Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 04:53 PM EDT

PDB ID	:	9B7J / pdb_00009b7j
EMDB ID	:	EMD-44306
Title	:	Cryo-EM structure of human dynactin complex bound to Chlamydia effector Dre1
Authors	:	Pawar, K.I.; Verba, K.A.
Deposited on	:	2024-03-27
Resolution	:	3.49 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:

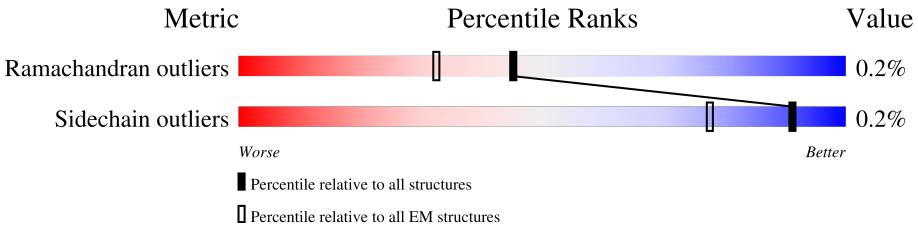
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	10% 95%
1	B	376	96%
1	C	376	98%
1	D	376	97%
1	E	376	96%
1	F	376	96%
1	G	376	96%
1	I	376	7% 97%
2	H	375	97%

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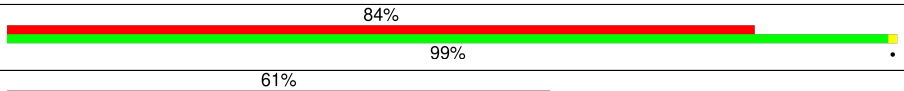
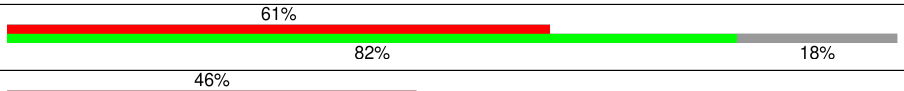
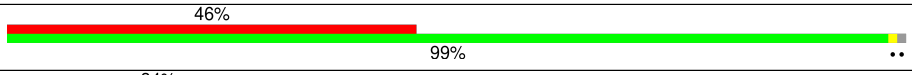
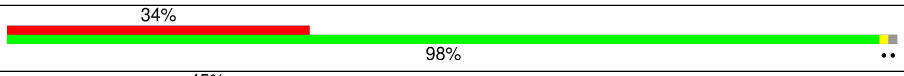
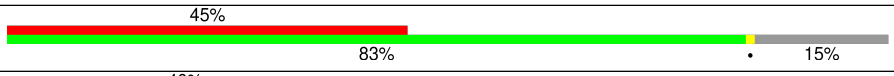
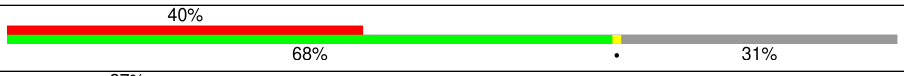
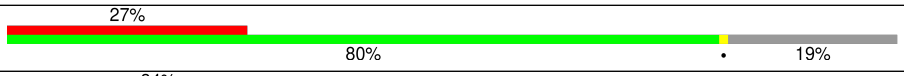
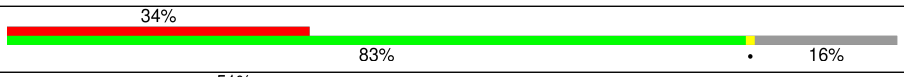
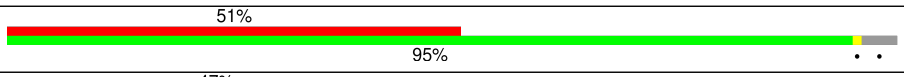
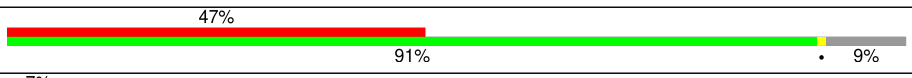
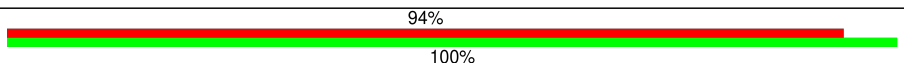
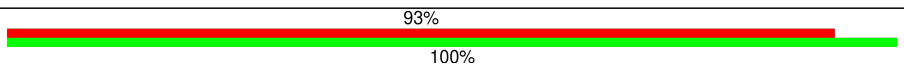
Mol	Chain	Length	Quality of chain
3	J	417	
4	K	460	
5	L	182	
6	M	190	
7	N	286	
8	O	272	
9	P	401	
9	Q	401	
9	p	401	
9	q	401	
10	R	186	
10	r	186	
11	S	1278	
12	T	83	
13	U	87	
14	s	1278	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 113042 atoms, of which 56723 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-centractin.

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

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

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

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

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

- Molecule 4 is a protein called Dynactin subunit 4.

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

- Molecule 5 is a protein called Dynactin subunit 5.

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

- Molecule 6 is a protein called Dynactin subunit 6.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	N	284	Total	C	H	N	O	S	0	0
			4532	1454	2221	402	449	6		

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

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

- Molecule 9 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	P	339	Total	C	H	N	O	S	0	0
			5411	1672	2739	462	533	5		
9	Q	278	Total	C	H	N	O	S	0	0
			4436	1373	2248	375	434	6		
9	p	326	Total	C	H	N	O	S	0	0
			5107	1581	2573	432	513	8		
9	q	337	Total	C	H	N	O	S	0	0
			5312	1651	2669	448	538	6		

- Molecule 10 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	179	Total	C	H	N	O	S	0	0
			2905	908	1475	249	269	4		
10	r	170	Total	C	H	N	O	S	0	0
			2786	872	1417	238	255	4		

- Molecule 11 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	S	154	Total	C	H	N	O	S	0	0
			2444	760	1234	218	229	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1282	ASP	SER	conflict	UNP Q14203

- Molecule 12 is a protein called Dynactin subunit 1, p150-glued.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	83	Total	C	H	N	O	0	0
			1079	332	581	83	83		

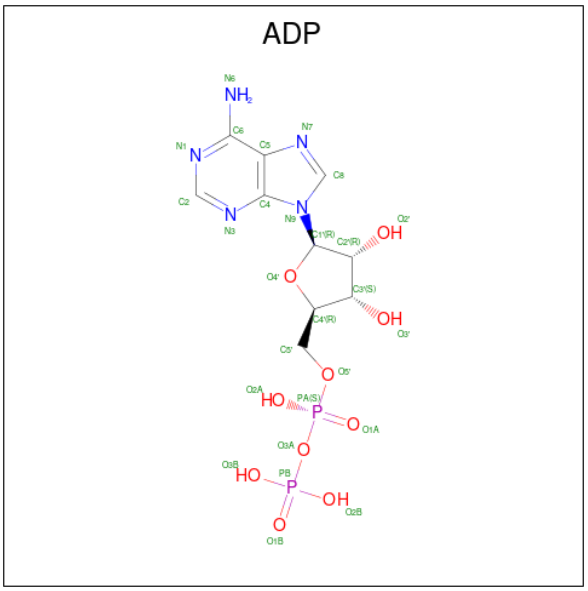
- Molecule 13 is a protein called Dynactin subunit 2, p50 dynamitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	87	Total	C	H	N	O	0	0
			1131	348	609	87	87		

- Molecule 14 is a protein called Dynactin subunit 1.

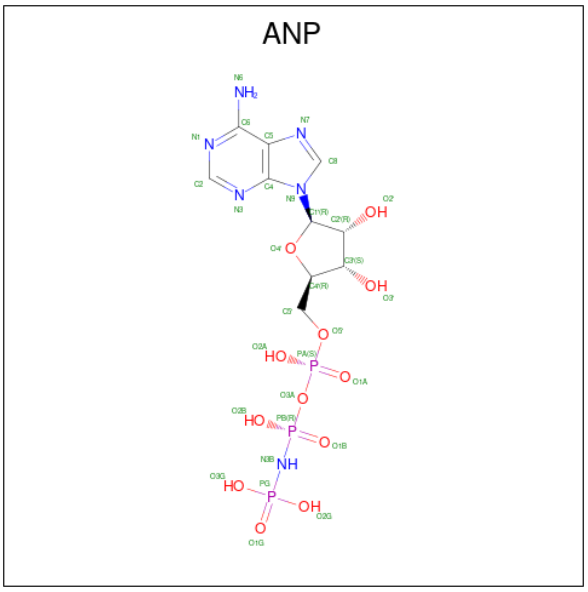
Mol	Chain	Residues	Atoms						AltConf	Trace
14	s	189	Total	C	H	N	O	S	0	0
			2940	910	1484	261	280	5		

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



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

- Molecule 16 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

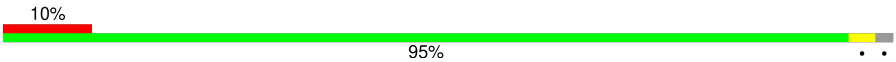
Mol	Chain	Residues	Atoms		AltConf
17	K	3	Total	Zn	0
			3	3	

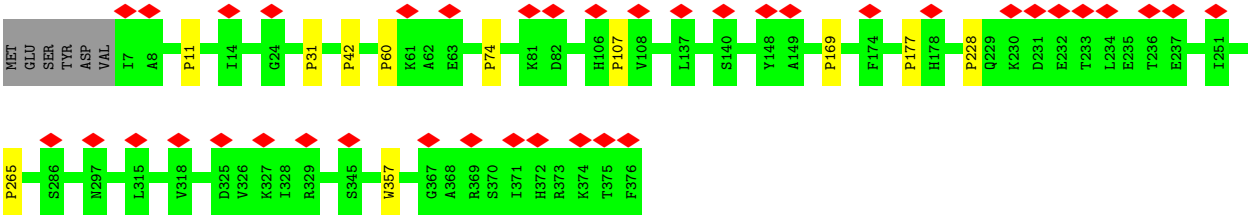
3 Residue-property plots (i)

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

• Molecule 1: Alpha-centractin

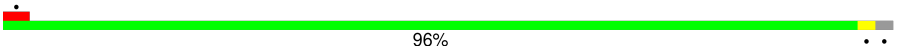
Chain A:

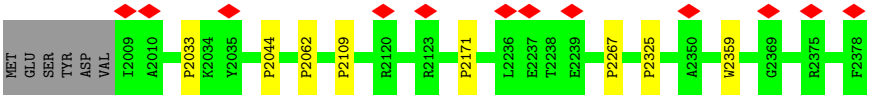




• Molecule 1: Alpha-centractin

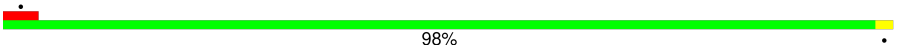
Chain B:

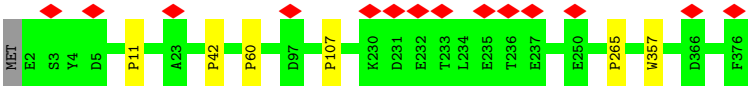




• Molecule 1: Alpha-centractin

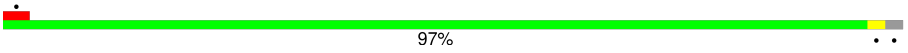
Chain C:

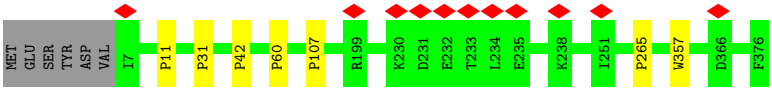




• Molecule 1: Alpha-centractin

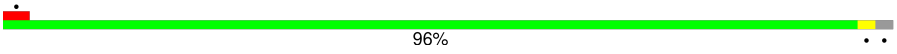
Chain D:

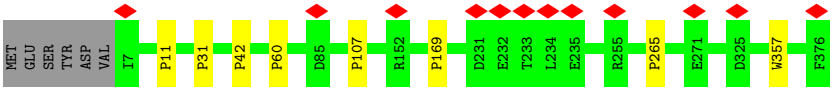




• Molecule 1: Alpha-centractin

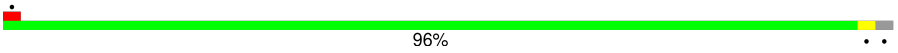
Chain E:





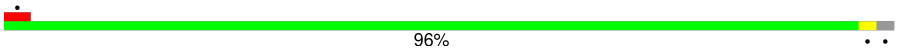
• Molecule 1: Alpha-centractin

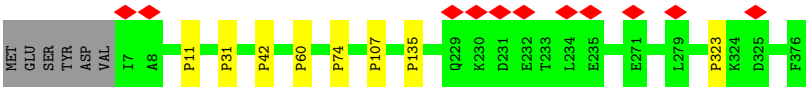
Chain F:



• Molecule 1: Alpha-centractin

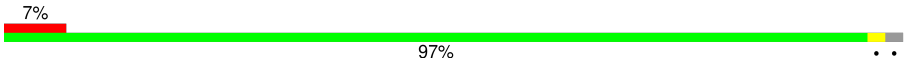
Chain G:

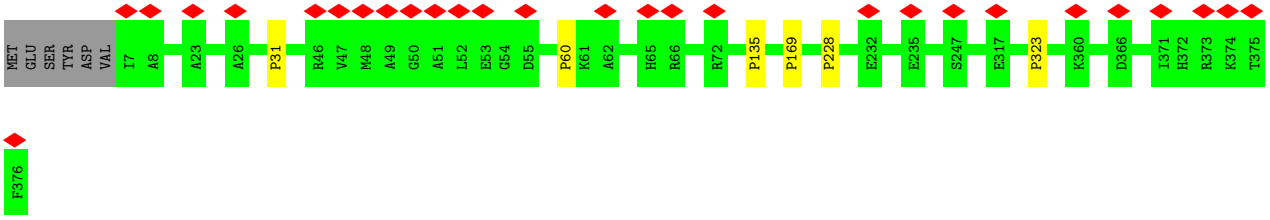




• Molecule 1: Alpha-centractin

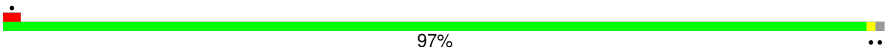
Chain I:

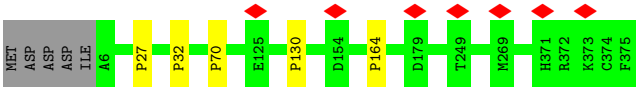




• Molecule 2: Actin, cytoplasmic 1

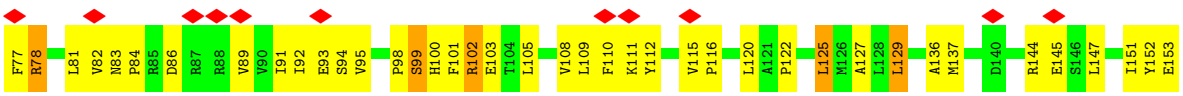
Chain H:

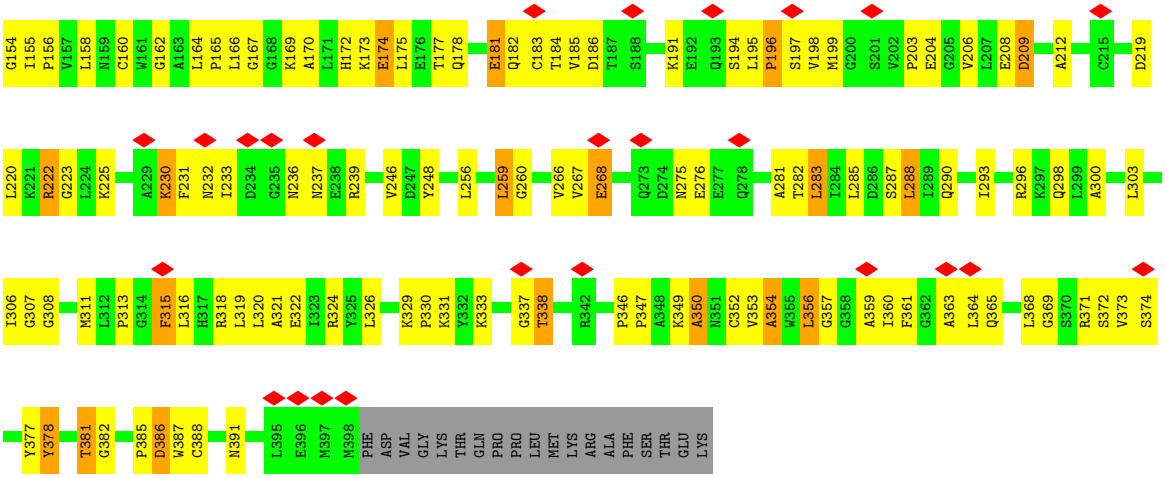




• Molecule 3: Actin-related protein 10

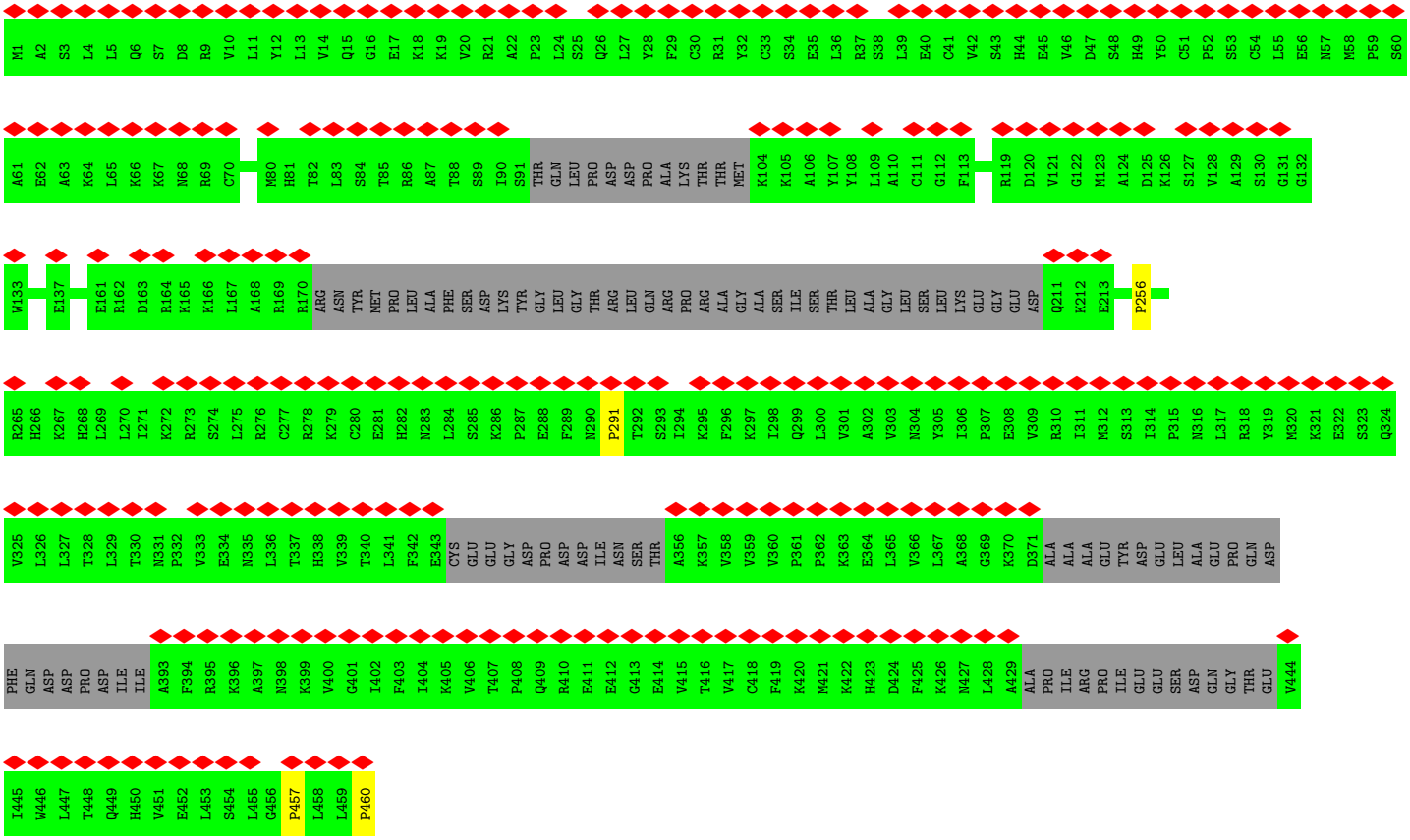
Chain J:





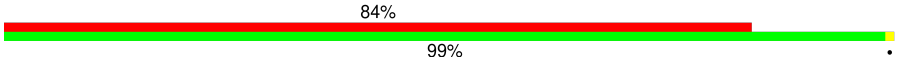
• Molecule 4: Dynactin subunit 4

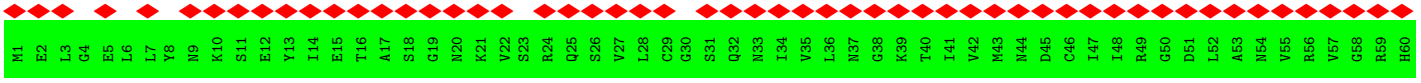
Chain K:

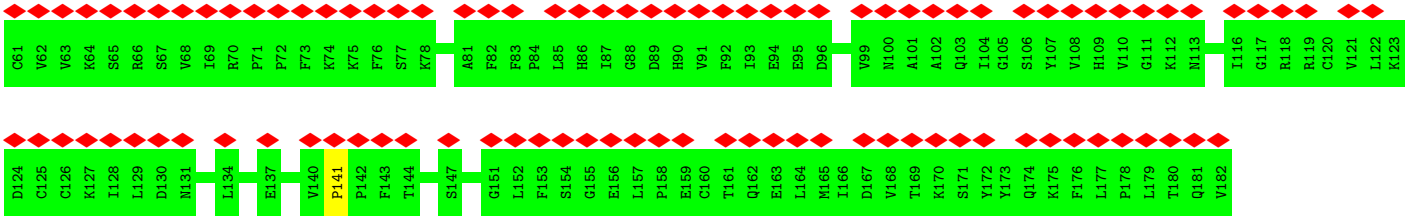


• Molecule 5: Dynactin subunit 5

Chain L:





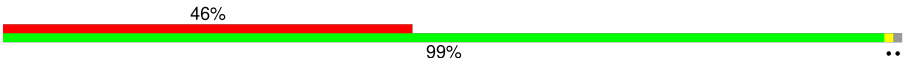


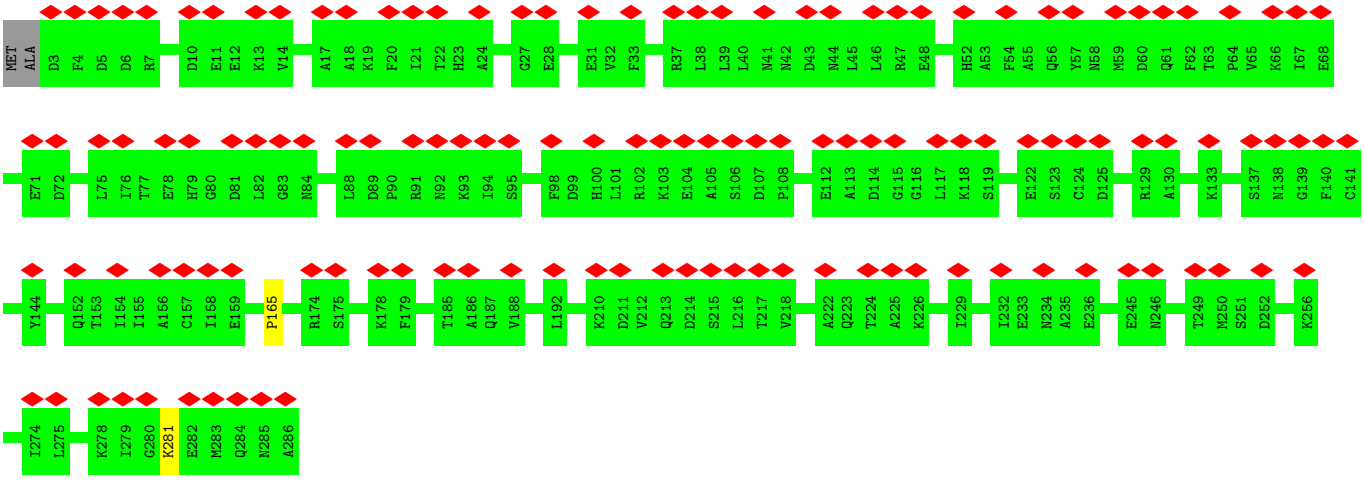
• Molecule 6: Dynactin subunit 6

Chain M:

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

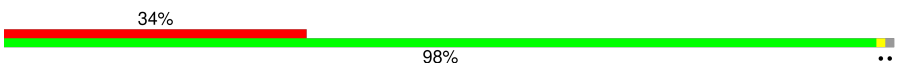
Chain N:

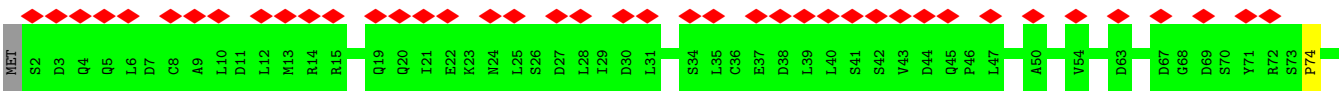


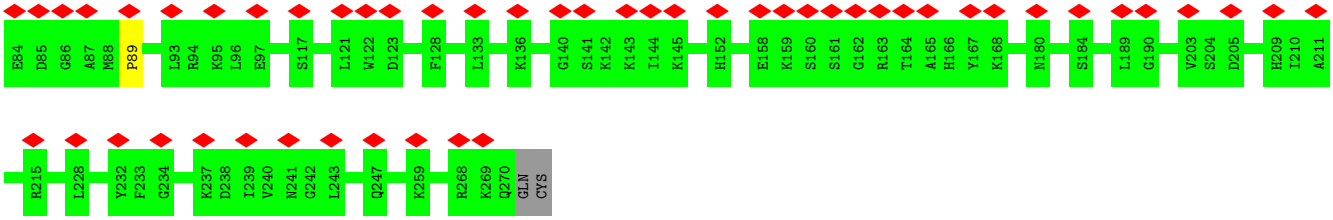


• Molecule 8: F-actin-capping protein subunit beta

Chain O:

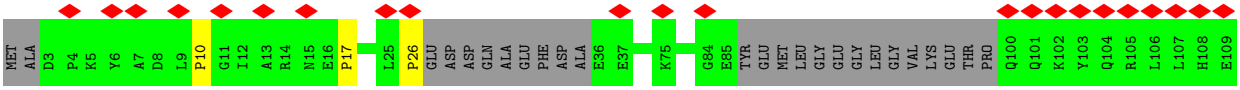


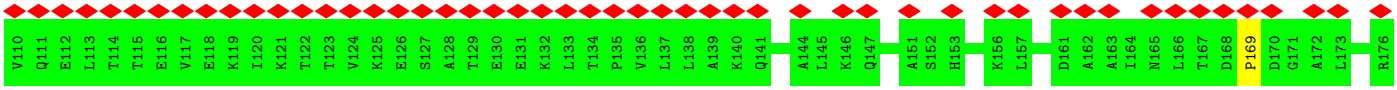


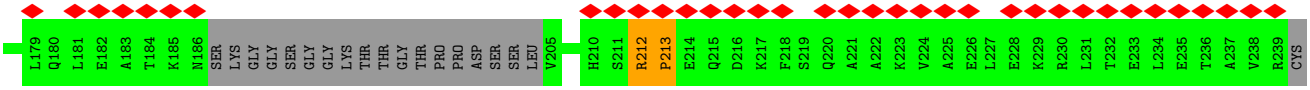


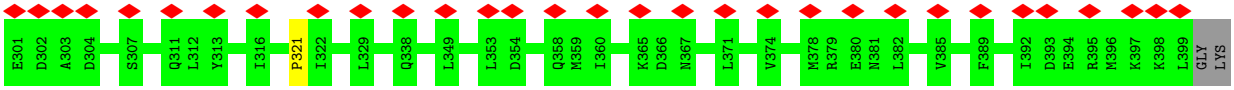
• Molecule 9: Dynactin subunit 2

Chain P:



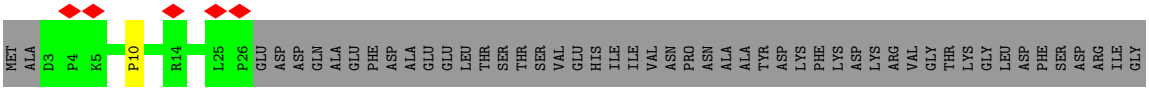


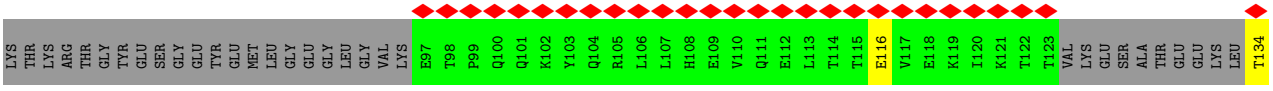


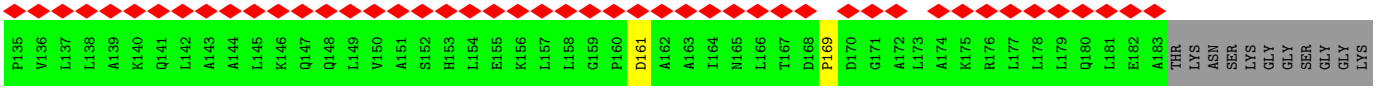


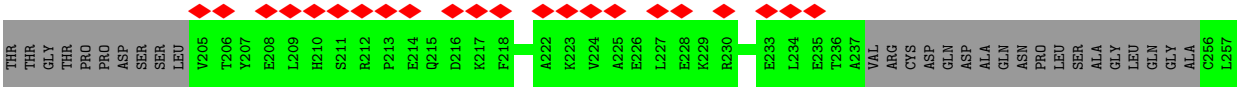
• Molecule 9: Dynactin subunit 2

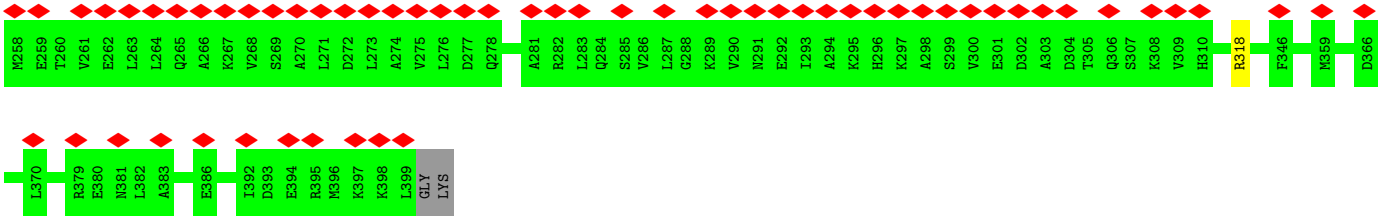
Chain Q:





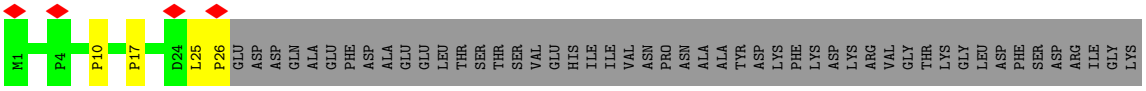


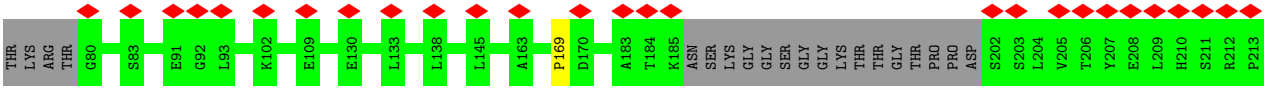


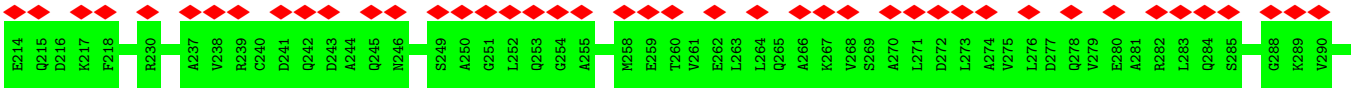


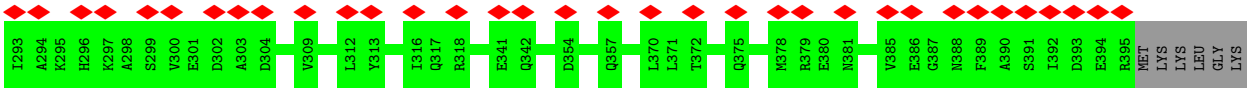
• Molecule 9: Dynactin subunit 2

Chain p:



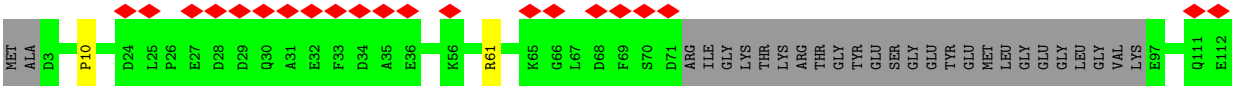


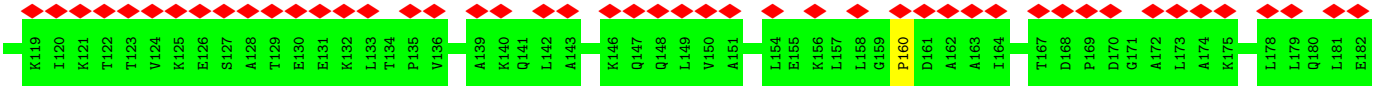


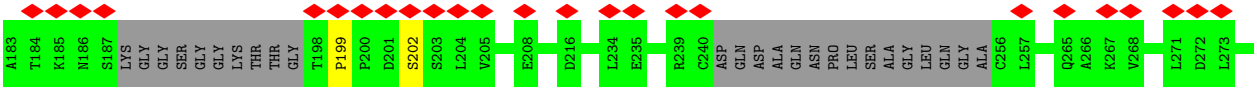


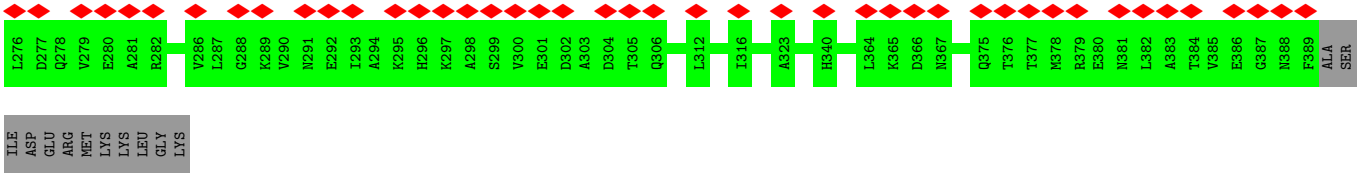
• Molecule 9: Dynactin subunit 2

Chain q:



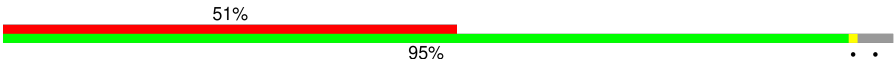


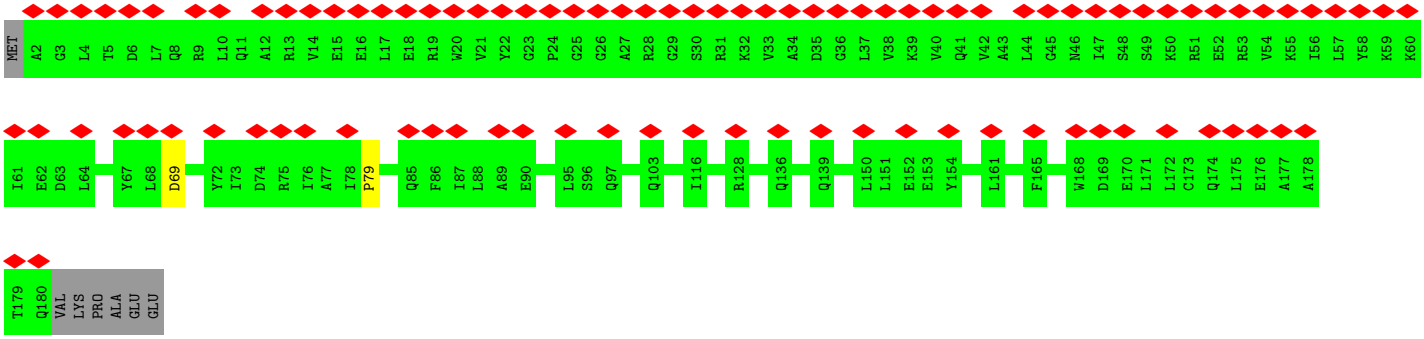




• Molecule 10: Dynactin subunit 3

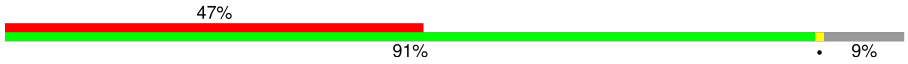
Chain R:

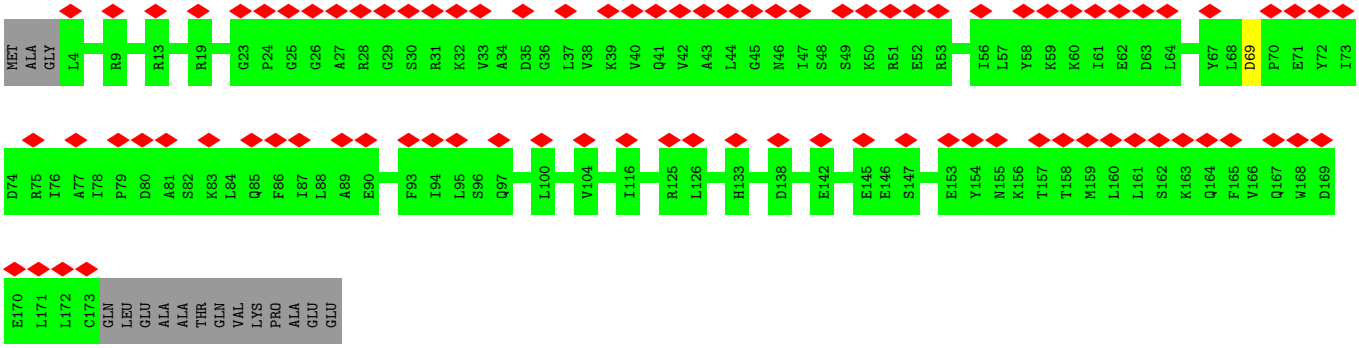




• Molecule 10: Dynactin subunit 3

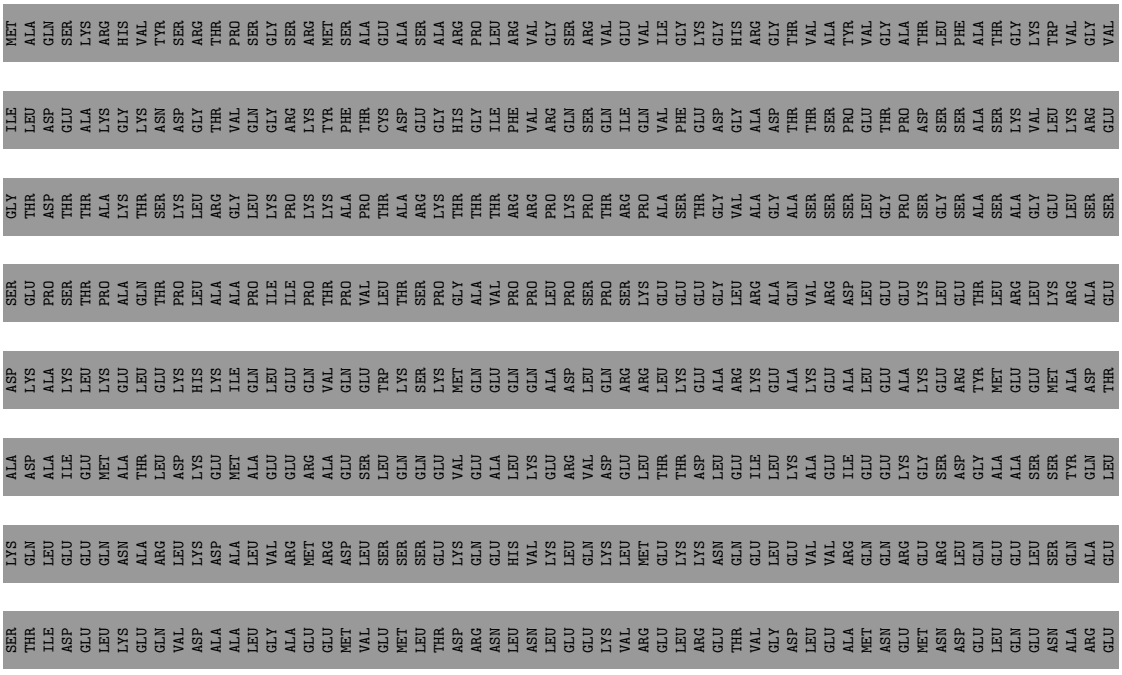
Chain r:

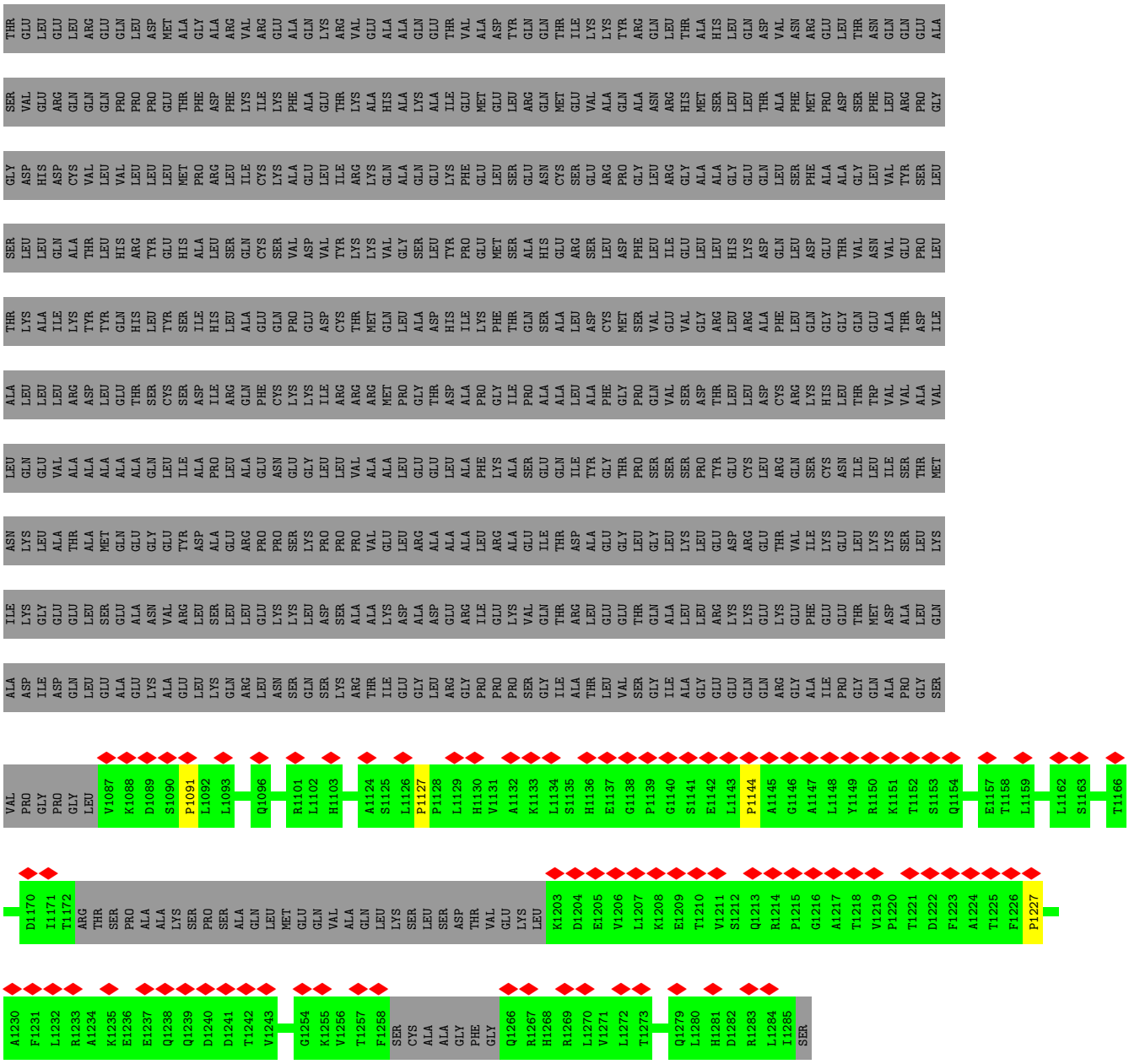




• Molecule 11: Dynactin subunit 1

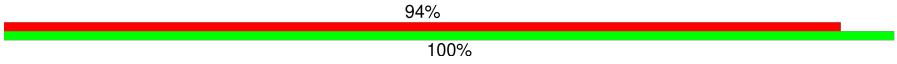
Chain S:





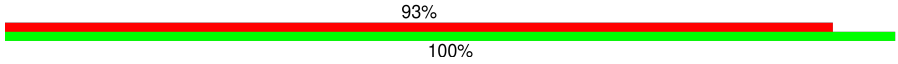
• Molecule 12: Dynactin subunit 1, p150-glued

Chain T:



• Molecule 13: Dynactin subunit 2, p50 dynamitin

Chain U:



X826 X827 X828 X829 X830 X831 X832 X833 X834 X835 X836 X837 X838 X839 X840 X841 X842 X843 X844 X845 X846 X847 X848 X849 X850 X851 X852 X853 X854 X855 X856 X857 X858 X859 X860 X861 X862 X863 X864 X865 X866 X867 X868 X869 X870 X871 X872 X873 X874 X875 X876 X877 X878 X879 X880 X881 X882 X883 X884 X885

X886 X887 X888 X889 X890 X891 X892 X893 X894 X895 X896 X897 X898 X899 X900 X901 X902 X903 X904 X905 X906 X907 X908 X909 X910 X911 X912

• Molecule 14: Dynactin subunit 1

Chain s: 5% 15% 85%

MET ALA GLN SER LYS ARG HIS VAL TYR SER ARG THR PRO SER GLY SER ARG MET SER ALA GLU ALA SER ALA ARG PRO LEU ARG VAL GLY SER ARG VAL GLU VAL ILE GLY LYS GLY HIS ARG GLY THR VAL ALA TYR VAL GLY ALA THR LEU PHE ALA THR GLY LYS TRP VAL GLY VAL

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

GLY THR ASP THR THR ALA LYS THR SER LYS LEU ARG GLY LEU LYS PRO LYS LYS LYS ALA PRO THR ALA ARG LYS THR THR THR ARG ARG PRO PRO LYS PRO THR ARG PRO ALA SER THR GLY VAL ALA ALA GLY ALA SER SER SER LEU GLY PRO SER GLY SER ALA SER ALA GLY GLU LEU SER SER

SER GLU PRO SER THR PRO ALA GLN LEU PRO LEU ALA ALA PRO ILE ILE PRO THR PRO VAL LEU THR SER PRO GLY ALA ALA PRO PRO LEU PRO SER PRO SER PRO LYS GLU GLU GLY GLY LEU ARG ALA GLN VAL ARG ASP LEU LEU GLU GLU LYS LEU GLU THR LEU ARG LEU LYS ARG ALA GLU

ASP LYS ALA LYS LEU LYS GLU LEU GLU LYS HIS LYS ILE GLN LEU GLU GLN VAL GLN GLU TRP LYS SER LYS MET GLN GLU GLN GLN ALA ASP LEU GLN ARG ARG LEU LYS GLU GLU ALA ARG LYS GLU ALA LYS GLU ALA LEU LEU GLU ALA LYS GLY SER ASP GLY ALA ALA SER SER TYR GLN LEU

ALA ASP ALA ILE GLU MET ALA THR LEU ASP LYS GLU ALA GLU GLU ARG ALA GLU SER LEU GLN GLN GLU VAL GLU ALA LEU LYS LYS GLU ALA ARG GLU ILE LEU LYS ALA GLU ILE GLU GLU GLU LYS GLY SER ASP GLY ARG TYR MET GLU GLU MET ALA ASP THR

LYS GLN LEU GLU GLN ASN ALA ARG LEU LYS ASP ALA LEU VAL ARG MET ARG ASP LEU SER SER SER GLU LYS GLN GLU VAL GLU ALA GLN GLU HIS VAL LYS LEU GLN LYS LEU MET GLU LYS LYS ASN GLN GLU LEU GLU VAL VAL ARG GLN GLN ARG GLU ARG LEU GLN GLU GLU LEU SER GLN ALA GLU

SER THR ILE ASP GLU LEU LYS GLU GLN VAL ASP ALA ALA LEU LEU GLY ALA GLU GLU MET VAL GLU MET LEU LEU THR ASP ARG ASN LEU ASN GLU GLU LYS VAL ARG GLU LEU ARG GLU THR VAL GLY ASP LEU GLU ALA MET ASN GLU MET ASN ASP GLU LEU GLN GLU ASN ALA ARG GLU

THR GLU LEU GLU LEU ARG GLU GLN LEU ASP MET ALA GLY ALA ARG VAL ALA GLU ARG GLU ALA ALA GLN LYS ARG VAL GLU ALA ALA ASP TYR GLN GLN THR ILE LYS LYS TYR ARG GLN LEU THR ALA HIS LEU LEU GLN ASP VAL ASN ARG GLU LEU THR ASN GLN GLU GLU ALA

SER VAL GLU ARG GLN GLN PRO PRO PRO PRO GLU THR PHE ASP PHE LYS ILE LYS PHE ALA GLU THR LYS ALA HIS ALA LYS ALA GLU ILE GLU GLU MET GLU LEU GLU ARG GLN MET GLU VAL ALA ASN ARG HIS MET SER LEU LEU LEU THR ALA PHE MET PRO ASP SER PHE LEU ARG PRO GLY

GLY ASP HIS ASP CYS VAL LEU VAL LEU LEU LEU MET PRO ARG LEU ILE CYS LYS ALA GLU LEU ILE ARG LYS GLN ALA GLU GLU LYS PHE GLU LEU SER GLU ASN CYS SER GLU ARG PRO GLY LEU ARG GLY ALA ALA GLU GLY LEU VAL TYR SER LEU

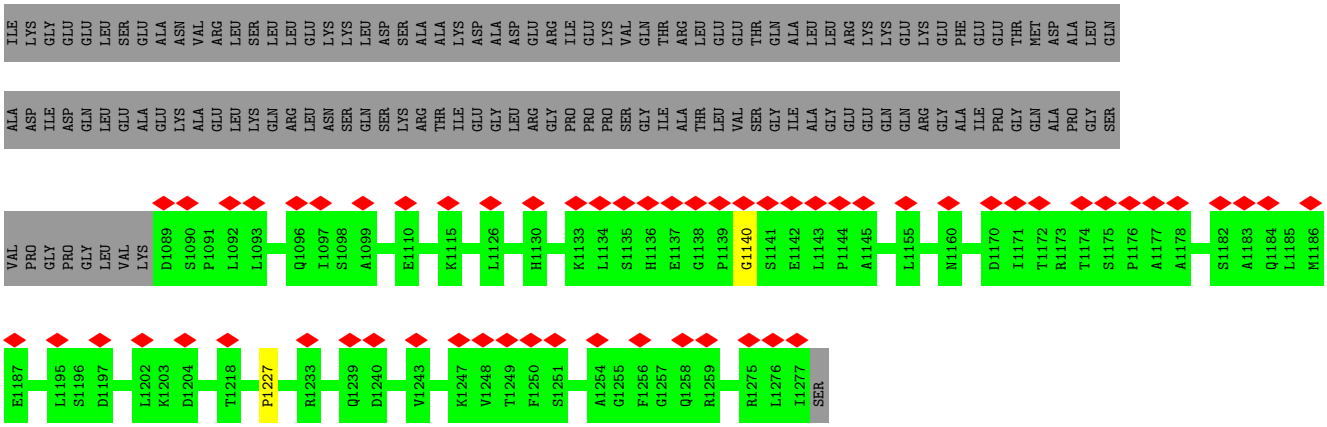
SER LEU LEU GLN LEU HIS ARG TYR GLU HIS ALA LEU SER GLN CYS SER VAL ASP VAL TYR LYS LYS VAL GLY SER LEU TYR PRO GLU MET SER ALA HIS GLU ARG SER LEU ASP PHE LEU ILE GLU GLU LEU HIS LYS ASP GLN LEU ASP GLU THR VAL ASN VAL GLU PRO LEU

THR LYS ALA ILE LYS TYR TYR GLN HIS LEU TYR SER ILE HIS LEU ALA GLU GLN PRO GLU ASP CYS THR MET GLN LEU ALA ASP HIS ILE LYS PHE THR GLN SER ALA LEU ASP CYS MET SER VAL GLU VAL GLY ARG LEU ARG ALA PHE LEU GLN GLY GLY GLN GLU ALA THR ASP ILE

ALA LEU LEU LEU ARG ASP LEU GLU THR SER CYS SER ASP ILE ARG GLN PHE CYS LYS LYS ILE ARG ARG MET PRO GLY THR ASP ALA PRO ALA ALA LEU ALA ALA PHE GLY PRO GLN VAL SER ASP THR LEU LEU ASP CYS ARG LYS HIS LEU THR TRP VAL VAL ALA LYS VAL

LEU GLN GLU VAL ALA ALA GLN LEU GLU GLU ALA ALA ALA GLU GLU ASN GLU GLY LEU GLU LEU ALA LEU VAL ALA ALA LEU GLU LEU LEU ALA PHE LYS ALA ALA SER GLU GLU GLN ILE ILE TYR GLY THR PRO SER SER SER PRO TYR GLU CYS LEU ARG GLN SER HIS CYS ASN ILE LEU LEU ILE SER THR MET

ASN LYS LEU ALA THR ALA MET GLN GLU GLY GLU TYR ASP ALA GLU ARG PRO PRO SER LYS PRO PRO PRO VAL GLU LEU ARG ALA ALA ALA LEU ARG GLU ILE THR ASP ALA GLU GLY LEU GLY LEU LYS LEU GLU ASP ARG GLU THR VAL ILE LYS GLU LEU LYS LYS SER LEU LYS


ILE LYS GLY GLU GLU LEU SER GLU ALA ASN VAL ARG LEU SER LEU LEU GLU LYS LYS LEU ASP SER ALA ALA LYS ASP ALA ASP GLU ARG ILE GLU LYS VAL GLN THR ARG LEU GLU GLU THR GLN ALA LEU LEU ARG LYS LYS GLU LYS GLU PHE GLU GLU THR MET ASP ALA LEU GLN
ALA ASP ILE ASP GLN LEU GLU GLU ALA GLU LYS ALA GLU LEU LYS GLN ARG LEU ASN SER GLN SER LYS ARG THR ILE GLU GLY LEU ARG GLY PRO PRO PRO SER GLY ILE ALA THR LEU VAL SER GLY ILE ALA GLY GLU GLU GLN GLN ARG GLY ALA ILE PRO GLY GLN ALA PRO GLY SER
VAL PRO GLY PRO GLY LEU VAL LYS D1089 S1090 P1091 L1092 L1093 Q1096 I1097 S1098 A1099 E1110 K1115 L1126 H1130 K1133 L1134 S1135 H1136 E1137 G1138 P1139 G1140 S1141 E1142 L1143 P1144 A1145 L1155 N1160 D1170 I1171 T1172 R1173 T1174 S1175 P1176 A1177 A1178 S1182 A1183 Q1184 L1185 M1186
E1187 L1195 S1196 D1197 L1202 K1203 D1204 T1218 P1227 R1233 Q1239 D1240 V1243 K1247 V1248 T1249 F1250 S1251 A1254 G1255 F1256 G1257 Q1258 R1259 R1275 L1276 I1277 SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45091	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 ($e^-/Å^2$)	57.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.993	Depositor
Minimum map value	-14.456	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.573	Depositor
Recommended contour level	6	Depositor
Map size (Å)	721.44, 721.44, 721.44	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.01	10/3025 (0.3%)	0.74	0/4085
1	B	0.99	7/3025 (0.2%)	0.74	0/4085
1	C	1.00	5/3068 (0.2%)	0.74	0/4144
1	D	0.99	6/3025 (0.2%)	0.74	0/4085
1	E	0.99	7/3025 (0.2%)	0.74	0/4085
1	F	1.00	8/3025 (0.3%)	0.74	0/4085
1	G	1.01	8/3025 (0.3%)	0.74	0/4085
1	I	1.00	6/3025 (0.2%)	0.74	0/4085
2	H	0.98	5/2948 (0.2%)	0.75	0/3991
3	J	2.01	106/3088 (3.4%)	2.22	203/4188 (4.8%)
4	K	0.76	4/2970 (0.1%)	0.59	0/4005
5	L	0.71	1/1435 (0.1%)	0.60	0/1941
6	M	0.71	0/1209	0.64	0/1641
7	N	0.75	1/2363 (0.0%)	0.57	0/3197
8	O	0.95	2/2156 (0.1%)	0.75	0/2906
9	P	0.86	5/2700 (0.2%)	0.76	1/3646 (0.0%)
9	Q	0.85	2/2211 (0.1%)	0.80	5/2993 (0.2%)
9	p	0.85	4/2562 (0.2%)	0.74	0/3469
9	q	0.84	2/2675 (0.1%)	0.77	0/3626
10	R	0.84	1/1449 (0.1%)	0.83	0/1957
10	r	0.80	0/1388	0.75	0/1874
11	S	0.86	3/1229 (0.2%)	0.83	1/1660 (0.1%)
14	s	0.76	1/1481 (0.1%)	0.72	0/2005
All	All	1.01	194/56107 (0.3%)	0.88	210/75838 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	29

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	102	ARG	N-CA	-11.59	1.23	1.46
3	J	330	PRO	N-CA	-10.70	1.29	1.47
3	J	206	VAL	CA-C	-9.83	1.27	1.52
3	J	318	ARG	CA-C	-9.20	1.29	1.52
9	P	213	PRO	N-CD	-9.09	1.35	1.47
3	J	331	LYS	N-CA	-8.87	1.28	1.46
11	S	1144	PRO	N-CD	-8.87	1.35	1.47
3	J	184	THR	C-O	8.73	1.40	1.23
3	J	356	LEU	C-N	-8.45	1.17	1.33
3	J	357	GLY	CA-C	8.43	1.65	1.51
3	J	186	ASP	N-CA	-8.13	1.30	1.46
3	J	167	GLY	N-CA	-7.82	1.34	1.46
3	J	183	CYS	N-CA	-7.79	1.30	1.46
1	I	135	PRO	N-CD	-7.54	1.37	1.47
3	J	329	LYS	C-N	-7.39	1.20	1.34
1	G	135	PRO	N-CD	-7.33	1.37	1.47
3	J	319	LEU	N-CA	-7.31	1.31	1.46
9	P	169	PRO	N-CD	-7.27	1.37	1.47
3	J	122	PRO	N-CD	-7.25	1.37	1.47
3	J	346	PRO	CA-C	-7.24	1.38	1.52
3	J	144	ARG	CA-C	-7.22	1.34	1.52
3	J	316	LEU	CA-C	-7.19	1.34	1.52
3	J	319	LEU	CA-C	-7.11	1.34	1.52
3	J	230	LYS	CA-C	-7.05	1.34	1.52
3	J	313	PRO	N-CA	-7.01	1.35	1.47
3	J	166	LEU	N-CA	-7.00	1.32	1.46
14	s	1227	PRO	N-CD	-6.97	1.38	1.47
9	p	26	PRO	N-CD	-6.93	1.38	1.47
3	J	364	LEU	N-CA	-6.93	1.32	1.46
3	J	276	GLU	N-CA	-6.93	1.32	1.46
3	J	313	PRO	CA-C	-6.82	1.39	1.52
3	J	377	TYR	CA-C	-6.81	1.35	1.52
3	J	322	GLU	CA-C	-6.71	1.35	1.52
3	J	77	PHE	N-CA	-6.69	1.32	1.46
1	D	107	PRO	N-CD	-6.64	1.38	1.47
1	A	265	PRO	N-CD	-6.64	1.38	1.47
4	K	256	PRO	N-CD	-6.62	1.38	1.47
3	J	172	HIS	N-CA	-6.60	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2109	PRO	N-CD	-6.58	1.38	1.47
4	K	460	PRO	N-CD	-6.58	1.38	1.47
3	J	382	GLY	CA-C	-6.52	1.41	1.51
1	I	60	PRO	N-CD	-6.50	1.38	1.47
1	A	228	PRO	N-CD	-6.46	1.38	1.47
1	C	107	PRO	N-CD	-6.44	1.38	1.47
3	J	182	GLN	C-O	6.43	1.35	1.23
8	O	74	PRO	N-CD	-6.42	1.38	1.47
3	J	109	LEU	CA-C	-6.40	1.36	1.52
11	S	1091	PRO	N-CD	-6.38	1.39	1.47
3	J	101	PHE	C-N	-6.36	1.19	1.34
3	J	156	PRO	CA-C	-6.35	1.40	1.52
1	A	107	PRO	N-CD	-6.32	1.39	1.47
3	J	311	MET	N-CA	-6.32	1.33	1.46
3	J	322	GLU	C-N	-6.32	1.19	1.34
3	J	185	VAL	C-N	-6.31	1.19	1.34
1	E	11	PRO	N-CD	-6.26	1.39	1.47
2	H	164	PRO	N-CD	-6.25	1.39	1.47
3	J	110	PHE	N-CA	-6.24	1.33	1.46
3	J	388	CYS	N-CA	-6.22	1.33	1.46
3	J	162	GLY	CA-C	6.21	1.61	1.51
2	H	130	PRO	N-CD	-6.18	1.39	1.47
1	A	60	PRO	N-CD	-6.17	1.39	1.47
11	S	1227	PRO	N-CD	-6.17	1.39	1.47
8	O	89	PRO	N-CD	-6.16	1.39	1.47
3	J	320	LEU	N-CA	-6.15	1.34	1.46
3	J	154	GLY	N-CA	-6.15	1.36	1.46
1	G	11	PRO	N-CD	-6.11	1.39	1.47
1	E	107	PRO	N-CD	-6.11	1.39	1.47
3	J	321	ALA	N-CA	-6.11	1.34	1.46
3	J	89	VAL	C-N	-6.11	1.20	1.34
3	J	101	PHE	CA-C	-6.11	1.37	1.52
1	F	60	PRO	N-CD	-6.07	1.39	1.47
1	G	60	PRO	N-CD	-6.06	1.39	1.47
1	F	169	PRO	N-CD	-6.05	1.39	1.47
3	J	65	TYR	CA-C	-6.05	1.37	1.52
3	J	37	CYS	N-CA	-6.04	1.34	1.46
3	J	248	TYR	C-N	-6.03	1.22	1.34
9	P	321	PRO	N-CD	-6.01	1.39	1.47
1	C	11	PRO	N-CD	-5.96	1.39	1.47
3	J	290	GLN	N-CA	-5.96	1.34	1.46
1	A	11	PRO	N-CD	-5.95	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	94	SER	CA-C	-5.95	1.37	1.52
3	J	209	ASP	CA-C	-5.95	1.37	1.52
3	J	98	PRO	N-CD	-5.94	1.39	1.47
3	J	93	GLU	N-CA	-5.94	1.34	1.46
1	B	2044	PRO	N-CD	-5.93	1.39	1.47
3	J	66	SER	N-CA	-5.92	1.34	1.46
1	D	60	PRO	N-CD	-5.92	1.39	1.47
3	J	318	ARG	N-CA	-5.92	1.34	1.46
1	D	42	PRO	N-CD	-5.92	1.39	1.47
3	J	137	MET	N-CA	5.92	1.58	1.46
3	J	231	PHE	N-CA	-5.91	1.34	1.46
1	I	169	PRO	N-CD	-5.88	1.39	1.47
1	C	60	PRO	N-CD	-5.88	1.39	1.47
3	J	74	ILE	C-N	-5.87	1.20	1.34
1	F	107	PRO	N-CD	-5.85	1.39	1.47
3	J	368	LEU	C-N	-5.84	1.22	1.33
1	E	42	PRO	N-CD	-5.84	1.39	1.47
1	C	42	PRO	N-CD	-5.80	1.39	1.47
1	B	2062	PRO	N-CD	-5.78	1.39	1.47
1	E	60	PRO	N-CD	-5.77	1.39	1.47
3	J	112	TYR	CA-C	-5.76	1.38	1.52
3	J	372	SER	N-CA	-5.71	1.34	1.46
3	J	324	ARG	C-N	-5.69	1.21	1.34
3	J	71	PHE	CA-C	-5.68	1.38	1.52
1	E	169	PRO	N-CD	-5.67	1.40	1.47
1	F	42	PRO	N-CD	-5.67	1.40	1.47
9	q	10	PRO	N-CD	-5.67	1.40	1.47
3	J	236	ASN	N-CA	-5.66	1.35	1.46
9	Q	10	PRO	N-CD	-5.66	1.40	1.47
3	J	347	PRO	N-CA	-5.66	1.37	1.47
3	J	209	ASP	C-N	-5.65	1.21	1.34
9	p	17	PRO	N-CD	-5.64	1.40	1.47
1	A	42	PRO	N-CD	-5.64	1.40	1.47
1	G	42	PRO	N-CD	-5.60	1.40	1.47
2	H	32	PRO	N-CD	-5.58	1.40	1.47
1	G	107	PRO	N-CD	-5.58	1.40	1.47
3	J	352	CYS	C-N	-5.57	1.21	1.34
10	R	79	PRO	N-CD	-5.57	1.40	1.47
2	H	70	PRO	N-CD	-5.57	1.40	1.47
1	C	265	PRO	N-CD	-5.57	1.40	1.47
1	A	169	PRO	N-CD	-5.56	1.40	1.47
3	J	120	LEU	N-CA	-5.56	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	24	PHE	C-N	-5.53	1.21	1.34
1	B	2267	PRO	N-CD	-5.53	1.40	1.47
3	J	346	PRO	C-N	-5.53	1.23	1.34
1	B	2325	PRO	N-CD	-5.53	1.40	1.47
3	J	368	LEU	CA-C	-5.53	1.38	1.52
3	J	266	VAL	N-CA	-5.52	1.35	1.46
1	D	11	PRO	N-CD	-5.50	1.40	1.47
3	J	83	ASN	CA-C	-5.50	1.38	1.52
3	J	36	ARG	C-N	-5.49	1.21	1.34
3	J	166	LEU	C-O	-5.48	1.12	1.23
9	q	160	PRO	N-CD	-5.47	1.40	1.47
3	J	109	LEU	C-N	-5.47	1.21	1.34
3	J	25	THR	CA-C	5.47	1.67	1.52
1	F	253	PRO	N-CD	-5.41	1.40	1.47
3	J	152	TYR	CA-C	-5.39	1.39	1.52
2	H	27	PRO	N-CD	-5.39	1.40	1.47
1	I	31	PRO	N-CD	-5.38	1.40	1.47
1	G	31	PRO	N-CD	-5.38	1.40	1.47
3	J	208	GLU	N-CA	-5.37	1.35	1.46
3	J	166	LEU	CA-C	-5.37	1.39	1.52
3	J	39	ILE	C-N	-5.37	1.24	1.34
3	J	307	GLY	CA-C	-5.36	1.43	1.51
3	J	82	VAL	C-N	5.36	1.46	1.34
3	J	329	LYS	CA-C	-5.35	1.39	1.52
1	A	74	PRO	N-CD	-5.35	1.40	1.47
1	F	74	PRO	N-CD	-5.34	1.40	1.47
1	A	31	PRO	N-CD	-5.33	1.40	1.47
1	G	74	PRO	N-CD	-5.33	1.40	1.47
7	N	165	PRO	N-CD	-5.32	1.40	1.47
3	J	360	ILE	CA-C	-5.30	1.39	1.52
1	I	228	PRO	N-CD	-5.30	1.40	1.47
3	J	316	LEU	N-CA	-5.29	1.35	1.46
1	B	2171	PRO	N-CD	-5.28	1.40	1.47
3	J	381	THR	CA-C	-5.27	1.39	1.52
3	J	91	ILE	CA-C	-5.27	1.39	1.52
3	J	102	ARG	CA-C	-5.25	1.39	1.52
3	J	25	THR	N-CA	-5.25	1.35	1.46
1	D	265	PRO	N-CD	-5.23	1.40	1.47
1	F	31	PRO	N-CD	-5.22	1.40	1.47
3	J	385	PRO	N-CD	-5.21	1.40	1.47
3	J	256	LEU	N-CA	-5.19	1.35	1.46
1	G	323	PRO	N-CD	-5.19	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	266	VAL	CA-C	-5.18	1.39	1.52
9	P	26	PRO	N-CD	-5.18	1.40	1.47
9	p	10	PRO	N-CD	-5.17	1.40	1.47
3	J	102	ARG	C-N	-5.16	1.22	1.34
3	J	203	PRO	N-CA	-5.15	1.38	1.47
3	J	93	GLU	C-N	-5.14	1.22	1.34
9	Q	169	PRO	N-CD	-5.14	1.40	1.47
3	J	300	ALA	CA-C	-5.13	1.39	1.52
3	J	230	LYS	C-O	-5.13	1.13	1.23
5	L	141	PRO	N-CD	-5.12	1.40	1.47
3	J	82	VAL	CA-C	5.11	1.66	1.52
3	J	153	GLU	N-CA	-5.10	1.36	1.46
1	E	31	PRO	N-CD	-5.10	1.40	1.47
3	J	166	LEU	C-N	-5.10	1.23	1.33
3	J	363	ALA	C-N	-5.10	1.22	1.34
3	J	164	LEU	CA-C	-5.09	1.39	1.52
1	F	265	PRO	N-CD	-5.09	1.40	1.47
9	P	17	PRO	N-CD	-5.09	1.40	1.47
4	K	457	PRO	N-CD	-5.08	1.40	1.47
3	J	155	ILE	CA-C	-5.07	1.39	1.52
1	I	323	PRO	N-CD	-5.05	1.40	1.47
3	J	371	ARG	C-N	-5.05	1.22	1.34
9	p	169	PRO	N-CD	-5.05	1.40	1.47
3	J	359	ALA	N-CA	-5.05	1.36	1.46
1	E	265	PRO	N-CD	-5.04	1.40	1.47
3	J	222	ARG	N-CA	-5.03	1.36	1.46
4	K	291	PRO	N-CD	-5.03	1.40	1.47
1	D	31	PRO	N-CD	-5.03	1.40	1.47
1	A	177	PRO	N-CD	-5.02	1.40	1.47
1	B	2033	PRO	N-CD	-5.02	1.40	1.47

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	144	ARG	O-C-N	27.02	165.94	122.70
3	J	196	PRO	C-N-CA	-23.71	62.42	121.70
3	J	144	ARG	CA-C-N	-20.73	71.60	117.20
3	J	308	GLY	C-N-CA	-13.14	88.85	121.70
3	J	356	LEU	C-N-CA	-12.52	96.00	122.30
3	J	144	ARG	CA-C-O	-12.27	94.34	120.10
3	J	368	LEU	C-N-CA	-12.06	96.97	122.30
3	J	230	LYS	C-N-CA	-11.42	93.14	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	237	ASN	C-N-CA	-11.42	93.16	121.70
3	J	182	GLN	C-N-CA	-11.09	93.99	121.70
3	J	352	CYS	C-N-CA	-10.72	94.89	121.70
3	J	23	ALA	C-N-CA	-10.54	95.36	121.70
3	J	17	VAL	C-N-CA	10.46	147.84	121.70
3	J	352	CYS	O-C-N	-9.76	107.08	122.70
3	J	173	LYS	C-N-CA	-9.56	97.81	121.70
3	J	322	GLU	C-N-CA	-9.52	97.91	121.70
3	J	230	LYS	N-CA-C	-9.40	85.61	111.00
3	J	158	LEU	C-N-CA	-9.37	98.28	121.70
3	J	313	PRO	C-N-CA	9.32	141.86	122.30
3	J	69	LYS	C-N-CA	-9.29	98.49	121.70
3	J	125	LEU	O-C-N	-8.98	108.33	122.70
3	J	23	ALA	O-C-N	-8.92	108.42	122.70
3	J	105	LEU	C-N-CA	-8.92	99.40	121.70
3	J	300	ALA	N-CA-C	-8.66	87.62	111.00
3	J	151	ILE	O-C-N	-8.61	108.93	122.70
3	J	19	ASP	C-N-CA	-8.57	100.26	121.70
3	J	109	LEU	C-N-CA	-8.53	100.37	121.70
3	J	165	PRO	N-CA-C	-8.48	90.05	112.10
3	J	195	LEU	C-N-CA	-8.41	86.66	122.00
3	J	219	ASP	C-N-CA	8.32	142.50	121.70
3	J	65	TYR	C-N-CA	-8.31	100.93	121.70
3	J	306	ILE	O-C-N	8.30	137.32	123.20
3	J	350	ALA	O-C-N	-8.26	109.49	122.70
3	J	18	ILE	C-N-CA	8.24	142.30	121.70
3	J	40	PRO	C-N-CA	-8.24	101.11	121.70
3	J	39	ILE	C-N-CD	8.17	145.56	128.40
3	J	268	GLU	C-N-CA	-8.15	101.33	121.70
3	J	248	TYR	C-N-CD	8.12	145.45	128.40
3	J	43	ILE	N-CA-C	-8.08	89.18	111.00
3	J	313	PRO	O-C-N	8.01	136.82	123.20
3	J	197	SER	N-CA-C	7.95	132.46	111.00
3	J	356	LEU	O-C-N	-7.89	109.79	123.20
3	J	152	TYR	C-N-CA	-7.82	102.14	121.70
3	J	40	PRO	N-CA-C	-7.81	91.80	112.10
3	J	46	ALA	C-N-CA	-7.69	106.15	122.30
3	J	100	HIS	N-CA-C	-7.64	90.38	111.00
3	J	330	PRO	C-N-CA	-7.59	102.73	121.70
3	J	110	PHE	N-CA-C	-7.53	90.68	111.00
3	J	144	ARG	N-CA-C	7.43	131.06	111.00
3	J	105	LEU	O-C-N	-7.37	110.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	318	ARG	O-C-N	7.33	134.43	122.70
3	J	22	GLU	N-CA-C	-7.33	91.21	111.00
3	J	170	ALA	O-C-N	7.31	134.39	122.70
3	J	232	ASN	N-CA-C	-7.25	91.41	111.00
3	J	115	VAL	C-N-CD	7.20	143.52	128.40
3	J	212	ALA	C-N-CA	-7.19	103.72	121.70
3	J	78	ARG	C-N-CA	-7.12	103.91	121.70
3	J	204	GLU	C-N-CA	-7.11	107.37	122.30
3	J	288	LEU	O-C-N	-7.10	111.34	122.70
3	J	31	GLY	N-CA-C	-7.09	95.37	113.10
9	Q	116	GLU	O-C-N	-7.09	111.36	122.70
3	J	298	GLN	O-C-N	7.05	133.99	122.70
9	P	212	ARG	C-N-CD	-7.04	105.11	120.60
3	J	391	ASN	C-N-CA	-6.98	104.25	121.70
3	J	296	ARG	CA-C-O	6.94	134.67	120.10
3	J	368	LEU	O-C-N	-6.92	111.43	123.20
3	J	329	LYS	C-N-CD	-6.86	105.51	120.60
3	J	69	LYS	O-C-N	-6.85	111.75	122.70
3	J	183	CYS	N-CA-C	6.83	129.43	111.00
3	J	125	LEU	CA-C-O	6.78	134.34	120.10
3	J	256	LEU	O-C-N	-6.77	111.87	122.70
3	J	175	LEU	C-N-CA	-6.75	104.83	121.70
3	J	275	ASN	C-N-CA	6.75	138.56	121.70
3	J	160	CYS	N-CA-C	-6.73	92.83	111.00
3	J	36	ARG	N-CA-C	-6.69	92.93	111.00
3	J	178	GLN	C-N-CA	-6.67	105.02	121.70
3	J	259	LEU	O-C-N	-6.62	111.94	123.20
3	J	34	GLY	C-N-CD	6.61	142.28	128.40
3	J	225	LYS	C-N-CA	-6.60	105.20	121.70
3	J	206	VAL	C-N-CA	-6.58	105.24	121.70
3	J	315	PHE	C-N-CA	-6.47	105.52	121.70
3	J	333	LYS	C-N-CA	-6.47	105.52	121.70
3	J	285	LEU	C-N-CA	-6.47	105.53	121.70
3	J	166	LEU	CA-C-N	6.47	129.13	116.20
3	J	71	PHE	O-C-N	6.46	133.03	122.70
3	J	315	PHE	CA-C-O	-6.45	106.56	120.10
3	J	125	LEU	C-N-CA	-6.44	105.59	121.70
3	J	195	LEU	CA-C-O	6.43	133.60	120.10
3	J	377	TYR	O-C-N	6.42	132.98	122.70
3	J	352	CYS	CA-C-O	6.42	133.58	120.10
3	J	37	CYS	CA-C-O	6.36	133.46	120.10
3	J	386	ASP	O-C-N	-6.32	112.59	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	136	ALA	C-N-CA	6.29	137.41	121.70
3	J	256	LEU	C-N-CA	-6.28	106.00	121.70
3	J	326	LEU	O-C-N	-6.25	112.70	122.70
3	J	16	VAL	C-N-CA	-6.23	106.13	121.70
3	J	378	TYR	C-N-CA	-6.14	106.35	121.70
3	J	16	VAL	N-CA-C	6.13	127.54	111.00
3	J	195	LEU	O-C-N	-6.13	109.46	121.10
3	J	306	ILE	N-CA-C	-6.11	94.49	111.00
3	J	74	ILE	CA-C-O	6.09	132.90	120.10
3	J	111	LYS	C-N-CA	-6.08	106.50	121.70
3	J	330	PRO	CA-N-CD	6.08	120.21	111.70
3	J	81	LEU	N-CA-C	-6.07	94.62	111.00
3	J	220	LEU	C-N-CA	-6.06	106.55	121.70
3	J	75	LEU	O-C-N	-6.05	113.02	122.70
3	J	266	VAL	C-N-CA	-6.04	106.59	121.70
3	J	76	TYR	C-N-CA	6.04	136.80	121.70
3	J	169	LYS	C-N-CA	-6.03	106.62	121.70
3	J	338	THR	O-C-N	-6.03	113.05	122.70
3	J	93	GLU	N-CA-C	-6.01	94.77	111.00
3	J	108	VAL	O-C-N	5.98	132.28	122.70
3	J	14	THR	C-N-CA	5.97	136.63	121.70
3	J	112	TYR	N-CA-C	-5.96	94.89	111.00
3	J	220	LEU	O-C-N	-5.95	113.17	122.70
3	J	109	LEU	N-CA-C	-5.95	94.95	111.00
3	J	319	LEU	C-N-CA	-5.94	106.86	121.70
3	J	103	GLU	O-C-N	5.93	132.18	122.70
3	J	373	VAL	O-C-N	-5.91	113.25	122.70
3	J	276	GLU	N-CA-C	-5.90	95.06	111.00
3	J	374	SER	O-C-N	5.89	132.13	122.70
3	J	166	LEU	N-CA-C	-5.88	95.14	111.00
3	J	357	GLY	N-CA-C	-5.86	98.44	113.10
3	J	72	ILE	C-N-CA	-5.86	107.05	121.70
3	J	173	LYS	N-CA-C	-5.86	95.18	111.00
3	J	337	GLY	N-CA-C	-5.86	98.45	113.10
3	J	184	THR	O-C-N	5.83	132.03	122.70
3	J	283	LEU	C-N-CA	-5.83	107.12	121.70
3	J	275	ASN	CA-C-N	-5.81	104.41	117.20
3	J	259	LEU	C-N-CA	-5.80	110.11	122.30
3	J	99	SER	CA-C-O	-5.80	107.92	120.10
9	Q	134	THR	CA-C-N	5.80	133.35	117.10
3	J	169	LYS	N-CA-C	-5.79	95.36	111.00
3	J	199	MET	C-N-CA	-5.78	110.16	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	116	GLU	CA-C-N	5.77	129.89	117.20
3	J	116	PRO	N-CA-C	-5.76	97.11	112.10
3	J	371	ARG	C-N-CA	5.76	136.09	121.70
3	J	349	LYS	CA-C-O	5.75	132.19	120.10
3	J	68	LEU	CA-C-O	5.75	132.17	120.10
3	J	95	VAL	N-CA-C	-5.75	95.49	111.00
3	J	361	PHE	C-N-CA	-5.72	110.29	122.30
3	J	84	PRO	O-C-N	-5.70	113.58	122.70
3	J	198	VAL	N-CA-C	-5.68	95.66	111.00
3	J	296	ARG	CA-C-N	-5.67	104.72	117.20
3	J	303	LEU	O-C-N	-5.66	113.64	122.70
3	J	223	GLY	N-CA-C	-5.65	98.99	113.10
3	J	122	PRO	N-CA-C	5.64	126.76	112.10
3	J	365	GLN	O-C-N	-5.63	113.68	122.70
3	J	122	PRO	O-C-N	-5.62	113.70	122.70
3	J	89	VAL	O-C-N	-5.61	113.73	122.70
3	J	167	GLY	C-N-CA	5.60	134.06	122.30
3	J	191	LYS	O-C-N	-5.56	113.81	122.70
3	J	194	SER	C-N-CA	-5.56	107.81	121.70
3	J	122	PRO	C-N-CA	-5.56	107.81	121.70
3	J	196	PRO	O-C-N	-5.55	113.82	122.70
3	J	177	THR	O-C-N	5.55	131.58	122.70
3	J	65	TYR	O-C-N	-5.54	113.83	122.70
3	J	281	ALA	C-N-CA	-5.54	107.85	121.70
3	J	387	TRP	C-N-CA	-5.54	107.85	121.70
3	J	337	GLY	C-N-CA	-5.52	107.90	121.70
3	J	322	GLU	O-C-N	-5.50	113.90	122.70
3	J	105	LEU	CA-C-O	5.49	131.62	120.10
3	J	129	LEU	O-C-N	-5.49	113.92	122.70
3	J	41	SER	N-CA-C	5.48	125.79	111.00
9	Q	116	GLU	C-N-CA	5.45	135.32	121.70
3	J	144	ARG	CB-CA-C	-5.44	99.51	110.40
3	J	233	ILE	C-N-CA	-5.43	108.13	121.70
3	J	300	ALA	N-CA-CB	5.43	117.70	110.10
3	J	246	VAL	O-C-N	-5.41	114.05	122.70
3	J	184	THR	CA-C-N	-5.39	105.34	117.20
3	J	318	ARG	C-N-CA	-5.39	108.23	121.70
3	J	357	GLY	C-N-CA	5.38	133.59	122.30
3	J	155	ILE	C-N-CD	5.37	139.68	128.40
3	J	209	ASP	O-C-N	-5.36	114.12	122.70
3	J	74	ILE	O-C-N	-5.35	114.14	122.70
3	J	129	LEU	CA-C-O	-5.33	108.91	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	86	ASP	N-CA-C	5.32	125.37	111.00
3	J	89	VAL	C-N-CA	-5.31	108.42	121.70
3	J	283	LEU	O-C-N	-5.29	114.24	122.70
3	J	267	VAL	N-CA-C	5.28	125.25	111.00
9	Q	116	GLU	N-CA-C	-5.28	96.75	111.00
3	J	350	ALA	C-N-CA	-5.27	108.54	121.70
3	J	331	LYS	C-N-CA	-5.25	108.58	121.70
3	J	184	THR	C-N-CA	-5.24	108.59	121.70
3	J	326	LEU	C-N-CA	-5.23	108.63	121.70
3	J	37	CYS	O-C-N	-5.22	114.34	122.70
3	J	147	LEU	O-C-N	-5.22	114.34	122.70
3	J	73	HIS	O-C-N	5.22	131.05	122.70
3	J	354	ALA	O-C-N	-5.21	114.36	122.70
3	J	43	ILE	C-N-CA	5.21	134.71	121.70
3	J	225	LYS	N-CA-C	-5.21	96.95	111.00
3	J	204	GLU	CA-C-O	5.20	131.02	120.10
11	S	1127	PRO	CA-C-N	5.20	131.65	117.10
3	J	369	GLY	O-C-N	-5.19	114.39	122.70
3	J	23	ALA	CA-C-O	5.17	130.97	120.10
3	J	204	GLU	O-C-N	-5.17	114.41	123.20
3	J	353	VAL	C-N-CA	-5.16	108.79	121.70
3	J	287	SER	C-N-CA	-5.15	108.83	121.70
3	J	174	GLU	CA-C-N	-5.14	105.89	117.20
3	J	378	TYR	O-C-N	-5.12	114.50	122.70
3	J	43	ILE	CA-C-O	-5.08	109.43	120.10
3	J	357	GLY	CA-C-O	-5.08	111.46	120.60
3	J	127	ALA	N-CA-C	5.07	124.69	111.00
3	J	248	TYR	C-N-CA	-5.07	100.72	122.00
3	J	75	LEU	CA-C-O	5.05	130.71	120.10
3	J	84	PRO	C-N-CA	-5.05	109.08	121.70
3	J	61	THR	O-C-N	5.04	130.77	122.70
3	J	320	LEU	O-C-N	5.03	130.74	122.70
3	J	17	VAL	O-C-N	-5.02	114.67	122.70
3	J	181	GLU	CA-C-O	-5.02	109.56	120.10

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	102	ARG	Mainchain
3	J	125	LEU	Mainchain
3	J	129	LEU	Mainchain

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

5.2 Too-close contacts

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

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%)	356 (97%)	12 (3%)	0	100	100
1	B	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	C	373/376 (99%)	364 (98%)	9 (2%)	0	100	100
1	D	368/376 (98%)	358 (97%)	10 (3%)	0	100	100
1	E	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	F	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	G	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	I	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
2	H	368/375 (98%)	356 (97%)	12 (3%)	0	100	100
3	J	379/417 (91%)	358 (94%)	18 (5%)	3 (1%)	16	51
4	K	349/460 (76%)	343 (98%)	6 (2%)	0	100	100
5	L	180/182 (99%)	176 (98%)	4 (2%)	0	100	100
6	M	152/190 (80%)	144 (95%)	8 (5%)	0	100	100
7	N	282/286 (99%)	278 (99%)	4 (1%)	0	100	100
8	O	267/272 (98%)	260 (97%)	7 (3%)	0	100	100
9	P	329/401 (82%)	312 (95%)	13 (4%)	4 (1%)	11	43
9	Q	268/401 (67%)	261 (97%)	6 (2%)	1 (0%)	30	64
9	p	320/401 (80%)	309 (97%)	10 (3%)	1 (0%)	37	68
9	q	329/401 (82%)	309 (94%)	18 (6%)	2 (1%)	22	56
10	R	177/186 (95%)	167 (94%)	9 (5%)	1 (1%)	22	56
10	r	168/186 (90%)	163 (97%)	4 (2%)	1 (1%)	22	56
11	S	146/1278 (11%)	140 (96%)	6 (4%)	0	100	100
14	s	187/1278 (15%)	180 (96%)	6 (3%)	1 (0%)	25	59
All	All	6850/9722 (70%)	6617 (97%)	219 (3%)	14 (0%)	45	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	283	LEU
9	P	213	PRO
9	p	25	LEU
9	q	202	SER
9	Q	161	ASP
10	R	69	ASP
3	J	23	ALA

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Mol	Chain	Res	Type
3	J	145	GLU
9	q	199	PRO
10	r	69	ASP
14	s	1140	GLY
9	P	10	PRO
9	P	268	VAL
9	P	212	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	318/324 (98%)	317 (100%)	1 (0%)	91 96
1	B	318/324 (98%)	317 (100%)	1 (0%)	91 96
1	C	323/324 (100%)	322 (100%)	1 (0%)	91 96
1	D	318/324 (98%)	317 (100%)	1 (0%)	91 96
1	E	318/324 (98%)	317 (100%)	1 (0%)	91 96
1	F	318/324 (98%)	317 (100%)	1 (0%)	91 96
1	G	318/324 (98%)	318 (100%)	0	100 100
1	I	318/324 (98%)	318 (100%)	0	100 100
2	H	313/318 (98%)	313 (100%)	0	100 100
3	J	339/363 (93%)	338 (100%)	1 (0%)	91 96
4	K	330/412 (80%)	330 (100%)	0	100 100
5	L	163/163 (100%)	163 (100%)	0	100 100
6	M	132/164 (80%)	132 (100%)	0	100 100
7	N	251/252 (100%)	250 (100%)	1 (0%)	89 95
8	O	238/241 (99%)	238 (100%)	0	100 100
9	P	298/343 (87%)	298 (100%)	0	100 100
9	Q	245/343 (71%)	244 (100%)	1 (0%)	89 95
9	p	281/343 (82%)	281 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	q	298/343 (87%)	297 (100%)	1 (0%)	91 96
10	R	154/160 (96%)	154 (100%)	0	100 100
10	r	149/160 (93%)	149 (100%)	0	100 100
11	S	137/1080 (13%)	137 (100%)	0	100 100
14	s	164/1080 (15%)	164 (100%)	0	100 100
All	All	6041/8357 (72%)	6031 (100%)	10 (0%)	91 97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	TRP
1	B	2359	TRP
1	C	357	TRP
1	D	357	TRP
1	E	357	TRP
1	F	357	TRP
3	J	239	ARG
7	N	281	LYS
9	Q	318	ARG
9	q	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2242	GLN
1	F	116	ASN
2	H	40	HIS
7	N	203	ASN
7	N	205	GLN
9	P	100	GLN
9	P	296	HIS
9	P	375	GLN
9	Q	278	GLN
11	S	1161	GLN
9	q	352	HIS
14	s	1184	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	ADP	D	800	-	24,29,29	0.74	0	29,45,45	0.71	1 (3%)
15	ADP	E	800	-	24,29,29	0.73	0	29,45,45	0.69	1 (3%)
15	ADP	F	800	-	24,29,29	0.72	0	29,45,45	0.70	1 (3%)
15	ADP	B	2401	-	24,29,29	0.74	0	29,45,45	0.70	1 (3%)
16	ANP	H	401	-	29,33,33	1.74	6 (20%)	31,52,52	1.57	7 (22%)
15	ADP	C	800	-	24,29,29	0.76	0	29,45,45	0.71	1 (3%)
15	ADP	G	800	-	24,29,29	0.71	0	29,45,45	0.70	1 (3%)
15	ADP	A	800	-	24,29,29	0.73	0	29,45,45	0.71	1 (3%)
15	ADP	I	800	-	24,29,29	0.71	0	29,45,45	0.73	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	D	800	-	-	4/12/32/32	0/3/3/3
15	ADP	E	800	-	-	4/12/32/32	0/3/3/3
15	ADP	F	800	-	-	4/12/32/32	0/3/3/3
15	ADP	B	2401	-	-	3/12/32/32	0/3/3/3
16	ANP	H	401	-	-	6/14/38/38	0/3/3/3
15	ADP	C	800	-	-	4/12/32/32	0/3/3/3
15	ADP	G	800	-	-	4/12/32/32	0/3/3/3
15	ADP	A	800	-	-	7/12/32/32	0/3/3/3
15	ADP	I	800	-	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	401	ANP	PG-N3B	4.37	1.74	1.63
16	H	401	ANP	PG-O1G	3.96	1.52	1.46
16	H	401	ANP	PB-N3B	3.56	1.72	1.63
16	H	401	ANP	PB-O1B	3.39	1.51	1.46
16	H	401	ANP	PB-O2B	-2.38	1.50	1.56
16	H	401	ANP	O4'-C1'	2.04	1.43	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	401	ANP	N3-C2-N1	-4.09	123.12	128.67
16	H	401	ANP	O1B-PB-N3B	-3.47	106.67	111.77
16	H	401	ANP	O1G-PG-N3B	-2.76	107.71	111.77
16	H	401	ANP	O2B-PB-O1B	2.65	115.55	109.87
16	H	401	ANP	O2A-PA-O1A	2.64	124.73	112.44
15	I	800	ADP	C5-C6-N6	2.30	123.81	120.31
15	D	800	ADP	C5-C6-N6	2.22	123.69	120.31
16	H	401	ANP	O3A-PB-N3B	2.22	112.75	106.59
15	C	800	ADP	C5-C6-N6	2.22	123.69	120.31
15	B	2401	ADP	C5-C6-N6	2.21	123.68	120.31
15	A	800	ADP	C5-C6-N6	2.19	123.65	120.31
15	F	800	ADP	C5-C6-N6	2.18	123.63	120.31
15	G	800	ADP	C5-C6-N6	2.16	123.61	120.31
15	E	800	ADP	C5-C6-N6	2.14	123.58	120.31
16	H	401	ANP	O2G-PG-O3G	2.05	113.09	107.59

There are no chirality outliers.

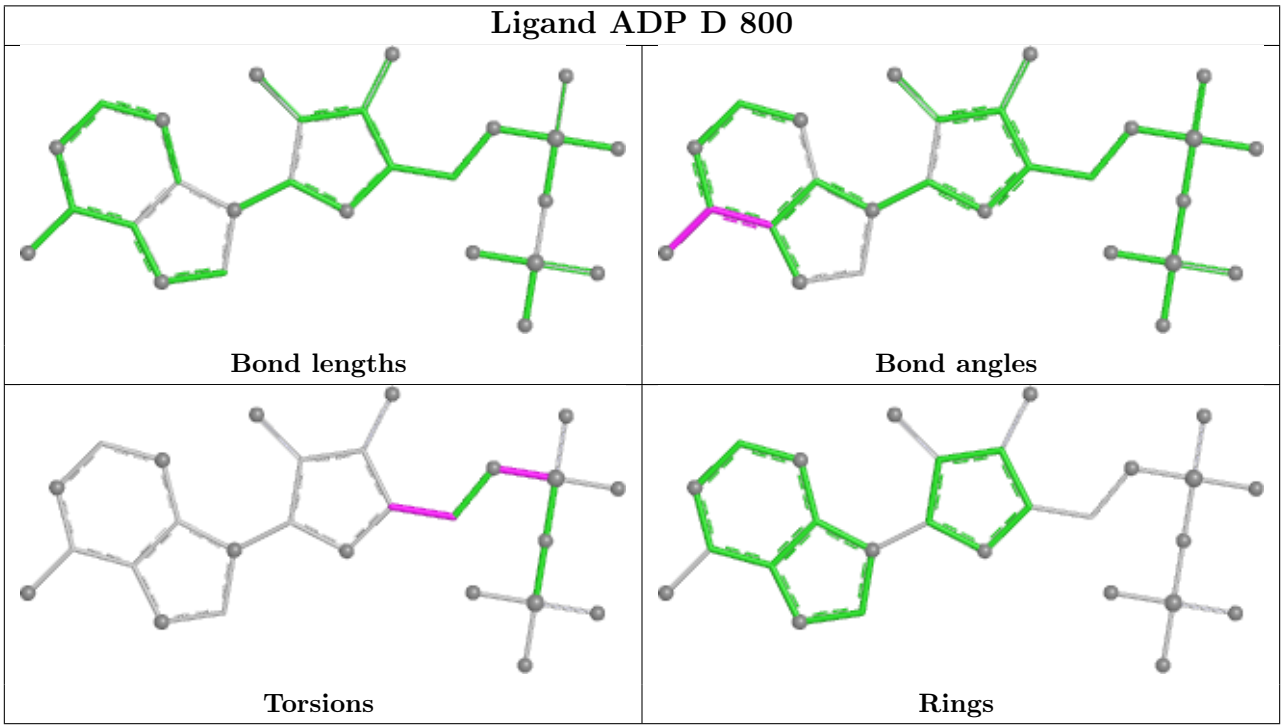
All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	800	ADP	PA-O3A-PB-O2B
15	A	800	ADP	PA-O3A-PB-O3B
15	A	800	ADP	C5'-O5'-PA-O1A
15	C	800	ADP	C5'-O5'-PA-O1A
15	C	800	ADP	C5'-O5'-PA-O3A
15	D	800	ADP	C5'-O5'-PA-O3A
15	E	800	ADP	C5'-O5'-PA-O1A
15	E	800	ADP	C5'-O5'-PA-O3A
15	F	800	ADP	C5'-O5'-PA-O1A
15	G	800	ADP	C5'-O5'-PA-O3A
15	I	800	ADP	C5'-O5'-PA-O1A
15	I	800	ADP	C5'-O5'-PA-O3A
16	H	401	ANP	PB-N3B-PG-O1G
16	H	401	ANP	PG-N3B-PB-O1B
16	H	401	ANP	PG-N3B-PB-O3A
15	A	800	ADP	C3'-C4'-C5'-O5'
15	D	800	ADP	C3'-C4'-C5'-O5'
15	E	800	ADP	C3'-C4'-C5'-O5'
15	F	800	ADP	C3'-C4'-C5'-O5'
15	G	800	ADP	C3'-C4'-C5'-O5'
15	I	800	ADP	C3'-C4'-C5'-O5'
15	B	2401	ADP	C3'-C4'-C5'-O5'
15	C	800	ADP	C3'-C4'-C5'-O5'
15	D	800	ADP	O4'-C4'-C5'-O5'
15	E	800	ADP	O4'-C4'-C5'-O5'
15	F	800	ADP	O4'-C4'-C5'-O5'
15	C	800	ADP	O4'-C4'-C5'-O5'
15	G	800	ADP	O4'-C4'-C5'-O5'
15	A	800	ADP	O4'-C4'-C5'-O5'
15	B	2401	ADP	O4'-C4'-C5'-O5'
15	I	800	ADP	O4'-C4'-C5'-O5'
16	H	401	ANP	PB-O3A-PA-O1A
16	H	401	ANP	O4'-C4'-C5'-O5'
15	A	800	ADP	C5'-O5'-PA-O3A
15	D	800	ADP	C5'-O5'-PA-O1A
15	F	800	ADP	C5'-O5'-PA-O3A
15	G	800	ADP	C5'-O5'-PA-O1A
16	H	401	ANP	PB-O3A-PA-O2A
15	B	2401	ADP	PA-O3A-PB-O1B
15	A	800	ADP	PA-O3A-PB-O1B

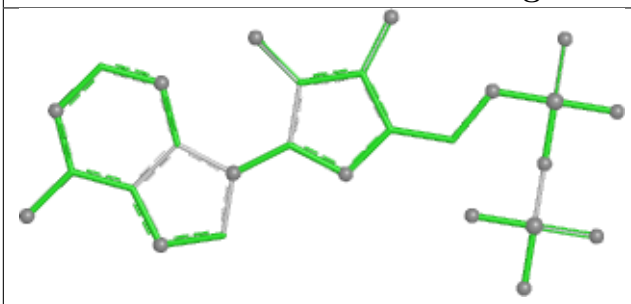
There are no ring outliers.

No monomer is involved in short contacts.

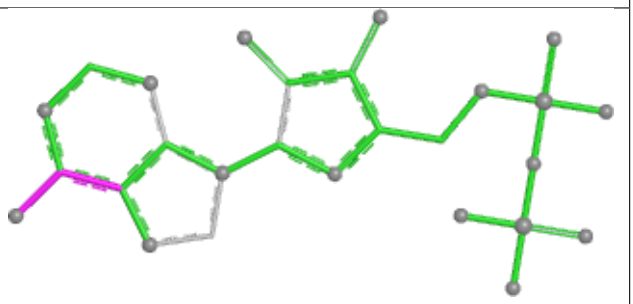
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



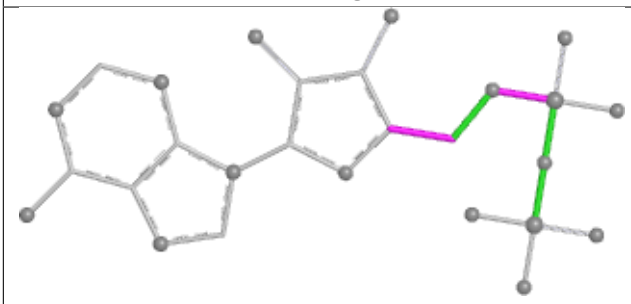
Ligand ADP E 800



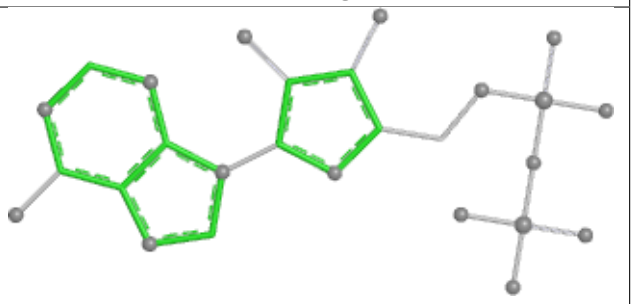
Bond lengths



Bond angles

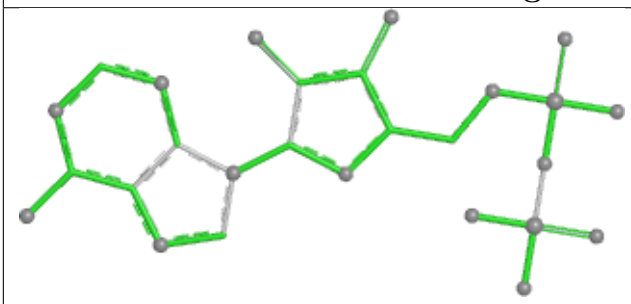


Torsions

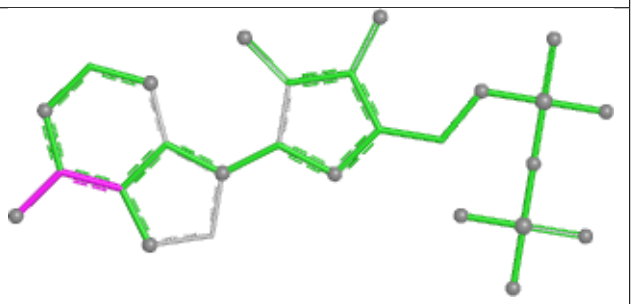


Rings

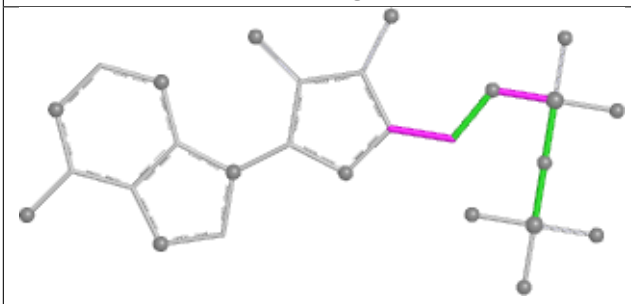
Ligand ADP F 800



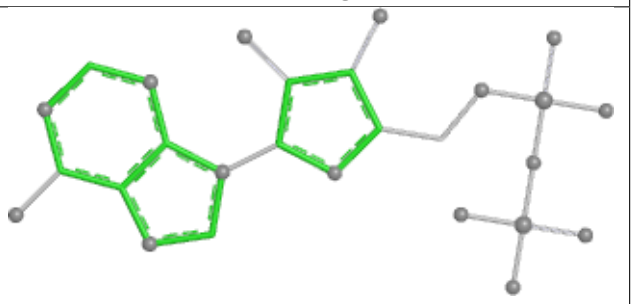
Bond lengths



Bond angles

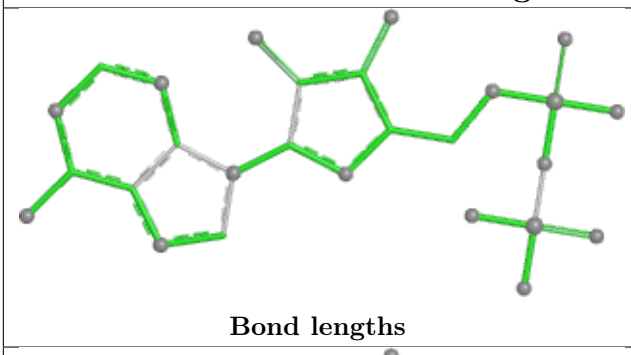


Torsions

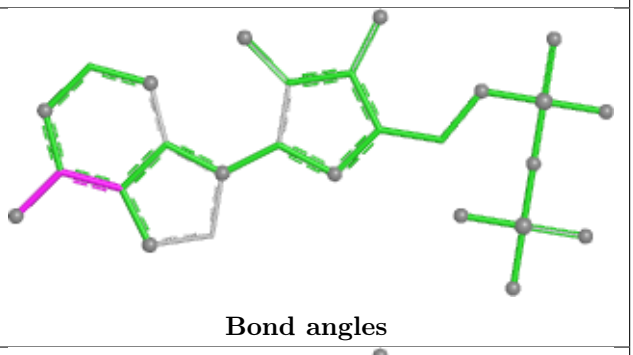


Rings

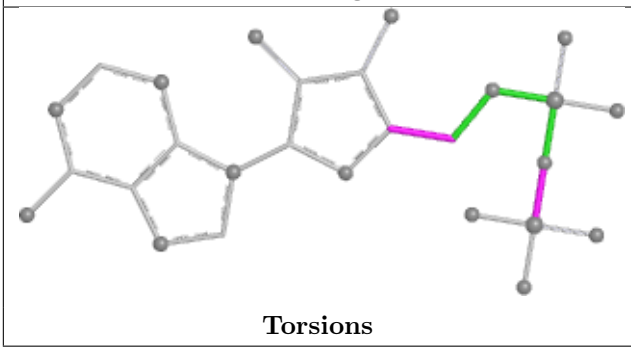
Ligand ADP B 2401



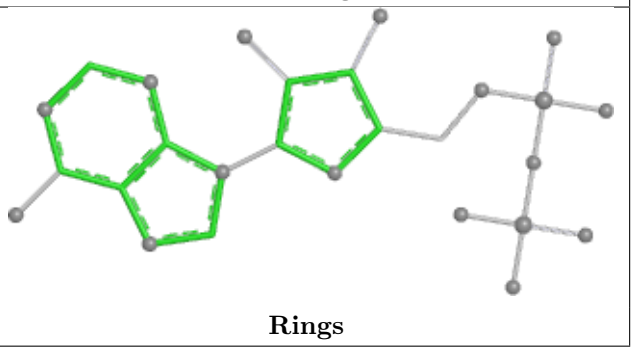
Bond lengths



Bond angles

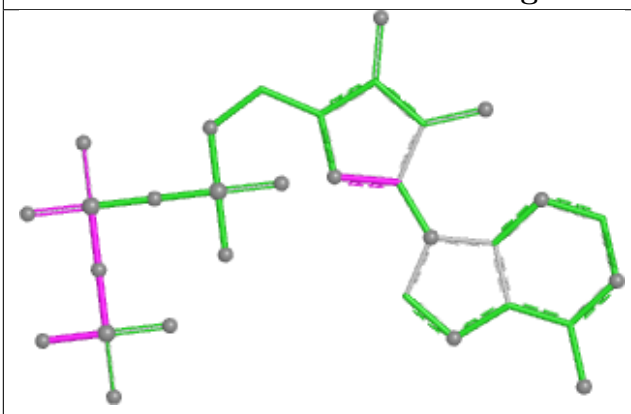


Torsions

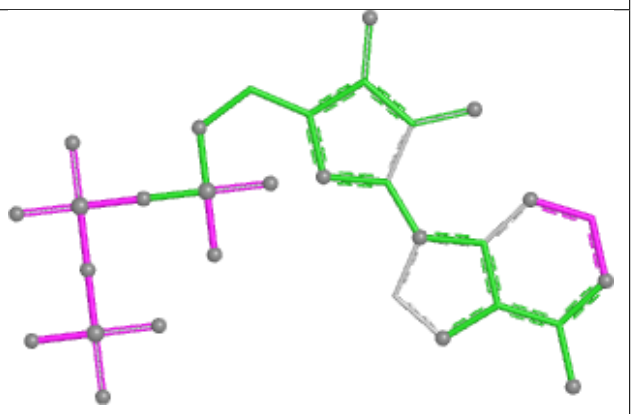


Rings

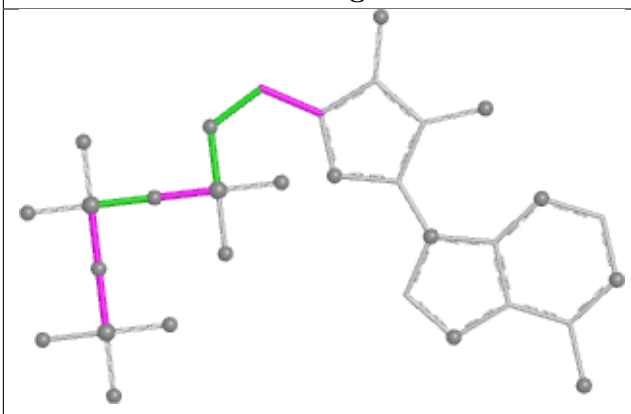
Ligand ANP H 401



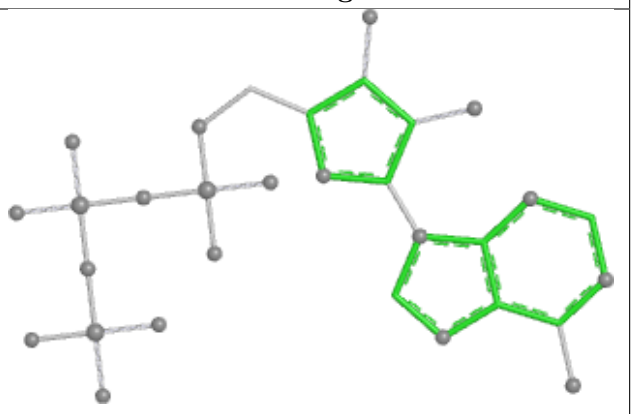
Bond lengths



Bond angles

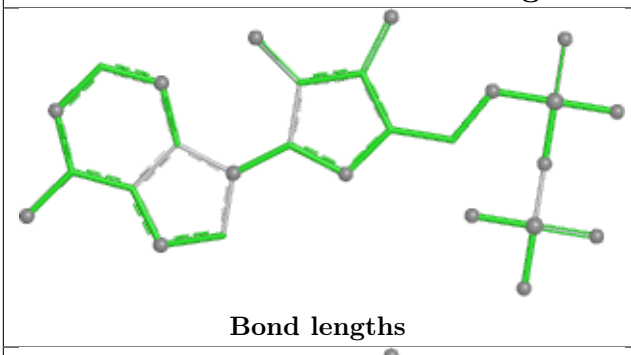


Torsions

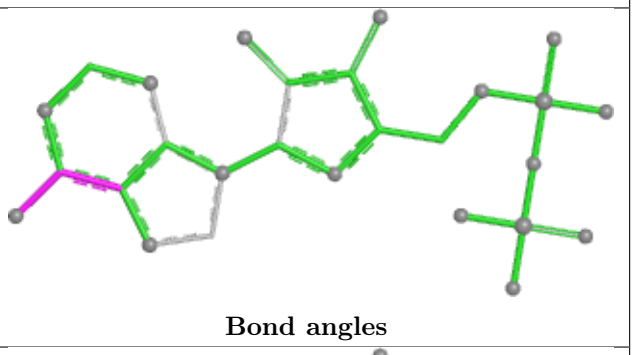


Rings

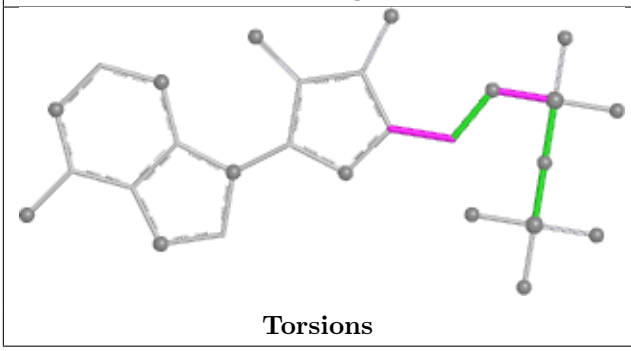
Ligand ADP C 800



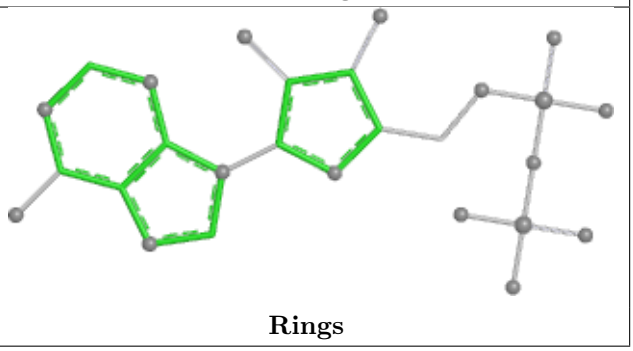
Bond lengths



Bond angles

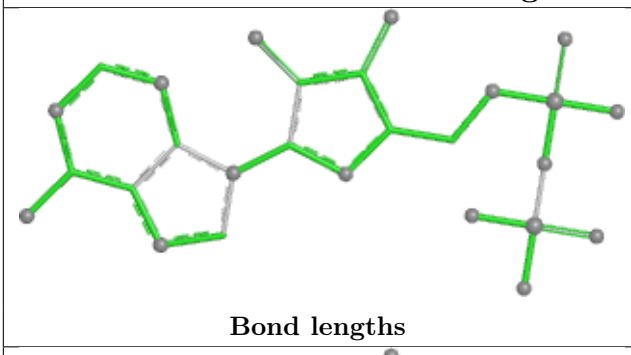


Torsions

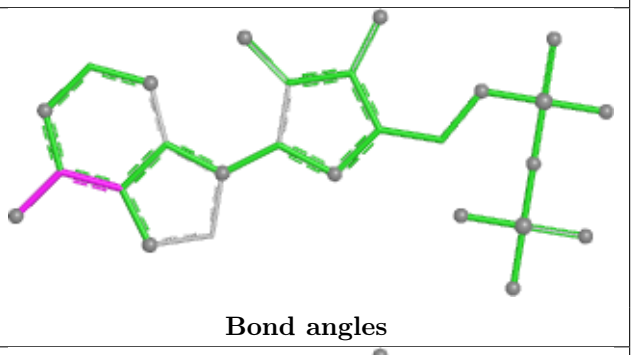


Rings

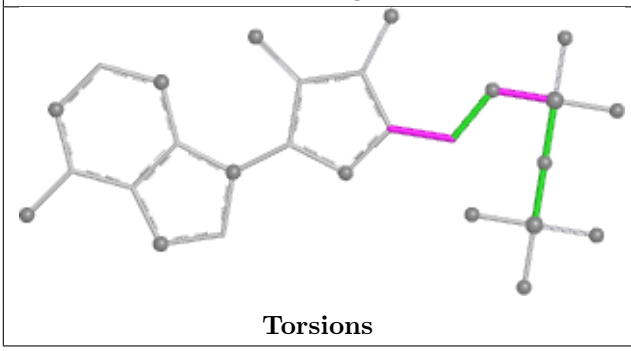
Ligand ADP G 800



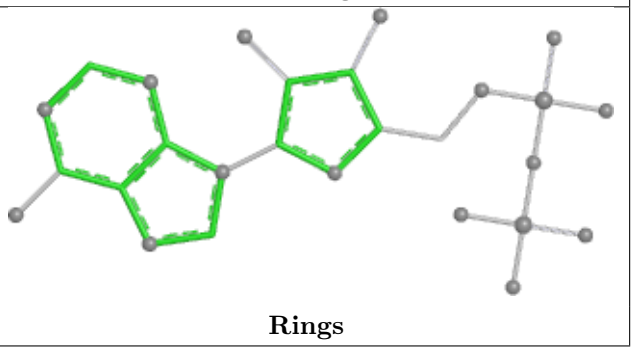
Bond lengths



Bond angles

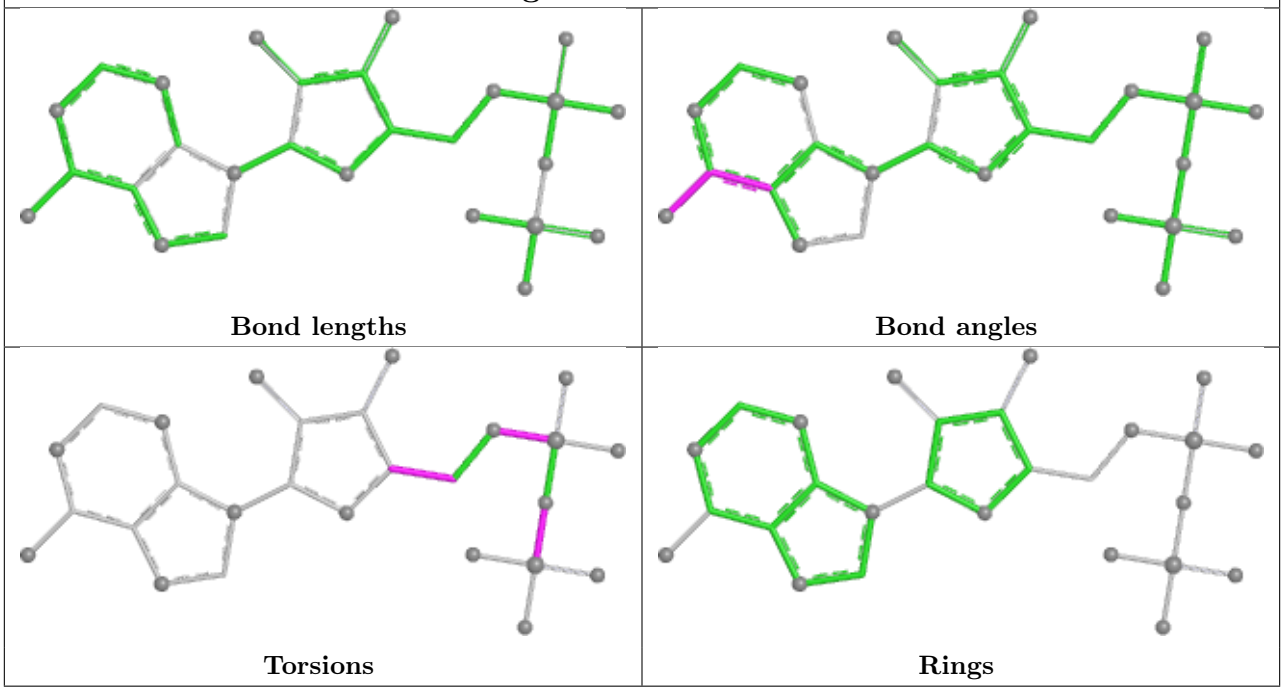


Torsions

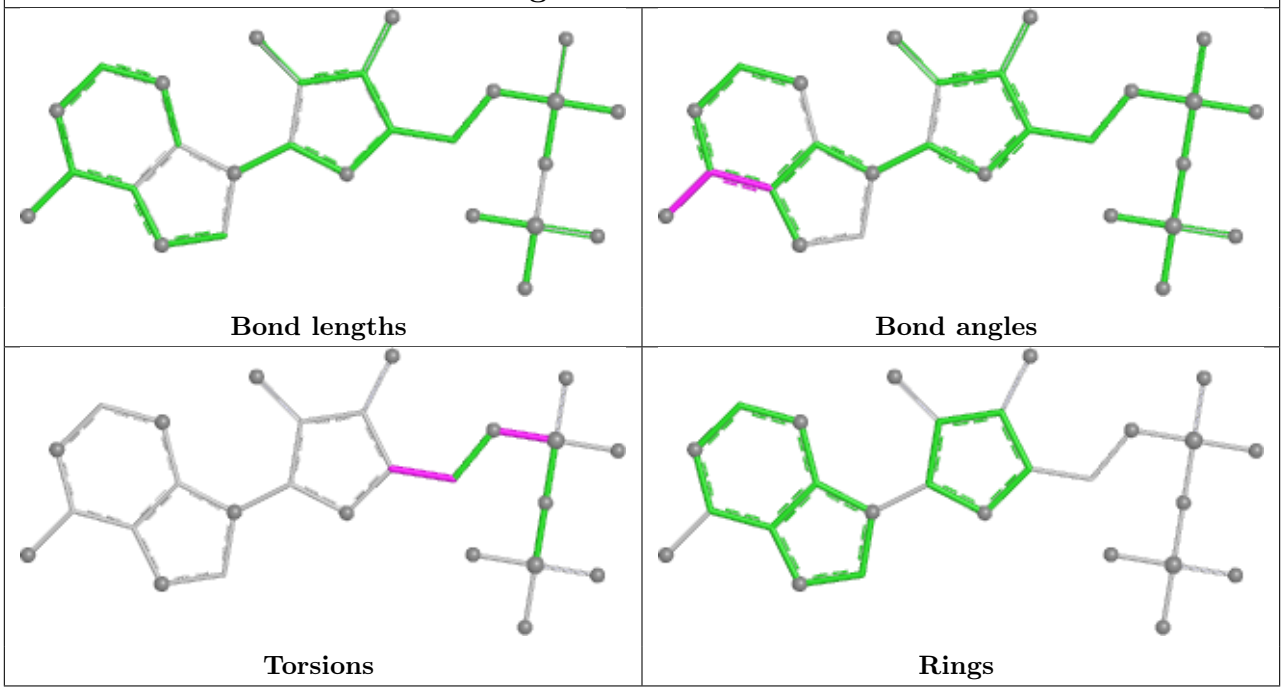


Rings

Ligand ADP A 800



Ligand ADP I 800



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	9
11	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	1243:VAL	C	1252:TYR	N	35.42
1	J	94:SER	C	95:VAL	N	3.81
1	J	116:PRO	C	117:SER	N	2.93
1	J	55:VAL	C	56:GLN	N	2.79
1	J	89:VAL	C	90:VAL	N	1.20
1	J	329:LYS	C	330:PRO	N	1.20
1	J	101:PHE	C	102:ARG	N	1.19
1	J	185:VAL	C	186:ASP	N	1.19
1	J	322:GLU	C	323:ILE	N	1.19
1	J	356:LEU	C	357:GLY	N	1.17

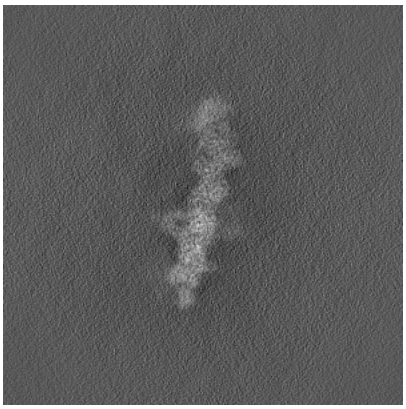
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44306. These allow visual inspection of the internal detail of the map and identification of artifacts.

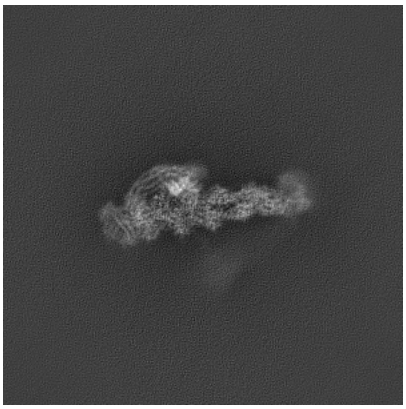
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

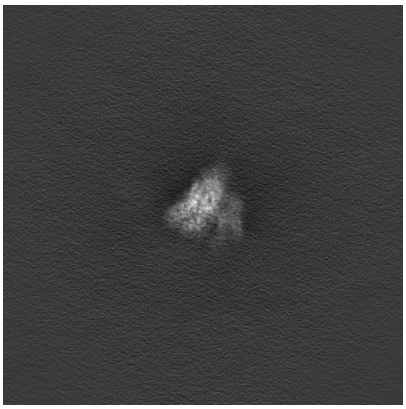
6.1.1 Primary map



X

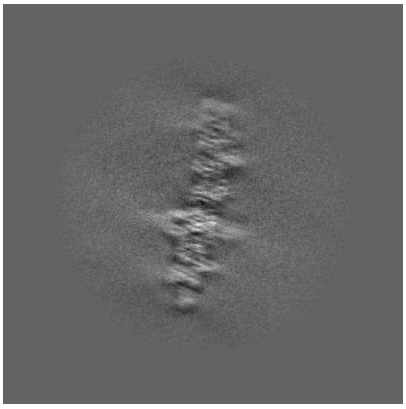


Y

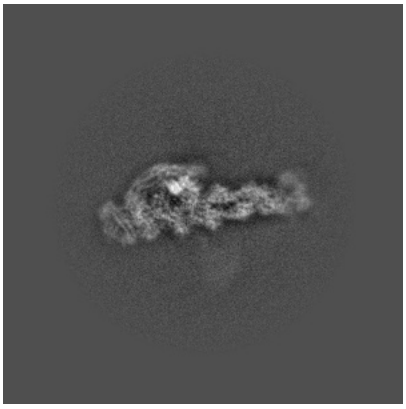


Z

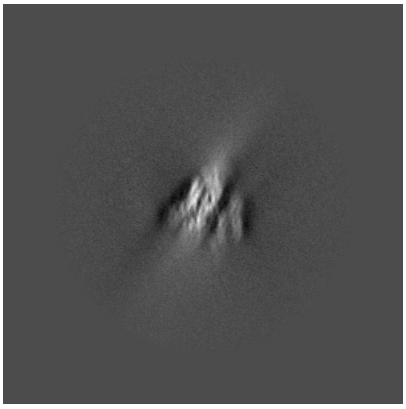
6.1.2 Raw map



X



Y

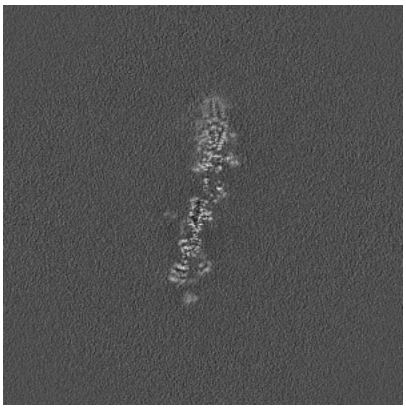


Z

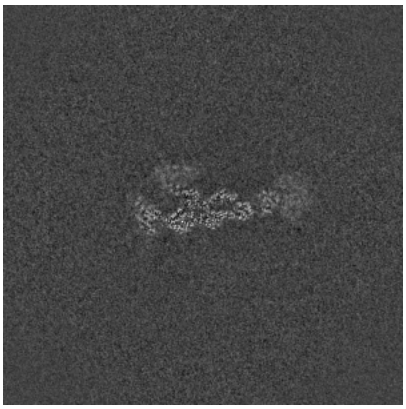
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

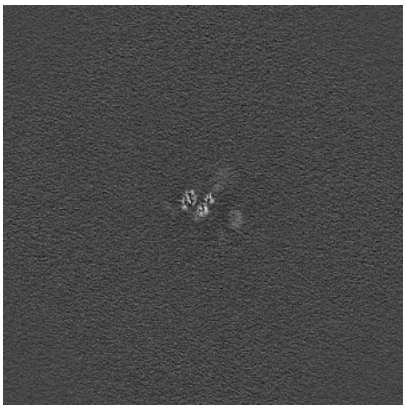
6.2.1 Primary map



X Index: 432

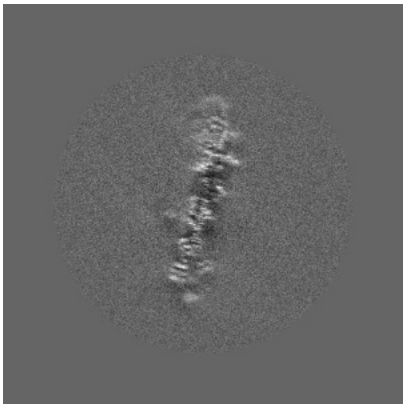


Y Index: 432

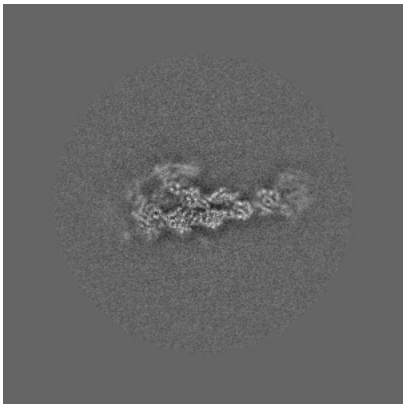


Z Index: 432

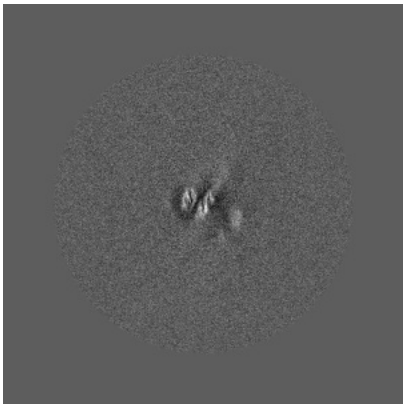
6.2.2 Raw map



X Index: 432



Y Index: 432

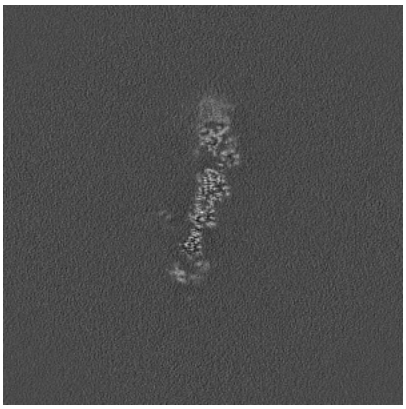


Z Index: 432

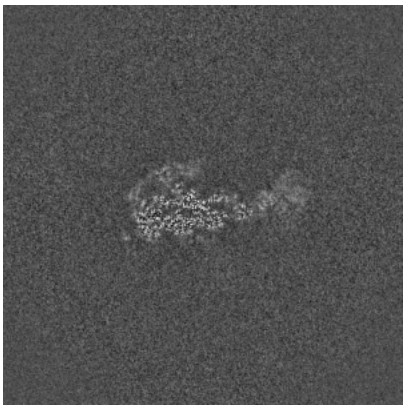
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

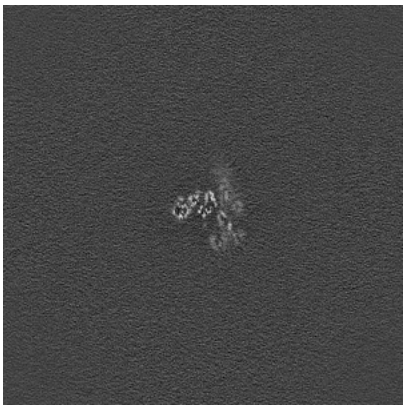
6.3.1 Primary map



X Index: 441

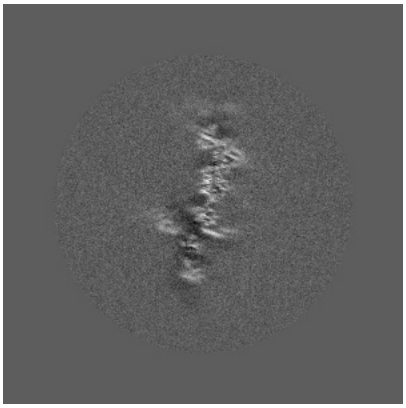


Y Index: 426

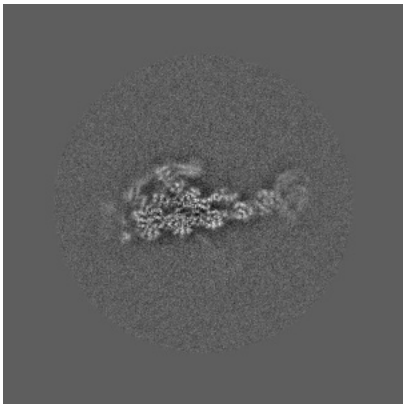


Z Index: 392

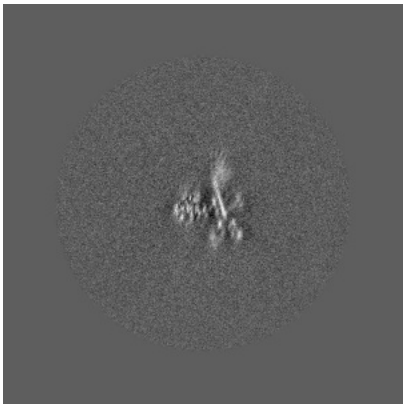
6.3.2 Raw map



X Index: 454



Y Index: 426

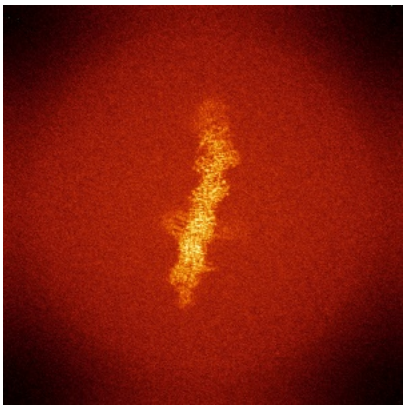


Z Index: 376

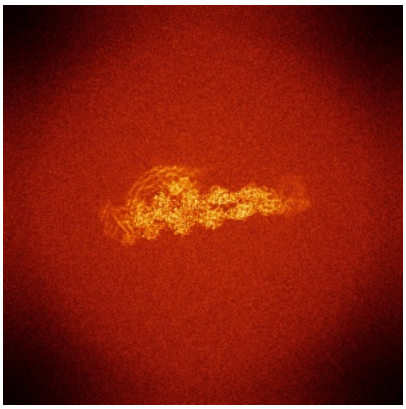
The images above show the largest variance slices of the map in three orthogonal directions.

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

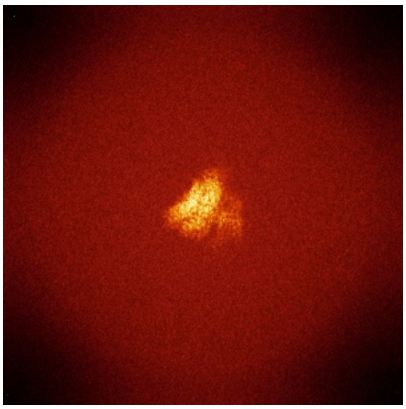
6.4.1 Primary map



X

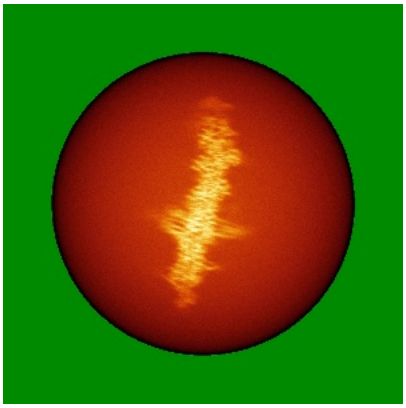


Y

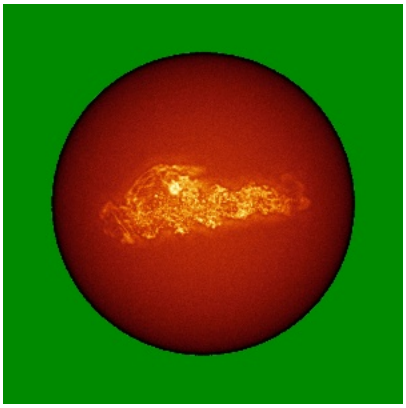


Z

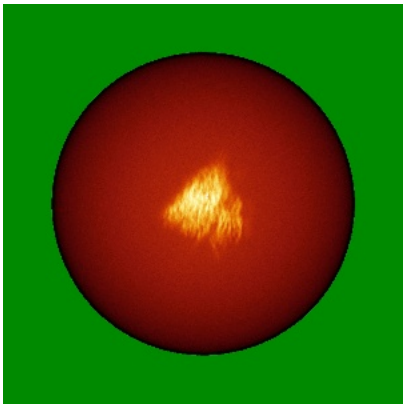
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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.

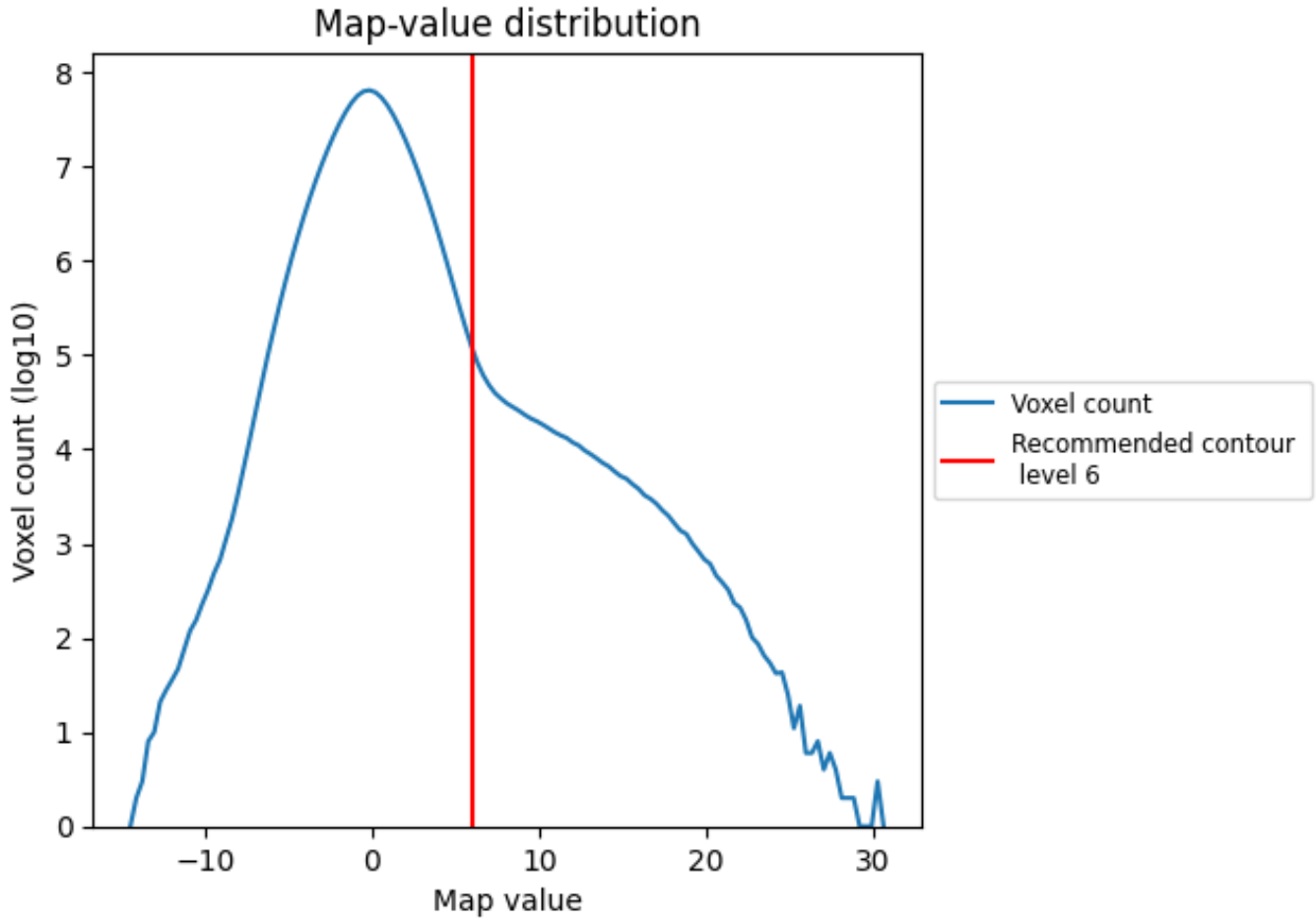
6.6 Mask visualisation (i)

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

7 Map analysis

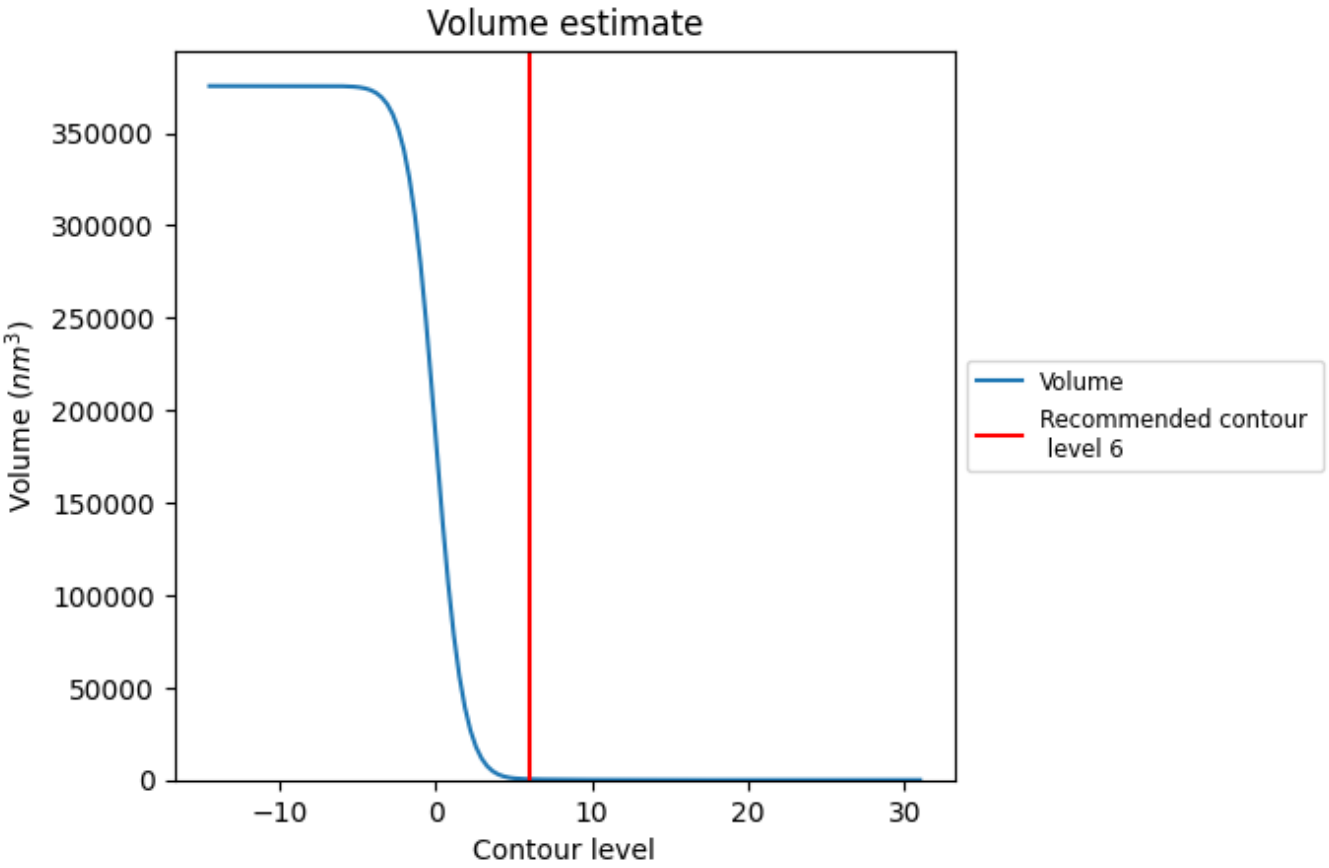
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

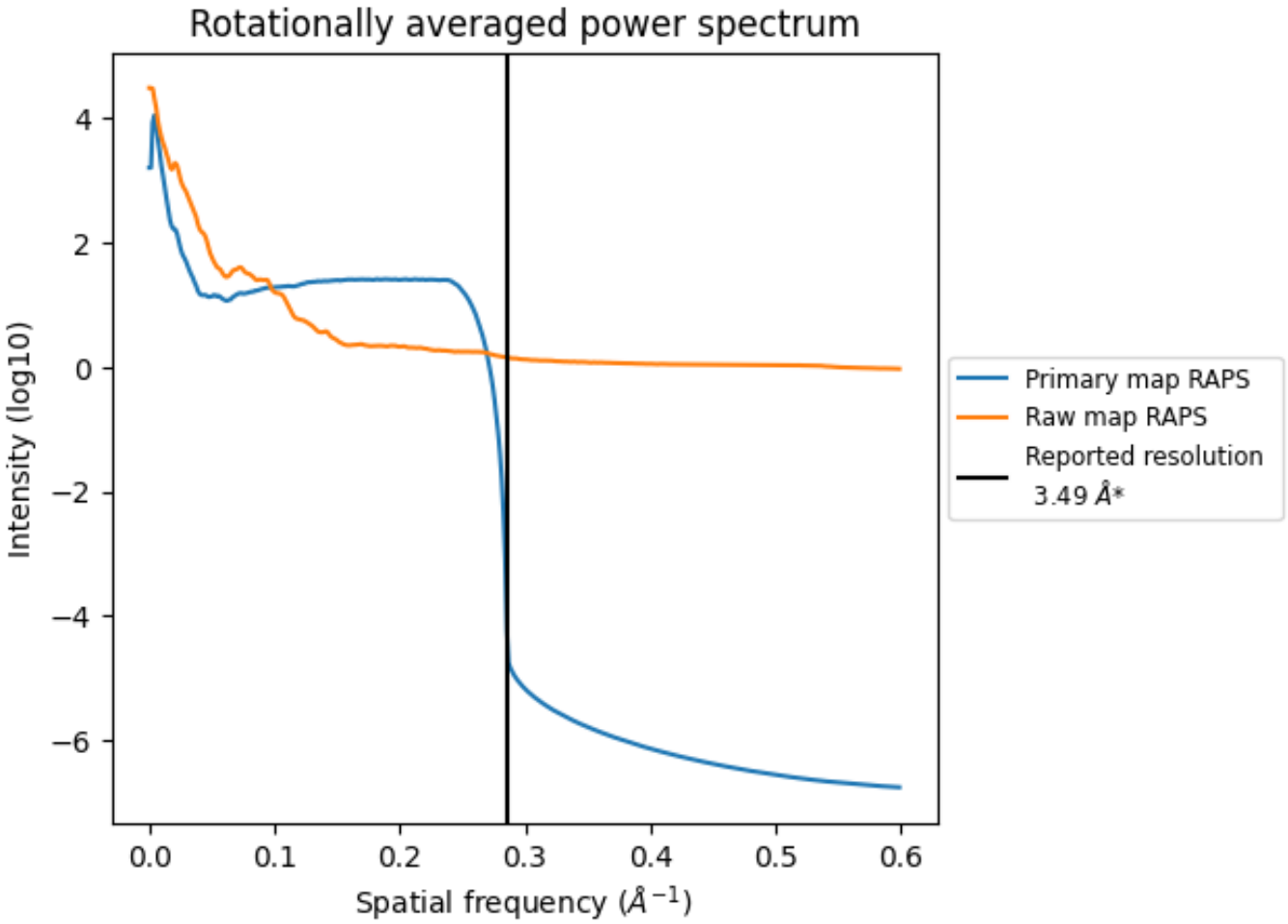
7.2 Volume estimate



The volume at the recommended contour level is 417 nm^3; this corresponds to an approximate mass of 376 kDa.

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

7.3 Rotationally averaged power spectrum (i)

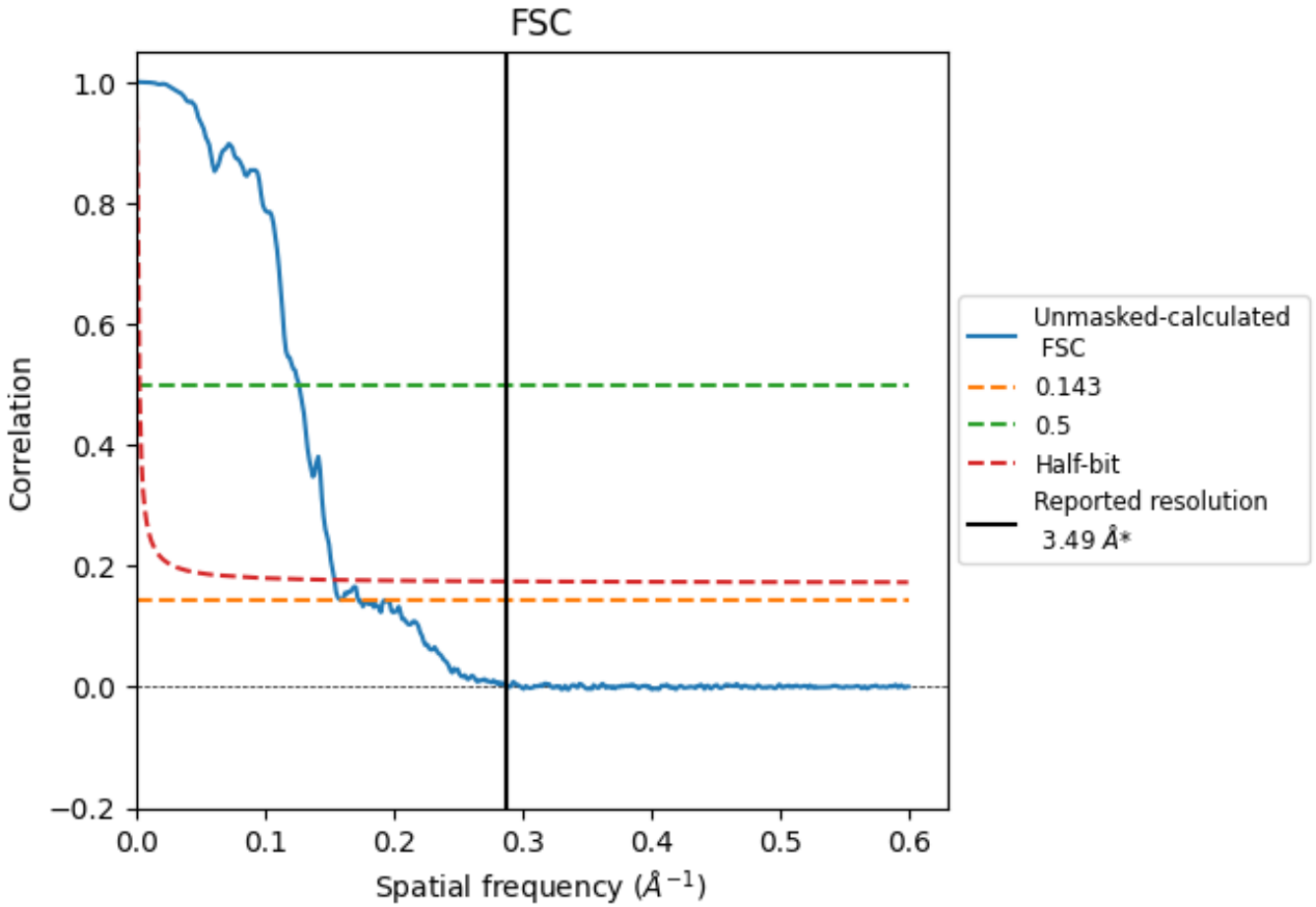


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8.2 Resolution estimates (i)

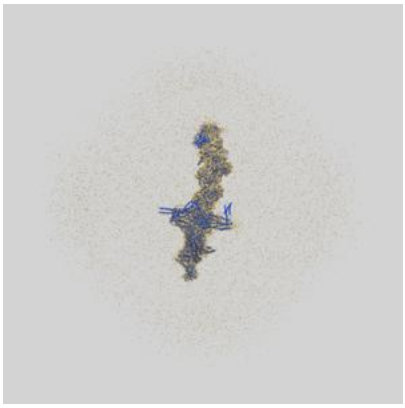
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.79	7.91	6.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.79 differs from the reported value 3.49 by more than 10 %

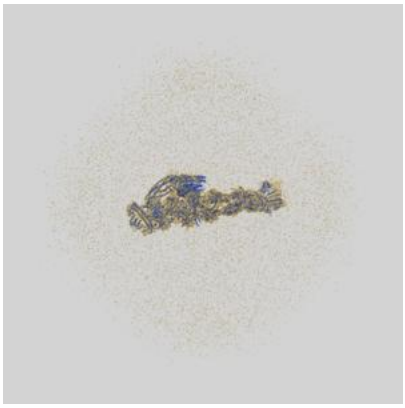
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44306 and PDB model 9B7J. Per-residue inclusion information can be found in section 3 on page 9.

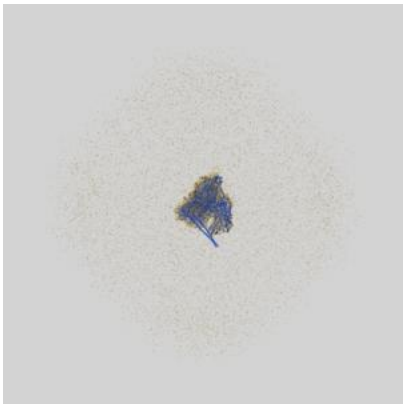
9.1 Map-model overlay



X



Y



Z

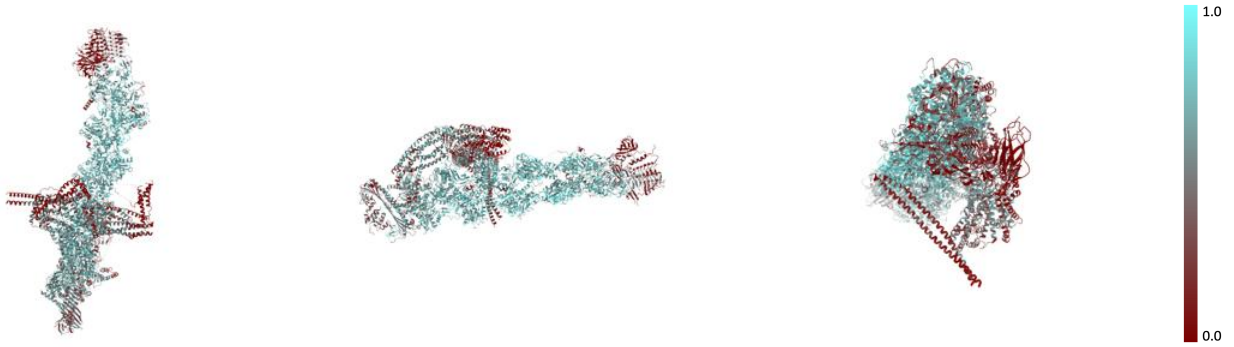
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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.

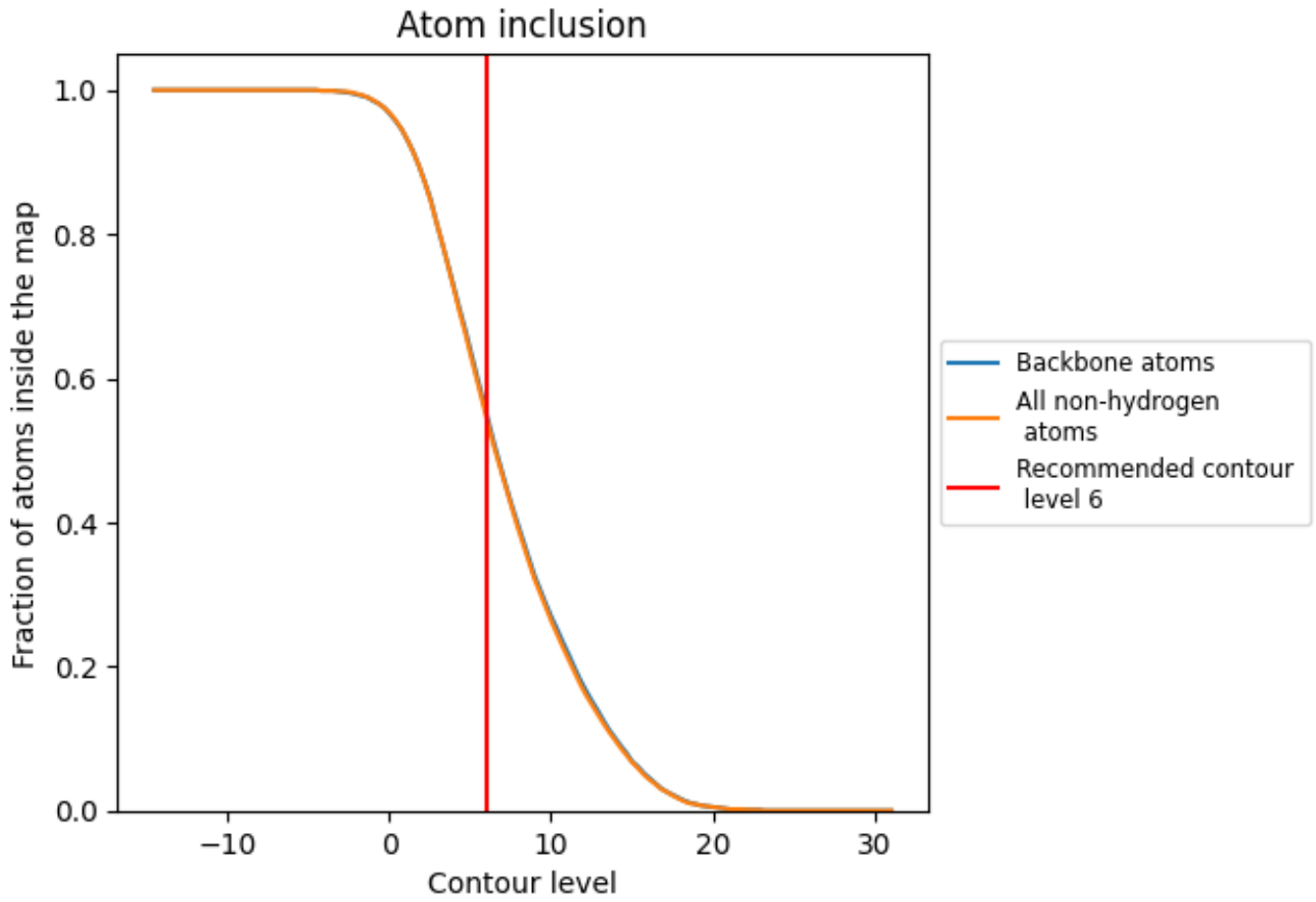
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (6).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 55% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.2800
A	0.6440	0.3200
B	0.7130	0.3640
C	0.7460	0.4090
D	0.7500	0.3870
E	0.7460	0.3880
F	0.7650	0.3890
G	0.7540	0.3930
H	0.7480	0.3770
I	0.6800	0.3300
J	0.6380	0.2850
K	0.2430	0.1450
L	0.1820	0.1210
M	0.2770	0.1510
N	0.4240	0.1870
O	0.5190	0.2220
P	0.3840	0.1820
Q	0.3310	0.1580
R	0.3610	0.1770
S	0.3390	0.1490
T	0.0980	0.1550
U	0.0900	0.1450
p	0.4950	0.2340
q	0.4520	0.2180
r	0.3930	0.1830
s	0.5030	0.2650