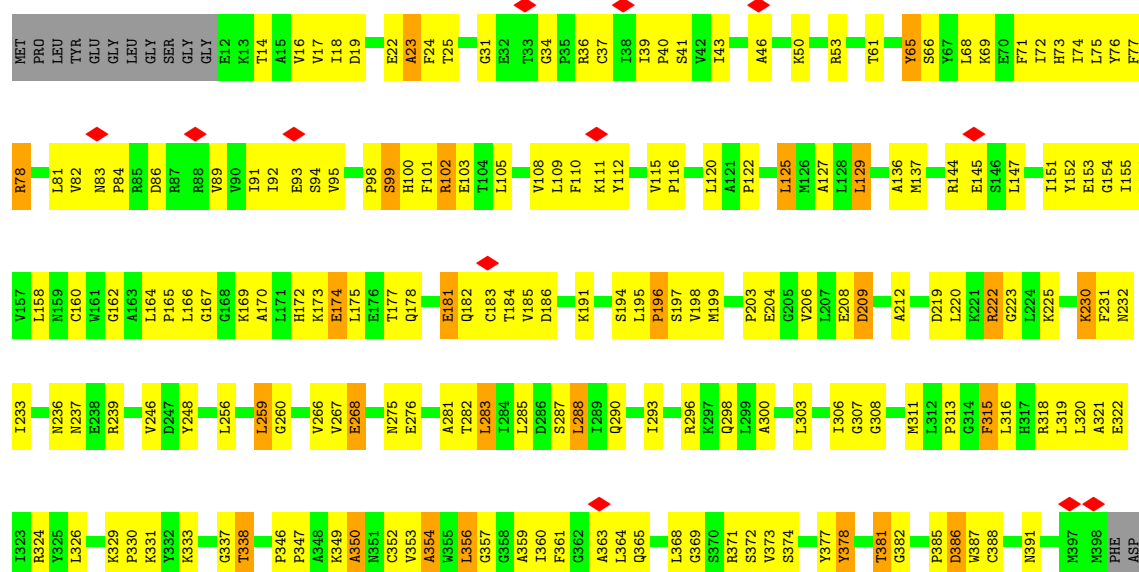
- Molecule 2: Actin, cytoplasmic 1

Chain H:  98%



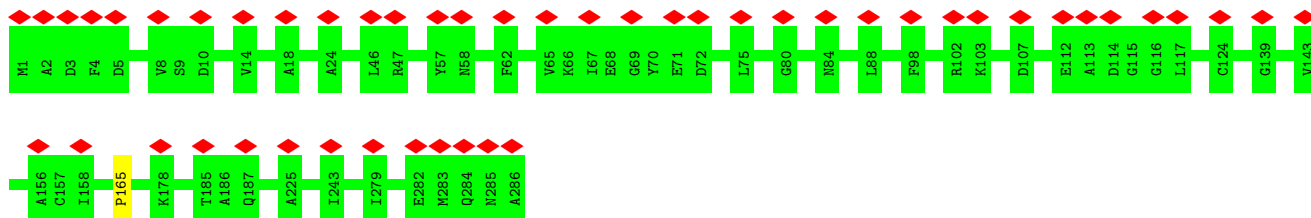
- Molecule 3: Actin-related protein 10

Chain J:  47%

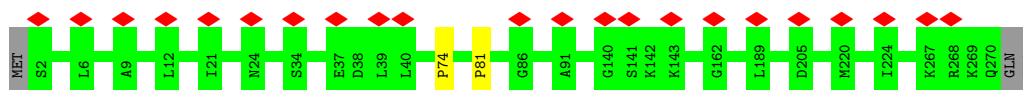


[illegible]

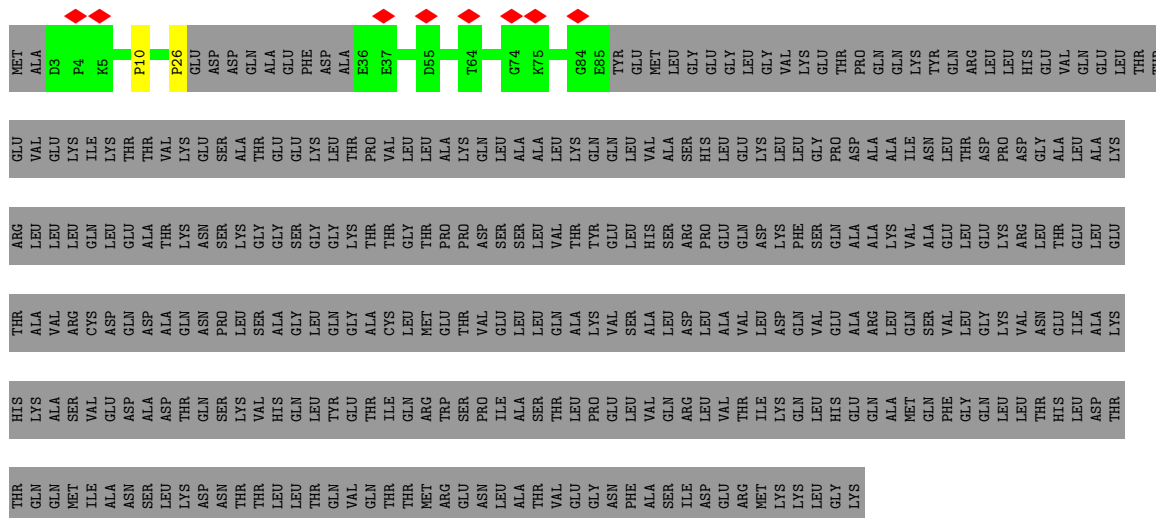
- Molecule 7: F-actin-capping protein subunit alpha-1



- Molecule 8: F-actin-capping protein subunit beta

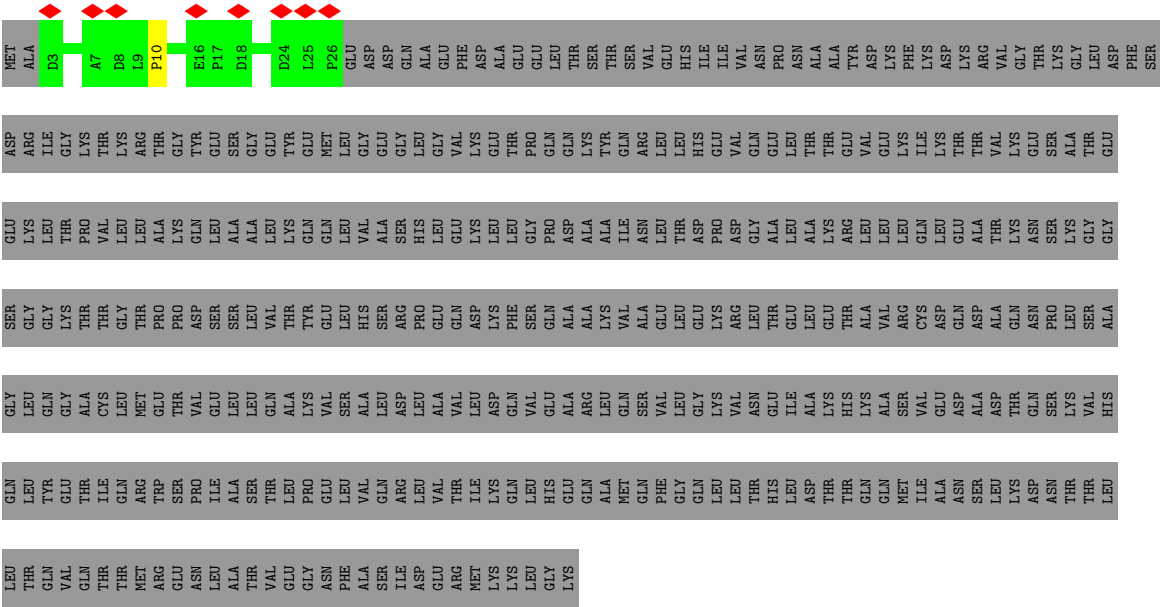


- Molecule 9: Dynactin subunit 2

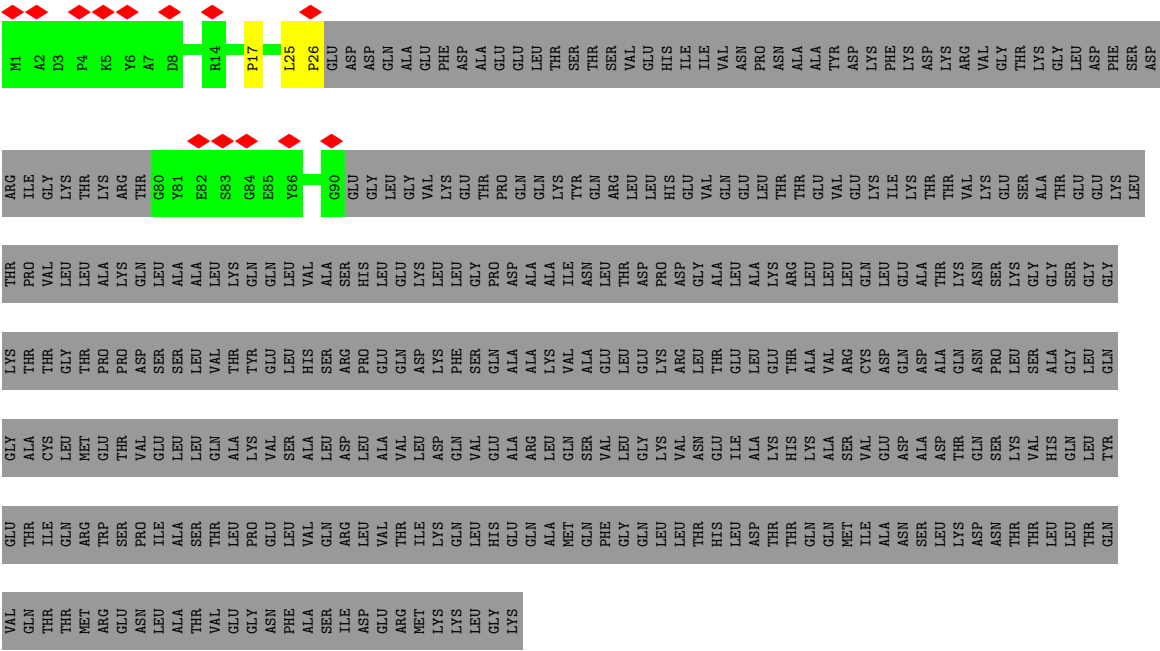


- Molecule 9: Dynactin subunit 2

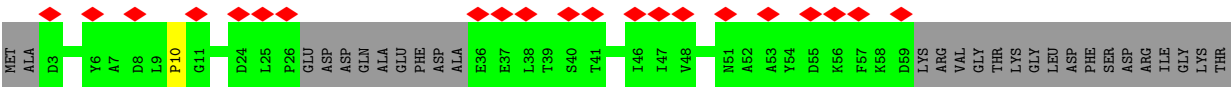




● Molecule 9: Dynactin subunit 2



● Molecule 9: Dynactin subunit 2



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	57.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	26.658	Depositor
Minimum map value	-12.272	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	1.217	Depositor
Recommended contour level	4	Depositor
Map size ( $\text{\AA}$ )	721.44, 721.44, 721.44	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.835, 0.835, 0.835	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, ANP, ZN

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	1.01	8/3025 (0.3%)	0.74	0/4085
1	B	0.99	5/3025 (0.2%)	0.74	0/4085
1	C	0.99	5/3068 (0.2%)	0.74	0/4144
1	D	0.98	5/3025 (0.2%)	0.74	0/4085
1	E	0.98	5/3025 (0.2%)	0.74	0/4085
1	F	1.00	8/3025 (0.3%)	0.74	0/4085
1	G	1.01	8/3025 (0.3%)	0.74	0/4085
1	I	1.00	7/3025 (0.2%)	0.74	0/4085
2	H	0.97	4/2948 (0.1%)	0.75	0/3991
3	J	2.01	106/3088 (3.4%)	2.22	204/4188 (4.9%)
4	K	0.77	5/2970 (0.2%)	0.59	0/4005
5	L	0.71	2/1435 (0.1%)	0.60	0/1941
6	M	0.71	0/1209	0.64	0/1641
7	N	0.75	1/2376 (0.0%)	0.57	0/3214
8	O	0.96	2/2156 (0.1%)	0.75	0/2906
9	P	0.93	1/591 (0.2%)	0.74	0/797
9	Q	1.01	1/193 (0.5%)	0.78	0/265
9	p	1.15	2/292 (0.7%)	0.87	0/395
9	q	0.92	1/387 (0.3%)	0.77	0/528
All	All	1.06	176/41888 (0.4%)	0.92	204/56610 (0.4%)

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
3	J	0	29

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	102	ARG	N-CA	-11.60	1.23	1.46
3	J	330	PRO	N-CA	-10.71	1.29	1.47
3	J	206	VAL	CA-C	-9.83	1.27	1.52
3	J	318	ARG	CA-C	-9.25	1.28	1.52
3	J	331	LYS	N-CA	-8.82	1.28	1.46
3	J	184	THR	C-O	8.73	1.40	1.23
3	J	357	GLY	CA-C	8.43	1.65	1.51
3	J	356	LEU	C-N	-8.37	1.18	1.33
3	J	186	ASP	N-CA	-8.15	1.30	1.46
3	J	167	GLY	N-CA	-7.84	1.34	1.46
3	J	183	CYS	N-CA	-7.80	1.30	1.46
1	G	228	PRO	N-CD	-7.58	1.37	1.47
3	J	319	LEU	N-CA	-7.40	1.31	1.46
3	J	329	LYS	C-N	-7.36	1.20	1.34
1	I	135	PRO	N-CD	-7.27	1.37	1.47
3	J	346	PRO	CA-C	-7.26	1.38	1.52
3	J	144	ARG	CA-C	-7.24	1.34	1.52
3	J	316	LEU	CA-C	-7.22	1.34	1.52
3	J	313	PRO	N-CA	-7.11	1.35	1.47
3	J	230	LYS	CA-C	-7.10	1.34	1.52
3	J	166	LEU	N-CA	-7.09	1.32	1.46
3	J	319	LEU	CA-C	-7.07	1.34	1.52
8	O	81	PRO	N-CD	-7.02	1.38	1.47
4	K	256	PRO	N-CD	-6.94	1.38	1.47
3	J	364	LEU	N-CA	-6.92	1.32	1.46
3	J	276	GLU	N-CA	-6.89	1.32	1.46
3	J	377	TYR	CA-C	-6.82	1.35	1.52
3	J	313	PRO	CA-C	-6.77	1.39	1.52
3	J	77	PHE	N-CA	-6.73	1.32	1.46
3	J	322	GLU	CA-C	-6.67	1.35	1.52
3	J	172	HIS	N-CA	-6.67	1.33	1.46
8	O	74	PRO	N-CD	-6.57	1.38	1.47
3	J	382	GLY	CA-C	-6.52	1.41	1.51
9	p	26	PRO	N-CD	-6.49	1.38	1.47
3	J	109	LEU	CA-C	-6.43	1.36	1.52
1	A	265	PRO	N-CD	-6.41	1.38	1.47
3	J	182	GLN	C-O	6.40	1.35	1.23
3	J	101	PHE	C-N	-6.37	1.19	1.34
3	J	322	GLU	C-N	-6.34	1.19	1.34
3	J	156	PRO	CA-C	-6.33	1.40	1.52
1	D	107	PRO	N-CD	-6.32	1.39	1.47
1	I	60	PRO	N-CD	-6.32	1.39	1.47
3	J	110	PHE	N-CA	-6.31	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	11	PRO	N-CD	-6.30	1.39	1.47
3	J	185	VAL	C-N	-6.29	1.19	1.34
3	J	311	MET	N-CA	-6.26	1.33	1.46
3	J	122	PRO	N-CD	-6.24	1.39	1.47
1	C	265	PRO	N-CD	-6.23	1.39	1.47
3	J	98	PRO	N-CD	-6.21	1.39	1.47
3	J	162	GLY	CA-C	6.21	1.61	1.51
3	J	388	CYS	N-CA	-6.21	1.33	1.46
1	F	107	PRO	N-CD	-6.17	1.39	1.47
1	A	228	PRO	N-CD	-6.16	1.39	1.47
4	K	460	PRO	N-CD	-6.16	1.39	1.47
3	J	321	ALA	N-CA	-6.15	1.34	1.46
1	B	2109	PRO	N-CD	-6.14	1.39	1.47
3	J	89	VAL	C-N	-6.14	1.20	1.34
3	J	320	LEU	N-CA	-6.12	1.34	1.46
3	J	101	PHE	CA-C	-6.09	1.37	1.52
3	J	37	CYS	N-CA	-6.05	1.34	1.46
1	A	107	PRO	N-CD	-6.04	1.39	1.47
1	C	107	PRO	N-CD	-6.04	1.39	1.47
3	J	65	TYR	CA-C	-6.04	1.37	1.52
3	J	290	GLN	N-CA	-6.04	1.34	1.46
3	J	154	GLY	N-CA	-6.03	1.37	1.46
3	J	248	TYR	C-N	-5.99	1.22	1.34
3	J	209	ASP	CA-C	-5.98	1.37	1.52
3	J	94	SER	CA-C	-5.97	1.37	1.52
1	A	60	PRO	N-CD	-5.94	1.39	1.47
3	J	231	PHE	N-CA	-5.94	1.34	1.46
3	J	93	GLU	N-CA	-5.94	1.34	1.46
3	J	66	SER	N-CA	-5.93	1.34	1.46
1	G	169	PRO	N-CD	-5.92	1.39	1.47
1	B	2044	PRO	N-CD	-5.91	1.39	1.47
3	J	318	ARG	N-CA	-5.91	1.34	1.46
3	J	137	MET	N-CA	5.90	1.58	1.46
3	J	74	ILE	C-N	-5.88	1.20	1.34
1	D	42	PRO	N-CD	-5.88	1.39	1.47
1	G	60	PRO	N-CD	-5.88	1.39	1.47
1	F	169	PRO	N-CD	-5.87	1.39	1.47
3	J	368	LEU	C-N	-5.86	1.22	1.33
4	K	139	PRO	N-CD	-5.84	1.39	1.47
1	E	42	PRO	N-CD	-5.80	1.39	1.47
9	p	17	PRO	N-CD	-5.79	1.39	1.47
1	E	60	PRO	N-CD	-5.78	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	372	SER	N-CA	-5.78	1.34	1.46
9	Q	10	PRO	N-CD	-5.78	1.39	1.47
1	C	42	PRO	N-CD	-5.76	1.39	1.47
1	F	60	PRO	N-CD	-5.76	1.39	1.47
3	J	112	TYR	CA-C	-5.75	1.38	1.52
3	J	71	PHE	CA-C	-5.75	1.38	1.52
1	F	42	PRO	N-CD	-5.72	1.39	1.47
1	A	42	PRO	N-CD	-5.72	1.39	1.47
3	J	236	ASN	N-CA	-5.71	1.34	1.46
3	J	324	ARG	C-N	-5.69	1.21	1.34
1	G	42	PRO	N-CD	-5.68	1.39	1.47
3	J	352	CYS	C-N	-5.67	1.21	1.34
1	E	169	PRO	N-CD	-5.66	1.40	1.47
9	q	10	PRO	N-CD	-5.63	1.40	1.47
1	D	60	PRO	N-CD	-5.61	1.40	1.47
1	I	169	PRO	N-CD	-5.61	1.40	1.47
1	E	107	PRO	N-CD	-5.60	1.40	1.47
1	A	11	PRO	N-CD	-5.60	1.40	1.47
3	J	347	PRO	N-CA	-5.60	1.37	1.47
3	J	209	ASP	C-N	-5.57	1.21	1.34
3	J	266	VAL	N-CA	-5.57	1.35	1.46
3	J	120	LEU	N-CA	-5.55	1.35	1.46
1	B	2062	PRO	N-CD	-5.54	1.40	1.47
2	H	130	PRO	N-CD	-5.51	1.40	1.47
5	L	141	PRO	N-CD	-5.51	1.40	1.47
3	J	166	LEU	C-O	-5.50	1.12	1.23
3	J	25	THR	CA-C	5.50	1.67	1.52
3	J	83	ASN	CA-C	-5.50	1.38	1.52
1	A	169	PRO	N-CD	-5.50	1.40	1.47
3	J	346	PRO	C-N	-5.49	1.23	1.34
3	J	24	PHE	C-N	-5.49	1.21	1.34
1	C	60	PRO	N-CD	-5.49	1.40	1.47
3	J	368	LEU	CA-C	-5.46	1.38	1.52
3	J	109	LEU	C-N	-5.43	1.21	1.34
3	J	152	TYR	CA-C	-5.39	1.39	1.52
3	J	36	ARG	C-N	-5.39	1.21	1.34
3	J	307	GLY	CA-C	-5.38	1.43	1.51
3	J	82	VAL	C-N	5.36	1.46	1.34
3	J	166	LEU	CA-C	-5.36	1.39	1.52
1	G	323	PRO	N-CD	-5.35	1.40	1.47
1	G	31	PRO	N-CD	-5.34	1.40	1.47
2	H	32	PRO	N-CD	-5.34	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	329	LYS	CA-C	-5.33	1.39	1.52
3	J	39	ILE	C-N	-5.33	1.24	1.34
3	J	360	ILE	CA-C	-5.31	1.39	1.52
1	F	31	PRO	N-CD	-5.31	1.40	1.47
3	J	208	GLU	N-CA	-5.30	1.35	1.46
1	G	107	PRO	N-CD	-5.30	1.40	1.47
1	I	31	PRO	N-CD	-5.30	1.40	1.47
1	D	11	PRO	N-CD	-5.29	1.40	1.47
4	K	291	PRO	N-CD	-5.29	1.40	1.47
1	A	31	PRO	N-CD	-5.28	1.40	1.47
3	J	91	ILE	CA-C	-5.28	1.39	1.52
2	H	70	PRO	N-CD	-5.27	1.40	1.47
5	L	142	PRO	N-CD	-5.26	1.40	1.47
1	B	2171	PRO	N-CD	-5.25	1.40	1.47
1	B	2325	PRO	N-CD	-5.25	1.40	1.47
3	J	102	ARG	CA-C	-5.25	1.39	1.52
3	J	381	THR	CA-C	-5.24	1.39	1.52
7	N	165	PRO	N-CD	-5.23	1.40	1.47
2	H	27	PRO	N-CD	-5.22	1.40	1.47
3	J	316	LEU	N-CA	-5.21	1.35	1.46
3	J	385	PRO	N-CD	-5.21	1.40	1.47
3	J	256	LEU	N-CA	-5.21	1.35	1.46
3	J	266	VAL	CA-C	-5.19	1.39	1.52
3	J	82	VAL	CA-C	5.17	1.66	1.52
3	J	93	GLU	C-N	-5.16	1.22	1.34
3	J	25	THR	N-CA	-5.16	1.36	1.46
3	J	300	ALA	CA-C	-5.15	1.39	1.52
3	J	230	LYS	C-O	-5.14	1.13	1.23
1	G	74	PRO	N-CD	-5.14	1.40	1.47
9	P	26	PRO	N-CD	-5.13	1.40	1.47
3	J	153	GLU	N-CA	-5.12	1.36	1.46
1	F	74	PRO	N-CD	-5.12	1.40	1.47
1	F	323	PRO	N-CD	-5.12	1.40	1.47
3	J	102	ARG	C-N	-5.12	1.22	1.34
1	I	228	PRO	N-CD	-5.12	1.40	1.47
3	J	203	PRO	N-CA	-5.09	1.38	1.47
3	J	363	ALA	C-N	-5.08	1.22	1.34
3	J	164	LEU	CA-C	-5.08	1.39	1.52
1	D	265	PRO	N-CD	-5.07	1.40	1.47
1	E	31	PRO	N-CD	-5.07	1.40	1.47
1	I	323	PRO	N-CD	-5.06	1.40	1.47
1	F	253	PRO	N-CD	-5.06	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	222	ARG	N-CA	-5.06	1.36	1.46
3	J	155	ILE	CA-C	-5.05	1.39	1.52
3	J	166	LEU	C-N	-5.04	1.24	1.33
1	C	323	PRO	N-CD	-5.04	1.40	1.47
3	J	371	ARG	C-N	-5.04	1.22	1.34
4	K	77	PRO	N-CD	-5.02	1.40	1.47
3	J	359	ALA	N-CA	-5.01	1.36	1.46

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	144	ARG	O-C-N	27.08	166.03	122.70
3	J	196	PRO	C-N-CA	-23.72	62.40	121.70
3	J	144	ARG	CA-C-N	-20.73	71.59	117.20
3	J	308	GLY	C-N-CA	-13.14	88.85	121.70
3	J	356	LEU	C-N-CA	-12.53	95.99	122.30
3	J	144	ARG	CA-C-O	-12.22	94.44	120.10
3	J	368	LEU	C-N-CA	-12.11	96.87	122.30
3	J	237	ASN	C-N-CA	-11.46	93.06	121.70
3	J	230	LYS	C-N-CA	-11.42	93.15	121.70
3	J	182	GLN	C-N-CA	-11.11	93.93	121.70
3	J	352	CYS	C-N-CA	-10.73	94.87	121.70
3	J	23	ALA	C-N-CA	-10.51	95.43	121.70
3	J	17	VAL	C-N-CA	10.45	147.84	121.70
3	J	352	CYS	O-C-N	-9.68	107.21	122.70
3	J	173	LYS	C-N-CA	-9.54	97.85	121.70
3	J	322	GLU	C-N-CA	-9.53	97.87	121.70
3	J	230	LYS	N-CA-C	-9.38	85.67	111.00
3	J	158	LEU	C-N-CA	-9.35	98.33	121.70
3	J	313	PRO	C-N-CA	9.32	141.88	122.30
3	J	69	LYS	C-N-CA	-9.30	98.44	121.70
3	J	23	ALA	O-C-N	-8.99	108.31	122.70
3	J	125	LEU	O-C-N	-8.97	108.35	122.70
3	J	105	LEU	C-N-CA	-8.89	99.48	121.70
3	J	300	ALA	N-CA-C	-8.67	87.60	111.00
3	J	151	ILE	O-C-N	-8.61	108.92	122.70
3	J	19	ASP	C-N-CA	-8.55	100.32	121.70
3	J	109	LEU	C-N-CA	-8.54	100.34	121.70
3	J	165	PRO	N-CA-C	-8.51	89.97	112.10
3	J	195	LEU	C-N-CA	-8.42	86.66	122.00
3	J	65	TYR	C-N-CA	-8.34	100.85	121.70
3	J	219	ASP	C-N-CA	8.28	142.41	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	306	ILE	O-C-N	8.27	137.25	123.20
3	J	18	ILE	C-N-CA	8.26	142.34	121.70
3	J	40	PRO	C-N-CA	-8.26	101.06	121.70
3	J	248	TYR	C-N-CD	8.21	145.64	128.40
3	J	350	ALA	O-C-N	-8.21	109.56	122.70
3	J	268	GLU	C-N-CA	-8.18	101.25	121.70
3	J	43	ILE	N-CA-C	-8.08	89.19	111.00
3	J	39	ILE	C-N-CD	8.07	145.36	128.40
3	J	313	PRO	O-C-N	8.00	136.79	123.20
3	J	197	SER	N-CA-C	7.94	132.43	111.00
3	J	356	LEU	O-C-N	-7.91	109.75	123.20
3	J	40	PRO	N-CA-C	-7.83	91.74	112.10
3	J	152	TYR	C-N-CA	-7.82	102.16	121.70
3	J	46	ALA	C-N-CA	-7.69	106.15	122.30
3	J	100	HIS	N-CA-C	-7.64	90.37	111.00
3	J	330	PRO	C-N-CA	-7.58	102.76	121.70
3	J	110	PHE	N-CA-C	-7.50	90.76	111.00
3	J	115	VAL	C-N-CD	7.47	144.09	128.40
3	J	144	ARG	N-CA-C	7.39	130.94	111.00
3	J	105	LEU	O-C-N	-7.38	110.89	122.70
3	J	170	ALA	O-C-N	7.35	134.46	122.70
3	J	22	GLU	N-CA-C	-7.33	91.21	111.00
3	J	318	ARG	O-C-N	7.26	134.32	122.70
3	J	232	ASN	N-CA-C	-7.26	91.40	111.00
3	J	212	ALA	C-N-CA	-7.18	103.75	121.70
3	J	78	ARG	C-N-CA	-7.11	103.93	121.70
3	J	288	LEU	O-C-N	-7.09	111.35	122.70
3	J	31	GLY	N-CA-C	-7.09	95.37	113.10
3	J	204	GLU	C-N-CA	-7.09	107.42	122.30
3	J	298	GLN	O-C-N	7.05	133.98	122.70
3	J	391	ASN	C-N-CA	-6.97	104.28	121.70
3	J	296	ARG	CA-C-O	6.89	134.57	120.10
3	J	69	LYS	O-C-N	-6.86	111.72	122.70
3	J	155	ILE	C-N-CD	6.86	142.80	128.40
3	J	368	LEU	O-C-N	-6.83	111.59	123.20
3	J	256	LEU	O-C-N	-6.81	111.80	122.70
3	J	183	CYS	N-CA-C	6.78	129.31	111.00
3	J	125	LEU	CA-C-O	6.77	134.32	120.10
3	J	329	LYS	C-N-CD	-6.75	105.76	120.60
3	J	175	LEU	C-N-CA	-6.73	104.86	121.70
3	J	160	CYS	N-CA-C	-6.73	92.83	111.00
3	J	275	ASN	C-N-CA	6.72	138.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	36	ARG	N-CA-C	-6.70	92.92	111.00
3	J	178	GLN	C-N-CA	-6.69	104.97	121.70
3	J	259	LEU	O-C-N	-6.62	111.95	123.20
3	J	206	VAL	C-N-CA	-6.60	105.21	121.70
3	J	225	LYS	C-N-CA	-6.58	105.24	121.70
3	J	34	GLY	C-N-CD	6.58	142.21	128.40
3	J	285	LEU	C-N-CA	-6.51	105.43	121.70
3	J	315	PHE	C-N-CA	-6.49	105.48	121.70
3	J	166	LEU	CA-C-N	6.47	129.13	116.20
3	J	333	LYS	C-N-CA	-6.46	105.56	121.70
3	J	125	LEU	C-N-CA	-6.44	105.59	121.70
3	J	315	PHE	CA-C-O	-6.43	106.60	120.10
3	J	71	PHE	O-C-N	6.41	132.95	122.70
3	J	195	LEU	CA-C-O	6.40	133.55	120.10
3	J	377	TYR	O-C-N	6.38	132.91	122.70
3	J	352	CYS	CA-C-O	6.37	133.47	120.10
3	J	37	CYS	CA-C-O	6.36	133.45	120.10
3	J	386	ASP	O-C-N	-6.34	112.55	122.70
3	J	256	LEU	C-N-CA	-6.28	106.01	121.70
3	J	136	ALA	C-N-CA	6.26	137.36	121.70
3	J	326	LEU	O-C-N	-6.23	112.73	122.70
3	J	16	VAL	C-N-CA	-6.23	106.13	121.70
3	J	378	TYR	C-N-CA	-6.14	106.34	121.70
3	J	195	LEU	O-C-N	-6.12	109.48	121.10
3	J	16	VAL	N-CA-C	6.11	127.49	111.00
3	J	306	ILE	N-CA-C	-6.10	94.52	111.00
3	J	111	LYS	C-N-CA	-6.10	106.46	121.70
3	J	220	LEU	C-N-CA	-6.07	106.52	121.70
3	J	81	LEU	N-CA-C	-6.06	94.63	111.00
3	J	74	ILE	CA-C-O	6.06	132.83	120.10
3	J	266	VAL	C-N-CA	-6.05	106.56	121.70
3	J	75	LEU	O-C-N	-6.05	113.02	122.70
3	J	93	GLU	N-CA-C	-6.04	94.69	111.00
3	J	76	TYR	C-N-CA	6.03	136.78	121.70
3	J	338	THR	O-C-N	-6.02	113.07	122.70
3	J	169	LYS	C-N-CA	-6.00	106.69	121.70
3	J	112	TYR	N-CA-C	-5.99	94.84	111.00
3	J	103	GLU	O-C-N	5.97	132.26	122.70
3	J	109	LEU	N-CA-C	-5.97	94.89	111.00
3	J	14	THR	C-N-CA	5.96	136.60	121.70
3	J	108	VAL	O-C-N	5.96	132.24	122.70
3	J	319	LEU	C-N-CA	-5.94	106.85	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	72	ILE	C-N-CA	-5.91	106.94	121.70
3	J	330	PRO	CA-N-CD	5.90	119.96	111.70
3	J	374	SER	O-C-N	5.89	132.12	122.70
3	J	276	GLU	N-CA-C	-5.88	95.12	111.00
3	J	220	LEU	O-C-N	-5.88	113.30	122.70
3	J	166	LEU	N-CA-C	-5.87	95.16	111.00
3	J	357	GLY	N-CA-C	-5.86	98.44	113.10
3	J	373	VAL	O-C-N	-5.86	113.32	122.70
3	J	173	LYS	N-CA-C	-5.86	95.17	111.00
3	J	337	GLY	N-CA-C	-5.84	98.50	113.10
3	J	275	ASN	CA-C-N	-5.83	104.37	117.20
3	J	99	SER	CA-C-O	-5.81	107.89	120.10
3	J	283	LEU	C-N-CA	-5.81	107.17	121.70
3	J	259	LEU	C-N-CA	-5.81	110.11	122.30
3	J	184	THR	O-C-N	5.80	131.98	122.70
3	J	199	MET	C-N-CA	-5.79	110.14	122.30
3	J	349	LYS	CA-C-O	5.77	132.22	120.10
3	J	169	LYS	N-CA-C	-5.76	95.44	111.00
3	J	371	ARG	C-N-CA	5.75	136.08	121.70
3	J	95	VAL	N-CA-C	-5.74	95.50	111.00
3	J	68	LEU	CA-C-O	5.72	132.12	120.10
3	J	116	PRO	N-CA-C	-5.71	97.24	112.10
3	J	361	PHE	C-N-CA	-5.71	110.31	122.30
3	J	198	VAL	N-CA-C	-5.69	95.64	111.00
3	J	365	GLN	O-C-N	-5.69	113.59	122.70
3	J	84	PRO	O-C-N	-5.68	113.61	122.70
3	J	223	GLY	N-CA-C	-5.66	98.95	113.10
3	J	296	ARG	CA-C-N	-5.64	104.80	117.20
3	J	303	LEU	O-C-N	-5.63	113.69	122.70
3	J	122	PRO	N-CA-C	5.62	126.71	112.10
3	J	194	SER	C-N-CA	-5.60	107.69	121.70
3	J	89	VAL	O-C-N	-5.57	113.79	122.70
3	J	167	GLY	C-N-CA	5.57	133.99	122.30
3	J	177	THR	O-C-N	5.57	131.60	122.70
3	J	122	PRO	C-N-CA	-5.56	107.80	121.70
3	J	281	ALA	C-N-CA	-5.55	107.83	121.70
3	J	191	LYS	O-C-N	-5.54	113.83	122.70
3	J	387	TRP	C-N-CA	-5.54	107.86	121.70
3	J	122	PRO	O-C-N	-5.53	113.85	122.70
3	J	129	LEU	O-C-N	-5.50	113.89	122.70
3	J	337	GLY	C-N-CA	-5.50	107.95	121.70
3	J	196	PRO	O-C-N	-5.49	113.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	41	SER	N-CA-C	5.49	125.83	111.00
3	J	233	ILE	C-N-CA	-5.47	108.02	121.70
3	J	144	ARG	CB-CA-C	-5.45	99.50	110.40
3	J	300	ALA	N-CA-CB	5.44	117.71	110.10
3	J	322	GLU	O-C-N	-5.44	114.00	122.70
3	J	65	TYR	O-C-N	-5.43	114.00	122.70
3	J	246	VAL	O-C-N	-5.43	114.02	122.70
3	J	105	LEU	CA-C-O	5.42	131.48	120.10
3	J	184	THR	CA-C-N	-5.39	105.35	117.20
3	J	318	ARG	C-N-CA	-5.38	108.24	121.70
3	J	357	GLY	C-N-CA	5.38	133.61	122.30
3	J	209	ASP	O-C-N	-5.38	114.09	122.70
3	J	129	LEU	CA-C-O	-5.32	108.92	120.10
3	J	74	ILE	O-C-N	-5.32	114.19	122.70
3	J	86	ASP	N-CA-C	5.32	125.37	111.00
3	J	89	VAL	C-N-CA	-5.31	108.42	121.70
3	J	267	VAL	N-CA-C	5.29	125.28	111.00
3	J	331	LYS	C-N-CA	-5.29	108.48	121.70
3	J	283	LEU	O-C-N	-5.28	114.25	122.70
3	J	350	ALA	C-N-CA	-5.27	108.53	121.70
3	J	184	THR	C-N-CA	-5.25	108.58	121.70
3	J	326	LEU	C-N-CA	-5.24	108.60	121.70
3	J	37	CYS	O-C-N	-5.23	114.33	122.70
3	J	147	LEU	O-C-N	-5.23	114.33	122.70
3	J	204	GLU	CA-C-O	5.22	131.06	120.10
3	J	43	ILE	C-N-CA	5.22	134.75	121.70
3	J	204	GLU	O-C-N	-5.20	114.36	123.20
3	J	225	LYS	N-CA-C	-5.20	96.97	111.00
3	J	73	HIS	O-C-N	5.19	131.01	122.70
3	J	354	ALA	O-C-N	-5.19	114.40	122.70
3	J	23	ALA	CA-C-O	5.18	130.99	120.10
3	J	369	GLY	O-C-N	-5.18	114.41	122.70
3	J	353	VAL	C-N-CA	-5.16	108.79	121.70
3	J	287	SER	C-N-CA	-5.16	108.81	121.70
3	J	378	TYR	O-C-N	-5.14	114.47	122.70
3	J	43	ILE	CA-C-O	-5.10	109.39	120.10
3	J	127	ALA	N-CA-C	5.09	124.75	111.00
3	J	174	GLU	CA-C-N	-5.08	106.01	117.20
3	J	61	THR	O-C-N	5.08	130.82	122.70
3	J	84	PRO	C-N-CA	-5.07	109.02	121.70
3	J	248	TYR	C-N-CA	-5.04	100.82	122.00
3	J	319	LEU	O-C-N	5.04	130.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	75	LEU	CA-C-O	5.02	130.65	120.10
3	J	181	GLU	CA-C-O	-5.01	109.58	120.10
3	J	357	GLY	CA-C-O	-5.01	111.59	120.60
3	J	175	LEU	O-C-N	-5.00	114.69	122.70
3	J	320	LEU	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	102	ARG	Mainchain
3	J	125	LEU	Mainchain
3	J	129	LEU	Mainchain
3	J	174	GLU	Mainchain
3	J	181	GLU	Mainchain
3	J	196	PRO	Mainchain
3	J	209	ASP	Mainchain
3	J	222	ARG	Mainchain
3	J	230	LYS	Mainchain
3	J	259	LEU	Mainchain
3	J	260	GLY	Mainchain
3	J	268	GLU	Mainchain
3	J	282	THR	Mainchain
3	J	288	LEU	Mainchain
3	J	293	ILE	Mainchain
3	J	315	PHE	Mainchain
3	J	338	THR	Mainchain
3	J	350	ALA	Mainchain
3	J	354	ALA	Mainchain
3	J	356	LEU	Mainchain
3	J	378	TYR	Mainchain
3	J	381	THR	Mainchain
3	J	386	ASP	Mainchain
3	J	50	LYS	Peptide
3	J	53	ARG	Mainchain
3	J	65	TYR	Mainchain
3	J	78	ARG	Mainchain
3	J	92	ILE	Mainchain
3	J	99	SER	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	B	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	C	373/376 (99%)	365 (98%)	8 (2%)	0	100	100
1	D	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	E	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	F	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	I	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
3	J	379/417 (91%)	357 (94%)	19 (5%)	3 (1%)	16	51
4	K	349/460 (76%)	342 (98%)	7 (2%)	0	100	100
5	L	180/182 (99%)	176 (98%)	3 (2%)	1 (1%)	22	55
6	M	152/190 (80%)	145 (95%)	7 (5%)	0	100	100
7	N	284/286 (99%)	279 (98%)	5 (2%)	0	100	100
8	O	267/272 (98%)	261 (98%)	6 (2%)	0	100	100
9	P	70/401 (18%)	65 (93%)	4 (6%)	1 (1%)	9	40
9	Q	22/401 (6%)	21 (96%)	1 (4%)	0	100	100
9	p	33/401 (8%)	28 (85%)	4 (12%)	1 (3%)	3	26
9	q	44/401 (11%)	42 (96%)	2 (4%)	0	100	100
All	All	5097/6794 (75%)	4935 (97%)	156 (3%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	283	LEU
9	p	25	LEU
3	J	23	ALA
3	J	145	GLU
5	L	179	LEU
9	P	10	PRO

### 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	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	B	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	C	323/324 (100%)	323 (100%)	0	100	100
1	D	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	E	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	F	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	G	318/324 (98%)	318 (100%)	0	100	100
1	I	318/324 (98%)	318 (100%)	0	100	100
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	339/363 (93%)	338 (100%)	1 (0%)	91	96
4	K	330/412 (80%)	330 (100%)	0	100	100
5	L	163/163 (100%)	163 (100%)	0	100	100
6	M	132/164 (80%)	132 (100%)	0	100	100
7	N	252/252 (100%)	252 (100%)	0	100	100
8	O	238/241 (99%)	238 (100%)	0	100	100
9	P	64/343 (19%)	64 (100%)	0	100	100
9	Q	21/343 (6%)	21 (100%)	0	100	100
9	p	30/343 (9%)	30 (100%)	0	100	100
9	q	43/343 (12%)	43 (100%)	0	100	100
All	All	4474/5877 (76%)	4468 (100%)	6 (0%)	92	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	TRP
1	B	2359	TRP
1	D	357	TRP
1	E	357	TRP
1	F	357	TRP
3	J	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	44	HIS
1	C	116	ASN
1	E	116	ASN
4	K	266	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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
11	ANP	H	401	-	29,33,33	1.74	6 (20%)	31,52,52	1.57	7 (22%)
10	ADP	G	800	-	24,29,29	0.71	0	29,45,45	0.70	1 (3%)
10	ADP	F	800	-	24,29,29	0.71	0	29,45,45	0.69	1 (3%)
10	ADP	E	800	-	24,29,29	0.72	0	29,45,45	0.70	1 (3%)
10	ADP	I	800	-	24,29,29	0.71	0	29,45,45	0.73	1 (3%)
10	ADP	C	800	-	24,29,29	0.76	0	29,45,45	0.72	1 (3%)
10	ADP	A	800	-	24,29,29	0.73	0	29,45,45	0.71	1 (3%)
10	ADP	D	800	-	24,29,29	0.72	0	29,45,45	0.70	1 (3%)
10	ADP	B	2401	-	24,29,29	0.75	0	29,45,45	0.70	1 (3%)

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
11	ANP	H	401	-	-	7/14/38/38	0/3/3/3
10	ADP	G	800	-	-	4/12/32/32	0/3/3/3
10	ADP	F	800	-	-	4/12/32/32	0/3/3/3
10	ADP	E	800	-	-	4/12/32/32	0/3/3/3
10	ADP	I	800	-	-	4/12/32/32	0/3/3/3
10	ADP	C	800	-	-	4/12/32/32	0/3/3/3
10	ADP	A	800	-	-	7/12/32/32	0/3/3/3
10	ADP	D	800	-	-	4/12/32/32	0/3/3/3
10	ADP	B	2401	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	401	ANP	PG-N3B	4.34	1.74	1.63
11	H	401	ANP	PG-O1G	3.93	1.52	1.46
11	H	401	ANP	PB-N3B	3.58	1.72	1.63
11	H	401	ANP	PB-O1B	3.43	1.51	1.46
11	H	401	ANP	PB-O2B	-2.38	1.50	1.56
11	H	401	ANP	O4'-C1'	2.07	1.43	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	401	ANP	N3-C2-N1	-4.09	123.13	128.67
11	H	401	ANP	O1B-PB-N3B	-3.48	106.65	111.77
11	H	401	ANP	O1G-PG-N3B	-2.76	107.70	111.77
11	H	401	ANP	O2A-PA-O1A	2.65	124.77	112.44
11	H	401	ANP	O2B-PB-O1B	2.64	115.52	109.87
10	I	800	ADP	C5-C6-N6	2.28	123.78	120.31
11	H	401	ANP	O3A-PB-N3B	2.23	112.77	106.59
10	D	800	ADP	C5-C6-N6	2.21	123.69	120.31
10	G	800	ADP	C5-C6-N6	2.21	123.68	120.31
10	C	800	ADP	C5-C6-N6	2.21	123.68	120.31
10	A	800	ADP	C5-C6-N6	2.19	123.65	120.31
10	B	2401	ADP	C5-C6-N6	2.19	123.65	120.31
10	E	800	ADP	C5-C6-N6	2.19	123.64	120.31
10	F	800	ADP	C5-C6-N6	2.08	123.47	120.31
11	H	401	ANP	O2G-PG-O3G	2.03	113.06	107.59

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	800	ADP	PA-O3A-PB-O2B
10	A	800	ADP	PA-O3A-PB-O3B
10	A	800	ADP	C5'-O5'-PA-O1A
10	A	800	ADP	C5'-O5'-PA-O3A
10	C	800	ADP	C5'-O5'-PA-O1A
10	C	800	ADP	C5'-O5'-PA-O3A
10	D	800	ADP	C5'-O5'-PA-O3A
10	E	800	ADP	C5'-O5'-PA-O1A
10	E	800	ADP	C5'-O5'-PA-O3A
10	F	800	ADP	C5'-O5'-PA-O1A
10	G	800	ADP	C5'-O5'-PA-O3A
10	I	800	ADP	C5'-O5'-PA-O1A
10	I	800	ADP	C5'-O5'-PA-O3A
11	H	401	ANP	PB-N3B-PG-O1G
11	H	401	ANP	PG-N3B-PB-O1B
11	H	401	ANP	PG-N3B-PB-O3A
11	H	401	ANP	C5'-O5'-PA-O2A
10	A	800	ADP	C3'-C4'-C5'-O5'
10	D	800	ADP	C3'-C4'-C5'-O5'
10	E	800	ADP	C3'-C4'-C5'-O5'
10	F	800	ADP	C3'-C4'-C5'-O5'
10	G	800	ADP	C3'-C4'-C5'-O5'
10	C	800	ADP	C3'-C4'-C5'-O5'

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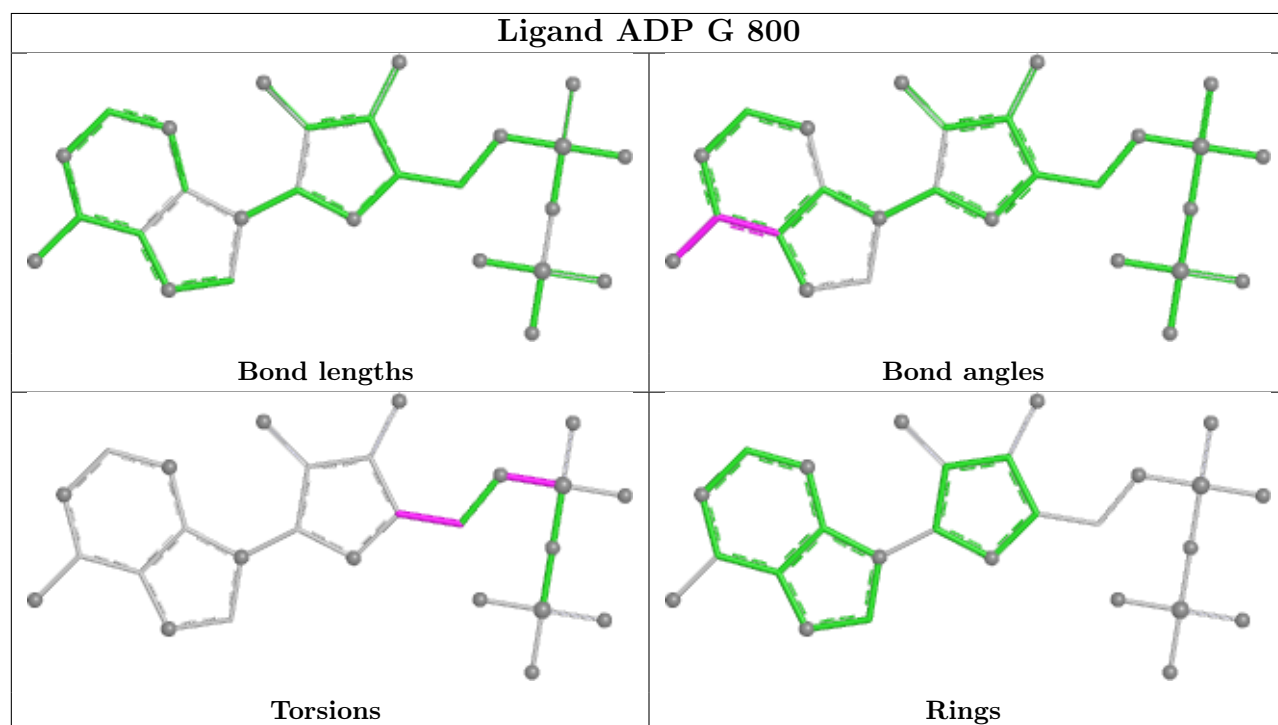
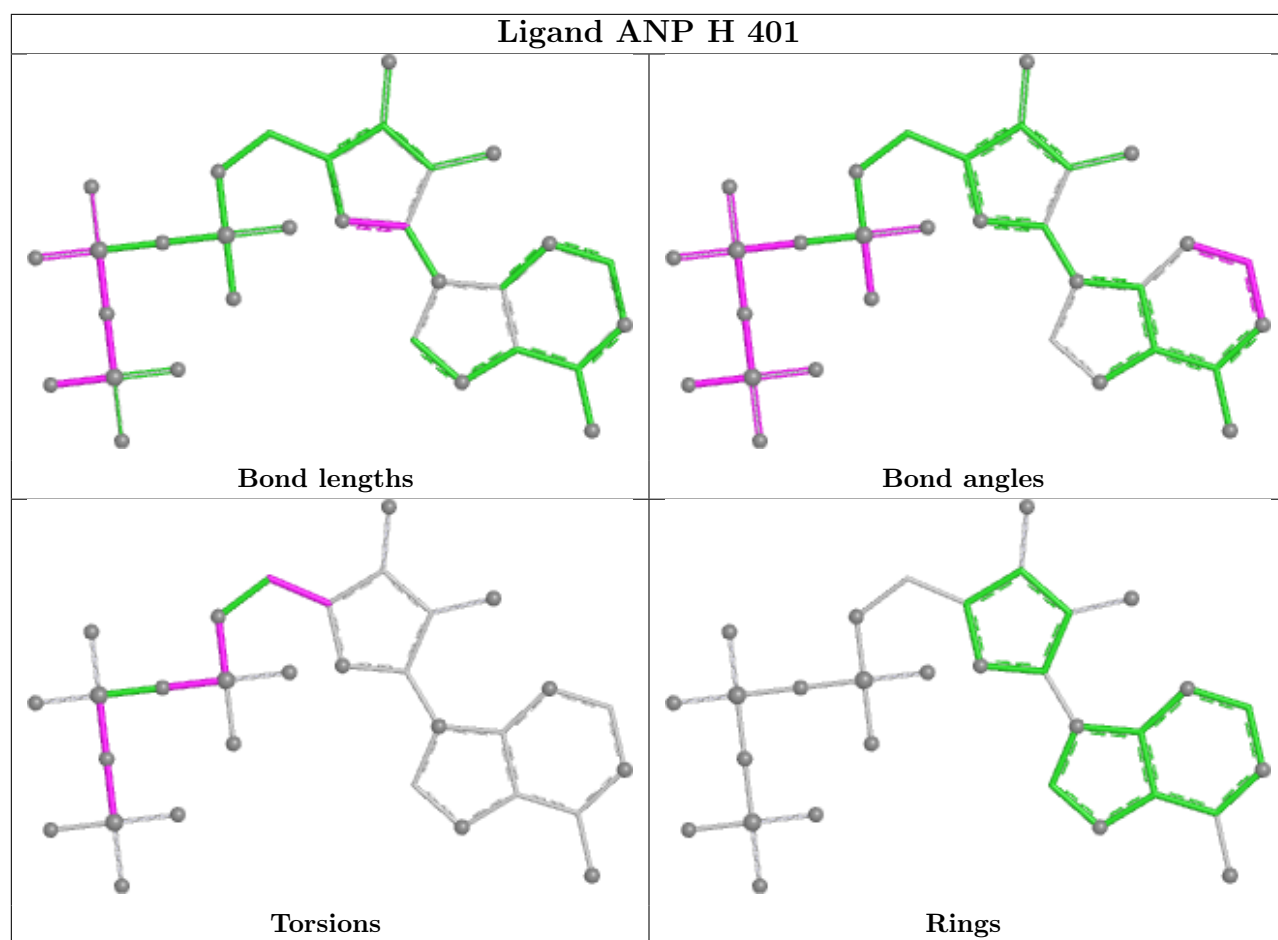
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Mol	Chain	Res	Type	Atoms
10	D	800	ADP	O4'-C4'-C5'-O5'
10	I	800	ADP	C3'-C4'-C5'-O5'
10	B	2401	ADP	C3'-C4'-C5'-O5'
11	H	401	ANP	PB-O3A-PA-O1A
10	E	800	ADP	O4'-C4'-C5'-O5'
10	F	800	ADP	O4'-C4'-C5'-O5'
10	A	800	ADP	O4'-C4'-C5'-O5'
10	C	800	ADP	O4'-C4'-C5'-O5'
10	G	800	ADP	O4'-C4'-C5'-O5'
10	I	800	ADP	O4'-C4'-C5'-O5'
10	B	2401	ADP	O4'-C4'-C5'-O5'
10	B	2401	ADP	PA-O3A-PB-O1B
10	D	800	ADP	C5'-O5'-PA-O1A
10	F	800	ADP	C5'-O5'-PA-O3A
10	G	800	ADP	C5'-O5'-PA-O1A
11	H	401	ANP	PB-O3A-PA-O2A
11	H	401	ANP	O4'-C4'-C5'-O5'
10	A	800	ADP	PA-O3A-PB-O1B

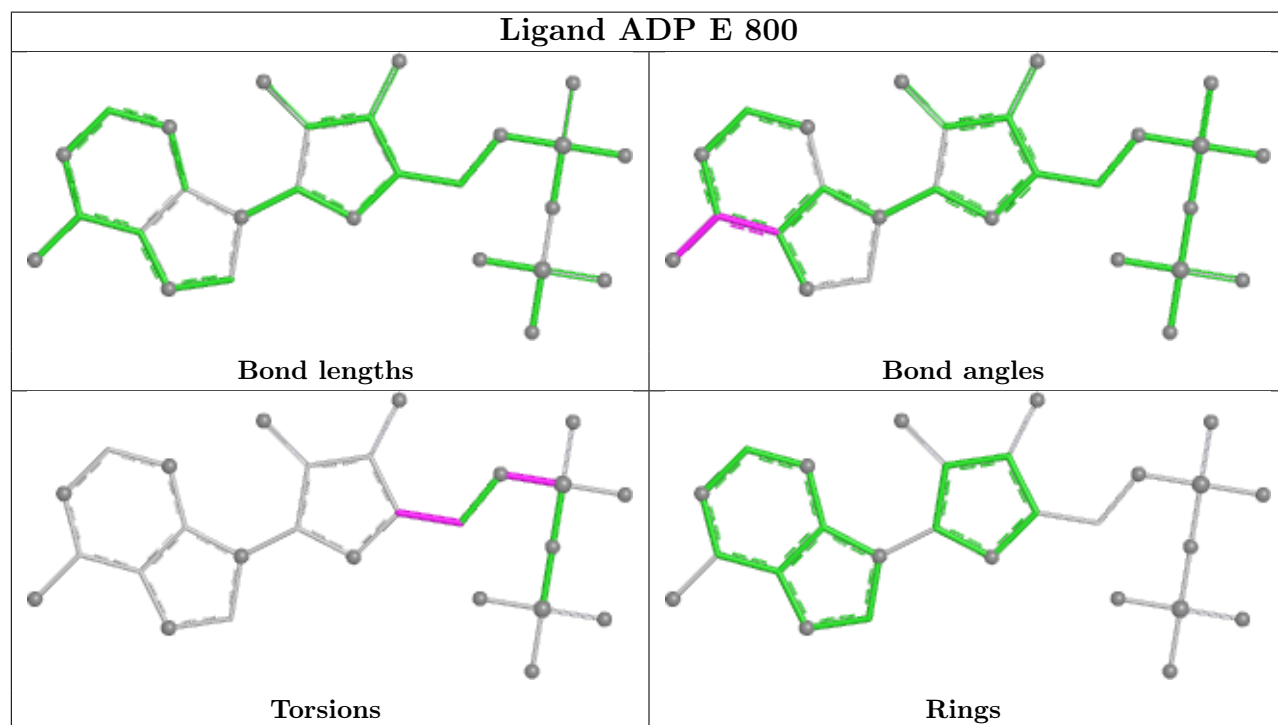
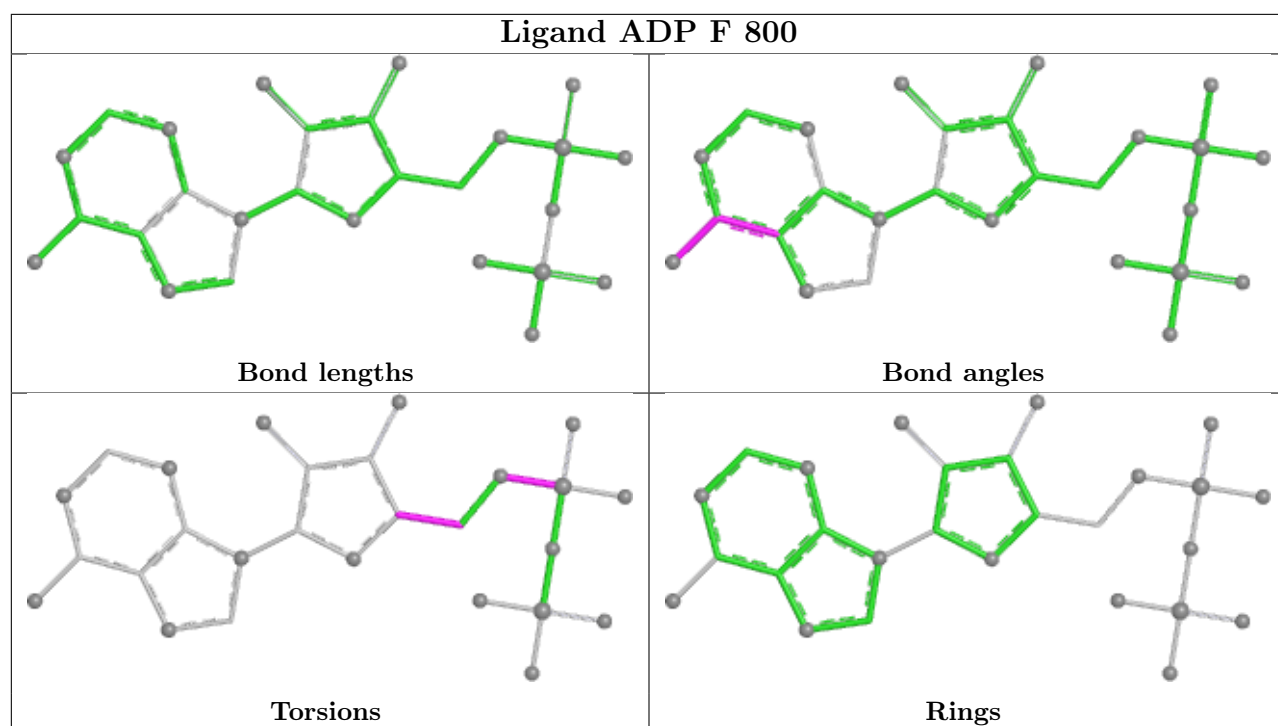
There are no ring outliers.

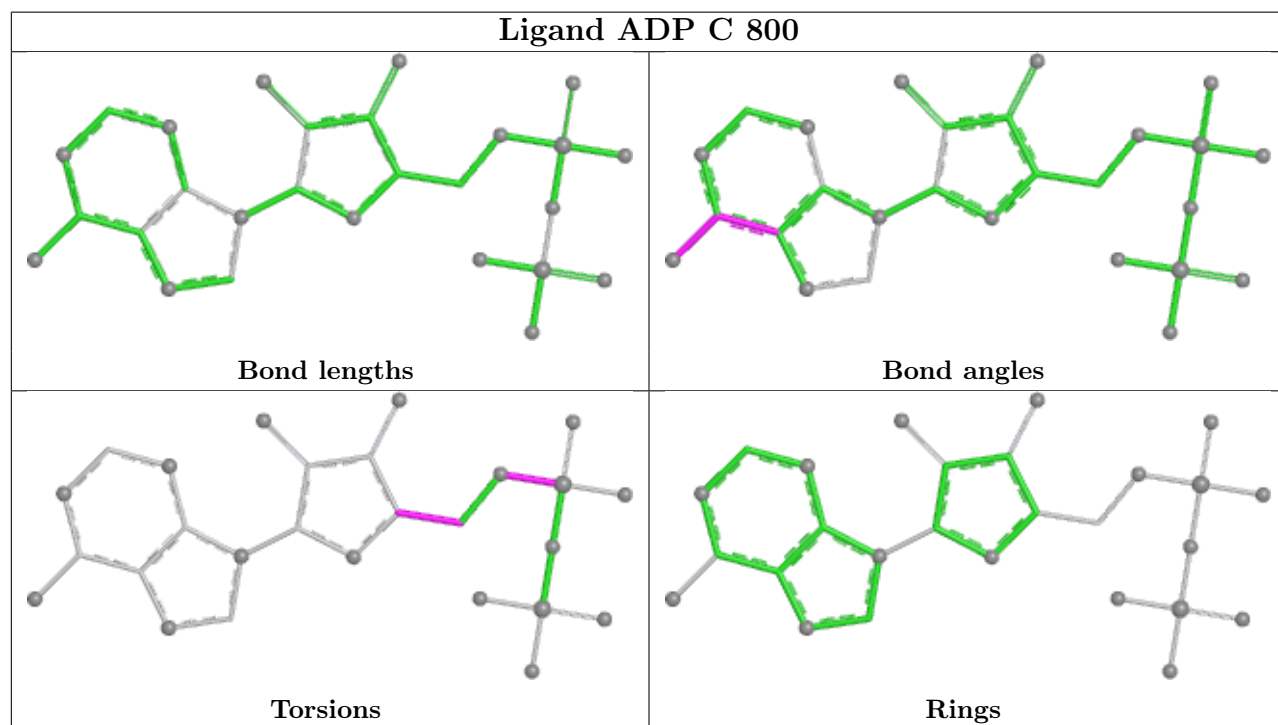
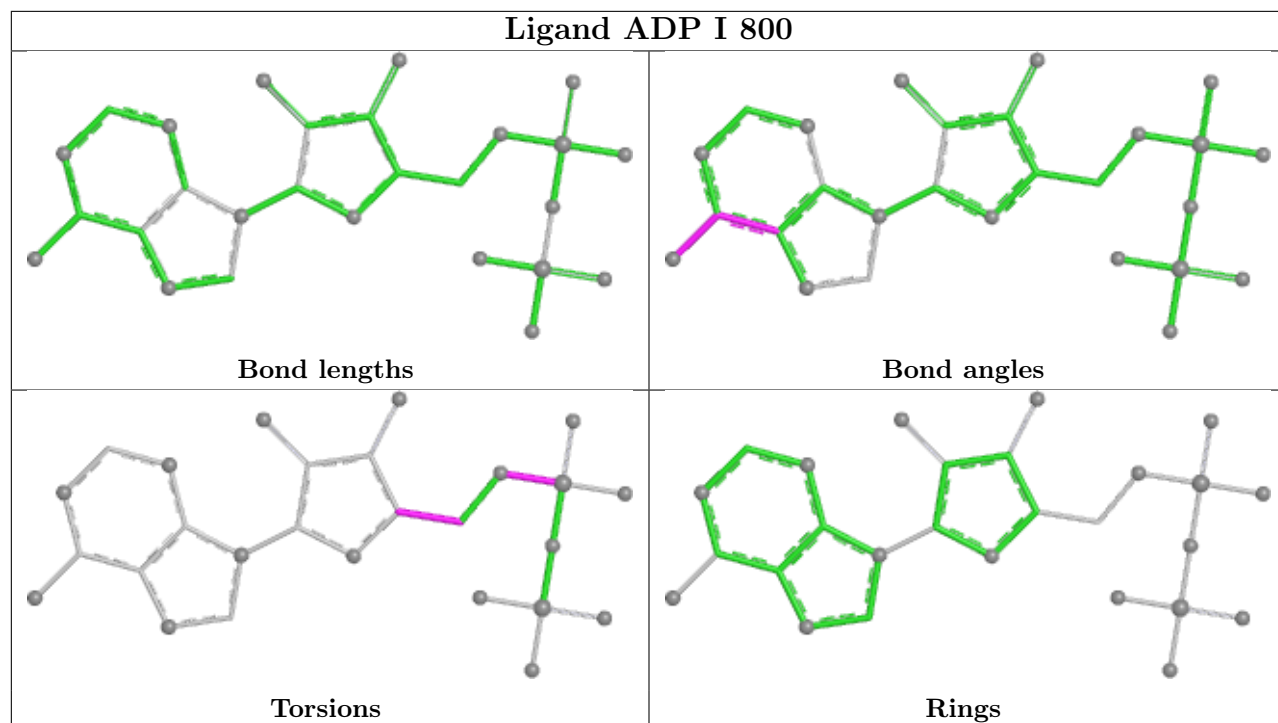
No monomer is involved in short contacts.

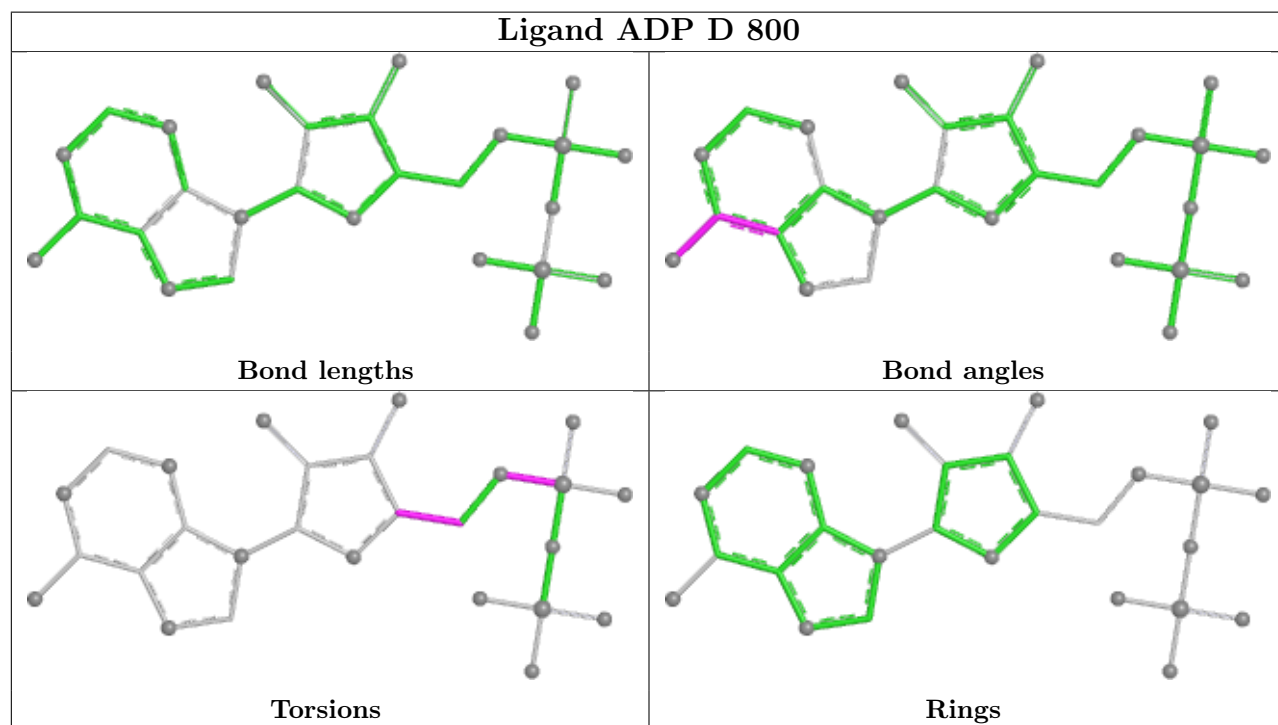
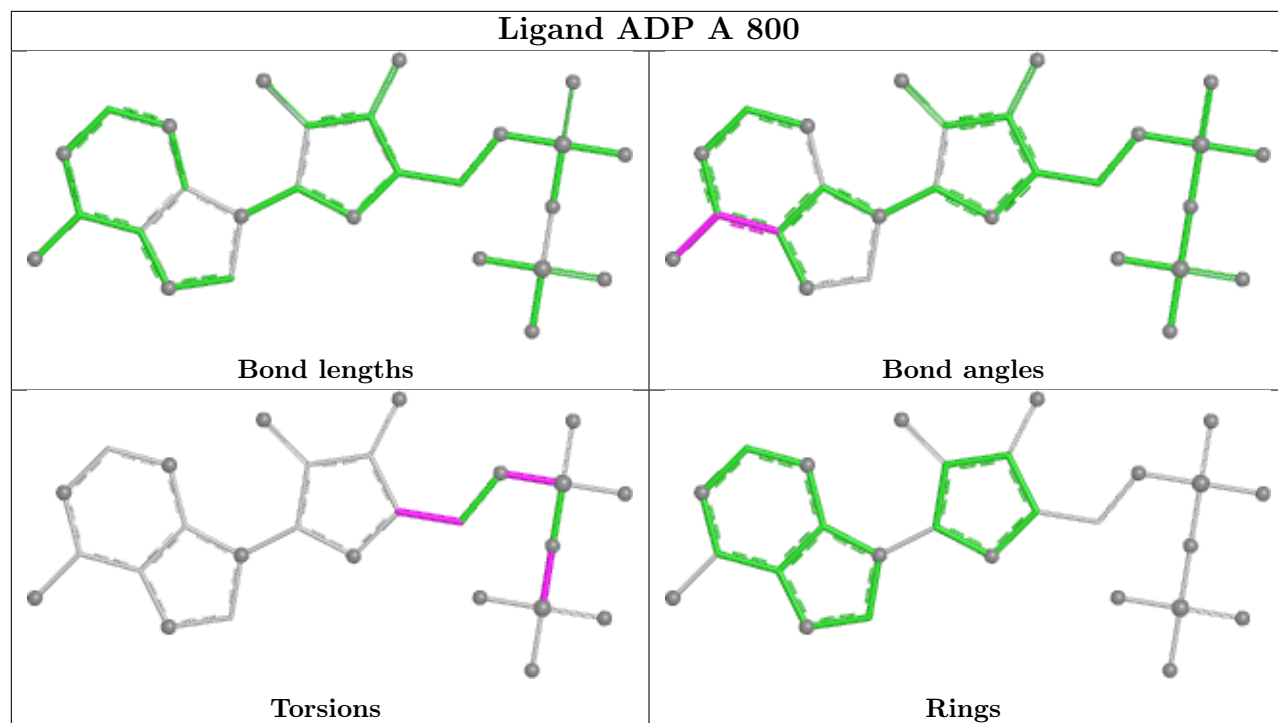
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

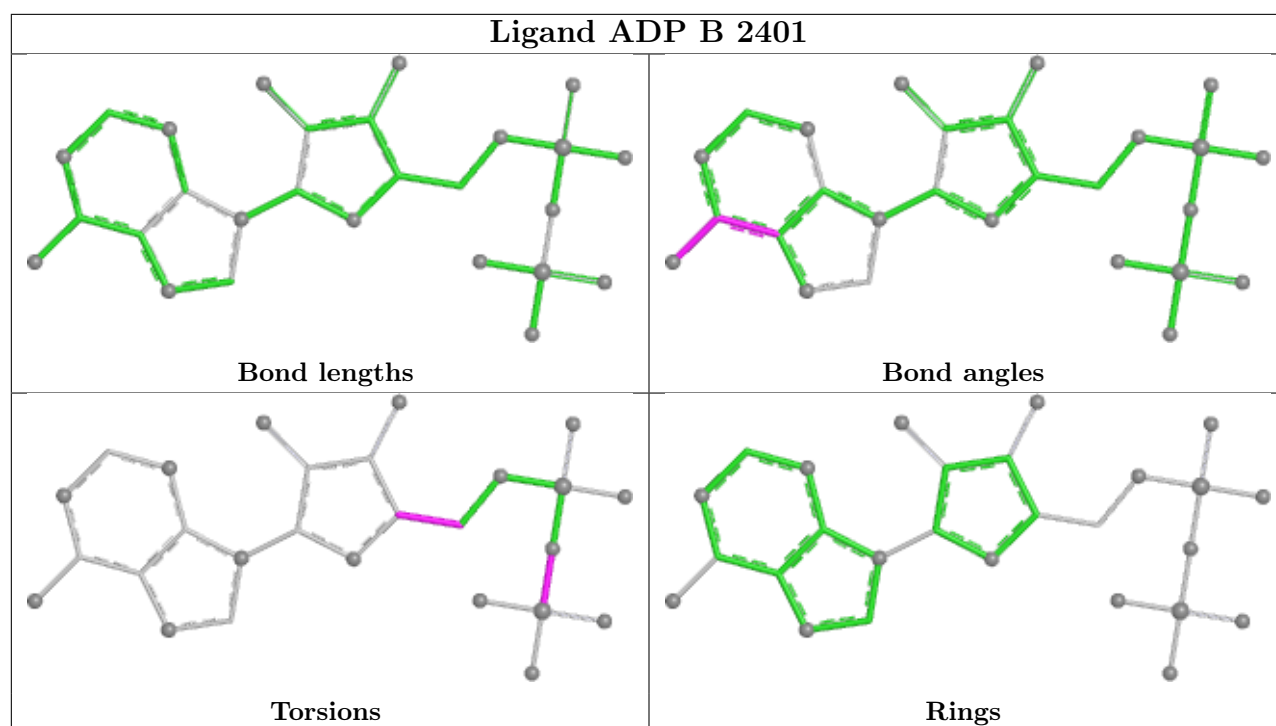












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	94:SER	C	95:VAL	N	3.80
1	J	116:PRO	C	117:SER	N	2.93
1	J	55:VAL	C	56:GLN	N	2.80
1	J	329:LYS	C	330:PRO	N	1.20
1	J	89:VAL	C	90:VAL	N	1.19
1	J	101:PHE	C	102:ARG	N	1.19
1	J	185:VAL	C	186:ASP	N	1.19
1	J	322:GLU	C	323:ILE	N	1.19
1	J	356:LEU	C	357:GLY	N	1.18

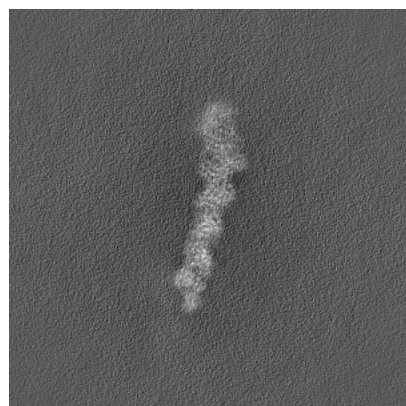
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44333. These allow visual inspection of the internal detail of the map and identification of artifacts.

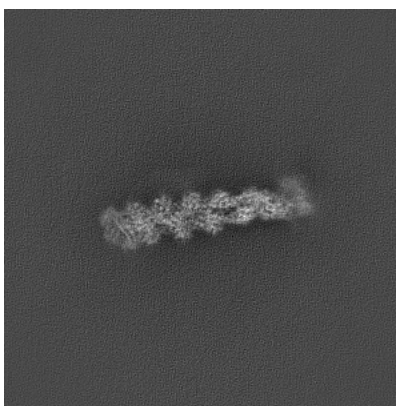
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

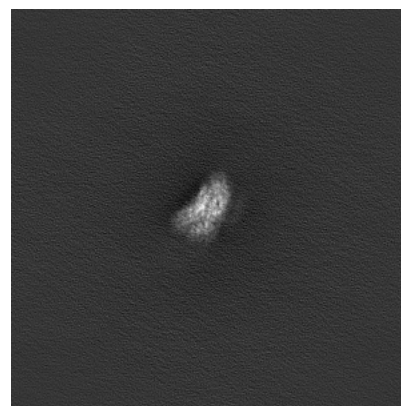
#### 6.1.1 Primary map



X

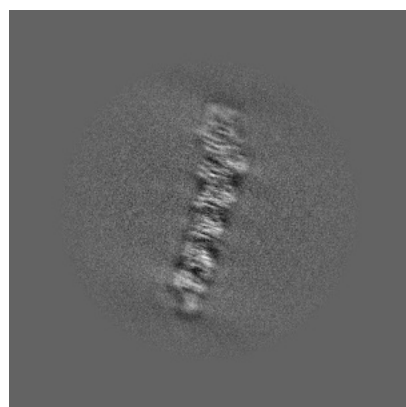


Y

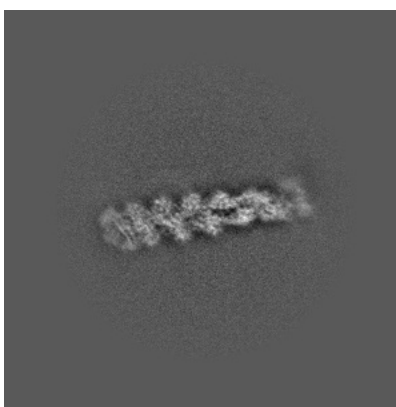


Z

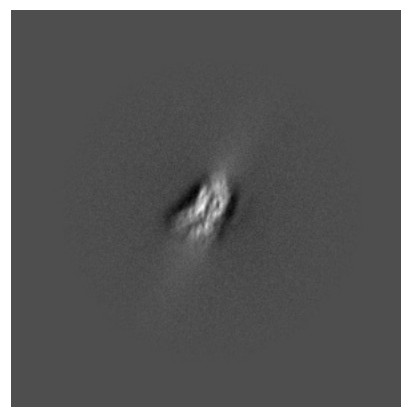
#### 6.1.2 Raw map



X



Y



Z

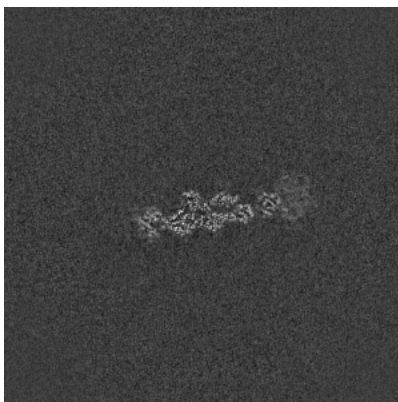
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

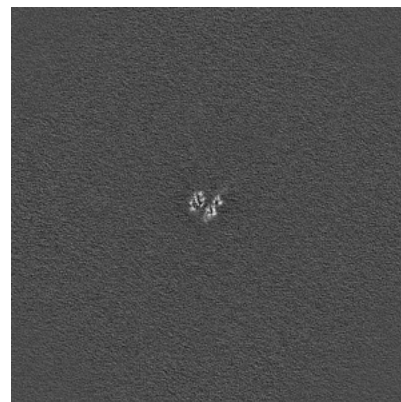
### 6.2.1 Primary map



X Index: 432

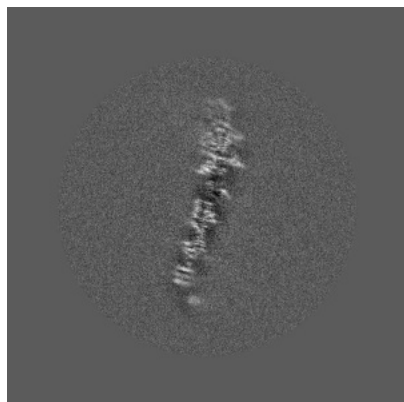


Y Index: 432

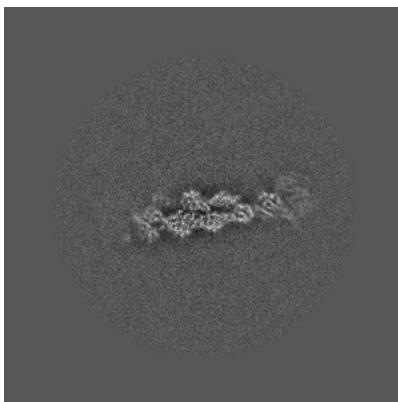


Z Index: 432

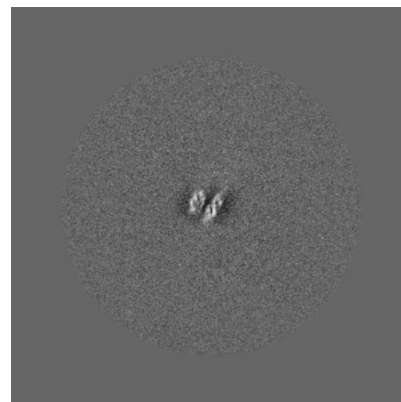
### 6.2.2 Raw map



X Index: 432



Y Index: 432



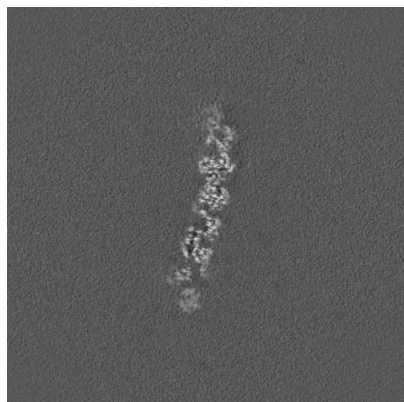
Z Index: 432

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

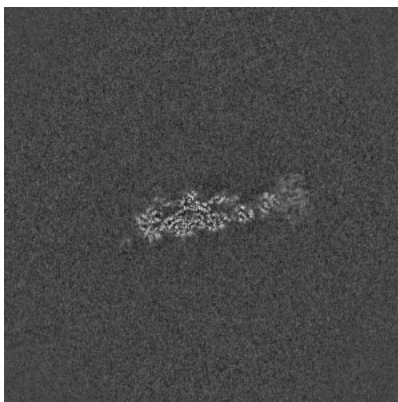


## 6.3 Largest variance slices [i](#)

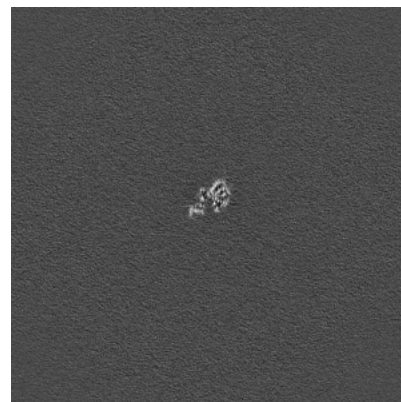
### 6.3.1 Primary map



X Index: 416

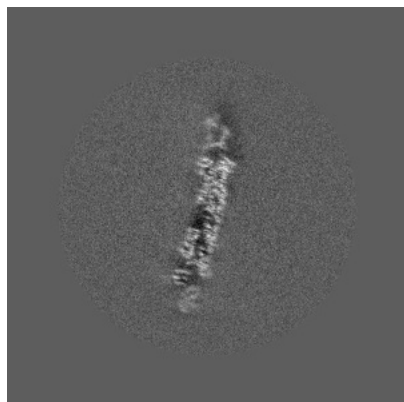


Y Index: 428

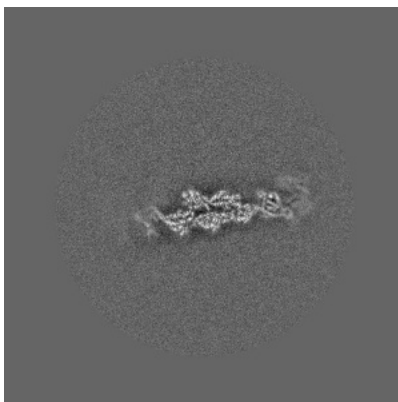


Z Index: 467

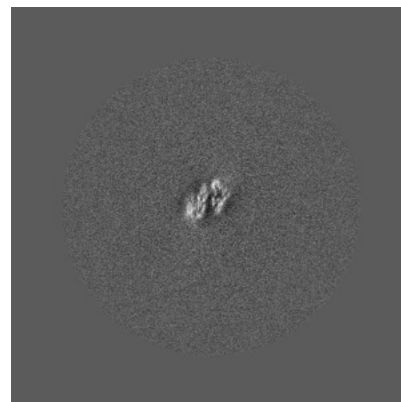
### 6.3.2 Raw map



X Index: 411



Y Index: 438

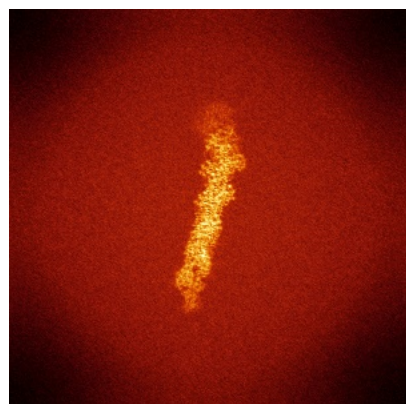


Z Index: 455

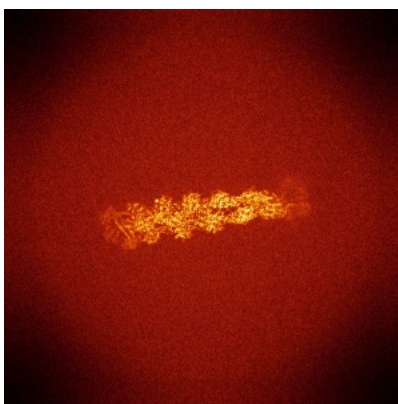
The images above show the largest variance slices of the map in three orthogonal directions.

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

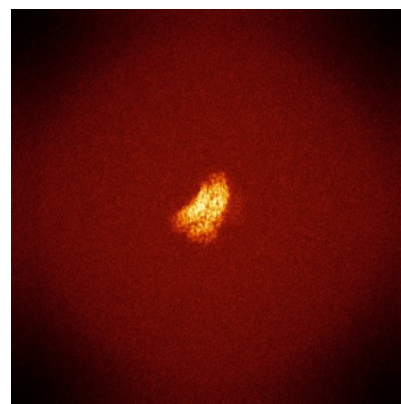
### 6.4.1 Primary map



X

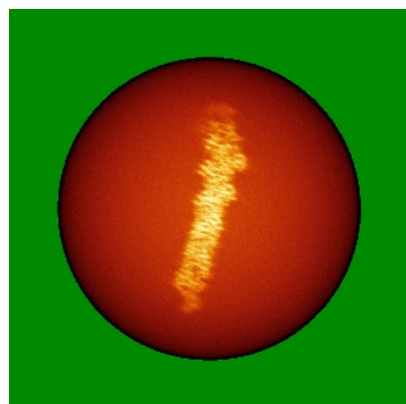


Y

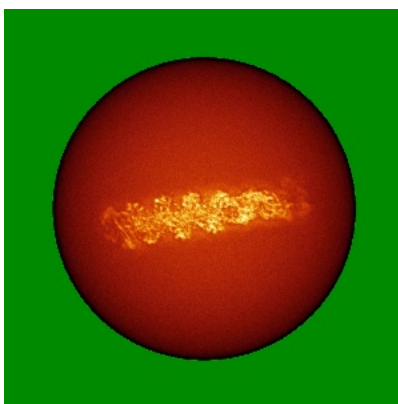


Z

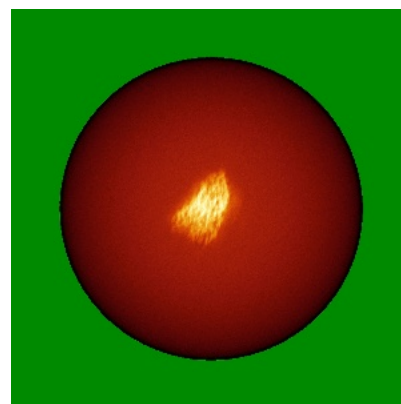
### 6.4.2 Raw map



X



Y



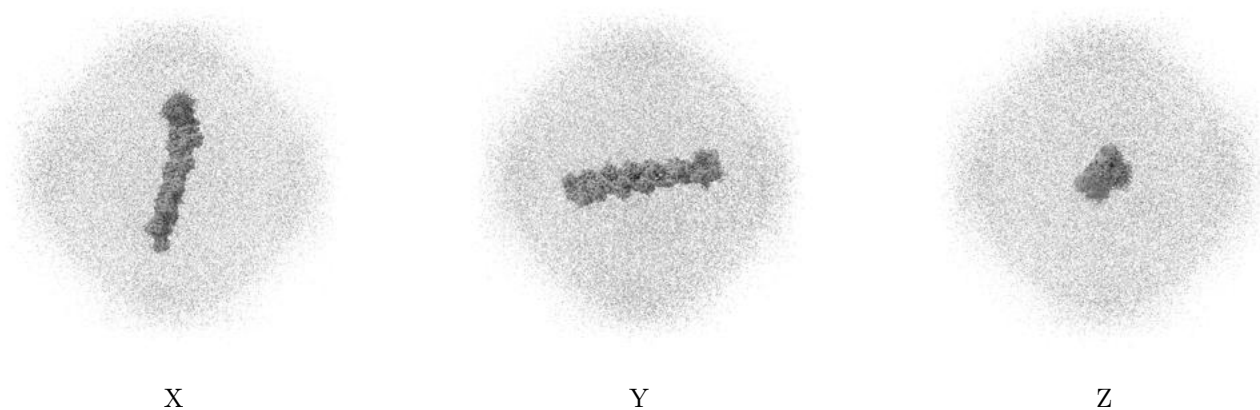
Z

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.



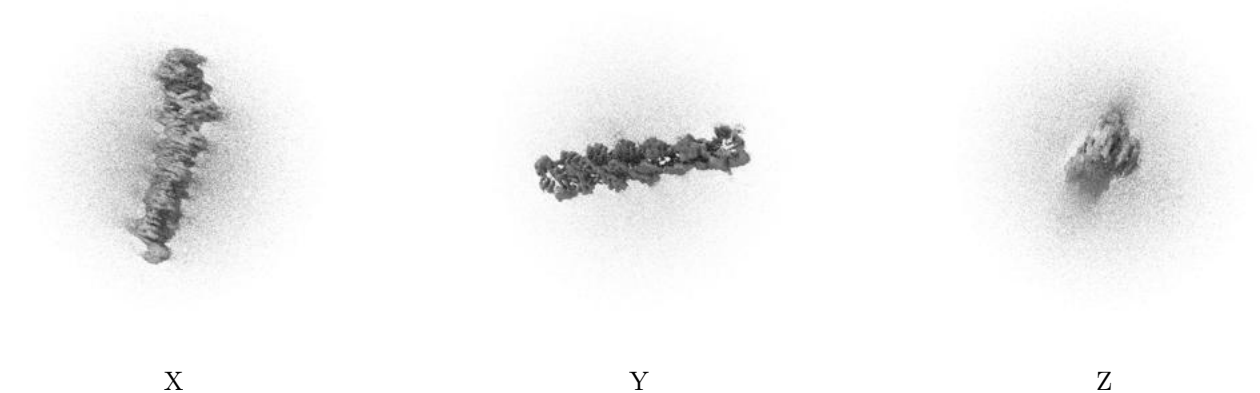
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

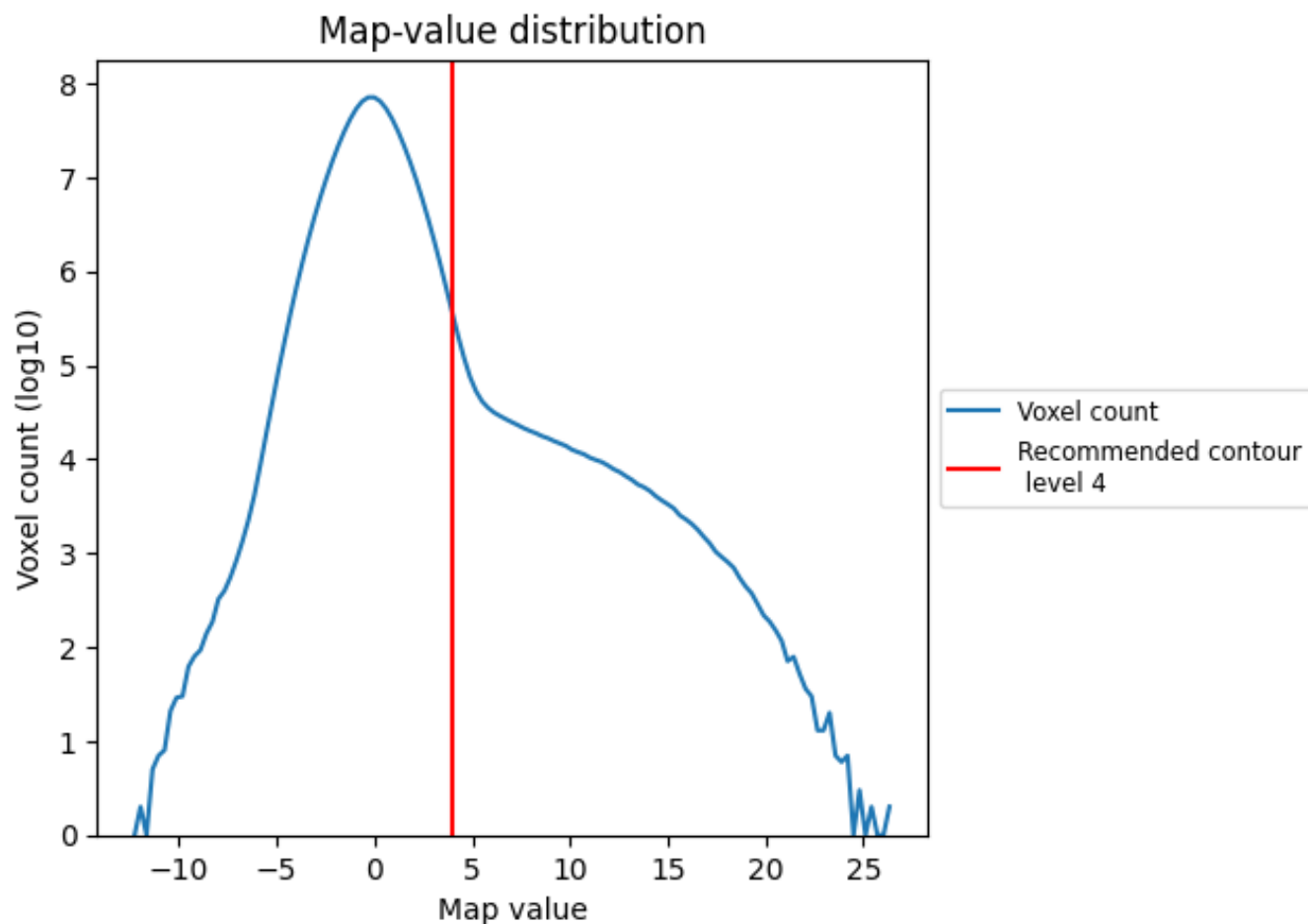
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

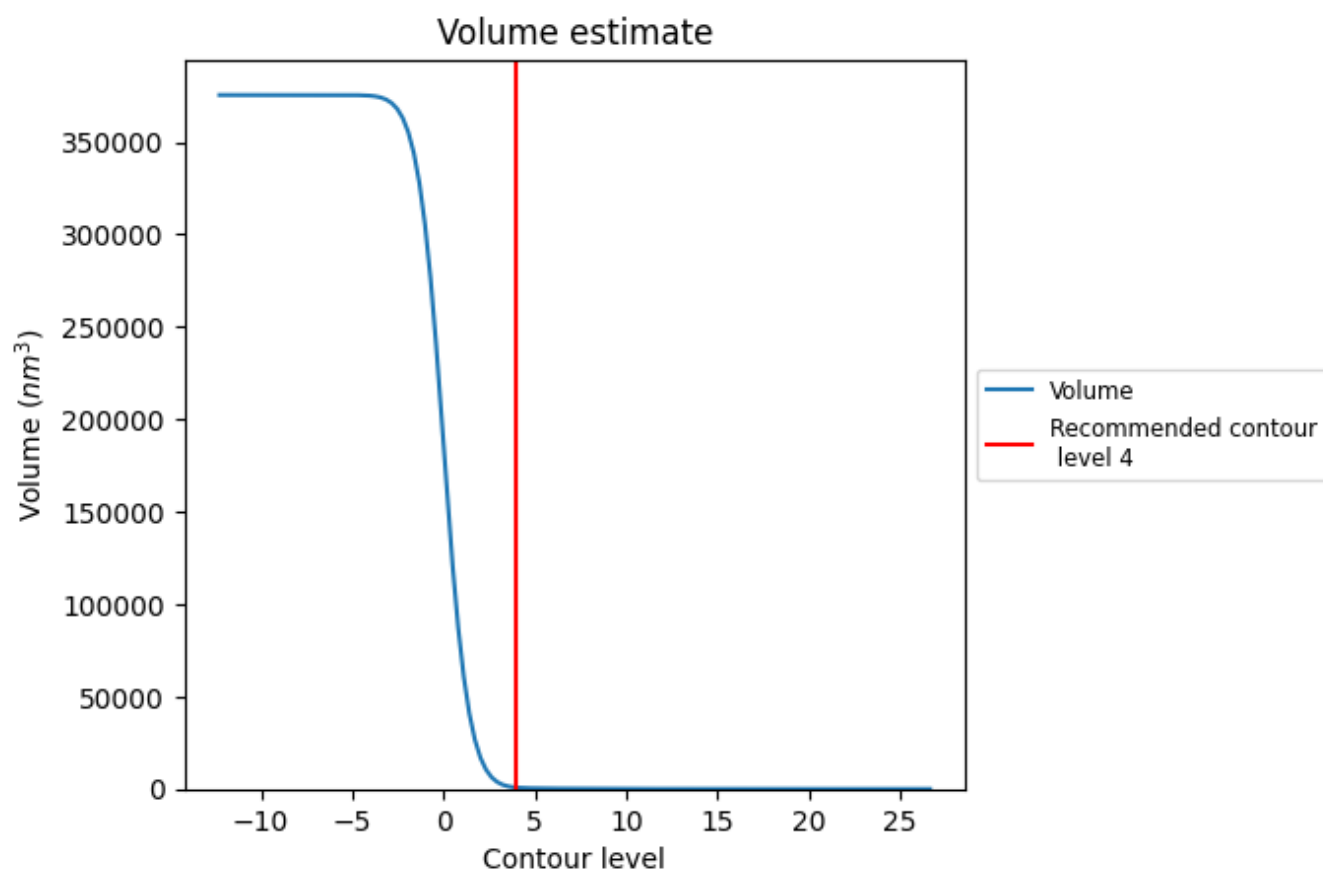
This section contains the results of statistical analysis of the map.

### 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.

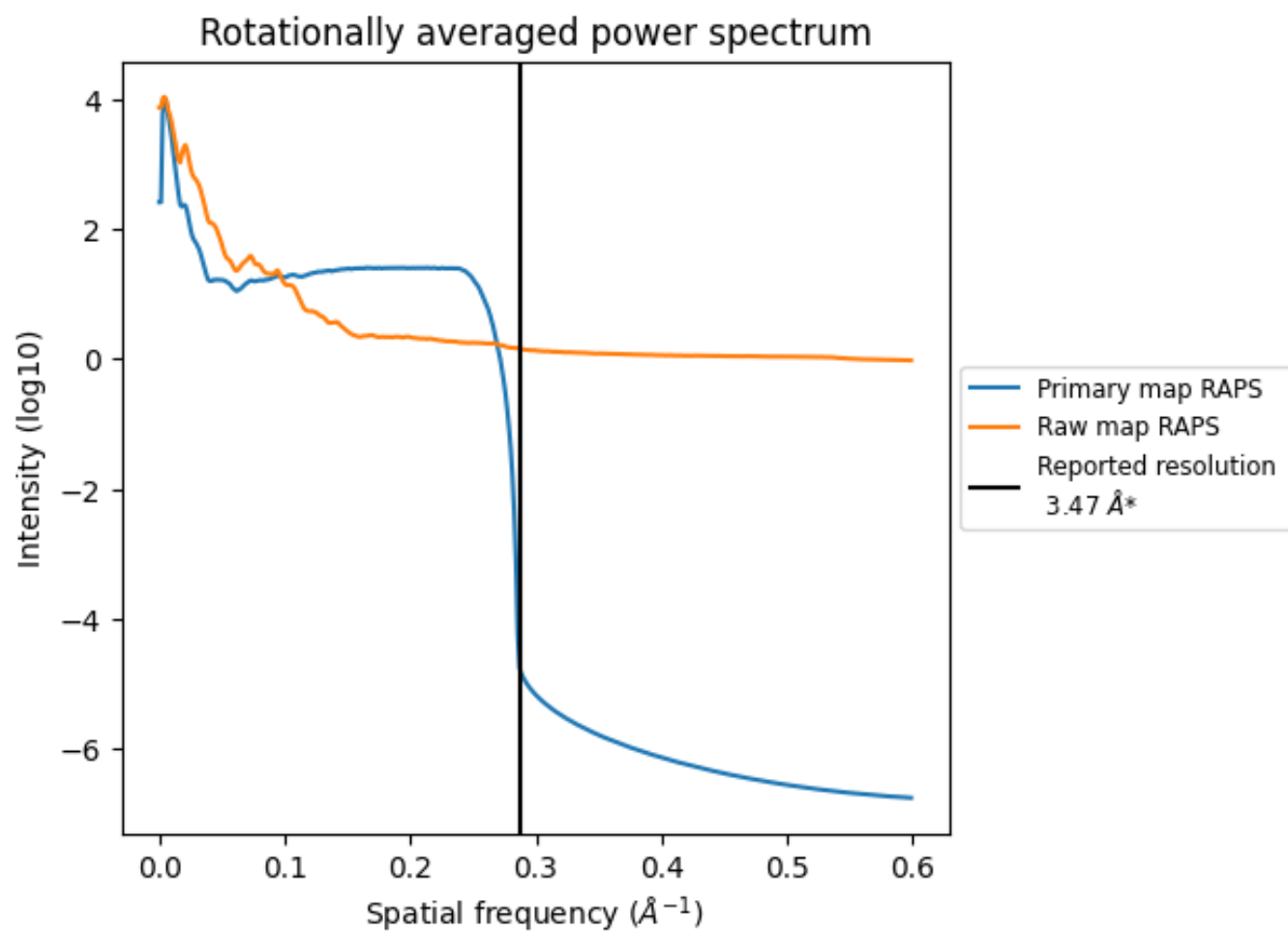
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 765  $\text{nm}^3$ ; this corresponds to an approximate mass of 691 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](#)

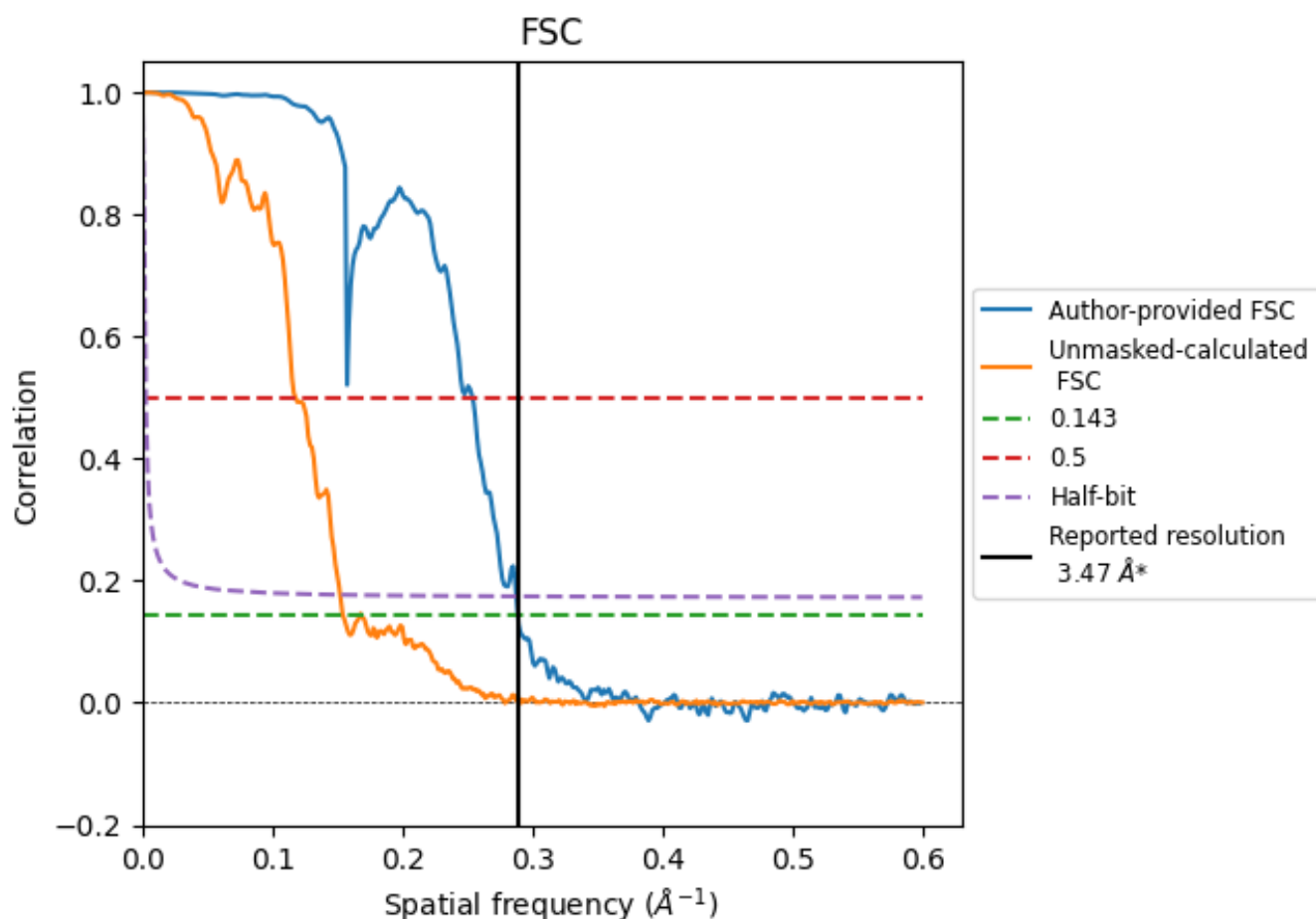


\*Reported resolution corresponds to spatial frequency of 0.288  $\text{\AA}^{-1}$

## 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  $0.288 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

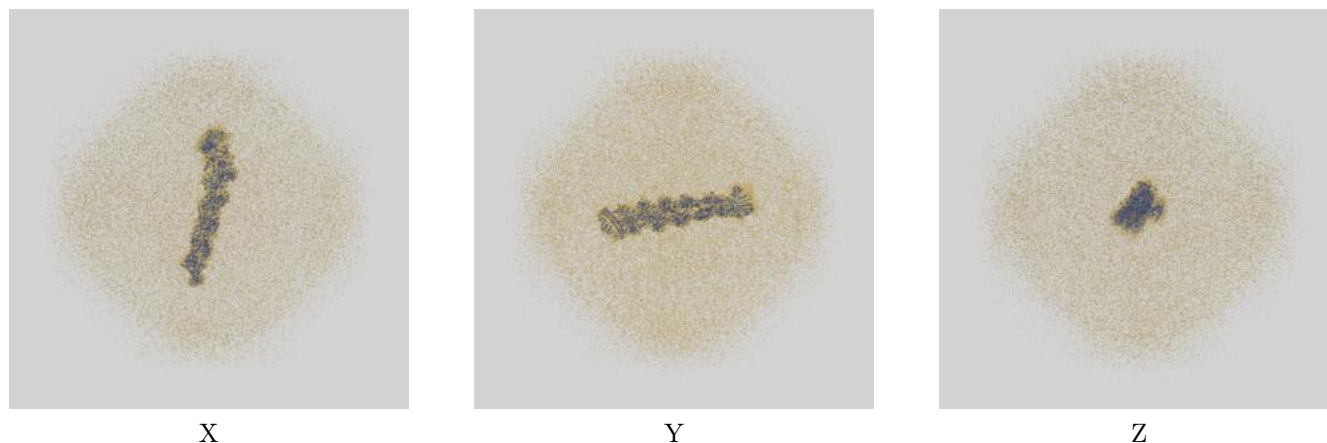
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.47	3.94	3.48
Unmasked-calculated*	6.49	8.50	6.58

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.49 differs from the reported value 3.47 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44333 and PDB model 9B85. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



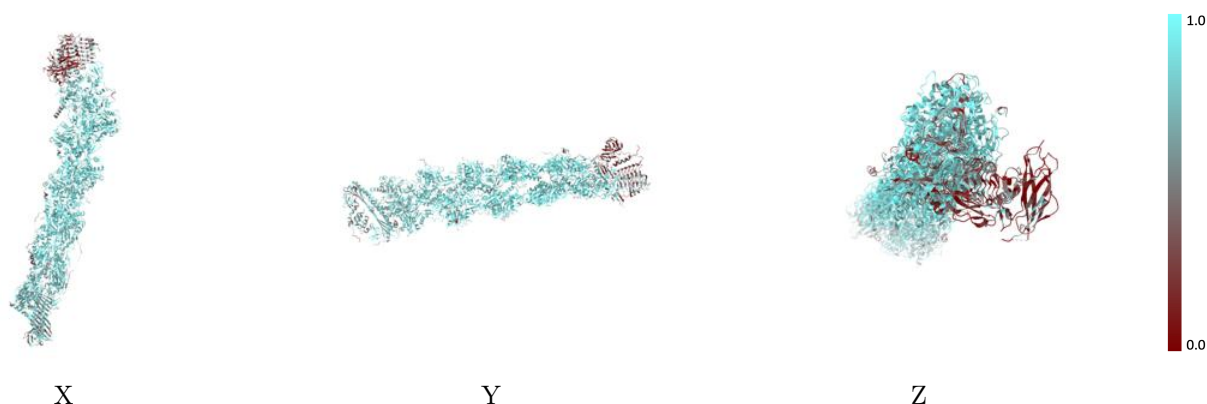
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

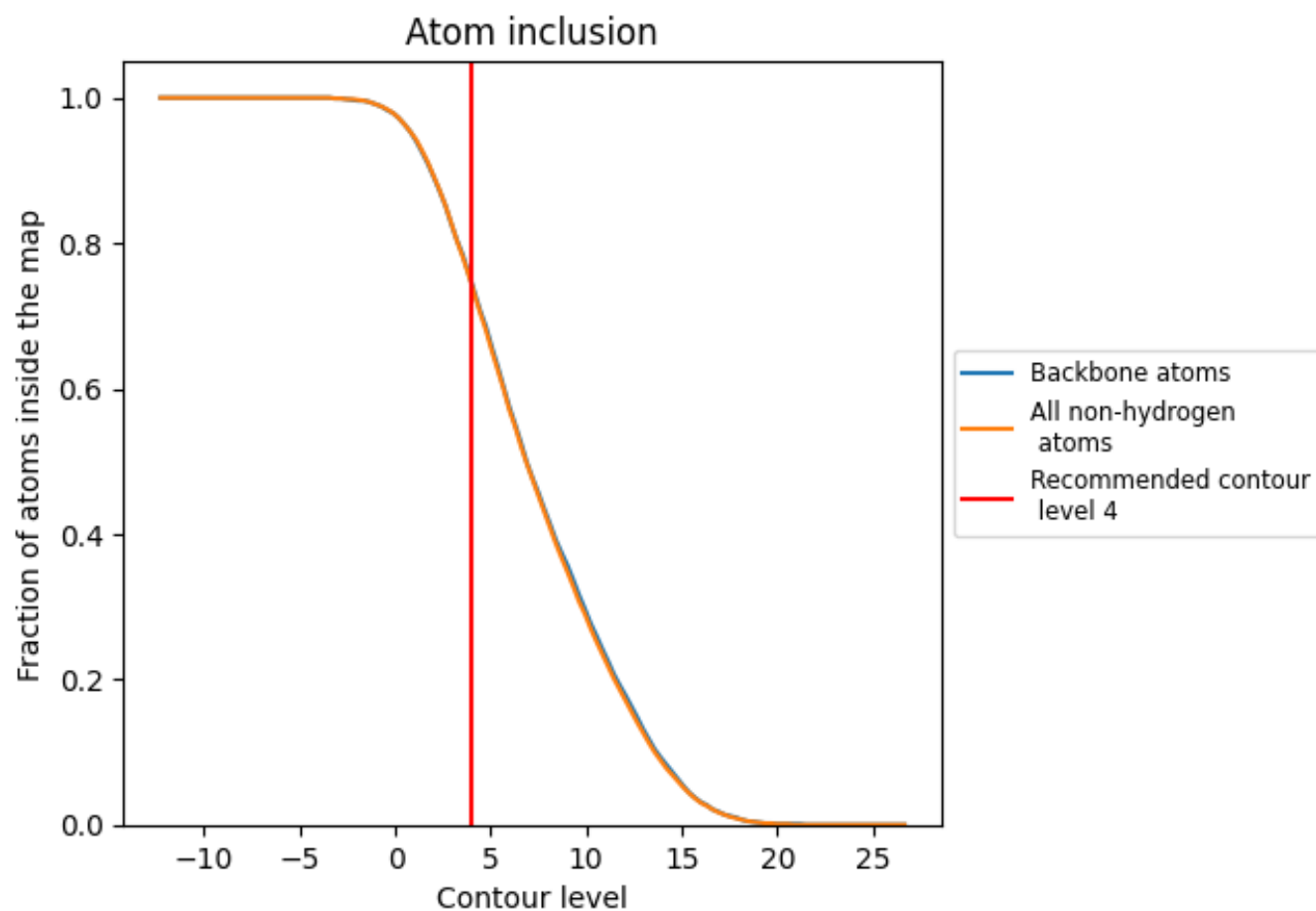
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (4).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.3060
A	 0.7800	 0.3070
B	 0.8140	 0.3470
C	 0.8420	 0.3770
D	 0.8680	 0.3910
E	 0.8560	 0.3800
F	 0.8700	 0.3870
G	 0.8630	 0.3920
H	 0.8650	 0.3760
I	 0.8220	 0.3250
J	 0.7910	 0.2870
K	 0.3990	 0.1340
L	 0.3250	 0.1000
M	 0.4630	 0.1350
N	 0.6200	 0.1810
O	 0.7150	 0.2340
P	 0.6710	 0.3050
Q	 0.4950	 0.2500
p	 0.4890	 0.2020
q	 0.4440	 0.2400

