



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:14 pm GMT

PDB ID : 6F1T  
EMDB ID : EMD-4168  
Title : Cryo-EM structure of two dynein tail domains bound to dynactin and BICDR1  
Authors : Urnavicius, L.; Lau, C.K.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.; Yildiz, A.; Carter, A.P.  
Deposited on : 2017-11-23  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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:

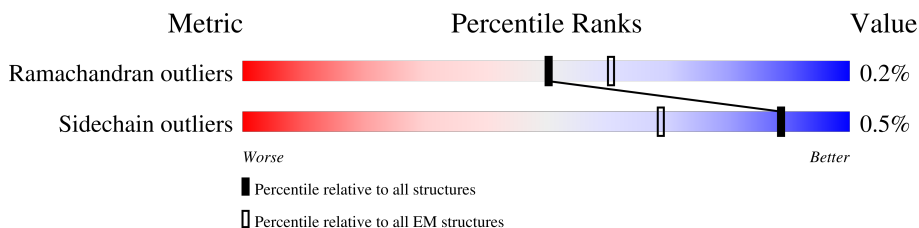
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	98% .
1	B	376	97% ..
1	C	376	98% ..
1	D	376	98% ..
1	E	376	98% .
1	F	376	97% ..
1	G	376	98% ..
1	I	376	98% .
2	H	375	99% .

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Mol	Chain	Length	Quality of chain
3	J	390	94% 5%
4	K	286	96%
5	L	272	99%
6	M	589	100%
7	N	618	100%
8	O	65	100%
8	P	65	100%
9	Q	87	46% 100%
9	R	87	100%
10	U	190	89% 9%
11	V	182	90% 9%
12	X	389	16% 73% 27%
13	Y	263	100%
14	Z	52	98%
15	a	66	79% 21%
16	b	89	84% 16%
17	c	50	74% 26%
18	d	26	88% 8%
19	e	1053	21% 88% 12%
19	f	1053	88% 12%
19	m	1053	86% 12%
19	n	1053	16% 87% 12%
20	g	612	6% 65% 35%
20	h	612	64% 35%
20	o	612	61% 35%

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Mol	Chain	Length	Quality of chain
20	p	612	
21	i	492	
21	j	492	
21	q	492	
21	r	492	
22	k	96	
22	l	96	
22	s	96	
22	t	96	
23	x	392	
24	z	53	

## 2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 92795 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	370	2956	1892	509	545	10	0	0
1	B	370	2956	1892	509	545	10	0	0
1	C	370	2956	1892	509	545	10	0	0
1	D	370	2956	1892	509	545	10	0	0
1	E	370	2956	1892	509	545	10	0	0
1	F	370	2956	1892	509	545	10	0	0
1	G	370	2956	1892	509	545	10	0	0
1	I	370	2956	1892	509	545	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	370	2885	1827	486	550	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	369	2883	1859	486	522	16	0	0

- Molecule 4 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	278	2264	1428	396	434	6	0	0

- Molecule 5 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	269	2122	1323	370	418	11	0	0

- Molecule 6 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	M	587	2935	1761	587	587	0	0

- Molecule 7 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	N	616	3080	1848	616	616	0	0

- Molecule 8 is a protein called Dynactin Subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	O	65	323	193	65	65	0	0
8	P	65	323	193	65	65	0	0

- Molecule 9 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Q	87	435	261	87	87	0	0
9	R	87	435	261	87	87	0	0

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	U	172	843	500	171	172	0	1

- Molecule 11 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	V	165	812	482	165	165	0	0

- Molecule 12 is a protein called BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICDR-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	X	285	1715	1028	340	346	1	0	0

- Molecule 13 is a protein called Dynactin Subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Y	263	1315	789	263	263	0	0

- Molecule 14 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	Z	52	260	156	52	52	0	0

- Molecule 15 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	a	52	405	255	64	86	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	37	LEU	GLN	conflict	UNP F1SKF9

- Molecule 16 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	b	75	585	365	99	121	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	37	LEU	GLN	conflict	UNP F1SKF9

- Molecule 17 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	c	37	256	159	42	54	1	0	0

- Molecule 18 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	d	24	188	118	29	41	0	0

- Molecule 19 is a protein called Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	e	926	5034	3049	982	1000	3	0	0
19	f	929	6939	4365	1267	1288	19	0	0
19	m	926	6260	3888	1182	1176	14	0	0
19	n	928	5730	3518	1099	1104	9	0	0

- Molecule 20 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			
20	g	397	1961	1167	397	397	0	0	
20	h	400	3010	1892	532	571	15	0	0
20	o	397	3126	1969	546	596	15	0	0
20	p	401	2116	1273	416	427	0	0	

There are 8 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
g	484	SER	THR	conflict	UNP Q13409
g	499	GLY	ASP	conflict	UNP Q13409
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409
o	484	SER	THR	conflict	UNP Q13409
o	499	GLY	ASP	conflict	UNP Q13409
p	484	SER	THR	conflict	UNP Q13409
p	499	GLY	ASP	conflict	UNP Q13409

- Molecule 21 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	268	Total	C	N	O	0	0	
			1327	791	268	268			
21	j	288	Total	C	N	O	S	0	0
			2284	1463	379	431	11		
21	q	268	Total	C	N	O	0	0	
			1327	791	268	268			
21	r	268	Total	C	N	O	0	0	
			1327	791	268	268			

- Molecule 22 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	93	Total	C	N	O	0	0	
			462	276	93	93			
22	l	93	Total	C	N	O	0	0	
			462	276	93	93			
22	s	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
22	t	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

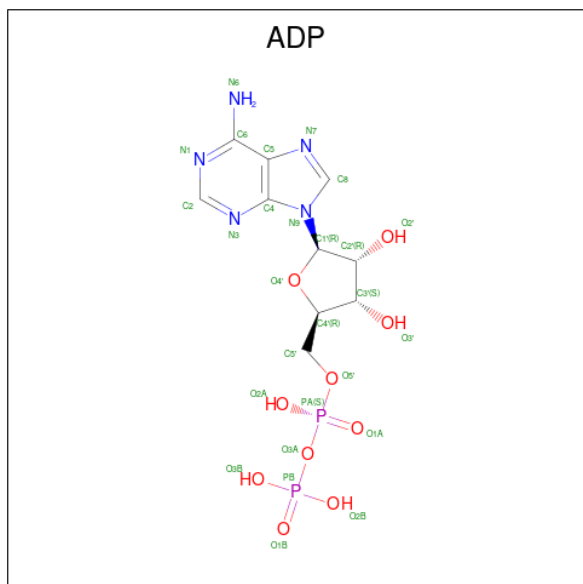
- Molecule 23 is a protein called BICD family-like cargo adapter 1, BICD family-like cargo adapter 1, BICD family-like cargo adapter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	288	Total	C	N	O	S	0	0
			1695	1018	336	340	1		

- Molecule 24 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	z	53	265	159	53	53	0	0

- Molecule 25 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

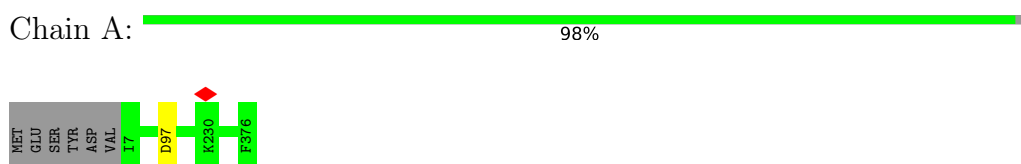
- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



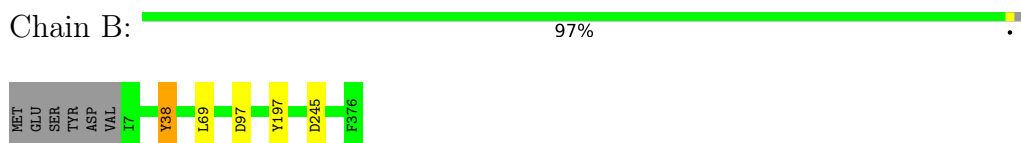
### 3 Residue-property plots [i](#)

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.

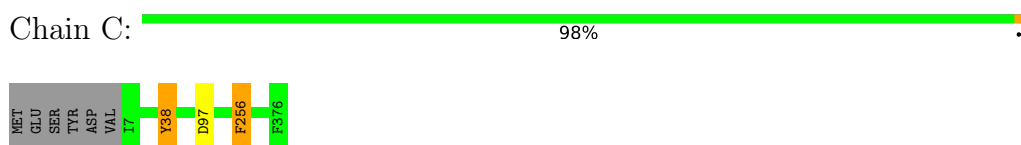
- Molecule 1: ARP1 actin related protein 1 homolog A



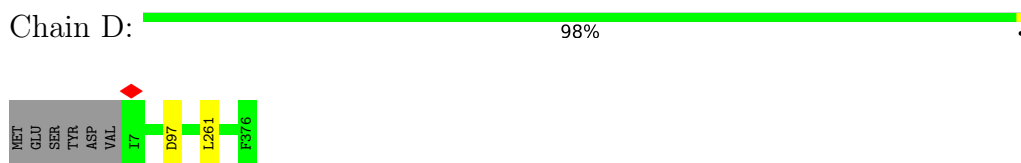
- Molecule 1: ARP1 actin related protein 1 homolog A



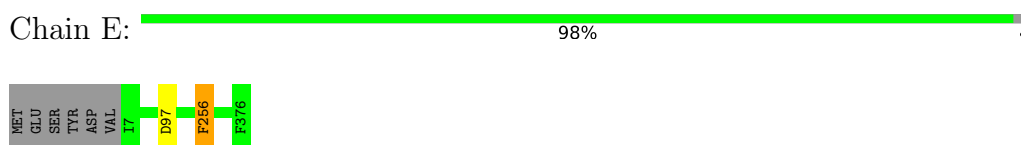
- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 1: ARP1 actin related protein 1 homolog A

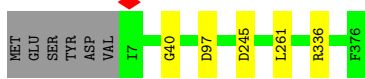


- Molecule 1: ARP1 actin related protein 1 homolog A



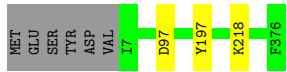
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain F:  97%



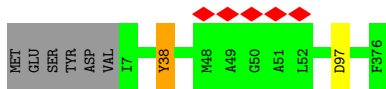
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain G:  98%



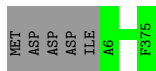
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain I:  98%



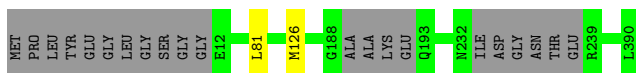
- Molecule 2: Actin, cytoplasmic 1

Chain H:  99%



- Molecule 3: Actin related protein 10 homolog

Chain J:  94% 5%



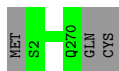
- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:  96%



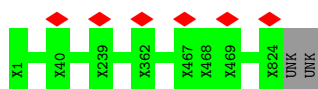
- Molecule 5: F-actin capping protein beta subunit

Chain L:  99%



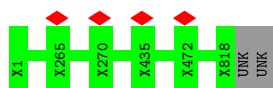
- Molecule 6: Dynactin Subunit 2

Chain M:  100%



- Molecule 7: Dynactin Subunit 2

Chain N:  100%



- Molecule 8: Dynactin Subunit 3

Chain O:  100%

There are no outlier residues recorded for this chain.

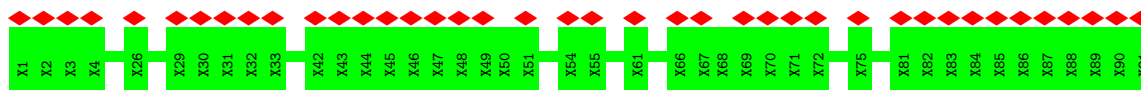
- Molecule 8: Dynactin Subunit 3

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Dynactin Subunit 2

Chain Q:  46% 100%




- Molecule 9: Dynactin Subunit 2

Chain R:  100%


There are no outlier residues recorded for this chain.

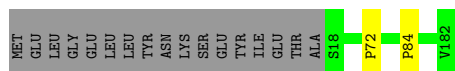
- Molecule 10: Dynactin 6

Chain U:  89% 9%

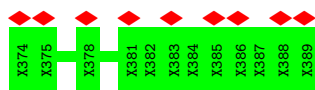
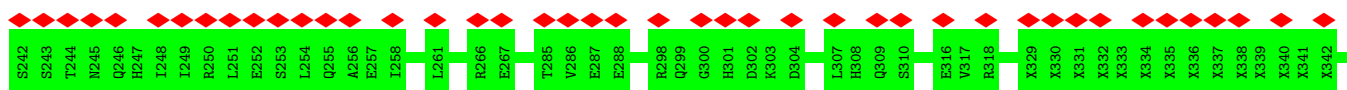
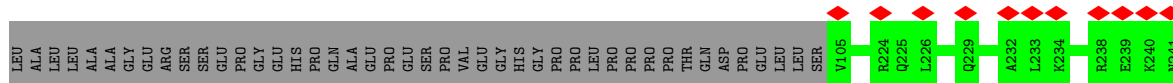
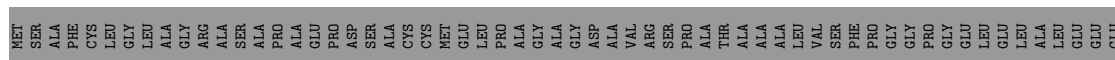
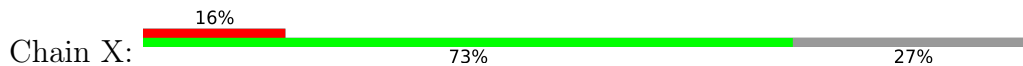


- Molecule 11: Dynactin subunit 5

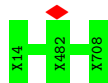
Chain V:  90% 9%



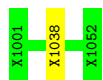
- Molecule 12: BICD family-like cargo adapter 1, BICD family-like cargo adapter 1, BICD family-like cargo adapter 1, BICDR-1



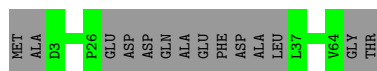
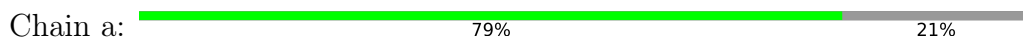
- Molecule 13: Dynactin Subunit 4



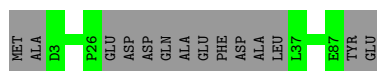
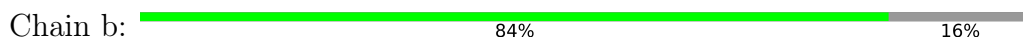
- Molecule 14: Dynactin Subunit 1



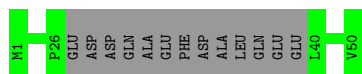
- Molecule 15: Dynactin subunit 2



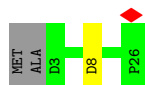
- Molecule 16: Dynactin subunit 2



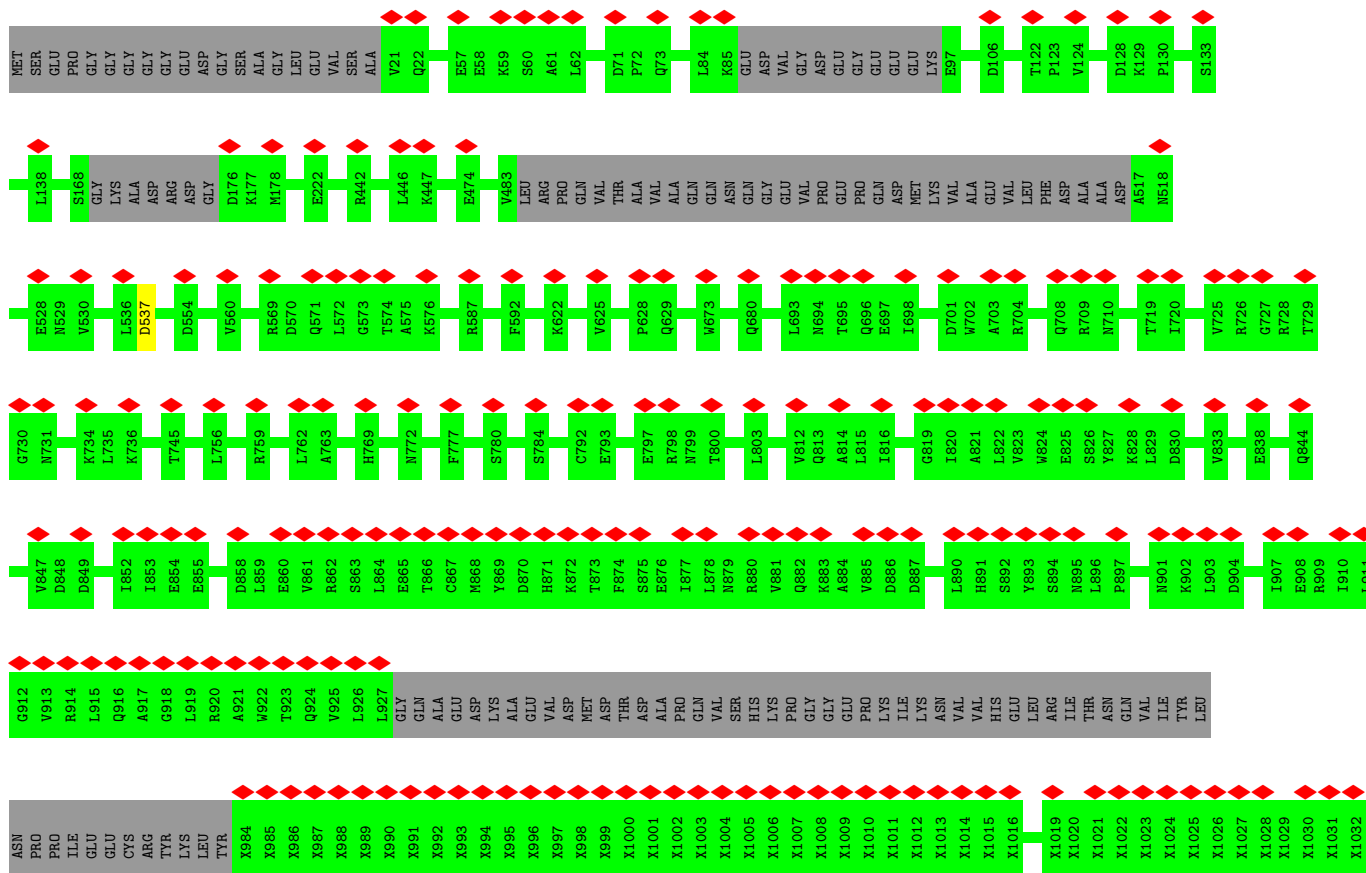
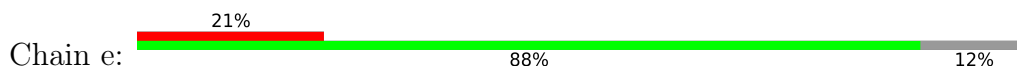
• Molecule 17: Dynactin subunit 2



• Molecule 18: Dynactin subunit 2

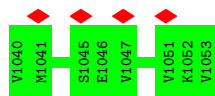


• Molecule 19: Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Dynein Heavy Chain, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Dynein Heavy Chain, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1

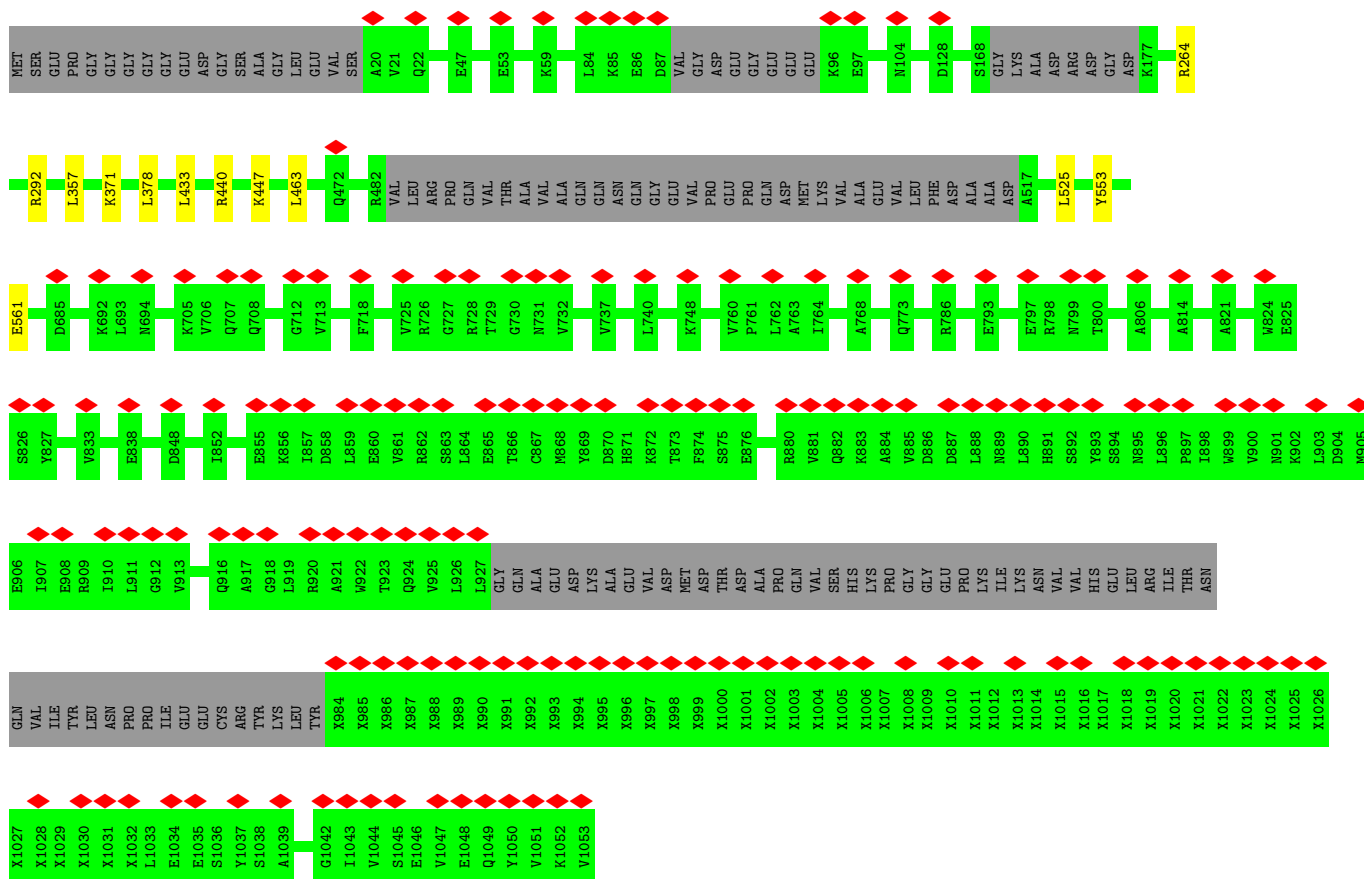
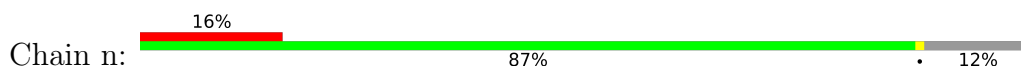




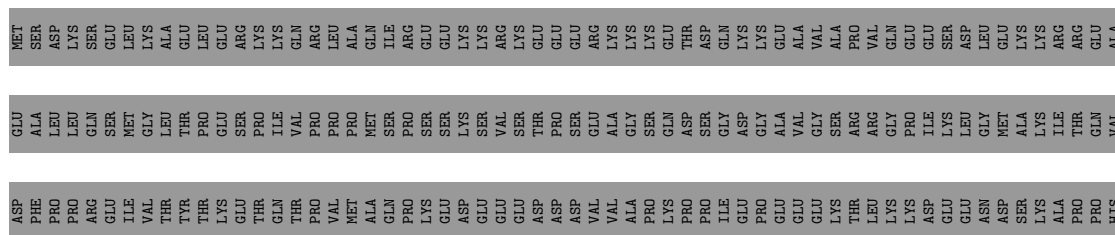


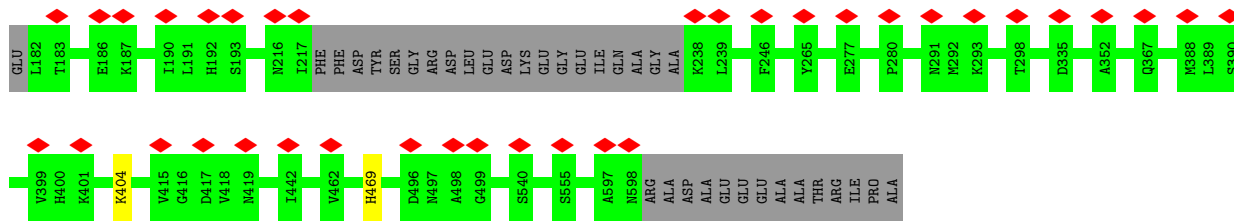


- Molecule 19: Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Dynein Heavy Chain, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Dynein Heavy Chain, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1

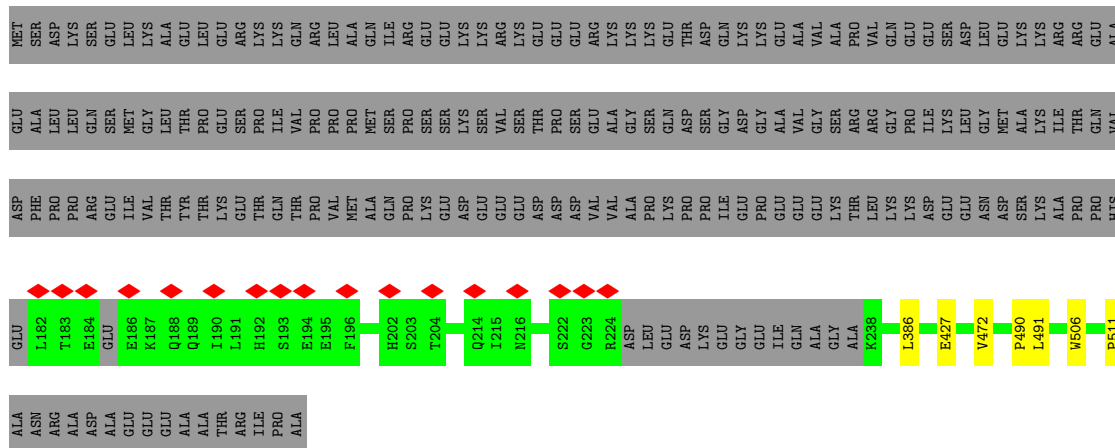


- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

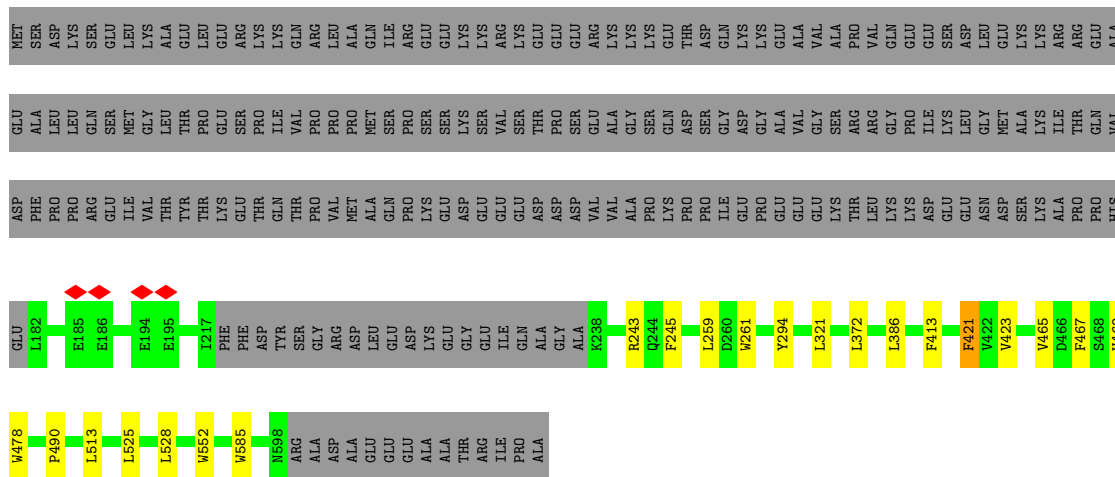




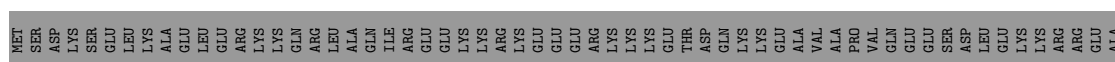
• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2



• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2



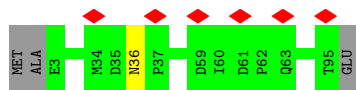
• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2



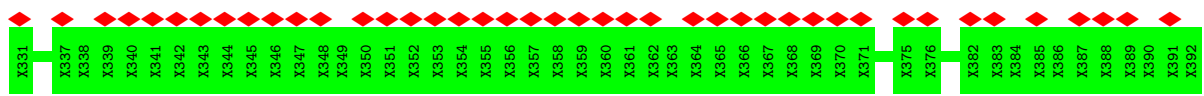
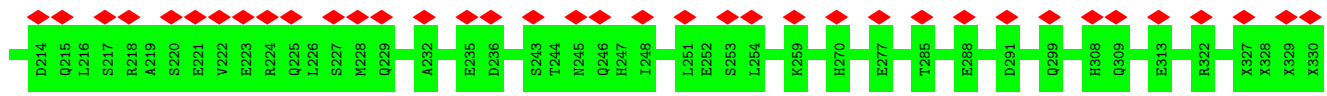
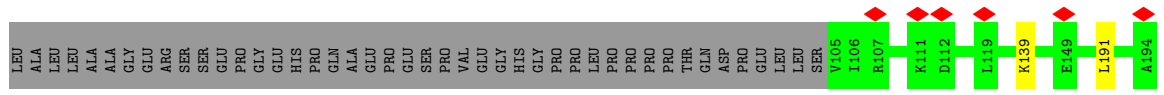
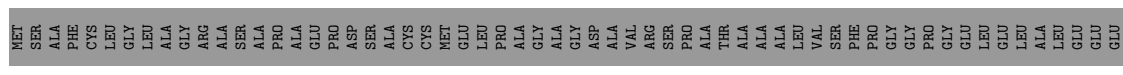




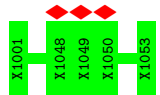




- Molecule 23: BICD family-like cargo adapter 1, BICD family-like cargo adapter 1, BICD family-like cargo adapter 1



- Molecule 24: Dynactin Subunit 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	205611	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 ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.440	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.046	Depositor
Map size (Å)	804.0, 804.0, 804.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.57	0/3025	0.67	1/4085 (0.0%)
1	B	0.82	0/3025	0.80	5/4085 (0.1%)
1	C	0.70	0/3025	0.77	6/4085 (0.1%)
1	D	0.83	0/3025	0.79	2/4085 (0.0%)
1	E	0.69	0/3025	0.73	3/4085 (0.1%)
1	F	0.89	1/3025 (0.0%)	0.84	3/4085 (0.1%)
1	G	0.61	0/3025	0.69	1/4085 (0.0%)
1	I	0.34	0/3025	0.66	4/4085 (0.1%)
2	H	0.49	0/2948	0.64	0/3991
3	J	0.35	0/2943	0.65	2/3992 (0.1%)
4	K	0.64	0/2316	0.78	3/3135 (0.1%)
5	L	0.63	0/2156	0.77	0/2906
10	U	0.38	0/841	0.65	0/1168
11	V	0.31	0/811	0.61	0/1126
12	X	0.39	0/1402	0.56	0/1914
15	a	0.39	0/413	0.65	0/563
16	b	0.43	0/595	0.69	0/803
17	c	0.57	0/260	0.78	0/356
18	d	0.79	1/193 (0.5%)	0.74	0/265
19	e	0.32	0/4807	0.62	0/6656
19	f	0.54	0/6791	0.82	7/9196 (0.1%)
19	m	0.61	5/6087 (0.1%)	0.84	14/8287 (0.2%)
19	n	0.42	1/5527 (0.0%)	0.74	8/7571 (0.1%)
20	g	0.37	0/1959	0.76	0/2725
20	h	0.68	2/3087 (0.1%)	0.88	2/4213 (0.0%)
20	o	0.78	5/3209 (0.2%)	1.03	14/4369 (0.3%)
20	p	0.32	0/2121	0.74	0/2933
21	i	0.26	0/1322	0.61	0/1835
21	j	0.61	1/2333 (0.0%)	1.07	13/3157 (0.4%)
21	q	0.29	0/1322	0.68	0/1835
21	r	0.28	0/1322	0.69	0/1835
22	k	0.33	0/461	0.81	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
22	l	0.31	0/461	0.69	0/642
22	s	0.28	0/752	0.57	0/1017
22	t	0.26	0/752	0.53	0/1017
23	x	0.37	0/1367	0.57	1/1870 (0.1%)
All	All	0.57	16/82758 (0.0%)	0.76	89/112699 (0.1%)

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
14	Z	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	n	553	TYR	CD1-CE1	-7.94	1.27	1.39
20	o	552	TRP	CB-CG	-7.30	1.37	1.50
19	m	702	TRP	CB-CG	-6.92	1.37	1.50
19	m	546	TRP	CB-CG	-6.77	1.38	1.50
19	m	749	GLU	CG-CD	-6.26	1.42	1.51
20	h	427	GLU	CG-CD	-5.82	1.43	1.51
20	h	506	TRP	CB-CG	-5.56	1.40	1.50
1	F	40	GLY	C-N	-5.46	1.21	1.34
19	m	749	GLU	CB-CG	-5.45	1.41	1.52
20	o	261	TRP	CB-CG	-5.45	1.40	1.50
19	m	702	TRP	CE3-CZ3	-5.41	1.29	1.38
18	d	8	ASP	C-N	-5.35	1.21	1.34
20	o	585	TRP	CE3-CZ3	-5.34	1.29	1.38
20	o	478	TRP	CB-CG	-5.22	1.40	1.50
20	o	423	VAL	CB-CG1	-5.07	1.42	1.52
21	j	58	LEU	CA-CB	-5.05	1.42	1.53

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	38	TYR	CB-CG-CD2	-10.52	114.69	121.00
20	o	513	LEU	CA-CB-CG	10.41	139.24	115.30
1	E	256	PHE	CB-CG-CD2	-10.13	113.71	120.80
1	C	38	TYR	CB-CG-CD2	-10.10	114.94	121.00
1	C	256	PHE	CB-CG-CD2	-9.94	113.84	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	o	421	PHE	CB-CG-CD2	-9.85	113.91	120.80
1	E	256	PHE	CB-CG-CD1	9.43	127.40	120.80
1	B	38	TYR	CB-CG-CD2	-9.14	115.51	121.00
1	C	256	PHE	CB-CG-CD1	8.81	126.97	120.80
20	o	259	LEU	CA-CB-CG	8.81	135.57	115.30
19	m	756	LEU	CB-CG-CD2	-8.72	96.18	111.00
19	m	601	ILE	CG1-CB-CG2	-8.35	93.04	111.40
19	m	694	ASN	C-N-CA	8.30	142.44	121.70
20	o	421	PHE	CB-CG-CD1	8.27	126.59	120.80
1	C	38	TYR	CB-CG-CD1	7.92	125.75	121.00
21	j	338	ASP	CB-CG-OD1	7.87	125.38	118.30
1	I	38	TYR	CB-CG-CD1	7.50	125.50	121.00
1	B	38	TYR	CB-CG-CD1	7.48	125.49	121.00
19	f	888	LEU	CB-CG-CD2	-7.48	98.28	111.00
20	o	528	LEU	CA-CB-CG	7.37	132.24	115.30
19	m	672	GLY	N-CA-C	-7.29	94.88	113.10
19	m	480	ILE	CG1-CB-CG2	-6.89	96.25	111.40
19	n	553	TYR	CA-CB-CG	-6.81	100.46	113.40
4	K	182	THR	N-CA-C	-6.64	93.07	111.00
21	j	280	LEU	CA-CB-CG	6.54	130.34	115.30
20	o	259	LEU	CB-CG-CD1	-6.53	99.90	111.00
19	f	762	LEU	CA-CB-CG	-6.52	100.30	115.30
19	f	1033	LEU	CA-CB-CG	6.47	130.18	115.30
20	o	294	TYR	CA-CB-CG	-6.42	101.20	113.40
1	B	38	TYR	CA-CB-CG	6.38	125.52	113.40
1	D	261	LEU	CA-CB-CG	6.38	129.97	115.30
20	h	386	LEU	CA-CB-CG	-6.28	100.85	115.30
20	o	386	LEU	CA-CB-CG	-6.26	100.91	115.30
19	m	433	LEU	CB-CG-CD1	-6.17	100.52	111.00
1	C	38	TYR	CA-CB-CG	5.95	124.71	113.40
21	j	240	LEU	CA-CB-CG	-5.94	101.63	115.30
19	n	433	LEU	CA-CB-CG	5.94	128.97	115.30
1	F	336	ARG	CB-CG-CD	-5.90	96.26	111.60
19	m	537	ASP	CB-CG-OD1	5.83	123.55	118.30
4	K	46	LEU	CA-CB-CG	5.80	128.63	115.30
3	J	81	LEU	CA-CB-CG	5.78	128.58	115.30
19	f	733	LEU	CA-CB-CG	5.73	128.49	115.30
20	o	372	LEU	CB-CG-CD2	-5.61	101.46	111.00
19	n	378	LEU	CA-CB-CG	-5.60	102.42	115.30
21	j	109	LEU	CA-CB-CG	5.57	128.12	115.30
19	m	619	LEU	CA-CB-CG	-5.53	102.58	115.30
3	J	126	MET	CA-CB-CG	-5.53	103.91	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	m	568	LEU	CA-CB-CG	-5.50	102.65	115.30
20	o	413	PHE	CB-CG-CD2	-5.46	116.98	120.80
20	o	490	PRO	N-CA-C	-5.43	97.98	112.10
4	K	149	ASP	CB-CG-OD1	5.38	123.15	118.30
19	n	371	LYS	C-N-CA	-5.38	108.25	121.70
1	F	261	LEU	CB-CG-CD2	-5.38	101.86	111.00
21	j	225	ILE	N-CA-C	-5.36	96.52	111.00
21	j	342	LYS	C-N-CD	5.34	139.62	128.40
21	j	363	LEU	CA-CB-CG	5.34	127.59	115.30
23	x	191	LEU	CA-CB-CG	-5.34	103.01	115.30
21	j	58	LEU	CB-CG-CD1	-5.32	101.96	111.00
19	n	463	LEU	CA-CB-CG	5.31	127.51	115.30
19	n	357	LEU	CA-CB-CG	5.30	127.49	115.30
1	I	38	TYR	CA-CB-CG	5.30	123.47	113.40
19	f	896	LEU	CB-CG-CD1	-5.30	101.99	111.00
19	m	740	LEU	N-CA-C	5.29	125.29	111.00
21	j	277	GLU	CA-CB-CG	-5.26	101.83	113.40
19	n	553	TYR	CB-CG-CD1	-5.26	117.84	121.00
19	m	758	PHE	CB-CG-CD2	-5.24	117.13	120.80
19	n	525	LEU	CA-CB-CG	5.24	127.36	115.30
1	F	97	ASP	CB-CG-OD2	5.23	123.01	118.30
21	j	86	LEU	CA-CB-CG	5.23	127.32	115.30
1	D	97	ASP	CB-CG-OD2	5.22	123.00	118.30
20	o	243	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	E	97	ASP	CB-CG-OD2	5.20	122.98	118.30
19	f	891	HIS	N-CA-C	-5.19	96.98	111.00
21	j	185	MET	CA-CB-CG	5.19	122.12	113.30
1	C	97	ASP	CB-CG-OD2	5.18	122.97	118.30
19	m	591	LEU	CA-CB-CG	-5.18	103.38	115.30
1	A	97	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	97	ASP	CB-CG-OD2	5.17	122.95	118.30
1	G	97	ASP	CB-CG-OD2	5.14	122.93	118.30
1	I	97	ASP	CB-CG-OD2	5.14	122.93	118.30
21	j	343	PRO	C-N-CD	5.14	139.19	128.40
19	m	167	GLU	N-CA-C	-5.14	97.13	111.00
21	j	186	GLU	N-CA-C	5.09	124.75	111.00
19	m	598	ARG	NE-CZ-NH2	-5.09	117.75	120.30
20	o	525	LEU	CA-CB-CG	5.06	126.94	115.30
20	h	506	TRP	CA-CB-CG	5.04	123.28	113.70
1	B	69	LEU	CA-CB-CG	-5.02	103.76	115.30
19	f	682	LEU	CB-CG-CD1	-5.01	102.49	111.00
20	o	321	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	Z	1038	UNK	Peptide

## 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%)	334 (91%)	34 (9%)	0	100	100
1	B	368/376 (98%)	338 (92%)	30 (8%)	0	100	100
1	C	368/376 (98%)	341 (93%)	27 (7%)	0	100	100
1	D	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	E	368/376 (98%)	335 (91%)	33 (9%)	0	100	100
1	F	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	G	368/376 (98%)	342 (93%)	26 (7%)	0	100	100
1	I	368/376 (98%)	342 (93%)	26 (7%)	0	100	100
2	H	368/375 (98%)	345 (94%)	23 (6%)	0	100	100
3	J	363/390 (93%)	336 (93%)	27 (7%)	0	100	100
4	K	276/286 (96%)	244 (88%)	32 (12%)	0	100	100
5	L	267/272 (98%)	233 (87%)	34 (13%)	0	100	100
10	U	169/190 (89%)	126 (75%)	41 (24%)	2 (1%)	13	50
11	V	163/182 (90%)	125 (77%)	36 (22%)	2 (1%)	13	50
12	X	220/389 (57%)	216 (98%)	4 (2%)	0	100	100
15	a	48/66 (73%)	43 (90%)	5 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	b	71/89 (80%)	58 (82%)	13 (18%)	0	100	100
17	c	33/50 (66%)	26 (79%)	7 (21%)	0	100	100
18	d	22/26 (85%)	16 (73%)	6 (27%)	0	100	100
19	e	868/1053 (82%)	807 (93%)	60 (7%)	1 (0%)	51	84
19	f	871/1053 (83%)	796 (91%)	75 (9%)	0	100	100
19	m	868/1053 (82%)	797 (92%)	70 (8%)	1 (0%)	51	84
19	n	870/1053 (83%)	797 (92%)	73 (8%)	0	100	100
20	g	393/612 (64%)	314 (80%)	77 (20%)	2 (0%)	29	68
20	h	394/612 (64%)	332 (84%)	59 (15%)	3 (1%)	19	58
20	o	393/612 (64%)	321 (82%)	70 (18%)	2 (0%)	29	68
20	p	397/612 (65%)	329 (83%)	68 (17%)	0	100	100
21	i	258/492 (52%)	226 (88%)	32 (12%)	0	100	100
21	j	280/492 (57%)	216 (77%)	60 (21%)	4 (1%)	11	46
21	q	258/492 (52%)	215 (83%)	43 (17%)	0	100	100
21	r	258/492 (52%)	217 (84%)	41 (16%)	0	100	100
22	k	91/96 (95%)	72 (79%)	19 (21%)	0	100	100
22	l	91/96 (95%)	76 (84%)	14 (15%)	1 (1%)	14	52
22	s	91/96 (95%)	82 (90%)	9 (10%)	0	100	100
22	t	91/96 (95%)	83 (91%)	8 (9%)	0	100	100
23	x	220/392 (56%)	218 (99%)	2 (1%)	0	100	100
All	All	11636/14727 (79%)	10362 (89%)	1256 (11%)	18 (0%)	50	81

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	U	79	PRO
20	o	467	PHE
20	h	491	LEU
21	j	246	TYR
20	o	469	HIS
19	e	537	ASP
20	h	511	PRO
21	j	103	ARG
19	m	455	ALA
20	g	404	LYS

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Mol	Chain	Res	Type
20	g	469	HIS
22	l	82	PRO
11	V	72	PRO
11	V	84	PRO
20	h	490	PRO
21	j	342	LYS
21	j	341	VAL
10	U	78	GLU

### 5.3.2 Protein sidechains [i](#)

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%)	318 (100%)	0	100	100
1	B	318/324 (98%)	315 (99%)	3 (1%)	78	90
1	C	318/324 (98%)	316 (99%)	2 (1%)	86	94
1	D	318/324 (98%)	318 (100%)	0	100	100
1	E	318/324 (98%)	317 (100%)	1 (0%)	92	97
1	F	318/324 (98%)	317 (100%)	1 (0%)	92	97
1	G	318/324 (98%)	316 (99%)	2 (1%)	86	94
1	I	318/324 (98%)	317 (100%)	1 (0%)	92	97
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	323/338 (96%)	323 (100%)	0	100	100
4	K	247/254 (97%)	247 (100%)	0	100	100
5	L	238/241 (99%)	238 (100%)	0	100	100
12	X	74/282 (26%)	74 (100%)	0	100	100
15	a	45/57 (79%)	45 (100%)	0	100	100
16	b	64/76 (84%)	64 (100%)	0	100	100
17	c	22/44 (50%)	22 (100%)	0	100	100
18	d	21/22 (96%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	e	125/891 (14%)	125 (100%)	0	100	100
19	f	643/891 (72%)	643 (100%)	0	100	100
19	m	453/891 (51%)	450 (99%)	3 (1%)	84	93
19	n	307/891 (34%)	302 (98%)	5 (2%)	62	83
20	h	307/531 (58%)	305 (99%)	2 (1%)	84	93
20	o	344/531 (65%)	341 (99%)	3 (1%)	78	90
20	p	37/531 (7%)	35 (95%)	2 (5%)	22	55
21	j	244/422 (58%)	242 (99%)	2 (1%)	81	91
22	s	87/89 (98%)	85 (98%)	2 (2%)	50	77
22	t	87/89 (98%)	86 (99%)	1 (1%)	73	88
23	x	64/282 (23%)	63 (98%)	1 (2%)	62	83
All	All	6589/10263 (64%)	6558 (100%)	31 (0%)	89	94

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	TYR
1	B	197	TYR
1	B	245	ASP
1	C	38	TYR
1	C	256	PHE
1	E	256	PHE
1	F	245	ASP
1	G	197	TYR
1	G	218	LYS
1	I	38	TYR
20	h	472	VAL
20	h	526	TRP
21	j	151	LYS
21	j	223	LEU
19	m	264	ARG
19	m	658	LEU
19	m	748	LYS
19	n	264	ARG
19	n	292	ARG
19	n	440	ARG
19	n	447	LYS
19	n	561	GLU

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Mol	Chain	Res	Type
20	o	245	PHE
20	o	421	PHE
20	o	465	VAL
20	p	185	GLU
20	p	216	ASN
22	s	36	ASN
22	s	70	ARG
22	t	36	ASN
23	x	139	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	116	ASN
1	B	98	GLN
1	B	133	ASN
1	C	116	ASN
1	C	133	ASN
1	D	10	GLN
1	D	133	ASN
1	E	98	GLN
1	E	116	ASN
1	E	120	ASN
1	F	9	ASN
1	F	44	HIS
1	F	297	ASN
1	G	98	GLN
1	G	116	ASN
2	H	12	ASN
2	H	88	HIS
2	H	161	HIS
1	I	98	GLN
1	I	116	ASN
1	I	133	ASN
1	I	372	HIS
3	J	58	ASN
3	J	273	GLN
5	L	20	GLN
12	X	161	ASN
16	b	47	HIS
19	f	215	ASN

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Mol	Chain	Res	Type
19	f	311	HIS
19	f	421	GLN
19	f	653	GLN
19	f	708	GLN
19	f	731	ASN
19	f	773	GLN
19	f	879	ASN
19	f	891	HIS
20	h	306	GLN
20	h	345	GLN
21	j	115	HIS
21	j	150	GLN
21	j	159	HIS
21	j	221	HIS
21	j	326	ASN
21	j	366	GLN
19	m	280	ASN
19	m	311	HIS
19	m	391	GLN
19	m	472	GLN
19	m	529	ASN
19	m	589	ASN
19	n	472	GLN
19	n	473	HIS
20	o	345	GLN
20	o	368	ASN
20	o	436	HIS
20	o	457	HIS
20	p	189	GLN
20	p	216	ASN
22	s	24	ASN
22	s	36	ASN
22	s	93	ASN
22	t	18	GLN
22	t	36	ASN
22	t	93	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands 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
25	ADP	B	800	-	24,29,29	1.17	2 (8%)	29,45,45	1.87	7 (24%)
25	ADP	I	800	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
25	ADP	A	800	-	24,29,29	1.01	1 (4%)	29,45,45	1.55	4 (13%)
25	ADP	C	800	-	24,29,29	1.07	1 (4%)	29,45,45	1.67	6 (20%)
25	ADP	E	800	-	24,29,29	1.07	1 (4%)	29,45,45	1.54	5 (17%)
25	ADP	F	800	-	24,29,29	1.17	1 (4%)	29,45,45	1.86	5 (17%)
25	ADP	D	800	-	24,29,29	1.24	3 (12%)	29,45,45	1.70	4 (13%)
25	ADP	J	800	-	24,29,29	0.93	1 (4%)	29,45,45	1.51	4 (13%)
25	ADP	G	800	-	24,29,29	1.10	1 (4%)	29,45,45	1.52	3 (10%)
26	ATP	H	401	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	6 (19%)

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
25	ADP	B	800	-	-	3/12/32/32	0/3/3/3
25	ADP	I	800	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	ADP	A	800	-	-	4/12/32/32	0/3/3/3
25	ADP	C	800	-	-	4/12/32/32	0/3/3/3
25	ADP	E	800	-	-	3/12/32/32	0/3/3/3
25	ADP	F	800	-	-	4/12/32/32	0/3/3/3
25	ADP	D	800	-	-	4/12/32/32	0/3/3/3
25	ADP	J	800	-	-	6/12/32/32	0/3/3/3
25	ADP	G	800	-	-	0/12/32/32	0/3/3/3
26	ATP	H	401	-	-	7/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	800	ADP	C2'-C1'	-3.11	1.49	1.53
25	F	800	ADP	C2'-C1'	-2.83	1.49	1.53
25	G	800	ADP	C2'-C1'	-2.75	1.49	1.53
25	D	800	ADP	C2'-C1'	-2.74	1.49	1.53
25	I	800	ADP	C5-C4	2.55	1.47	1.40
25	J	800	ADP	C5-C4	2.54	1.47	1.40
25	D	800	ADP	C4-N3	-2.40	1.32	1.35
25	A	800	ADP	C2'-C1'	-2.38	1.50	1.53
26	H	401	ATP	C5-C4	2.32	1.47	1.40
25	C	800	ADP	C2'-C1'	-2.31	1.50	1.53
25	E	800	ADP	C2'-C1'	-2.11	1.50	1.53
25	B	800	ADP	C4-N3	-2.09	1.32	1.35
25	D	800	ADP	C5-N7	-2.02	1.32	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	F	800	ADP	PA-O3A-PB	-6.65	110.00	132.83
25	B	800	ADP	PA-O3A-PB	-5.71	113.24	132.83
25	D	800	ADP	PA-O3A-PB	-5.17	115.09	132.83
25	C	800	ADP	PA-O3A-PB	-4.75	116.53	132.83
25	G	800	ADP	PA-O3A-PB	-4.18	118.49	132.83
25	J	800	ADP	PA-O3A-PB	-4.15	118.58	132.83
25	E	800	ADP	PA-O3A-PB	-4.11	118.72	132.83
25	A	800	ADP	PA-O3A-PB	-4.10	118.76	132.83
25	I	800	ADP	PA-O3A-PB	-3.79	119.82	132.83
25	D	800	ADP	C3'-C2'-C1'	3.71	106.56	100.98
25	B	800	ADP	C3'-C2'-C1'	3.60	106.40	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	E	800	ADP	C3'-C2'-C1'	3.60	106.40	100.98
25	A	800	ADP	N3-C2-N1	-3.56	123.12	128.68
25	I	800	ADP	C3'-C2'-C1'	3.54	106.31	100.98
26	H	401	ATP	PA-O3A-PB	-3.32	121.43	132.83
25	C	800	ADP	N3-C2-N1	-3.32	123.49	128.68
25	J	800	ADP	N3-C2-N1	-3.17	123.72	128.68
25	G	800	ADP	C3'-C2'-C1'	3.04	105.56	100.98
25	F	800	ADP	C4-C5-N7	-3.03	106.24	109.40
25	F	800	ADP	N3-C2-N1	-3.02	123.96	128.68
25	B	800	ADP	N3-C2-N1	-2.97	124.03	128.68
26	H	401	ATP	N3-C2-N1	-2.97	124.04	128.68
26	H	401	ATP	PB-O3B-PG	-2.86	123.02	132.83
25	J	800	ADP	C3'-C2'-C1'	2.84	105.26	100.98
26	H	401	ATP	C4-C5-N7	-2.84	106.44	109.40
25	E	800	ADP	N3-C2-N1	-2.73	124.41	128.68
25	E	800	ADP	C4-C5-N7	-2.67	106.62	109.40
25	A	800	ADP	C4-C5-N7	-2.67	106.62	109.40
25	I	800	ADP	N3-C2-N1	-2.62	124.58	128.68
25	I	800	ADP	C4-C5-N7	-2.57	106.72	109.40
25	C	800	ADP	C4-C5-N7	-2.56	106.73	109.40
25	J	800	ADP	C4-C5-N7	-2.54	106.75	109.40
26	H	401	ATP	C3'-C2'-C1'	2.53	104.79	100.98
25	B	800	ADP	C4-C5-N7	-2.49	106.80	109.40
25	D	800	ADP	O2'-C2'-C3'	-2.48	103.79	111.82
25	G	800	ADP	C4-C5-N7	-2.43	106.86	109.40
25	B	800	ADP	O2A-PA-O1A	2.38	124.03	112.24
25	F	800	ADP	O3B-PB-O1B	2.28	119.61	110.68
25	C	800	ADP	O2A-PA-O1A	2.26	123.44	112.24
25	E	800	ADP	O2A-PA-O1A	2.24	123.32	112.24
25	B	800	ADP	C2'-C3'-C4'	2.24	107.00	102.64
25	D	800	ADP	O4'-C1'-C2'	-2.20	103.72	106.93
25	C	800	ADP	C3'-C2'-C1'	2.18	104.27	100.98
25	B	800	ADP	O3B-PB-O2B	2.08	115.59	107.64
25	A	800	ADP	C2-N1-C6	2.07	122.29	118.75
25	F	800	ADP	C3'-C2'-C1'	2.05	104.07	100.98
25	C	800	ADP	O3B-PB-O2B	2.04	115.44	107.64
26	H	401	ATP	O3G-PG-O2G	2.03	115.39	107.64

There are no chirality outliers.

All (35) torsion outliers are listed below:

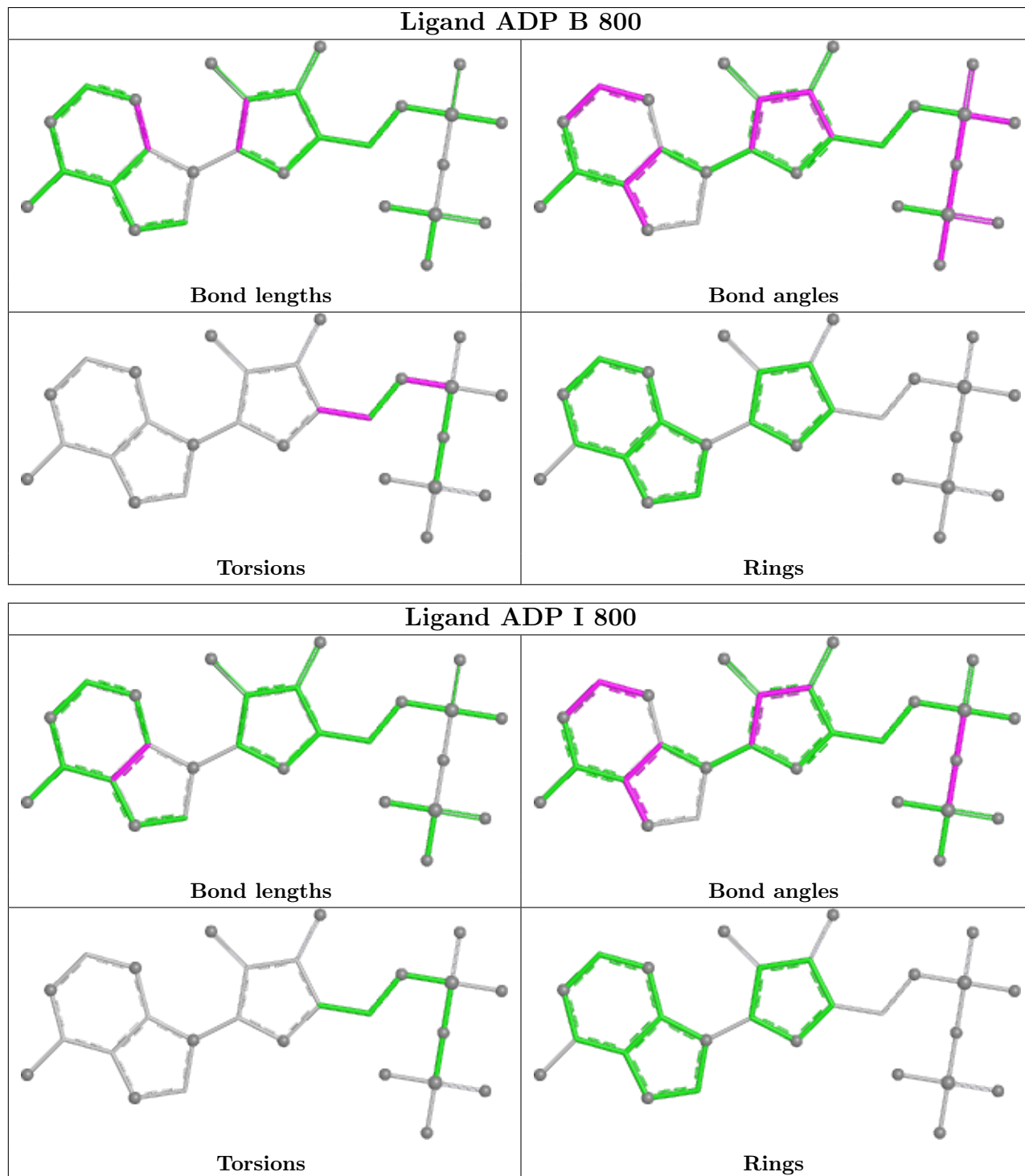
Mol	Chain	Res	Type	Atoms
25	A	800	ADP	C5'-O5'-PA-O2A
25	A	800	ADP	C5'-O5'-PA-O3A
25	A	800	ADP	O4'-C4'-C5'-O5'
25	A	800	ADP	C3'-C4'-C5'-O5'
25	B	800	ADP	C3'-C4'-C5'-O5'
25	C	800	ADP	C5'-O5'-PA-O3A
25	D	800	ADP	C5'-O5'-PA-O1A
25	D	800	ADP	C5'-O5'-PA-O3A
25	E	800	ADP	C5'-O5'-PA-O1A
25	F	800	ADP	C5'-O5'-PA-O3A
25	F	800	ADP	C3'-C4'-C5'-O5'
25	J	800	ADP	PA-O3A-PB-O3B
25	J	800	ADP	C5'-O5'-PA-O1A
25	J	800	ADP	C5'-O5'-PA-O2A
26	H	401	ATP	C5'-O5'-PA-O1A
26	H	401	ATP	C5'-O5'-PA-O2A
26	H	401	ATP	C3'-C4'-C5'-O5'
25	D	800	ADP	O4'-C4'-C5'-O5'
25	D	800	ADP	C3'-C4'-C5'-O5'
26	H	401	ATP	O4'-C4'-C5'-O5'
25	F	800	ADP	O4'-C4'-C5'-O5'
25	B	800	ADP	O4'-C4'-C5'-O5'
25	C	800	ADP	C3'-C4'-C5'-O5'
25	J	800	ADP	C3'-C4'-C5'-O5'
26	H	401	ATP	PA-O3A-PB-O1B
25	C	800	ADP	O4'-C4'-C5'-O5'
25	J	800	ADP	O4'-C4'-C5'-O5'
25	E	800	ADP	C5'-O5'-PA-O3A
25	J	800	ADP	C5'-O5'-PA-O3A
25	C	800	ADP	C5'-O5'-PA-O1A
25	F	800	ADP	C5'-O5'-PA-O2A
26	H	401	ATP	PA-O3A-PB-O2B
26	H	401	ATP	C5'-O5'-PA-O3A
25	B	800	ADP	C5'-O5'-PA-O1A
25	E	800	ADP	C5'-O5'-PA-O2A

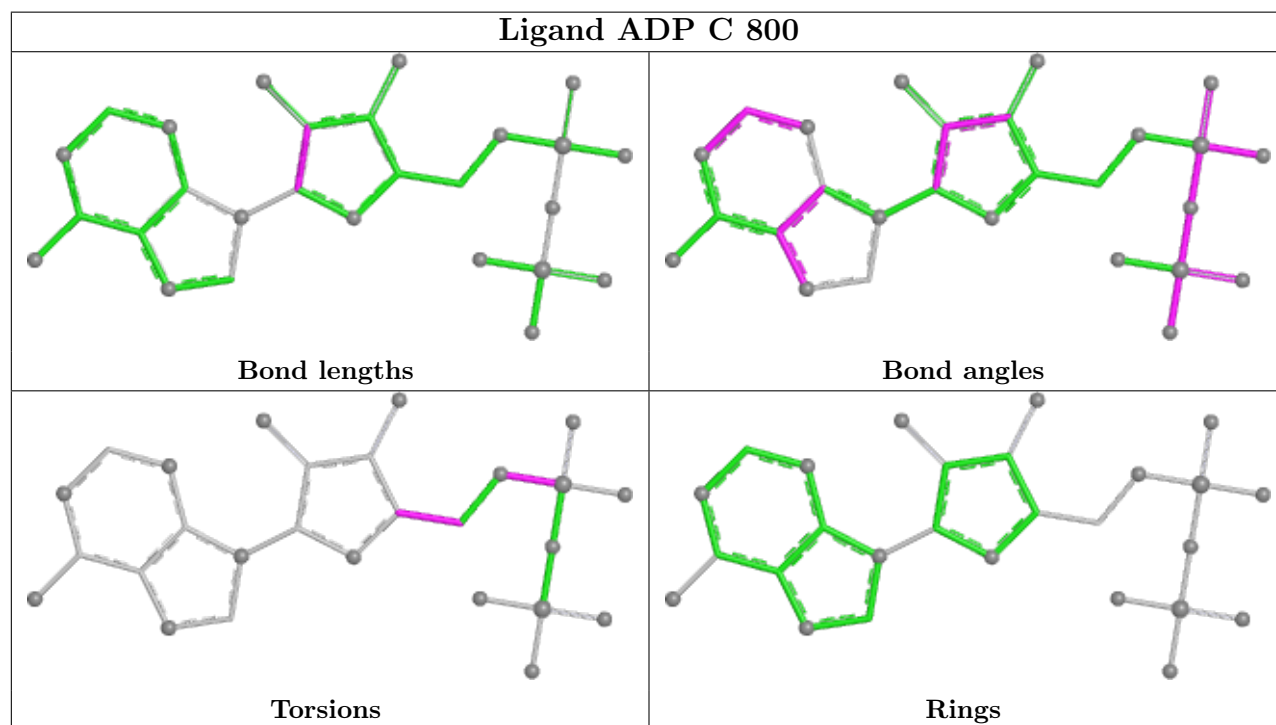
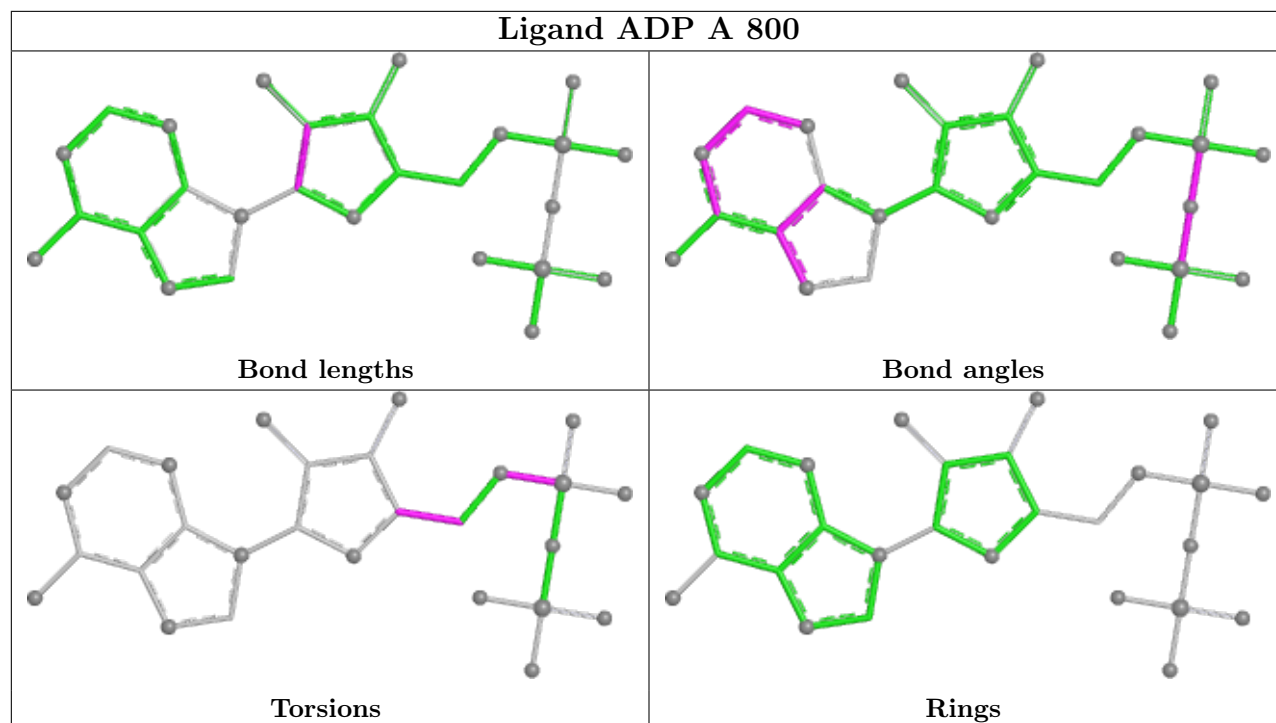
There are no ring outliers.

No monomer is involved in short contacts.

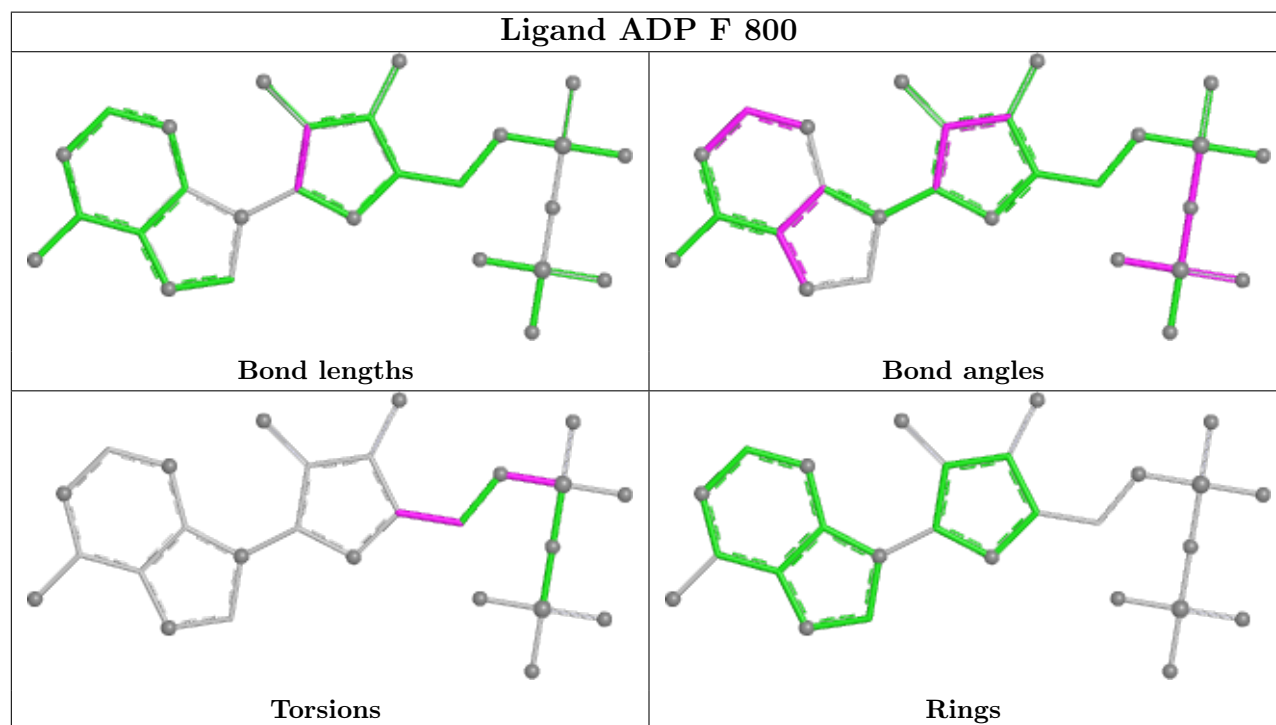
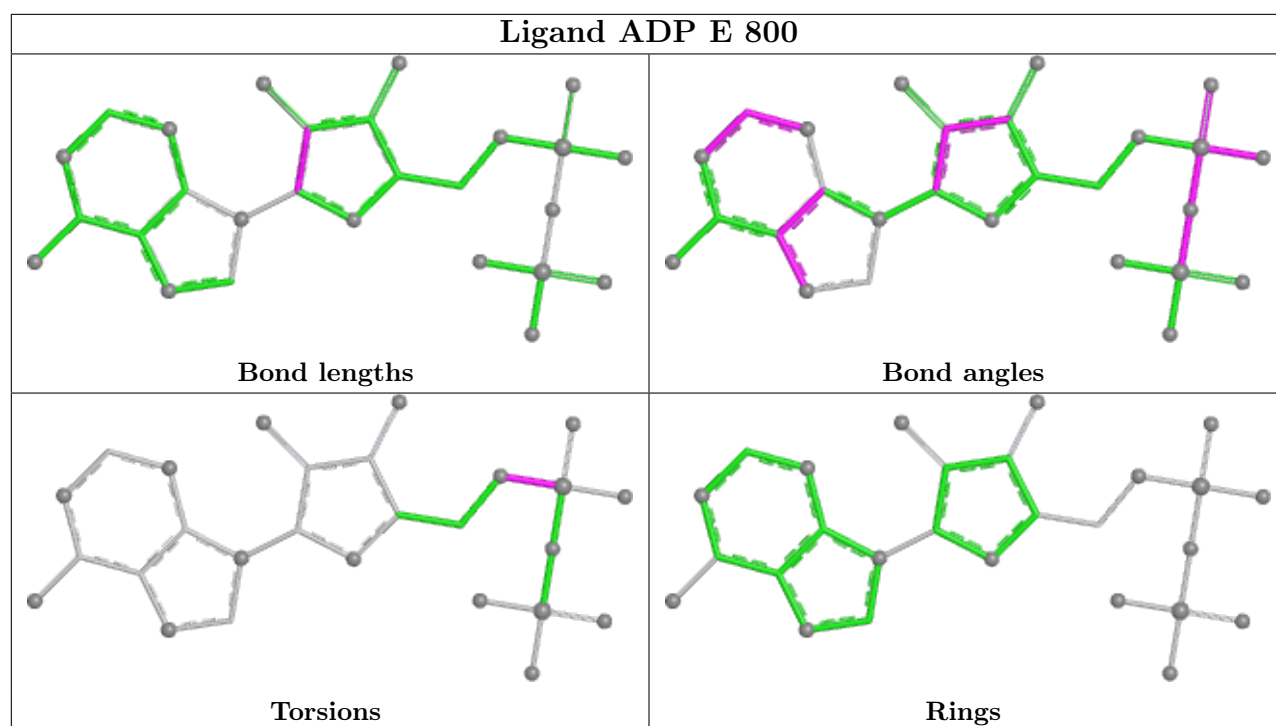
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

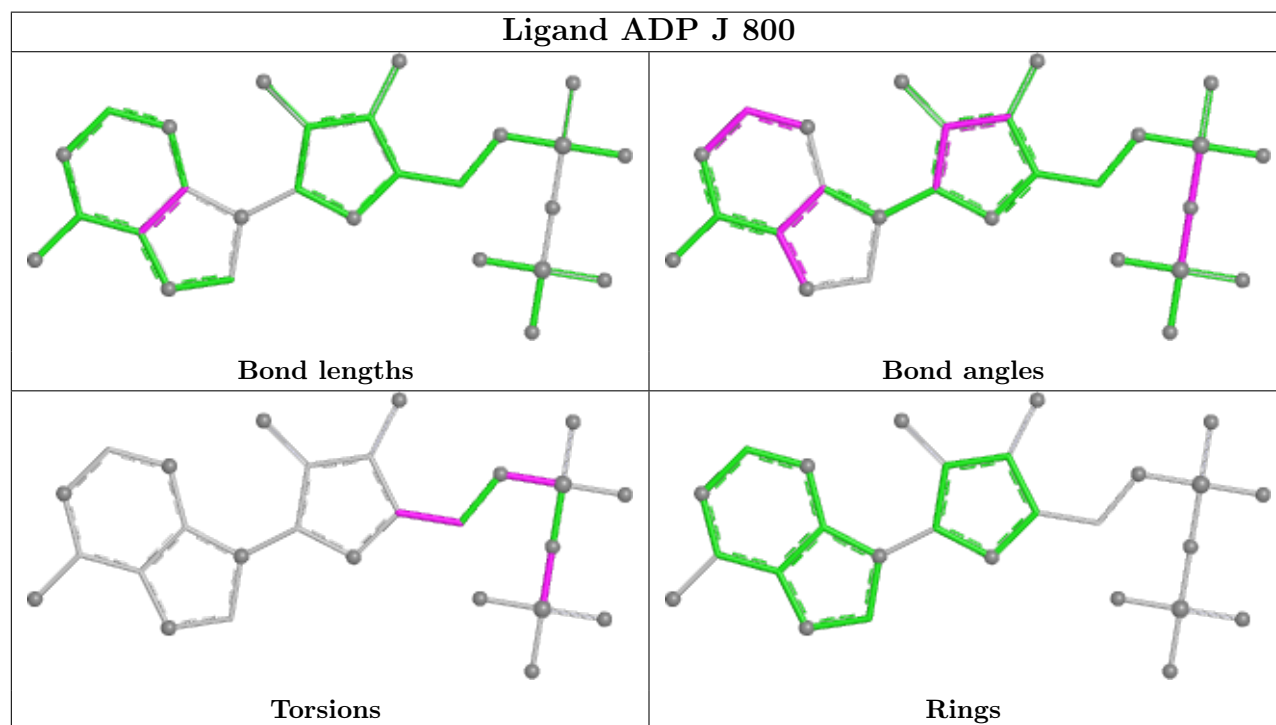
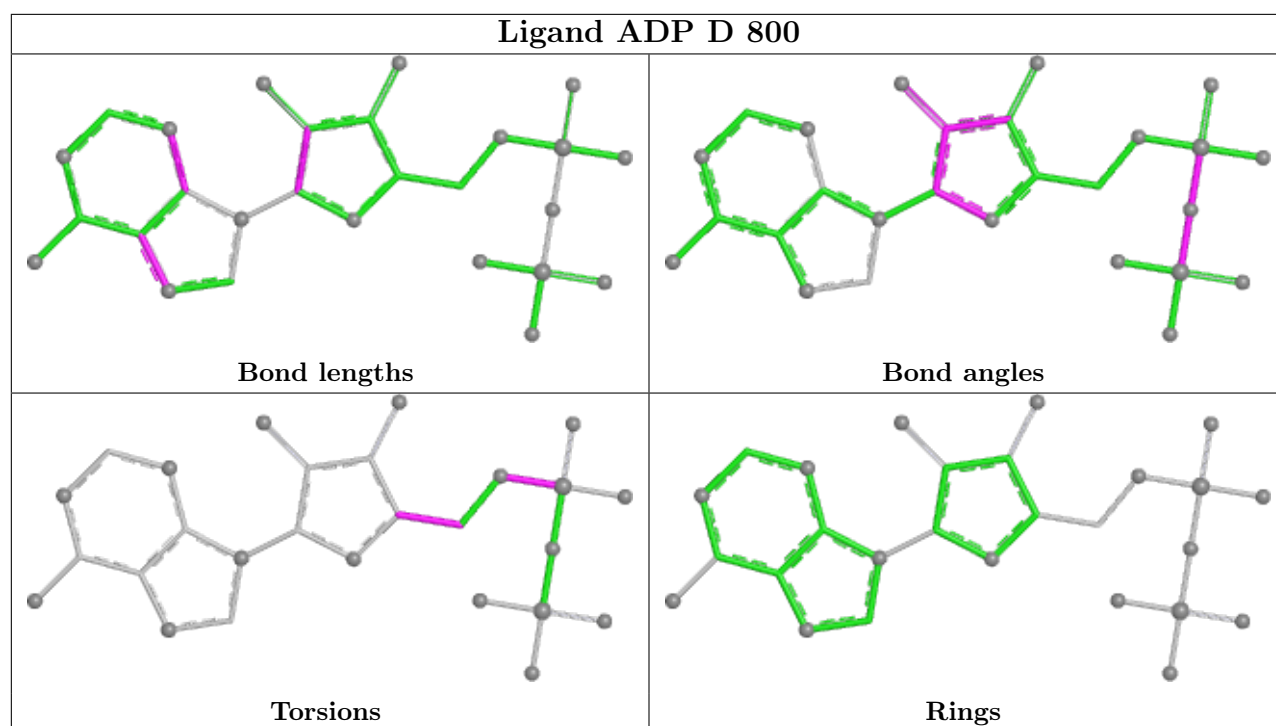
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

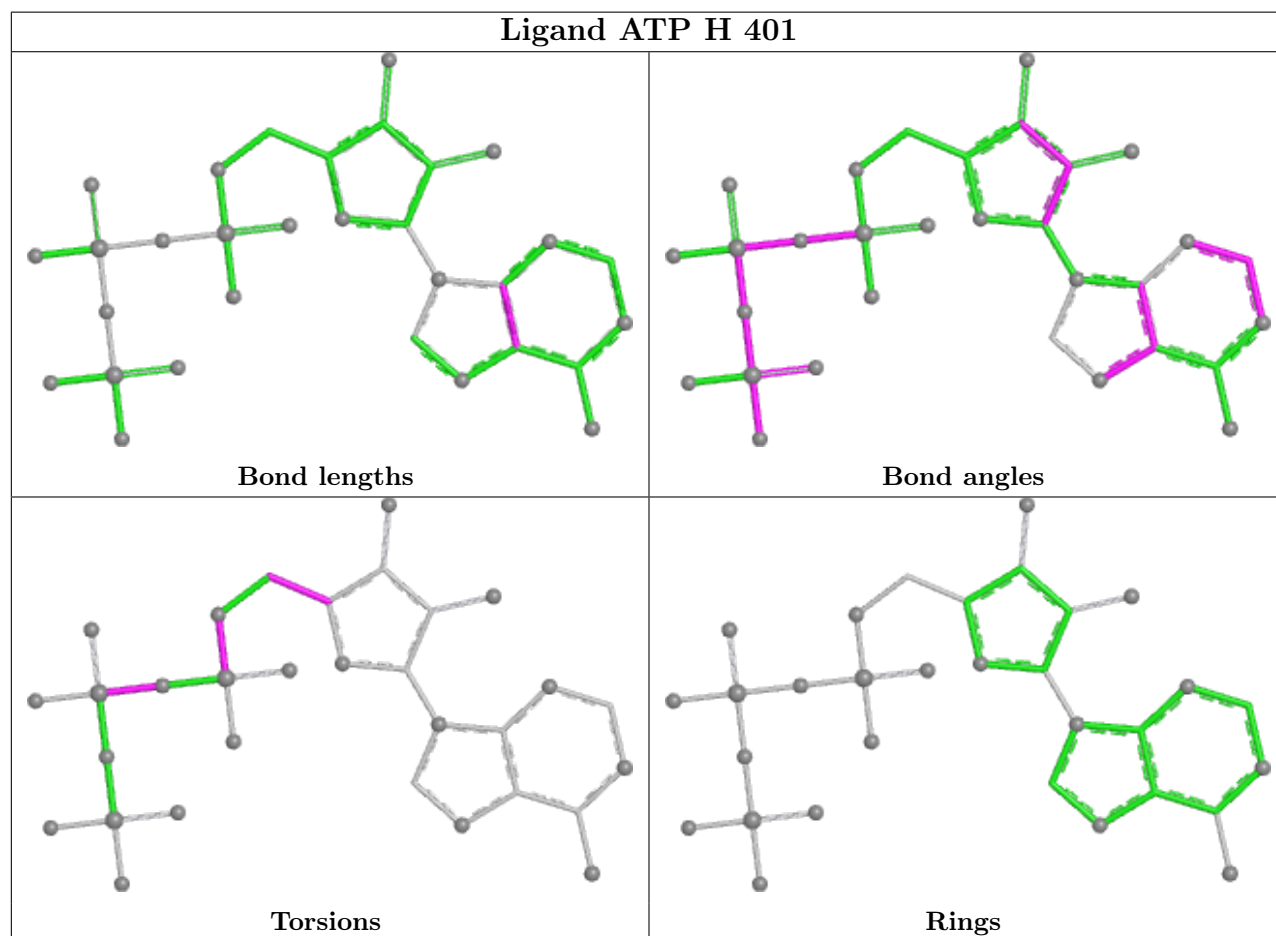
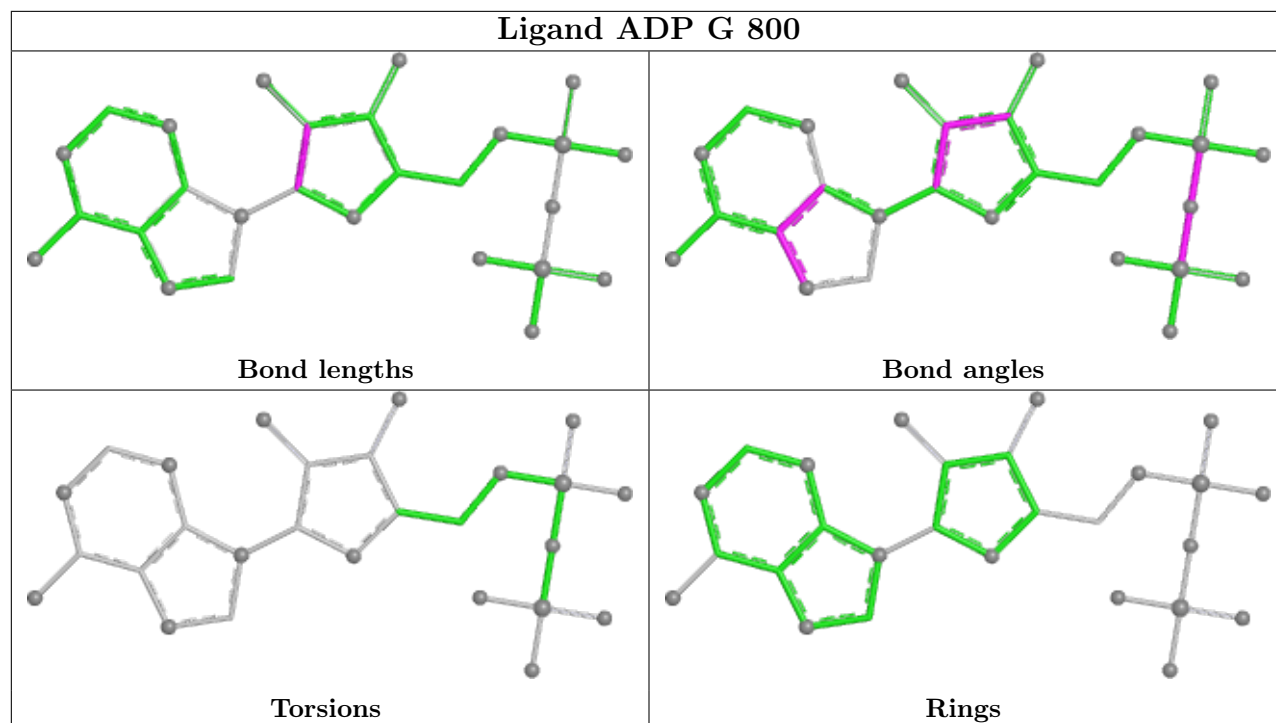












## 5.7 Other polymers [i](#)

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
13	Y	11
7	N	5
6	M	5
8	O	3
8	P	3
9	R	2
9	Q	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	171:UNK	C	201:UNK	N	99.45
1	M	171:UNK	C	201:UNK	N	95.63
1	N	367:UNK	C	401:UNK	N	94.83
1	M	367:UNK	C	401:UNK	N	83.96
1	M	625:UNK	C	701:UNK	N	67.24
1	N	634:UNK	C	701:UNK	N	66.59
1	Y	26:UNK	C	155:UNK	N	62.21
1	Y	500:UNK	C	508:UNK	N	61.14
1	R	38:UNK	C	42:UNK	N	56.24
1	Q	38:UNK	C	42:UNK	N	55.28
1	Y	359:UNK	C	415:UNK	N	40.71
1	M	741:UNK	C	801:UNK	N	36.38
1	N	768:UNK	C	801:UNK	N	34.80
1	Y	193:UNK	C	282:UNK	N	28.70
1	N	559:UNK	C	602:UNK	N	26.73
1	O	41:UNK	C	64:UNK	N	26.59
1	M	559:UNK	C	601:UNK	N	23.98
1	P	41:UNK	C	64:UNK	N	22.87
1	Y	160:UNK	C	181:UNK	N	21.87
1	Y	620:UNK	C	703:UNK	N	21.61
1	P	78:UNK	C	80:UNK	N	17.18
1	O	78:UNK	C	80:UNK	N	16.31
1	O	94:UNK	C	96:UNK	N	15.75
1	P	94:UNK	C	96:UNK	N	15.58

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	62:UNK	C	64:UNK	N	15.43
1	Q	62:UNK	C	64:UNK	N	13.22
1	Y	535:UNK	C	580:UNK	N	12.88
1	Y	611:UNK	C	615:UNK	N	12.25
1	Y	421:UNK	C	423:UNK	N	8.61
1	Y	586:UNK	C	588:UNK	N	6.92
1	Y	597:UNK	C	601:UNK	N	4.97

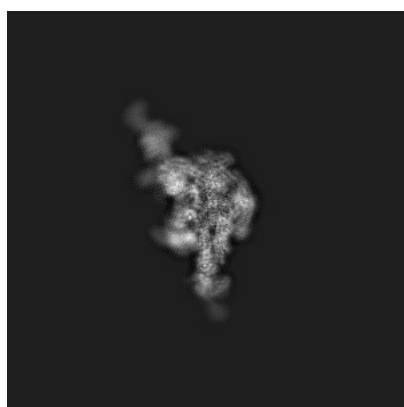
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4168. These allow visual inspection of the internal detail of the map and identification of artifacts.

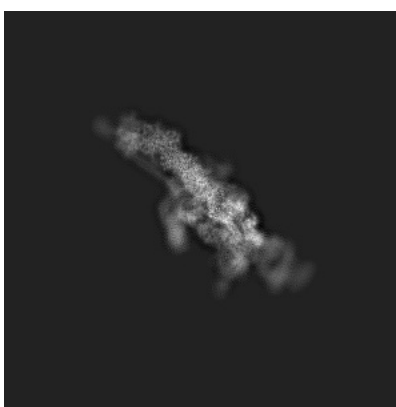
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

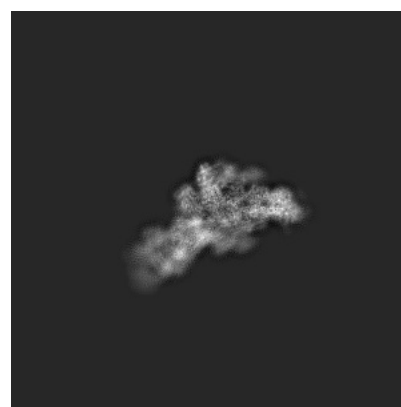
#### 6.1.1 Primary map



X



Y

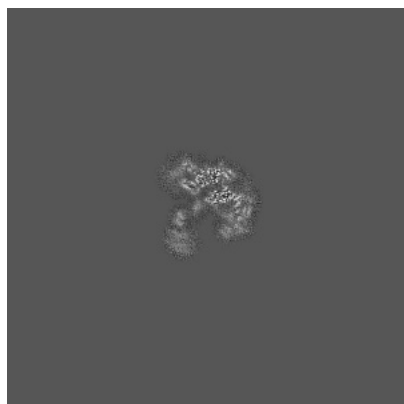


Z

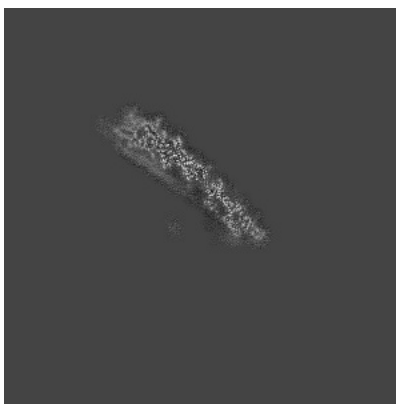
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

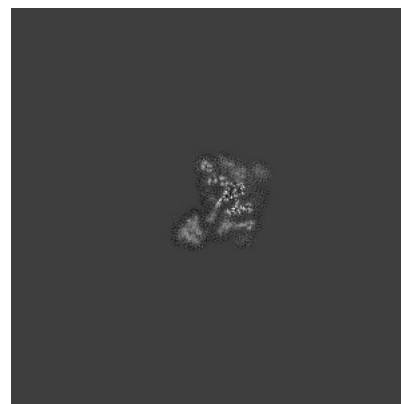
#### 6.2.1 Primary map



X Index: 300



Y Index: 300

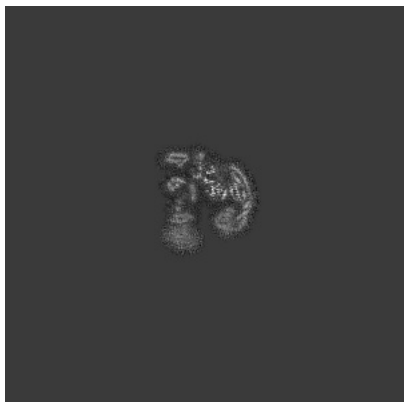


Z Index: 300

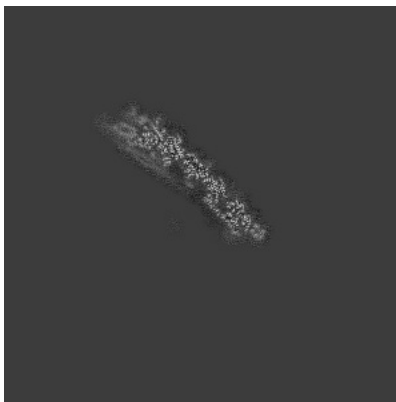
The images above show central slices of the map in three orthogonal directions.

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

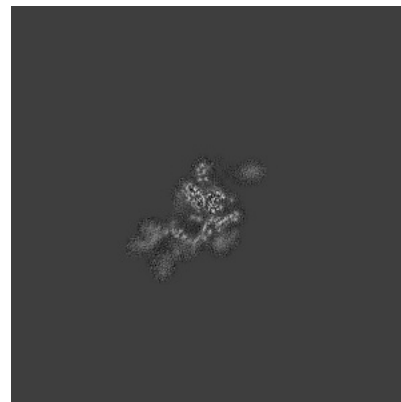
### 6.3.1 Primary map



X Index: 288



Y Index: 302

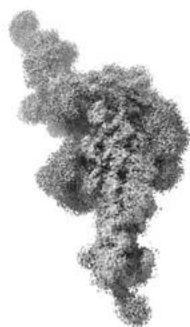


Z Index: 336

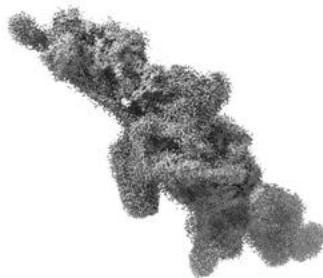
The images above show the largest variance slices of the map in three orthogonal directions.

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

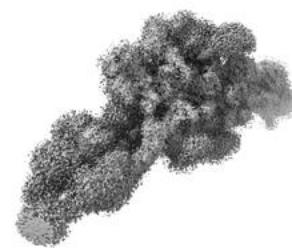
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.046. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

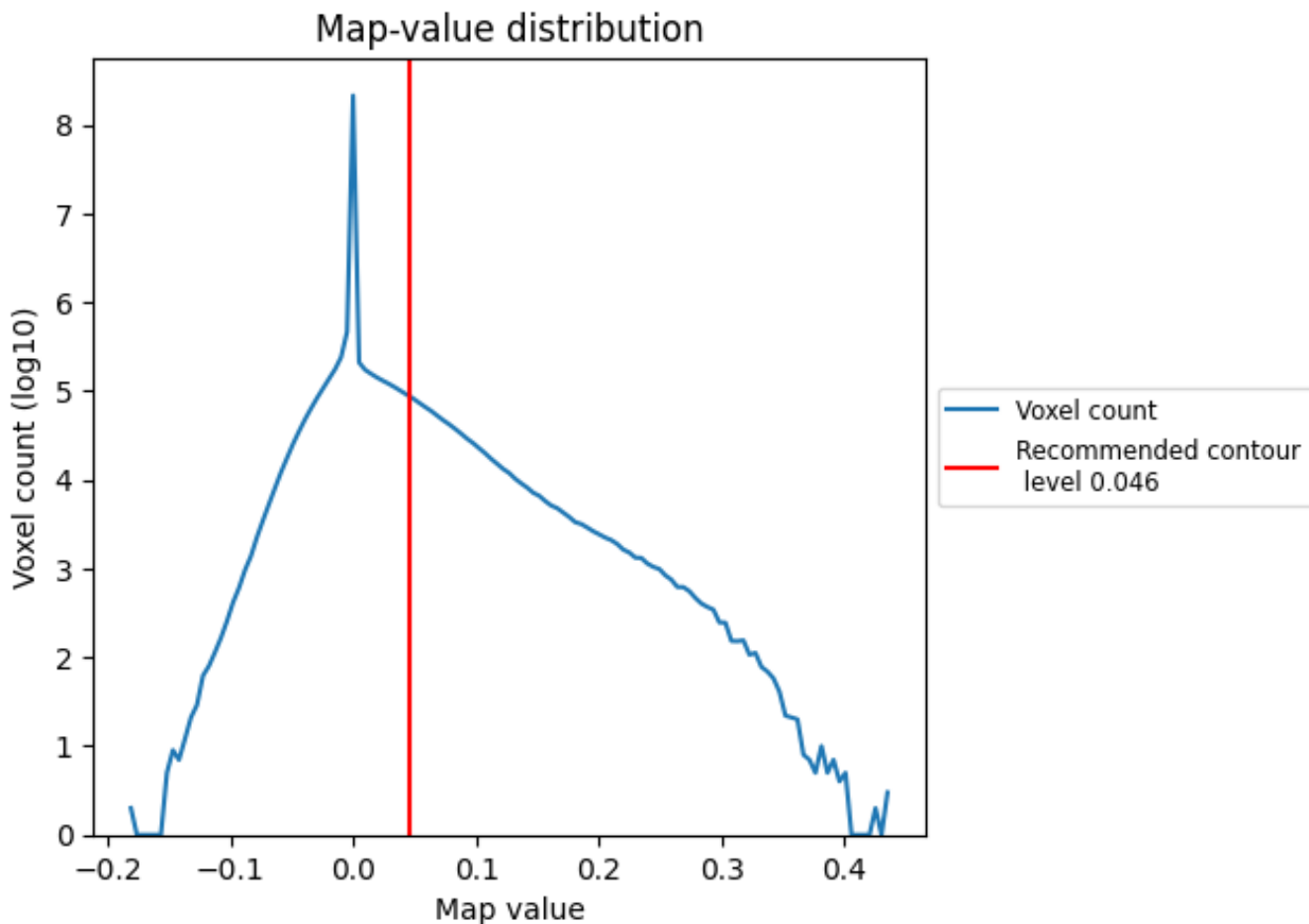
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

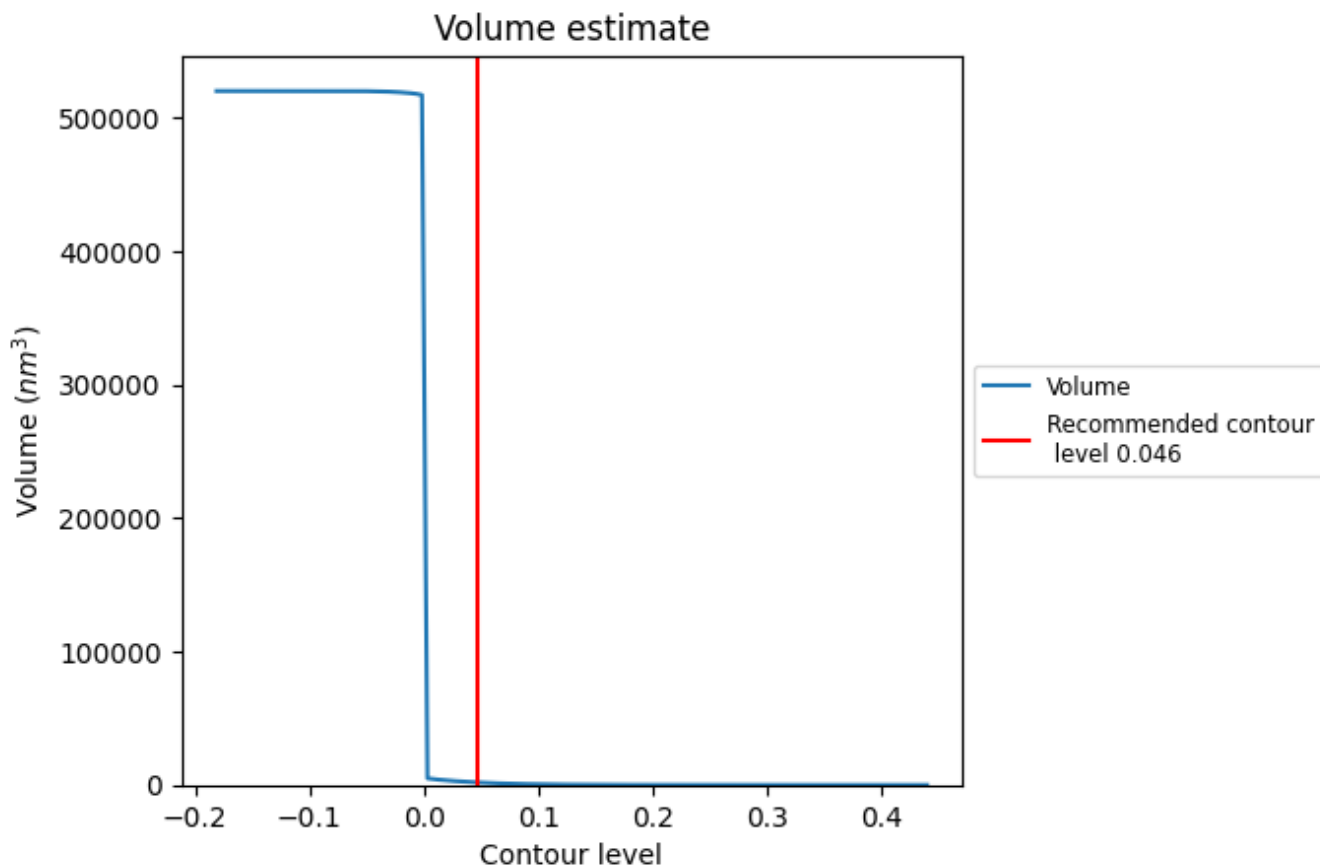
This section contains the results of statistical analysis of the map.

### 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.

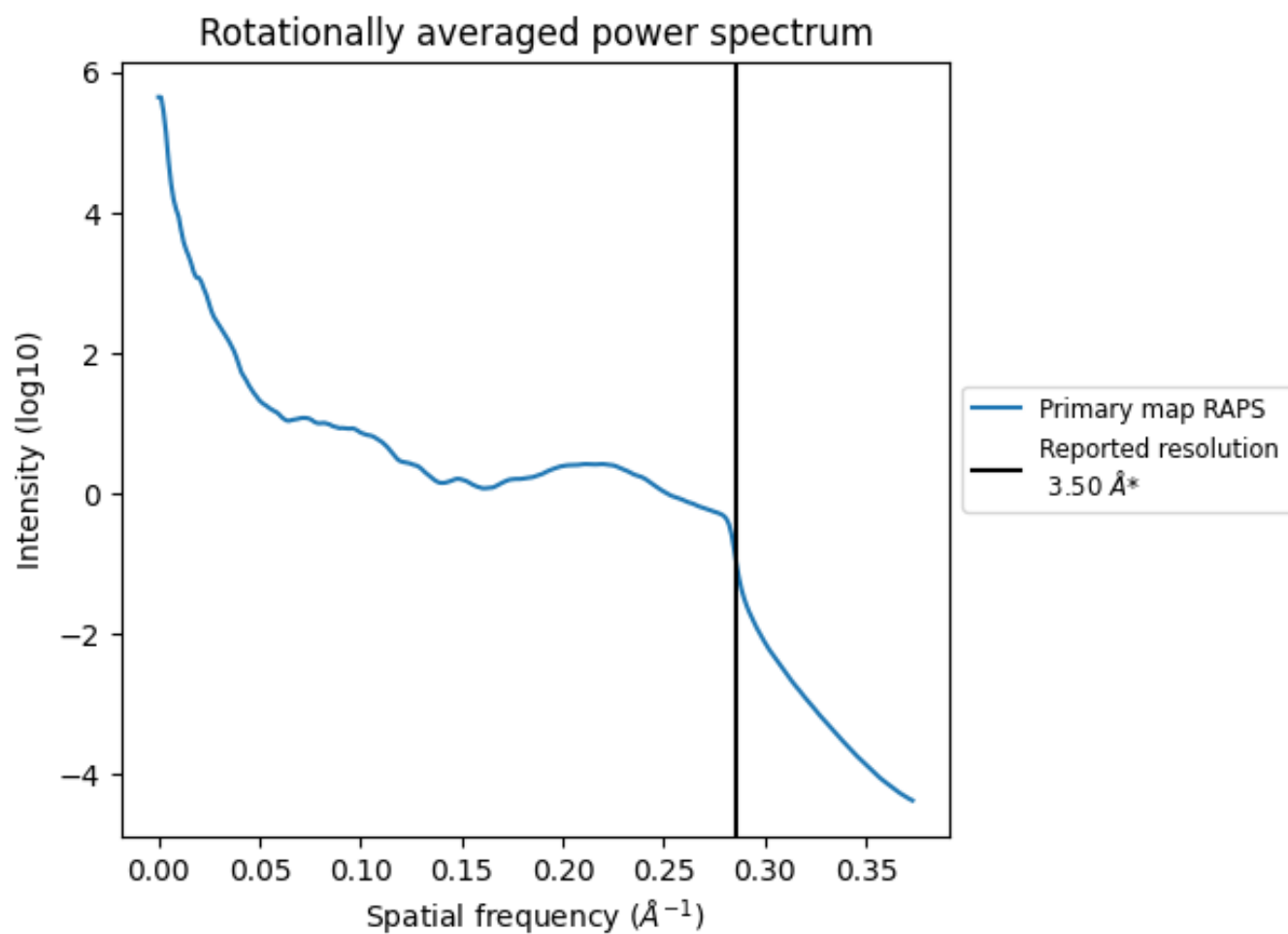
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1916 nm<sup>3</sup>; this corresponds to an approximate mass of 1731 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  $0.286 \text{\AA}^{-1}$

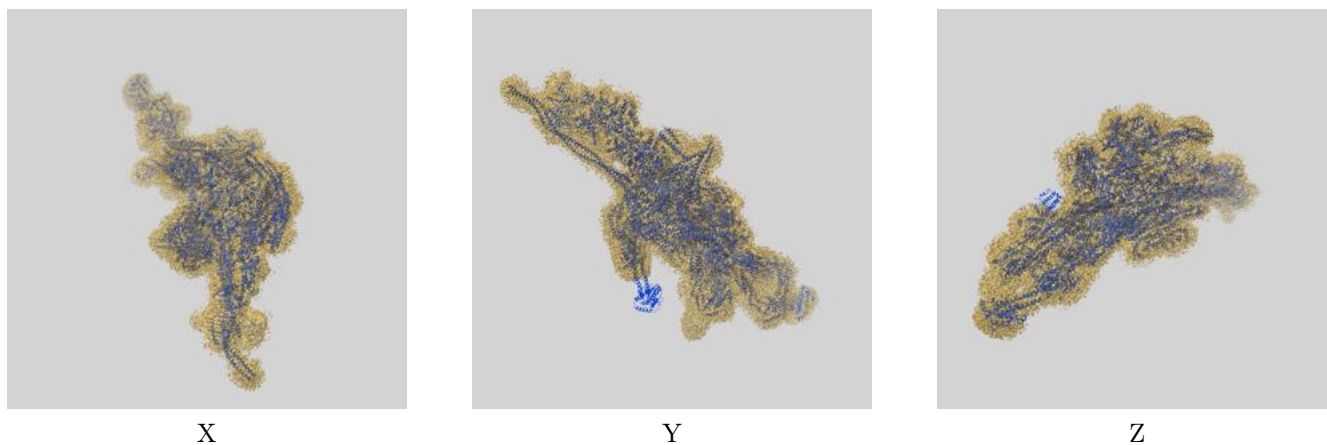
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

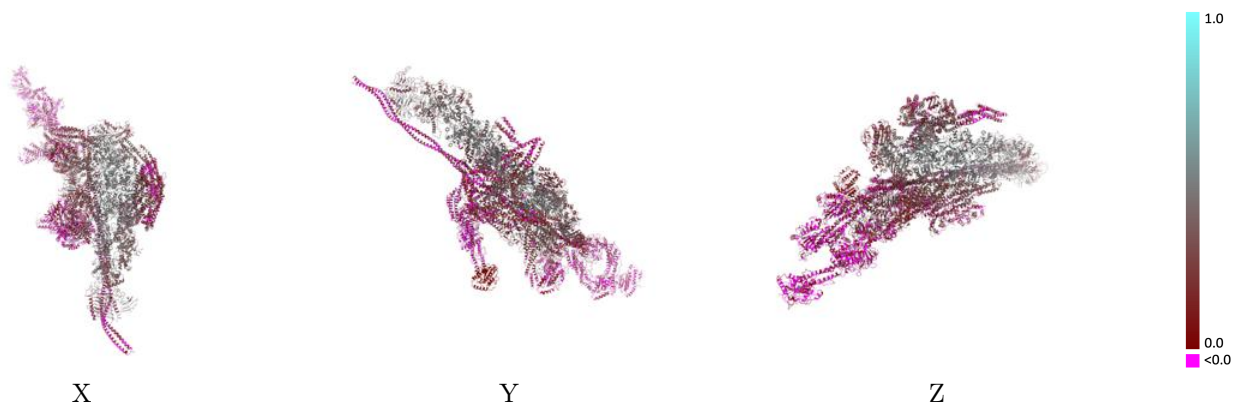
This section contains information regarding the fit between EMDB map EMD-4168 and PDB model 6F1T. Per-residue inclusion information can be found in section 3 on page 12.

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



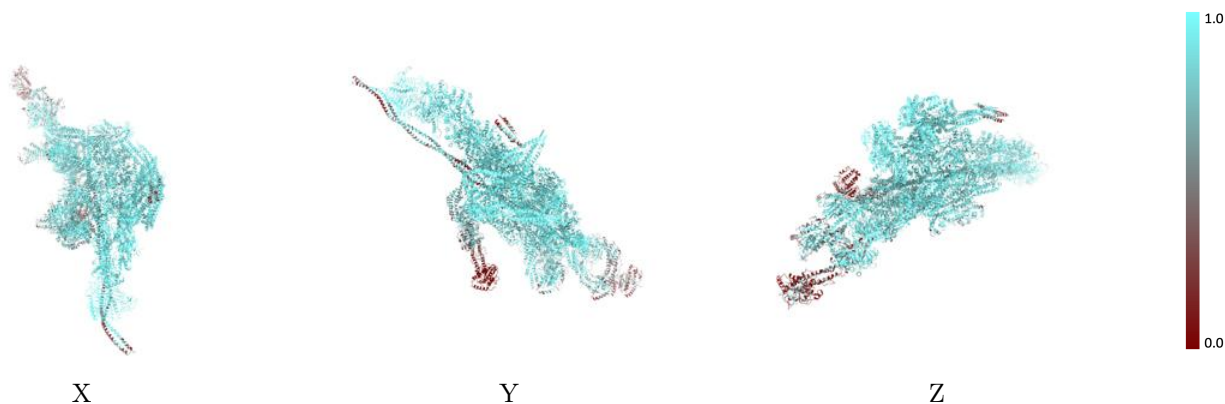
The images above show the 3D surface view of the map at the recommended contour level 0.046 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



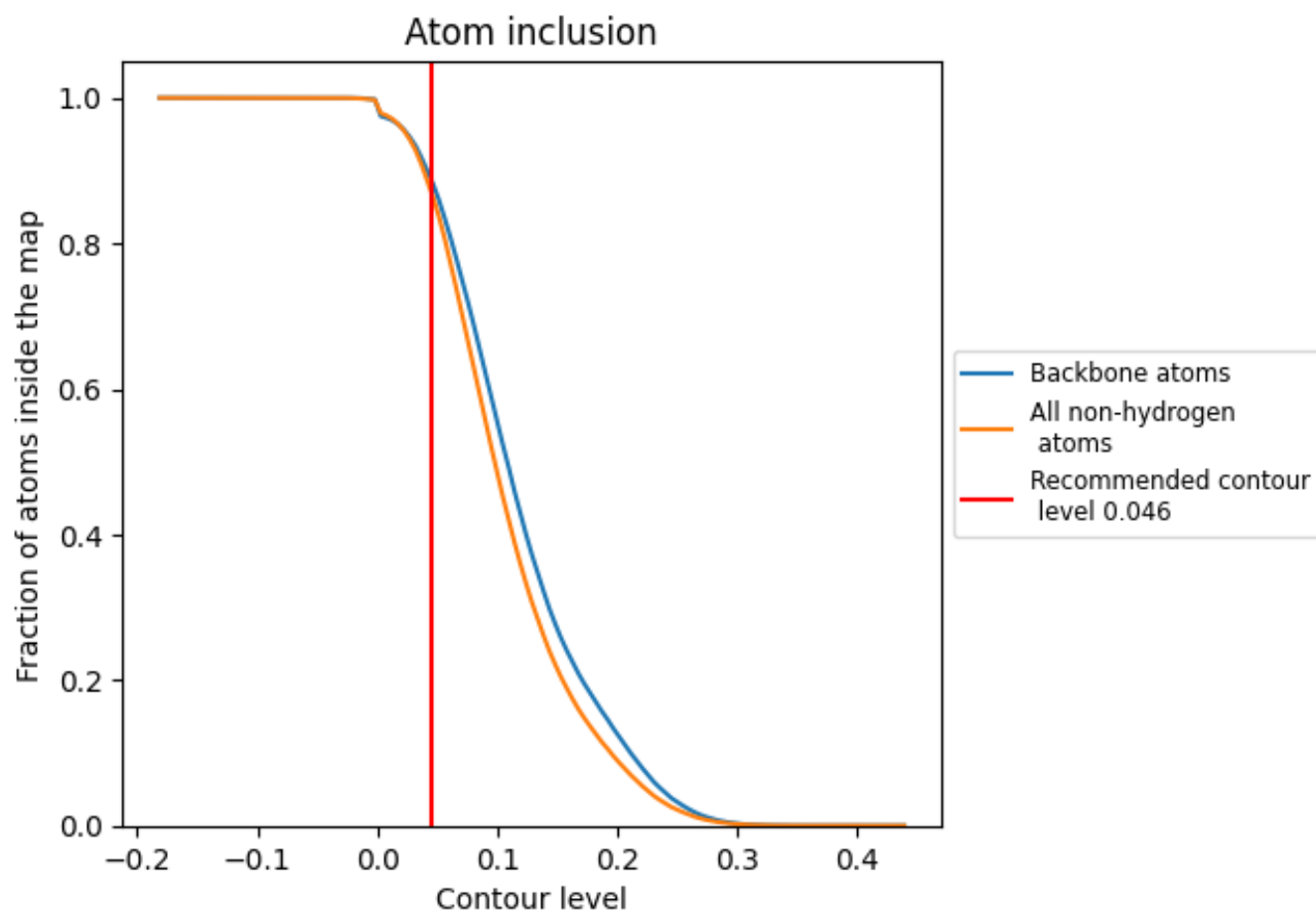
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.046).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.046) and Q-score for the entire model and for each chain.























Chain	Atom inclusion	Q-score
All	 0.8680	 0.2690
A	 0.9403	 0.4110
B	 0.9626	 0.4730
C	 0.9461	 0.4780
D	 0.9602	 0.4650
E	 0.9523	 0.4730
F	 0.9571	 0.4600
G	 0.9599	 0.4500
H	 0.9616	 0.4520
I	 0.9461	 0.3910
J	 0.9489	 0.3890
K	 0.9482	 0.2900
L	 0.9414	 0.3630
M	 0.9642	 0.1830
N	 0.9718	 0.2050
O	 0.9907	 0.1940
P	 0.9876	 0.2470
Q	 0.4943	 0.1760
R	 0.9931	 0.4040
U	 0.9620	 0.3030
V	 0.9988	 0.3820
X	 0.7123	 0.1100
Y	 0.9878	 0.3960
Z	 0.9923	 0.3400
a	 0.9250	 0.4390
b	 0.9319	 0.4050
c	 0.9444	 0.4200
d	 0.9130	 0.3730
e	 0.7293	 0.1310
f	 0.9010	 0.2120
g	 0.8225	 0.0460
h	 0.9155	 0.2420
i	 0.0234	 -0.0000
j	 0.8073	 0.0720
k	 0.6515	 0.0120



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Chain	Atom inclusion	Q-score
l	 0.6905	 0.0350
m	 0.8989	 0.2480
n	 0.7840	 0.1680
o	 0.9147	 0.2180
p	 0.8286	 0.0500
q	 0.6217	 0.0260
r	 0.2969	 0.0000
s	 0.7740	 0.0320
t	 0.7904	 0.0600
x	 0.6842	 0.1050
z	 0.9321	 0.3110