



## Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 01:33 PM EDT

PDB ID : 9DGU / pdb\_00009dgu  
EMDB ID : EMD-46848  
Title : structure of dynactin, dynein tail with two BICDR from dynein-dynactin-BI  
CDR on microtubules  
Authors : Rao, Q.; Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
Resolution : 7.10 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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

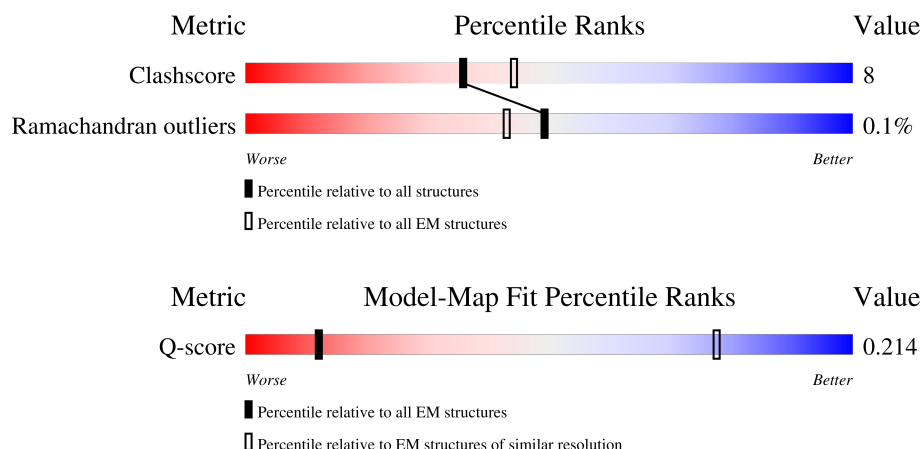
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.10 Å.

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





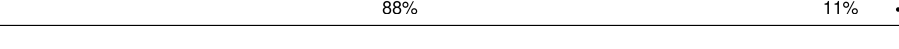
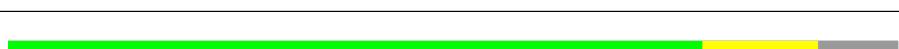

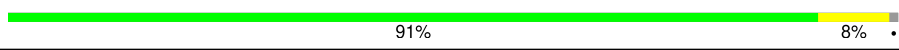

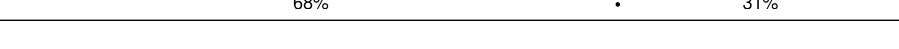



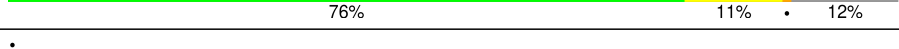




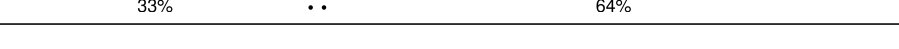
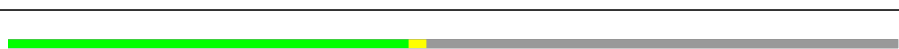






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	464 ( 6.60 - 7.60 )

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	 84% 14% •
1	B	376	 84% 14% •
1	C	376	 86% 14%
1	D	376	 82% 16% •
1	E	376	 86% 12% •

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Mol	Chain	Length	Quality of chain
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	P	405	
6	Q	405	
7	O	186	
7	R	186	
8	U	190	
9	V	182	
10	W	1281	
10	Z	1281	
11	Y	467	
12	a	577	
12	b	577	
12	c	577	
12	d	577	
13	e	4646	
13	f	4646	
13	m	4646	

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Mol	Chain	Length	Quality of chain
13	n	4646	<div><div></div><div>15%</div><div></div><div>84%</div></div>
14	g	612	<div><div></div><div>51%</div><div>7%</div><div>42%</div></div>
14	h	612	<div><div></div><div>50%</div><div>9%</div><div>42%</div></div>
14	o	612	<div><div></div><div>50%</div><div>8%</div><div>42%</div></div>
14	p	612	<div><div></div><div>52%</div><div>6%</div><div>42%</div></div>
15	j	492	<div><div></div><div>97%</div></div>
15	q	492	<div><div></div><div>97%</div></div>

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 61911 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 Alpha-centractin.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	B	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	C	375	Total	C	N	O	0	0
			1847	1097	375	375		
1	D	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	E	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	F	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	G	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	I	370	Total	C	N	O	0	0
			1822	1082	370	370		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	370	Total	C	N	O	0	0
			1822	1082	370	370		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	379	Total	C	N	O	0	0
			1868	1110	379	379		

- Molecule 4 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	278	Total	C	N	O	0	0
			1378	822	278	278		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	269	Total	C	N	O	0	0
			1327	789	269	269		

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	340	Total	C	N	O	0	0
			1689	1009	340	340		
6	N	280	Total	C	N	O	0	0
			1394	834	280	280		
6	P	325	Total	C	N	O	0	0
			1612	962	325	325		
6	Q	343	Total	C	N	O	0	0
			1707	1021	343	343		

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	179	Total	C	N	O	0	0
			888	530	179	179		
7	R	170	Total	C	N	O	0	0
			844	504	170	170		

- Molecule 8 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	167	Total	C	N	O	0	0
			822	488	167	167		

- Molecule 9 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	179	Total	C	N	O	0	0
			881	523	179	179		

- Molecule 10 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	152	Total	C	N	O	0	0
			754	450	152	152		
10	Z	192	Total	C	N	O	0	0
			952	568	192	192		

- Molecule 11 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	410	Total	C	N	O	0	0
			2038	1218	410	410		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	a	207	Total	C	N	O	0	0
			1030	616	207	207		
12	b	207	Total	C	N	O	0	0
			1030	616	207	207		
12	c	240	Total	C	N	O	0	0
			1194	714	240	240		
12	d	269	Total	C	N	O	0	0
			1339	801	269	269		

- Molecule 13 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	798	Total	C	N	O	0	0
			3959	2363	798	798		
13	f	808	Total	C	N	O	0	0
			4009	2393	808	808		
13	m	792	Total	C	N	O	0	0
			3750	2166	792	792		
13	n	755	Total	C	N	O	0	0
			3566	2056	755	755		

- Molecule 14 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	g	358	Total	C	N	O	0	0
			1767	1051	358	358		
14	h	358	Total	C	N	O	0	0
			1767	1051	358	358		

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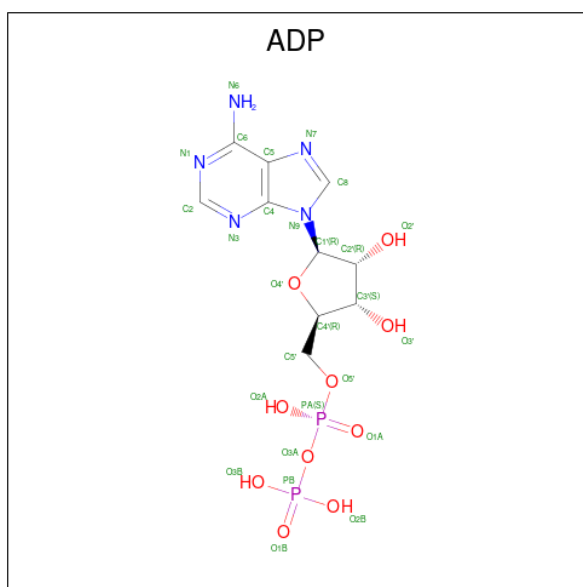
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Mol	Chain	Residues	Atoms				AltConf	Trace
14	o	358	Total	C	N	O	0	0
			1767	1051	358	358		
14	p	358	Total	C	N	O	0	0
			1767	1051	358	358		

- Molecule 15 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	j	14	Total	C	N	O	0	0
			56	28	14	14		
15	q	14	Total	C	N	O	0	0
			56	28	14	14		

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

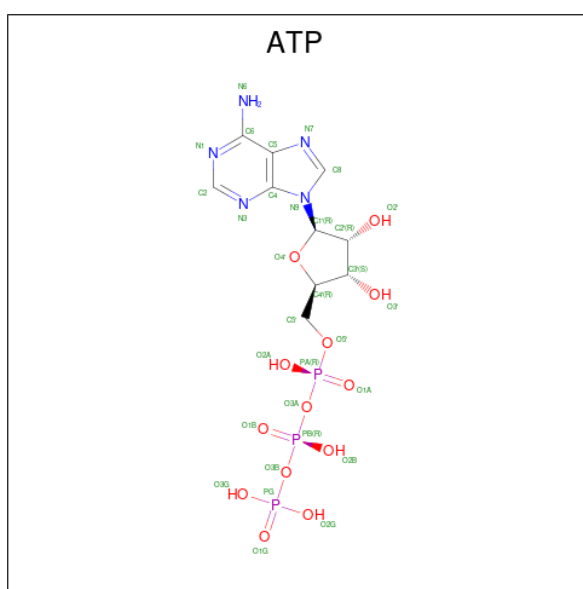




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Mol	Chain	Residues	Atoms					AltConf
16	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
17	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

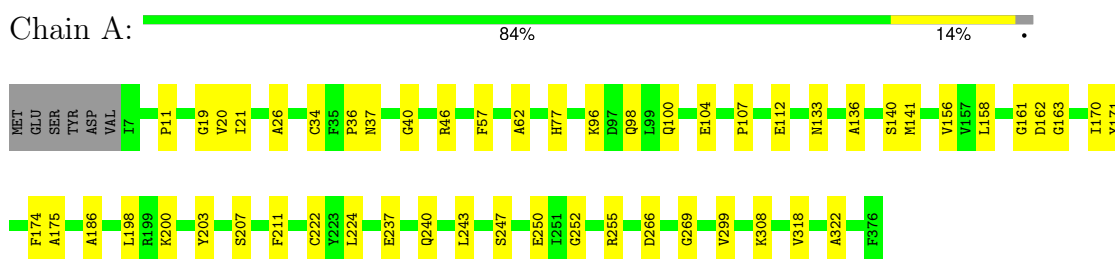
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
18	Y	3	Total	Zn	0
			3	3	

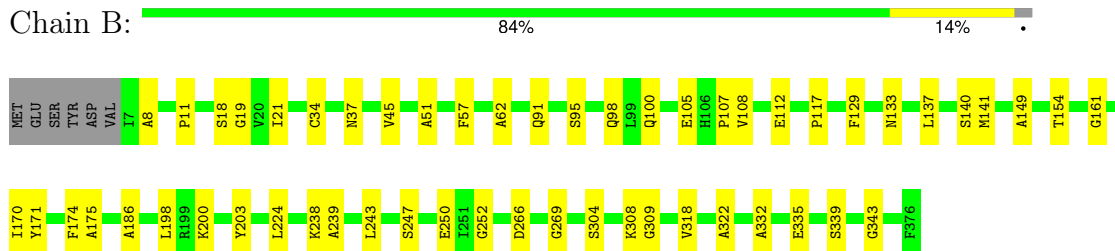
### 3 Residue-property plots [i](#)

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.

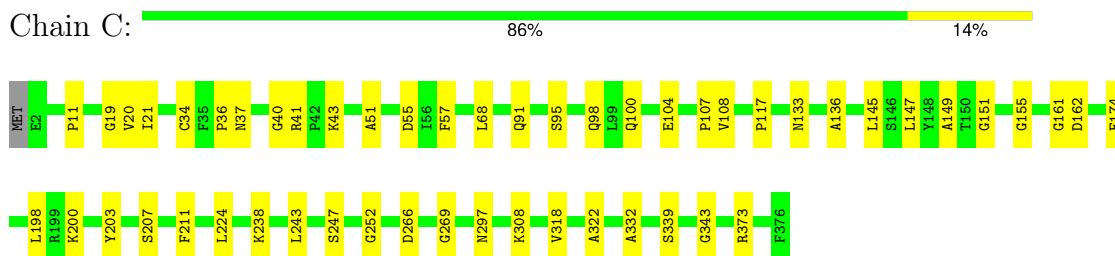
- Molecule 1: Alpha-centractin



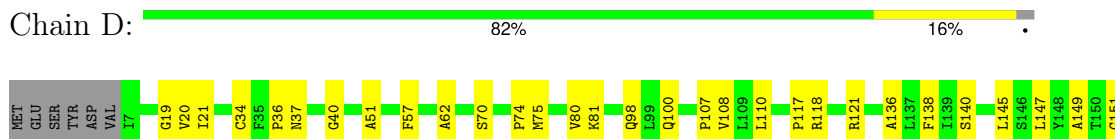
- Molecule 1: Alpha-centractin



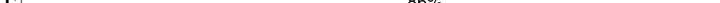
- Molecule 1: Alpha-centractin



- Molecule 1: Alpha-centractin

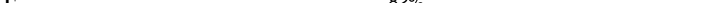


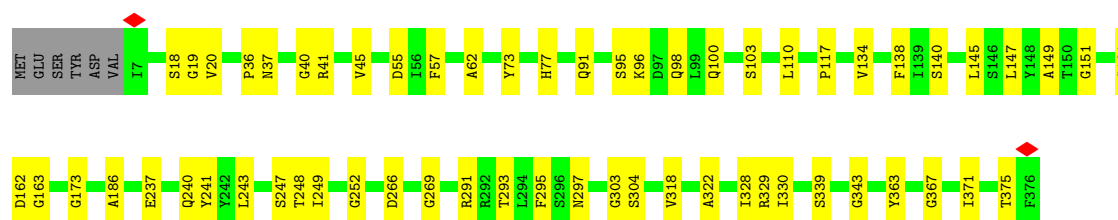
- Molecule 1: Alpha-centractin

Chain E:  86% 12% •




- Molecule 1: Alpha-centractin

Chain F:  82% 16% .



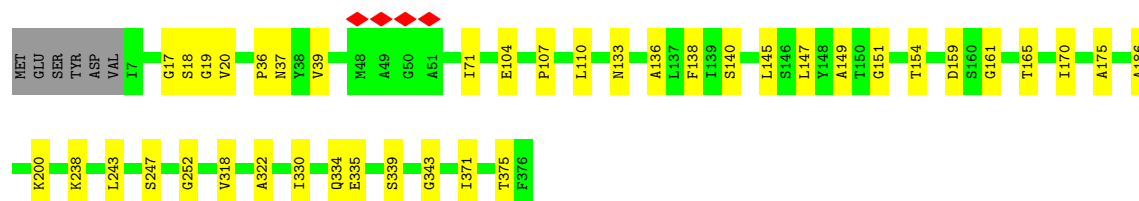
- Molecule 1: Alpha-centractin

Chain G:  86% 13%

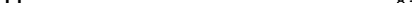


- Molecule 1: Alpha-centractin

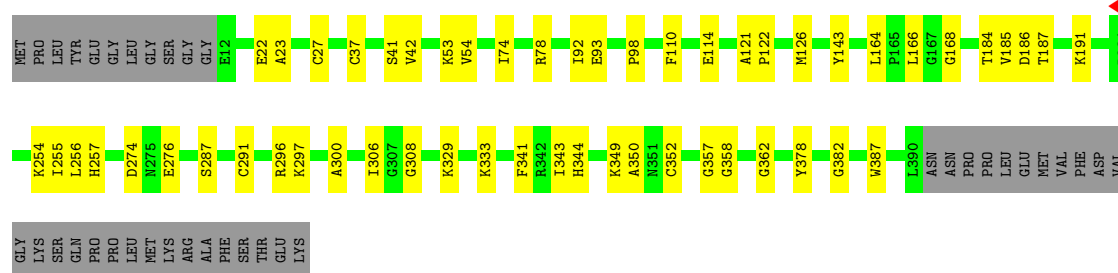
Chain I:  88% 11% .



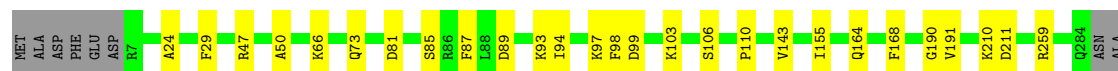
- Molecule 2: Actin, cytoplasmic 1

Chain H:  83% 15%

- Molecule 3: Actin-related protein 10



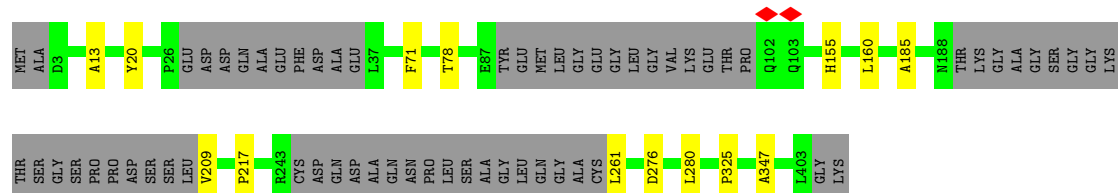
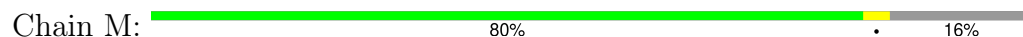
- Molecule 4: F-actin-capping protein subunit alpha-1



- Molecule 5: F-actin-capping protein subunit beta

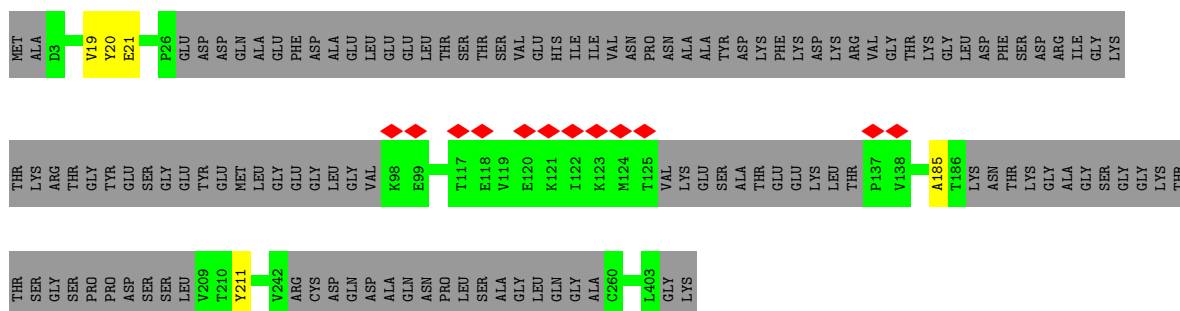


- Molecule 6: Dynactin subunit 2



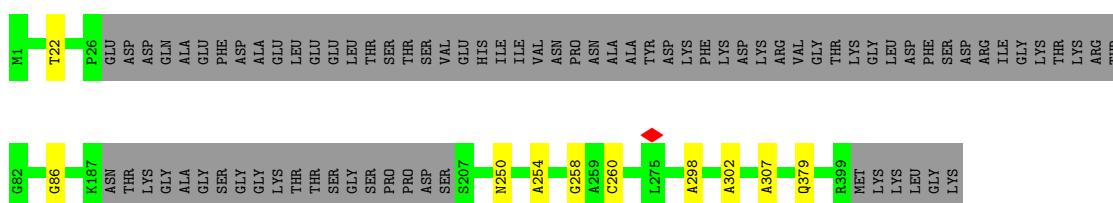
- Molecule 6: Dynactin subunit 2





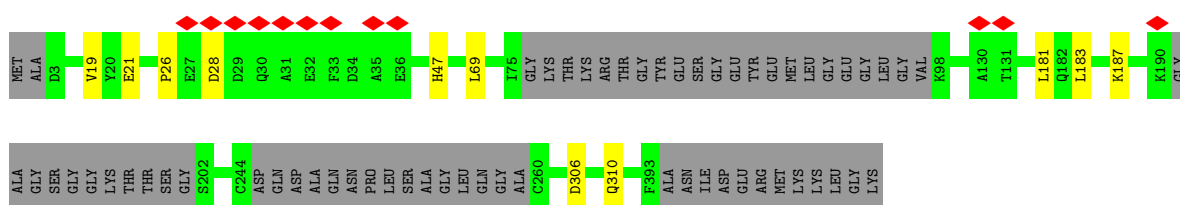
• Molecule 6: Dynactin subunit 2

Chain P: 78% 20%



• Molecule 6: Dynactin subunit 2

Chain Q: 82% 15%



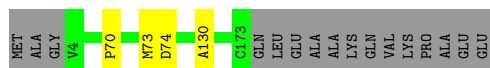
• Molecule 7: Dynactin subunit 3

Chain O: 90% 6%



• Molecule 7: Dynactin subunit 3

Chain R: 89% 9%



• Molecule 8: Dynactin subunit 6

Chain U: 76% 11% 12%



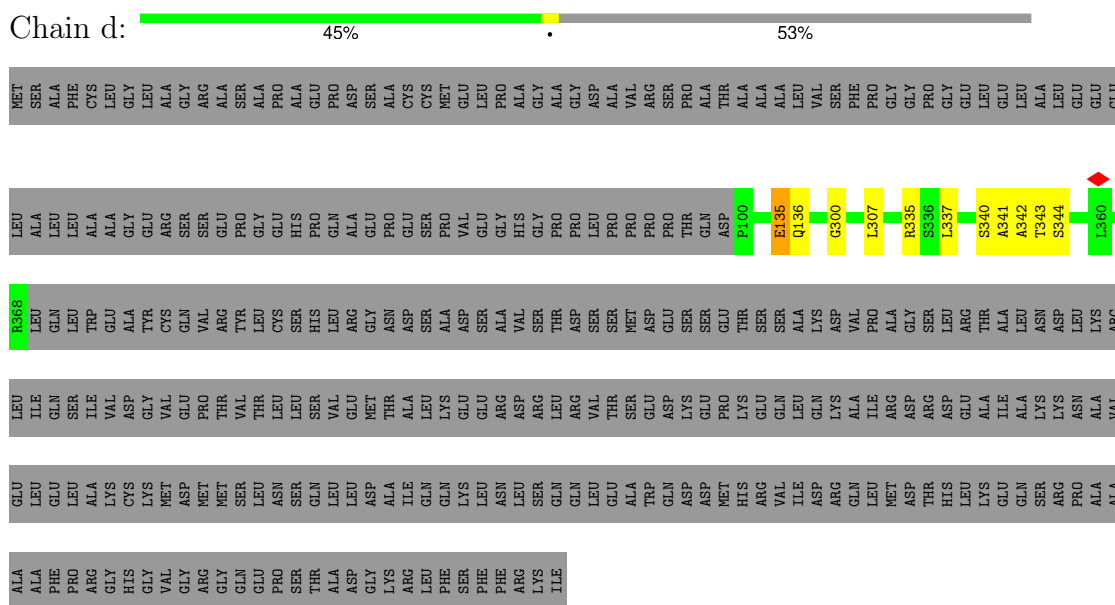




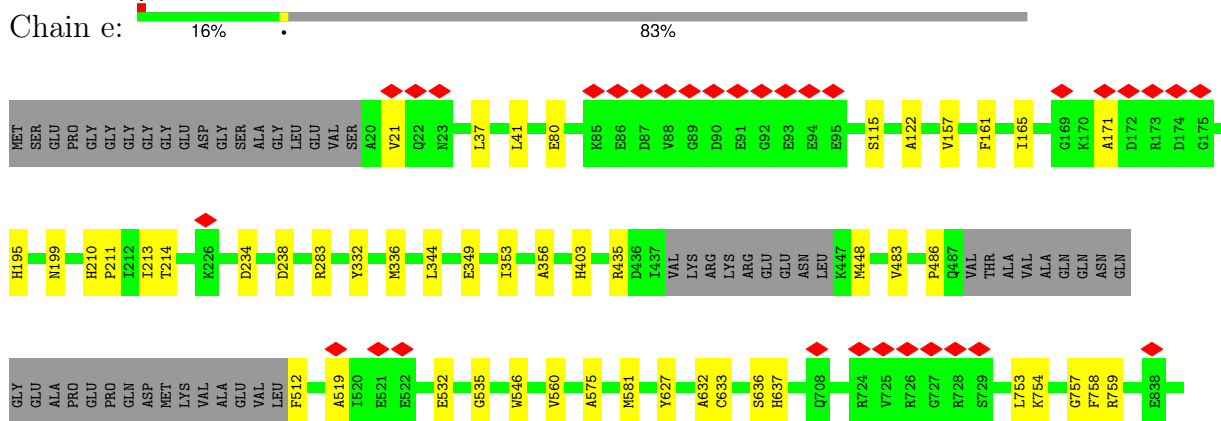




- Molecule 12: BICD family-like cargo adapter 1



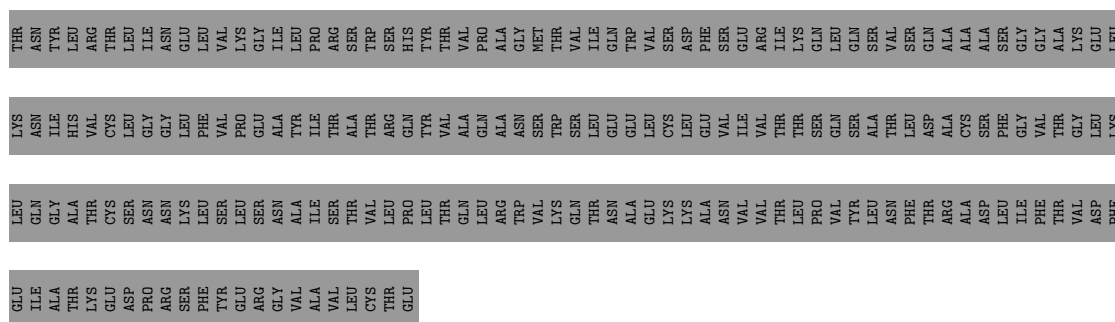
- Molecule 13: Cytoplasmic dynein 1 heavy chain 1



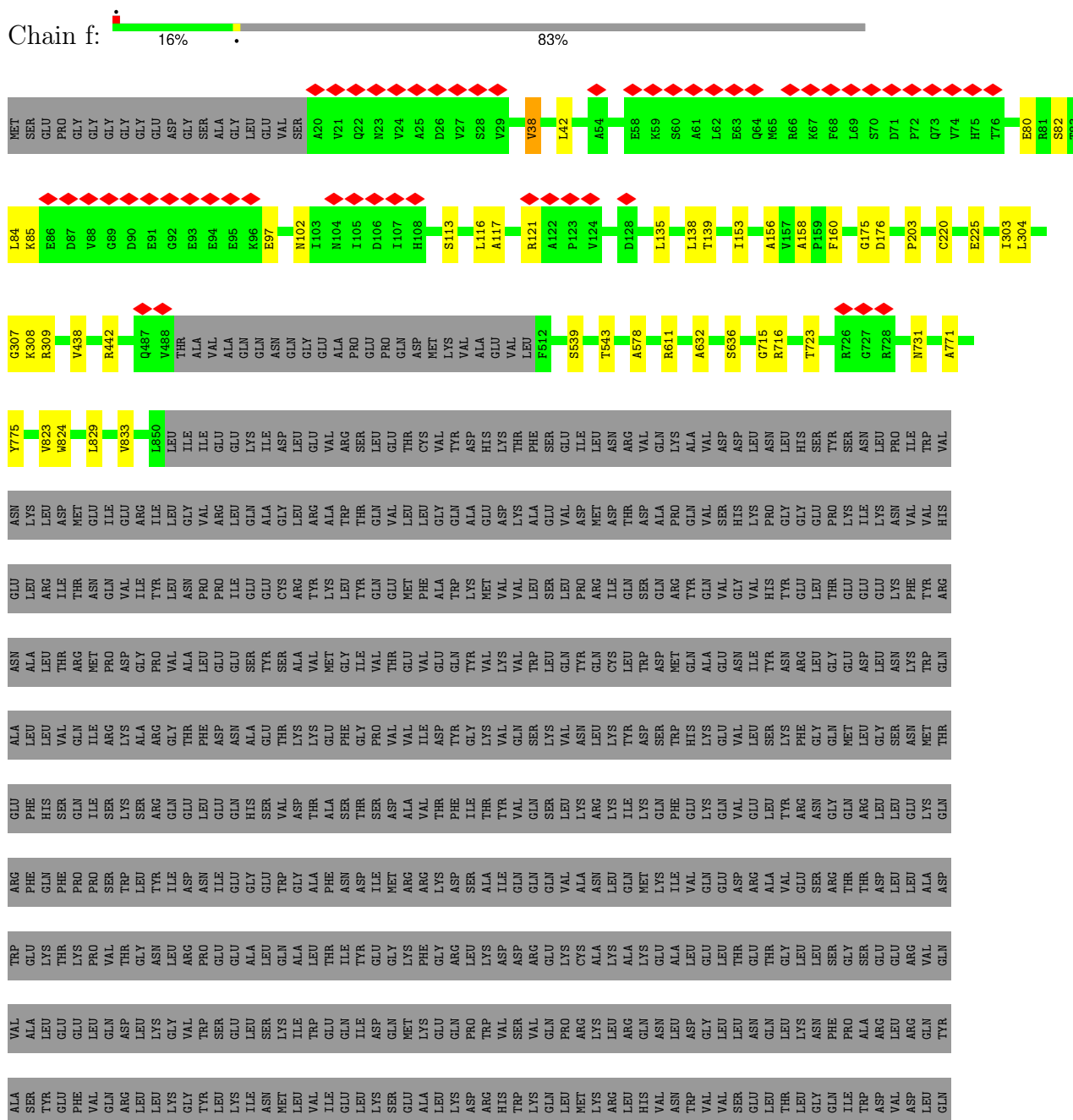








- Molecule 13: Cytoplasmic dynein 1 heavy chain 1





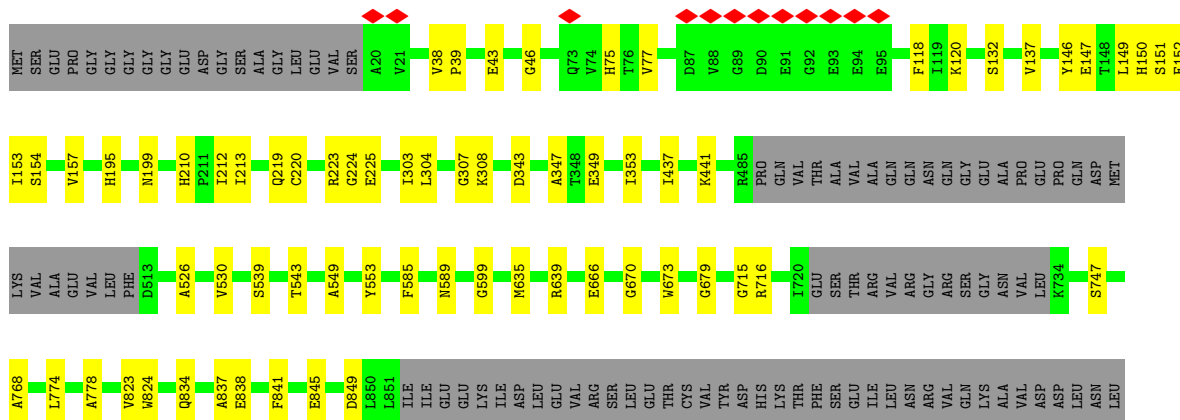




[illegible]

- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

Chain m:  16% . 83%









LEU ASN PHE THR ARG ALA ASP LEU ILE PHE THR VAL ASP PHE GLU ILE ALA THR LYS GLU ASP PRO ARG SER PHE TYR GLU ARG GLY VAL ALA VAL LEU CYS THR GLU

Chain n:  15% • 84%







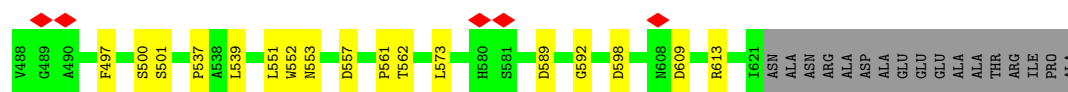
[illegible]

- Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

Chain g: 

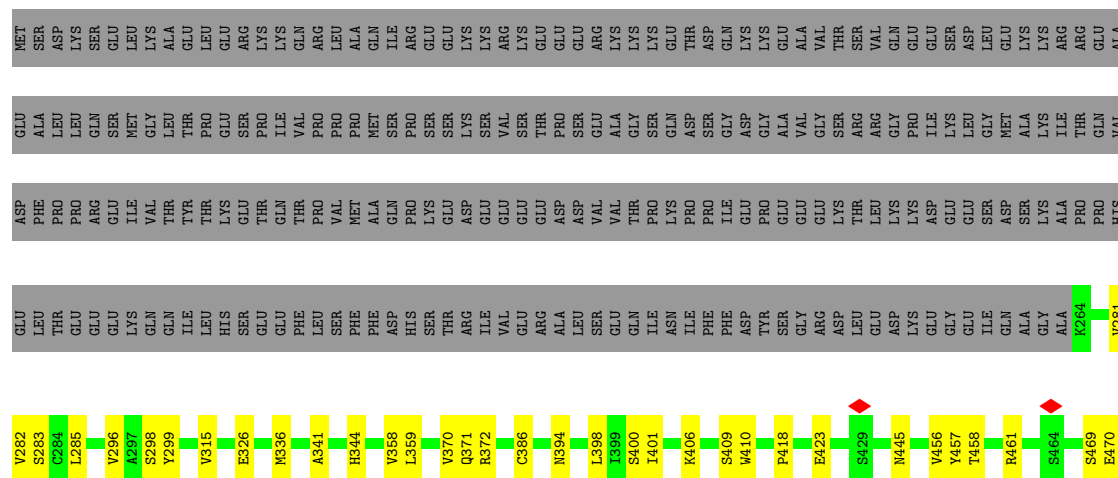
[illegible]





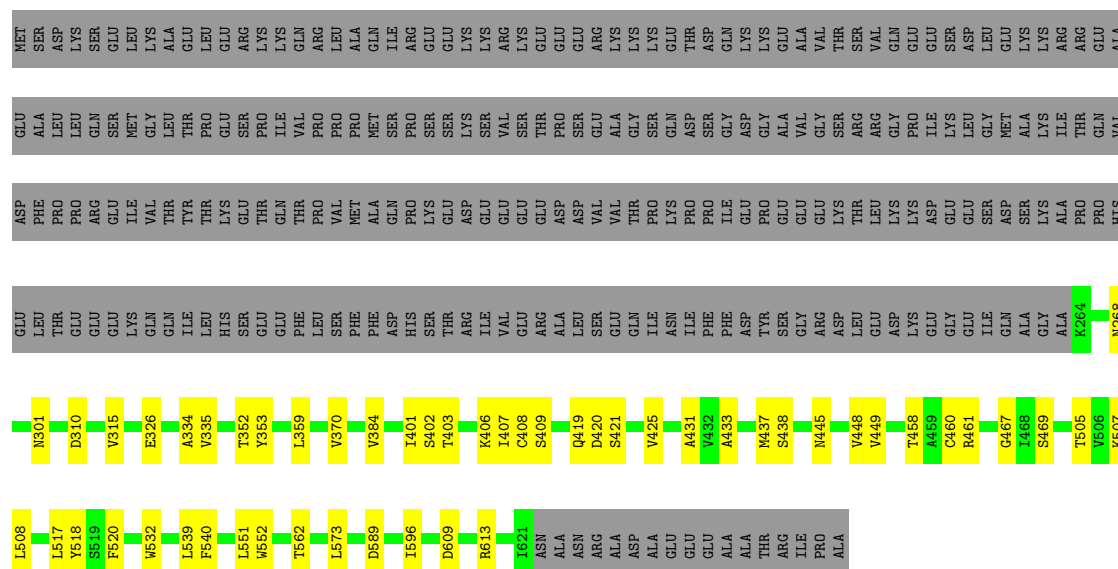
• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

Chain h: 50% 9% 42%



• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

Chain o: 50% 8% 42%



• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

Chain p: 52% 6% 42%



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.461	Depositor
Minimum map value	-0.215	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	666.62396, 666.62396, 666.62396	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.736, 1.736, 1.736	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, ATP, 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	0.25	0/1821	0.47	0/2531
1	B	0.28	0/1821	0.53	0/2531
1	C	0.26	0/1846	0.52	0/2566
1	D	0.26	0/1821	0.51	0/2531
1	E	0.25	0/1821	0.52	0/2531
1	F	0.32	1/1821 (0.1%)	0.56	0/2531
1	G	0.26	0/1821	0.51	0/2531
1	I	0.23	0/1821	0.50	0/2531
2	H	0.26	0/1821	0.49	2/2531 (0.1%)
3	J	0.23	0/1867	0.47	0/2596
4	K	0.24	0/1377	0.44	0/1919
5	L	0.25	0/1326	0.47	0/1844
6	M	0.18	0/1684	0.40	1/2343 (0.0%)
6	N	0.22	0/1389	0.42	0/1933
6	P	0.22	0/1609	0.45	0/2240
6	Q	0.21	0/1703	0.41	0/2373
7	O	0.20	0/887	0.42	0/1236
7	R	0.19	0/843	0.47	0/1175
8	U	0.40	1/821 (0.1%)	0.59	0/1140
9	V	0.36	0/880	0.82	5/1222 (0.4%)
10	W	0.17	0/750	0.36	0/1040
10	Z	0.26	0/951	0.47	0/1325
11	Y	0.25	0/2035	0.50	0/2837
12	a	0.28	0/1029	0.56	0/1436
12	b	1.19	3/1029 (0.3%)	1.26	6/1436 (0.4%)
12	c	0.25	0/1193	0.55	0/1665
12	d	0.32	0/1338	0.73	1/1868 (0.1%)
13	e	0.16	0/3956	0.39	0/5515
13	f	0.23	0/4007	0.52	0/5588
13	m	0.22	0/3747	0.46	0/5115
13	n	0.21	0/3562	0.41	0/4855
14	g	0.14	0/1766	0.32	0/2457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
14	h	0.24	0/1766	0.50	0/2457
14	o	0.25	0/1766	0.48	0/2457
14	p	0.19	0/1766	0.46	0/2457
15	j	0.11	0/55	0.15	0/67
15	q	0.11	0/55	0.32	0/67
All	All	0.28	5/61571 (0.0%)	0.51	15/85477 (0.0%)

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
8	U	0	2
9	V	0	3
12	b	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	282	LEU	C-N	31.58	1.72	1.33
12	b	283	GLN	N-CA	14.76	1.63	1.46
8	U	71	THR	C-O	-7.34	1.20	1.23
1	F	73	TYR	C-N	-6.43	1.28	1.33
12	b	282	LEU	CA-C	5.51	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	282	LEU	CA-C-N	23.93	152.24	120.65
12	b	282	LEU	C-N-CA	23.93	152.24	120.65
12	b	282	LEU	CA-C-O	-11.71	108.01	120.42
12	b	283	GLN	N-CA-C	7.36	118.99	110.97
9	V	74	LYS	N-CA-C	6.94	117.80	108.23
12	b	282	LEU	N-CA-C	6.39	118.33	111.36
9	V	82	PHE	CA-C-N	-6.32	115.81	122.89
9	V	82	PHE	C-N-CA	-6.32	115.81	122.89
2	H	100	GLU	CA-C-N	-5.84	105.43	122.21
2	H	100	GLU	C-N-CA	-5.84	105.43	122.21
12	b	299	GLN	N-CA-CB	-5.62	101.57	110.22
12	d	135	GLU	N-CA-CB	5.51	117.95	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	78	THR	CB-CA-C	-5.27	108.94	115.89
9	V	80	VAL	CA-C-N	-5.26	114.70	123.33
9	V	80	VAL	C-N-CA	-5.26	114.70	123.33

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	U	169	LYS	Peptide
8	U	170	ILE	Peptide
9	V	74	LYS	Peptide
9	V	75	LYS	Peptide
9	V	82	PHE	Peptide
12	b	294	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1822	0	820	31	0
1	B	1822	0	820	34	0
1	C	1847	0	830	32	0
1	D	1822	0	820	41	0
1	E	1822	0	820	28	0
1	F	1822	0	820	38	0
1	G	1822	0	820	29	0
1	I	1822	0	820	25	0
2	H	1822	0	835	32	0
3	J	1868	0	823	35	0
4	K	1378	0	611	16	0
5	L	1327	0	585	16	0
6	M	1689	0	765	11	0
6	N	1394	0	632	6	0
6	P	1612	0	747	7	0
6	Q	1707	0	769	8	0
7	O	888	0	413	7	0
7	R	844	0	385	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	U	822	0	370	13	0
9	V	881	0	379	29	0
10	W	754	0	336	6	0
10	Z	952	0	434	6	0
11	Y	2038	0	886	44	0
12	a	1030	0	445	2	0
12	b	1030	0	444	21	0
12	c	1194	0	512	3	0
12	d	1339	0	579	20	0
13	e	3959	0	1773	30	0
13	f	4009	0	1794	27	0
13	m	3750	0	1534	37	0
13	n	3566	0	1454	24	0
14	g	1767	0	796	26	0
14	h	1767	0	796	29	0
14	o	1767	0	796	26	0
14	p	1767	0	796	20	0
15	j	56	0	15	1	0
15	q	56	0	15	1	0
16	A	27	0	12	1	0
16	B	27	0	12	3	0
16	C	27	0	12	2	0
16	D	27	0	12	3	0
16	E	27	0	12	2	0
16	F	27	0	12	5	0
16	G	27	0	12	2	0
16	I	27	0	12	1	0
16	J	27	0	12	5	0
17	H	31	0	12	3	0
18	Y	3	0	0	0	0
All	All	61911	0	27409	683	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (683) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:282:LEU:C	12:b:283:GLN:N	1.72	1.43
9:V:32:GLN:N	12:d:343:THR:H	1.60	0.99
9:V:32:GLN:H	12:d:343:THR:H	1.15	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:g:265:LEU:HA	14:g:598:ASP:O	1.73	0.88
9:V:33:ASN:H	12:d:343:THR:N	1.72	0.88
2:H:149:THR:HA	2:H:165:ILE:O	1.74	0.87
9:V:34:ILE:H	12:d:343:THR:HA	1.41	0.85
1:G:371:ILE:O	1:G:375:THR:N	2.11	0.83
14:h:505:THR:HA	14:h:520:PHE:O	1.79	0.83
14:h:315:VAL:O	14:h:326:GLU:N	2.14	0.81
1:C:243:LEU:N	1:C:247:SER:O	2.12	0.81
11:Y:107:TYR:HA	12:b:285:THR:N	1.97	0.80
13:f:82:SER:HA	13:f:113:SER:HA	1.64	0.79
3:J:27:CYS:CB	3:J:37:CYS:CB	2.62	0.77
14:o:315:VAL:O	14:o:326:GLU:N	2.17	0.77
3:J:344:HIS:HA	11:Y:228:ALA:HA	1.65	0.76
13:e:403:HIS:HA	13:e:532:GLU:HA	1.66	0.76
13:m:150:HIS:O	13:m:154:SER:N	2.17	0.76
14:o:505:THR:HA	14:o:520:PHE:O	1.87	0.75
13:e:37:LEU:O	13:e:41:LEU:N	2.16	0.74
13:e:344:LEU:HA	13:e:356:ALA:HB1	1.69	0.74
13:m:303:ILE:O	13:m:307:GLY:N	2.20	0.74
10:Z:1227:VAL:N	10:Z:1234:PHE:O	2.19	0.74
1:D:371:ILE:O	1:D:375:THR:N	2.20	0.74
9:V:32:GLN:H	12:d:343:THR:N	1.86	0.73
3:J:143:TYR:N	16:J:800:ADP:O3B	2.20	0.73
1:A:170:ILE:HA	1:A:175:ALA:HA	1.69	0.73
9:V:118:ARG:O	9:V:137:GLU:N	2.22	0.73
2:H:157:ASP:N	17:H:401:ATP:O2B	2.20	0.73
11:Y:50:TYR:O	11:Y:277:LEU:N	2.20	0.72
1:C:51:ALA:HB2	1:E:173:GLY:HA3	1.71	0.72
1:D:20:VAL:N	16:D:800:ADP:O1A	2.20	0.72
9:V:52:LEU:N	12:d:341:ALA:O	2.22	0.72
11:Y:107:TYR:CB	12:b:280:ASP:O	2.37	0.72
1:G:60:PRO:O	1:G:63:GLU:N	2.23	0.71
1:E:241:TYR:O	1:E:248:THR:HA	1.90	0.71
11:Y:107:TYR:CA	12:b:285:THR:H	2.04	0.71
13:f:716:ARG:HA	13:f:823:VAL:HA	1.71	0.71
1:E:20:VAL:HA	1:E:36:PRO:HA	1.72	0.71
13:f:723:THR:O	13:f:731:ASN:HA	1.92	0.70
13:m:834:GLN:O	13:m:837:ALA:HB3	1.90	0.70
1:B:154:THR:HA	1:B:170:ILE:O	1.91	0.70
2:H:291:LYS:O	2:H:295:ALA:N	2.24	0.70
13:e:21:VAL:HA	13:e:122:ALA:HB1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:g:315:VAL:O	14:g:326:GLU:N	2.24	0.69
13:m:146:TYR:O	13:m:150:HIS:N	2.18	0.69
14:h:406:LYS:HA	14:h:423:GLU:HA	1.73	0.69
13:f:85:LYS:HA	13:f:97:GLU:HA	1.75	0.69
1:E:147:LEU:O	1:E:151:GLY:N	2.26	0.69
13:e:283:ARG:HA	13:f:175:GLY:HA3	1.74	0.69
14:p:573:LEU:HA	14:p:589:ASP:HA	1.75	0.69
14:g:551:LEU:O	14:g:562:THR:N	2.24	0.69
13:f:117:ALA:N	13:f:138:LEU:O	2.20	0.68
14:g:539:LEU:HA	14:g:553:ASN:HA	1.75	0.68
14:o:437:MET:HA	14:o:449:VAL:HA	1.75	0.68
1:I:39:VAL:O	1:I:71:ILE:HA	1.94	0.68
13:m:530:VAL:HA	13:m:549:ALA:HB1	1.76	0.68
1:A:243:LEU:N	1:A:247:SER:O	2.27	0.68
1:G:20:VAL:HA	1:G:36:PRO:HA	1.73	0.68
11:Y:107:TYR:HA	12:b:285:THR:H	1.57	0.67
1:B:170:ILE:HA	1:B:175:ALA:HA	1.77	0.67
3:J:185:VAL:HA	3:J:256:LEU:HA	1.77	0.67
14:h:398:LEU:O	14:h:409:SER:HA	1.95	0.66
13:n:303:ILE:O	13:n:307:GLY:N	2.28	0.66
14:g:359:LEU:O	14:g:370:VAL:N	2.27	0.66
1:I:20:VAL:HA	1:I:36:PRO:HA	1.75	0.66
7:O:47:ILE:O	7:O:51:ARG:N	2.28	0.66
13:e:754:LYS:HA	13:e:759:ARG:HA	1.78	0.66
1:C:147:LEU:O	1:C:151:GLY:N	2.28	0.66
1:D:110:LEU:O	1:D:140:SER:N	2.28	0.66
13:f:220:CYS:O	13:f:225:GLU:N	2.29	0.66
5:L:52:ASP:O	5:L:56:GLY:N	2.28	0.66
8:U:53:GLY:HA3	8:U:87:ASN:H	1.59	0.66
1:E:291:ARG:O	1:E:295:PHE:N	2.29	0.66
13:n:68:PHE:O	13:n:125:ILE:N	2.26	0.65
13:m:845:GLU:O	13:m:849:ASP:N	2.28	0.65
1:C:43:LYS:N	1:C:68:LEU:O	2.26	0.65
2:H:16:MET:N	17:H:401:ATP:O1B	2.27	0.65
1:F:291:ARG:O	1:F:295:PHE:N	2.26	0.65
13:m:585:PHE:O	13:m:589:ASN:N	2.29	0.65
2:H:19:ALA:O	2:H:28:ARG:N	2.29	0.65
4:K:97:LYS:N	4:K:106:SER:O	2.31	0.64
14:p:505:THR:HA	14:p:520:PHE:O	1.96	0.64
2:H:153:MET:N	2:H:298:VAL:O	2.30	0.64
13:e:234:ASP:O	13:e:238:ASP:N	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:384:VAL:HA	14:o:402:SER:HA	1.78	0.64
5:L:52:ASP:O	5:L:56:GLY:CA	2.46	0.64
13:e:165:ILE:O	13:e:171:ALA:N	2.30	0.64
11:Y:360:ASN:N	11:Y:423:THR:O	2.28	0.64
13:m:343:ASP:O	13:m:347:ALA:N	2.31	0.64
1:A:46:ARG:HA	1:C:174:PHE:HA	1.79	0.63
11:Y:107:TYR:CB	12:b:281:LEU:O	2.46	0.63
14:h:445:ASN:O	14:h:461:ARG:N	2.23	0.63
13:m:715:GLY:O	13:m:824:TRP:N	2.31	0.63
6:M:209:VAL:HA	10:W:1258:PHE:HA	1.81	0.63
14:o:268:ASN:N	14:o:596:ILE:O	2.32	0.63
13:m:77:VAL:O	13:m:118:PHE:N	2.26	0.63
11:Y:87:ALA:HB1	12:b:285:THR:HA	1.81	0.63
1:F:19:GLY:N	16:F:800:ADP:O1A	2.19	0.63
9:V:58:GLY:HA3	9:V:89:ASP:HA	1.81	0.63
1:F:363:TYR:O	1:F:367:GLY:N	2.29	0.62
4:K:164:GLN:O	4:K:168:PHE:N	2.32	0.62
1:D:147:LEU:O	1:D:151:GLY:N	2.32	0.62
1:G:147:LEU:O	1:G:151:GLY:N	2.31	0.62
13:e:627:TYR:HA	13:e:632:ALA:HB3	1.81	0.62
13:n:315:SER:O	13:n:319:ASP:N	2.30	0.62
4:K:89:ASP:O	4:K:93:LYS:HA	1.99	0.62
1:F:240:GLN:HA	1:F:249:ILE:O	1.98	0.62
1:E:19:GLY:N	16:E:800:ADP:O1A	2.28	0.62
6:N:211:TYR:O	10:W:1256:VAL:N	2.30	0.62
13:f:771:ALA:O	13:f:775:TYR:N	2.32	0.62
13:e:632:ALA:O	13:e:636:SER:N	2.25	0.61
10:W:1159:LYS:O	10:W:1163:LEU:N	2.33	0.61
13:e:575:ALA:HB1	13:e:581:MET:HA	1.82	0.61
1:F:57:PHE:C	1:F:62:ALA:HB2	2.26	0.61
14:o:301:ASN:HA	14:o:310:ASP:HA	1.83	0.61
13:e:483:VAL:O	13:e:512:PHE:N	2.33	0.61
1:D:162:ASP:N	16:D:800:ADP:O1B	2.23	0.61
14:h:551:LEU:O	14:h:562:THR:N	2.34	0.61
13:m:152:PHE:O	13:m:157:VAL:N	2.33	0.61
1:E:145:LEU:O	1:E:343:GLY:HA3	2.01	0.60
1:F:110:LEU:N	1:F:138:PHE:O	2.33	0.60
8:U:141:THR:HA	8:U:153:GLN:HA	1.82	0.60
9:V:32:GLN:C	12:d:342:ALA:H	2.09	0.60
14:o:409:SER:O	14:o:419:GLN:N	2.33	0.60
13:n:333:ASN:O	13:n:337:LYS:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:p:315:VAL:O	14:p:326:GLU:N	2.34	0.60
1:F:20:VAL:HA	1:F:36:PRO:HA	1.81	0.60
14:p:539:LEU:HA	14:p:552:TRP:O	2.02	0.60
1:E:318:VAL:O	1:E:322:ALA:N	2.35	0.60
3:J:306:ILE:HA	3:J:350:ALA:HB1	1.82	0.60
2:H:240:TYR:O	2:H:247:VAL:HA	2.01	0.60
3:J:308:GLY:HA3	16:J:800:ADP:C8	2.35	0.60
13:m:195:HIS:O	13:m:199:ASN:N	2.35	0.60
14:g:334:ALA:O	14:g:353:TYR:N	2.31	0.60
15:q:435:SER:O	15:q:439:LYS:N	2.29	0.60
14:o:335:VAL:HA	14:o:352:THR:HA	1.81	0.60
2:H:214:GLU:HA	17:H:401:ATP:C2	2.37	0.59
2:H:290:ARG:O	2:H:294:TYR:N	2.28	0.59
9:V:32:GLN:N	12:d:343:THR:N	2.40	0.59
14:g:409:SER:O	14:g:419:GLN:N	2.35	0.59
4:K:191:VAL:HA	4:K:210:LYS:O	2.02	0.59
1:F:318:VAL:O	1:F:322:ALA:N	2.34	0.59
14:o:551:LEU:O	14:o:562:THR:N	2.35	0.59
14:h:401:ILE:HA	14:h:406:LYS:O	2.02	0.59
1:A:112:GLU:N	1:A:140:SER:O	2.36	0.58
13:f:82:SER:O	13:f:84:LEU:N	2.36	0.58
4:K:190:GLY:O	4:K:211:ASP:HA	2.03	0.58
6:Q:306:ASP:O	6:Q:310:GLN:N	2.35	0.58
11:Y:87:ALA:HB2	12:b:284:GLY:O	2.02	0.58
14:g:438:SER:N	14:g:448:VAL:O	2.34	0.58
14:o:573:LEU:HA	14:o:589:ASP:HA	1.85	0.58
1:F:19:GLY:O	1:F:37:ASN:N	2.31	0.58
1:I:335:GLU:O	1:I:339:SER:N	2.37	0.58
5:L:52:ASP:O	5:L:56:GLY:HA2	2.04	0.58
11:Y:87:ALA:CB	12:b:285:THR:HA	2.33	0.58
1:C:108:VAL:N	1:C:136:ALA:O	2.28	0.58
4:K:97:LYS:O	4:K:106:SER:N	2.26	0.58
14:g:609:ASP:O	14:g:613:ARG:N	2.27	0.58
14:h:527:VAL:HA	14:h:544:ASP:HA	1.84	0.58
13:f:121:ARG:H	13:f:135:LEU:HA	1.68	0.58
1:I:334:GLN:HA	6:M:13:ALA:HB3	1.85	0.58
3:J:23:ALA:N	16:J:800:ADP:O1B	2.27	0.58
9:V:38:GLY:HA3	9:V:59:ARG:HA	1.86	0.58
10:W:1189:SER:O	10:W:1193:GLY:N	2.32	0.58
13:e:633:CYS:O	13:e:637:HIS:N	2.35	0.58
8:U:103:ASP:O	8:U:121:SER:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:VAL:O	1:G:322:ALA:N	2.36	0.57
4:K:99:ASP:O	4:K:103:LYS:N	2.36	0.57
1:E:240:GLN:HA	1:E:249:ILE:O	2.04	0.57
1:E:243:LEU:N	1:E:247:SER:O	2.37	0.57
2:H:317:ILE:O	2:H:321:ALA:N	2.27	0.57
14:h:480:THR:H	14:h:501:SER:HA	1.68	0.57
1:A:20:VAL:HA	1:A:36:PRO:HA	1.86	0.57
14:g:335:VAL:HA	14:g:352:THR:HA	1.86	0.57
7:O:70:PRO:O	7:O:74:ASP:N	2.30	0.57
9:V:33:ASN:H	12:d:343:THR:CA	2.17	0.57
14:h:386:CYS:O	14:h:400:SER:HA	2.05	0.57
1:D:318:VAL:O	1:D:322:ALA:N	2.29	0.56
14:g:487:ALA:HB3	14:g:537:PRO:HA	1.85	0.56
1:F:110:LEU:O	1:F:140:SER:N	2.37	0.56
9:V:39:LYS:N	9:V:59:ARG:O	2.37	0.56
1:B:51:ALA:HB2	1:D:173:GLY:HA3	1.86	0.56
1:C:145:LEU:O	1:C:343:GLY:HA3	2.06	0.56
1:F:241:TYR:O	1:F:248:THR:HA	2.05	0.56
1:F:243:LEU:N	1:F:247:SER:O	2.25	0.56
4:K:85:SER:O	4:K:98:PHE:N	2.34	0.56
14:p:268:ASN:N	14:p:596:ILE:O	2.38	0.56
13:e:80:GLU:HA	13:e:115:SER:HA	1.87	0.56
14:o:508:LEU:O	14:o:517:LEU:N	2.38	0.56
1:B:112:GLU:N	1:B:140:SER:O	2.24	0.56
6:M:155:HIS:O	6:M:160:LEU:N	2.30	0.56
11:Y:28:TYR:HA	11:Y:308:VAL:HA	1.87	0.56
12:d:135:GLU:O	12:d:136:GLN:C	2.48	0.56
13:m:716:ARG:HA	13:m:823:VAL:HA	1.88	0.56
13:e:195:HIS:O	13:e:199:ASN:N	2.21	0.56
1:E:329:ARG:HA	6:Q:21:GLU:HA	1.88	0.56
1:B:332:ALA:H	6:P:86:GLY:HA3	1.70	0.56
1:E:335:GLU:O	1:E:339:SER:N	2.38	0.55
1:G:363:TYR:O	1:G:367:GLY:N	2.38	0.55
11:Y:363:ALA:HA	11:Y:413:VAL:HA	1.88	0.55
13:e:283:ARG:CA	13:f:176:ASP:H	2.18	0.55
13:e:486:PRO:HA	13:e:512:PHE:HA	1.86	0.55
14:g:553:ASN:O	14:g:557:ASP:N	2.37	0.55
14:h:394:ASN:O	13:m:599:GLY:HA3	2.06	0.55
1:G:224:LEU:N	1:G:308:LYS:O	2.34	0.55
7:R:70:PRO:O	7:R:74:ASP:N	2.32	0.55
1:A:222:CYS:HA	1:A:255:ARG:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:181:LYS:O	5:L:185:GLY:N	2.39	0.55
3:J:186:ASP:HA	3:J:191:LYS:O	2.06	0.55
11:Y:344:THR:N	11:Y:429:LYS:O	2.25	0.55
14:p:437:MET:HA	14:p:449:VAL:HA	1.88	0.55
1:F:91:GLN:O	1:F:95:SER:N	2.40	0.55
3:J:187:THR:HA	3:J:254:LYS:HA	1.88	0.55
1:F:77:HIS:HA	1:F:163:GLY:C	2.32	0.55
1:G:243:LEU:N	1:G:247:SER:O	2.24	0.55
5:L:124:LEU:H	5:L:128:PHE:HA	1.72	0.55
7:O:33:VAL:O	7:O:37:LEU:N	2.38	0.55
9:V:121:VAL:O	9:V:139:VAL:HA	2.07	0.55
11:Y:428:LEU:O	11:Y:455:THR:HA	2.06	0.55
13:e:753:LEU:O	13:e:757:GLY:N	2.40	0.55
14:g:438:SER:O	14:g:448:VAL:N	2.29	0.55
13:m:774:LEU:O	13:m:778:ALA:N	2.34	0.55
1:I:318:VAL:O	1:I:322:ALA:N	2.39	0.54
14:p:551:LEU:O	14:p:562:THR:N	2.39	0.54
13:m:673:TRP:O	13:m:679:GLY:HA3	2.07	0.54
1:I:147:LEU:O	1:I:151:GLY:N	2.33	0.54
1:E:104:GLU:HA	1:E:133:ASN:O	2.07	0.54
1:G:19:GLY:O	1:G:37:ASN:N	2.34	0.54
9:V:111:GLY:N	9:V:128:ILE:O	2.40	0.54
14:h:539:LEU:HA	14:h:553:ASN:HA	1.88	0.54
1:D:369:ARG:O	1:D:373:ARG:CB	2.55	0.54
5:L:151:ILE:O	5:L:171:SER:HA	2.07	0.54
14:p:266:SER:O	14:p:598:ASP:N	2.27	0.54
11:Y:110:ALA:HA	11:Y:117:THR:HA	1.87	0.54
1:G:104:GLU:HA	1:G:133:ASN:O	2.07	0.54
14:p:508:LEU:O	14:p:517:LEU:N	2.41	0.54
13:m:38:VAL:O	13:m:43:GLU:N	2.28	0.54
1:F:329:ARG:HA	6:N:21:GLU:HA	1.90	0.54
10:W:1130:ALA:O	10:W:1134:LEU:N	2.39	0.54
11:Y:400:ALA:N	11:Y:408:GLY:O	2.37	0.53
13:f:438:VAL:O	13:f:442:ARG:N	2.42	0.53
14:o:407:ILE:O	14:o:421:SER:HA	2.08	0.53
10:W:1159:LYS:O	10:W:1164:LEU:N	2.35	0.53
1:A:200:LYS:O	1:B:117:PRO:HA	2.09	0.53
6:M:276:ASP:O	6:M:280:LEU:N	2.32	0.53
13:e:283:ARG:HA	13:f:176:ASP:H	1.73	0.53
1:A:77:HIS:HA	1:A:163:GLY:O	2.09	0.53
1:B:171:TYR:N	1:B:174:PHE:O	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:LEU:O	1:G:343:GLY:HA3	2.08	0.53
1:G:295:PHE:O	1:G:328:ILE:HA	2.09	0.53
13:f:715:GLY:O	13:f:824:TRP:N	2.21	0.53
2:H:107:GLU:O	2:H:136:ILE:HA	2.09	0.53
3:J:184:THR:O	3:J:257:HIS:N	2.26	0.53
13:f:304:LEU:O	13:f:309:ARG:N	2.37	0.53
1:E:200:LYS:O	1:F:117:PRO:HA	2.09	0.53
10:Z:1186:ALA:O	10:Z:1188:SER:N	2.40	0.53
13:f:303:ILE:O	13:f:307:GLY:N	2.33	0.53
14:o:539:LEU:HA	14:o:552:TRP:O	2.09	0.53
14:p:301:ASN:HA	14:p:310:ASP:HA	1.90	0.53
1:C:318:VAL:O	1:C:322:ALA:N	2.42	0.52
1:G:373:ARG:O	6:M:71:PHE:N	2.36	0.52
1:I:19:GLY:O	1:I:37:ASN:N	2.26	0.52
13:m:526:ALA:HB1	13:m:553:TYR:HA	1.91	0.52
8:U:169:LYS:O	12:b:302:ASP:O	2.27	0.52
11:Y:343:LEU:HA	11:Y:430:HIS:HA	1.90	0.52
14:h:359:LEU:N	14:h:371:GLN:O	2.42	0.52
1:I:159:ASP:O	1:I:165:THR:HA	2.09	0.52
1:B:21:ILE:O	1:B:34:CYS:HA	2.09	0.52
1:C:332:ALA:O	6:Q:47:HIS:HA	2.09	0.52
1:G:159:ASP:O	1:G:165:THR:HA	2.10	0.52
3:J:358:GLY:O	3:J:362:GLY:N	2.41	0.52
5:L:109:ASP:HA	5:L:114:GLY:H	1.74	0.52
13:f:578:ALA:HB2	13:f:611:ARG:C	2.35	0.52
1:B:198:LEU:O	1:B:203:TYR:N	2.39	0.52
1:C:200:LYS:O	1:D:117:PRO:HA	2.10	0.52
4:K:81:ASP:HA	4:K:87:PHE:HA	1.92	0.52
11:Y:387:ALA:O	11:Y:392:PHE:N	2.34	0.52
14:g:480:THR:N	14:g:500:SER:O	2.43	0.52
1:A:11:PRO:O	1:A:26:ALA:N	2.43	0.52
8:U:122:GLY:C	8:U:140:ASN:HA	2.35	0.52
6:Q:26:PRO:O	6:Q:28:ASP:N	2.42	0.52
9:V:127:LYS:O	9:V:145:VAL:HA	2.10	0.52
13:m:539:SER:O	13:m:543:THR:N	2.33	0.52
14:o:507:LYS:HA	14:o:518:TYR:O	2.10	0.52
1:A:171:TYR:N	1:A:174:PHE:O	2.43	0.51
2:H:334:GLU:O	2:H:338:SER:N	2.43	0.51
11:Y:398:VAL:O	11:Y:409:VAL:HA	2.10	0.51
1:A:198:LEU:O	1:A:203:TYR:N	2.40	0.51
1:F:103:SER:O	1:F:134:VAL:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:185:ALA:HB1	6:P:379:GLN:HA	1.92	0.51
11:Y:400:ALA:HB3	11:Y:408:GLY:HA3	1.92	0.51
13:f:304:LEU:O	13:f:308:LYS:N	2.43	0.51
14:h:458:THR:O	14:h:469:SER:N	2.39	0.51
14:p:405:GLY:O	14:p:424:LEU:N	2.28	0.51
5:L:109:ASP:O	5:L:113:GLU:HA	2.11	0.51
1:D:51:ALA:HB2	1:F:173:GLY:HA3	1.92	0.51
1:D:238:LYS:HA	1:D:252:GLY:CA	2.41	0.51
3:J:42:VAL:HA	3:J:53:LYS:HA	1.92	0.51
8:U:102:GLY:N	8:U:119:LEU:O	2.33	0.51
13:f:153:ILE:O	13:f:158:ALA:N	2.43	0.51
14:o:532:TRP:HA	14:o:540:PHE:CB	2.41	0.51
2:H:53:TYR:O	2:H:58:ALA:HB2	2.11	0.51
1:B:243:LEU:N	1:B:247:SER:O	2.30	0.51
1:G:373:ARG:C	6:M:71:PHE:H	2.19	0.51
1:I:154:THR:HA	1:I:170:ILE:O	2.11	0.51
6:P:307:ALA:HB1	7:R:73:MET:O	2.10	0.51
11:Y:332:VAL:O	11:Y:408:GLY:HA2	2.10	0.51
1:A:156:VAL:O	1:A:299:VAL:N	2.37	0.51
1:B:11:PRO:HA	1:B:107:PRO:O	2.09	0.51
1:G:41:ARG:O	1:G:70:SER:N	2.44	0.51
6:P:258:GLY:O	6:P:260:CYS:N	2.43	0.51
1:A:112:GLU:O	1:A:141:MET:HA	2.11	0.51
1:G:42:PRO:HA	1:G:69:LEU:HA	1.92	0.51
14:g:552:TRP:HA	14:g:561:PRO:HA	1.93	0.51
13:m:75:HIS:O	13:m:120:LYS:N	2.44	0.51
13:e:157:VAL:O	13:e:161:PHE:N	2.31	0.50
1:C:162:ASP:HA	16:C:800:ADP:H4'	1.91	0.50
1:G:200:LYS:O	2:H:112:PRO:HA	2.11	0.50
6:Q:183:LEU:O	6:Q:187:LYS:N	2.44	0.50
9:V:33:ASN:H	12:d:342:ALA:C	2.17	0.50
13:e:332:TYR:O	13:e:336:MET:N	2.38	0.50
1:A:19:GLY:O	1:A:37:ASN:N	2.36	0.50
1:B:112:GLU:O	1:B:141:MET:HA	2.11	0.50
1:C:40:GLY:N	1:C:57:PHE:O	2.41	0.50
1:I:110:LEU:N	1:I:138:PHE:O	2.44	0.50
14:o:445:ASN:O	14:o:461:ARG:N	2.39	0.50
13:m:39:PRO:O	13:m:46:GLY:N	2.42	0.50
1:D:20:VAL:HA	1:D:36:PRO:HA	1.94	0.50
3:J:92:ILE:HA	3:J:121:ALA:HB3	1.93	0.50
5:L:108:ARG:O	5:L:113:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:O	1:C:203:TYR:N	2.40	0.50
2:H:237:GLU:HA	2:H:251:GLY:HA2	1.93	0.50
9:V:71:PRO:CB	9:V:84:PRO:HA	2.42	0.50
3:J:93:GLU:N	3:J:121:ALA:O	2.32	0.49
5:L:70:SER:HA	5:L:80:ASP:O	2.12	0.49
11:Y:111:CYS:N	11:Y:116:TRP:O	2.45	0.49
1:F:96:LYS:HA	1:F:100:GLN:CB	2.42	0.49
1:F:266:ASP:C	1:F:269:GLY:H	2.20	0.49
3:J:186:ASP:N	3:J:255:ILE:O	2.45	0.49
14:g:280:ARG:O	14:g:592:GLY:N	2.44	0.49
14:h:282:VAL:HA	14:h:298:SER:O	2.11	0.49
13:m:149:LEU:O	13:m:153:ILE:N	2.34	0.49
13:m:437:ILE:O	13:m:441:LYS:N	2.45	0.49
1:I:371:ILE:O	1:I:375:THR:N	2.45	0.49
11:Y:107:TYR:HA	12:b:284:GLY:C	2.37	0.49
13:m:132:SER:H	13:n:41:LEU:C	2.20	0.49
1:F:45:VAL:O	2:H:170:ALA:N	2.44	0.49
2:H:219:VAL:N	2:H:307:PRO:O	2.42	0.49
3:J:378:TYR:O	3:J:382:GLY:N	2.41	0.49
14:o:401:ILE:HA	14:o:406:LYS:O	2.13	0.49
1:E:19:GLY:O	1:E:37:ASN:N	2.29	0.49
1:F:149:ALA:HB2	1:F:339:SER:O	2.12	0.49
2:H:42:GLY:HA3	3:J:387:TRP:HA	1.93	0.49
5:L:73:SER:O	5:L:77:ASN:N	2.46	0.49
5:L:138:GLY:HA3	5:L:146:GLY:H	1.77	0.49
11:Y:127:SER:O	12:b:277:GLU:HA	2.11	0.49
1:C:21:ILE:O	1:C:34:CYS:HA	2.13	0.49
1:I:238:LYS:HA	1:I:252:GLY:N	2.27	0.49
2:H:370:VAL:O	2:H:374:CYS:N	2.46	0.49
14:p:267:LEU:HA	14:p:597:TYR:HA	1.95	0.49
1:A:98:GLN:O	1:A:100:GLN:N	2.46	0.49
1:F:330:ILE:N	6:N:20:TYR:O	2.46	0.49
2:H:124:PHE:O	2:H:128:ASN:HA	2.13	0.49
1:B:161:GLY:O	1:B:186:ALA:HB1	2.12	0.49
1:I:170:ILE:HA	1:I:175:ALA:HA	1.95	0.49
13:e:435:ARG:HA	13:e:448:MET:H	1.77	0.49
14:p:359:LEU:N	14:p:371:GLN:O	2.43	0.49
1:D:361:LYS:O	1:D:364:GLU:N	2.46	0.48
11:Y:107:TYR:HA	12:b:284:GLY:HA3	1.95	0.48
12:c:307:LEU:HA	12:d:307:LEU:HA	1.94	0.48
13:m:666:GLU:O	13:m:670:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLY:O	1:C:37:ASN:N	2.38	0.48
1:D:266:ASP:C	1:D:269:GLY:H	2.20	0.48
1:F:330:ILE:O	6:N:19:VAL:HA	2.12	0.48
1:I:18:SER:N	16:I:800:ADP:O3B	2.32	0.48
13:n:666:GLU:O	13:n:670:GLY:N	2.46	0.48
11:Y:11:LEU:O	11:Y:458:VAL:HA	2.13	0.48
14:h:359:LEU:O	14:h:370:VAL:N	2.46	0.48
3:J:41:SER:O	3:J:54:VAL:N	2.34	0.48
4:K:94:ILE:HA	4:K:110:PRO:HA	1.95	0.48
1:C:41:ARG:HA	1:C:55:ASP:O	2.14	0.48
11:Y:43:SER:H	11:Y:284:CYS:HA	1.78	0.48
1:B:335:GLU:O	1:B:339:SER:N	2.46	0.48
1:D:370:SER:O	1:D:374:LYS:N	2.43	0.48
1:G:161:GLY:O	1:G:186:ALA:HB1	2.13	0.48
11:Y:107:TYR:CB	12:b:284:GLY:N	2.77	0.48
13:n:75:HIS:O	13:n:120:LYS:N	2.47	0.48
1:A:266:ASP:C	1:A:269:GLY:H	2.22	0.48
1:F:40:GLY:O	1:F:57:PHE:N	2.45	0.48
13:e:435:ARG:HA	13:e:448:MET:N	2.28	0.48
13:m:747:SER:HA	13:m:768:ALA:HB1	1.95	0.48
2:H:132:MET:O	2:H:357:ILE:N	2.28	0.48
13:n:58:GLU:O	13:n:62:LEU:N	2.32	0.48
4:K:47:ARG:HA	4:K:50:ALA:HB3	1.95	0.48
9:V:35:VAL:O	9:V:56:ARG:HA	2.13	0.48
11:Y:422:VAL:O	11:Y:462:LEU:N	2.47	0.48
13:f:80:GLU:N	13:f:102:ASN:O	2.40	0.48
14:h:285:LEU:HA	14:h:296:VAL:O	2.13	0.48
13:m:137:VAL:O	13:n:139:THR:N	2.46	0.48
1:D:75:MET:HA	1:D:80:VAL:HA	1.96	0.47
3:J:349:LYS:O	3:J:352:CYS:N	2.47	0.47
12:b:166:TRP:O	12:b:169:ARG:N	2.47	0.47
1:A:318:VAL:O	1:A:322:ALA:N	2.43	0.47
1:B:129:PHE:O	1:B:133:ASN:HA	2.15	0.47
6:P:250:ASN:O	6:P:254:ALA:N	2.46	0.47
1:D:239:ALA:O	1:D:250:GLU:HA	2.14	0.47
1:G:18:SER:N	16:G:800:ADP:O3B	2.34	0.47
2:H:72:GLU:O	2:H:75:ILE:N	2.41	0.47
3:J:308:GLY:H	16:J:800:ADP:H5'1	1.80	0.47
13:n:748:LYS:O	13:n:752:ASN:N	2.45	0.47
1:A:104:GLU:HA	1:A:133:ASN:O	2.14	0.47
1:C:238:LYS:HA	1:C:252:GLY:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LEU:O	1:E:203:TYR:N	2.45	0.47
14:g:410:TRP:HA	14:g:419:GLN:H	1.79	0.47
13:e:349:GLU:O	13:e:353:ILE:N	2.41	0.47
13:m:219:GLN:O	13:m:223:ARG:N	2.39	0.47
1:B:8:ALA:HB1	1:B:105:GLU:O	2.15	0.47
1:B:318:VAL:O	1:B:322:ALA:N	2.26	0.47
1:G:103:SER:O	1:G:134:VAL:HA	2.14	0.47
4:K:66:LYS:HA	4:K:73:GLN:HA	1.97	0.47
11:Y:435:LEU:H	11:Y:449:ALA:HB1	1.79	0.47
14:h:532:TRP:HA	14:h:540:PHE:CB	2.45	0.47
14:o:425:VAL:HA	14:o:431:ALA:HA	1.97	0.47
1:A:162:ASP:HA	16:A:800:ADP:H4'	1.97	0.47
13:m:220:CYS:O	13:m:225:GLU:N	2.35	0.47
14:p:311:GLY:O	14:p:330:HIS:HA	2.14	0.47
1:A:207:SER:O	1:A:211:PHE:N	2.46	0.47
1:D:57:PHE:C	1:D:62:ALA:HB2	2.40	0.47
1:I:330:ILE:O	6:M:20:TYR:N	2.47	0.47
8:U:82:MET:HA	8:U:99:MET:O	2.15	0.46
14:g:484:CYS:HA	14:g:497:PHE:HA	1.96	0.46
13:f:156:ALA:O	13:f:160:PHE:N	2.31	0.46
13:n:119:ILE:O	13:n:136:ARG:N	2.47	0.46
4:K:259:ARG:HA	5:L:112:PHE:HA	1.97	0.46
14:o:334:ALA:O	14:o:353:TYR:N	2.48	0.46
1:A:21:ILE:O	1:A:34:CYS:HA	2.15	0.46
1:B:238:LYS:HA	1:B:252:GLY:N	2.30	0.46
11:Y:250:THR:N	11:Y:264:ILE:O	2.44	0.46
1:A:224:LEU:N	1:A:308:LYS:O	2.21	0.46
1:E:161:GLY:O	1:E:186:ALA:HB1	2.14	0.46
1:A:40:GLY:O	1:A:57:PHE:N	2.47	0.46
1:D:158:LEU:O	1:D:301:SER:N	2.48	0.46
1:F:18:SER:N	16:F:800:ADP:O1A	2.49	0.46
3:J:22:GLU:N	16:J:800:ADP:O1B	2.49	0.46
6:Q:181:LEU:C	6:Q:183:LEU:H	2.24	0.46
1:G:57:PHE:O	1:G:62:ALA:HB2	2.16	0.46
14:h:341:ALA:HB3	14:h:344:HIS:O	2.16	0.46
13:n:169:GLY:O	13:n:173:ARG:N	2.48	0.46
13:n:539:SER:O	13:n:543:THR:N	2.35	0.46
1:A:237:GLU:O	1:A:252:GLY:HA2	2.16	0.46
1:F:304:SER:N	16:F:800:ADP:O4'	2.48	0.46
2:H:71:ILE:HA	2:H:75:ILE:O	2.16	0.46
9:V:52:LEU:HA	12:d:340:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:N	1:D:138:PHE:O	2.37	0.46
1:D:198:LEU:O	1:D:203:TYR:N	2.47	0.46
1:G:238:LYS:HA	1:G:252:GLY:N	2.30	0.46
2:H:90:PHE:O	2:H:95:ARG:N	2.48	0.46
13:m:147:GLU:O	13:m:151:SER:N	2.33	0.46
13:n:121:ARG:H	13:n:134:GLN:C	2.24	0.46
7:O:114:ALA:O	7:O:118:ALA:N	2.49	0.46
13:n:837:ALA:O	13:n:841:PHE:N	2.31	0.46
11:Y:434:ASN:N	11:Y:449:ALA:HB1	2.31	0.45
13:n:67:LYS:O	13:n:71:ASP:N	2.49	0.45
1:D:156:VAL:O	1:D:299:VAL:N	2.46	0.45
1:E:153:THR:CB	1:E:172:GLU:HA	2.46	0.45
2:H:122:ILE:O	2:H:126:THR:N	2.49	0.45
1:I:145:LEU:O	1:I:343:GLY:HA3	2.16	0.45
1:A:57:PHE:C	1:A:62:ALA:HB2	2.42	0.45
1:B:91:GLN:O	1:B:95:SER:N	2.50	0.45
1:G:198:LEU:O	1:G:203:TYR:N	2.50	0.45
3:J:93:GLU:O	3:J:122:PRO:HA	2.16	0.45
3:J:343:ILE:O	11:Y:229:VAL:N	2.37	0.45
9:V:102:ALA:HB2	9:V:119:ARG:HA	1.97	0.45
14:g:330:HIS:N	14:g:367:ARG:O	2.27	0.45
13:n:674:GLU:HA	13:n:679:GLY:HA3	1.98	0.45
1:C:161:GLY:HA2	16:C:800:ADP:O3A	2.17	0.45
1:D:198:LEU:O	1:D:202:GLY:N	2.49	0.45
12:b:294:LEU:HA	12:b:297:GLU:H	1.81	0.45
1:C:11:PRO:HA	1:C:107:PRO:O	2.16	0.45
4:K:89:ASP:O	4:K:93:LYS:CA	2.63	0.45
12:a:163:GLU:O	12:a:166:TRP:N	2.46	0.45
1:F:161:GLY:O	1:F:186:ALA:HB1	2.16	0.45
1:I:17:GLY:HA3	1:I:20:VAL:O	2.16	0.45
1:I:161:GLY:O	1:I:186:ALA:HB1	2.17	0.45
10:Z:1126:ALA:O	10:Z:1130:ALA:N	2.48	0.45
13:n:220:CYS:O	13:n:225:GLU:N	2.33	0.45
1:F:41:ARG:HA	1:F:55:ASP:O	2.17	0.45
14:h:358:VAL:HA	14:h:372:ARG:HA	1.98	0.45
1:B:266:ASP:C	1:B:269:GLY:H	2.25	0.45
1:E:149:ALA:HB2	1:E:339:SER:O	2.17	0.45
2:H:106:THR:HA	2:H:135:ALA:O	2.17	0.45
1:A:161:GLY:O	1:A:186:ALA:HB1	2.16	0.45
1:B:239:ALA:O	1:B:250:GLU:HA	2.17	0.45
1:C:155:GLY:HA2	1:C:297:ASN:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:GLY:HA2	1:D:70:SER:O	2.16	0.45
1:E:304:SER:N	16:E:800:ADP:O4'	2.50	0.45
1:F:162:ASP:HA	16:F:800:ADP:H4'	1.98	0.45
6:P:298:ALA:O	6:P:302:ALA:N	2.50	0.45
13:m:210:HIS:O	13:m:213:ILE:N	2.49	0.45
14:o:438:SER:N	14:o:448:VAL:O	2.42	0.45
14:o:609:ASP:O	14:o:613:ARG:N	2.27	0.45
1:C:149:ALA:HB2	1:C:339:SER:O	2.17	0.45
1:D:74:PRO:O	1:D:81:LYS:N	2.50	0.45
2:H:369:ILE:O	2:H:373:LYS:N	2.45	0.45
13:e:211:PRO:O	13:e:213:ILE:N	2.44	0.45
13:n:526:ALA:HB1	13:n:553:TYR:HA	1.98	0.45
1:C:98:GLN:C	1:C:100:GLN:H	2.26	0.44
9:V:50:GLY:O	12:d:342:ALA:HA	2.17	0.44
9:V:60:HIS:O	9:V:90:HIS:HA	2.17	0.44
1:D:21:ILE:O	1:D:34:CYS:HA	2.17	0.44
1:D:145:LEU:O	1:D:343:GLY:HA3	2.16	0.44
1:D:153:THR:O	1:D:173:GLY:N	2.35	0.44
8:U:170:ILE:O	8:U:172:PRO:N	2.50	0.44
10:Z:1150:GLU:HA	10:Z:1153:ALA:HB3	1.98	0.44
14:h:456:VAL:O	14:h:472:PHE:N	2.47	0.44
13:n:678:GLU:O	13:n:682:LEU:N	2.51	0.44
1:B:57:PHE:C	1:B:62:ALA:HB2	2.43	0.44
3:J:143:TYR:O	3:J:168:GLY:N	2.50	0.44
9:V:33:ASN:C	12:d:344:SER:H	2.26	0.44
13:m:210:HIS:O	13:m:212:ILE:N	2.50	0.44
13:m:838:GLU:O	13:m:841:PHE:CB	2.64	0.44
8:U:43:ALA:HB1	8:U:47:PRO:HA	2.00	0.44
11:Y:107:TYR:HA	12:b:284:GLY:CA	2.47	0.44
1:C:104:GLU:HA	1:C:133:ASN:O	2.18	0.44
14:g:437:MET:HA	14:g:449:VAL:HA	2.00	0.44
14:h:410:TRP:HA	14:h:418:PRO:HA	2.00	0.44
14:o:460:CYS:O	14:o:467:GLY:N	2.33	0.44
1:B:18:SER:N	16:B:800:ADP:O1A	2.50	0.44
1:C:224:LEU:N	1:C:308:LYS:O	2.44	0.44
1:D:118:ARG:O	1:D:121:ARG:N	2.51	0.44
2:H:362:TYR:O	2:H:366:GLY:N	2.44	0.44
5:L:153:VAL:O	5:L:169:LEU:HA	2.18	0.44
11:Y:43:SER:CB	11:Y:283:ARG:O	2.66	0.44
1:A:96:LYS:HA	1:A:100:GLN:CB	2.48	0.44
3:J:329:LYS:O	3:J:333:LYS:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:124:LEU:N	5:L:128:PHE:HA	2.33	0.44
1:A:158:LEU:N	1:A:299:VAL:O	2.35	0.44
3:J:300:ALA:O	3:J:341:PHE:HA	2.17	0.44
12:c:300:GLY:HA2	12:d:300:GLY:HA2	2.00	0.44
14:g:277:SER:O	14:g:592:GLY:HA3	2.18	0.44
1:C:91:GLN:O	1:C:95:SER:N	2.51	0.43
1:F:328:ILE:O	6:N:21:GLU:HA	2.17	0.43
2:H:265:SER:C	2:H:268:GLY:H	2.26	0.43
14:h:568:GLU:C	14:h:570:ASN:H	2.26	0.43
1:B:200:LYS:O	1:C:117:PRO:HA	2.18	0.43
3:J:126:MET:O	3:J:357:GLY:HA3	2.18	0.43
11:Y:49:HIS:O	11:Y:57:ASN:HA	2.17	0.43
14:p:403:THR:O	14:p:433:ALA:HA	2.19	0.43
1:B:304:SER:N	16:B:800:ADP:O4'	2.51	0.43
1:D:98:GLN:C	1:D:100:GLN:H	2.26	0.43
1:D:108:VAL:N	1:D:136:ALA:O	2.34	0.43
11:Y:107:TYR:CA	12:b:284:GLY:HA3	2.48	0.43
12:d:335:ARG:C	12:d:337:LEU:H	2.27	0.43
1:D:238:LYS:HA	1:D:252:GLY:N	2.33	0.43
14:g:573:LEU:HA	14:g:589:ASP:HA	2.00	0.43
13:m:220:CYS:O	13:m:224:GLY:N	2.52	0.43
6:M:185:ALA:HB2	7:R:130:ALA:HB3	2.00	0.43
9:V:33:ASN:N	12:d:343:THR:N	2.54	0.43
14:g:391:GLY:HA3	14:g:396:HIS:HA	2.01	0.43
14:h:493:PHE:O	14:h:496:LEU:N	2.50	0.43
14:h:609:ASP:O	14:h:613:ARG:N	2.38	0.43
1:F:293:THR:O	1:F:297:ASN:N	2.33	0.43
1:D:19:GLY:O	1:D:37:ASN:N	2.37	0.43
3:J:296:ARG:O	3:J:300:ALA:N	2.44	0.43
12:a:163:GLU:O	12:a:164:GLY:C	2.61	0.43
1:D:160:SER:N	1:D:301:SER:O	2.35	0.43
1:E:158:LEU:O	1:E:301:SER:N	2.52	0.43
3:J:164:LEU:O	3:J:166:LEU:N	2.45	0.43
9:V:134:LEU:HA	9:V:151:GLY:HA3	2.00	0.43
14:h:457:TYR:HA	14:h:470:GLU:O	2.19	0.43
14:p:311:GLY:HA2	14:p:335:VAL:H	1.84	0.43
1:D:57:PHE:O	1:D:62:ALA:HB2	2.19	0.42
11:Y:344:THR:HA	11:Y:369:PRO:HA	1.99	0.42
15:j:426:GLU:C	15:j:430:ALA:H	2.27	0.42
14:p:401:ILE:HA	14:p:406:LYS:O	2.18	0.42
1:D:107:PRO:CB	1:D:136:ALA:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:519:ALA:HB1	13:e:560:VAL:HA	2.00	0.42
1:B:19:GLY:N	16:B:800:ADP:O1A	2.30	0.42
1:G:224:LEU:O	1:G:309:GLY:HA3	2.20	0.42
1:I:243:LEU:N	1:I:247:SER:O	2.35	0.42
11:Y:435:LEU:H	11:Y:449:ALA:CB	2.32	0.42
13:f:539:SER:O	13:f:543:THR:N	2.38	0.42
1:B:149:ALA:HB2	1:B:343:GLY:N	2.34	0.42
1:B:238:LYS:HA	1:B:252:GLY:CA	2.48	0.42
1:F:145:LEU:O	1:F:343:GLY:HA3	2.19	0.42
1:I:104:GLU:HA	1:I:133:ASN:C	2.44	0.42
1:I:149:ALA:HB2	1:I:339:SER:O	2.19	0.42
14:g:480:THR:H	14:g:501:SER:HA	1.84	0.42
1:C:207:SER:O	1:C:211:PHE:N	2.49	0.42
2:H:239:SER:HA	2:H:248:ILE:O	2.18	0.42
6:M:261:LEU:N	7:O:21:VAL:O	2.52	0.42
14:g:359:LEU:N	14:g:371:GLN:O	2.52	0.42
14:g:439:PHE:HA	14:g:447:PHE:HA	2.02	0.42
4:K:24:ALA:HB1	4:K:29:PHE:HA	2.02	0.42
14:h:281:VAL:O	14:h:299:TYR:HA	2.20	0.42
1:D:304:SER:N	16:D:800:ADP:O4'	2.53	0.42
1:E:222:CYS:HA	1:E:255:ARG:O	2.20	0.42
3:J:110:PHE:O	3:J:114:GLU:HA	2.20	0.42
6:M:347:ALA:HB1	7:O:115:HIS:C	2.44	0.42
11:Y:326:TYR:HA	11:Y:415:PRO:O	2.20	0.42
13:n:117:ALA:H	13:n:138:LEU:C	2.28	0.42
14:o:408:CYS:HA	14:o:420:ASP:O	2.19	0.42
14:o:458:THR:O	14:o:469:SER:N	2.39	0.42
12:b:302:ASP:O	12:b:303:LYS:C	2.62	0.42
3:J:274:ASP:C	3:J:276:GLU:H	2.27	0.42
3:J:287:SER:O	3:J:291:CYS:N	2.53	0.42
1:D:328:ILE:O	6:P:22:THR:N	2.32	0.41
8:U:15:ALA:N	8:U:31:PRO:O	2.53	0.41
8:U:52:GLU:O	8:U:86:THR:HA	2.19	0.41
13:e:283:ARG:N	13:f:176:ASP:H	2.17	0.41
1:C:238:LYS:HA	1:C:252:GLY:N	2.34	0.41
1:F:147:LEU:O	1:F:151:GLY:N	2.53	0.41
13:m:304:LEU:O	13:m:308:LYS:N	2.52	0.41
13:n:343:ASP:O	13:n:347:ALA:N	2.51	0.41
1:B:45:VAL:O	1:D:174:PHE:HA	2.20	0.41
1:E:223:TYR:O	1:E:256:PHE:HA	2.20	0.41
1:G:109:LEU:HA	1:G:138:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:107:TYR:CB	12:b:281:LEU:C	2.92	0.41
13:e:535:GLY:HA2	13:e:546:TRP:HA	2.02	0.41
1:E:57:PHE:O	1:E:62:ALA:HB2	2.21	0.41
1:I:200:LYS:O	3:J:98:PRO:HA	2.20	0.41
13:e:210:HIS:O	13:e:214:THR:N	2.49	0.41
13:f:632:ALA:O	13:f:636:SER:N	2.50	0.41
14:h:283:SER:CB	14:h:336:MET:HA	2.51	0.41
1:A:40:GLY:N	1:A:57:PHE:O	2.43	0.41
1:C:40:GLY:O	1:C:57:PHE:N	2.53	0.41
1:E:242:TYR:HA	1:E:247:SER:O	2.21	0.41
1:F:98:GLN:O	1:F:100:GLN:N	2.53	0.41
7:O:16:GLU:O	7:O:20:TRP:N	2.54	0.41
8:U:169:LYS:O	12:b:306:GLN:N	2.52	0.41
13:e:753:LEU:O	13:e:758:PHE:N	2.53	0.41
13:n:530:VAL:HA	13:n:549:ALA:HB1	2.01	0.41
1:B:108:VAL:O	1:B:137:LEU:HA	2.21	0.41
1:B:224:LEU:O	1:B:309:GLY:HA3	2.21	0.41
1:F:303:GLY:HA3	16:F:800:ADP:H5'1	2.02	0.41
14:o:403:THR:O	14:o:433:ALA:HA	2.21	0.41
5:L:80:ASP:HA	5:L:81:PRO:C	2.45	0.41
14:o:359:LEU:O	14:o:370:VAL:N	2.53	0.41
14:p:504:TRP:HA	14:p:525:ASP:O	2.21	0.41
1:A:240:GLN:HA	1:A:250:GLU:HA	2.03	0.41
1:B:98:GLN:C	1:B:100:GLN:H	2.29	0.41
1:B:224:LEU:N	1:B:308:LYS:O	2.50	0.41
1:C:20:VAL:HA	1:C:36:PRO:HA	2.03	0.41
1:C:266:ASP:C	1:C:269:GLY:H	2.29	0.41
1:C:373:ARG:HA	6:Q:69:LEU:C	2.46	0.41
1:D:149:ALA:HB2	1:D:339:SER:O	2.20	0.41
1:G:219:GLU:HA	16:G:800:ADP:C2	2.55	0.41
1:I:107:PRO:CB	1:I:136:ALA:HB3	2.51	0.41
3:J:74:ILE:O	3:J:78:ARG:N	2.51	0.41
4:K:143:VAL:HA	4:K:155:ILE:O	2.21	0.41
6:M:325:PRO:O	10:Z:1121:GLY:HA3	2.20	0.41
11:Y:78:GLY:HA2	11:Y:254:GLN:CB	2.51	0.41
14:h:487:ALA:HB3	14:h:537:PRO:HA	2.03	0.41
2:H:104:LEU:HA	2:H:133:TYR:O	2.21	0.41
9:V:33:ASN:N	12:d:342:ALA:N	2.68	0.41
1:F:237:GLU:O	1:F:252:GLY:HA2	2.21	0.40
12:c:159:PHE:O	12:c:162:ARG:N	2.54	0.40
1:D:75:MET:HA	1:D:81:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:VAL:O	1:G:174:PHE:HA	2.22	0.40
1:E:330:ILE:O	6:Q:19:VAL:HA	2.21	0.40
1:I:104:GLU:HA	1:I:133:ASN:O	2.21	0.40
1:I:110:LEU:O	1:I:140:SER:N	2.54	0.40
10:Z:1141:LEU:O	10:Z:1145:GLU:N	2.55	0.40
13:f:38:VAL:O	13:f:42:LEU:N	2.40	0.40
13:f:829:LEU:O	13:f:833:VAL:N	2.33	0.40
13:m:349:GLU:O	13:m:353:ILE:N	2.49	0.40
14:p:280:ARG:O	14:p:592:GLY:N	2.54	0.40
1:B:19:GLY:O	1:B:37:ASN:N	2.46	0.40
9:V:16:THR:HA	9:V:21:LYS:HA	2.03	0.40
13:n:373:PRO:O	13:n:377:ALA:N	2.42	0.40
2:H:89:THR:O	2:H:94:LEU:N	2.27	0.40
3:J:297:LYS:O	3:J:300:ALA:HB3	2.20	0.40
9:V:33:ASN:N	12:d:342:ALA:H	2.19	0.40
13:m:635:MET:O	13:m:639:ARG:N	2.46	0.40
1:A:107:PRO:CB	1:A:136:ALA:HB3	2.51	0.40
1:E:266:ASP:C	1:E:269:GLY:H	2.28	0.40
1:F:371:ILE:O	1:F:375:THR:N	2.55	0.40
1:G:238:LYS:HA	1:G:252:GLY:CA	2.52	0.40
8:U:122:GLY:HA2	8:U:158:GLN:H	1.86	0.40
11:Y:28:TYR:HA	11:Y:309:ALA:H	1.86	0.40
13:f:116:LEU:HA	13:f:139:THR:HA	2.03	0.40
14:p:337:SER:O	14:p:350:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	368/376 (98%)	347 (94%)	21 (6%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
1	C	373/376 (99%)	354 (95%)	19 (5%)	0	100	100
1	D	368/376 (98%)	350 (95%)	18 (5%)	0	100	100
1	E	368/376 (98%)	348 (95%)	20 (5%)	0	100	100
1	F	368/376 (98%)	344 (94%)	24 (6%)	0	100	100
1	G	368/376 (98%)	350 (95%)	18 (5%)	0	100	100
1	I	368/376 (98%)	346 (94%)	22 (6%)	0	100	100
2	H	368/375 (98%)	346 (94%)	22 (6%)	0	100	100
3	J	377/417 (90%)	349 (93%)	28 (7%)	0	100	100
4	K	276/286 (96%)	261 (95%)	15 (5%)	0	100	100
5	L	267/272 (98%)	252 (94%)	15 (6%)	0	100	100
6	M	330/405 (82%)	310 (94%)	19 (6%)	1 (0%)	36	72
6	N	270/405 (67%)	258 (96%)	12 (4%)	0	100	100
6	P	319/405 (79%)	308 (97%)	11 (3%)	0	100	100
6	Q	335/405 (83%)	322 (96%)	13 (4%)	0	100	100
7	O	177/186 (95%)	169 (96%)	8 (4%)	0	100	100
7	R	168/186 (90%)	158 (94%)	10 (6%)	0	100	100
8	U	165/190 (87%)	146 (88%)	19 (12%)	0	100	100
9	V	177/182 (97%)	153 (86%)	23 (13%)	1 (1%)	21	59
10	W	144/1281 (11%)	135 (94%)	8 (6%)	1 (1%)	18	56
10	Z	190/1281 (15%)	179 (94%)	11 (6%)	0	100	100
11	Y	404/467 (86%)	358 (89%)	44 (11%)	2 (0%)	24	63
12	a	205/577 (36%)	203 (99%)	2 (1%)	0	100	100
12	b	205/577 (36%)	198 (97%)	6 (3%)	1 (0%)	24	63
12	c	238/577 (41%)	234 (98%)	4 (2%)	0	100	100
12	d	267/577 (46%)	256 (96%)	11 (4%)	0	100	100
13	e	792/4646 (17%)	748 (94%)	44 (6%)	0	100	100
13	f	804/4646 (17%)	757 (94%)	45 (6%)	2 (0%)	43	78
13	m	786/4646 (17%)	751 (96%)	35 (4%)	0	100	100
13	n	747/4646 (16%)	714 (96%)	32 (4%)	1 (0%)	48	83
14	g	356/612 (58%)	348 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	h	356/612 (58%)	335 (94%)	21 (6%)	0	100	100
14	o	356/612 (58%)	333 (94%)	23 (6%)	0	100	100
14	p	356/612 (58%)	337 (95%)	19 (5%)	0	100	100
15	j	12/492 (2%)	12 (100%)	0	0	100	100
15	q	12/492 (2%)	12 (100%)	0	0	100	100
All	All	12408/34075 (36%)	11734 (95%)	665 (5%)	9 (0%)	49	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
10	W	1142	PRO
11	Y	175	PRO
11	Y	441	PRO
12	b	166	TRP
13	f	38	VAL
13	f	203	PRO
13	n	21	VAL
9	V	75	LYS

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	ATP	H	401	-	32,33,33	0.52	1 (3%)	48,52,52	0.35	0
16	ADP	C	800	-	28,29,29	1.37	5 (17%)	43,45,45	1.78	8 (18%)
16	ADP	I	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.85	10 (23%)
16	ADP	E	800	-	28,29,29	1.40	5 (17%)	43,45,45	1.83	11 (25%)
16	ADP	J	800	-	28,29,29	1.42	6 (21%)	43,45,45	1.83	11 (25%)
16	ADP	G	800	-	28,29,29	1.38	4 (14%)	43,45,45	1.85	12 (27%)
16	ADP	B	800	-	28,29,29	1.38	4 (14%)	43,45,45	1.81	8 (18%)
16	ADP	A	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	8 (18%)
16	ADP	F	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	10 (23%)
16	ADP	D	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ATP	H	401	-	-	10/22/38/38	0/3/3/3
16	ADP	C	800	-	-	3/16/32/32	0/3/3/3
16	ADP	I	800	-	-	0/16/32/32	0/3/3/3
16	ADP	E	800	-	-	1/16/32/32	0/3/3/3
16	ADP	J	800	-	-	7/16/32/32	0/3/3/3
16	ADP	G	800	-	-	0/16/32/32	0/3/3/3
16	ADP	B	800	-	-	1/16/32/32	0/3/3/3
16	ADP	A	800	-	-	0/16/32/32	0/3/3/3
16	ADP	F	800	-	-	3/16/32/32	0/3/3/3
16	ADP	D	800	-	-	7/16/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	800	ADP	C5-C4	4.67	1.47	1.39
16	D	800	ADP	C5-C4	4.66	1.47	1.39
16	F	800	ADP	C5-C4	4.64	1.47	1.39
16	A	800	ADP	C5-C4	4.62	1.47	1.39
16	I	800	ADP	C5-C4	4.58	1.47	1.39
16	B	800	ADP	C5-C4	4.56	1.47	1.39
16	C	800	ADP	C5-C4	4.55	1.47	1.39
16	G	800	ADP	C5-C4	4.53	1.47	1.39
16	J	800	ADP	C5-C4	4.51	1.47	1.39
16	I	800	ADP	C5-C6	2.74	1.48	1.41
16	A	800	ADP	C5-C6	2.72	1.48	1.41
16	F	800	ADP	C5-C6	2.71	1.48	1.41
16	G	800	ADP	C5-C6	2.71	1.48	1.41
16	D	800	ADP	C5-C6	2.71	1.48	1.41
16	J	800	ADP	C5-C6	2.68	1.48	1.41
16	E	800	ADP	C5-C6	2.66	1.48	1.41
16	B	800	ADP	C5-C6	2.65	1.48	1.41
16	C	800	ADP	C5-C6	2.62	1.48	1.41
16	J	800	ADP	C8-N7	2.41	1.36	1.31
16	C	800	ADP	C5-N7	-2.38	1.34	1.39
16	B	800	ADP	C5-N7	-2.37	1.34	1.39
16	A	800	ADP	C5-N7	-2.36	1.34	1.39
16	E	800	ADP	C5-N7	-2.35	1.34	1.39
16	G	800	ADP	C8-N7	2.33	1.36	1.31
16	G	800	ADP	C5-N7	-2.33	1.34	1.39
16	D	800	ADP	C5-N7	-2.32	1.34	1.39
16	F	800	ADP	C5-N7	-2.31	1.34	1.39
16	I	800	ADP	C5-N7	-2.30	1.34	1.39
16	F	800	ADP	C8-N7	2.29	1.36	1.31
16	E	800	ADP	C8-N7	2.25	1.36	1.31
16	A	800	ADP	C8-N7	2.24	1.36	1.31
16	I	800	ADP	C8-N7	2.24	1.36	1.31
16	D	800	ADP	C8-N7	2.24	1.36	1.31
17	H	401	ATP	PB-O3B	-2.22	1.57	1.59
16	J	800	ADP	C5-N7	-2.21	1.35	1.39
16	B	800	ADP	C8-N7	2.19	1.35	1.31
16	C	800	ADP	C8-N7	2.18	1.35	1.31
16	J	800	ADP	C4-N9	-2.12	1.33	1.37
16	C	800	ADP	C4-N9	-2.11	1.33	1.37
16	E	800	ADP	C4-N9	-2.01	1.33	1.37
16	J	800	ADP	PA-O3A	2.00	1.61	1.59

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	800	ADP	C5-C4-N3	-6.10	118.32	126.72
16	F	800	ADP	C5-C4-N3	-6.03	118.42	126.72
16	D	800	ADP	C5-C4-N3	-5.99	118.47	126.72
16	A	800	ADP	C5-C4-N3	-5.94	118.54	126.72
16	B	800	ADP	C5-C4-N3	-5.89	118.60	126.72
16	E	800	ADP	C5-C4-N3	-5.88	118.62	126.72
16	G	800	ADP	C5-C4-N3	-5.85	118.67	126.72
16	C	800	ADP	C5-C4-N3	-5.78	118.77	126.72
16	J	800	ADP	C5-C4-N3	-5.41	119.27	126.72
16	I	800	ADP	N3-C4-N9	4.79	135.31	127.17
16	F	800	ADP	N3-C4-N9	4.70	135.16	127.17
16	A	800	ADP	N3-C4-N9	4.65	135.07	127.17
16	C	800	ADP	N3-C4-N9	4.63	135.05	127.17
16	E	800	ADP	N3-C4-N9	4.63	135.04	127.17
16	B	800	ADP	N3-C4-N9	4.62	135.03	127.17
16	D	800	ADP	N3-C4-N9	4.61	135.02	127.17
16	G	800	ADP	N3-C4-N9	4.52	134.86	127.17
16	J	800	ADP	N3-C4-N9	4.22	134.35	127.17
16	G	800	ADP	C4-C5-N7	-3.71	106.34	110.58
16	F	800	ADP	C4-C5-N7	-3.65	106.41	110.58
16	J	800	ADP	C2-N3-C4	3.62	120.67	111.83
16	D	800	ADP	C4-C5-N7	-3.62	106.45	110.58
16	E	800	ADP	C4-C5-N7	-3.61	106.45	110.58
16	I	800	ADP	C2-N3-C4	3.61	120.64	111.83
16	I	800	ADP	C4-C5-N7	-3.58	106.49	110.58
16	D	800	ADP	C2-N3-C4	3.54	120.47	111.83
16	A	800	ADP	C2-N3-C4	3.52	120.44	111.83
16	J	800	ADP	C4-C5-N7	-3.49	106.59	110.58
16	B	800	ADP	C2-N3-C4	3.48	120.32	111.83
16	B	800	ADP	C4-C5-N7	-3.46	106.62	110.58
16	F	800	ADP	C2-N3-C4	3.46	120.28	111.83
16	A	800	ADP	C4-C5-N7	-3.46	106.63	110.58
16	G	800	ADP	C2-N3-C4	3.43	120.22	111.83
16	E	800	ADP	C2-N3-C4	3.41	120.16	111.83
16	J	800	ADP	N3-C2-N1	-3.39	123.45	128.58
16	C	800	ADP	C4-C5-N7	-3.36	106.75	110.58
16	C	800	ADP	C2-N3-C4	3.33	119.96	111.83
16	A	800	ADP	C2'-C1'-N9	-3.23	105.28	113.30
16	J	800	ADP	C4-N9-C8	3.00	108.88	105.74
16	B	800	ADP	C2'-C1'-N9	-2.86	106.21	113.30
16	C	800	ADP	C4-N9-C8	2.80	108.68	105.74
16	D	800	ADP	C2'-C1'-N9	-2.80	106.35	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	800	ADP	C4-N9-C8	2.77	108.64	105.74
16	E	800	ADP	C4-N9-C8	2.76	108.64	105.74
16	I	800	ADP	C4-N9-C8	2.69	108.56	105.74
16	G	800	ADP	C5-N7-C8	2.69	107.68	103.45
16	F	800	ADP	C5-N7-C8	2.67	107.64	103.45
16	F	800	ADP	C4-N9-C8	2.65	108.52	105.74
16	A	800	ADP	N3-C2-N1	-2.64	124.58	128.58
16	D	800	ADP	N3-C2-N1	-2.62	124.61	128.58
16	I	800	ADP	N3-C2-N1	-2.60	124.64	128.58
16	E	800	ADP	C5-N7-C8	2.60	107.54	103.45
16	J	800	ADP	C5-N7-C8	2.59	107.52	103.45
16	B	800	ADP	C4-N9-C8	2.57	108.44	105.74
16	I	800	ADP	C5-N7-C8	2.56	107.48	103.45
16	D	800	ADP	C5-N7-C8	2.55	107.46	103.45
16	B	800	ADP	N3-C2-N1	-2.54	124.73	128.58
16	B	800	ADP	C5-N7-C8	2.51	107.40	103.45
16	F	800	ADP	C2'-C1'-N9	-2.51	107.07	113.30
16	A	800	ADP	C4-N9-C8	2.50	108.36	105.74
16	A	800	ADP	C5-N7-C8	2.47	107.33	103.45
16	D	800	ADP	C4-N9-C8	2.44	108.31	105.74
16	G	800	ADP	N3-C2-N1	-2.44	124.89	128.58
16	C	800	ADP	C5-N7-C8	2.43	107.27	103.45
16	E	800	ADP	N3-C2-N1	-2.39	124.96	128.58
16	F	800	ADP	N3-C2-N1	-2.34	125.04	128.58
16	J	800	ADP	C6-C5-N7	2.34	136.60	132.09
16	G	800	ADP	C3'-C2'-C1'	2.34	105.88	101.46
16	J	800	ADP	N9-C8-N7	-2.32	110.65	113.94
16	C	800	ADP	N3-C2-N1	-2.28	125.14	128.58
16	C	800	ADP	C2'-C1'-N9	-2.27	107.67	113.30
16	J	800	ADP	C3'-C2'-C1'	2.25	105.71	101.46
16	I	800	ADP	C3'-C2'-C1'	2.19	105.61	101.46
16	G	800	ADP	N9-C8-N7	-2.17	110.86	113.94
16	G	800	ADP	C6-C5-N7	2.16	136.26	132.09
16	E	800	ADP	C2'-C1'-N9	-2.08	108.13	113.30
16	F	800	ADP	N9-C8-N7	-2.06	111.01	113.94
16	E	800	ADP	C3'-C2'-C1'	2.06	105.36	101.46
16	E	800	ADP	C6-C5-N7	2.05	136.05	132.09
16	G	800	ADP	O3B-PB-O2B	2.05	115.49	107.80
16	E	800	ADP	N9-C8-N7	-2.05	111.03	113.94
16	D	800	ADP	C6-C5-N7	2.02	135.99	132.09
16	F	800	ADP	C6-C5-N7	2.02	135.99	132.09
16	G	800	ADP	C2'-C1'-N9	-2.02	108.29	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	800	ADP	C6-C5-N7	2.01	135.97	132.09
16	J	800	ADP	C2-N1-C6	2.00	122.02	118.73
16	I	800	ADP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	800	ADP	C5'-O5'-PA-O3A
16	C	800	ADP	C5'-O5'-PA-O3A
16	D	800	ADP	PA-O3A-PB-O2B
16	D	800	ADP	PA-O3A-PB-O3B
16	D	800	ADP	C5'-O5'-PA-O2A
16	D	800	ADP	C5'-O5'-PA-O3A
16	F	800	ADP	C5'-O5'-PA-O1A
16	F	800	ADP	C5'-O5'-PA-O2A
16	J	800	ADP	PA-O3A-PB-O3B
16	J	800	ADP	C5'-O5'-PA-O1A
16	J	800	ADP	C5'-O5'-PA-O2A
16	J	800	ADP	C5'-O5'-PA-O3A
17	H	401	ATP	C5'-O5'-PA-O1A
17	H	401	ATP	C5'-O5'-PA-O2A
17	H	401	ATP	C5'-O5'-PA-O3A
17	H	401	ATP	O4'-C4'-C5'-O5'
17	H	401	ATP	C3'-C4'-C5'-O5'
16	J	800	ADP	O4'-C4'-C5'-O5'
16	J	800	ADP	C3'-C4'-C5'-O5'
17	H	401	ATP	PB-O3B-PG-O1G
17	H	401	ATP	PB-O3A-PA-O1A
17	H	401	ATP	PB-O3B-PG-O2G
16	C	800	ADP	C5'-O5'-PA-O1A
16	D	800	ADP	C5'-O5'-PA-O1A
16	F	800	ADP	C5'-O5'-PA-O3A
17	H	401	ATP	PA-O3A-PB-O2B
16	E	800	ADP	O4'-C4'-C5'-O5'
17	H	401	ATP	PB-O3A-PA-O5'
16	J	800	ADP	PA-O3A-PB-O2B
16	D	800	ADP	O4'-C4'-C5'-O5'
16	D	800	ADP	PA-O3A-PB-O1B
16	C	800	ADP	PB-O3A-PA-O1A

There are no ring outliers.

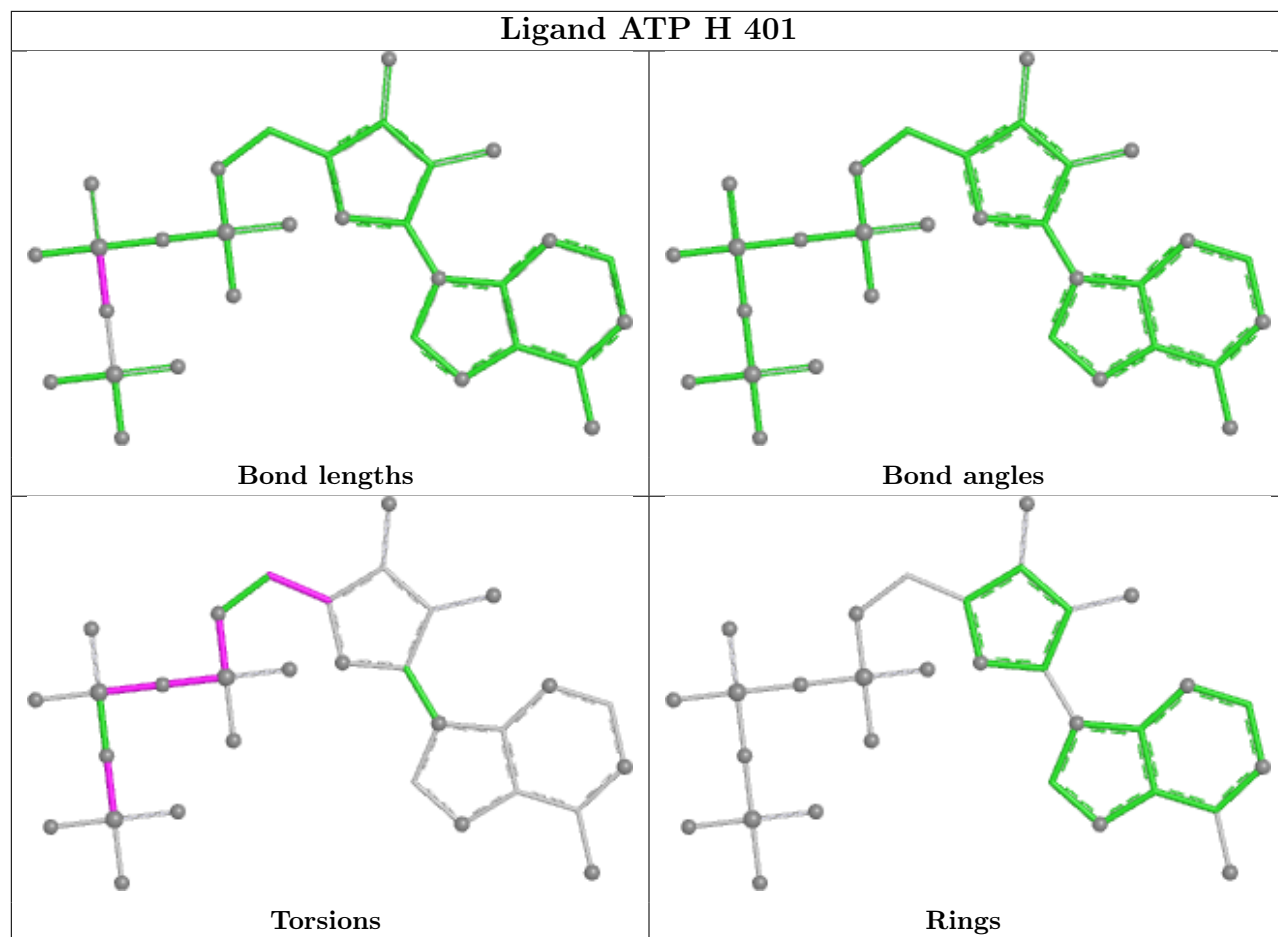


10 monomers are involved in 27 short contacts:

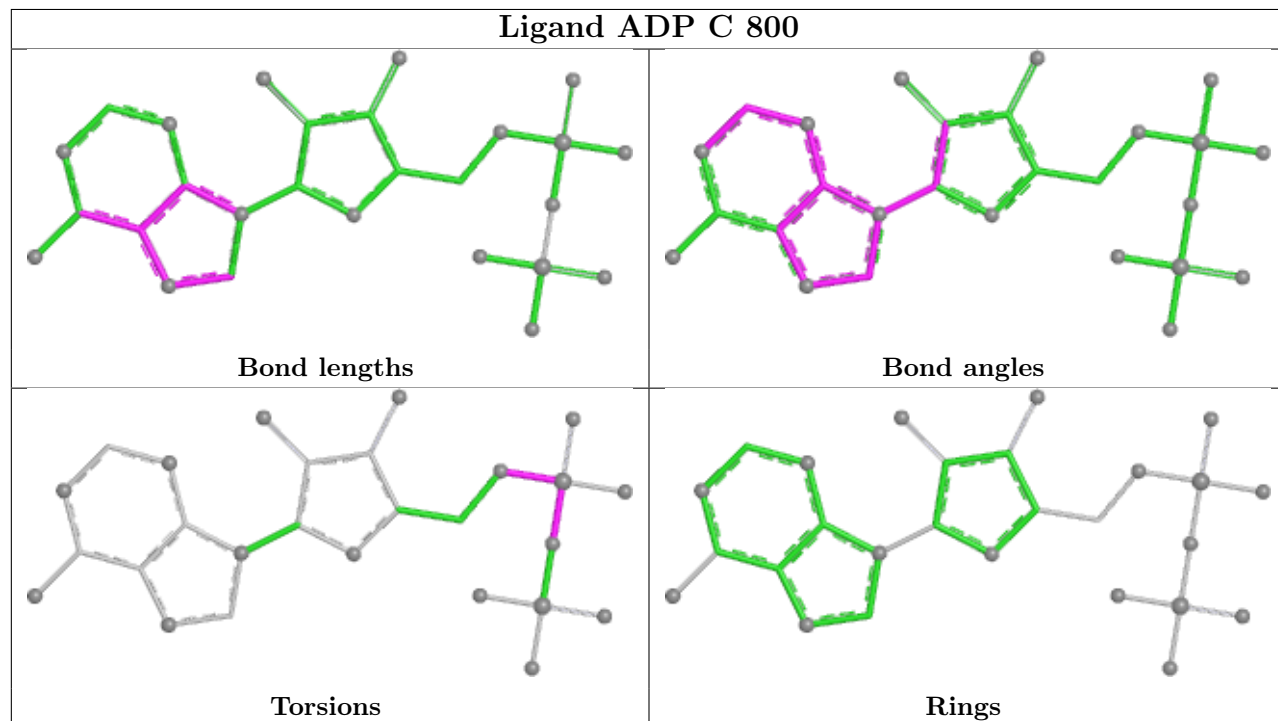
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	401	ATP	3	0
16	C	800	ADP	2	0
16	I	800	ADP	1	0
16	E	800	ADP	2	0
16	J	800	ADP	5	0
16	G	800	ADP	2	0
16	B	800	ADP	3	0
16	A	800	ADP	1	0
16	F	800	ADP	5	0
16	D	800	ADP	3	0

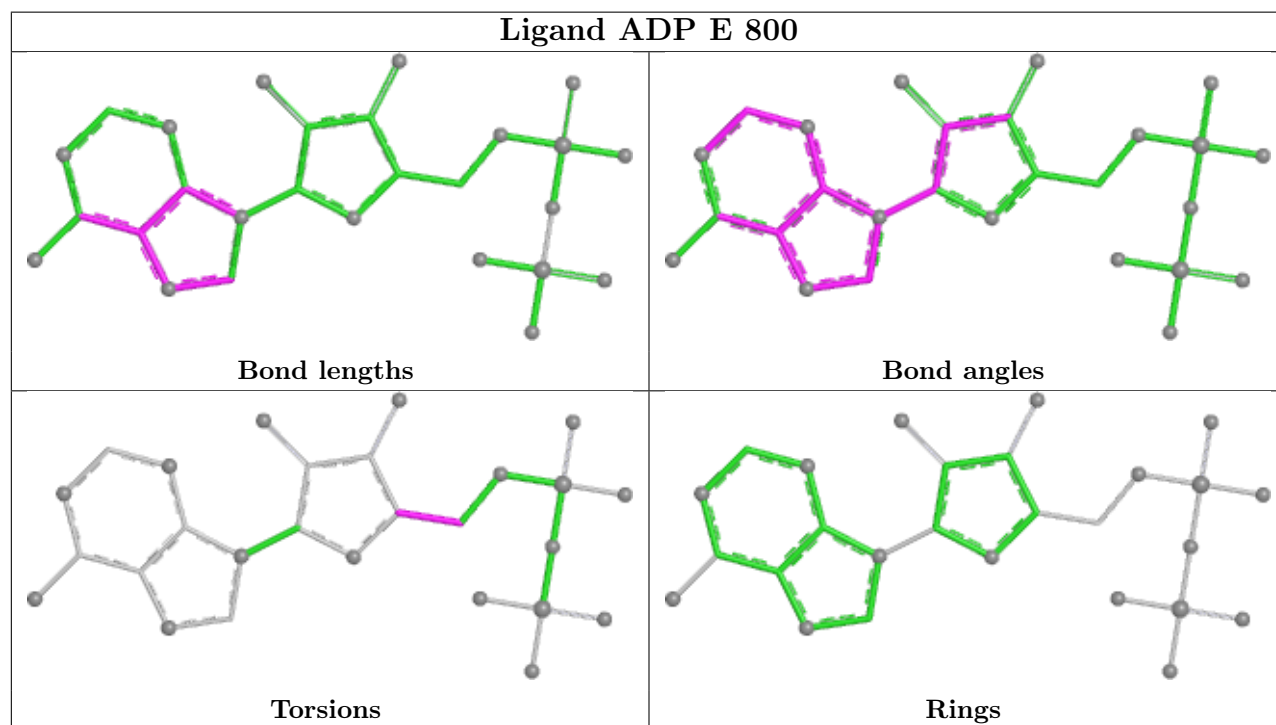
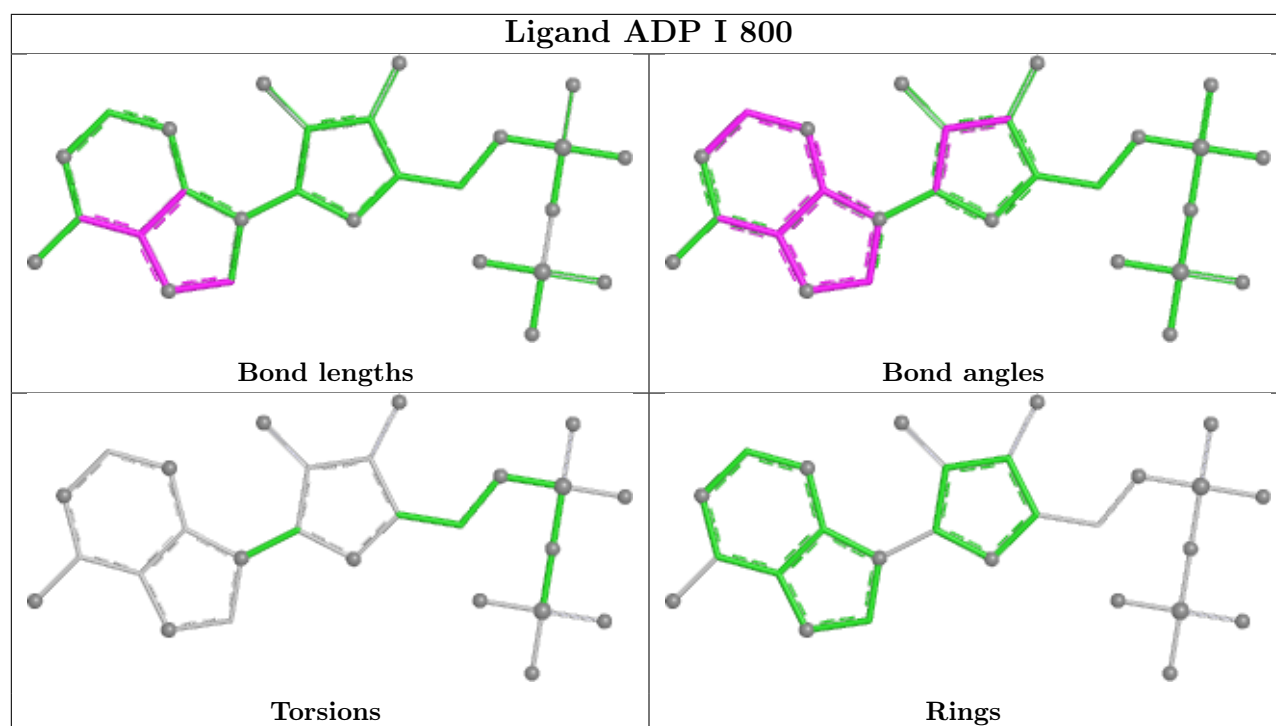
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

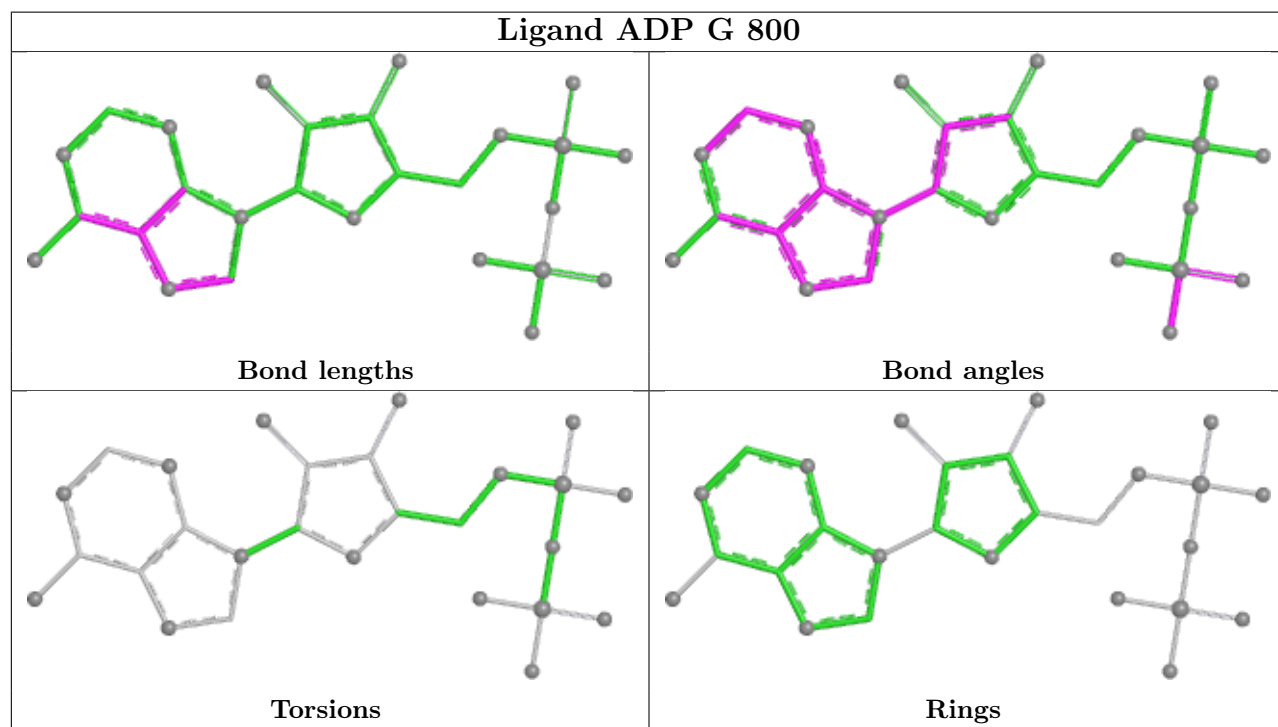
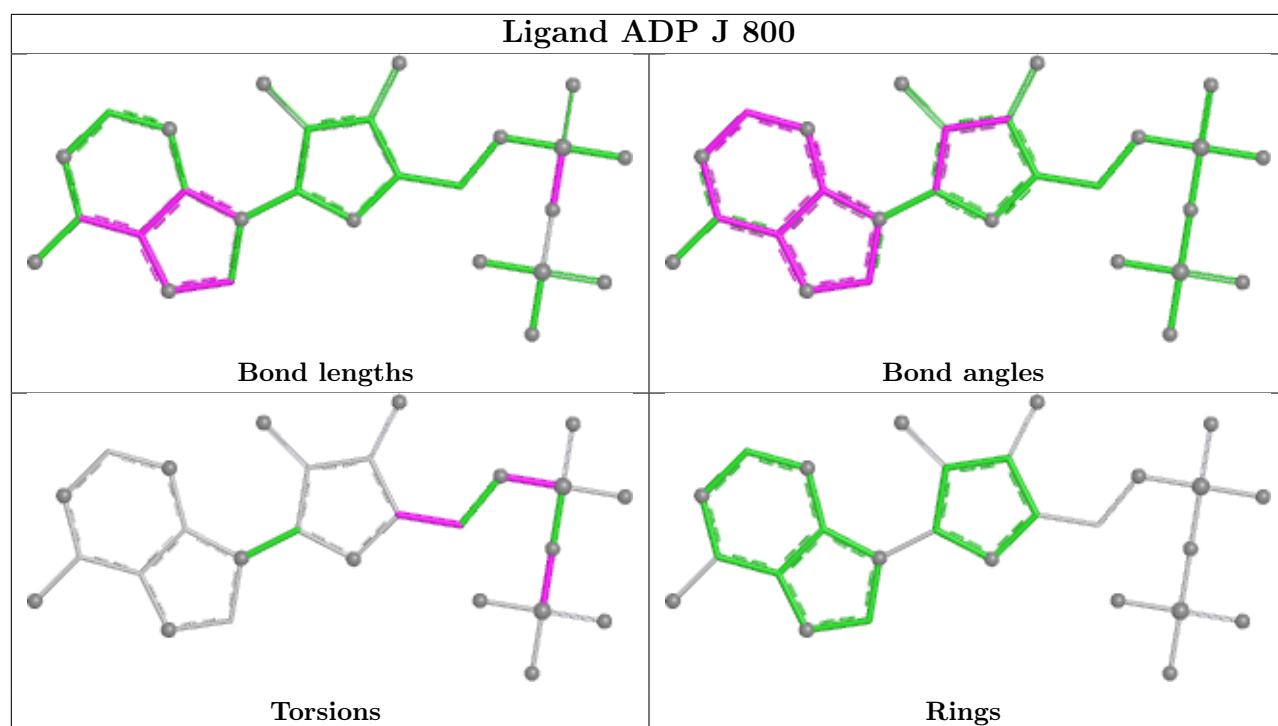
## Ligand ATP H 401

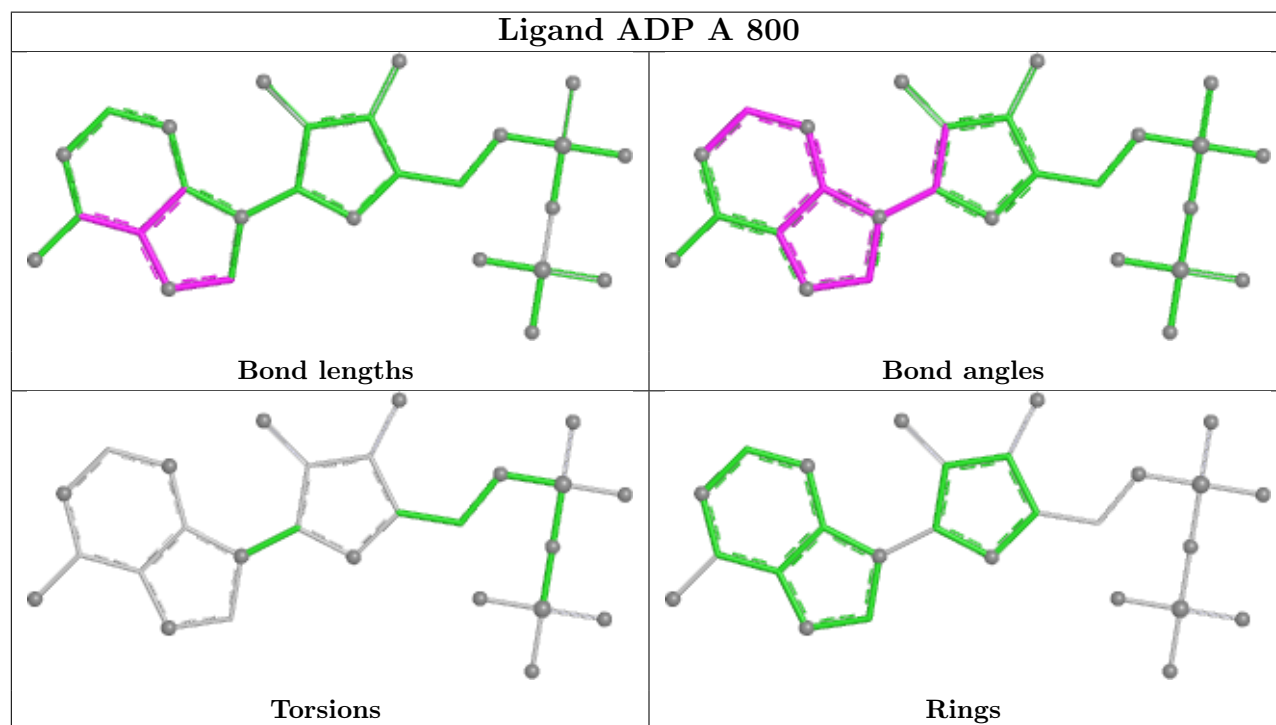
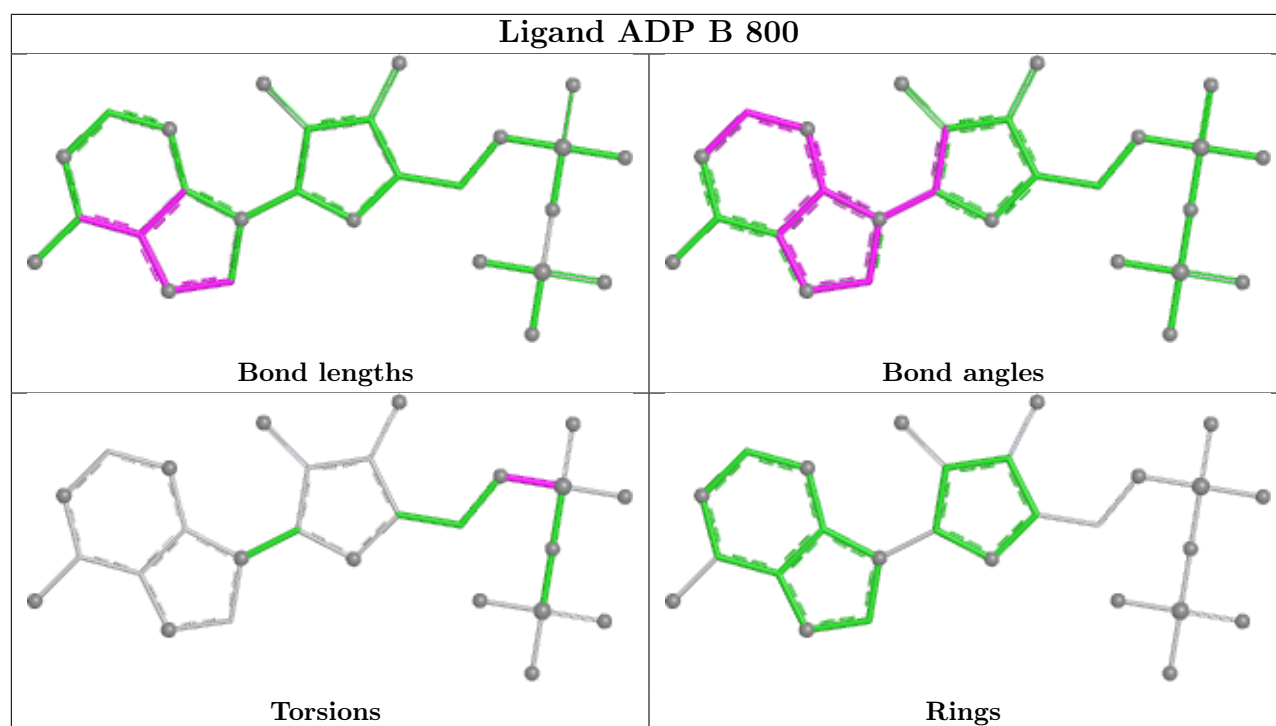


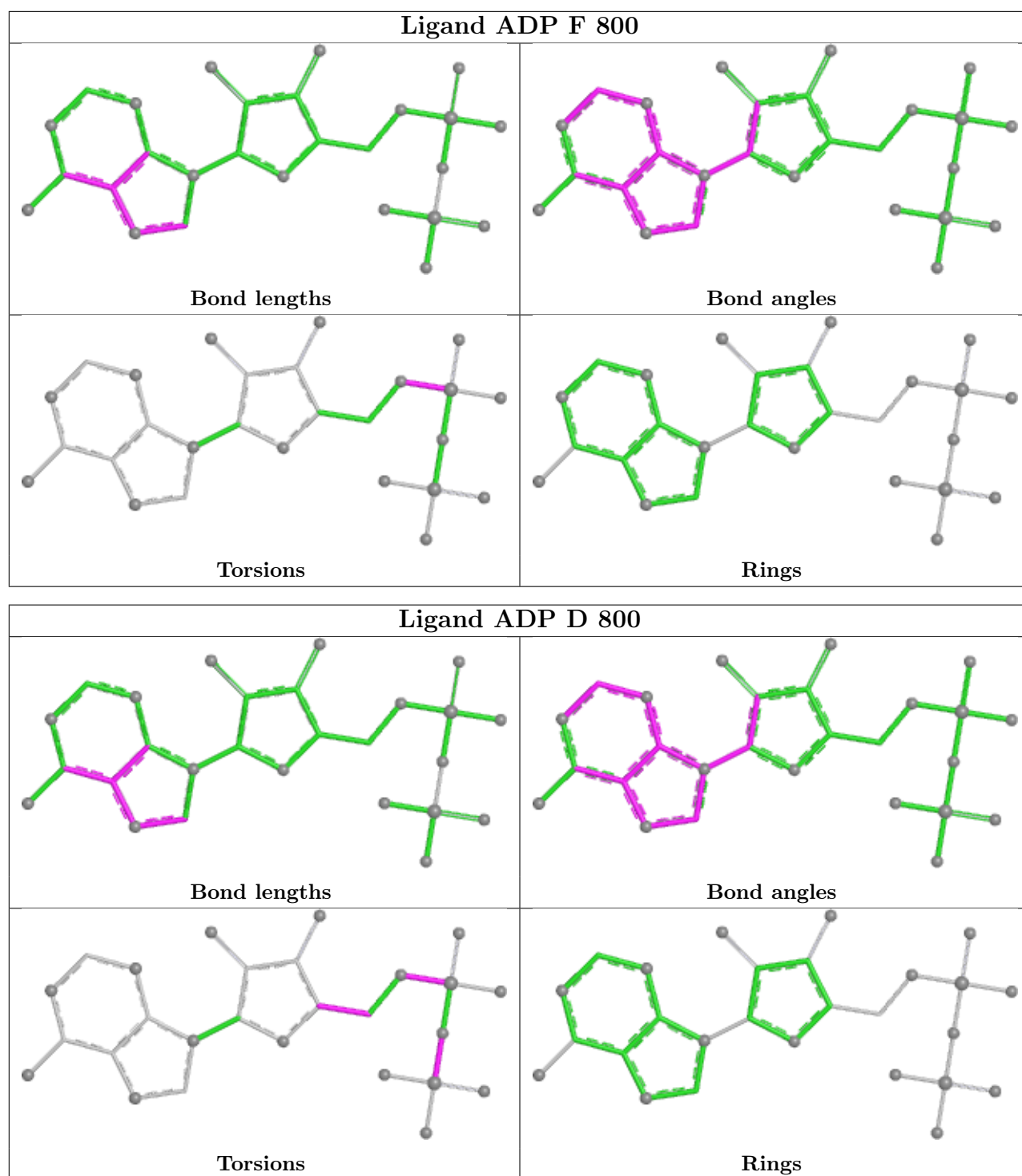
## Ligand ADP C 800











## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	282:LEU	C	283:GLN	N	1.72

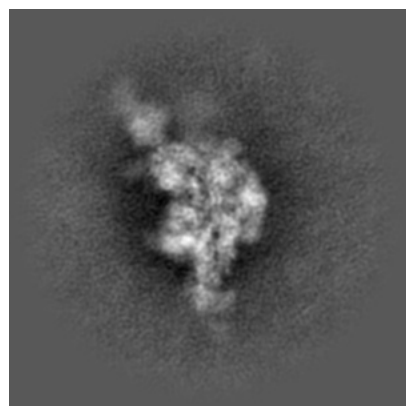
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46848. These allow visual inspection of the internal detail of the map and identification of artifacts.

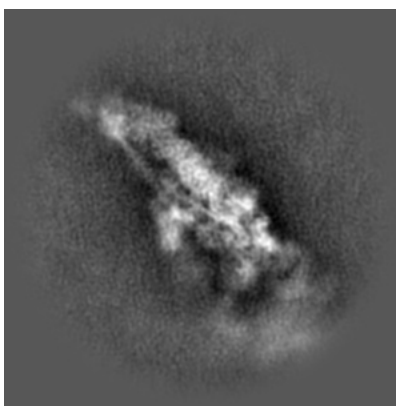
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

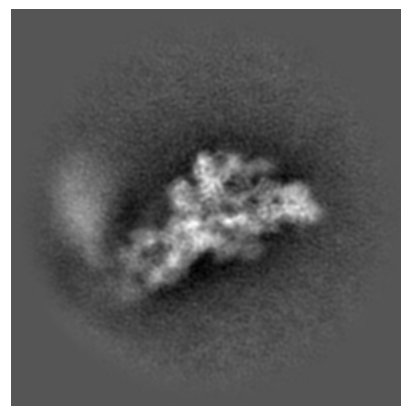
#### 6.1.1 Primary map



X

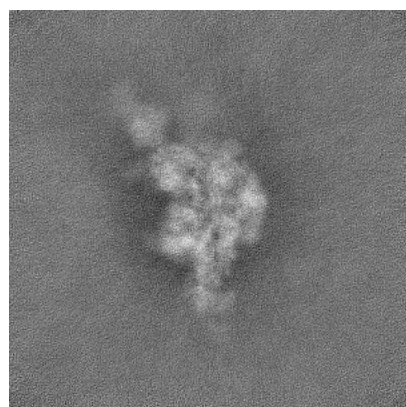


Y

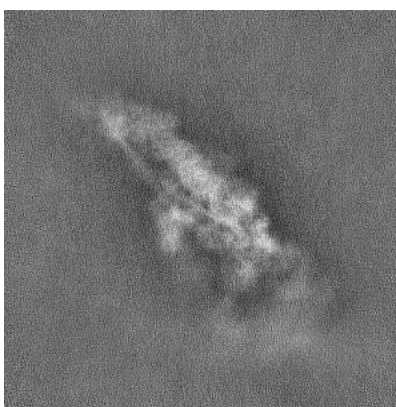


Z

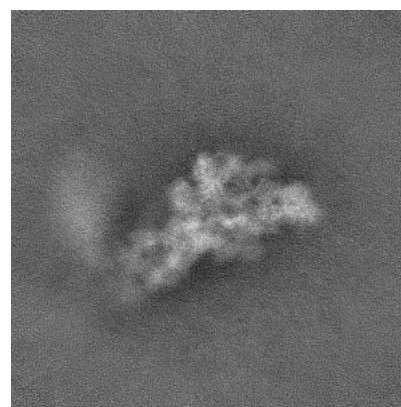
#### 6.1.2 Raw map



X



Y



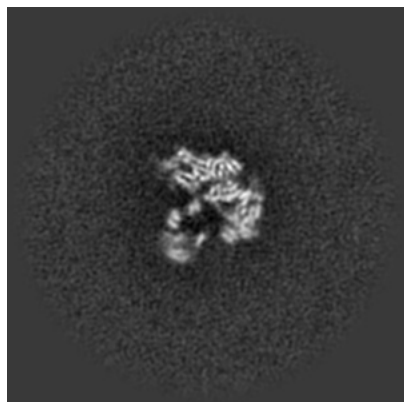
Z

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

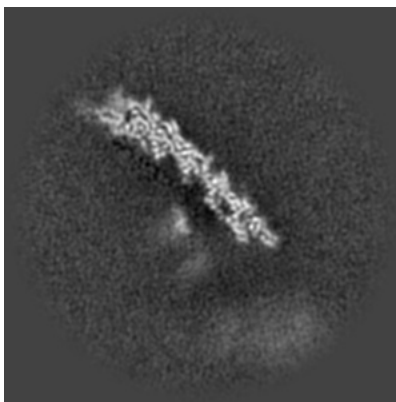


## 6.2 Central slices [i](#)

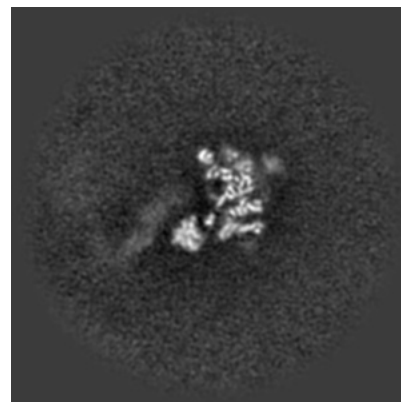
### 6.2.1 Primary map



X Index: 192

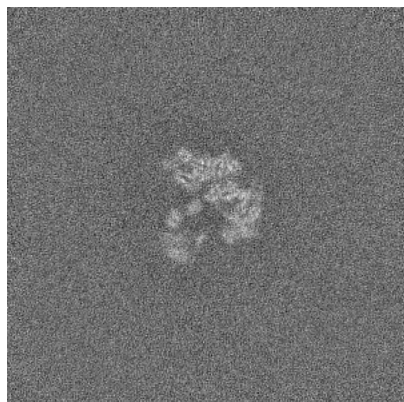


Y Index: 192

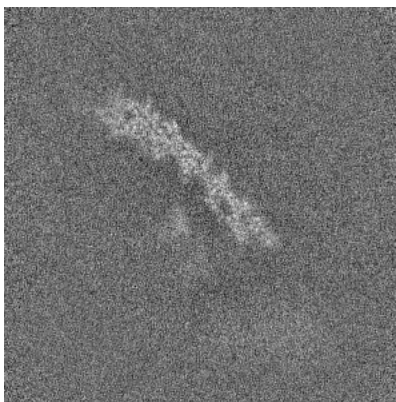


Z Index: 192

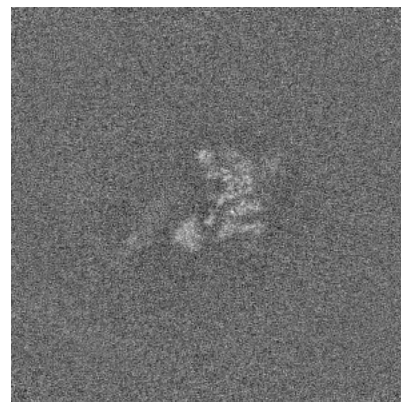
### 6.2.2 Raw map



X Index: 192



Y Index: 192

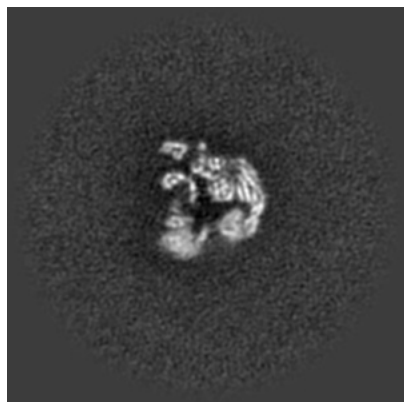


Z Index: 192

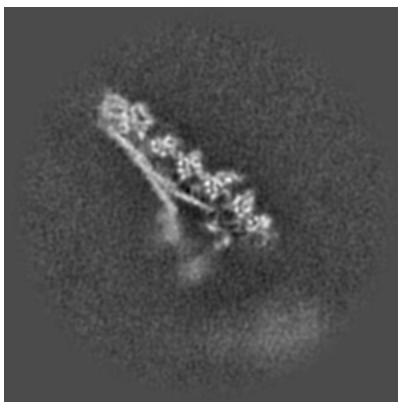
The images above show central slices of the map in three orthogonal directions.

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

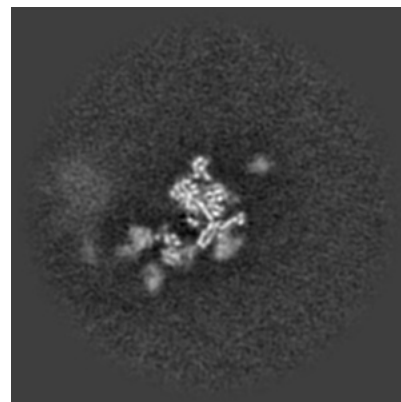
### 6.3.1 Primary map



X Index: 184

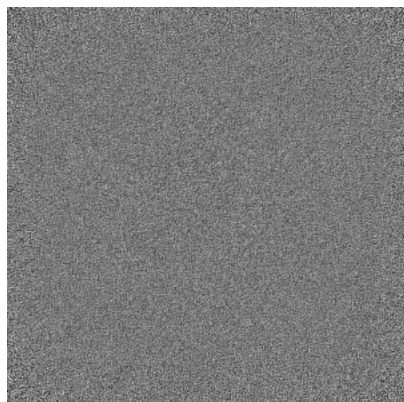


Y Index: 184

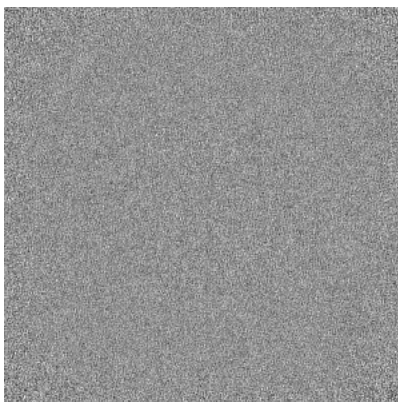


Z Index: 222

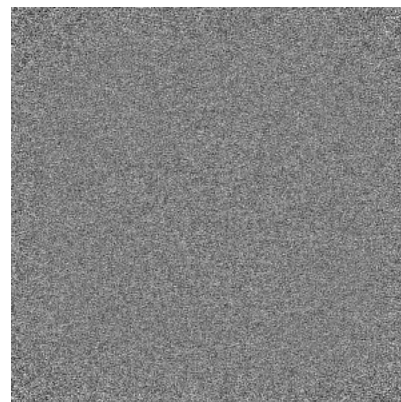
### 6.3.2 Raw map



X Index: 0



Y Index: 0

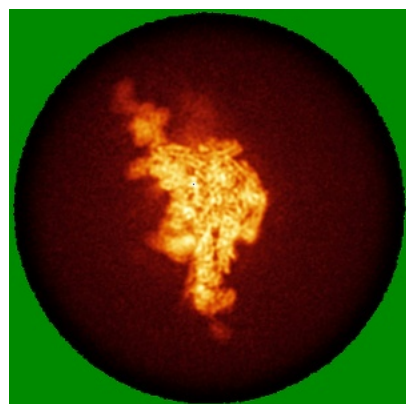


Z Index: 0

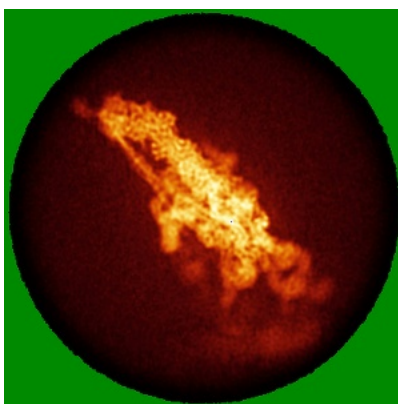
The images above show the largest variance slices of the map in three orthogonal directions.

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

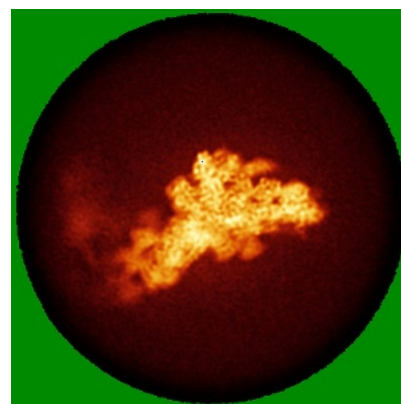
### 6.4.1 Primary map



X

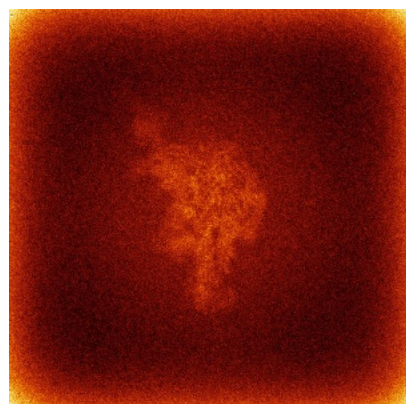


Y

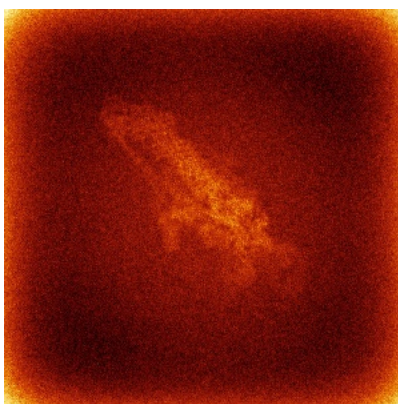


Z

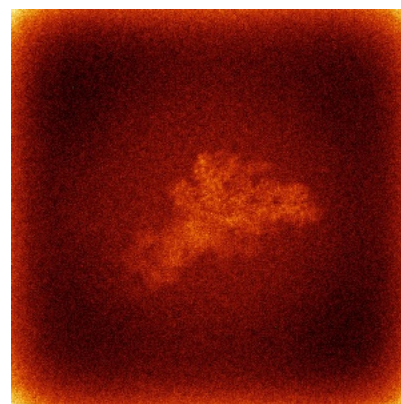
### 6.4.2 Raw map



X



Y



Z

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



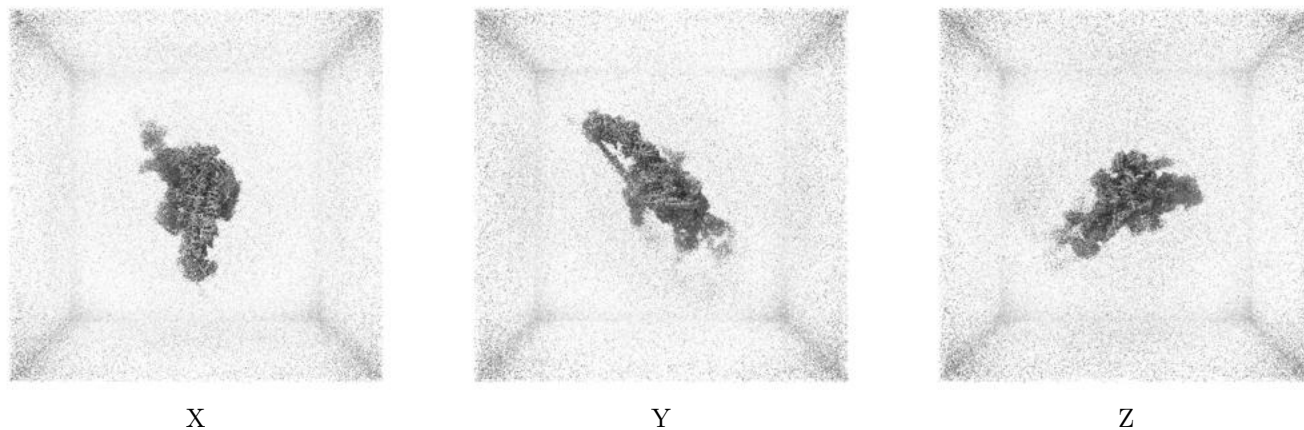
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

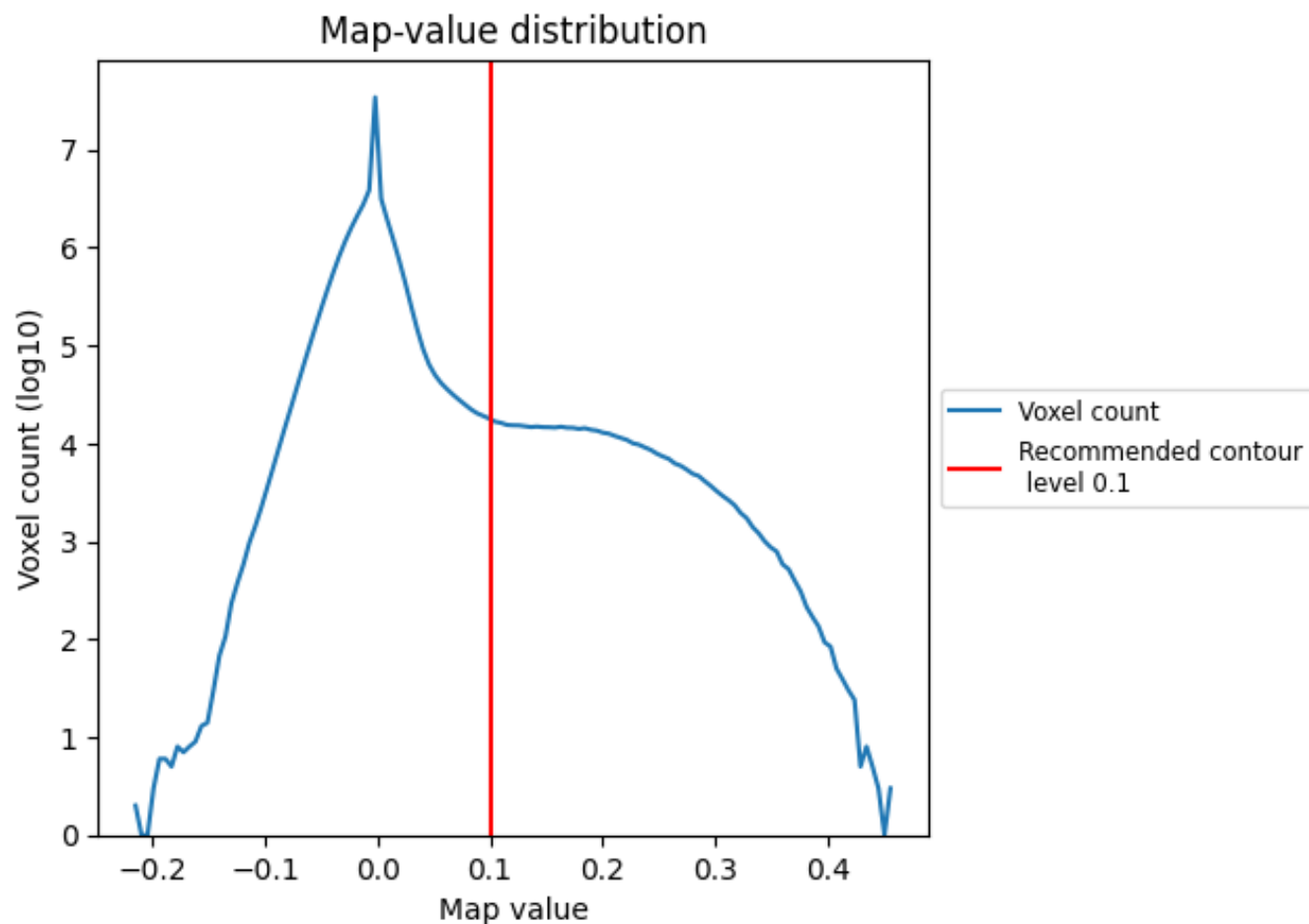
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

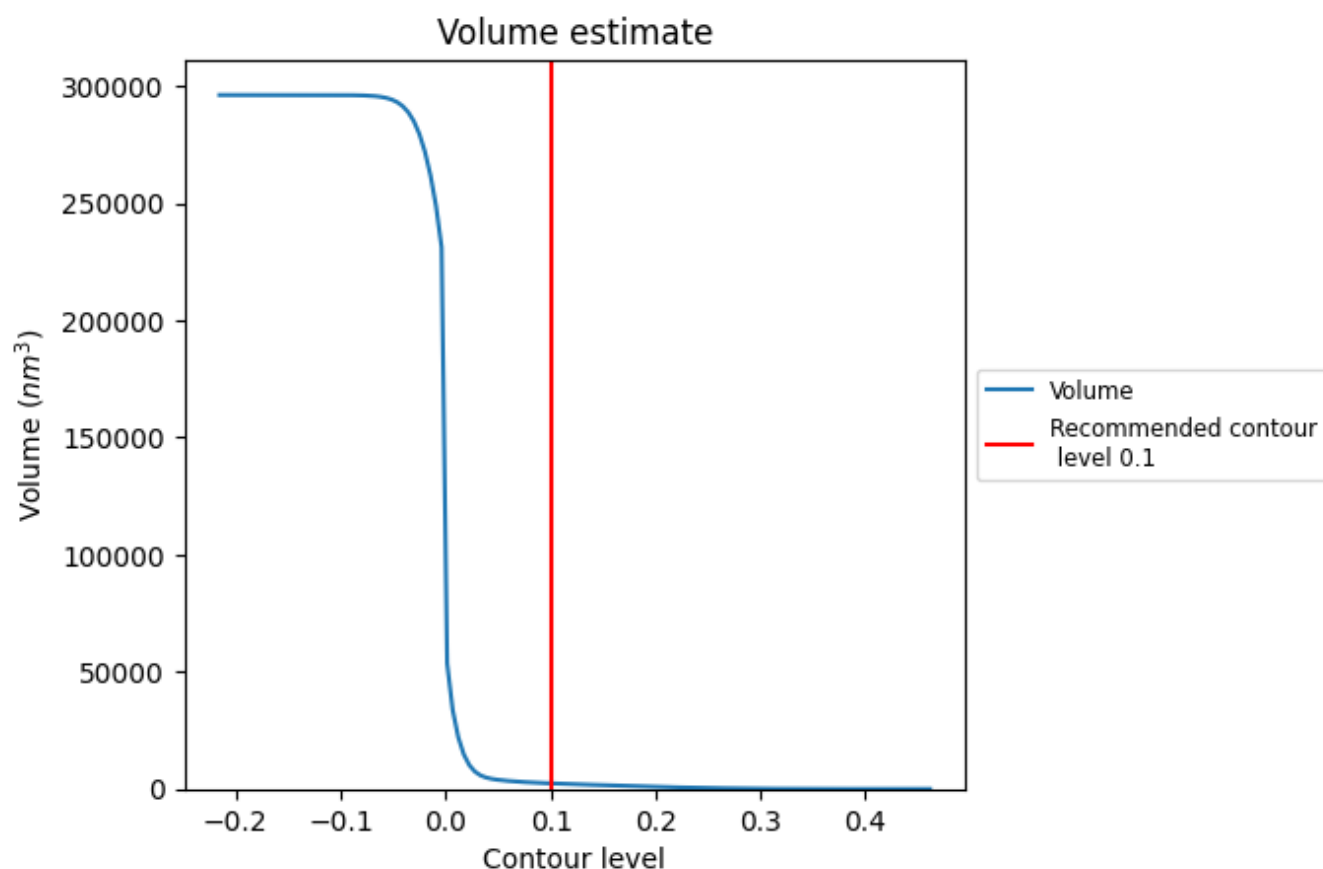
This section contains the results of statistical analysis of the map.

### 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.

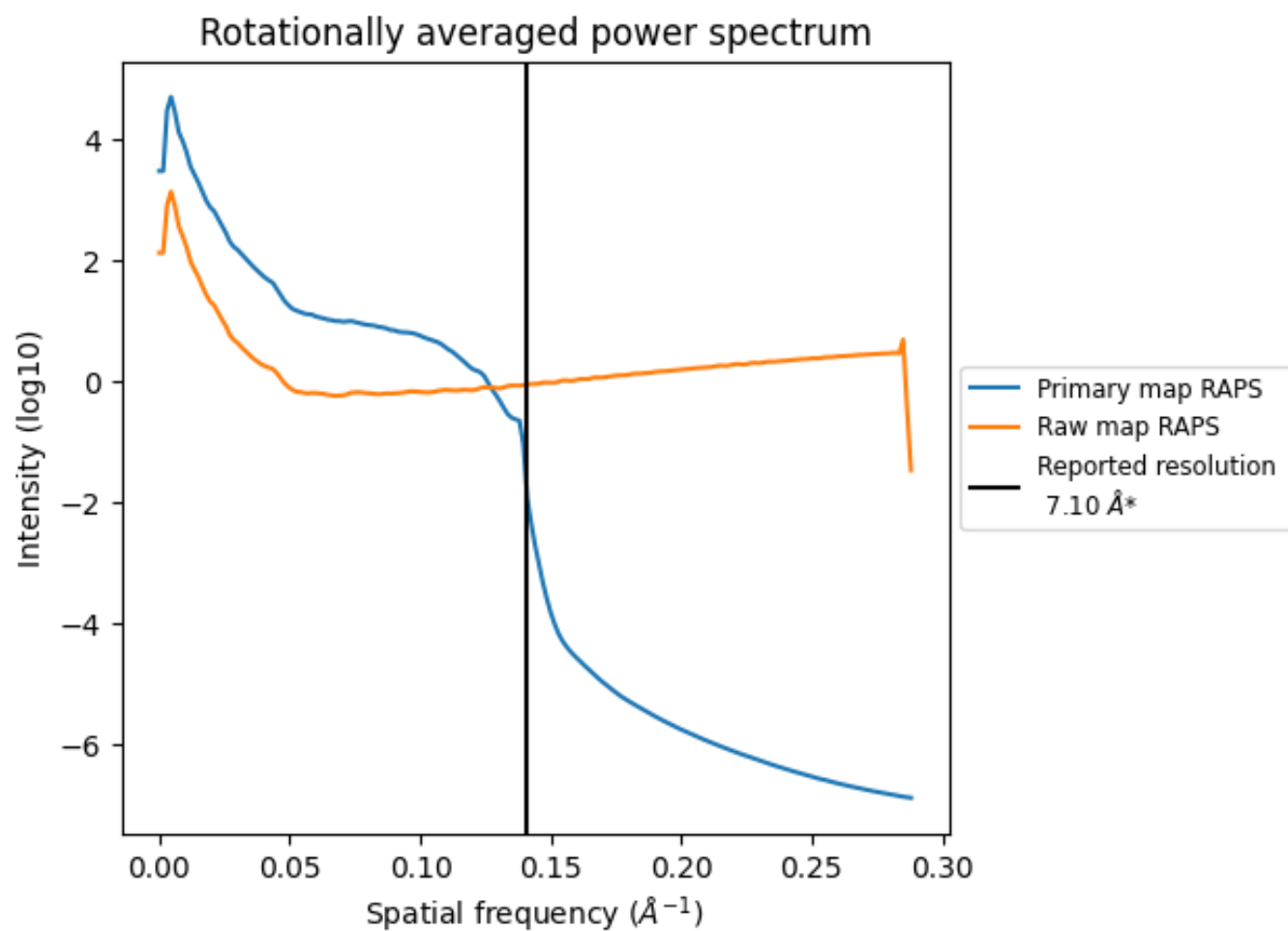
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2389 nm<sup>3</sup>; this corresponds to an approximate mass of 2158 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](#)

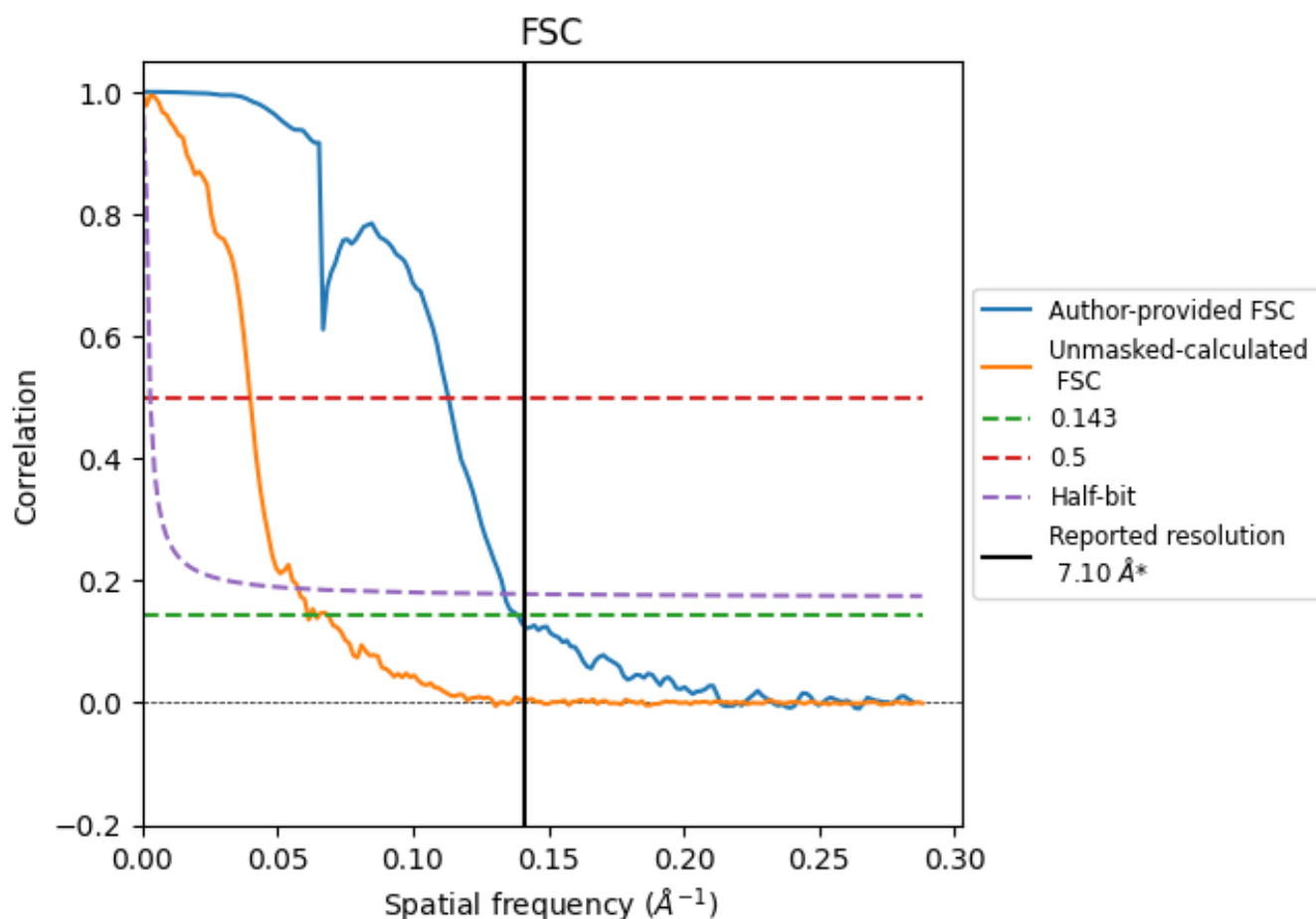


\*Reported resolution corresponds to spatial frequency of 0.141 Å<sup>-1</sup>

## 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 0.141 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

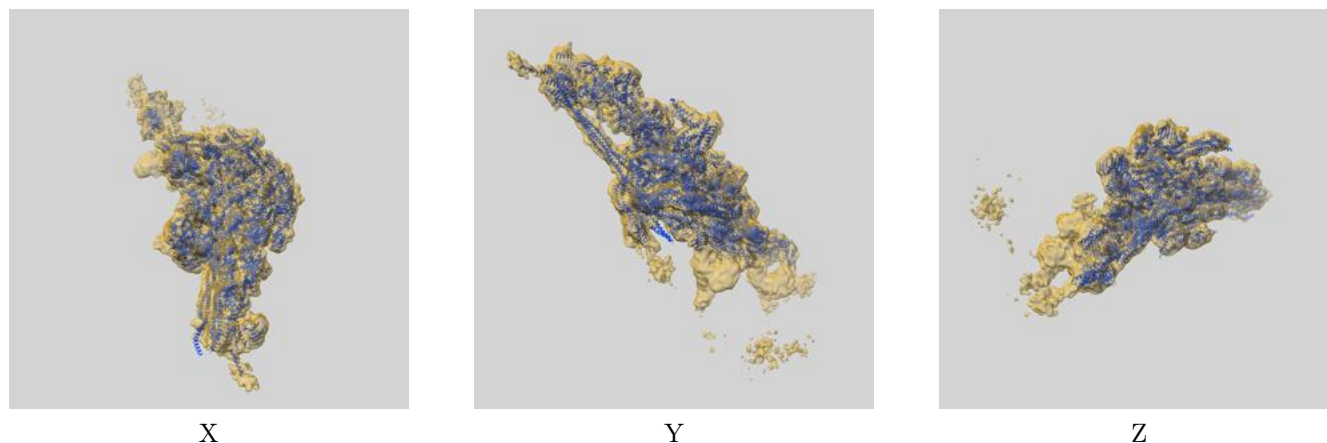
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	7.21	8.85	7.48
Unmasked-calculated*	16.34	25.13	17.39

\*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 16.34 differs from the reported value 7.1 by more than 10 %

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

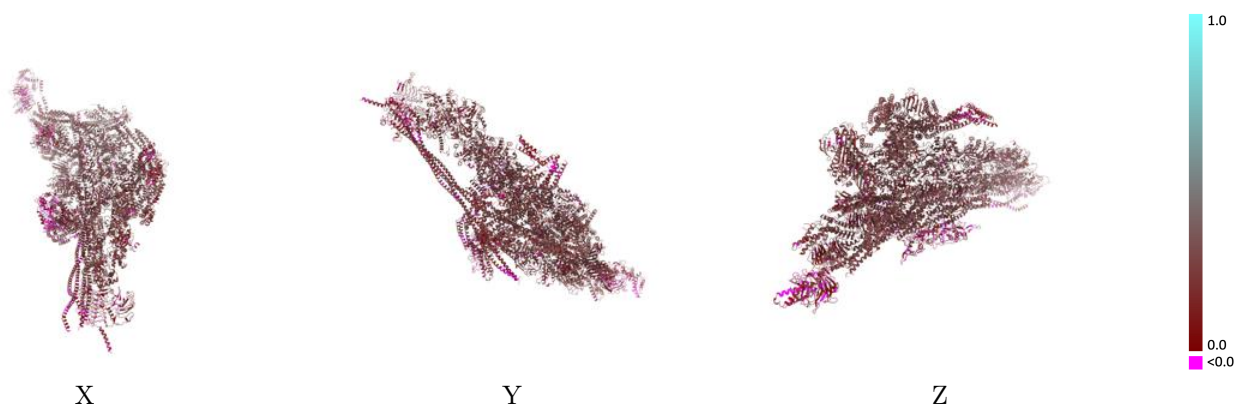
This section contains information regarding the fit between EMDB map EMD-46848 and PDB model 9DGU. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



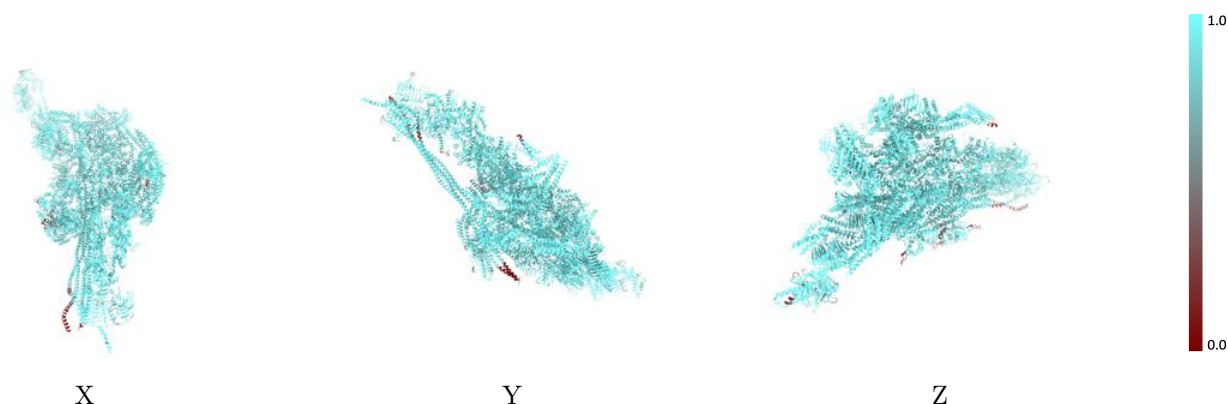
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



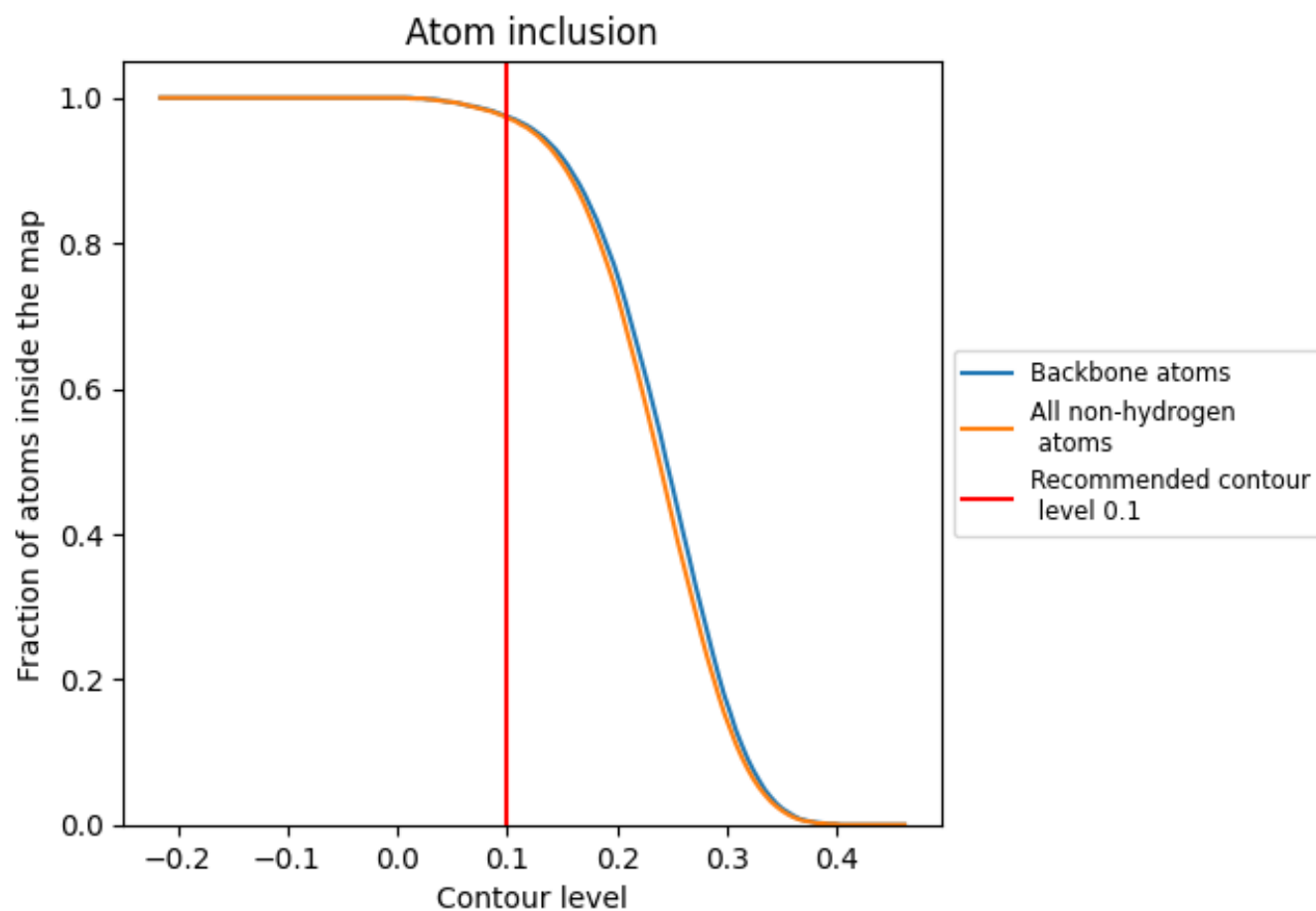
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9730	 0.2140
A	 0.9980	 0.2410
B	 1.0000	 0.2500
C	 0.9990	 0.2550
D	 1.0000	 0.2490
E	 0.9990	 0.2580
F	 0.9950	 0.2520
G	 1.0000	 0.2590
H	 1.0000	 0.2560
I	 0.9910	 0.2330
J	 0.9930	 0.2400
K	 1.0000	 0.2440
L	 0.9960	 0.2480
M	 0.9940	 0.2260
N	 0.9560	 0.2210
O	 0.9990	 0.2380
P	 0.9940	 0.2510
Q	 0.9590	 0.2480
R	 0.9990	 0.2160
U	 0.9680	 0.1570
V	 0.9900	 0.1490
W	 0.9630	 0.2170
Y	 0.9340	 0.1750
Z	 0.9960	 0.2480
a	 0.7410	 0.1150
b	 0.8060	 0.1640
c	 0.9950	 0.2470
d	 0.9930	 0.2340
e	 0.9530	 0.1520
f	 0.9320	 0.2020
g	 0.9610	 0.1180
h	 0.9960	 0.1870
j	 1.0000	 0.2460
m	 0.9830	 0.2450
n	 0.9730	 0.2170



*Continued on next page...*

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Chain	Atom inclusion	Q-score
o	 0.9970	 0.1990
p	 0.9490	 0.0810
q	 0.9460	 0.2230