



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:02 PM UTC

PDB ID : 6F38 / pdb_00006f38
EMDB ID : EMD-4177
Title : Cryo-EM structure of two dynein tail domains bound to dynactin and HOOK3
Authors : Lau, C.K.; Urnavicius, L.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.; Yildiz, A.; Carter, A.P.
Deposited on : 2017-11-28
Resolution : 6.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

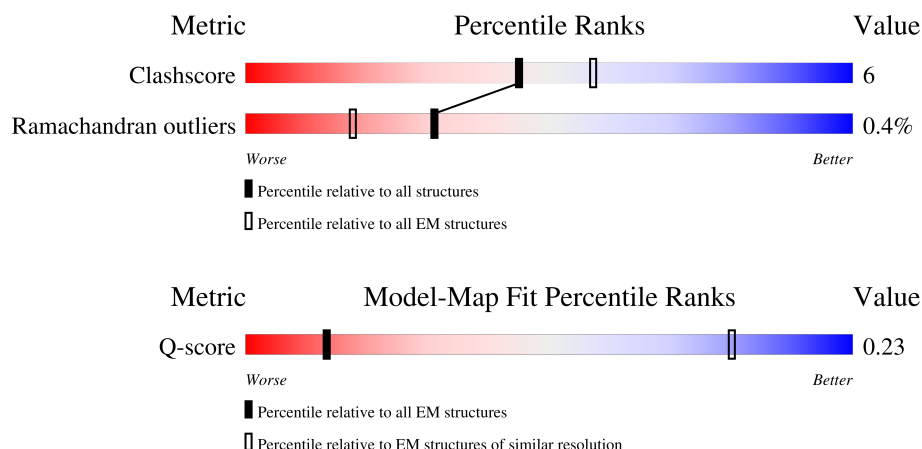
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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.



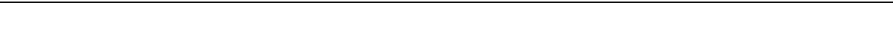
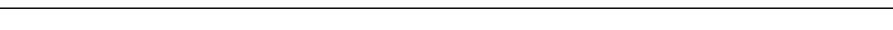
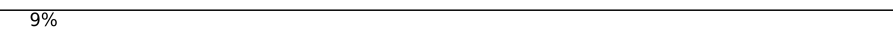
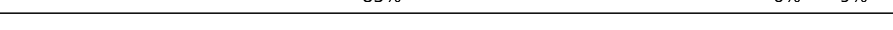
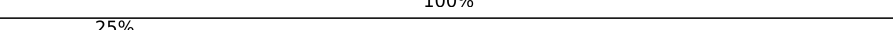
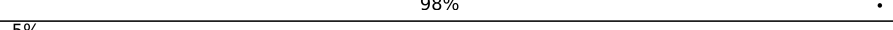
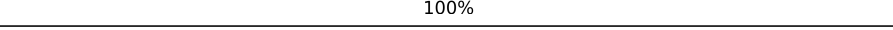
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	523 (6.20 - 7.20)

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

Mol	Chain	Length	Quality of chain
1	A	376	90% 9% .
1	B	376	88% 10% ..
1	C	376	89% 10% .
1	D	376	89% 9% .
1	E	376	86% 11% ..

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Mol	Chain	Length	Quality of chain
1	F	376	 89% 9%
1	G	376	 84% 14%
1	I	376	 87% 11%
2	H	375	 86% 12%
3	J	390	 86% 9% 5%
4	K	286	 82% 15%
5	L	272	 82% 17%
6	M	587	 97%
7	N	616	 98%
8	O	65	 89% 11%
8	P	65	 77% 23%
9	Q	87	 54% 94% 6%
9	R	87	 98%
10	U	190	 9% 85% 6% 9%
11	V	182	 70% 20% 9%
12	X	223	 26% 100%
12	x	223	 25% 98%
13	Y	264	 5% 89% 11%
14	Z	52	 100%
15	a	68	 72% 24%
16	b	90	 74% 9% 17%
17	c	50	 6% 62% 10% 26%
18	d	29	 7% 83% 17%
19	e	1455	 19% 61% 36%
19	f	1455	 9% 60% 36%

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Mol	Chain	Length	Quality of chain
19	m	1455	
19	n	1455	
20	g	612	
20	h	612	
20	o	612	
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	z	53	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 68864 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
1	A	370	Total	C	N	O	0	0
			1821	1082	369	370		
1	B	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	C	370	Total	C	N	O	0	0
			1822	1082	370	370		
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 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	369	Total	C	N	O	0	0
			1819	1081	369	369		

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

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	587	Total	C	N	O	0	0
			2935	1761	587	587		

- Molecule 7 is a protein called Dynactin Subunit 2.

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

- Molecule 8 is a protein called Dynactin Subunit 3.

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

- Molecule 9 is a protein called Dynactin Subunit 2.

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

- Molecule 10 is a protein called Dynactin 6.

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

- Molecule 11 is a protein called Dynactin subunit 5.

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

- Molecule 12 is a protein called HOOK3.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	223	Total	C	N	O	0	0
			1115	669	223	223		
12	x	222	Total	C	N	O	0	0
			1110	666	222	222		

- Molecule 13 is a protein called Dynactin Subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Y	264	Total	C	N	O	0	0
			1320	792	264	264		

- Molecule 14 is a protein called Dynactin Subunit 1.

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

- Molecule 15 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	a	52	Total	C	N	O	0	0
			259	155	52	52		

- Molecule 16 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	75	Total	C	N	O	0	0
			369	219	75	75		

- Molecule 17 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	c	37	Total	C	N	O	0	0
			184	110	37	37		

- Molecule 18 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	d	24	Total	C	N	O	0	0
			119	71	24	24		

- Molecule 19 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	e	926	Total	C	N	O	0	0
			4598	2746	926	926		
19	f	929	Total	C	N	O	0	0
			4613	2755	929	929		
19	m	926	Total	C	N	O	0	0
			4598	2746	926	926		
19	n	928	Total	C	N	O	0	0
			4608	2752	928	928		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
20	g	397	Total	C	N	O	0	0
			1961	1167	397	397		
20	h	400	Total	C	N	O	0	0
			1975	1175	400	400		
20	o	397	Total	C	N	O	0	0
			1961	1167	397	397		
20	p	401	Total	C	N	O	0	1
			1977	1176	401	400		

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	275	Total	C	N	O	0	0
			1362	812	275	275		
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		

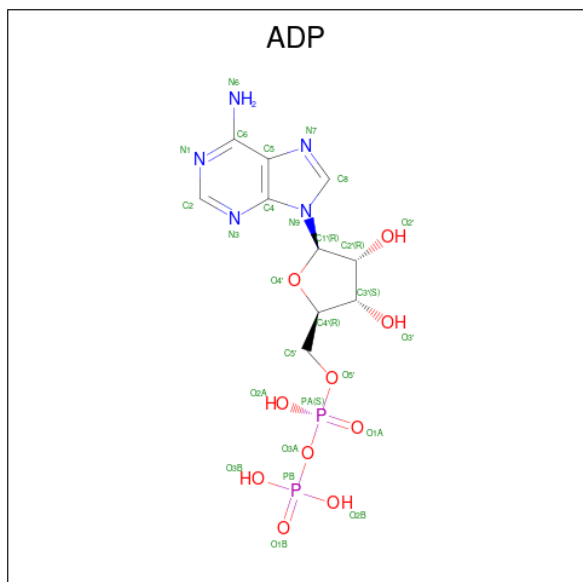
- Molecule 22 is a protein called Dynein light chain roadblock-type 1.

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	0	0
			462	276	93	93		
22	t	93	Total	C	N	O	0	0
			462	276	93	93		

- Molecule 23 is a protein called Dynactin Subunit 1.

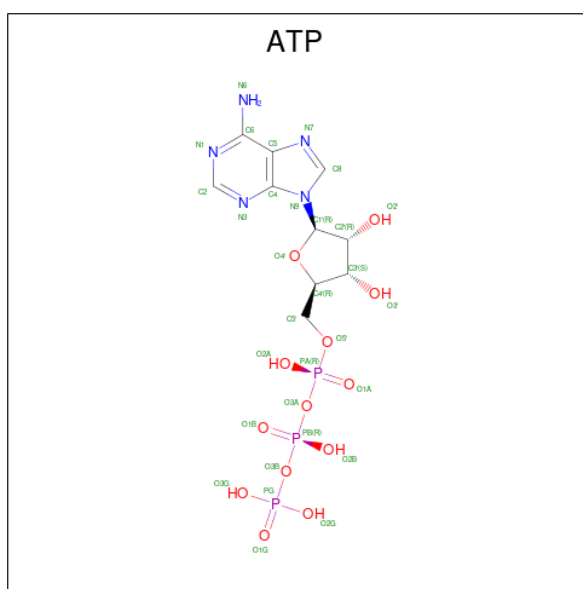
Mol	Chain	Residues	Atoms				AltConf	Trace
23	z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 24 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 25 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

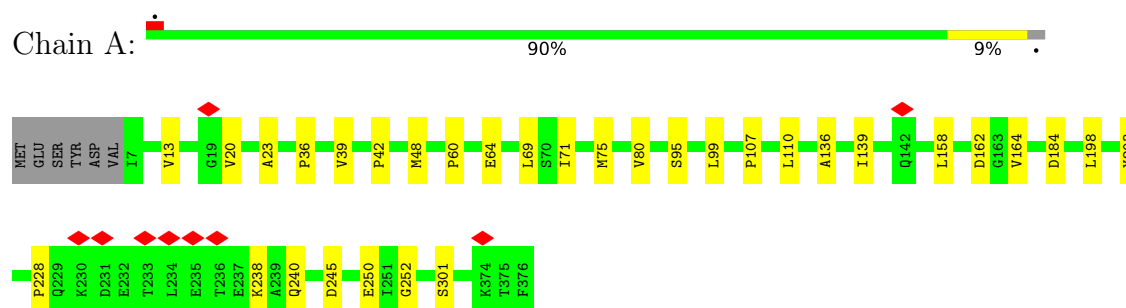


Mol	Chain	Residues	Atoms					AltConf
25	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

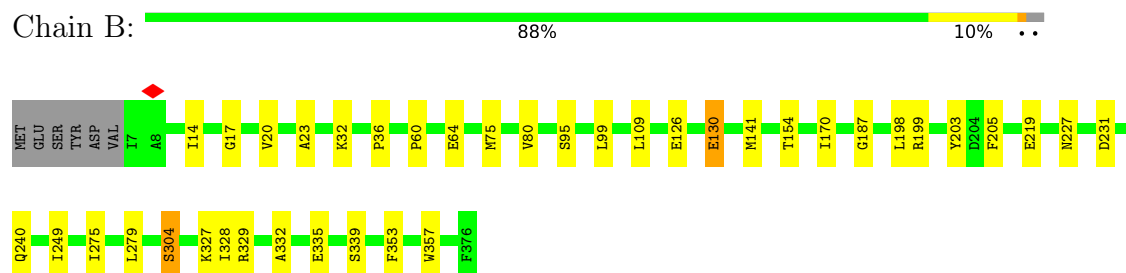
3 Residue-property plots

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

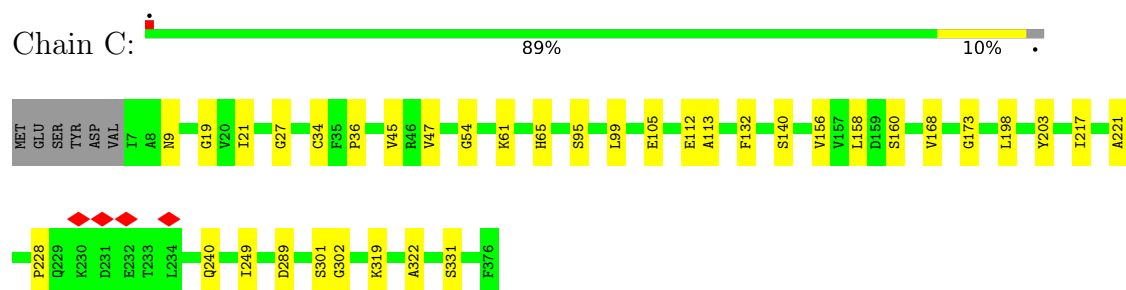
- Molecule 1: ARP1 actin related protein 1 homolog A



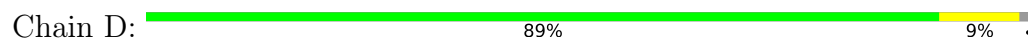
- Molecule 1: ARP1 actin related protein 1 homolog A

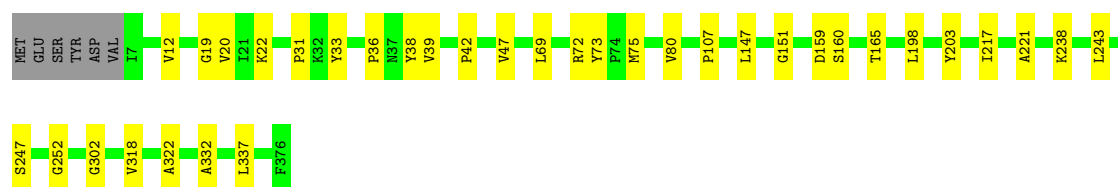


- Molecule 1: ARP1 actin related protein 1 homolog A

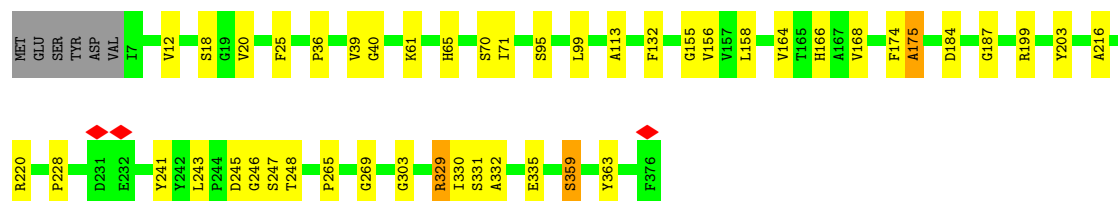
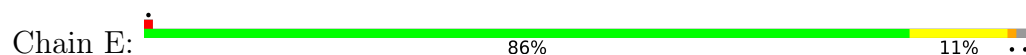


- Molecule 1: ARP1 actin related protein 1 homolog A

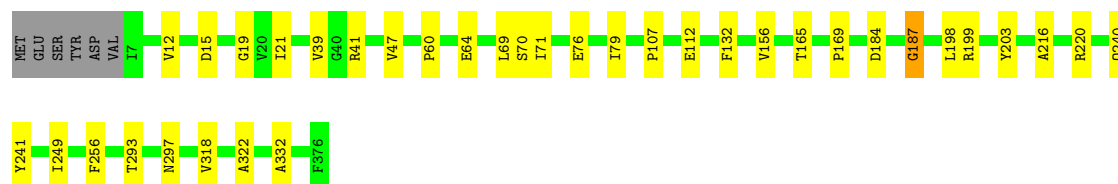




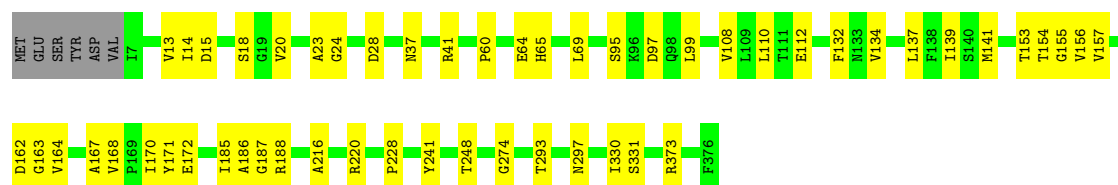
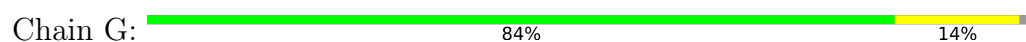
- Molecule 1: ARP1 actin related protein 1 homolog A



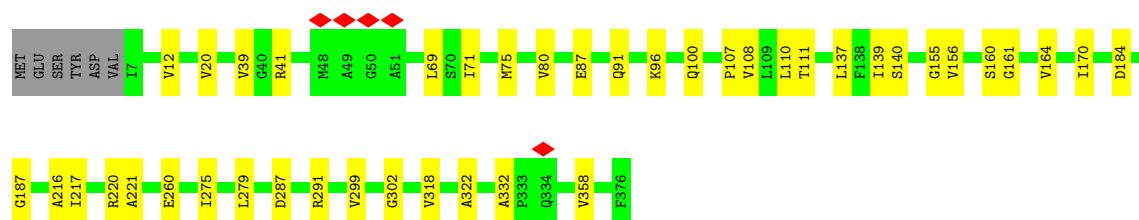
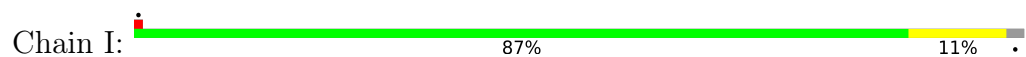
- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 1: ARP1 actin related protein 1 homolog A

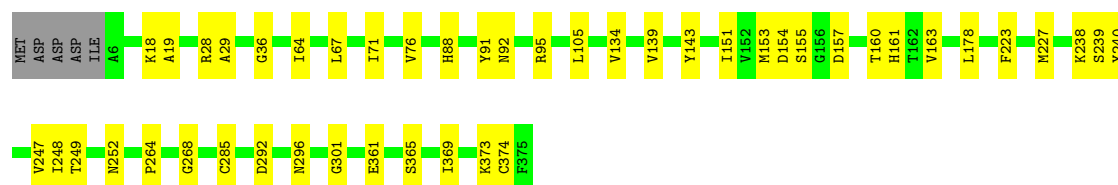


- Molecule 1: ARP1 actin related protein 1 homolog A



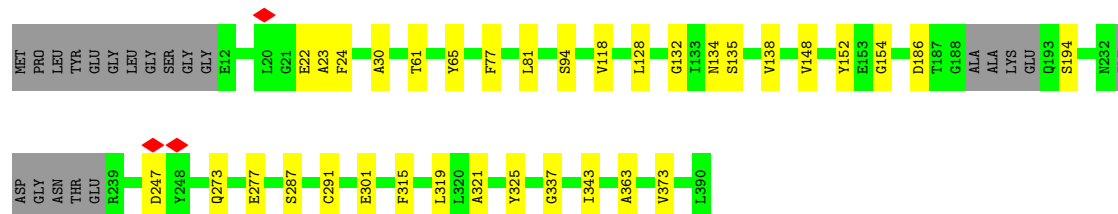
- Molecule 2: Actin, cytoplasmic 1

Chain H:  86% 12% .



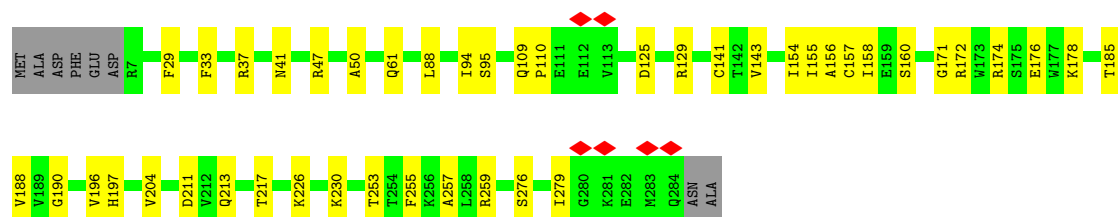
- Molecule 3: Actin related protein 10 homolog

Chain J:  86% 9% 5%



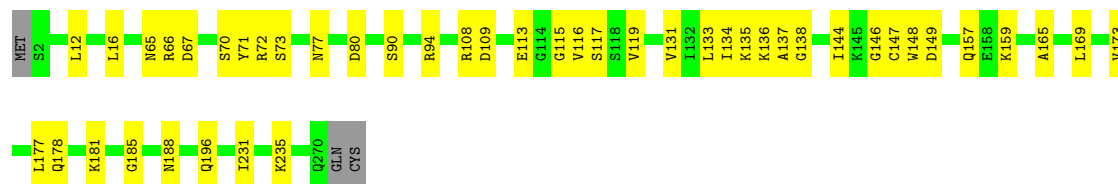
- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:  82% 15% .

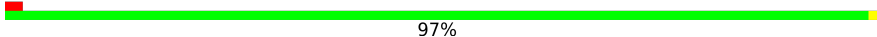


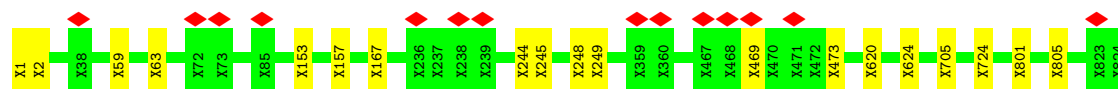
- Molecule 5: F-actin capping protein beta subunit

Chain L:  82% 17% .

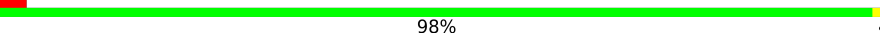


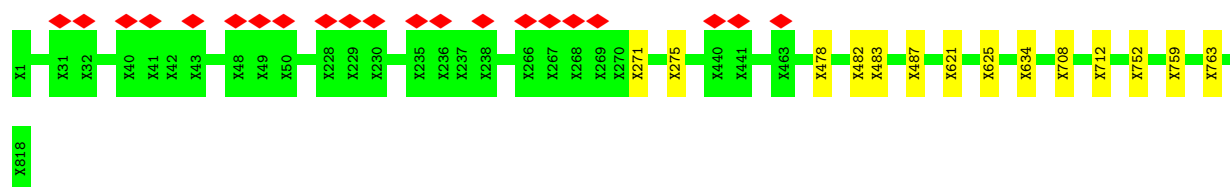
- Molecule 6: Dynactin Subunit 2

Chain M:  97% .



- Molecule 7: Dynactin Subunit 2

Chain N:  98%



- Molecule 8: Dynactin Subunit 3

Chain O:  89% 11%

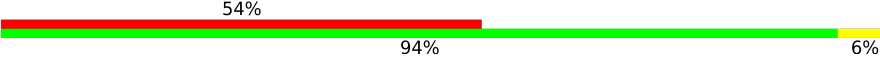


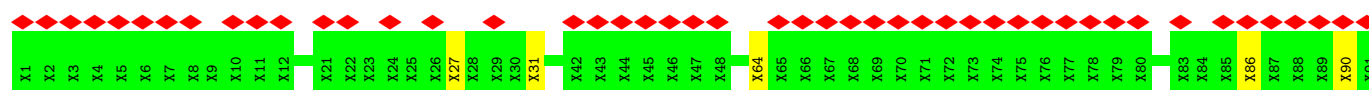
- Molecule 8: Dynactin Subunit 3

Chain P:  77% 23%

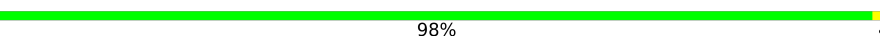


- Molecule 9: Dynactin Subunit 2

Chain Q:  54% 94% 6%



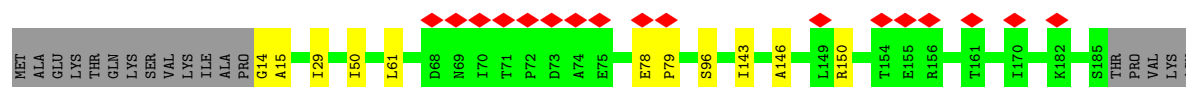
- Molecule 9: Dynactin Subunit 2

Chain R:  98%



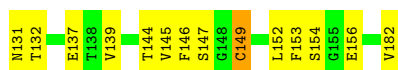
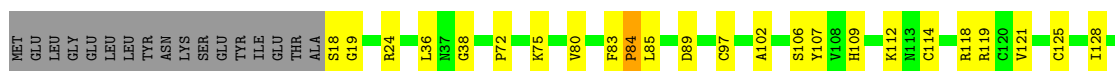
- Molecule 10: Dynactin 6

Chain U:  9% 85% 6% 9%

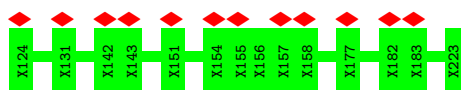
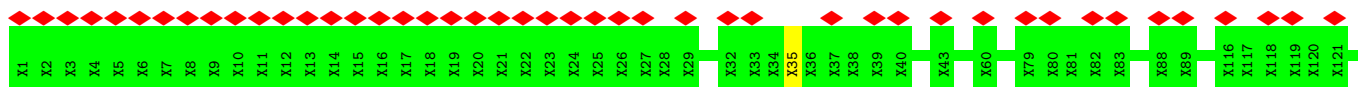


- Molecule 11: Dynactin subunit 5

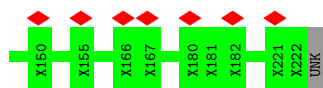
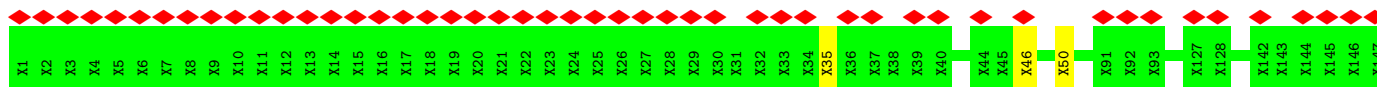
Chain V:  70% 20% 9%



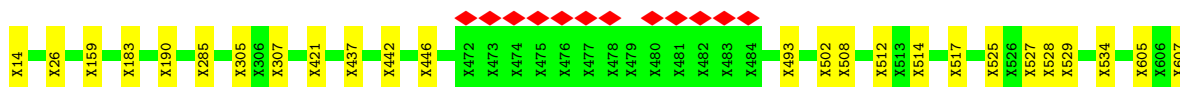
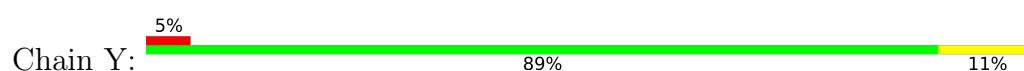
- Molecule 12: HOOK3



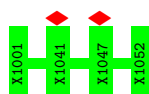
- Molecule 12: HOOK3



- Molecule 13: Dynactin Subunit 4

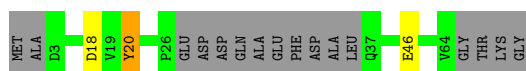


- Molecule 14: Dynactin Subunit 1

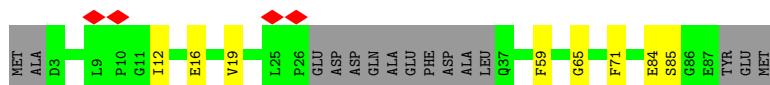
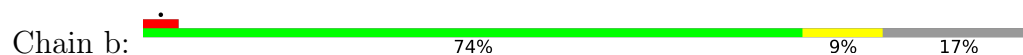


- Molecule 15: Dynactin subunit 2

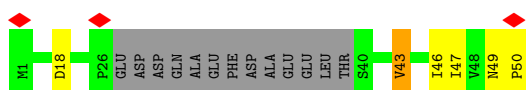




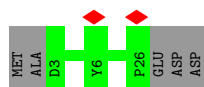
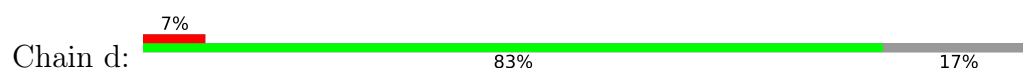
• Molecule 16: Dynactin subunit 2



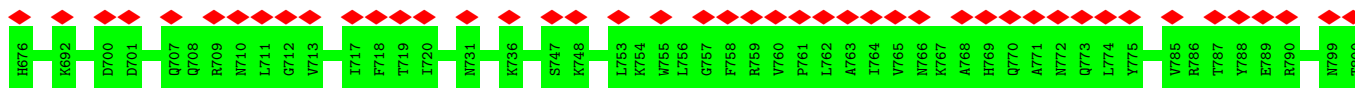
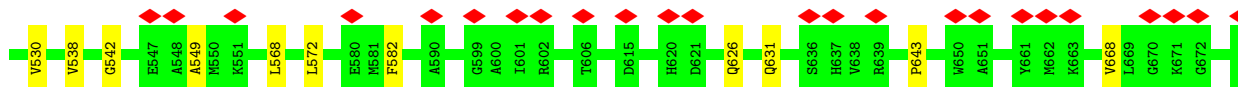
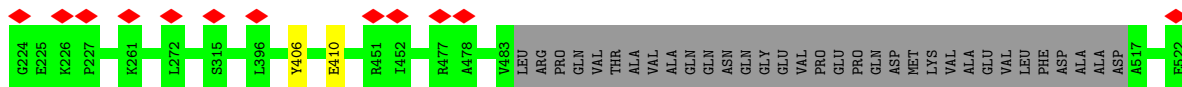
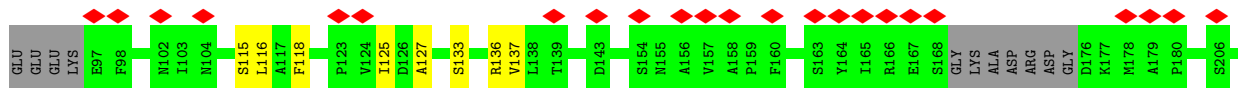
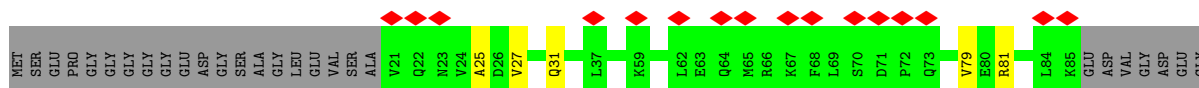
• Molecule 17: Dynactin subunit 2

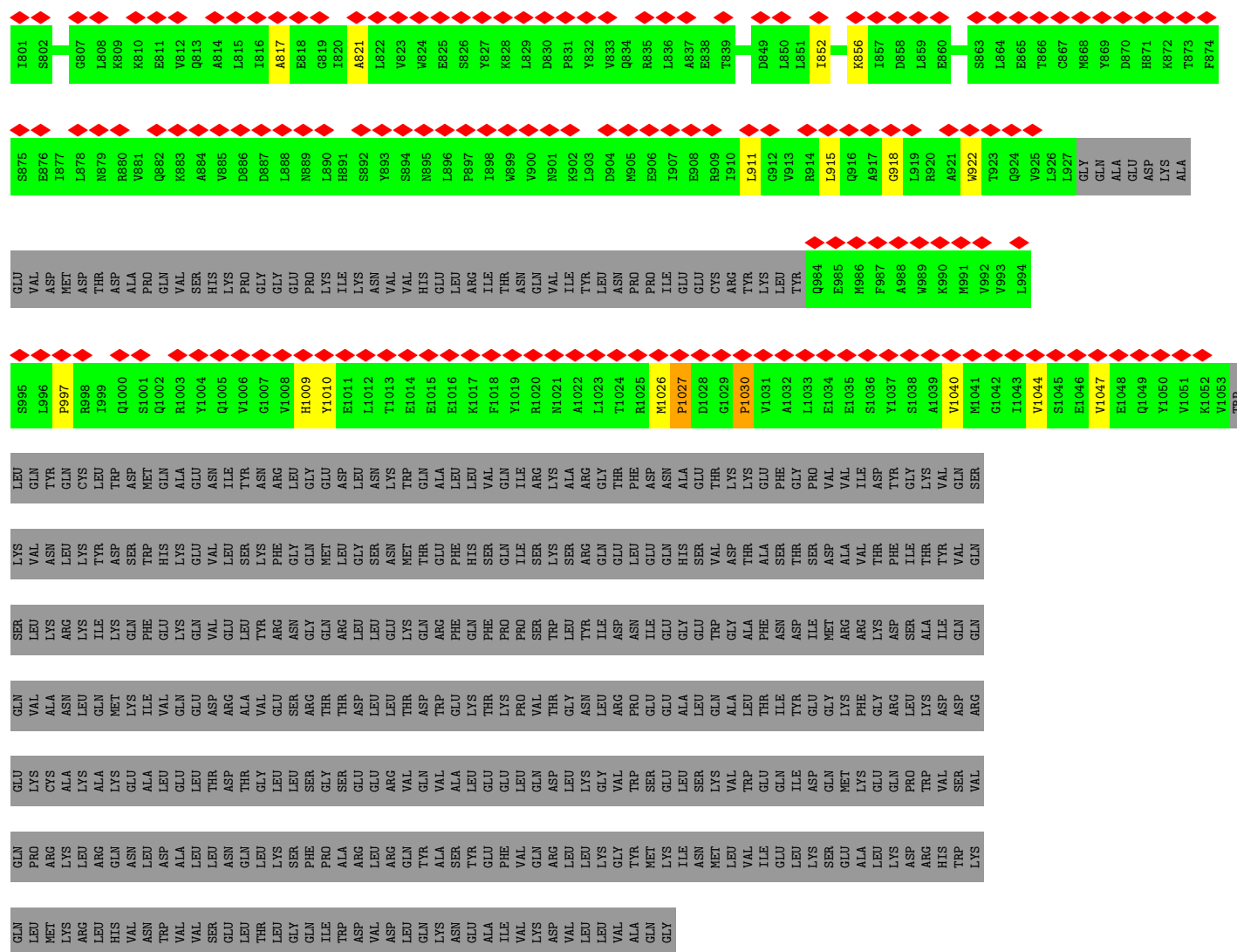


• Molecule 18: Dynactin subunit 2

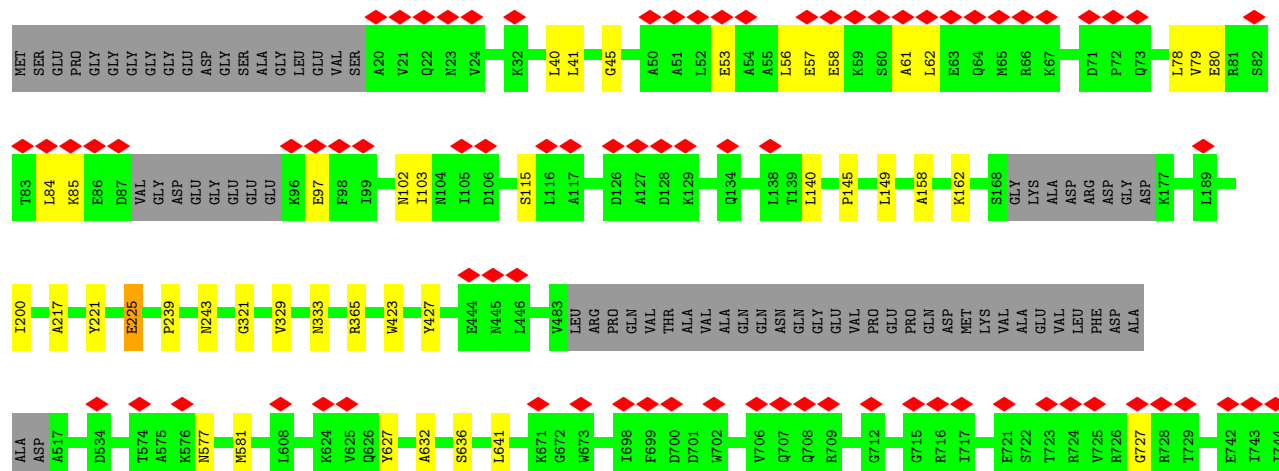


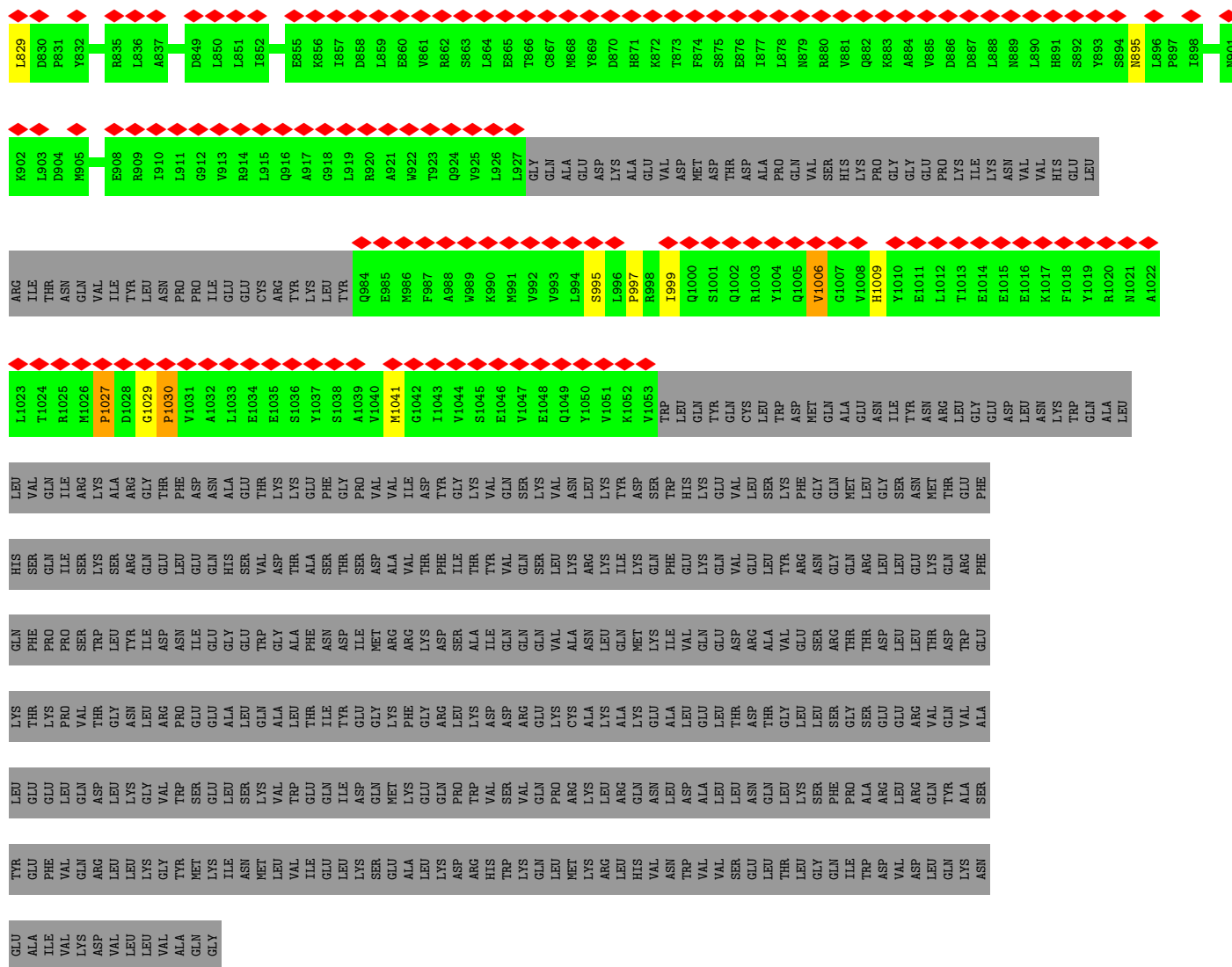
• Molecule 19: Cytoplasmic dynein 1 heavy chain 1



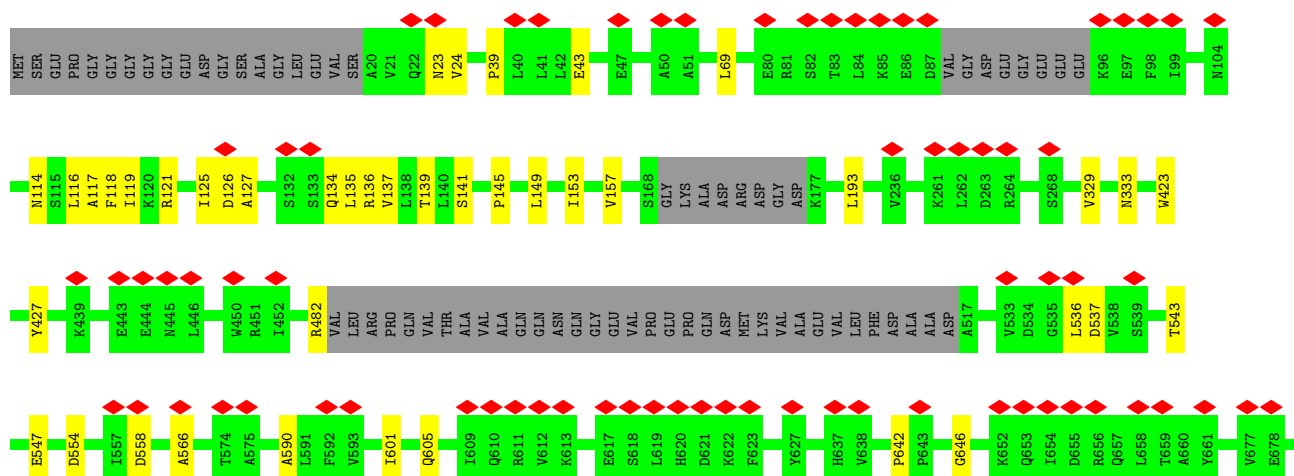


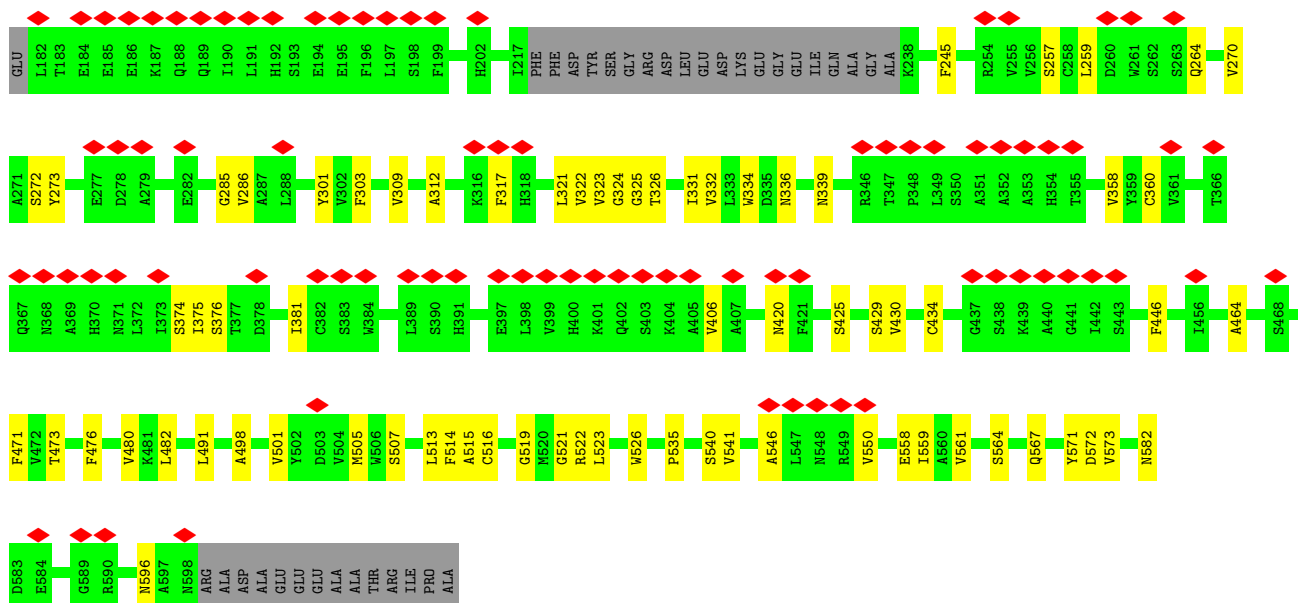
• Molecule 19: Cytoplasmic dynein 1 heavy chain 1



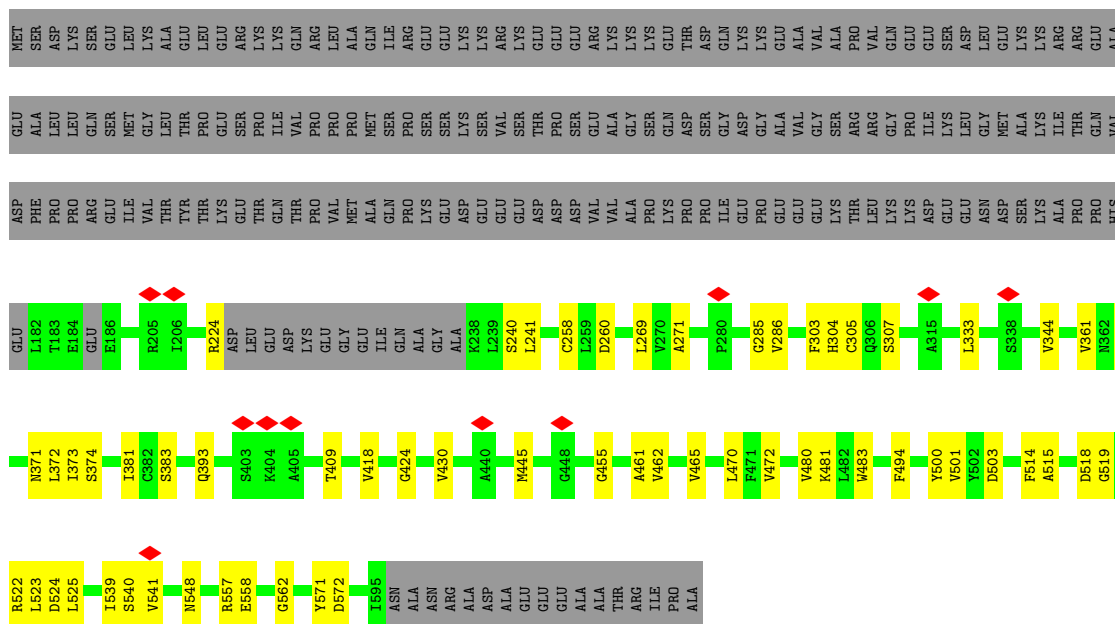


● Molecule 19: Cytoplasmic dynein 1 heavy chain 1

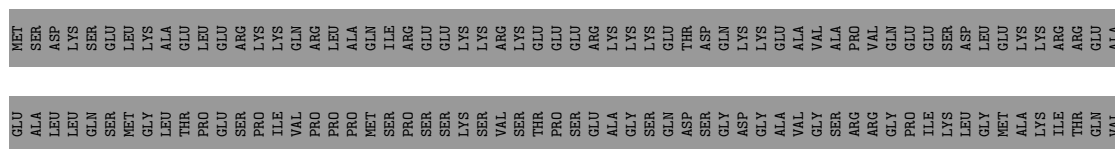


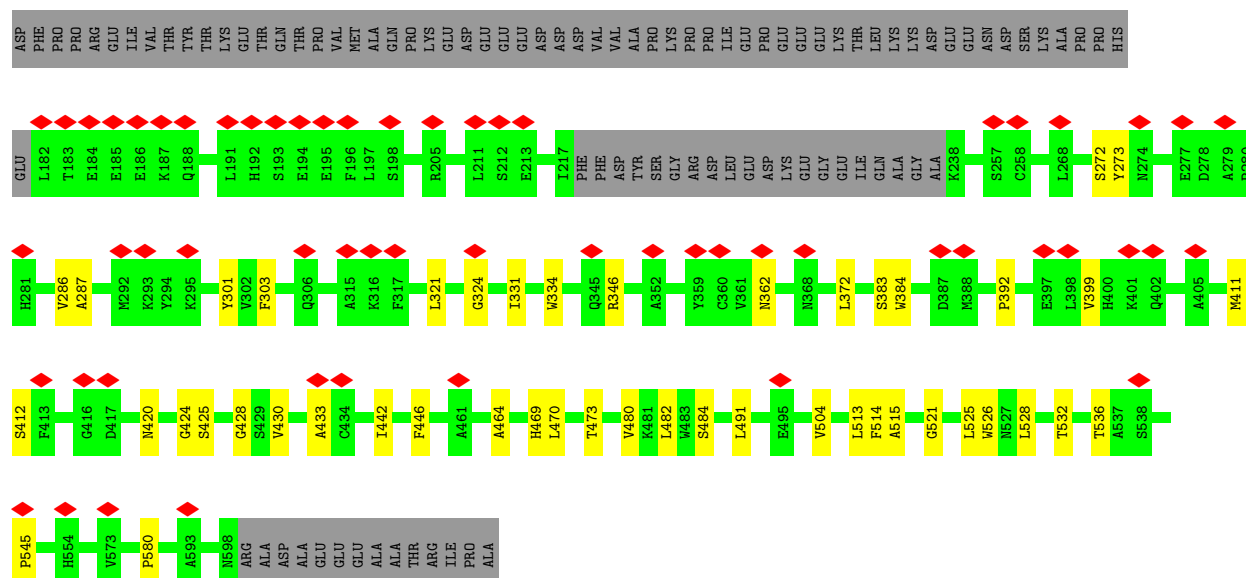


- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

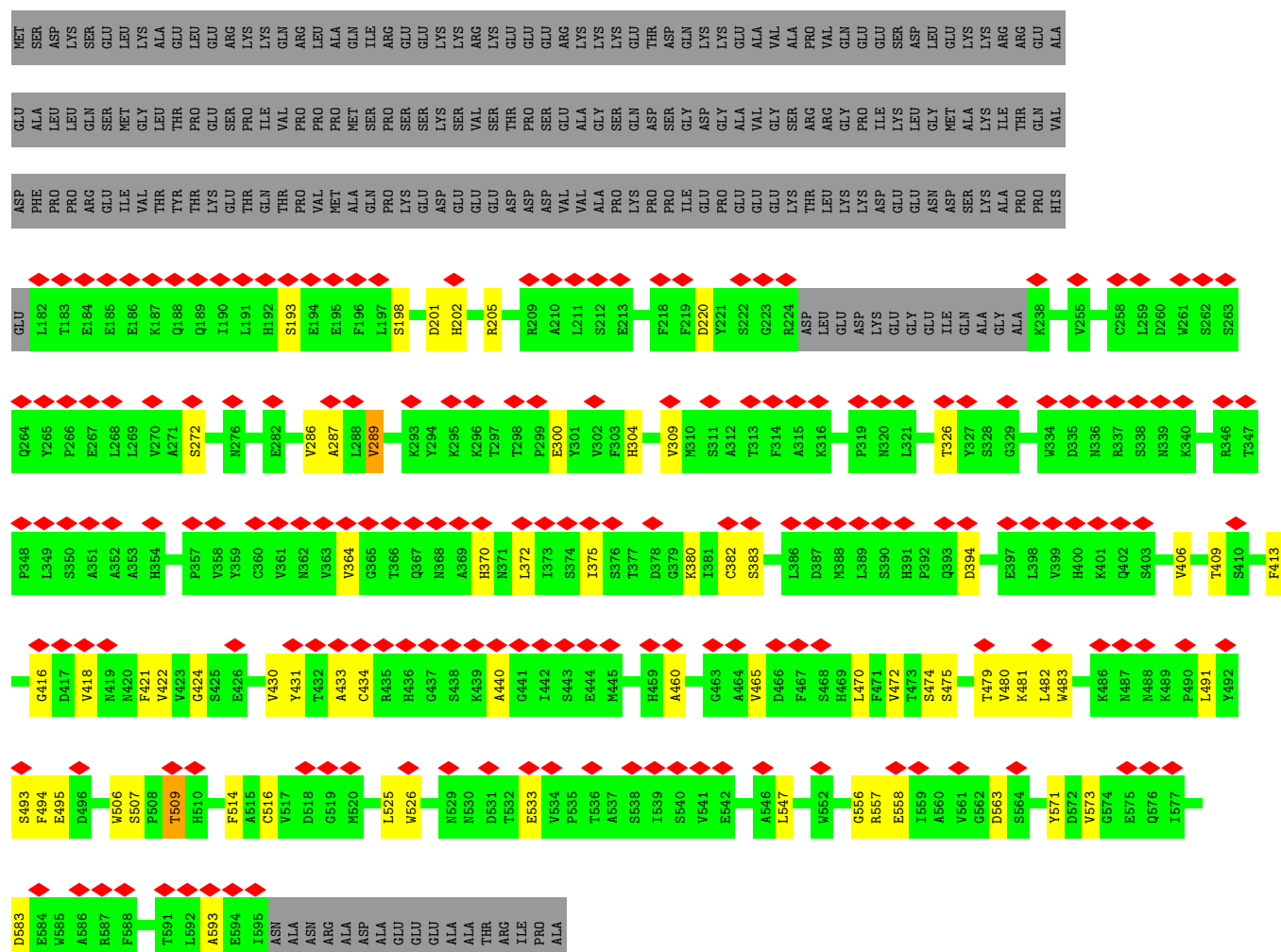


- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

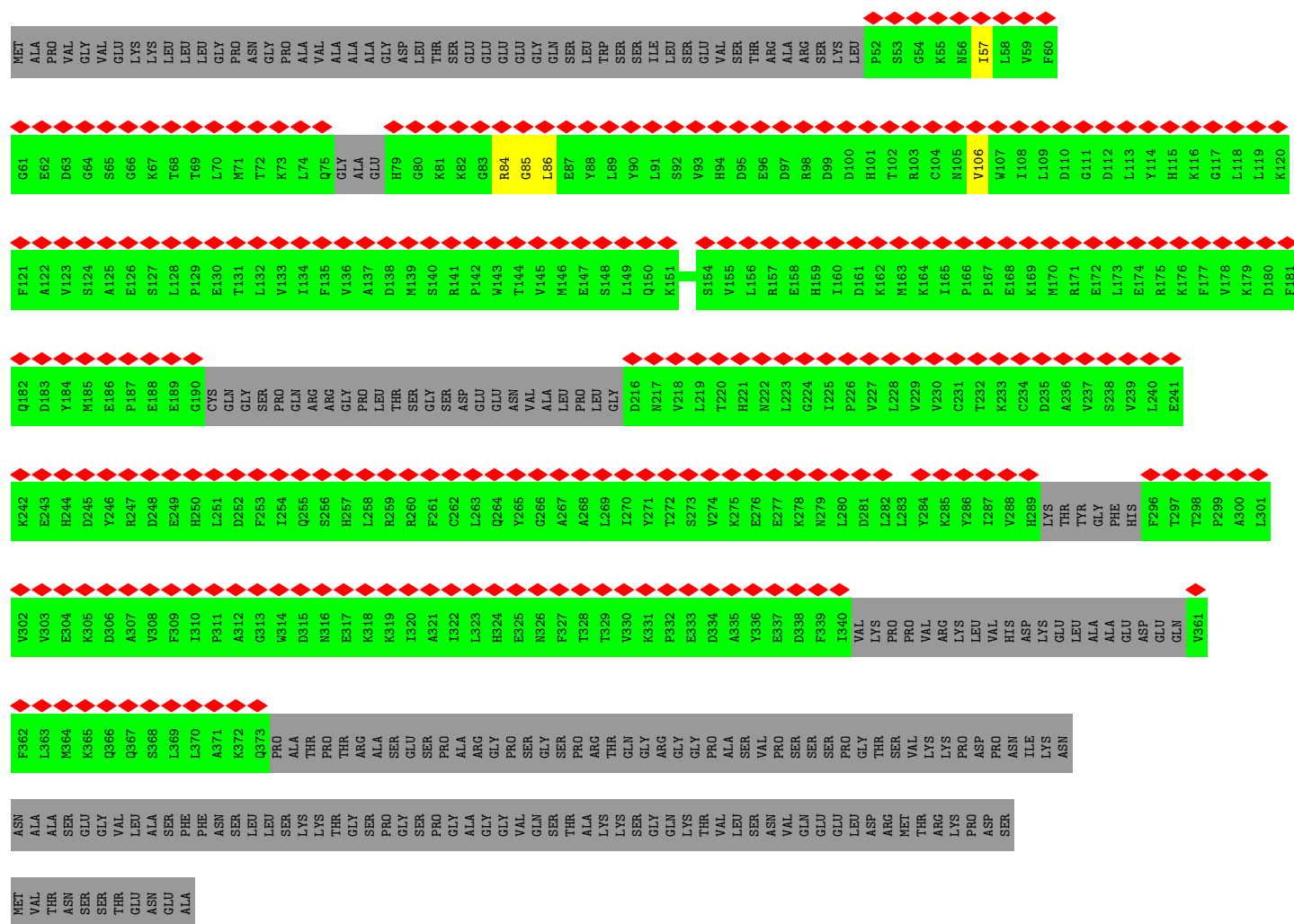




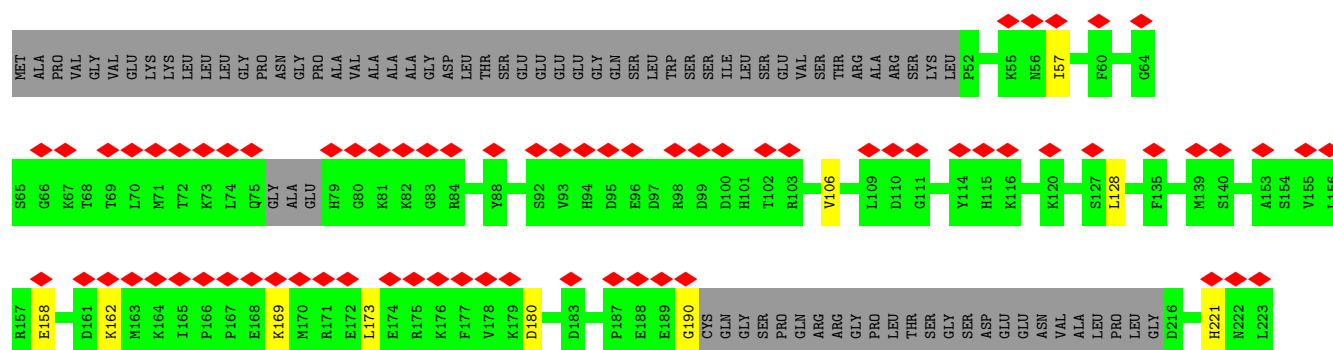
• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

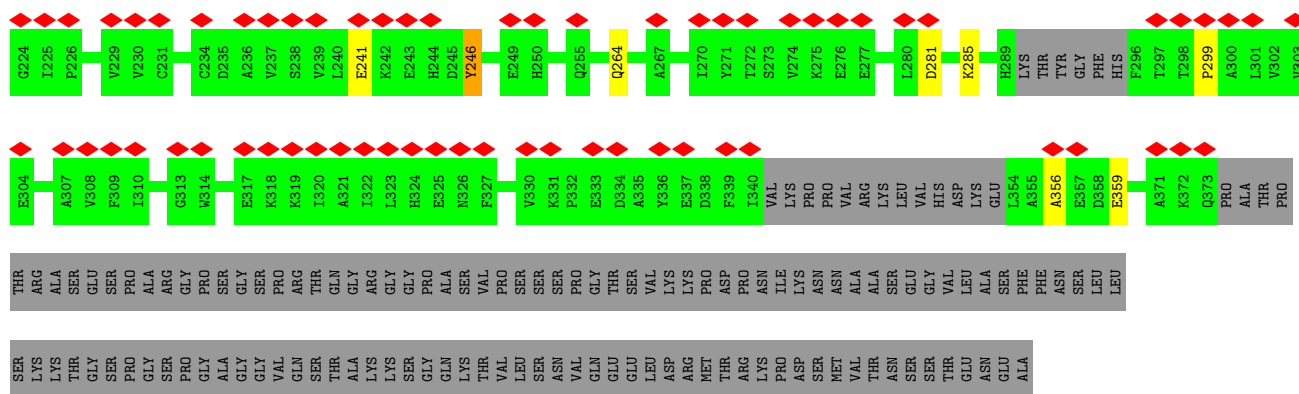


• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

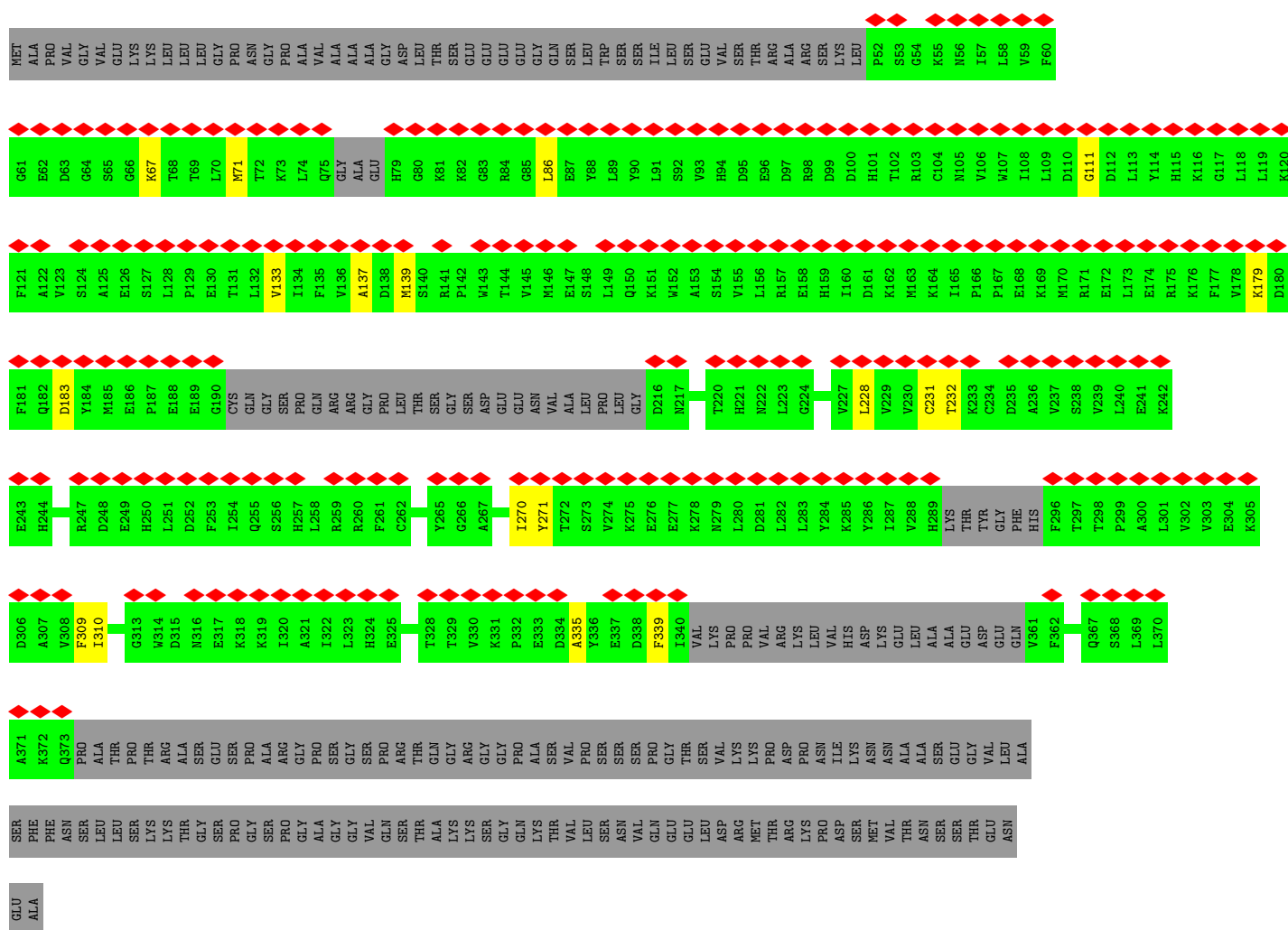


• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2



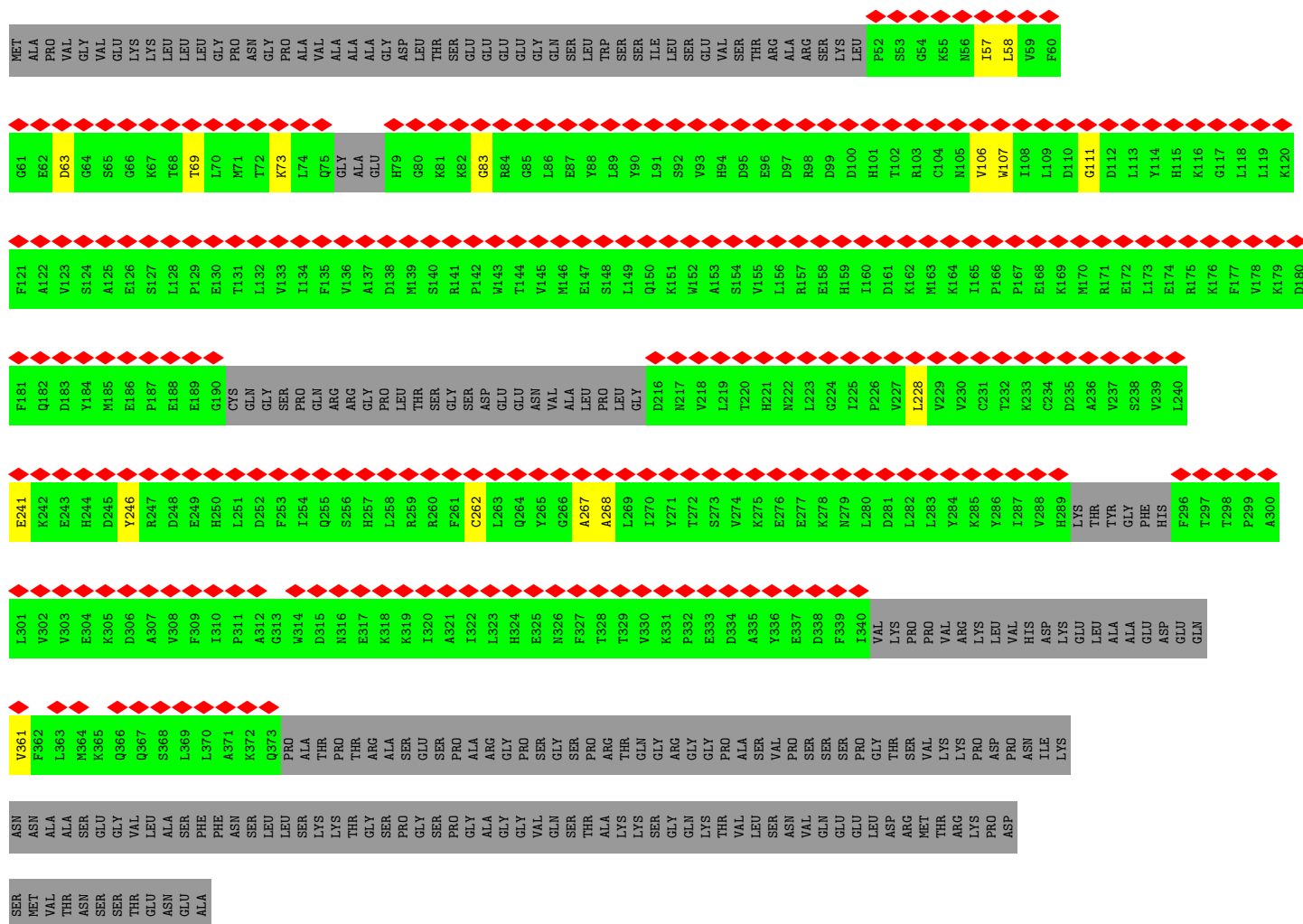


• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

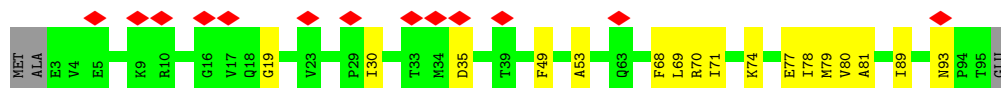


• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

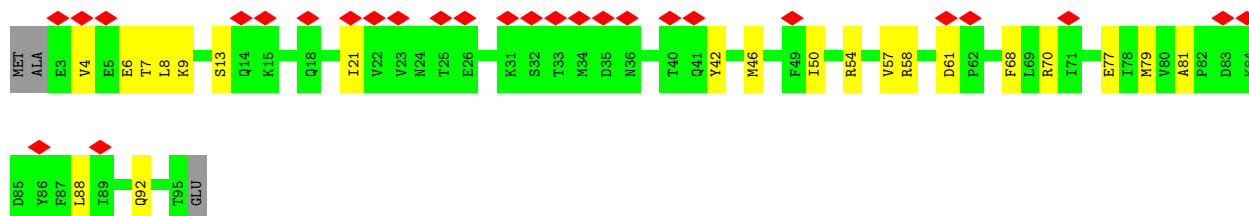
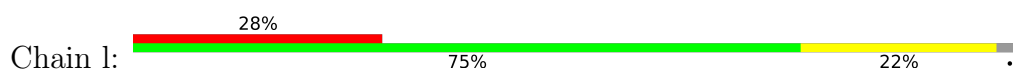




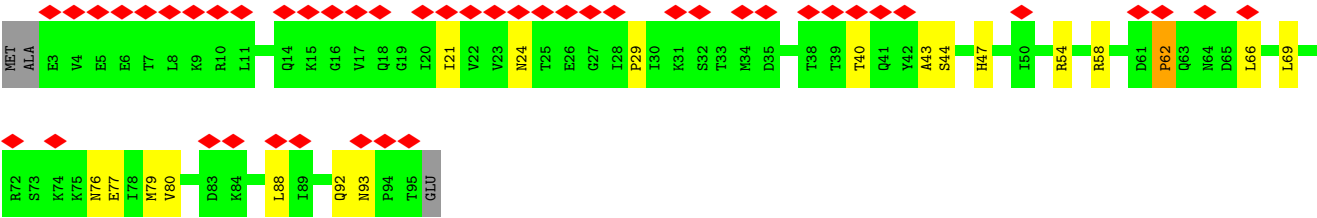
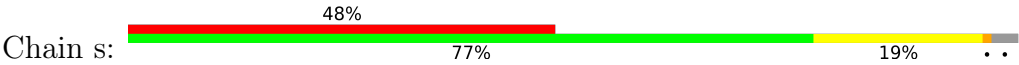
• Molecule 22: Dynein light chain roadblock-type 1



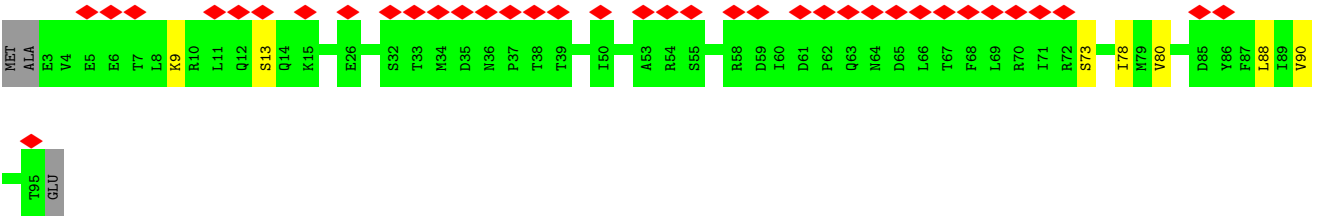
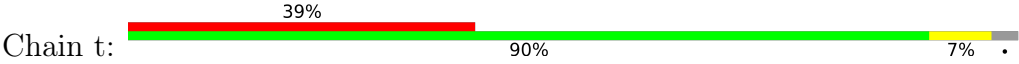
• Molecule 22: Dynein light chain roadblock-type 1



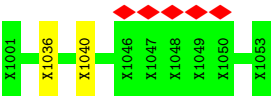
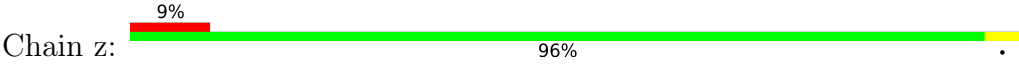
• Molecule 22: Dynein light chain roadblock-type 1



• Molecule 22: Dynein light chain roadblock-type 1



• Molecule 23: Dynactin Subunit 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23407	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.237	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	852.0, 852.0, 852.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.42, 1.42, 1.42	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	0/1820	1.09	2/2529 (0.1%)
1	B	0.59	0/1821	1.16	8/2531 (0.3%)
1	C	0.58	0/1821	1.19	5/2531 (0.2%)
1	D	0.60	0/1821	1.15	4/2531 (0.2%)
1	E	0.61	0/1821	1.22	10/2531 (0.4%)
1	F	0.61	0/1821	1.17	8/2531 (0.3%)
1	G	0.68	1/1821 (0.1%)	1.25	10/2531 (0.4%)
1	I	0.55	0/1821	1.14	2/2531 (0.1%)
2	H	0.58	0/1821	1.11	6/2531 (0.2%)
3	J	0.56	0/1816	1.25	5/2522 (0.2%)
4	K	0.47	0/1377	1.12	3/1919 (0.2%)
5	L	0.54	0/1326	1.06	1/1844 (0.1%)
10	U	0.43	0/841	0.92	0/1168
11	V	0.28	0/811	0.82	1/1126 (0.1%)
15	a	0.53	0/257	1.27	1/356 (0.3%)
16	b	0.59	0/367	1.25	4/507 (0.8%)
17	c	0.45	0/182	1.11	1/251 (0.4%)
18	d	0.37	0/118	1.04	0/163
19	e	0.30	0/4593	0.79	6/6403 (0.1%)
19	f	0.39	0/4608	1.03	11/6424 (0.2%)
19	m	0.39	0/4593	0.97	23/6403 (0.4%)
19	n	0.34	0/4603	0.88	8/6417 (0.1%)
20	g	0.29	0/1959	0.97	0/2725
20	h	0.38	0/1972	1.13	6/2741 (0.2%)
20	o	0.38	1/1959 (0.1%)	1.12	7/2725 (0.3%)
20	p	0.35	0/1975	1.00	5/2747 (0.2%)
21	i	0.27	0/1322	0.73	0/1835
21	j	0.41	0/1357	1.14	2/1884 (0.1%)
21	q	0.28	0/1322	0.81	0/1835
21	r	0.29	0/1322	0.85	2/1835 (0.1%)
22	k	0.29	0/461	0.84	4/642 (0.6%)
22	l	0.35	0/461	0.84	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	s	0.49	0/461	1.12	2/642 (0.3%)
22	t	0.37	0/461	0.99	0/642
All	All	0.45	2/56912 (0.0%)	1.04	147/79175 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	65	HIS	CA-CB	-11.55	1.35	1.53
20	o	301	TYR	CA-CB	-6.00	1.44	1.53

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	247	ASP	CA-C-N	17.02	144.06	120.39
3	J	247	ASP	C-N-CA	17.02	144.06	120.39
20	o	412	SER	CA-C-N	12.93	153.34	121.80
20	o	412	SER	C-N-CA	12.93	153.34	121.80
1	F	47	VAL	N-CA-C	-9.91	103.79	111.62
19	m	1030	PRO	N-CA-CB	9.18	112.88	103.25
1	E	155	GLY	N-CA-C	9.11	121.28	112.08
19	m	799	ASN	N-CA-C	8.89	120.66	110.97
19	f	1030	PRO	N-CA-CB	8.82	112.51	103.25
19	n	1030	PRO	N-CA-CB	8.82	112.51	103.25
2	H	252	ASN	CA-C-N	8.53	133.61	120.82
2	H	252	ASN	C-N-CA	8.53	133.61	120.82
1	F	112	GLU	CA-C-N	7.97	140.96	122.31
1	F	112	GLU	C-N-CA	7.97	140.96	122.31
19	e	1030	PRO	N-CA-CB	7.91	111.55	103.25
19	m	1027	PRO	N-CA-CB	7.67	111.31	103.25
19	f	1033	LEU	N-CA-C	7.50	119.36	111.03
1	G	331	SER	CA-C-N	7.49	140.07	121.80
1	G	331	SER	C-N-CA	7.49	140.07	121.80
1	B	17	GLY	N-CA-C	-7.29	102.17	112.37
19	f	1027	PRO	N-CA-CB	7.21	110.81	103.25
1	G	330	ILE	CA-C-N	7.19	134.67	122.15
1	G	330	ILE	C-N-CA	7.19	134.67	122.15
20	h	418	VAL	CA-C-N	7.13	135.16	121.54
20	h	418	VAL	C-N-CA	7.13	135.16	121.54
1	D	47	VAL	N-CA-C	-7.13	106.13	112.12
19	e	997	PRO	N-CA-CB	7.09	110.06	103.46
1	G	28	ASP	CA-C-N	7.04	131.38	120.82
1	G	28	ASP	C-N-CA	7.04	131.38	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	97	ASP	N-CA-C	-7.03	104.35	114.12
20	h	557	ARG	CA-C-N	6.98	134.87	121.54
20	h	557	ARG	C-N-CA	6.98	134.87	121.54
11	V	149	CYS	N-CA-C	-6.96	103.03	112.35
20	h	364	VAL	N-CA-C	-6.93	106.74	113.53
19	e	1027	PRO	N-CA-CB	6.90	110.50	103.25
19	m	997	PRO	N-CA-CB	6.86	110.45	103.25
20	p	418	VAL	N-CA-C	-6.79	106.10	112.83
19	n	566	ALA	N-CA-C	6.75	118.64	111.28
19	m	309	ARG	CA-C-N	6.75	130.23	120.38
19	m	309	ARG	C-N-CA	6.75	130.23	120.38
1	F	132	PHE	N-CA-C	-6.69	101.52	110.55
17	c	50	PRO	N-CA-CB	6.69	110.36	103.00
19	n	1027	PRO	N-CA-CB	6.65	110.57	103.52
19	n	997	PRO	N-CA-CB	6.64	110.22	103.25
19	f	200	ILE	N-CA-C	-6.53	104.28	110.42
19	f	823	VAL	N-CA-C	6.51	113.18	106.21
20	h	558	GLU	N-CA-C	-6.32	97.34	110.80
19	m	1009	HIS	CA-C-N	6.30	133.58	121.54
19	m	1009	HIS	C-N-CA	6.30	133.58	121.54
1	F	256	PHE	N-CA-C	-6.22	107.53	114.62
19	e	626	GLN	CA-C-N	6.18	128.74	120.58
19	e	626	GLN	C-N-CA	6.18	128.74	120.58
19	f	85	LYS	CA-C-N	6.18	131.37	122.35
19	f	85	LYS	C-N-CA	6.18	131.37	122.35
20	o	425	SER	CA-C-N	6.12	130.00	120.82
20	o	425	SER	C-N-CA	6.12	130.00	120.82
1	C	54	GLY	N-CA-C	-6.11	98.71	113.18
1	E	113	ALA	N-CA-C	-6.03	100.86	109.24
1	G	274	GLY	N-CA-C	-6.03	98.89	113.18
19	f	997	PRO	N-CA-CB	6.00	110.16	103.44
1	A	250	GLU	CA-C-N	-5.97	116.83	123.16
1	A	250	GLU	C-N-CA	-5.97	116.83	123.16
20	p	289	VAL	CA-C-N	5.96	130.19	121.31
20	p	289	VAL	C-N-CA	5.96	130.19	121.31
21	r	83	GLY	CA-C-N	5.96	132.92	121.54
21	r	83	GLY	C-N-CA	5.96	132.92	121.54
3	J	94	SER	N-CA-C	-5.89	97.24	107.49
3	J	301	GLU	N-CA-C	-5.86	104.82	111.14
1	G	331	SER	N-CA-C	5.83	117.59	109.31
1	D	31	PRO	N-CA-C	-5.82	100.48	112.47
1	C	113	ALA	CA-C-N	-5.75	113.77	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ALA	C-N-CA	-5.75	113.77	119.92
1	E	132	PHE	N-CA-C	-5.73	102.03	110.52
1	B	130	GLU	N-CA-C	-5.72	104.45	112.12
2	H	64	ILE	N-CA-C	-5.68	107.35	112.12
1	B	141	MET	CA-C-N	5.67	128.45	120.28
1	B	141	MET	C-N-CA	5.67	128.45	120.28
22	k	30	ILE	N-CA-C	-5.67	107.14	111.62
1	F	187	GLY	N-CA-C	5.65	126.58	113.18
19	n	1029	GLY	CA-C-N	5.65	126.90	119.84
19	n	1029	GLY	C-N-CA	5.65	126.90	119.84
1	C	132	PHE	N-CA-C	-5.61	102.21	110.52
22	k	35	ASP	CA-C-N	5.59	127.96	120.58
22	k	35	ASP	C-N-CA	5.59	127.96	120.58
20	o	428	GLY	N-CA-C	-5.58	99.95	113.18
22	s	62	PRO	N-CA-C	5.57	123.95	112.47
20	p	509	THR	N-CA-C	-5.57	106.65	113.50
1	I	260	GLU	CA-C-N	5.55	132.15	121.54
1	I	260	GLU	C-N-CA	5.55	132.15	121.54
22	s	21	ILE	N-CA-CB	-5.50	106.78	112.28
16	b	59	PHE	N-CA-C	-5.47	101.99	109.71
5	L	157	GLN	N-CA-C	-5.42	101.49	109.62
1	E	329	ARG	N-CA-C	-5.42	100.59	109.80
1	G	37	ASN	N-CA-C	5.41	117.33	109.71
21	j	128	LEU	N-CA-C	5.40	121.74	109.81
19	m	372	TYR	CA-C-N	5.39	125.69	119.93
19	m	372	TYR	C-N-CA	5.39	125.69	119.93
1	B	205	PHE	CA-C-N	5.37	128.22	120.38
1	B	205	PHE	C-N-CA	5.37	128.22	120.38
1	F	241	TYR	N-CA-C	-5.35	102.84	110.59
2	H	374	CYS	CA-C-N	5.34	131.32	121.70
2	H	374	CYS	C-N-CA	5.34	131.32	121.70
19	m	1029	GLY	CA-C-N	5.33	126.50	119.84
19	m	1029	GLY	C-N-CA	5.33	126.50	119.84
4	K	61	GLN	CA-C-O	-5.33	111.02	119.23
19	m	1006	VAL	CA-C-N	5.32	131.84	121.41
19	m	1006	VAL	C-N-CA	5.32	131.84	121.41
1	E	359	SER	CA-C-N	5.31	131.68	121.54
1	E	359	SER	C-N-CA	5.31	131.68	121.54
19	n	536	LEU	CA-C-N	5.30	131.67	121.54
19	n	536	LEU	C-N-CA	5.30	131.67	121.54
19	m	131	VAL	N-CA-C	5.28	115.42	110.30
1	F	332	ALA	N-CA-C	5.26	121.44	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	e	136	ARG	N-CA-C	-5.26	101.57	109.15
19	m	1041	MET	CA-C-N	5.26	129.79	120.74
19	m	1041	MET	C-N-CA	5.26	129.79	120.74
4	K	276	SER	CA-C-N	5.26	131.58	121.54
4	K	276	SER	C-N-CA	5.26	131.58	121.54
20	p	193	SER	N-CA-C	-5.25	101.22	109.25
21	j	180	ASP	N-CA-C	-5.24	104.95	112.13
19	m	222	GLU	CA-C-N	5.24	131.55	121.54
19	m	222	GLU	C-N-CA	5.24	131.55	121.54
2	H	285	CYS	N-CA-C	5.21	114.92	108.19
20	o	346	ARG	CA-C-N	5.21	127.88	120.49
20	o	346	ARG	C-N-CA	5.21	127.88	120.49
3	J	337	GLY	N-CA-C	-5.18	100.91	113.18
1	E	330	ILE	N-CA-C	5.17	116.16	108.46
19	f	1051	VAL	N-CA-C	-5.15	107.32	111.91
1	E	335	GLU	CA-C-N	5.15	131.38	121.54
1	E	335	GLU	C-N-CA	5.15	131.38	121.54
1	E	175	ALA	N-CA-C	5.15	117.32	110.53
19	f	727	GLY	N-CA-C	5.14	125.37	113.18
1	B	304	SER	CA-C-N	5.14	133.54	121.52
1	B	304	SER	C-N-CA	5.14	133.54	121.52
22	k	19	GLY	N-CA-C	-5.13	101.02	113.18
16	b	19	VAL	N-CA-C	-5.11	102.26	109.21
19	m	829	LEU	CA-C-N	5.11	129.64	121.62
19	m	829	LEU	C-N-CA	5.11	129.64	121.62
1	D	337	LEU	CA-C-N	5.10	127.83	120.38
1	D	337	LEU	C-N-CA	5.10	127.83	120.38
1	C	36	PRO	N-CA-C	5.09	118.60	111.33
16	b	12	ILE	CA-C-N	5.09	128.30	120.82
16	b	12	ILE	C-N-CA	5.09	128.30	120.82
19	f	321	GLY	N-CA-C	-5.06	101.19	113.18
19	m	76	THR	N-CA-C	5.04	117.19	109.07
19	m	405	ALA	N-CA-C	-5.04	100.57	108.63
15	a	20	TYR	CB-CA-C	-5.03	104.57	112.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1821	0	819	17	0
1	B	1822	0	820	21	0
1	C	1822	0	820	19	0
1	D	1822	0	820	18	0
1	E	1822	0	820	26	0
1	F	1822	0	820	17	0
1	G	1822	0	820	24	0
1	I	1822	0	820	23	0
2	H	1822	0	835	22	0
3	J	1819	0	794	18	0
4	K	1378	0	611	22	0
5	L	1327	0	585	26	0
6	M	2935	0	603	11	0
7	N	3080	0	634	8	0
8	O	323	0	76	6	0
8	P	323	0	76	10	0
9	Q	435	0	94	3	0
9	R	435	0	93	1	0
10	U	843	0	376	5	0
11	V	812	0	344	20	0
12	X	1115	0	225	1	0
12	x	1110	0	224	2	0
13	Y	1320	0	353	19	0
14	Z	260	0	56	0	0
15	a	259	0	110	4	0
16	b	369	0	161	4	0
17	c	184	0	80	5	0
18	d	119	0	50	0	0
19	e	4598	0	2028	21	0
19	f	4613	0	2037	29	0
19	m	4598	0	2028	18	0
19	n	4608	0	2035	25	0
20	g	1961	0	883	43	0
20	h	1975	0	886	32	0
20	o	1961	0	883	23	0
20	p	1977	0	888	39	0
21	i	1327	0	574	5	0
21	j	1362	0	594	8	0
21	q	1327	0	574	10	0
21	r	1327	0	574	9	0
22	k	462	0	192	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	l	462	0	192	15	0
22	s	462	0	192	9	0
22	t	462	0	192	4	0
23	z	265	0	59	1	0
24	A	27	0	12	1	0
24	B	27	0	12	2	0
24	C	27	0	12	1	0
24	D	27	0	12	2	0
24	E	27	0	12	2	0
24	F	27	0	12	2	0
24	G	27	0	12	2	0
24	I	27	0	12	1	0
24	J	27	0	12	3	0
25	H	31	0	12	1	0
All	All	68864	0	27870	613	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 6.

All (613) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:VAL:O	1:F:71:ILE:HA	1.55	1.05
8:O:37:UNK:HA	8:O:73:UNK:O	1.61	0.99
21:r:57:ILE:O	21:r:106:VAL:HA	1.61	0.99
2:H:154:ASP:O	2:H:160:THR:HA	1.65	0.97
8:P:64:UNK:HA	8:P:76:UNK:O	1.64	0.96
11:V:85:LEU:HA	11:V:102:ALA:O	1.65	0.95
1:E:40:GLY:HA2	1:E:70:SER:O	1.66	0.95
22:s:80:VAL:HA	22:s:88:LEU:O	1.66	0.95
8:P:33:UNK:HA	8:P:77:UNK:O	1.69	0.92
20:o:321:LEU:HA	20:o:334:TRP:O	1.68	0.92
20:g:360:CYS:O	20:g:374:SER:HA	1.70	0.90
20:g:505:MET:O	20:g:515:ALA:HB3	1.71	0.90
20:p:364:VAL:O	20:p:370:HIS:HA	1.73	0.89
11:V:97:CYS:HA	11:V:114:CYS:O	1.73	0.89
1:F:240:GLN:HA	1:F:249:ILE:O	1.73	0.88
4:K:158:ILE:O	4:K:174:ARG:HA	1.71	0.88
20:o:372:LEU:O	20:o:383:SER:HA	1.73	0.88
4:K:143:VAL:HA	4:K:155:ILE:O	1.73	0.88
22:k:70:ARG:HA	22:k:78:ILE:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:119:VAL:HA	5:L:131:VAL:O	1.74	0.87
20:h:372:LEU:O	20:h:383:SER:HA	1.75	0.86
5:L:177:LEU:O	5:L:188:ASN:HA	1.76	0.84
4:K:188:VAL:O	4:K:213:GLN:HA	1.78	0.84
20:h:470:LEU:HA	20:h:483:TRP:O	1.77	0.83
1:F:41:ARG:O	1:F:69:LEU:HA	1.77	0.83
19:e:1044:VAL:N	21:i:84:ARG:CB	2.40	0.82
20:p:470:LEU:HA	20:p:483:TRP:O	1.78	0.82
1:E:39:VAL:O	1:E:71:ILE:HA	1.79	0.81
1:B:240:GLN:HA	1:B:249:ILE:O	1.80	0.81
1:B:154:THR:HA	1:B:170:ILE:O	1.80	0.80
2:H:18:LYS:HA	2:H:29:ALA:O	1.81	0.80
1:G:108:VAL:O	1:G:137:LEU:HA	1.81	0.79
1:A:110:LEU:O	1:A:139:ILE:HA	1.82	0.79
22:t:80:VAL:HA	22:t:88:LEU:O	1.83	0.79
5:L:70:SER:HA	5:L:80:ASP:O	1.83	0.77
20:p:382:CYS:HA	20:p:394:ASP:O	1.85	0.77
1:G:41:ARG:O	1:G:69:LEU:HA	1.85	0.77
22:t:78:ILE:HA	22:t:90:VAL:O	1.86	0.76
4:K:156:ALA:O	4:K:176:GLU:HA	1.85	0.75
19:e:817:ALA:O	19:e:821:ALA:HB2	1.85	0.75
20:o:420:ASN:HA	20:o:433:ALA:O	1.86	0.75
1:I:108:VAL:O	1:I:137:LEU:HA	1.86	0.75
20:h:514:PHE:O	20:h:525:LEU:HA	1.87	0.74
19:e:1047:VAL:CB	21:i:86:LEU:O	2.36	0.74
4:K:197:HIS:HA	4:K:204:VAL:O	1.88	0.73
2:H:105:LEU:O	2:H:134:VAL:HA	1.89	0.73
1:I:39:VAL:O	1:I:71:ILE:HA	1.88	0.73
8:P:65:UNK:O	8:P:75:UNK:HA	1.88	0.73
20:o:473:THR:O	20:o:480:VAL:HA	1.88	0.73
1:B:20:VAL:HA	1:B:36:PRO:HA	1.71	0.72
1:E:243:LEU:N	1:E:247:SER:O	2.21	0.72
5:L:144:ILE:HA	5:L:178:GLN:O	1.90	0.72
1:G:156:VAL:HA	1:G:168:VAL:O	1.89	0.71
22:l:21:ILE:O	22:l:88:LEU:HA	1.90	0.71
20:g:471:PHE:O	20:g:482:LEU:HA	1.89	0.71
1:G:157:VAL:O	1:G:167:ALA:HA	1.92	0.70
20:p:474:SER:HA	20:p:480:VAL:HA	1.74	0.70
21:r:63:ASP:H	21:r:111:GLY:H	1.40	0.69
1:G:241:TYR:O	1:G:248:THR:HA	1.93	0.69
1:E:303:GLY:H	24:E:800:ADP:H5'2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:528:UNK:O	13:Y:605:UNK:HA	1.93	0.69
10:U:146:ALA:HB2	11:V:149:CYS:CB	2.23	0.68
20:g:245:PHE:O	20:g:567:GLN:HA	1.93	0.68
20:g:358:VAL:HA	20:g:376:SER:HA	1.75	0.68
20:g:324:GLY:O	20:g:331:ILE:HA	1.94	0.68
20:g:285:GLY:HA2	20:g:309:VAL:H	1.58	0.68
20:o:504:VAL:HA	20:o:515:ALA:O	1.93	0.68
1:I:110:LEU:O	1:I:139:ILE:HA	1.93	0.67
1:D:160:SER:H	1:D:302:GLY:HA3	1.60	0.67
5:L:73:SER:O	5:L:77:ASN:N	2.27	0.67
20:g:309:VAL:HA	20:g:326:THR:HA	1.75	0.66
1:E:332:ALA:H	15:a:18:ASP:HA	1.60	0.66
1:E:95:SER:O	1:E:99:LEU:N	2.27	0.66
20:p:494:PHE:HA	20:p:533:GLU:HA	1.76	0.66
20:h:286:VAL:HA	20:h:303:PHE:O	1.96	0.66
1:E:156:VAL:HA	1:E:168:VAL:O	1.95	0.66
19:f:221:TYR:HA	19:f:225:GLU:HA	1.77	0.65
20:h:260:ASP:O	20:h:269:LEU:HA	1.96	0.65
20:p:481:LYS:HA	20:p:493:SER:HA	1.78	0.65
22:k:69:LEU:O	22:k:79:MET:HA	1.96	0.65
20:g:522:ARG:HA	20:g:540:SER:HA	1.78	0.64
19:e:631:GLN:H	20:g:546:ALA:H	1.45	0.64
1:A:20:VAL:HA	1:A:36:PRO:HA	1.78	0.64
20:h:515:ALA:HA	20:h:524:ASP:O	1.97	0.64
20:p:516:CYS:H	20:p:525:LEU:HA	1.63	0.64
13:Y:517:UNK:O	13:Y:525:UNK:N	2.31	0.64
13:Y:508:UNK:N	13:Y:534:UNK:O	2.32	0.63
20:h:472:VAL:HA	20:h:481:LYS:O	1.99	0.63
20:g:498:ALA:HB3	20:g:519:GLY:H	1.64	0.62
20:p:272:SER:HA	20:p:287:ALA:HA	1.80	0.62
20:g:558:GLU:HA	20:g:573:VAL:H	1.63	0.62
1:E:241:TYR:O	1:E:248:THR:HA	2.00	0.62
11:V:146:PHE:HA	11:V:153:PHE:HA	1.82	0.62
20:g:513:LEU:HA	20:g:526:TRP:O	1.98	0.62
5:L:159:LYS:H	5:L:165:ALA:HA	1.65	0.61
22:s:69:LEU:O	22:s:79:MET:HA	1.99	0.61
3:J:186:ASP:HA	3:J:194:SER:HA	1.81	0.61
20:g:286:VAL:HA	20:g:303:PHE:O	2.00	0.61
4:K:154:ILE:O	4:K:178:LYS:HA	2.01	0.61
19:m:114:ASN:HA	19:m:141:SER:HA	1.83	0.61
1:I:41:ARG:O	1:I:69:LEU:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:559:ILE:H	20:g:572:ASP:HA	1.66	0.61
1:C:95:SER:O	1:C:99:LEU:N	2.34	0.60
2:H:88:HIS:O	2:H:92:ASN:CB	2.49	0.60
1:G:95:SER:O	1:G:99:LEU:N	2.31	0.60
1:G:216:ALA:O	1:G:220:ARG:CB	2.49	0.60
2:H:91:TYR:HA	2:H:95:ARG:HA	1.82	0.60
1:D:42:PRO:HA	1:D:69:LEU:HA	1.83	0.60
1:C:160:SER:H	1:C:302:GLY:HA3	1.65	0.60
19:f:1013:THR:HA	19:f:1033:LEU:HA	1.81	0.60
1:E:243:LEU:C	1:E:245:ASP:H	2.10	0.60
20:h:285:GLY:N	20:h:305:CYS:O	2.35	0.60
20:o:362:ASN:O	20:o:372:LEU:HA	2.02	0.60
20:h:522:ARG:HA	20:h:540:SER:HA	1.83	0.60
19:n:69:LEU:HA	19:n:125:ILE:H	1.67	0.60
1:F:156:VAL:HA	1:F:169:PRO:HA	1.83	0.59
1:B:332:ALA:HB3	17:c:43:VAL:HA	1.84	0.59
19:f:40:LEU:HA	19:f:45:GLY:HA2	1.84	0.59
19:f:911:LEU:O	19:f:915:LEU:CB	2.50	0.59
21:q:271:TYR:H	21:q:309:PHE:HA	1.67	0.59
20:h:258:CYS:O	20:h:271:ALA:HA	2.03	0.59
1:D:20:VAL:HA	1:D:36:PRO:HA	1.85	0.59
5:L:136:LYS:O	5:L:148:TRP:CB	2.50	0.59
20:g:406:VAL:HA	20:g:425:SER:HA	1.84	0.59
1:I:111:THR:HA	1:I:140:SER:H	1.66	0.59
20:h:548:ASN:N	20:h:562:GLY:O	2.35	0.58
20:g:464:ALA:HB1	20:g:582:ASN:HA	1.85	0.58
22:k:80:VAL:HA	22:k:89:ILE:HA	1.84	0.58
1:B:219:GLU:O	24:B:800:ADP:N6	2.36	0.58
2:H:19:ALA:O	2:H:28:ARG:N	2.36	0.58
8:P:25:UNK:HA	8:P:36:UNK:HA	1.85	0.58
22:l:77:GLU:CB	22:l:92:GLN:O	2.52	0.58
20:g:257:SER:N	20:g:272:SER:O	2.37	0.58
19:f:847:VAL:O	19:f:851:LEU:CB	2.51	0.58
4:K:171:GLY:HA2	4:K:196:VAL:HA	1.86	0.58
1:G:293:THR:O	1:G:297:ASN:N	2.36	0.57
1:I:216:ALA:O	1:I:220:ARG:CB	2.52	0.57
21:i:57:ILE:O	21:i:106:VAL:HA	2.03	0.57
20:p:424:GLY:HA2	20:p:430:VAL:HA	1.86	0.57
1:B:329:ARG:HA	17:c:46:ILE:HA	1.85	0.57
2:H:153:MET:HA	2:H:161:HIS:O	2.04	0.57
19:f:80:GLU:HA	19:f:115:SER:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:176:ASP:N	19:n:193:LEU:O	2.38	0.57
19:m:145:PRO:O	19:m:149:LEU:CB	2.52	0.57
20:g:559:ILE:CB	20:g:571:TYR:O	2.53	0.57
1:G:18:SER:N	24:G:800:ADP:O3B	2.37	0.57
20:g:550:VAL:HA	20:g:561:VAL:HA	1.85	0.57
20:h:455:GLY:HA3	20:h:503:ASP:HA	1.86	0.57
5:L:169:LEU:O	5:L:196:GLN:HA	2.04	0.57
19:n:24:VAL:HA	19:n:126:ASP:HA	1.87	0.57
19:f:84:LEU:O	19:f:97:GLU:HA	2.05	0.57
20:o:470:LEU:HA	20:o:484:SER:HA	1.86	0.57
21:q:137:ALA:HB3	21:q:231:CYS:HA	1.87	0.57
20:p:416:GLY:HA3	20:p:460:ALA:HA	1.87	0.57
4:K:255:PHE:O	4:K:259:ARG:N	2.37	0.56
5:L:149:ASP:O	5:L:173:VAL:HA	2.05	0.56
8:P:26:UNK:O	8:P:35:UNK:N	2.38	0.56
20:p:422:VAL:HA	20:p:431:TYR:O	2.03	0.56
1:I:160:SER:H	1:I:302:GLY:HA2	1.70	0.56
19:n:754:LYS:HA	20:p:406:VAL:HA	1.86	0.56
1:F:60:PRO:O	1:F:64:GLU:CB	2.53	0.56
5:L:115:GLY:HA2	5:L:135:LYS:O	2.05	0.56
19:f:217:ALA:O	19:f:221:TYR:CB	2.53	0.56
19:n:145:PRO:O	19:n:149:LEU:CB	2.53	0.56
2:H:160:THR:CB	2:H:178:LEU:O	2.54	0.56
2:H:264:PRO:O	2:H:268:GLY:N	2.39	0.56
20:h:461:ALA:HB3	20:h:465:VAL:H	1.71	0.56
3:J:30:ALA:HB1	3:J:363:ALA:HA	1.86	0.56
19:n:39:PRO:O	19:n:43:GLU:N	2.34	0.56
1:E:20:VAL:HA	1:E:36:PRO:HA	1.86	0.56
19:e:538:VAL:O	19:e:542:GLY:N	2.39	0.56
19:n:642:PRO:O	19:n:646:GLY:N	2.39	0.56
2:H:240:TYR:O	2:H:247:VAL:HA	2.06	0.56
1:B:60:PRO:O	1:B:64:GLU:CB	2.54	0.56
1:C:331:SER:N	15:a:46:GLU:O	2.33	0.56
1:G:373:ARG:O	16:b:71:PHE:N	2.39	0.56
4:K:185:THR:HA	4:K:217:THR:HA	1.86	0.56
4:K:141:CYS:HA	4:K:157:CYS:O	2.05	0.56
20:h:241:LEU:HA	20:h:571:TYR:HA	1.88	0.56
19:n:114:ASN:HA	19:n:141:SER:HA	1.86	0.56
1:C:156:VAL:HA	1:C:168:VAL:O	2.06	0.55
3:J:134:ASN:O	3:J:154:GLY:N	2.36	0.55
3:J:315:PHE:O	3:J:319:LEU:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:68:PHE:HA	22:k:81:ALA:HA	1.88	0.55
19:m:594:ARG:O	19:m:598:ARG:N	2.39	0.55
20:p:482:LEU:O	20:p:491:LEU:N	2.38	0.55
10:U:14:GLY:O	10:U:15:ALA:N	2.39	0.55
22:l:57:VAL:O	22:l:61:ASP:N	2.37	0.55
1:D:243:LEU:N	1:D:247:SER:O	2.39	0.55
1:G:153:THR:O	1:G:172:GLU:N	2.38	0.55
3:J:343:ILE:O	13:Y:493:UNK:N	2.40	0.55
19:m:995:SER:O	19:m:999:ILE:N	2.38	0.55
1:E:243:LEU:C	1:E:245:ASP:N	2.63	0.55
20:g:375:ILE:HA	20:g:381:ILE:HA	1.87	0.55
20:o:525:LEU:O	20:o:536:THR:N	2.40	0.55
5:L:12:LEU:O	5:L:16:LEU:N	2.40	0.55
19:e:852:ILE:O	19:e:856:LYS:CB	2.55	0.55
1:G:13:VAL:O	1:G:24:GLY:N	2.35	0.55
20:p:547:LEU:HA	20:p:563:ASP:HA	1.89	0.55
13:Y:14:UNK:N	13:Y:437:UNK:O	2.40	0.55
19:n:733:LEU:H	21:r:361:VAL:HA	1.72	0.55
3:J:343:ILE:N	13:Y:493:UNK:O	2.38	0.54
1:A:198:LEU:O	1:A:203:TYR:N	2.39	0.54
1:E:243:LEU:O	1:E:245:ASP:N	2.41	0.54
2:H:151:ILE:HA	2:H:163:VAL:O	2.07	0.54
20:p:286:VAL:HA	20:p:304:HIS:HA	1.90	0.54
21:r:241:GLU:HA	21:r:246:TYR:H	1.71	0.54
4:K:88:LEU:HA	4:K:94:ILE:O	2.08	0.54
19:e:118:PHE:HA	19:e:137:VAL:HA	1.89	0.54
19:n:117:ALA:O	19:n:137:VAL:HA	2.07	0.54
1:B:199:ARG:HA	1:B:203:TYR:H	1.73	0.54
1:C:21:ILE:O	1:C:34:CYS:HA	2.07	0.54
7:N:478:UNK:O	7:N:482:UNK:N	2.41	0.54
19:n:119:ILE:O	19:n:135:LEU:HA	2.08	0.54
1:G:162:ASP:O	1:G:188:ARG:N	2.33	0.54
21:j:221:HIS:N	21:j:264:GLN:O	2.37	0.54
22:t:9:LYS:O	22:t:13:SER:CB	2.56	0.54
4:K:253:THR:O	4:K:257:ALA:N	2.37	0.54
20:g:257:SER:H	20:g:273:TYR:HA	1.72	0.54
1:G:155:GLY:O	1:G:170:ILE:N	2.41	0.53
1:I:12:VAL:O	1:I:108:VAL:HA	2.08	0.53
11:V:109:HIS:O	11:V:128:ILE:N	2.41	0.53
22:s:76:ASN:HA	22:s:93:ASN:HA	1.90	0.53
20:g:420:ASN:HA	20:g:434:CYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:PRO:O	1:G:64:GLU:CB	2.57	0.53
4:K:95:SER:O	4:K:109:GLN:N	2.42	0.53
7:N:708:UNK:O	7:N:712:UNK:N	2.41	0.53
20:h:383:SER:O	20:h:393:GLN:N	2.41	0.53
20:p:198:SER:O	20:p:202:HIS:CB	2.57	0.53
21:r:228:LEU:HA	21:r:268:ALA:H	1.73	0.53
5:L:115:GLY:CA	5:L:135:LYS:O	2.56	0.53
19:e:582:PHE:HA	19:e:668:VAL:HA	1.91	0.53
1:B:23:ALA:O	1:B:32:LYS:N	2.42	0.53
1:G:110:LEU:O	1:G:139:ILE:HA	2.09	0.53
5:L:137:ALA:HA	5:L:147:CYS:HA	1.91	0.53
5:L:181:LYS:O	5:L:185:GLY:N	2.42	0.53
19:n:23:ASN:O	19:n:127:ALA:N	2.40	0.53
6:M:1:UNK:N	8:O:41:UNK:O	2.38	0.53
6:M:167:UNK:HA	6:M:705:UNK:HA	1.90	0.53
22:l:46:MET:O	22:l:50:ILE:CB	2.57	0.53
19:n:482:ARG:H	19:n:590:ALA:HB3	1.74	0.53
19:n:829:LEU:O	19:n:833:VAL:CB	2.57	0.52
11:V:112:LYS:O	11:V:131:ASN:N	2.36	0.52
21:j:158:GLU:O	21:j:162:LYS:CB	2.58	0.52
21:q:139:MET:N	21:q:232:THR:O	2.40	0.52
22:s:40:THR:O	22:s:44:SER:CB	2.57	0.52
5:L:66:ARG:HA	5:L:71:TYR:HA	1.91	0.52
5:L:117:SER:HA	5:L:133:LEU:O	2.09	0.52
1:G:154:THR:HA	1:G:171:TYR:HA	1.91	0.52
13:Y:517:UNK:N	13:Y:525:UNK:O	2.42	0.52
20:h:470:LEU:CA	20:h:483:TRP:O	2.54	0.52
1:B:275:ILE:O	1:B:279:LEU:CB	2.58	0.52
1:I:137:LEU:O	1:I:358:VAL:N	2.42	0.52
16:b:65:GLY:N	16:b:85:SER:O	2.40	0.52
13:Y:159:UNK:HA	13:Y:190:UNK:HA	1.91	0.52
20:g:312:ALA:HA	20:g:325:GLY:H	1.75	0.52
1:B:75:MET:HA	1:B:80:VAL:HA	1.92	0.52
19:e:406:TYR:O	19:e:410:GLU:CB	2.58	0.52
19:n:118:PHE:HA	19:n:136:ARG:O	2.10	0.52
7:N:483:UNK:O	7:N:487:UNK:N	2.43	0.52
19:f:53:GLU:O	19:f:57:GLU:CB	2.58	0.52
20:p:409:THR:N	20:p:424:GLY:O	2.43	0.52
20:p:465:VAL:HA	20:p:583:ASP:HA	1.92	0.52
2:H:361:GLU:O	2:H:365:SER:CB	2.58	0.51
19:f:802:SER:O	19:f:806:ALA:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:l:9:LYS:O	22:l:13:SER:HA	2.09	0.51
1:F:19:GLY:N	24:F:800:ADP:O1B	2.44	0.51
5:L:73:SER:O	5:L:77:ASN:CA	2.58	0.51
19:e:133:SER:HA	19:f:41:LEU:HA	1.92	0.51
19:f:158:ALA:O	19:f:162:LYS:CB	2.58	0.51
20:p:470:LEU:CA	20:p:483:TRP:O	2.53	0.51
22:s:43:ALA:O	22:s:47:HIS:CB	2.58	0.51
1:F:199:ARG:HA	1:F:203:TYR:H	1.74	0.51
6:M:153:UNK:O	6:M:157:UNK:N	2.43	0.51
19:e:568:LEU:O	19:e:572:LEU:CB	2.59	0.51
21:q:86:LEU:N	21:q:111:GLY:O	2.43	0.51
1:A:48:MET:H	1:C:173:GLY:HA3	1.76	0.51
1:B:304:SER:HA	24:B:800:ADP:H1'	1.93	0.51
20:g:264:GLN:H	20:g:317:PHE:HA	1.75	0.51
21:j:190:GLY:HA2	21:j:299:PRO:HA	1.91	0.51
22:l:42:TYR:O	22:l:46:MET:CB	2.58	0.51
19:m:78:LEU:HA	19:m:117:ALA:HA	1.92	0.51
1:B:327:LYS:HA	17:c:49:ASN:H	1.74	0.51
20:g:323:VAL:HA	20:g:332:VAL:O	2.11	0.51
19:m:696:GLN:O	19:m:700:ASP:CB	2.58	0.51
1:D:217:ILE:O	1:D:221:ALA:N	2.44	0.51
8:P:37:UNK:HA	8:P:73:UNK:O	2.11	0.51
16:b:65:GLY:O	16:b:84:GLU:N	2.42	0.51
19:m:40:LEU:HA	19:m:45:GLY:HA2	1.92	0.51
21:r:58:LEU:HA	21:r:107:TRP:O	2.11	0.51
1:B:227:ASN:O	1:B:231:ASP:N	2.38	0.51
19:n:329:VAL:O	19:n:333:ASN:CB	2.59	0.51
20:o:287:ALA:O	20:o:303:PHE:CB	2.59	0.51
20:p:372:LEU:O	20:p:383:SER:HA	2.10	0.51
5:L:90:SER:O	5:L:94:ARG:N	2.43	0.51
13:Y:307:UNK:N	13:Y:421:UNK:O	2.44	0.51
2:H:239:SER:HA	2:H:248:ILE:O	2.10	0.51
5:L:116:VAL:O	5:L:134:ILE:HA	2.11	0.51
20:h:374:SER:O	20:h:381:ILE:HA	2.11	0.51
6:M:801:UNK:O	6:M:805:UNK:N	2.43	0.50
11:V:75:LYS:HA	11:V:80:VAL:HA	1.94	0.50
13:Y:508:UNK:H	13:Y:534:UNK:H	1.58	0.50
20:g:491:LEU:HA	20:g:596:ASN:HA	1.92	0.50
21:j:241:GLU:HA	21:j:246:TYR:H	1.76	0.50
1:C:45:VAL:O	1:E:175:ALA:N	2.44	0.50
1:E:216:ALA:O	1:E:220:ARG:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:322:VAL:CB	20:g:334:TRP:O	2.60	0.50
20:h:430:VAL:O	20:h:445:MET:HA	2.12	0.50
1:B:14:ILE:N	1:B:109:LEU:O	2.40	0.50
1:A:75:MET:HA	1:A:80:VAL:HA	1.92	0.50
1:C:240:GLN:HA	1:C:249:ILE:O	2.11	0.50
7:N:634:UNK:O	8:O:96:UNK:N	2.44	0.50
1:I:217:ILE:O	1:I:221:ALA:N	2.45	0.50
3:J:321:ALA:O	3:J:325:TYR:CB	2.59	0.50
11:V:114:CYS:HA	11:V:132:THR:O	2.11	0.50
20:p:289:VAL:O	20:p:300:GLU:N	2.35	0.50
12:x:46:UNK:O	12:x:50:UNK:CB	2.60	0.50
1:A:107:PRO:HA	1:A:136:ALA:O	2.11	0.50
4:K:29:PHE:O	4:K:33:PHE:CB	2.60	0.50
19:e:25:ALA:HA	19:e:127:ALA:HB2	1.94	0.50
19:e:530:VAL:HA	19:e:549:ALA:HB1	1.93	0.50
1:D:19:GLY:N	24:D:800:ADP:O1B	2.45	0.50
1:I:287:ASP:O	1:I:291:ARG:N	2.37	0.50
11:V:118:ARG:O	11:V:137:GLU:N	2.41	0.50
20:o:482:LEU:O	20:o:491:LEU:N	2.44	0.50
5:L:67:ASP:N	5:L:70:SER:O	2.41	0.50
7:N:759:UNK:O	7:N:763:UNK:N	2.44	0.50
11:V:145:VAL:O	11:V:154:SER:N	2.45	0.50
20:g:425:SER:H	20:g:430:VAL:HA	1.77	0.49
20:o:384:TRP:HA	20:o:392:PRO:HA	1.94	0.49
20:p:375:ILE:HA	20:p:380:LYS:O	2.11	0.49
8:P:26:UNK:N	8:P:35:UNK:O	2.45	0.49
1:A:60:PRO:O	1:A:64:GLU:CB	2.61	0.49
5:L:108:ARG:O	5:L:113:GLU:N	2.45	0.49
5:L:231:ILE:O	5:L:235:LYS:CB	2.60	0.49
13:Y:512:UNK:HA	13:Y:529:UNK:O	2.12	0.49
20:g:516:CYS:O	20:g:523:LEU:HA	2.13	0.49
20:h:224:ARG:HA	22:k:74:LYS:HA	1.92	0.49
19:m:24:VAL:HA	19:m:126:ASP:HA	1.94	0.49
20:o:411:MET:HA	20:o:424:GLY:H	1.77	0.49
20:p:421:PHE:O	20:p:433:ALA:HB3	2.12	0.49
1:C:27:GLY:O	7:N:752:UNK:N	2.45	0.49
6:M:469:UNK:O	6:M:473:UNK:CB	2.61	0.49
20:g:521:GLY:O	20:g:541:VAL:N	2.46	0.49
21:q:335:ALA:O	21:q:339:PHE:CB	2.60	0.49
4:K:190:GLY:O	4:K:211:ASP:HA	2.13	0.49
19:f:79:VAL:HA	19:f:102:ASN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:333:LEU:O	20:h:344:VAL:N	2.45	0.49
22:l:68:PHE:HA	22:l:81:ALA:HA	1.94	0.49
6:M:620:UNK:O	6:M:624:UNK:CB	2.60	0.49
20:h:521:GLY:O	20:h:541:VAL:N	2.46	0.49
21:r:69:THR:O	21:r:73:LYS:CB	2.60	0.49
1:B:95:SER:O	1:B:99:LEU:N	2.41	0.49
1:B:335:GLU:O	1:B:339:SER:N	2.45	0.49
4:K:47:ARG:HA	4:K:50:ALA:HB3	1.95	0.49
7:N:621:UNK:O	7:N:625:UNK:CB	2.60	0.49
20:o:514:PHE:O	20:o:525:LEU:HA	2.12	0.49
11:V:83:PHE:H	11:V:119:ARG:HA	1.78	0.49
20:h:500:TYR:O	20:h:519:GLY:N	2.46	0.49
22:l:54:ARG:O	22:l:58:ARG:CB	2.61	0.49
19:e:81:ARG:H	19:e:115:SER:HA	1.77	0.48
19:f:802:SER:O	19:f:806:ALA:HB2	2.13	0.48
9:Q:27:UNK:O	9:Q:31:UNK:CB	2.61	0.48
11:V:147:SER:N	11:V:152:LEU:O	2.42	0.48
20:h:523:LEU:CB	20:h:539:ILE:O	2.61	0.48
19:m:801:ILE:O	19:m:805:VAL:CB	2.61	0.48
19:n:554:ASP:O	19:n:558:ASP:N	2.33	0.48
1:D:238:LYS:HA	1:D:252:GLY:H	1.78	0.48
8:O:38:UNK:O	8:O:73:UNK:CB	2.61	0.48
1:F:19:GLY:H	24:F:800:ADP:PB	2.36	0.48
21:r:228:LEU:HA	21:r:267:ALA:HB1	1.94	0.48
1:C:112:GLU:N	1:C:140:SER:O	2.46	0.48
1:D:198:LEU:O	1:D:203:TYR:N	2.47	0.48
3:J:61:THR:O	3:J:65:TYR:CB	2.62	0.48
4:K:95:SER:N	4:K:109:GLN:O	2.40	0.48
19:f:751:ARG:O	19:f:755:TRP:CB	2.62	0.48
1:A:95:SER:O	1:A:99:LEU:N	2.46	0.48
22:k:77:GLU:H	22:k:93:ASN:HA	1.79	0.48
8:P:24:UNK:N	8:P:37:UNK:O	2.46	0.48
5:L:73:SER:O	5:L:77:ASN:HA	2.14	0.48
19:e:1047:VAL:CB	21:i:85:GLY:O	2.61	0.48
3:J:23:ALA:N	24:J:800:ADP:O3B	2.36	0.48
13:Y:26:UNK:O	13:Y:502:UNK:N	2.37	0.48
1:D:39:VAL:CB	1:D:72:ARG:O	2.62	0.47
13:Y:285:UNK:O	13:Y:620:UNK:N	2.47	0.47
20:h:480:VAL:O	20:h:494:PHE:N	2.46	0.47
3:J:24:PHE:N	24:J:800:ADP:O1B	2.41	0.47
4:K:37:ARG:O	4:K:41:ASN:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:p:491:LEU:HA	20:p:593:ALA:HB2	1.96	0.47
1:A:164:VAL:HA	1:A:184:ASP:HA	1.96	0.47
1:D:22:LYS:HA	1:D:33:TYR:O	2.14	0.47
1:F:318:VAL:O	1:F:322:ALA:N	2.42	0.47
20:g:339:ASN:O	22:l:6:GLU:N	2.41	0.47
20:h:240:SER:N	20:h:572:ASP:O	2.48	0.47
22:k:49:PHE:O	22:k:53:ALA:CB	2.62	0.47
20:o:430:VAL:CB	20:o:446:PHE:O	2.62	0.47
1:D:159:ASP:O	1:D:165:THR:HA	2.14	0.47
7:N:271:UNK:O	7:N:275:UNK:N	2.47	0.47
1:A:162:ASP:N	24:A:800:ADP:O3A	2.48	0.47
1:B:328:ILE:O	17:c:47:ILE:N	2.47	0.47
4:K:94:ILE:HA	4:K:110:PRO:HA	1.96	0.47
1:G:15:ASP:H	1:G:23:ALA:HA	1.80	0.47
11:V:121:VAL:H	11:V:139:VAL:HA	1.80	0.47
22:s:66:LEU:HA	22:t:73:SER:HA	1.96	0.47
1:G:14:ILE:HA	1:G:23:ALA:HA	1.97	0.47
1:I:161:GLY:N	1:I:164:VAL:O	2.43	0.47
1:I:318:VAL:O	1:I:322:ALA:N	2.34	0.47
19:e:25:ALA:N	19:e:125:ILE:O	2.44	0.47
19:f:58:GLU:O	19:f:62:LEU:N	2.48	0.47
19:f:239:PRO:O	19:f:243:ASN:CB	2.63	0.47
19:f:636:SER:O	19:f:641:LEU:N	2.48	0.47
20:g:505:MET:O	20:g:515:ALA:CB	2.55	0.47
1:F:216:ALA:O	1:F:220:ARG:CB	2.62	0.47
1:I:275:ILE:O	1:I:279:LEU:CB	2.63	0.47
4:K:226:LYS:O	4:K:230:LYS:CB	2.63	0.47
20:p:558:GLU:HA	20:p:571:TYR:O	2.15	0.47
1:D:38:TYR:HA	1:D:73:TYR:HA	1.96	0.47
11:V:84:PRO:O	11:V:102:ALA:N	2.48	0.47
20:g:473:THR:O	20:g:480:VAL:HA	2.15	0.47
19:m:82:SER:HA	19:m:113:SER:HA	1.97	0.47
1:E:243:LEU:O	1:E:246:GLY:N	2.43	0.47
2:H:369:ILE:O	2:H:373:LYS:CB	2.62	0.47
6:M:245:UNK:O	6:M:249:UNK:CB	2.63	0.47
20:h:285:GLY:O	20:h:305:CYS:N	2.48	0.47
19:n:601:ILE:O	19:n:605:GLN:CB	2.63	0.47
20:p:506:TRP:HA	20:p:514:PHE:HA	1.97	0.47
1:C:47:VAL:H	1:E:174:PHE:HA	1.78	0.46
1:E:265:PRO:O	1:E:269:GLY:N	2.47	0.46
13:Y:527:UNK:HA	13:Y:607:UNK:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:911:LEU:O	19:e:915:LEU:CB	2.63	0.46
1:D:332:ALA:N	17:c:18:ASP:O	2.49	0.46
11:V:18:SER:N	11:V:36:LEU:O	2.48	0.46
20:g:339:ASN:HA	22:l:7:THR:H	1.79	0.46
1:A:42:PRO:HA	1:A:69:LEU:HA	1.96	0.46
1:E:18:SER:N	24:E:800:ADP:O2B	2.39	0.46
6:M:2:UNK:N	8:O:41:UNK:O	2.48	0.46
10:U:61:LEU:O	10:U:96:SER:N	2.46	0.46
19:f:78:LEU:O	19:f:103:ILE:HA	2.15	0.46
19:f:806:ALA:HB1	21:j:359:GLU:H	1.80	0.46
21:j:281:ASP:O	21:j:285:LYS:CB	2.64	0.46
1:C:61:LYS:O	1:C:65:HIS:N	2.39	0.46
20:g:301:TYR:HA	22:l:7:THR:HA	1.97	0.46
20:g:526:TRP:HA	20:g:535:PRO:HA	1.98	0.46
19:m:344:LEU:HA	19:m:347:ALA:HB2	1.96	0.46
20:o:273:TYR:N	20:o:286:VAL:O	2.49	0.46
11:V:106:SER:O	11:V:125:CYS:N	2.35	0.46
1:B:126:GLU:O	1:B:130:GLU:CB	2.64	0.46
1:C:198:LEU:O	1:C:203:TYR:N	2.48	0.46
1:E:199:ARG:HA	1:E:203:TYR:H	1.81	0.46
19:n:423:TRP:O	19:n:427:TYR:CB	2.64	0.46
11:V:89:ASP:O	11:V:107:TYR:N	2.40	0.46
19:f:115:SER:O	19:f:140:LEU:N	2.49	0.46
22:k:70:ARG:N	22:l:70:ARG:O	2.49	0.46
23:z:1036:UNK:O	23:z:1040:UNK:CB	2.64	0.46
1:E:158:LEU:HA	1:E:166:HIS:O	2.16	0.46
2:H:223:PHE:O	2:H:227:MET:CB	2.64	0.46
19:f:423:TRP:O	19:f:427:TYR:CB	2.64	0.45
19:m:718:PHE:HA	19:m:824:TRP:HA	1.97	0.45
1:A:158:LEU:O	1:A:301:SER:N	2.49	0.45
2:H:139:VAL:O	2:H:143:TYR:CB	2.65	0.45
1:G:163:GLY:N	1:G:186:ALA:HB3	2.31	0.45
3:J:128:LEU:O	3:J:132:GLY:N	2.40	0.45
21:q:179:LYS:O	21:q:183:ASP:CB	2.64	0.45
3:J:77:PHE:HA	3:J:81:LEU:HA	1.97	0.45
20:o:399:VAL:O	20:o:442:ILE:N	2.47	0.45
20:p:413:PHE:HA	20:p:421:PHE:HA	1.96	0.45
22:s:77:GLU:CB	22:s:92:GLN:O	2.64	0.45
1:D:20:VAL:N	24:D:800:ADP:O1B	2.49	0.45
1:C:217:ILE:O	1:C:221:ALA:N	2.47	0.45
1:C:319:LYS:HA	1:C:322:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:MET:HA	1:I:80:VAL:HA	1.97	0.45
10:U:29:ILE:HA	10:U:50:ILE:H	1.82	0.45
19:f:56:LEU:HA	19:f:61:ALA:HB1	1.99	0.45
20:g:476:PHE:HA	20:g:501:VAL:H	1.80	0.45
19:e:1040:VAL:O	21:i:84:ARG:CB	2.65	0.45
20:p:475:SER:N	20:p:479:THR:O	2.48	0.45
19:e:79:VAL:N	19:e:116:LEU:O	2.44	0.45
21:q:133:VAL:O	21:q:228:LEU:N	2.48	0.45
22:s:24:ASN:H	22:s:29:PRO:HA	1.82	0.45
22:s:54:ARG:O	22:s:58:ARG:CB	2.65	0.45
1:C:19:GLY:HA3	24:C:800:ADP:H5'1	1.99	0.45
19:f:329:VAL:O	19:f:333:ASN:CB	2.65	0.45
21:q:67:LYS:O	21:q:71:MET:CB	2.65	0.45
1:D:318:VAL:O	1:D:322:ALA:N	2.51	0.44
2:H:36:GLY:HA2	2:H:67:LEU:HA	1.99	0.44
19:f:627:TYR:HA	19:f:632:ALA:HB3	2.00	0.44
1:E:329:ARG:H	15:a:20:TYR:C	2.25	0.44
2:H:157:ASP:N	25:H:401:ATP:O2B	2.50	0.44
6:M:724:UNK:O	9:Q:64:UNK:N	2.50	0.44
20:g:259:LEU:HA	20:g:270:VAL:O	2.17	0.44
21:q:270:ILE:HA	21:q:310:ILE:H	1.83	0.44
1:G:20:VAL:N	24:G:800:ADP:O1B	2.40	0.44
1:I:156:VAL:O	1:I:299:VAL:N	2.50	0.44
8:O:89:UNK:O	8:O:94:UNK:N	2.51	0.44
20:o:464:ALA:HB3	20:o:580:PRO:HA	2.00	0.44
11:V:24:ARG:N	11:V:182:VAL:O	2.43	0.44
19:e:27:VAL:O	19:e:31:GLN:CB	2.65	0.44
20:h:409:THR:N	20:h:424:GLY:O	2.50	0.44
21:j:57:ILE:O	21:j:106:VAL:HA	2.17	0.44
1:E:331:SER:HA	15:a:18:ASP:HA	1.99	0.44
1:G:164:VAL:HA	1:G:185:ILE:H	1.83	0.44
1:I:164:VAL:HA	1:I:184:ASP:HA	1.99	0.44
3:J:138:VAL:O	3:J:148:VAL:HA	2.17	0.44
1:C:158:LEU:O	1:C:301:SER:N	2.50	0.44
19:f:145:PRO:O	19:f:149:LEU:CB	2.66	0.44
22:l:70:ARG:HA	22:l:79:MET:HA	1.99	0.44
3:J:273:GLN:HA	3:J:277:GLU:HA	2.00	0.44
13:Y:442:UNK:O	13:Y:446:UNK:N	2.51	0.44
13:Y:611:UNK:N	13:Y:705:UNK:O	2.51	0.44
20:p:509:THR:N	20:p:556:GLY:HA3	2.33	0.44
1:A:13:VAL:O	1:A:23:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:O	1:A:71:ILE:HA	2.18	0.44
20:h:286:VAL:HA	20:h:304:HIS:HA	1.98	0.44
9:R:57:UNK:O	9:R:62:UNK:N	2.51	0.43
12:X:35:UNK:HA	12:x:35:UNK:HA	2.00	0.43
19:f:577:ASN:O	19:f:581:MET:N	2.49	0.43
1:D:12:VAL:N	1:D:107:PRO:O	2.49	0.43
2:H:292:ASP:O	2:H:296:ASN:N	2.36	0.43
1:I:332:ALA:H	16:b:16:GLU:HA	1.82	0.43
13:Y:183:UNK:N	13:Y:616:UNK:O	2.51	0.43
20:p:201:ASP:O	20:p:205:ARG:CB	2.66	0.43
1:A:245:ASP:HA	1:C:289:ASP:HA	2.00	0.43
20:g:507:SER:H	20:g:514:PHE:HA	1.82	0.43
20:p:434:CYS:H	20:p:440:ALA:HA	1.83	0.43
1:I:87:GLU:O	1:I:91:GLN:CB	2.66	0.43
21:j:169:LYS:O	21:j:173:LEU:CB	2.66	0.43
19:m:78:LEU:O	19:m:103:ILE:HA	2.17	0.43
20:o:528:LEU:HA	20:o:532:THR:HA	2.00	0.43
1:F:165:THR:H	1:F:184:ASP:HA	1.83	0.43
1:F:198:LEU:O	1:F:203:TYR:N	2.52	0.43
1:I:12:VAL:N	1:I:107:PRO:O	2.51	0.43
19:f:846:LYS:O	19:f:850:LEU:CB	2.67	0.43
3:J:135:SER:HA	3:J:152:TYR:HA	2.01	0.43
20:g:429:SER:HA	20:g:446:PHE:O	2.18	0.43
20:p:309:VAL:HA	20:p:326:THR:HA	2.01	0.43
5:L:109:ASP:HA	5:L:113:GLU:HA	2.01	0.43
1:G:112:GLU:O	1:G:141:MET:HA	2.19	0.43
20:h:501:VAL:HA	20:h:518:ASP:HA	1.99	0.43
19:n:543:THR:O	19:n:547:GLU:CB	2.67	0.43
20:p:383:SER:O	20:p:394:ASP:CB	2.67	0.43
20:p:514:PHE:CB	20:p:526:TRP:O	2.67	0.43
8:P:35:UNK:HA	8:P:76:UNK:HA	2.00	0.43
1:F:76:GLU:N	1:F:79:ILE:O	2.51	0.42
1:F:293:THR:O	1:F:297:ASN:N	2.45	0.42
1:I:20:VAL:N	24:I:800:ADP:O1B	2.51	0.42
3:J:22:GLU:N	24:J:800:ADP:O3B	2.52	0.42
9:Q:86:UNK:O	9:Q:90:UNK:CB	2.68	0.42
22:l:50:ILE:O	22:l:54:ARG:CB	2.67	0.42
19:m:804:LEU:HA	19:m:895:ASN:H	1.84	0.42
1:B:353:PHE:O	1:B:357:TRP:N	2.52	0.42
11:V:19:GLY:H	11:V:38:GLY:HA2	1.84	0.42
13:Y:305:UNK:O	13:Y:421:UNK:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:l:4:VAL:O	22:l:8:LEU:CB	2.67	0.42
19:n:116:LEU:HA	19:n:139:THR:HA	2.00	0.42
2:H:71:ILE:HA	2:H:76:VAL:HA	2.01	0.42
6:M:59:UNK:O	6:M:63:UNK:CB	2.67	0.42
8:P:89:UNK:O	8:P:93:UNK:CB	2.67	0.42
20:o:324:GLY:O	20:o:331:ILE:HA	2.18	0.42
20:p:421:PHE:CB	20:p:433:ALA:O	2.67	0.42
21:q:270:ILE:HA	21:q:309:PHE:HA	2.02	0.42
1:D:147:LEU:O	1:D:151:GLY:N	2.52	0.42
1:E:61:LYS:O	1:E:65:HIS:N	2.51	0.42
1:F:15:ASP:O	1:F:21:ILE:HA	2.20	0.42
19:n:121:ARG:N	19:n:134:GLN:O	2.51	0.42
1:F:41:ARG:H	1:F:70:SER:H	1.66	0.42
20:o:513:LEU:HA	20:o:526:TRP:O	2.19	0.42
1:I:96:LYS:HA	1:I:100:GLN:HA	2.02	0.42
20:h:285:GLY:N	20:h:307:SER:O	2.52	0.42
1:G:132:PHE:O	1:G:134:VAL:N	2.52	0.42
1:D:75:MET:HA	1:D:80:VAL:HA	2.00	0.42
20:p:495:GLU:N	20:p:533:GLU:O	2.43	0.42
1:E:359:SER:O	1:E:363:TYR:N	2.42	0.41
20:h:361:VAL:HA	20:h:373:ILE:O	2.20	0.41
1:B:198:LEU:O	1:B:203:TYR:N	2.53	0.41
6:M:244:UNK:O	6:M:248:UNK:CB	2.68	0.41
1:A:238:LYS:O	1:A:240:GLN:N	2.54	0.41
1:E:12:VAL:HA	1:E:25:PHE:HA	2.02	0.41
1:F:12:VAL:N	1:F:107:PRO:O	2.49	0.41
2:H:238:LYS:O	2:H:249:THR:HA	2.20	0.41
13:Y:514:UNK:HA	13:Y:528:UNK:HA	2.03	0.41
20:g:482:LEU:O	20:g:491:LEU:N	2.33	0.41
1:A:238:LYS:HA	1:A:252:GLY:H	1.85	0.41
20:o:272:SER:HA	20:o:287:ALA:HA	2.03	0.41
21:r:262:CYS:HA	21:r:267:ALA:HB3	2.02	0.41
11:V:144:THR:HA	11:V:156:GLU:HA	2.03	0.41
20:o:521:GLY:N	20:o:545:PRO:O	2.54	0.41
20:p:472:VAL:HA	20:p:482:LEU:HA	2.02	0.41
3:J:118:VAL:O	3:J:373:VAL:N	2.54	0.41
4:K:125:ASP:O	4:K:129:ARG:CB	2.69	0.41
20:p:507:SER:H	20:p:514:PHE:HA	1.85	0.41
5:L:138:GLY:N	5:L:146:GLY:O	2.44	0.41
19:e:918:GLY:O	19:e:922:TRP:CB	2.69	0.41
19:f:771:ALA:O	19:f:775:TYR:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:568:LEU:O	19:m:572:LEU:CB	2.69	0.41
1:E:164:VAL:HA	1:E:184:ASP:HA	2.03	0.41
1:I:155:GLY:N	1:I:170:ILE:O	2.54	0.41
22:k:71:ILE:O	22:k:77:GLU:HA	2.20	0.41
3:J:287:SER:O	3:J:291:CYS:N	2.54	0.41
20:h:363:VAL:HA	20:h:371:ASN:O	2.20	0.41
5:L:65:ASN:O	5:L:72:ARG:N	2.54	0.40
20:g:321:LEU:N	20:g:336:ASN:H	2.19	0.40
22:k:49:PHE:O	22:k:53:ALA:HB2	2.21	0.40
19:m:312:ALA:O	19:m:316:PHE:CB	2.69	0.40
1:C:9:ASN:CB	1:C:105:GLU:O	2.69	0.40
19:n:718:PHE:O	19:n:824:TRP:N	2.53	0.40
20:o:526:TRP:HA	20:o:536:THR:H	1.86	0.40
2:H:155:SER:H	2:H:301:GLY:HA3	1.86	0.40
19:n:836:LEU:O	19:n:840:VAL:CB	2.69	0.40
20:p:557:ARG:O	20:p:573:VAL:N	2.54	0.40
4:K:160:SER:O	4:K:172:ARG:HA	2.21	0.40
10:U:143:ILE:HA	10:U:150:ARG:O	2.21	0.40
19:m:562:THR:O	19:m:566:ALA:CB	2.69	0.40
19:n:153:ILE:O	19:n:157:VAL:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	311 (84%)	56 (15%)	1 (0%)	36	72
1	B	368/376 (98%)	318 (86%)	49 (13%)	1 (0%)	36	72
1	C	368/376 (98%)	315 (86%)	52 (14%)	1 (0%)	36	72
1	D	368/376 (98%)	316 (86%)	52 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	368/376 (98%)	315 (86%)	51 (14%)	2 (0%)	24	63
1	F	368/376 (98%)	310 (84%)	57 (16%)	1 (0%)	36	72
1	G	368/376 (98%)	308 (84%)	58 (16%)	2 (0%)	24	63
1	I	368/376 (98%)	308 (84%)	59 (16%)	1 (0%)	36	72
2	H	368/375 (98%)	316 (86%)	52 (14%)	0	100	100
3	J	363/390 (93%)	296 (82%)	67 (18%)	0	100	100
4	K	276/286 (96%)	240 (87%)	35 (13%)	1 (0%)	30	67
5	L	267/272 (98%)	232 (87%)	35 (13%)	0	100	100
10	U	169/190 (89%)	126 (75%)	41 (24%)	2 (1%)	10	44
11	V	163/182 (90%)	115 (71%)	46 (28%)	2 (1%)	10	44
15	a	48/68 (71%)	33 (69%)	15 (31%)	0	100	100
16	b	71/90 (79%)	51 (72%)	20 (28%)	0	100	100
17	c	33/50 (66%)	25 (76%)	7 (21%)	1 (3%)	3	22
18	d	22/29 (76%)	17 (77%)	5 (23%)	0	100	100
19	e	916/1455 (63%)	770 (84%)	140 (15%)	6 (1%)	18	56
19	f	919/1455 (63%)	786 (86%)	130 (14%)	3 (0%)	36	72
19	m	916/1455 (63%)	787 (86%)	125 (14%)	4 (0%)	30	67
19	n	918/1455 (63%)	798 (87%)	114 (12%)	6 (1%)	18	56
20	g	393/612 (64%)	296 (75%)	96 (24%)	1 (0%)	36	72
20	h	394/612 (64%)	305 (77%)	88 (22%)	1 (0%)	36	72
20	o	393/612 (64%)	301 (77%)	91 (23%)	1 (0%)	36	72
20	p	397/612 (65%)	274 (69%)	122 (31%)	1 (0%)	36	72
21	i	258/492 (52%)	225 (87%)	33 (13%)	0	100	100
21	j	265/492 (54%)	206 (78%)	57 (22%)	2 (1%)	16	54
21	q	258/492 (52%)	202 (78%)	56 (22%)	0	100	100
21	r	258/492 (52%)	204 (79%)	54 (21%)	0	100	100
22	k	91/96 (95%)	64 (70%)	27 (30%)	0	100	100
22	l	91/96 (95%)	66 (72%)	25 (28%)	0	100	100
22	s	91/96 (95%)	69 (76%)	21 (23%)	1 (1%)	11	46
22	t	91/96 (95%)	75 (82%)	16 (18%)	0	100	100
All	All	11373/15560 (73%)	9380 (82%)	1952 (17%)	41 (0%)	31	67

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	U	79	PRO
19	e	1026	MET
19	e	1027	PRO
19	e	1030	PRO
19	f	1030	PRO
19	m	1030	PRO
19	n	1006	VAL
19	n	1026	MET
19	n	1030	PRO
1	G	187	GLY
1	I	187	GLY
4	K	279	ILE
19	f	225	GLU
20	g	564	SER
21	j	356	ALA
19	m	1006	VAL
1	E	187	GLY
19	e	1009	HIS
19	m	1027	PRO
21	j	246	TYR
19	m	539	SER
19	n	537	ASP
20	p	220	ASP
1	C	228	PRO
1	E	228	PRO
1	F	187	GLY
1	G	228	PRO
19	e	643	PRO
19	e	1010	TYR
19	f	365	ARG
11	V	84	PRO
19	n	1009	HIS
20	o	469	HIS
1	B	187	GLY
19	n	1007	GLY
17	c	43	VAL
20	h	462	VAL
22	s	62	PRO
1	A	228	PRO
10	U	78	GLU
11	V	72	PRO

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 [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	$\# Z > 2$
24	ADP	C	800	-	28,29,29	1.29	5 (17%)	43,45,45	2.06	13 (30%)
24	ADP	G	800	-	28,29,29	1.38	5 (17%)	43,45,45	1.85	10 (23%)
24	ADP	B	800	-	28,29,29	1.31	5 (17%)	43,45,45	2.19	15 (34%)
24	ADP	E	800	-	28,29,29	1.37	5 (17%)	43,45,45	1.93	10 (23%)
25	ATP	H	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.84	9 (18%)
24	ADP	I	800	-	28,29,29	1.41	4 (14%)	43,45,45	1.90	12 (27%)
24	ADP	F	800	-	28,29,29	1.34	5 (17%)	43,45,45	2.00	11 (25%)
24	ADP	D	800	-	28,29,29	1.32	5 (17%)	43,45,45	1.93	12 (27%)
24	ADP	J	800	-	28,29,29	1.39	5 (17%)	43,45,45	1.98	13 (30%)
24	ADP	A	800	-	28,29,29	1.35	5 (17%)	43,45,45	1.94	12 (27%)

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
24	ADP	C	800	-	-	6/16/32/32	0/3/3/3
24	ADP	G	800	-	-	5/16/32/32	0/3/3/3
24	ADP	B	800	-	-	1/16/32/32	0/3/3/3
24	ADP	E	800	-	-	2/16/32/32	0/3/3/3
25	ATP	H	401	-	-	7/22/38/38	0/3/3/3
24	ADP	I	800	-	-	7/16/32/32	0/3/3/3
24	ADP	F	800	-	-	5/16/32/32	0/3/3/3
24	ADP	D	800	-	-	4/16/32/32	0/3/3/3
24	ADP	J	800	-	-	4/16/32/32	0/3/3/3
24	ADP	A	800	-	-	4/16/32/32	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	800	ADP	C5-C4	4.29	1.46	1.39
24	J	800	ADP	C5-C4	4.23	1.46	1.39
24	I	800	ADP	C5-C4	4.22	1.46	1.39
24	E	800	ADP	C5-C4	4.09	1.46	1.39
24	G	800	ADP	C5-C4	4.07	1.46	1.39
24	B	800	ADP	C5-C4	3.91	1.46	1.39
25	H	401	ATP	C5-C4	3.83	1.45	1.39
24	F	800	ADP	C5-C4	3.82	1.45	1.39
24	D	800	ADP	C5-C4	3.74	1.45	1.39
24	C	800	ADP	C5-C4	3.74	1.45	1.39
24	D	800	ADP	C4-N9	-2.81	1.31	1.37
24	I	800	ADP	C5-N7	-2.81	1.34	1.39
25	H	401	ATP	C4-N9	-2.70	1.32	1.37
24	C	800	ADP	C4-N9	-2.66	1.32	1.37
24	E	800	ADP	C5-N7	-2.63	1.34	1.39
24	J	800	ADP	C5-C6	2.60	1.48	1.41
24	A	800	ADP	C5-C6	2.56	1.48	1.41
25	H	401	ATP	C5-N7	-2.56	1.34	1.39
24	C	800	ADP	C5-N7	-2.53	1.34	1.39
24	G	800	ADP	C5-N7	-2.53	1.34	1.39
24	F	800	ADP	C5-N7	-2.52	1.34	1.39
24	B	800	ADP	C5-N7	-2.49	1.34	1.39
24	J	800	ADP	C4-N9	-2.48	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	800	ADP	C5-N7	-2.48	1.34	1.39
24	J	800	ADP	C5-N7	-2.46	1.34	1.39
24	F	800	ADP	C4-N9	-2.46	1.32	1.37
24	F	800	ADP	C5-C6	2.43	1.47	1.41
24	E	800	ADP	C5-C6	2.41	1.47	1.41
24	G	800	ADP	C5-C6	2.39	1.47	1.41
25	H	401	ATP	C5-C6	2.38	1.47	1.41
24	I	800	ADP	C4-N9	-2.38	1.32	1.37
24	I	800	ADP	C5-C6	2.36	1.47	1.41
24	B	800	ADP	C5-C6	2.36	1.47	1.41
24	D	800	ADP	C5-C6	2.32	1.47	1.41
24	A	800	ADP	C5-N7	-2.31	1.34	1.39
24	E	800	ADP	C4-N9	-2.30	1.32	1.37
24	C	800	ADP	C8-N7	2.25	1.36	1.31
24	A	800	ADP	C4-N9	-2.23	1.33	1.37
24	J	800	ADP	C8-N7	2.22	1.36	1.31
24	F	800	ADP	C8-N7	2.20	1.35	1.31
24	B	800	ADP	C8-N7	2.19	1.35	1.31
24	C	800	ADP	C5-C6	2.18	1.47	1.41
25	H	401	ATP	C8-N9	-2.17	1.33	1.37
24	G	800	ADP	C4-N9	-2.16	1.33	1.37
24	D	800	ADP	C8-N7	2.15	1.35	1.31
24	A	800	ADP	C8-N7	2.13	1.35	1.31
24	G	800	ADP	C8-N7	2.11	1.35	1.31
24	E	800	ADP	C8-N7	2.11	1.35	1.31
24	B	800	ADP	C4-N9	-2.11	1.33	1.37

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	F	800	ADP	C5-C4-N3	-6.10	118.31	126.72
25	H	401	ATP	C5-C4-N3	-6.04	118.41	126.72
24	I	800	ADP	C5-C4-N3	-5.95	118.52	126.72
24	B	800	ADP	C5-C4-N3	-5.87	118.64	126.72
24	E	800	ADP	C5-C4-N3	-5.64	118.94	126.72
24	G	800	ADP	C5-C4-N3	-5.53	119.10	126.72
24	A	800	ADP	C5-C4-N3	-5.43	119.25	126.72
24	J	800	ADP	C5-C4-N3	-5.38	119.31	126.72
25	H	401	ATP	N3-C4-N9	5.22	136.05	127.17
24	C	800	ADP	O4'-C1'-N9	5.05	117.79	108.09
24	B	800	ADP	N3-C4-N9	4.85	135.42	127.17
24	C	800	ADP	C5-C4-N3	-4.72	120.22	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	I	800	ADP	N3-C4-N9	4.66	135.10	127.17
24	A	800	ADP	N3-C4-N9	4.66	135.09	127.17
24	G	800	ADP	N3-C4-N9	4.57	134.94	127.17
24	D	800	ADP	C5-C4-N3	-4.56	120.44	126.72
24	F	800	ADP	N3-C4-N9	4.53	134.87	127.17
24	E	800	ADP	N3-C4-N9	4.52	134.85	127.17
24	F	800	ADP	C2-N3-C4	4.40	122.58	111.83
24	J	800	ADP	N3-C4-N9	4.02	134.01	127.17
24	D	800	ADP	C4-N9-C8	4.00	109.94	105.74
24	B	800	ADP	C2-N3-C4	3.99	121.58	111.83
24	F	800	ADP	N3-C2-N1	-3.98	122.55	128.58
25	H	401	ATP	C4-N9-C8	3.92	109.85	105.74
24	J	800	ADP	C4-C5-N7	-3.91	106.11	110.58
24	C	800	ADP	N3-C2-N1	-3.90	122.67	128.58
24	D	800	ADP	N3-C4-N9	3.80	133.63	127.17
25	H	401	ATP	C2-N3-C4	3.80	121.10	111.83
24	B	800	ADP	N3-C2-N1	-3.76	122.89	128.58
24	J	800	ADP	C2-N3-C4	3.73	120.95	111.83
24	C	800	ADP	N3-C4-N9	3.71	133.47	127.17
24	G	800	ADP	C2-N3-C4	3.70	120.87	111.83
24	A	800	ADP	C4-N9-C8	3.64	109.56	105.74
24	F	800	ADP	C4-C5-N7	-3.63	106.43	110.58
24	B	800	ADP	C4'-O4'-C1'	-3.62	101.47	109.47
24	E	800	ADP	C2-N3-C4	3.58	120.56	111.83
24	J	800	ADP	N3-C2-N1	-3.57	123.17	128.58
24	C	800	ADP	C2-N3-C4	3.57	120.55	111.83
24	I	800	ADP	C4-C5-N7	-3.56	106.51	110.58
24	B	800	ADP	C4-N9-C8	3.56	109.48	105.74
24	A	800	ADP	C2-N3-C4	3.49	120.36	111.83
24	B	800	ADP	C4-C5-N7	-3.44	106.65	110.58
24	C	800	ADP	C4-N9-C8	3.43	109.34	105.74
24	D	800	ADP	N3-C2-N1	-3.39	123.46	128.58
24	D	800	ADP	C2-N3-C4	3.38	120.10	111.83
24	E	800	ADP	C4-C5-N7	-3.35	106.75	110.58
24	G	800	ADP	N3-C2-N1	-3.34	123.53	128.58
24	C	800	ADP	C4-C5-N7	-3.32	106.79	110.58
24	D	800	ADP	C4-C5-N7	-3.29	106.83	110.58
24	I	800	ADP	C2-N3-C4	3.25	119.78	111.83
24	G	800	ADP	C4-C5-N7	-3.24	106.88	110.58
24	A	800	ADP	C4-C5-N7	-3.21	106.91	110.58
24	G	800	ADP	C4-N9-C8	3.20	109.10	105.74
24	E	800	ADP	N3-C2-N1	-3.11	123.88	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	E	800	ADP	C4-N9-C8	3.09	108.98	105.74
25	H	401	ATP	C4-C5-N7	-3.09	107.05	110.58
24	J	800	ADP	C4-N9-C8	3.04	108.93	105.74
24	C	800	ADP	C4'-O4'-C1'	-3.02	102.80	109.47
24	A	800	ADP	N3-C2-N1	-3.00	124.03	128.58
24	J	800	ADP	O4'-C1'-N9	2.90	113.66	108.09
24	D	800	ADP	N9-C8-N7	-2.90	109.82	113.94
24	I	800	ADP	C3'-C2'-C1'	2.83	106.82	101.46
24	B	800	ADP	C5-N7-C8	2.82	107.89	103.45
25	H	401	ATP	N3-C2-N1	-2.79	124.36	128.58
24	J	800	ADP	C5-N7-C8	2.78	107.83	103.45
24	B	800	ADP	N9-C8-N7	-2.75	110.03	113.94
24	J	800	ADP	C4'-O4'-C1'	-2.74	103.41	109.47
24	B	800	ADP	C2'-C1'-N9	2.74	120.12	113.30
24	B	800	ADP	O5'-C5'-C4'	-2.72	99.74	108.99
24	F	800	ADP	C4-N9-C8	2.71	108.58	105.74
24	D	800	ADP	C6-C5-N7	2.67	137.24	132.09
24	C	800	ADP	N9-C8-N7	-2.66	110.16	113.94
24	A	800	ADP	C2'-C1'-N9	-2.66	106.70	113.30
24	I	800	ADP	C4-N9-C8	2.65	108.52	105.74
24	J	800	ADP	C6-C5-N7	2.63	137.16	132.09
24	I	800	ADP	C5-N7-C8	2.62	107.57	103.45
24	C	800	ADP	C6-C5-N7	2.62	137.14	132.09
24	F	800	ADP	C6-C5-N7	2.62	137.14	132.09
25	H	401	ATP	N9-C8-N7	-2.58	110.28	113.94
24	E	800	ADP	C5-N7-C8	2.57	107.50	103.45
24	D	800	ADP	C5-N7-C8	2.56	107.48	103.45
24	I	800	ADP	C2'-C1'-N9	-2.56	106.94	113.30
24	C	800	ADP	C4-N9-C1'	-2.55	120.67	126.63
24	G	800	ADP	C5-N7-C8	2.54	107.44	103.45
24	A	800	ADP	C5-N7-C8	2.52	107.41	103.45
24	C	800	ADP	C5-N7-C8	2.52	107.40	103.45
24	F	800	ADP	C5-N7-C8	2.51	107.40	103.45
24	B	800	ADP	O4'-C1'-N9	2.47	112.84	108.09
24	J	800	ADP	N9-C8-N7	-2.47	110.43	113.94
24	A	800	ADP	N9-C8-N7	-2.45	110.46	113.94
25	H	401	ATP	C5-N7-C8	2.44	107.29	103.45
24	I	800	ADP	N3-C2-N1	-2.38	124.97	128.58
24	E	800	ADP	C3'-C2'-C1'	2.37	105.95	101.46
24	E	800	ADP	N9-C8-N7	-2.35	110.60	113.94
24	G	800	ADP	N9-C8-N7	-2.34	110.61	113.94
24	A	800	ADP	O2A-PA-O1A	2.31	123.18	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	800	ADP	C6-C5-N7	2.31	136.53	132.09
24	C	800	ADP	C2-N1-C6	2.30	122.51	118.73
24	D	800	ADP	O2A-PA-O1A	2.26	122.96	112.44
24	F	800	ADP	N9-C8-N7	-2.24	110.76	113.94
24	A	800	ADP	C6-C5-N7	2.22	136.37	132.09
24	G	800	ADP	C6-C5-N7	2.22	136.36	132.09
24	J	800	ADP	C2-N1-C6	2.19	122.32	118.73
24	A	800	ADP	C3'-C2'-C1'	2.14	105.51	101.46
25	H	401	ATP	O2B-PB-O1B	2.13	122.36	112.44
24	B	800	ADP	O2A-PA-O1A	2.11	122.25	112.44
24	E	800	ADP	C6-C5-N7	2.10	136.13	132.09
24	B	800	ADP	O3B-PB-O2B	2.09	115.65	107.80
24	I	800	ADP	N9-C8-N7	-2.06	111.02	113.94
24	G	800	ADP	O2A-PA-O1A	2.05	121.99	112.44
24	F	800	ADP	C5'-C4'-C3'	-2.04	107.87	115.21
24	I	800	ADP	O4'-C4'-C3'	2.03	109.18	105.15
24	I	800	ADP	O2A-PA-O1A	2.02	121.84	112.44
24	J	800	ADP	O2A-PA-O1A	2.01	121.79	112.44
24	D	800	ADP	O3B-PB-O2B	2.01	115.32	107.80
24	F	800	ADP	O2A-PA-O1A	2.00	121.75	112.44
24	D	800	ADP	O4'-C1'-N9	2.00	111.93	108.09

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	800	ADP	C5'-O5'-PA-O2A
24	B	800	ADP	C5'-O5'-PA-O2A
24	C	800	ADP	C5'-O5'-PA-O2A
24	C	800	ADP	C5'-O5'-PA-O3A
24	E	800	ADP	C3'-C4'-C5'-O5'
24	F	800	ADP	O4'-C4'-C5'-O5'
24	F	800	ADP	C3'-C4'-C5'-O5'
24	F	800	ADP	C2'-C1'-N9-C8
24	G	800	ADP	C5'-O5'-PA-O1A
24	G	800	ADP	C5'-O5'-PA-O3A
24	I	800	ADP	C5'-O5'-PA-O1A
24	I	800	ADP	C5'-O5'-PA-O3A
25	H	401	ATP	PB-O3A-PA-O5'
25	H	401	ATP	C5'-O5'-PA-O2A
25	H	401	ATP	C5'-O5'-PA-O3A
24	D	800	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
24	G	800	ADP	C3'-C4'-C5'-O5'
24	A	800	ADP	O4'-C4'-C5'-O5'
24	C	800	ADP	O4'-C4'-C5'-O5'
24	E	800	ADP	O4'-C4'-C5'-O5'
24	G	800	ADP	O4'-C4'-C5'-O5'
24	I	800	ADP	C3'-C4'-C5'-O5'
24	J	800	ADP	O4'-C4'-C5'-O5'
24	F	800	ADP	C2'-C1'-N9-C4
24	A	800	ADP	C3'-C4'-C5'-O5'
24	C	800	ADP	C3'-C4'-C5'-O5'
24	D	800	ADP	O4'-C4'-C5'-O5'
24	J	800	ADP	C3'-C4'-C5'-O5'
25	H	401	ATP	C3'-C4'-C5'-O5'
25	H	401	ATP	C4'-C5'-O5'-PA
24	I	800	ADP	O4'-C4'-C5'-O5'
24	C	800	ADP	C4'-C5'-O5'-PA
24	J	800	ADP	C2'-C1'-N9-C8
24	D	800	ADP	C4'-C5'-O5'-PA
24	A	800	ADP	C5'-O5'-PA-O3A
24	D	800	ADP	C5'-O5'-PA-O2A
24	G	800	ADP	C5'-O5'-PA-O2A
24	I	800	ADP	C5'-O5'-PA-O2A
25	H	401	ATP	O4'-C4'-C5'-O5'
25	H	401	ATP	PA-O3A-PB-O1B
24	J	800	ADP	O4'-C1'-N9-C8
24	I	800	ADP	PB-O3A-PA-O1A
24	I	800	ADP	PB-O3A-PA-O2A
24	F	800	ADP	C4'-C5'-O5'-PA
24	C	800	ADP	PB-O3A-PA-O2A

There are no ring outliers.

10 monomers are involved in 17 short contacts:

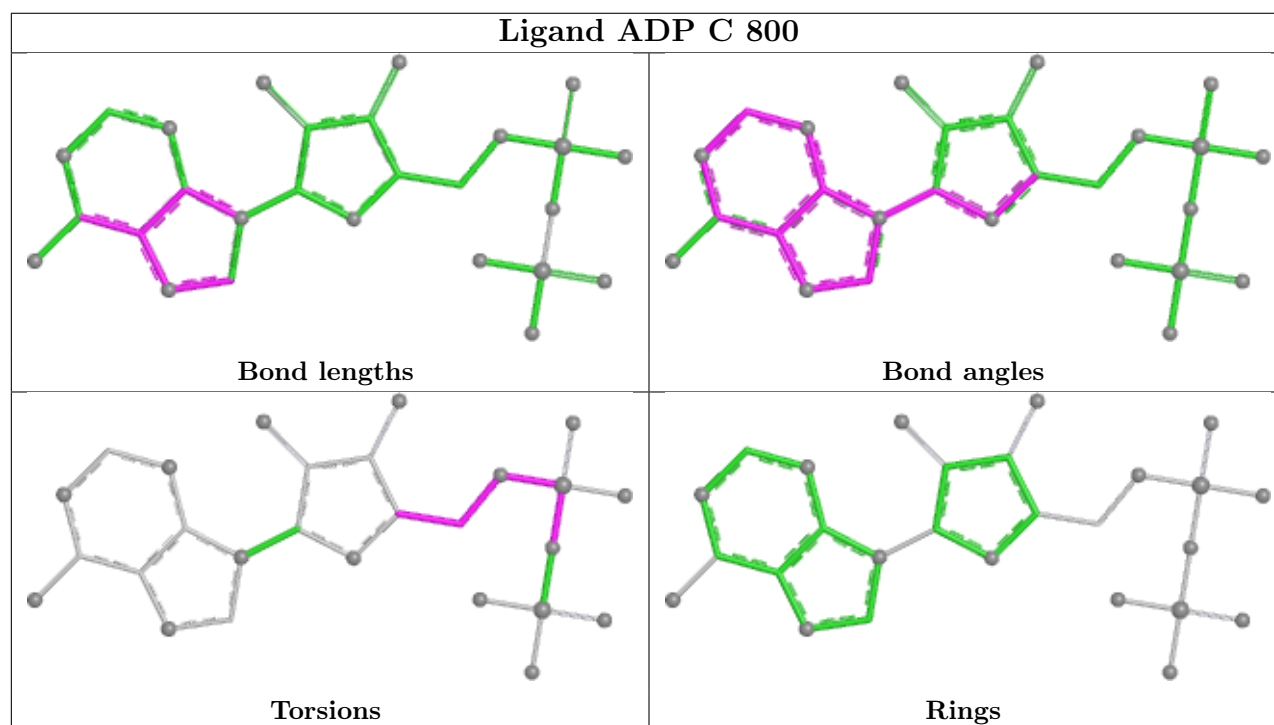
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	800	ADP	1	0
24	G	800	ADP	2	0
24	B	800	ADP	2	0
24	E	800	ADP	2	0
25	H	401	ATP	1	0
24	I	800	ADP	1	0
24	F	800	ADP	2	0
24	D	800	ADP	2	0

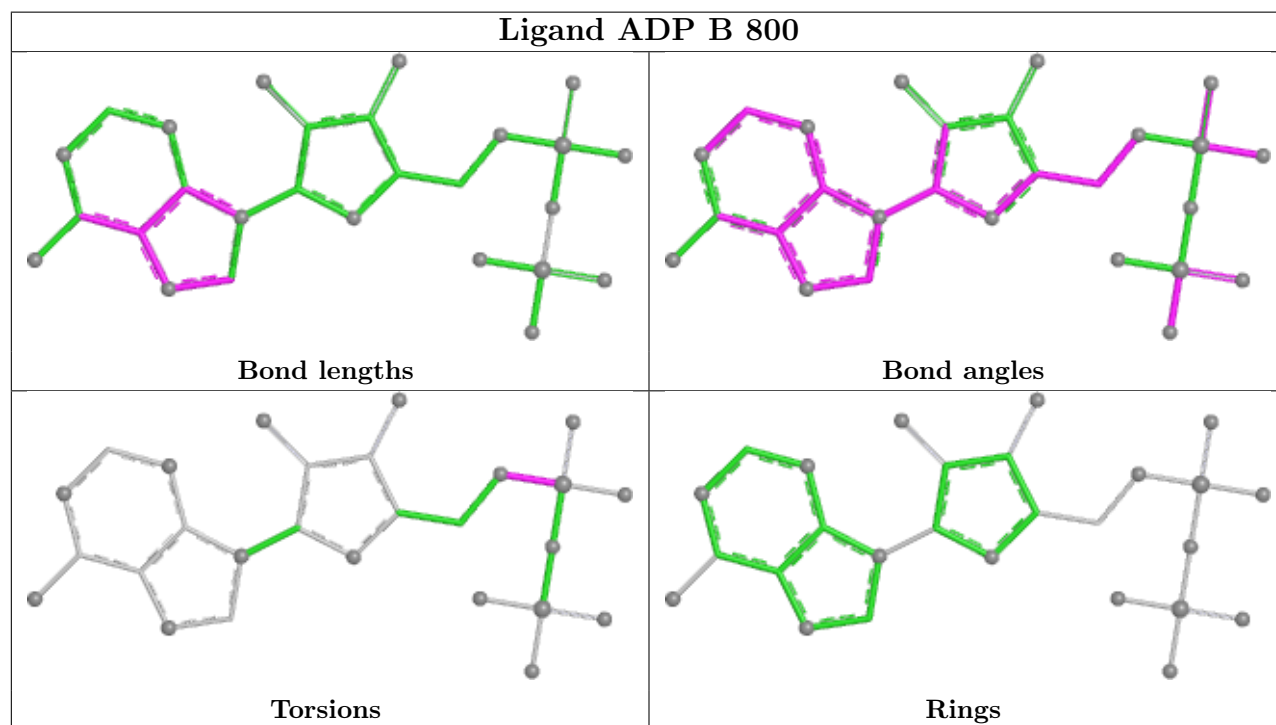
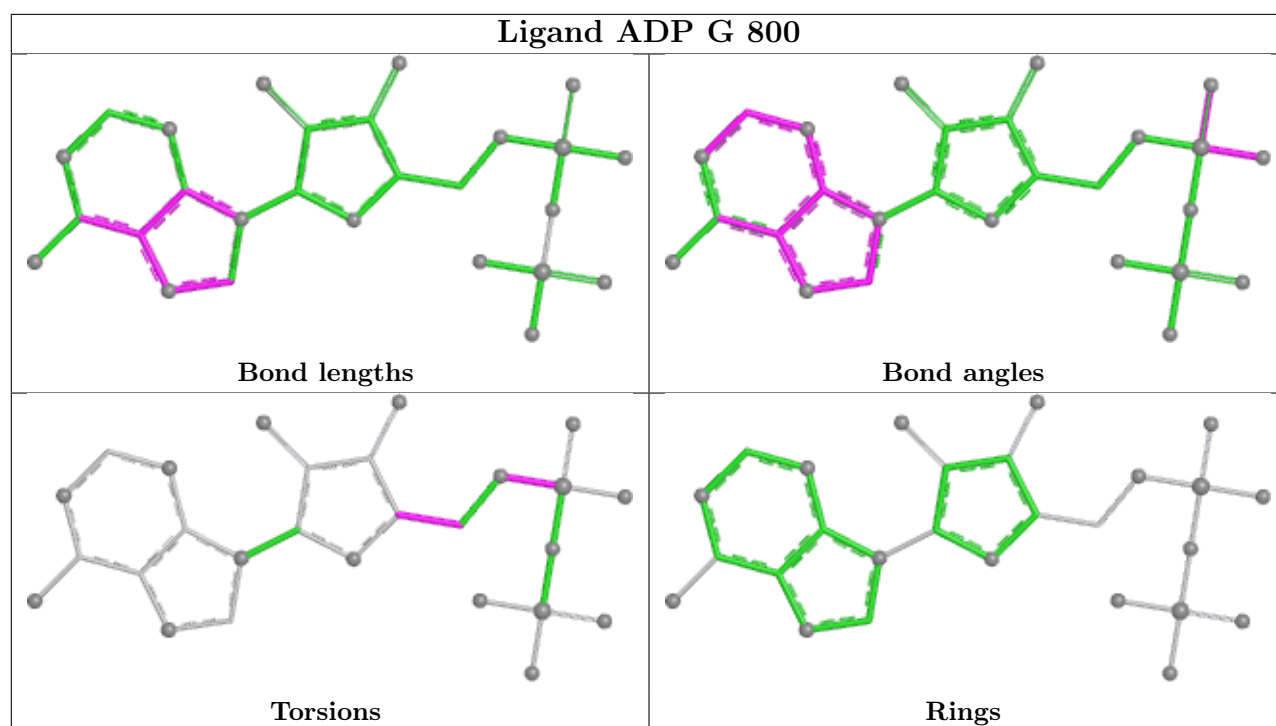
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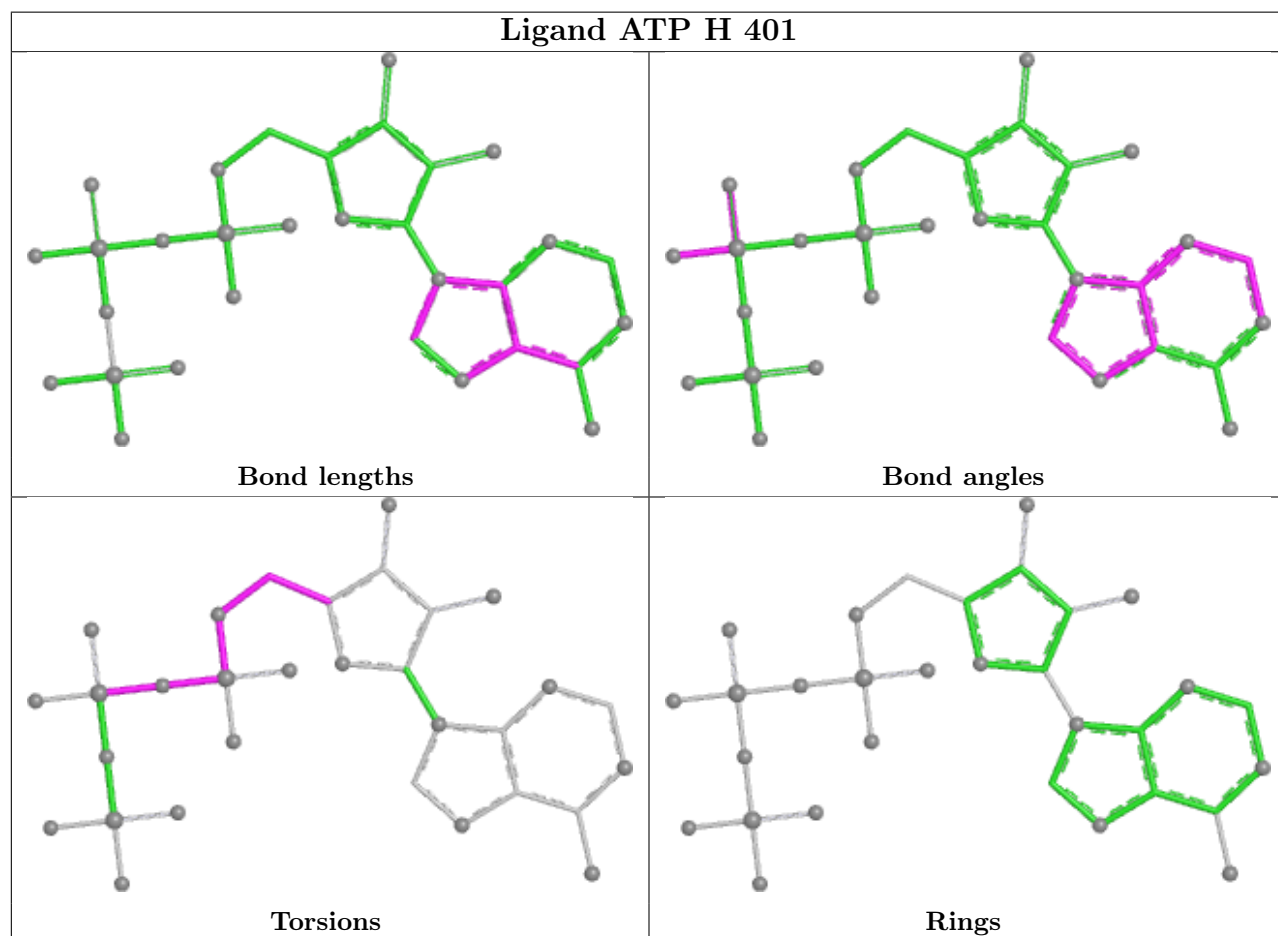
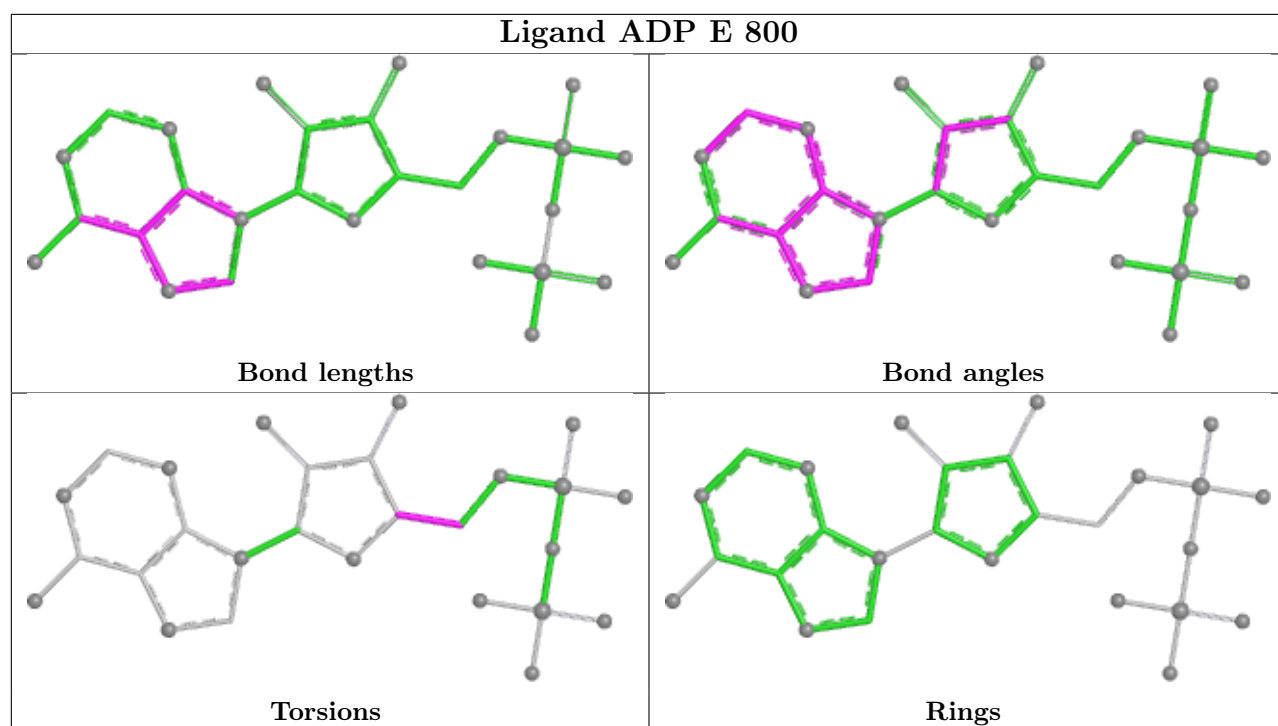
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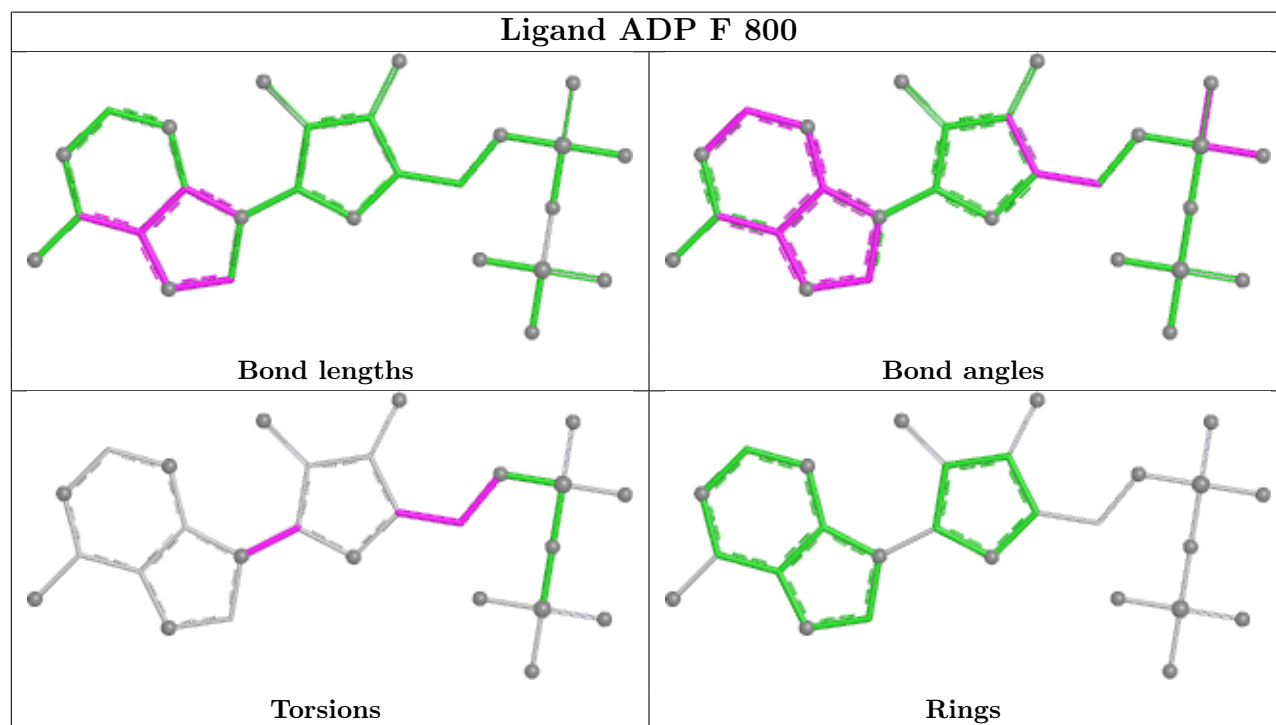
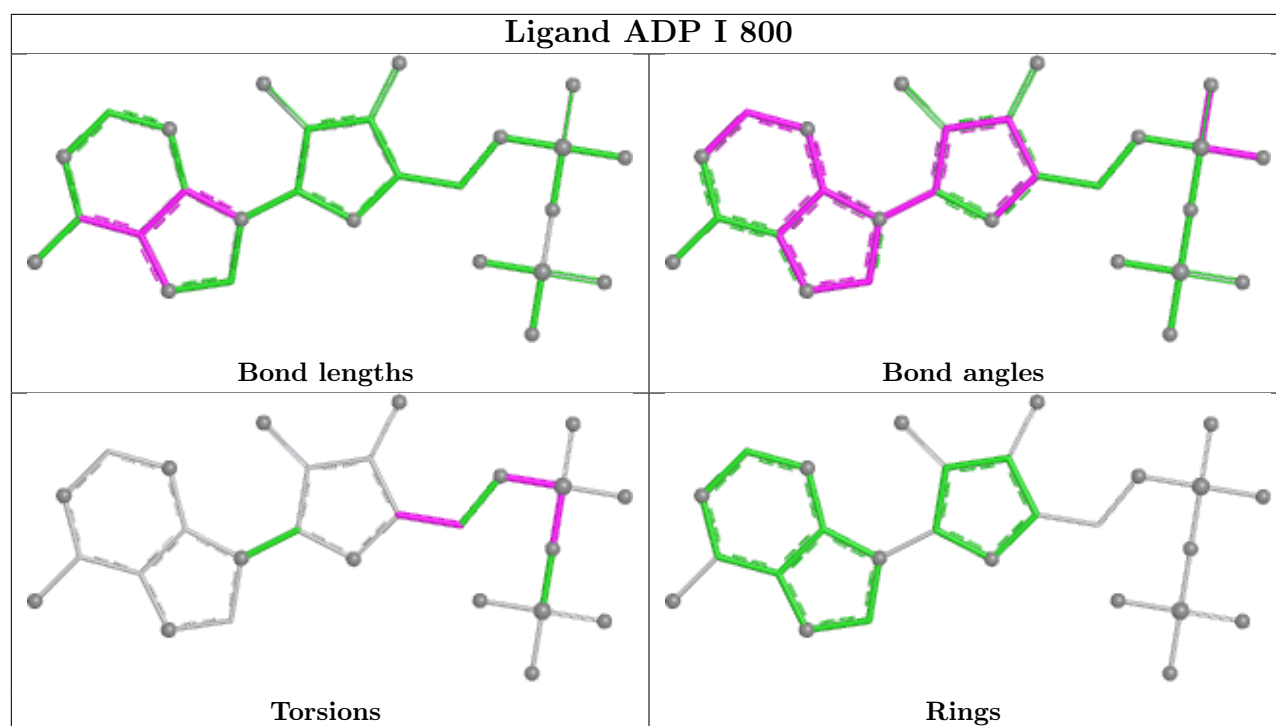
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	J	800	ADP	3	0
24	A	800	ADP	1	0

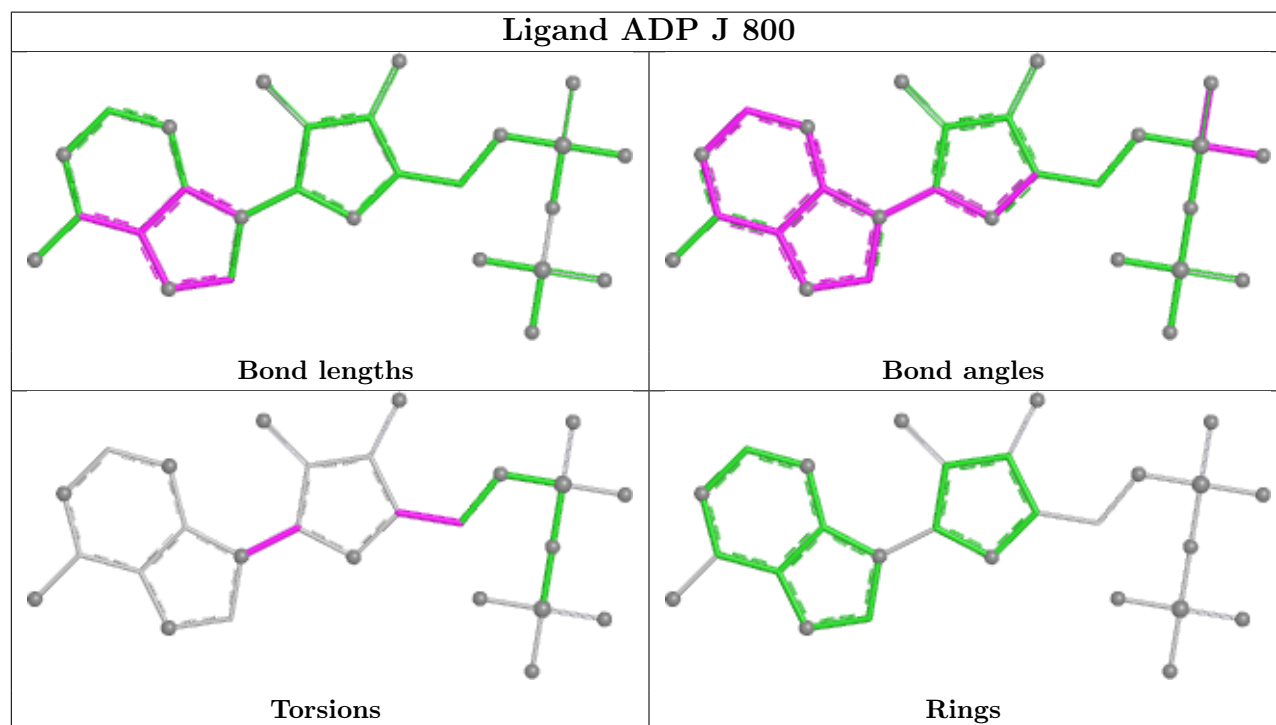
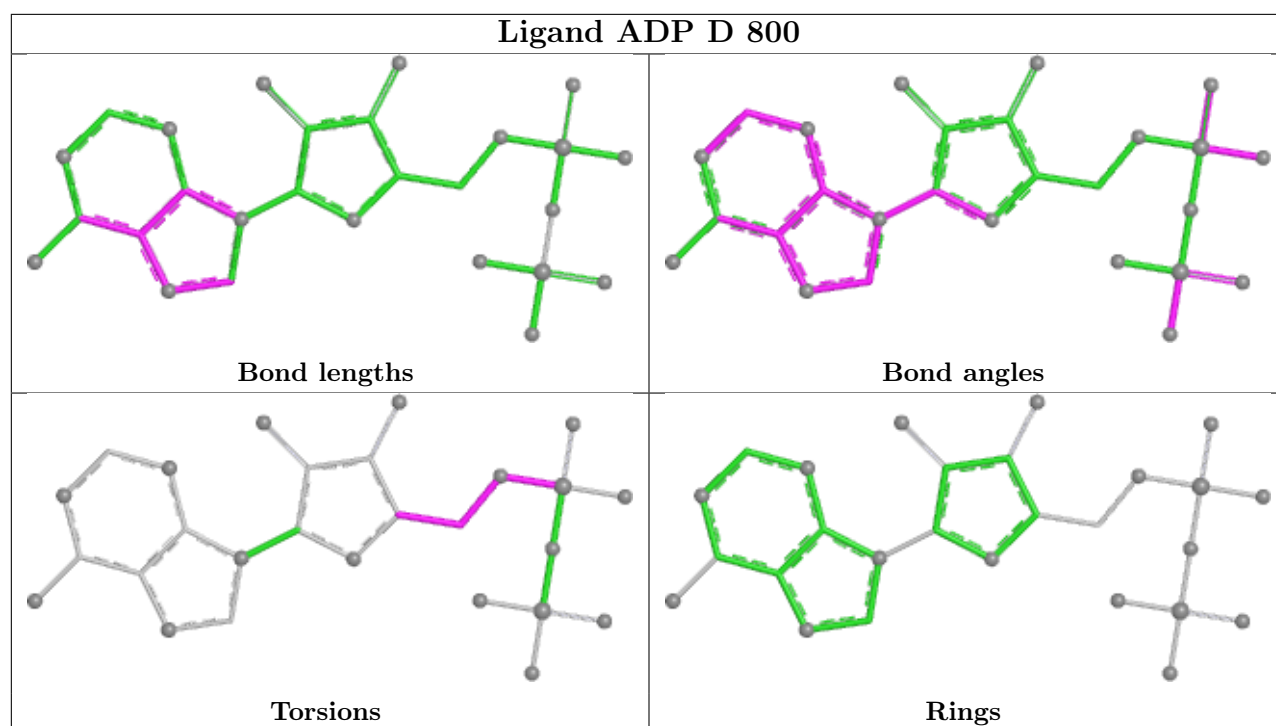
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

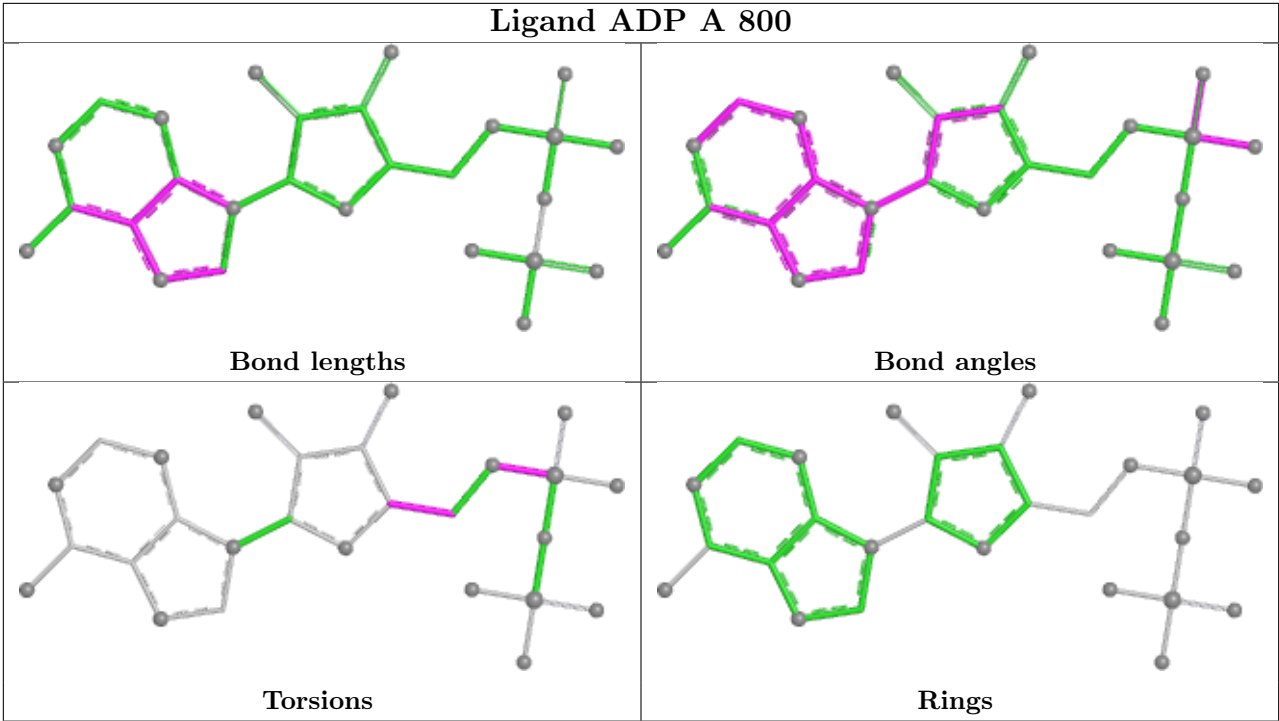












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	Y	12
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	367:UNK	C	401:UNK	N	98.98
1	N	171:UNK	C	201:UNK	N	96.72
1	M	171:UNK	C	201:UNK	N	91.43
1	M	367:UNK	C	401:UNK	N	84.01

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	625:UNK	C	701:UNK	N	69.30
1	N	634:UNK	C	701:UNK	N	65.16
1	Y	502:UNK	C	508:UNK	N	64.57
1	Y	26:UNK	C	155:UNK	N	61.57
1	R	38:UNK	C	42:UNK	N	57.41
1	Q	38:UNK	C	42:UNK	N	56.33
1	Y	359:UNK	C	415:UNK	N	42.89
1	M	741:UNK	C	801:UNK	N	38.70
1	N	768:UNK	C	801:UNK	N	35.08
1	Y	193:UNK	C	282:UNK	N	30.03
1	M	559:UNK	C	601:UNK	N	27.26
1	O	41:UNK	C	64:UNK	N	25.18
1	N	559:UNK	C	602:UNK	N	24.22
1	Y	620:UNK	C	703:UNK	N	23.20
1	P	41:UNK	C	64:UNK	N	21.70
1	Y	160:UNK	C	181:UNK	N	21.23
1	R	62:UNK	C	64:UNK	N	18.98
1	Q	62:UNK	C	64:UNK	N	17.17
1	Y	535:UNK	C	580:UNK	N	16.25
1	P	78:UNK	C	80:UNK	N	16.03
1	P	94:UNK	C	96:UNK	N	14.66
1	O	94:UNK	C	96:UNK	N	13.83
1	Y	611:UNK	C	615:UNK	N	13.79
1	O	78:UNK	C	80:UNK	N	13.01
1	Y	586:UNK	C	588:UNK	N	9.70
1	Y	421:UNK	C	423:UNK	N	8.75
1	Y	597:UNK	C	601:UNK	N	3.93
1	Y	298:UNK	C	300:UNK	N	3.19

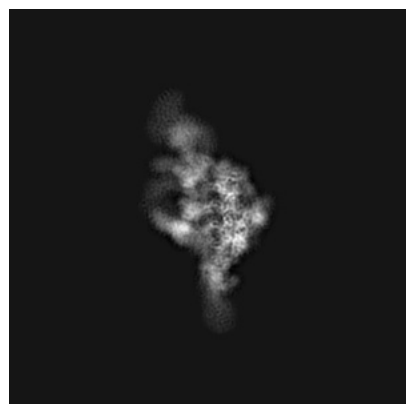
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4177. These allow visual inspection of the internal detail of the map and identification of artifacts.

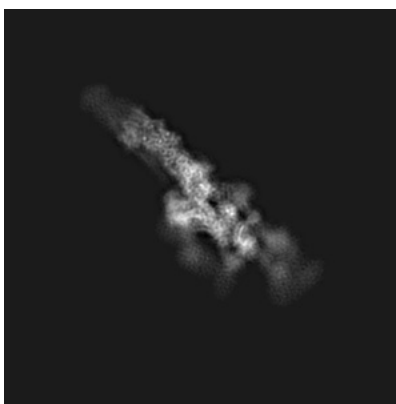
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

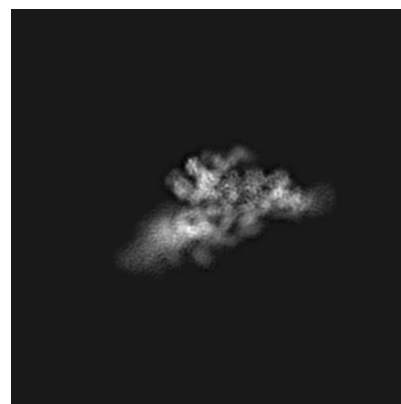
6.1.1 Primary map



X

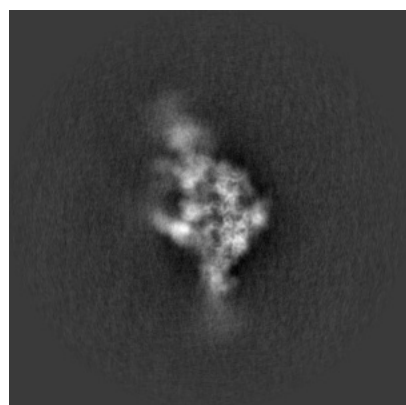


Y

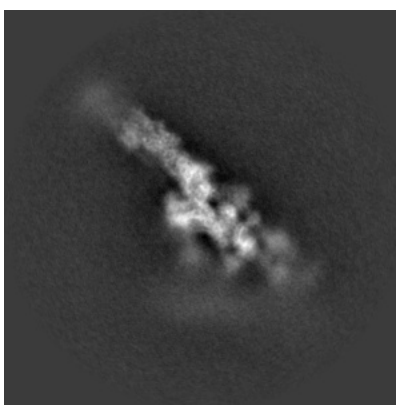


Z

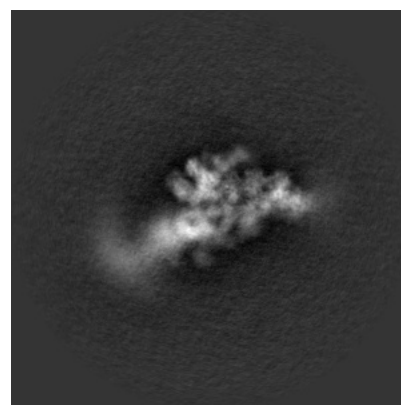
6.1.2 Raw map



X



Y



Z

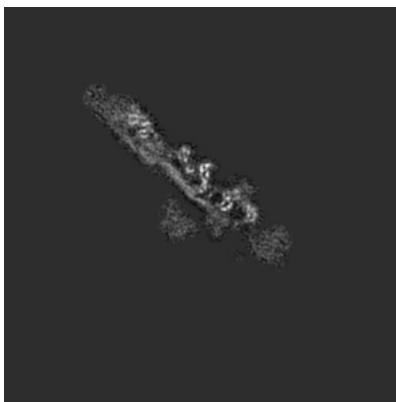
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

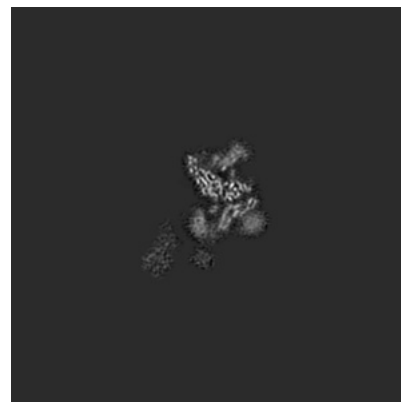
6.2.1 Primary map



X Index: 300

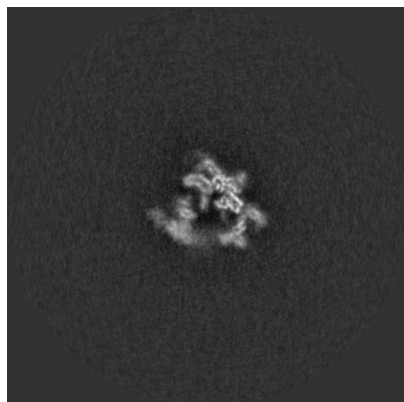


Y Index: 300

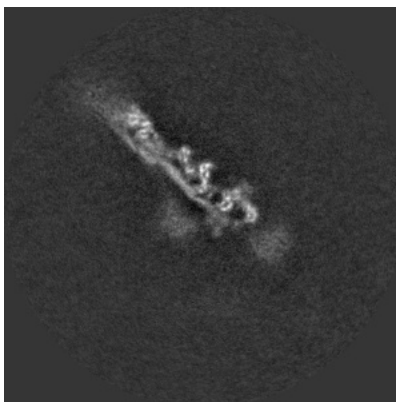


Z Index: 300

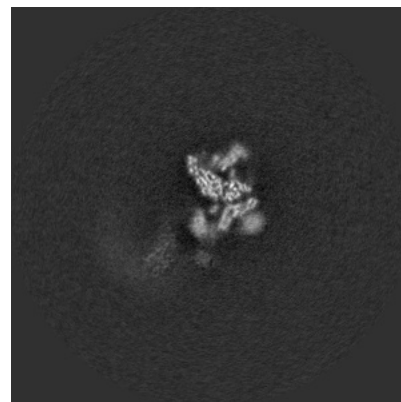
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

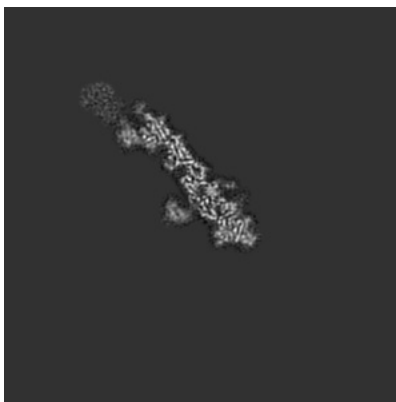
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 288

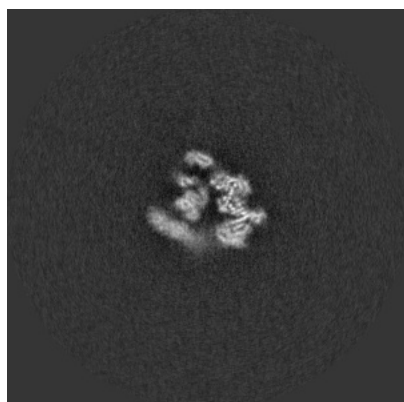


Y Index: 325

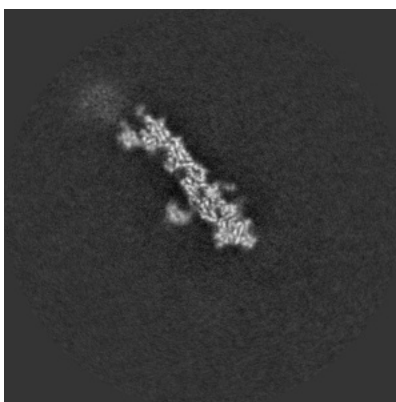


Z Index: 274

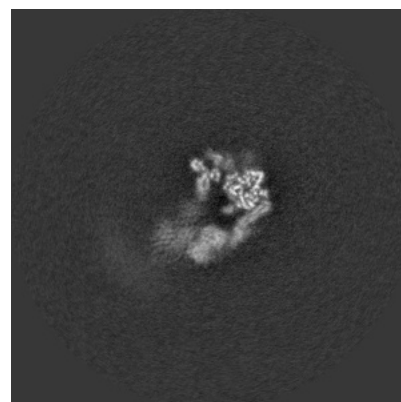
6.3.2 Raw map



X Index: 289



Y Index: 325

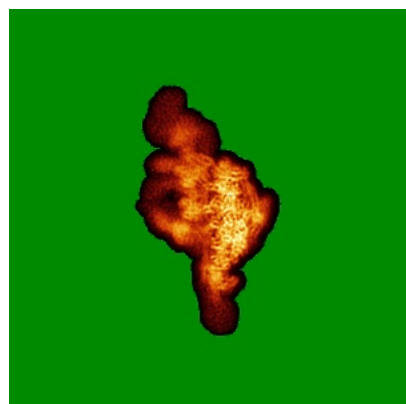


Z Index: 274

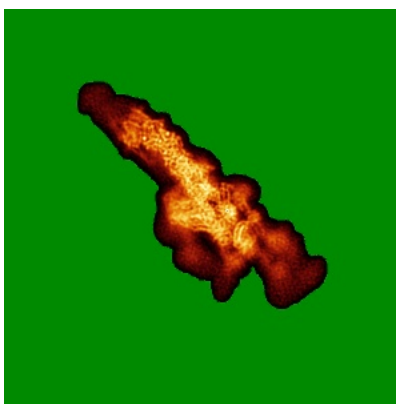
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

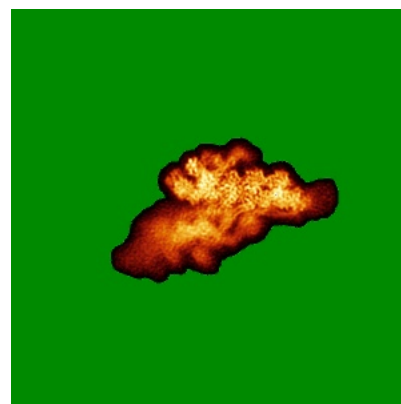
6.4.1 Primary map



X



Y



Z

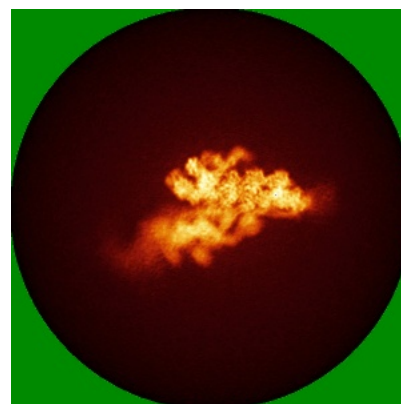
6.4.2 Raw map



X



Y

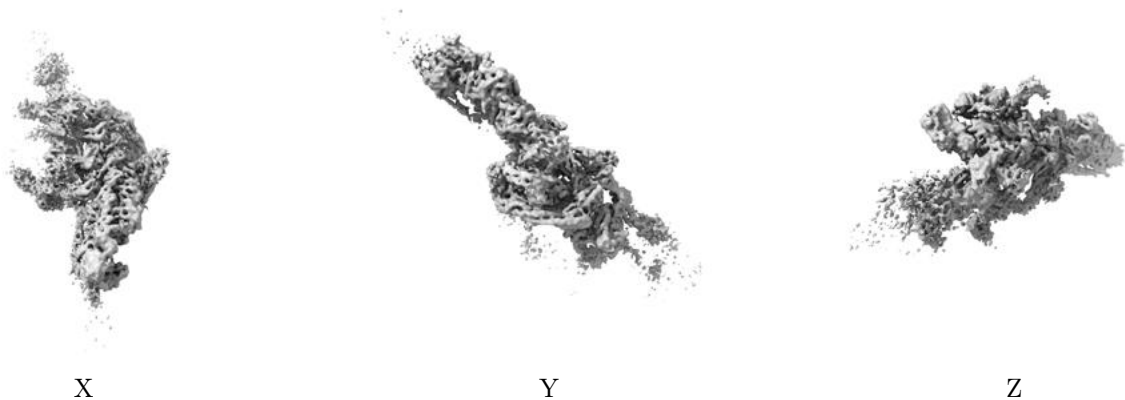


Z

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.

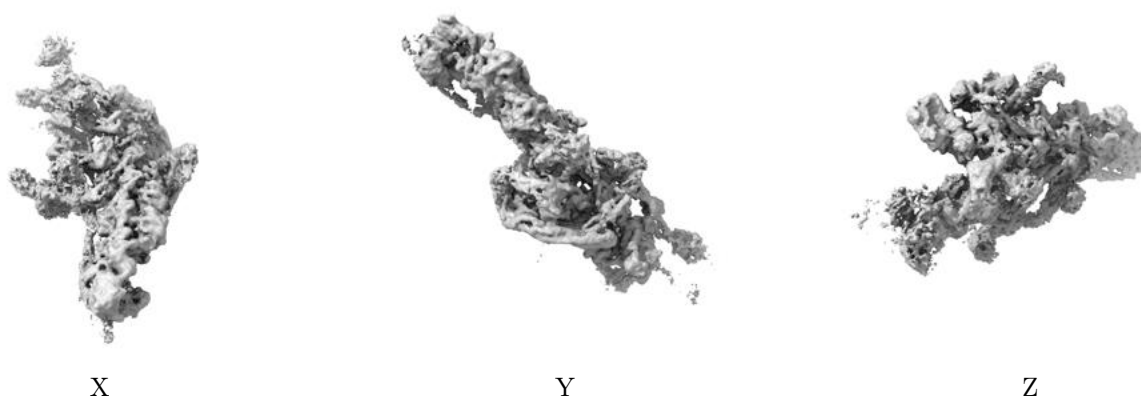
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

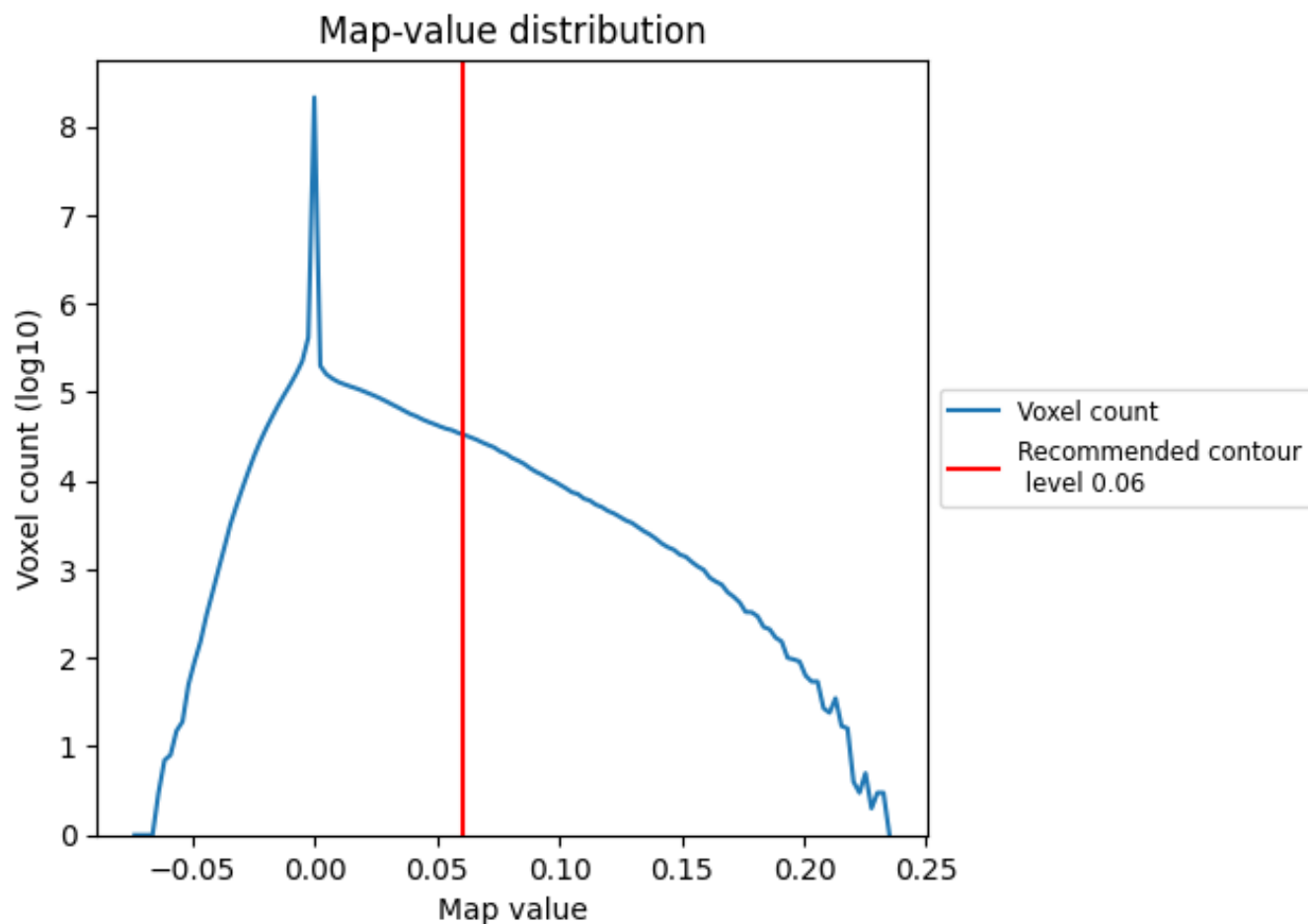
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

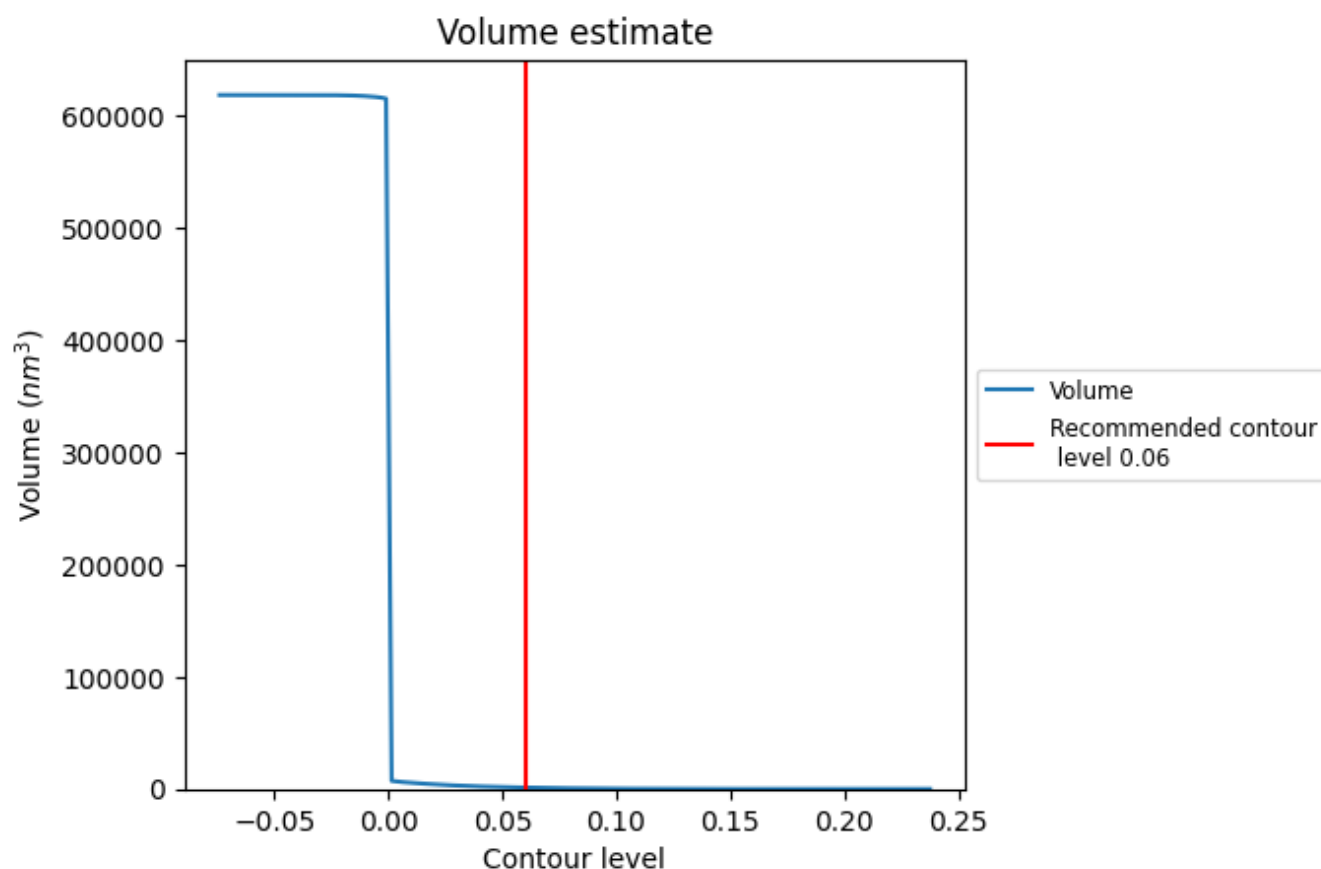
This section contains the results of statistical analysis of the map.

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.

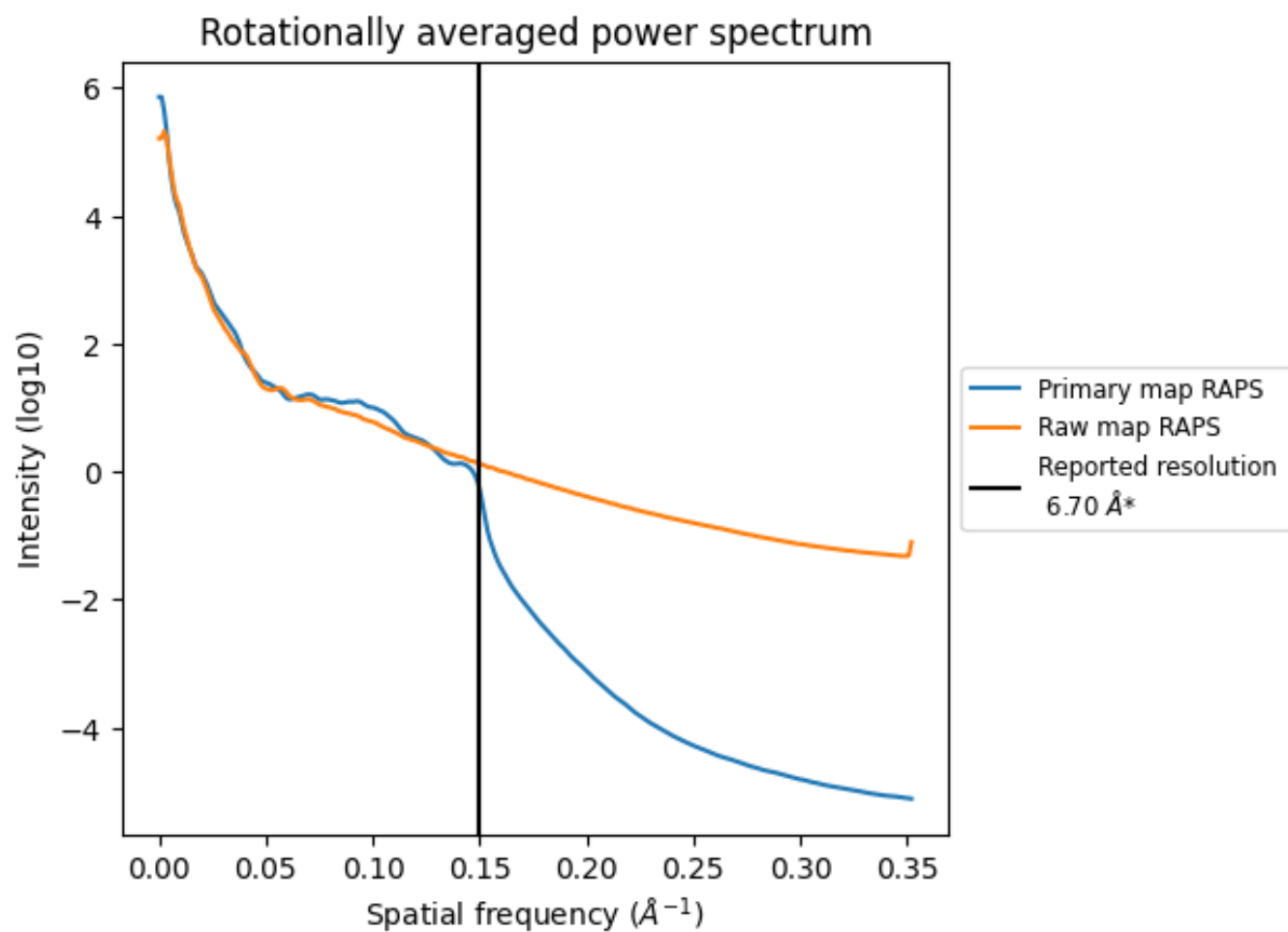
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1246 nm³; this corresponds to an approximate mass of 1125 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

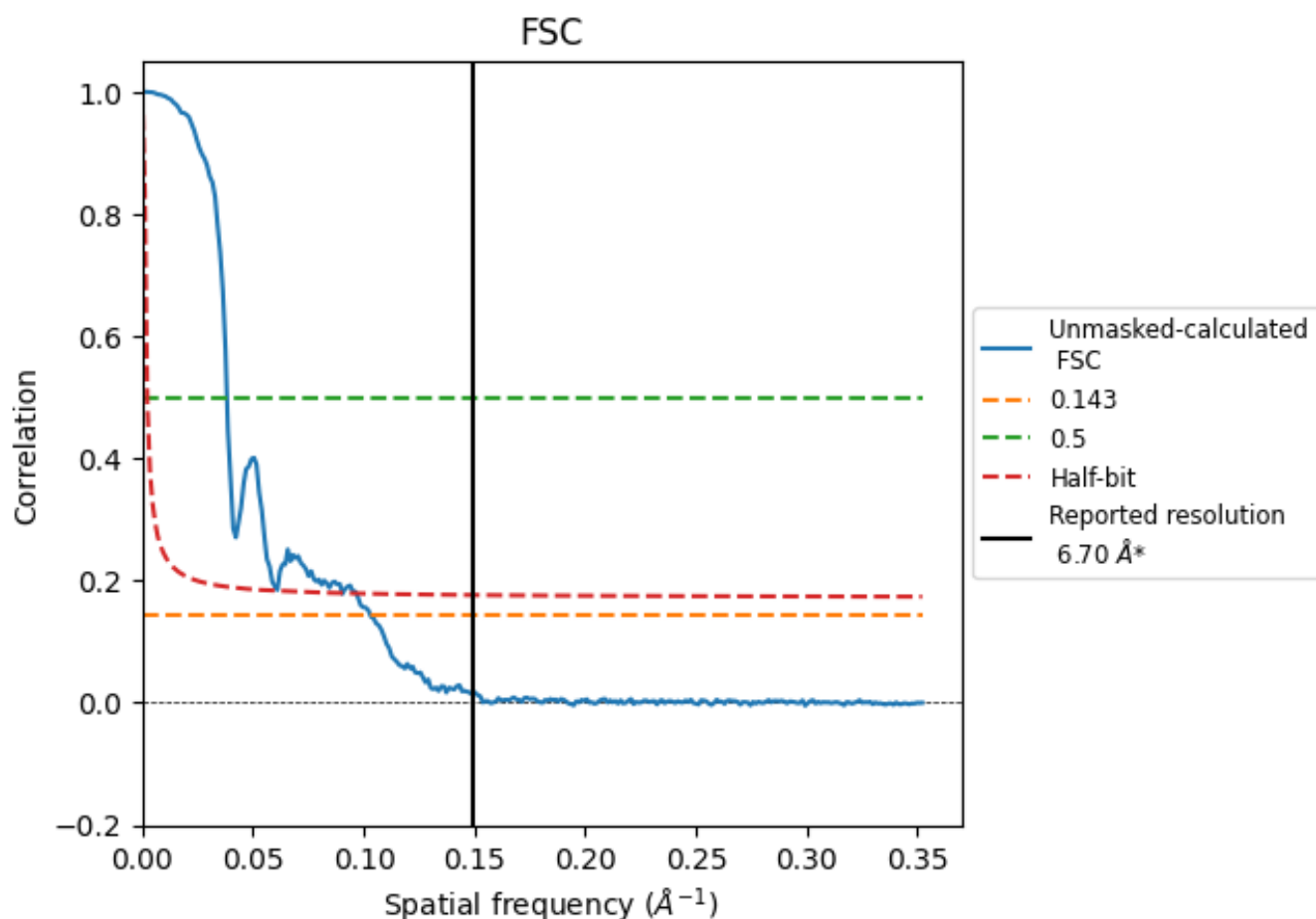


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.149 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

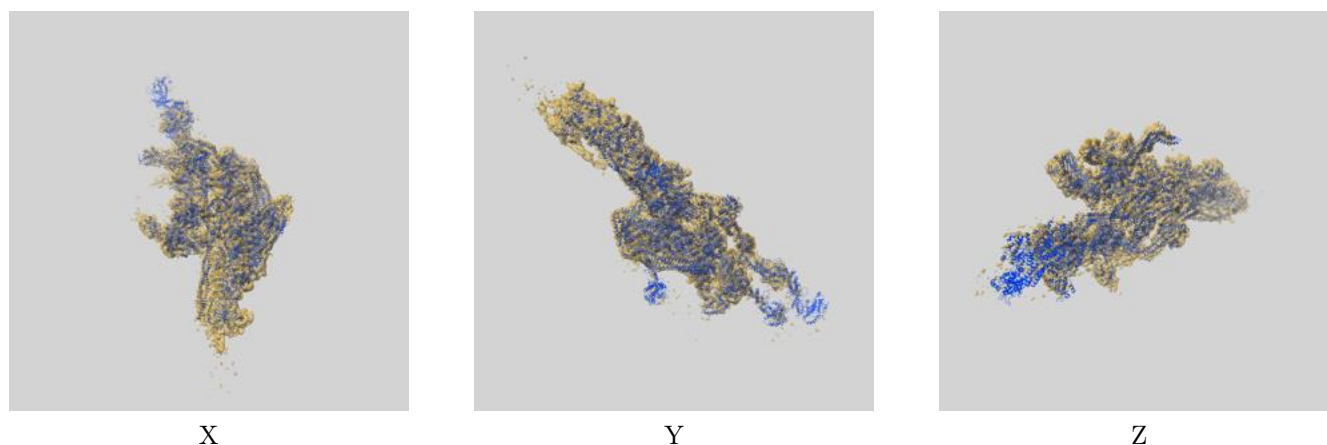
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.71	26.18	11.07

*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 9.71 differs from the reported value 6.7 by more than 10 %

9 Map-model fit [i](#)

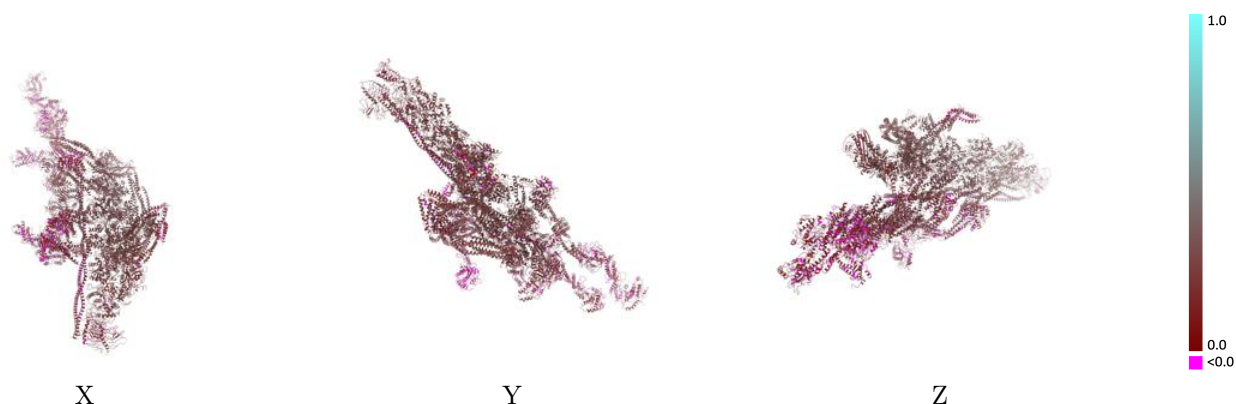
This section contains information regarding the fit between EMDB map EMD-4177 and PDB model 6F38. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



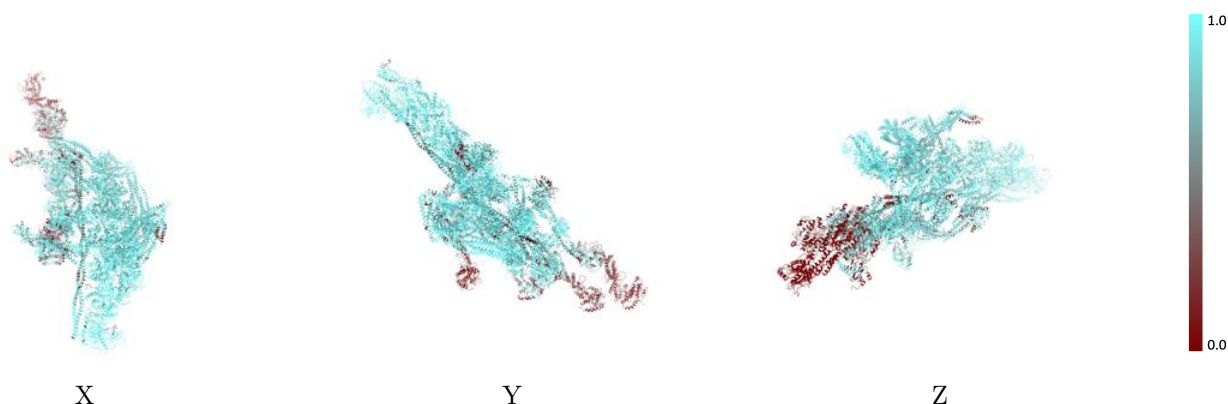
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



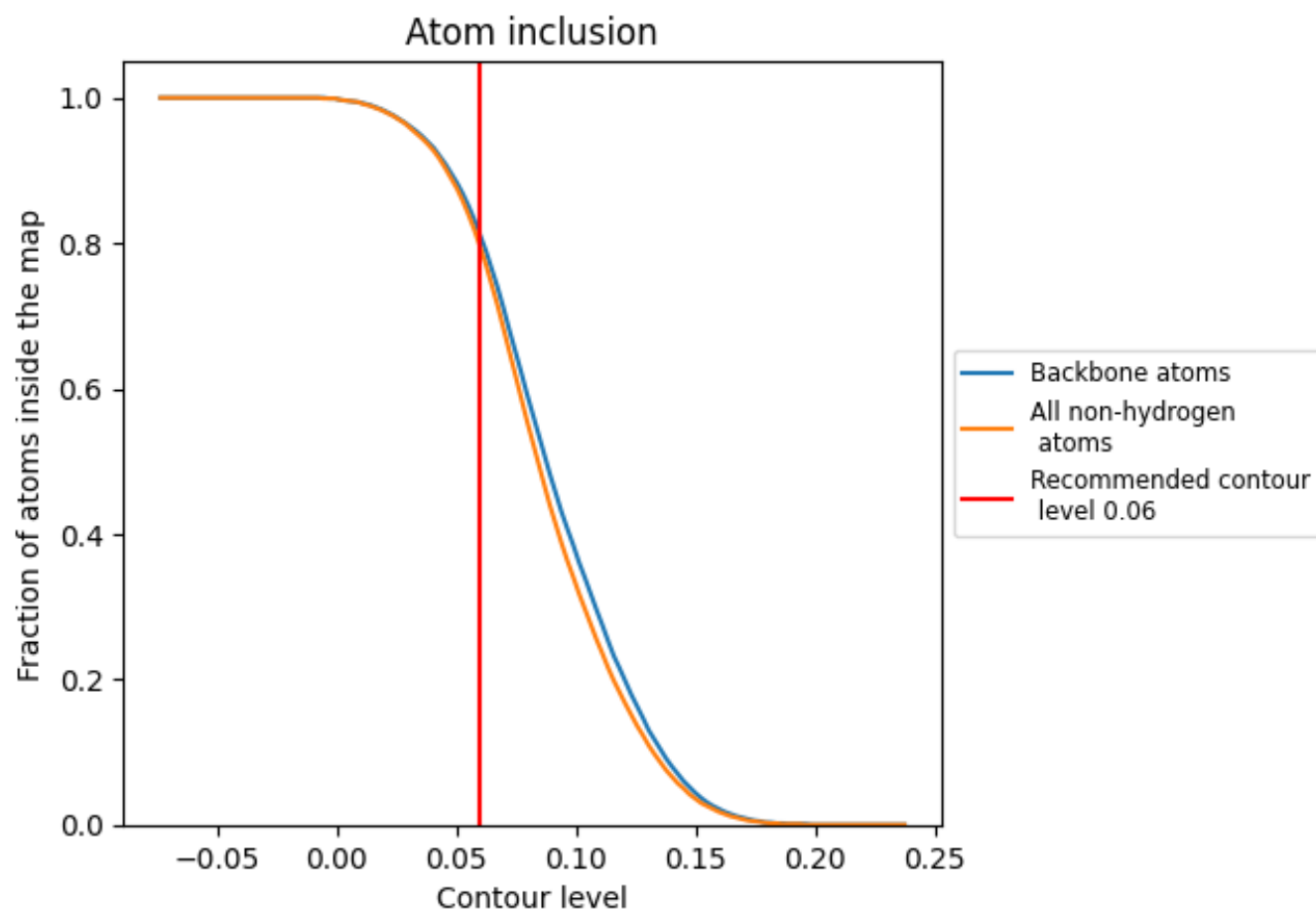
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.2300
A	 0.9710	 0.2770
B	 0.9850	 0.2960
C	 0.9660	 0.2910
D	 0.9870	 0.2990
E	 0.9790	 0.2990
F	 0.9910	 0.3010
G	 0.9920	 0.2930
H	 0.9930	 0.2970
I	 0.9820	 0.2740
J	 0.9830	 0.2810
K	 0.9740	 0.2600
L	 0.9890	 0.2780
M	 0.9580	 0.2450
N	 0.9530	 0.2620
O	 0.9910	 0.3010
P	 0.9970	 0.2980
Q	 0.4530	 0.1500
R	 0.9910	 0.2830
U	 0.8770	 0.1760
V	 0.9910	 0.2640
X	 0.7040	 0.2110
Y	 0.9540	 0.3210
Z	 0.9540	 0.2960
a	 0.9500	 0.2980
b	 0.9270	 0.2800
c	 0.8970	 0.3030
d	 0.8990	 0.3020
e	 0.6710	 0.1900
f	 0.8410	 0.2310
g	 0.7660	 0.1410
h	 0.9450	 0.2210
i	 0.0140	 0.0040
j	 0.4950	 0.1510
k	 0.8510	 0.1460



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Chain	Atom inclusion	Q-score
l	 0.7040	 0.1570
m	 0.6970	 0.2240
n	 0.6130	 0.2010
o	 0.8210	 0.1830
p	 0.5110	 0.1360
q	 0.1370	 0.1770
r	 0.0140	 0.1610
s	 0.4980	 0.1090
t	 0.6280	 0.1230
x	 0.7010	 0.1930
z	 0.8910	 0.2550