Full wwPDB EM Validation Report

Dec 9, 2024 – 02:34 PM JST

PDB ID	:	8JRT
EMDB ID	:	EMD-36605
Title	:	Cryo-EM structure of human 26S proteasomal RP subcomplex (Ea state) bound to K11/K48-branched ubiquitin (Ub) chain composed of three Ub.
Authors	:	Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on	:	2023-06-17
Resolution	:	3.60 Å(reported)
Based on initial model	:	6MSB

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 (i) 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 (1)) were used in the production of this report:

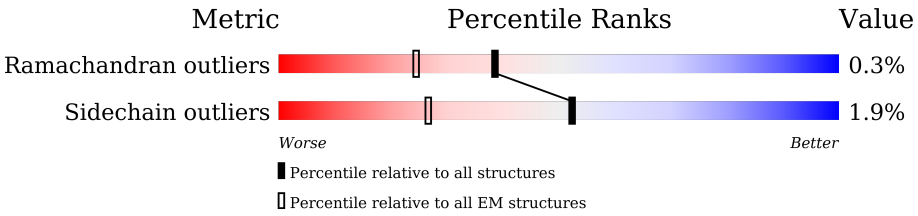
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.60 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	433	90% 9%
2	B	440	5% 87% 13%
3	C	406	92% 7%
4	D	418	89% 9%
5	G	246	98%
6	H	234	99%
7	I	261	96%
8	J	248	95%
9	K	241	96%

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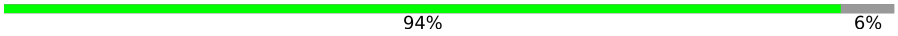
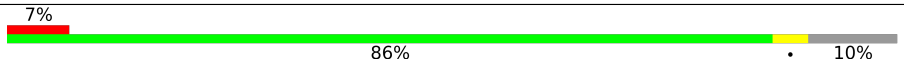
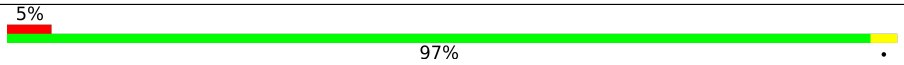
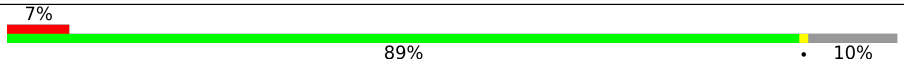
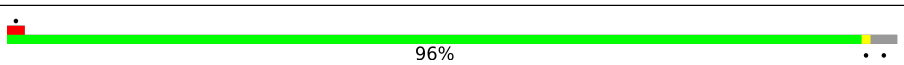
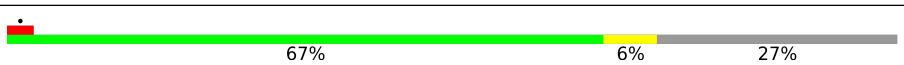
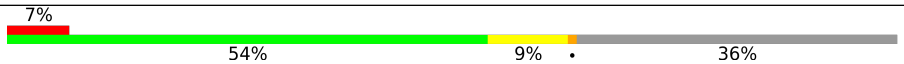
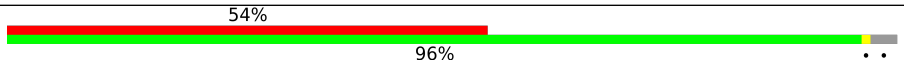
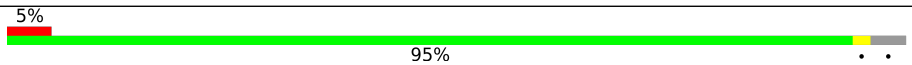
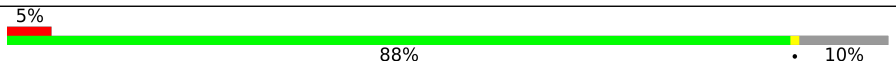
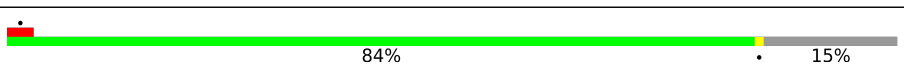
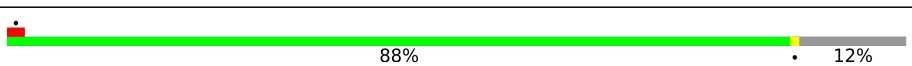
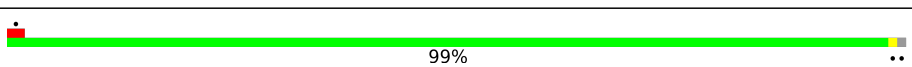
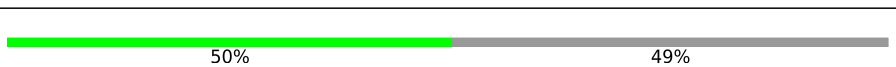
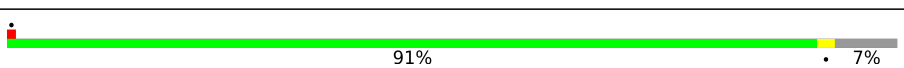
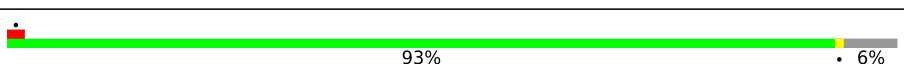
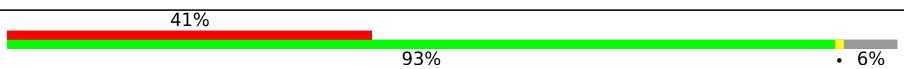
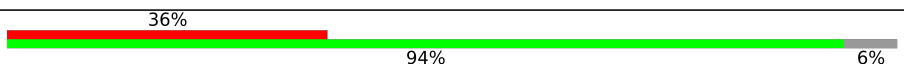
Mol	Chain	Length	Quality of chain
10	L	263	
11	M	255	
12	V	534	
13	W	456	
14	X	422	
15	Y	389	
16	d	350	
17	e	70	
18	f	908	
19	E	389	
20	F	439	
21	U	953	
22	Z	324	
23	a	376	
24	b	377	
25	c	310	
26	u	81	
26	v	81	
26	w	81	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 66765 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 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	394	2998	1887	531	562	18	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	384	2851	1786	493	560	12	0	0

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	379	2948	1856	531	545	16	0	0

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3039	1923	524	579	13	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	240	1826	1160	305	348	13	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	232	1708	1081	289	333	5	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		

- Molecule 9 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	234	Total	C	N	O	S	0	0
			1759	1102	290	356	11		

- Molecule 10 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 11 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V	479	Total	C	N	O	S	0	0
			3313	2078	619	609	7		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	456	Total	C	N	O	S	0	0
			3364	2118	592	639	15		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	380	Total	C	N	O	S	0	0
			2958	1882	504	560	12		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	257	Total	C	N	O	S	0	0
			1956	1261	327	361	7		

- Molecule 17 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	45	Total	C	N	O	S	0	0
			331	197	57	76	1		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	f	881	Total	C	N	O	0	0
			4343	2581	881	881		

- Molecule 19 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	375	Total	C	N	O	S	0	0
			2979	1875	529	559	16		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	395	Total	C	N	O	S	0	0
			3093	1943	535	598	17		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	808	Total	C	N	O	S	0	0
			6304	4003	1074	1183	44		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	373	Total	C	N	O	S	0	0
			2557	1598	462	486	11		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 26 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
26	u	76	Total	C	N	O	S	0	0
			604	378	107	118	1		
26	w	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-4	GLY	-	linker	UNP P0CG47
v	-3	SER	-	linker	UNP P0CG47

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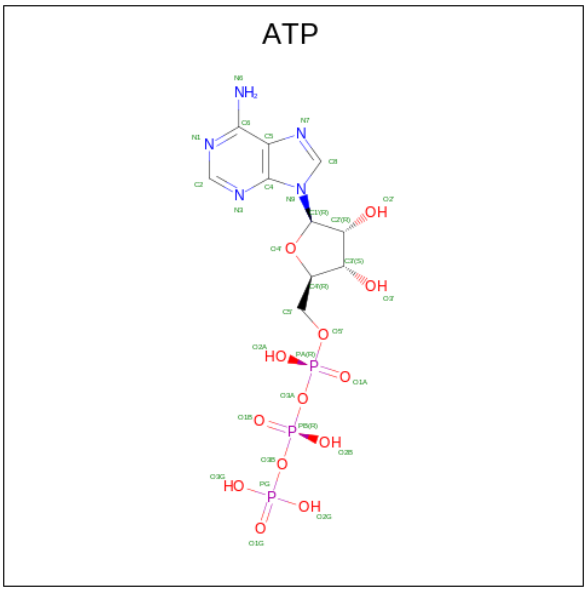
Chain	Residue	Modelled	Actual	Comment	Reference
v	-2	GLY	-	linker	UNP P0CG47
v	-1	GLY	-	linker	UNP P0CG47
v	0	SER	-	linker	UNP P0CG47
v	63	ARG	LYS	engineered mutation	UNP P0CG47
u	-4	GLY	-	linker	UNP P0CG47
u	-3	SER	-	linker	UNP P0CG47
u	-2	GLY	-	linker	UNP P0CG47
u	-1	GLY	-	linker	UNP P0CG47
u	0	SER	-	linker	UNP P0CG47
u	63	ARG	LYS	engineered mutation	UNP P0CG47
w	-4	GLY	-	linker	UNP P0CG47
w	-3	SER	-	linker	UNP P0CG47
w	-2	GLY	-	linker	UNP P0CG47
w	-1	GLY	-	linker	UNP P0CG47
w	0	SER	-	linker	UNP P0CG47
w	63	ARG	LYS	engineered mutation	UNP P0CG47

- Molecule 27 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
27	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
27	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

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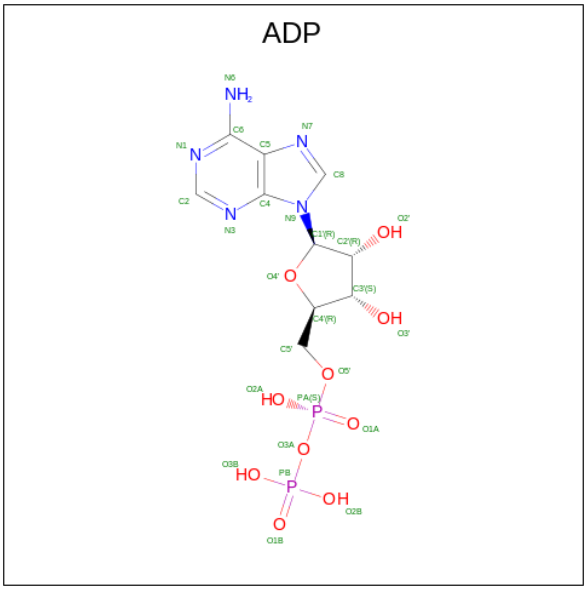
Mol	Chain	Residues	Atoms					AltConf
27	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Mg	0
			1	1	
28	B	1	Total	Mg	0
			1	1	
28	D	1	Total	Mg	0
			1	1	
28	E	1	Total	Mg	0
			1	1	
28	F	1	Total	Mg	0
			1	1	

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



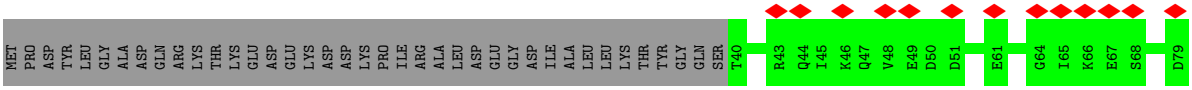
Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
29	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

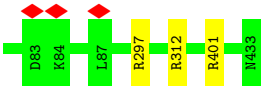
3 Residue-property plots (i)

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: 26S protease regulatory subunit 7

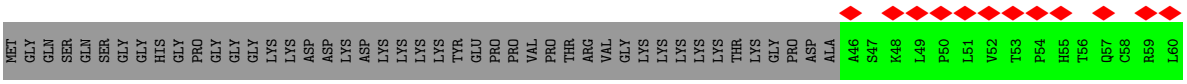
Chain A:

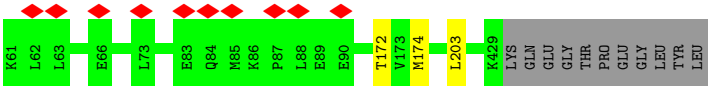




• Molecule 2: 26S protease regulatory subunit 4

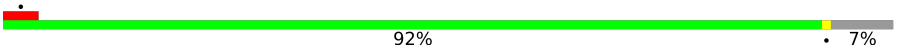
Chain B:

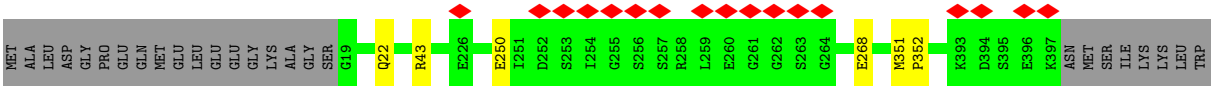




• Molecule 3: 26S protease regulatory subunit 8

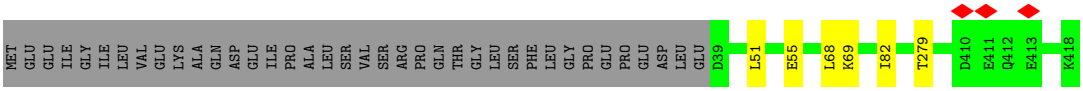
Chain C:



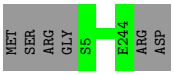


• Molecule 4: 26S protease regulatory subunit 6B

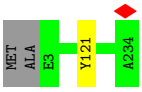
Chain D:



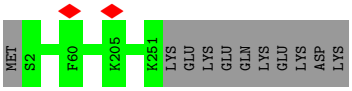
• Molecule 5: Proteasome subunit alpha type-6



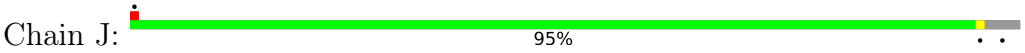
• Molecule 6: Proteasome subunit alpha type-2



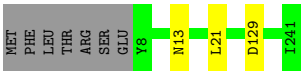
• Molecule 7: Proteasome subunit alpha type-4



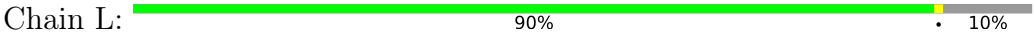
• Molecule 8: Proteasome subunit alpha type-7

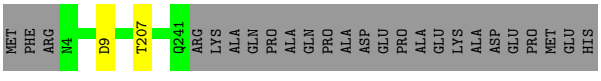


• Molecule 9: Proteasome subunit alpha type-5



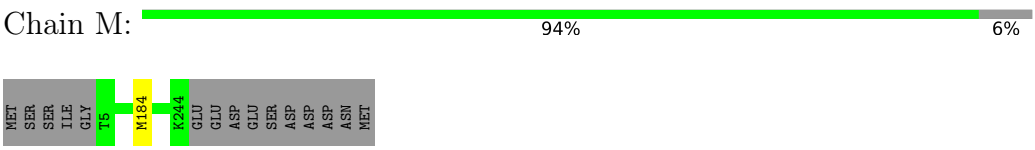
• Molecule 10: Proteasome subunit alpha type-1





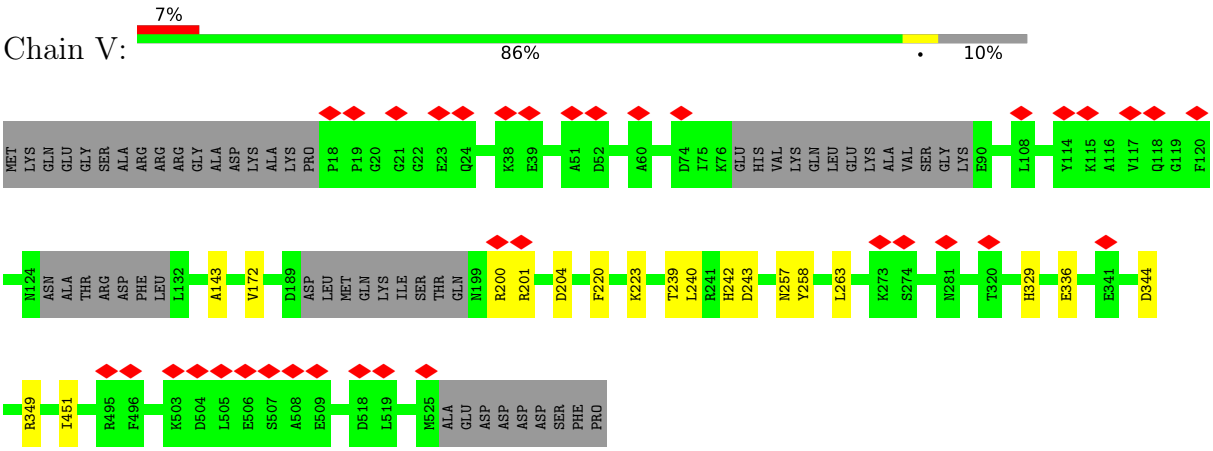
• Molecule 11: Proteasome subunit alpha type-3

Chain M:



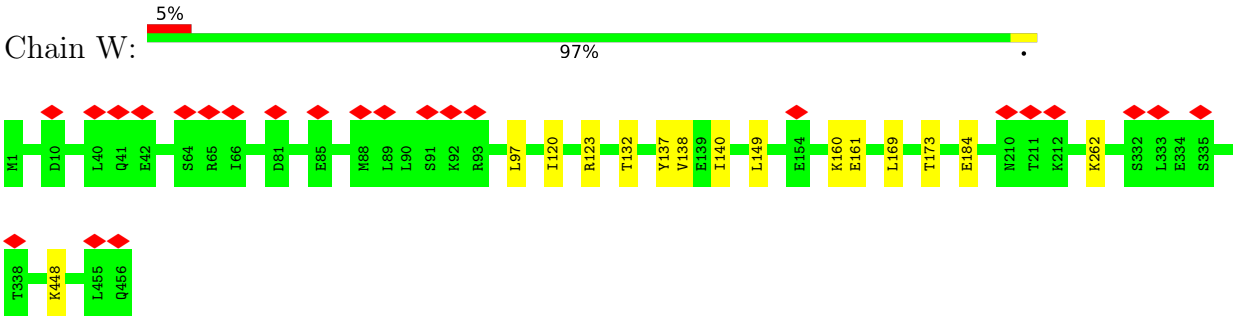
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



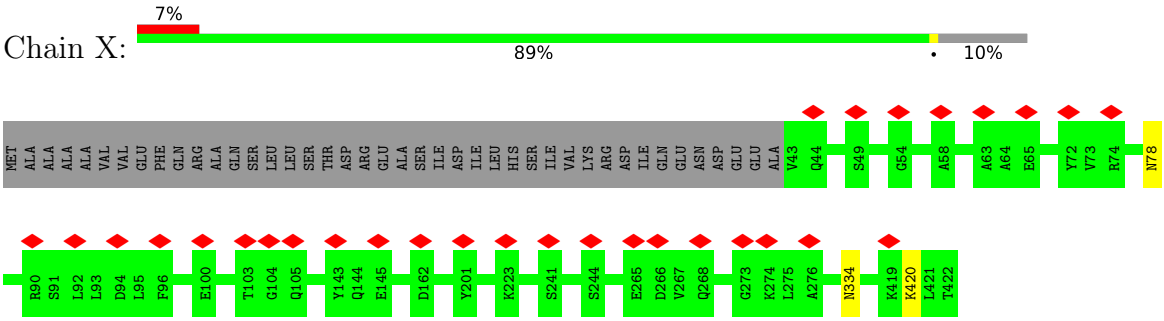
• Molecule 13: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



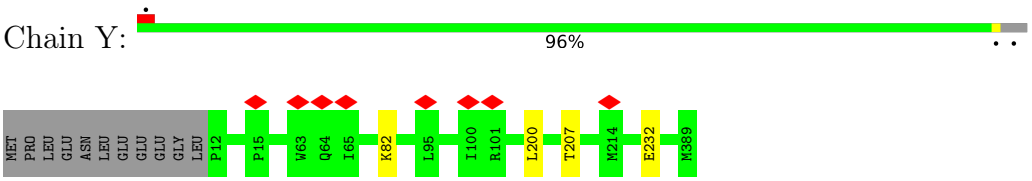
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



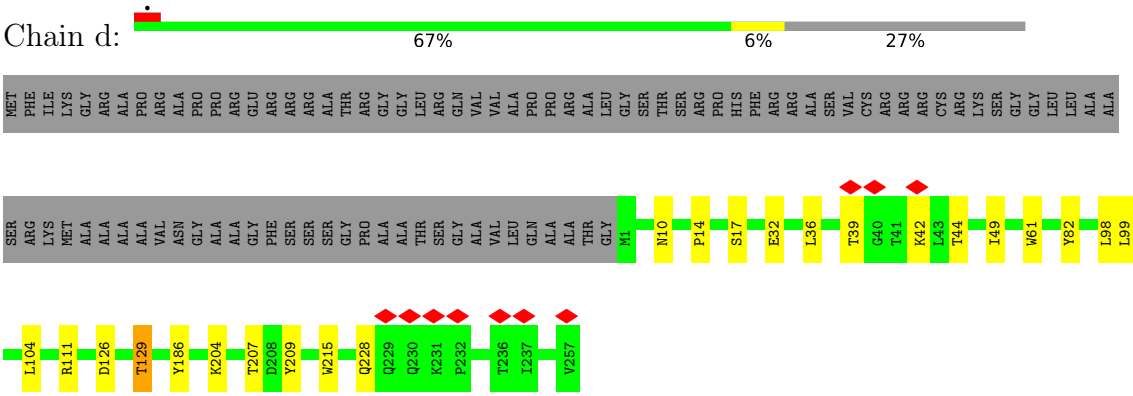
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



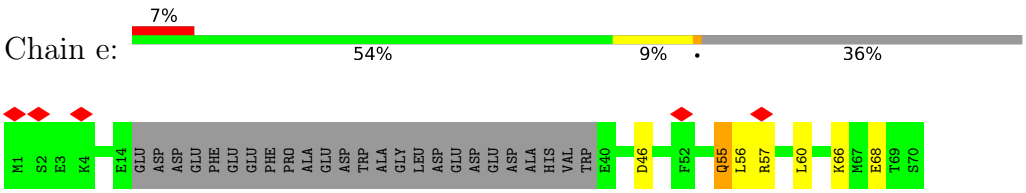
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



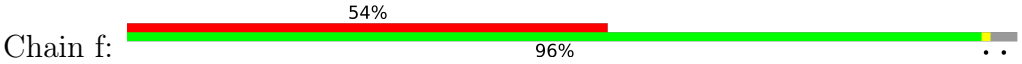
• Molecule 17: 26S proteasome complex subunit DSS1

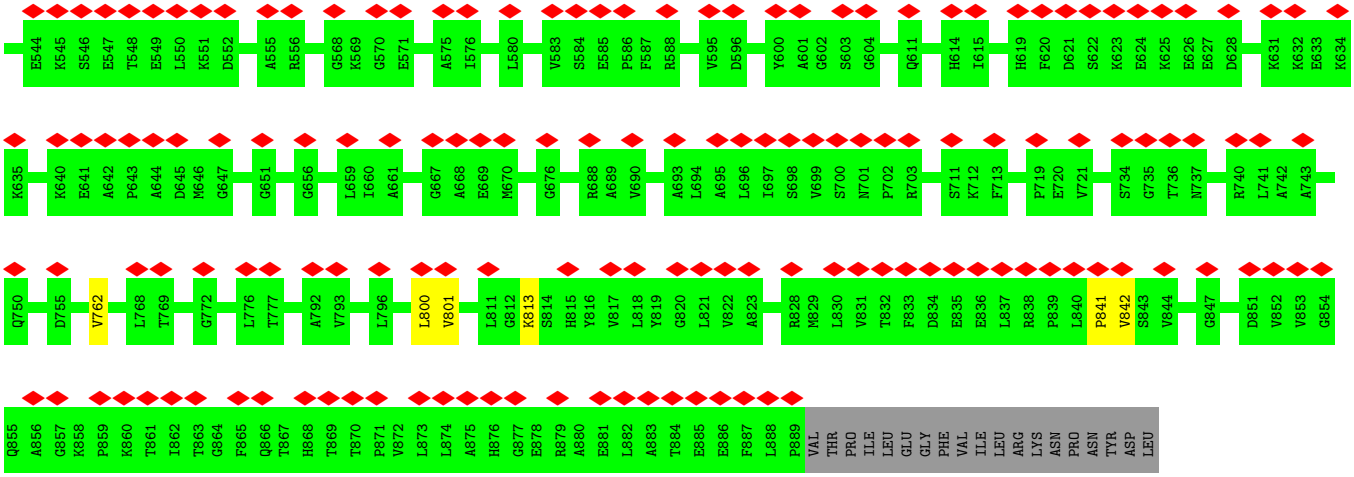
Chain e:



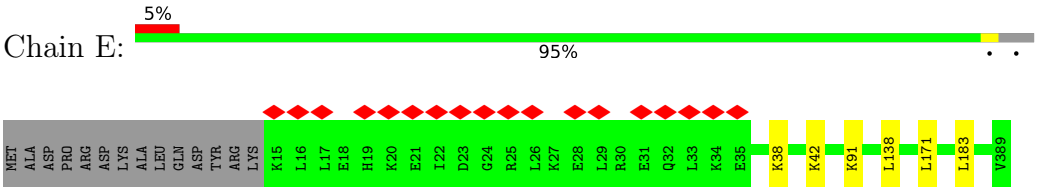
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2

Chain f:

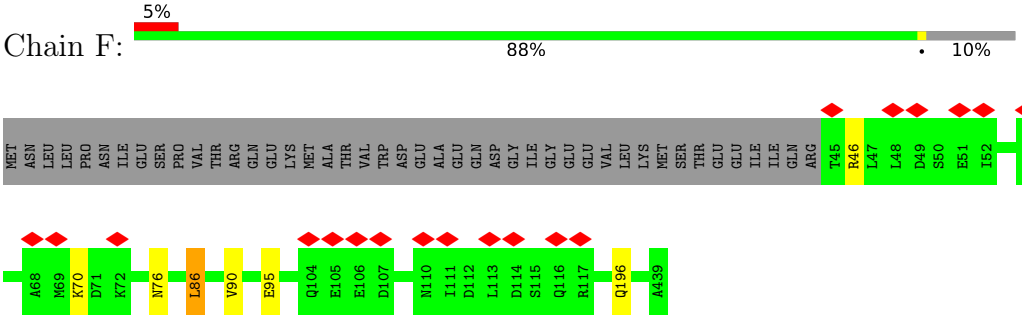




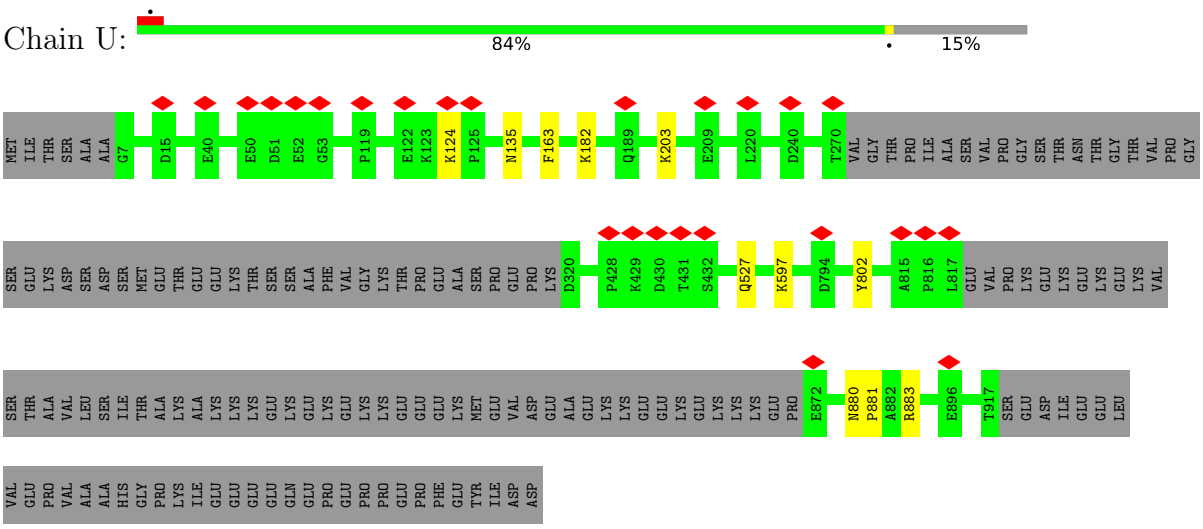
• Molecule 19: 26S protease regulatory subunit 10B



• Molecule 20: 26S protease regulatory subunit 6A

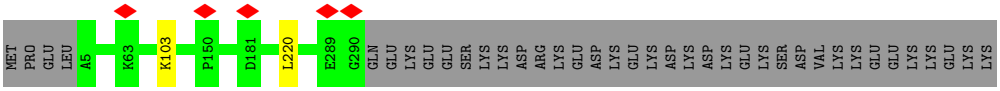


• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



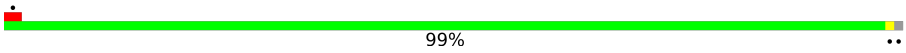
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 7

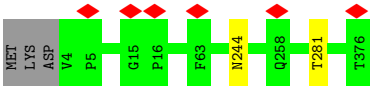
Chain Z:



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 13

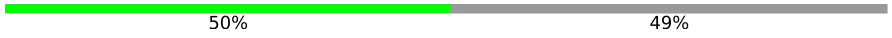
Chain a:

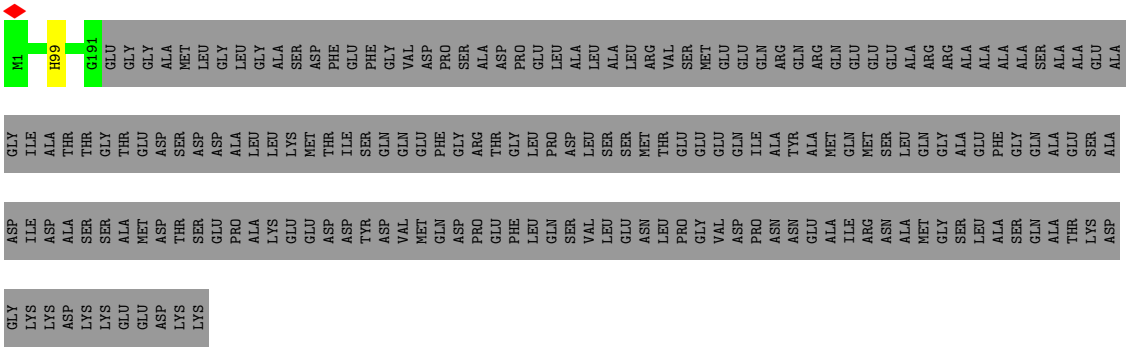




• Molecule 24: 26S proteasome non-ATPase regulatory subunit 4

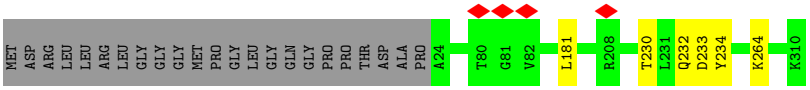
Chain b:





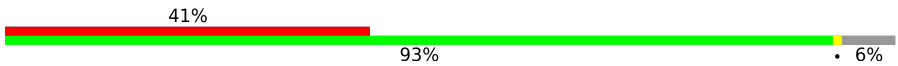
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 14

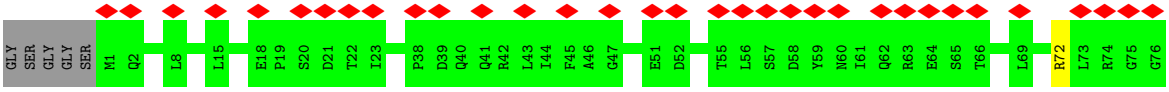
Chain c:



• Molecule 26: Polyubiquitin-B

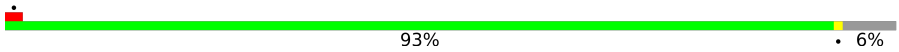
Chain v:

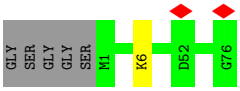




• Molecule 26: Polyubiquitin-B

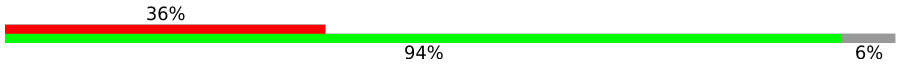
Chain u:

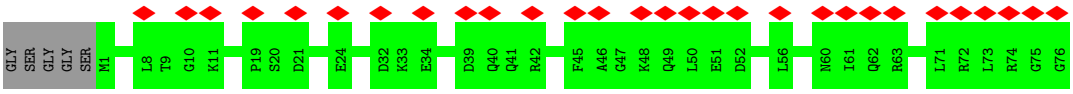




• Molecule 26: Polyubiquitin-B

Chain w:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54794	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 ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	70000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	42.355	Depositor
Minimum map value	-20.615	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	560.0, 560.0, 560.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.41	0/3049	0.59	0/4126
2	B	0.37	0/2888	0.55	0/3912
3	C	0.36	0/2987	0.58	0/4021
4	D	0.38	0/3089	0.58	0/4168
5	G	0.38	0/1859	0.52	0/2523
6	H	0.39	0/1743	0.51	0/2372
7	I	0.36	0/1942	0.54	0/2628
8	J	0.38	0/1737	0.56	0/2369
9	K	0.37	0/1786	0.54	0/2419
10	L	0.37	0/1885	0.57	0/2552
11	M	0.37	0/1891	0.53	0/2552
12	V	0.30	0/3359	0.53	0/4573
13	W	0.29	0/3406	0.52	0/4609
14	X	0.28	0/3002	0.49	0/4051
15	Y	0.35	0/3173	0.56	0/4273
16	d	0.30	0/1994	0.53	0/2704
17	e	0.29	0/334	0.58	0/449
18	f	0.24	0/4341	0.43	0/6037
19	E	0.37	0/3025	0.60	0/4073
20	F	0.38	0/3134	0.59	0/4225
21	U	0.27	0/6417	0.49	0/8684
22	Z	0.32	0/2324	0.53	0/3150
23	a	0.27	0/2592	0.50	0/3531
24	b	0.28	0/1478	0.54	0/2001
25	c	0.32	0/2302	0.55	0/3110
26	u	0.25	0/610	0.58	0/819
26	v	0.24	0/609	0.54	0/819
26	w	0.25	0/609	0.59	0/819
All	All	0.33	0/67565	0.54	0/91569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/433 (90%)	343 (88%)	49 (12%)	0	100	100
2	B	382/440 (87%)	355 (93%)	27 (7%)	0	100	100
3	C	377/406 (93%)	336 (89%)	39 (10%)	2 (0%)	25	59
4	D	378/418 (90%)	337 (89%)	41 (11%)	0	100	100
5	G	238/246 (97%)	228 (96%)	10 (4%)	0	100	100
6	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
7	I	248/261 (95%)	228 (92%)	20 (8%)	0	100	100
8	J	237/248 (96%)	218 (92%)	17 (7%)	2 (1%)	16	51
9	K	232/241 (96%)	222 (96%)	10 (4%)	0	100	100
10	L	236/263 (90%)	220 (93%)	16 (7%)	0	100	100
11	M	238/255 (93%)	223 (94%)	15 (6%)	0	100	100
12	V	471/534 (88%)	427 (91%)	42 (9%)	2 (0%)	30	63
13	W	454/456 (100%)	418 (92%)	35 (8%)	1 (0%)	44	73
14	X	378/422 (90%)	356 (94%)	22 (6%)	0	100	100
15	Y	376/389 (97%)	349 (93%)	27 (7%)	0	100	100
16	d	255/350 (73%)	218 (86%)	31 (12%)	6 (2%)	5	30
17	e	41/70 (59%)	38 (93%)	2 (5%)	1 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	f	877/908 (97%)	735 (84%)	135 (15%)	7 (1%)	16 51
19	E	373/389 (96%)	361 (97%)	12 (3%)	0	100 100
20	F	393/439 (90%)	368 (94%)	24 (6%)	1 (0%)	37 67
21	U	802/953 (84%)	771 (96%)	30 (4%)	1 (0%)	48 79
22	Z	284/324 (88%)	267 (94%)	17 (6%)	0	100 100
23	a	371/376 (99%)	357 (96%)	14 (4%)	0	100 100
24	b	189/377 (50%)	173 (92%)	16 (8%)	0	100 100
25	c	285/310 (92%)	269 (94%)	15 (5%)	1 (0%)	30 63
26	u	74/81 (91%)	71 (96%)	3 (4%)	0	100 100
26	v	74/81 (91%)	71 (96%)	3 (4%)	0	100 100
26	w	74/81 (91%)	70 (95%)	4 (5%)	0	100 100
All	All	8959/9985 (90%)	8249 (92%)	686 (8%)	24 (0%)	38 67

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	V	143	ALA
16	d	32	GLU
16	d	129	THR
18	f	472	HIS
18	f	801	VAL
25	c	234	TYR
3	C	352	PRO
18	f	800	LEU
18	f	813	LYS
18	f	841	PRO
21	U	881	PRO
16	d	17	SER
20	F	86	LEU
12	V	172	VAL
13	W	97	LEU
16	d	10	ASN
3	C	268	GLU
8	J	52	LYS
17	e	55	GLN
8	J	97	THR
16	d	228	GLN
18	f	762	VAL

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Mol	Chain	Res	Type
16	d	14	PRO
18	f	842	VAL

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	308/372 (83%)	305 (99%)	3 (1%)	73 85
2	B	292/385 (76%)	289 (99%)	3 (1%)	73 85
3	C	317/352 (90%)	313 (99%)	4 (1%)	65 81
4	D	333/366 (91%)	327 (98%)	6 (2%)	54 74
5	G	193/210 (92%)	193 (100%)	0	100 100
6	H	164/191 (86%)	163 (99%)	1 (1%)	84 92
7	I	193/221 (87%)	193 (100%)	0	100 100
8	J	154/211 (73%)	153 (99%)	1 (1%)	84 92
9	K	189/203 (93%)	186 (98%)	3 (2%)	58 76
10	L	198/224 (88%)	196 (99%)	2 (1%)	73 85
11	M	192/212 (91%)	191 (100%)	1 (0%)	86 93
12	V	255/460 (55%)	238 (93%)	17 (7%)	13 41
13	W	312/416 (75%)	298 (96%)	14 (4%)	23 53
14	X	310/362 (86%)	307 (99%)	3 (1%)	73 85
15	Y	334/344 (97%)	330 (99%)	4 (1%)	67 82
16	d	185/294 (63%)	167 (90%)	18 (10%)	6 29
17	e	29/63 (46%)	22 (76%)	7 (24%)	0 4
19	E	329/341 (96%)	323 (98%)	6 (2%)	54 74
20	F	339/379 (89%)	332 (98%)	7 (2%)	48 71
21	U	688/816 (84%)	678 (98%)	10 (2%)	60 78
22	Z	257/295 (87%)	255 (99%)	2 (1%)	79 88
23	a	202/336 (60%)	200 (99%)	2 (1%)	73 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	b	167/312 (54%)	166 (99%)	1 (1%)	84 92
25	c	252/268 (94%)	247 (98%)	5 (2%)	50 72
26	u	68/70 (97%)	67 (98%)	1 (2%)	60 78
26	v	68/70 (97%)	67 (98%)	1 (2%)	60 78
26	w	68/70 (97%)	68 (100%)	0	100 100
All	All	6396/7843 (82%)	6274 (98%)	122 (2%)	52 73

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	ARG
1	A	312	ARG
1	A	401	ARG
2	B	172	THR
2	B	174	MET
2	B	203	LEU
3	C	22	GLN
3	C	43	ARG
3	C	250	GLU
3	C	351	MET
4	D	51	LEU
4	D	55	GLU
4	D	68	LEU
4	D	69	LYS
4	D	82	ILE
4	D	279	THR
6	H	121	TYR
8	J	118	TYR
9	K	13	ASN
9	K	21	LEU
9	K	129	ASP
10	L	9	ASP
10	L	207	THR
11	M	184	MET
12	V	200	ARG
12	V	201	ARG
12	V	204	ASP
12	V	220	PHE
12	V	223	LYS
12	V	239	THR

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Mol	Chain	Res	Type
12	V	240	LEU
12	V	242	HIS
12	V	243	ASP
12	V	257	ASN
12	V	258	TYR
12	V	263	LEU
12	V	329	HIS
12	V	336	GLU
12	V	344	ASP
12	V	349	ARG
12	V	451	ILE
13	W	120	ILE
13	W	123	ARG
13	W	132	THR
13	W	137	TYR
13	W	138	VAL
13	W	140	ILE
13	W	149	LEU
13	W	160	LYS
13	W	161	GLU
13	W	169	LEU
13	W	173	THR
13	W	184	GLU
13	W	262	LYS
13	W	448	LYS
14	X	78	ASN
14	X	334	ASN
14	X	420	LYS
15	Y	82	LYS
15	Y	200	LEU
15	Y	207	THR
15	Y	232	GLU
16	d	36	LEU
16	d	39	THR
16	d	42	LYS
16	d	44	THR
16	d	49	ILE
16	d	61	TRP
16	d	82	TYR
16	d	98	LEU
16	d	99	LEU
16	d	104	LEU

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Mol	Chain	Res	Type
16	d	111	ARG
16	d	126	ASP
16	d	129	THR
16	d	186	TYR
16	d	204	LYS
16	d	207	THR
16	d	209	TYR
16	d	215	TRP
17	e	46	ASP
17	e	55	GLN
17	e	56	LEU
17	e	57	ARG
17	e	60	LEU
17	e	66	LYS
17	e	68	GLU
19	E	38	LYS
19	E	42	LYS
19	E	91	LYS
19	E	138	LEU
19	E	171	LEU
19	E	183	LEU
20	F	46	ARG
20	F	70	LYS
20	F	76	ASN
20	F	86	LEU
20	F	90	VAL
20	F	95	GLU
20	F	196	GLN
21	U	124	LYS
21	U	135	ASN
21	U	163	PHE
21	U	182	LYS
21	U	203	LYS
21	U	527	GLN
21	U	597	LYS
21	U	802	TYR
21	U	880	ASN
21	U	883	ARG
22	Z	103	LYS
22	Z	220	LEU
23	a	244	ASN
23	a	281	THR

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Mol	Chain	Res	Type
24	b	99	HIS
25	c	181	LEU
25	c	230	THR
25	c	232	GLN
25	c	233	ASP
25	c	264	LYS
26	v	72	ARG
26	u	6	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	343	ASN
13	W	444	HIS
15	Y	365	GLN
21	U	171	ASN
23	a	244	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
29	ADP	C	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
27	ATP	A	501	28	26,33,33	0.75	0	31,52,52	0.79	1 (3%)
27	ATP	E	401	28	26,33,33	0.71	0	31,52,52	0.81	2 (6%)
29	ADP	F	501	28	24,29,29	0.99	2 (8%)	29,45,45	1.59	4 (13%)
27	ATP	B	501	28	26,33,33	0.71	0	31,52,52	0.79	1 (3%)
27	ATP	D	501	28	26,33,33	0.73	0	31,52,52	0.85	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
29	ADP	C	501	-	-	1/12/32/32	0/3/3/3
27	ATP	A	501	28	-	1/18/38/38	0/3/3/3
27	ATP	E	401	28	-	8/18/38/38	0/3/3/3
29	ADP	F	501	28	-	3/12/32/32	0/3/3/3
27	ATP	B	501	28	-	2/18/38/38	0/3/3/3
27	ATP	D	501	28	-	6/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	501	ADP	C5-C4	2.22	1.46	1.40
29	C	501	ADP	C5-C4	2.09	1.46	1.40
29	F	501	ADP	C2'-C1'	-2.06	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	501	ADP	PA-O3A-PB	-4.85	116.20	132.83
29	C	501	ADP	PA-O3A-PB	-3.78	119.85	132.83
29	C	501	ADP	C3'-C2'-C1'	3.19	105.78	100.98
29	F	501	ADP	N3-C2-N1	-3.09	123.85	128.68
29	C	501	ADP	N3-C2-N1	-3.09	123.85	128.68
29	F	501	ADP	C3'-C2'-C1'	2.37	104.54	100.98
29	F	501	ADP	C4-C5-N7	-2.30	107.01	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	501	ATP	C5-C6-N6	2.29	123.84	120.35
27	E	401	ATP	C5-C6-N6	2.28	123.82	120.35
27	B	501	ATP	C5-C6-N6	2.27	123.80	120.35
27	A	501	ATP	C5-C6-N6	2.25	123.77	120.35
29	C	501	ADP	C4-C5-N7	-2.23	107.07	109.40
27	E	401	ATP	PB-O3B-PG	2.02	139.76	132.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	D	501	ATP	C5'-O5'-PA-O3A
27	D	501	ATP	O4'-C4'-C5'-O5'
27	E	401	ATP	C5'-O5'-PA-O2A
27	E	401	ATP	C5'-O5'-PA-O3A
27	E	401	ATP	O4'-C4'-C5'-O5'
27	E	401	ATP	C3'-C4'-C5'-O5'
29	F	501	ADP	O4'-C4'-C5'-O5'
29	F	501	ADP	C3'-C4'-C5'-O5'
27	B	501	ATP	O4'-C4'-C5'-O5'
27	B	501	ATP	C3'-C4'-C5'-O5'
27	D	501	ATP	C3'-C4'-C5'-O5'
29	F	501	ADP	C4'-C5'-O5'-PA
27	D	501	ATP	C5'-O5'-PA-O1A
27	D	501	ATP	C5'-O5'-PA-O2A
27	E	401	ATP	C5'-O5'-PA-O1A
29	C	501	ADP	O4'-C4'-C5'-O5'
27	E	401	ATP	PG-O3B-PB-O1B
27	A	501	ATP	O4'-C4'-C5'-O5'
27	D	501	ATP	PA-O3A-PB-O1B
27	E	401	ATP	PB-O3A-PA-O1A
27	E	401	ATP	PB-O3A-PA-O2A

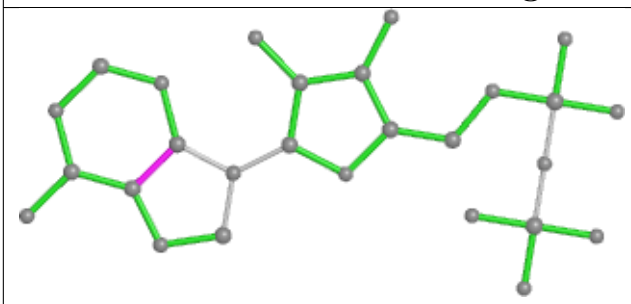
There are no ring outliers.

No monomer is involved in short contacts.

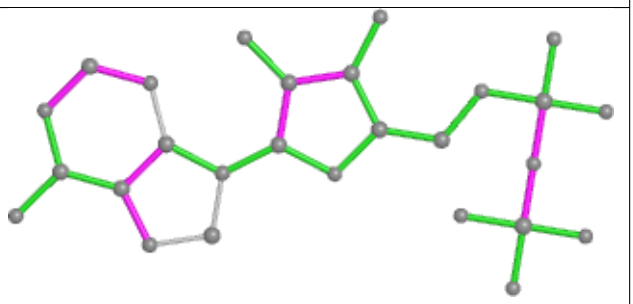
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

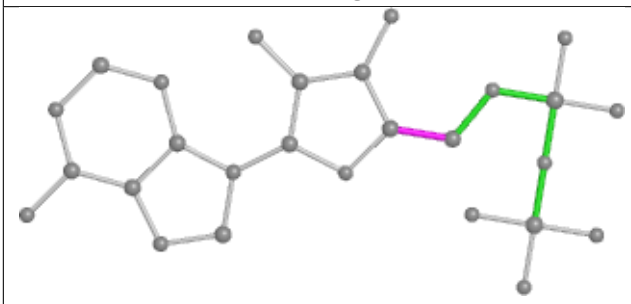
Ligand ADP C 501



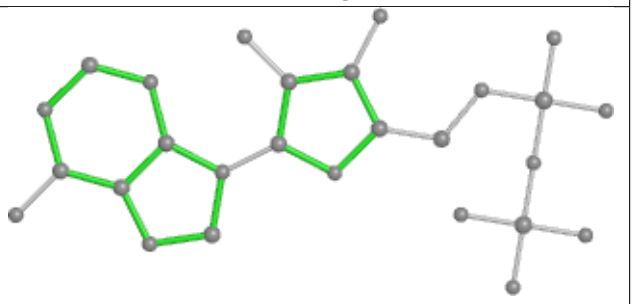
Bond lengths



Bond angles

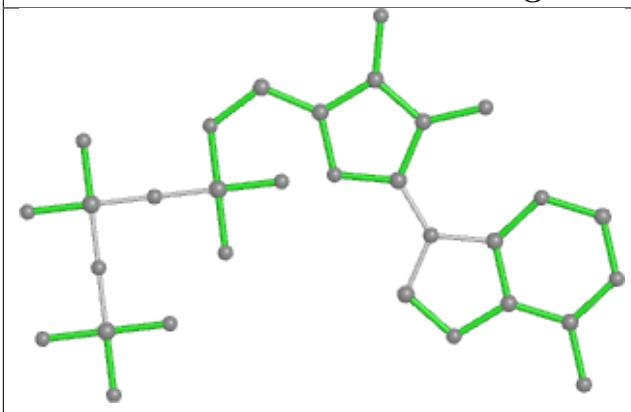


Torsions

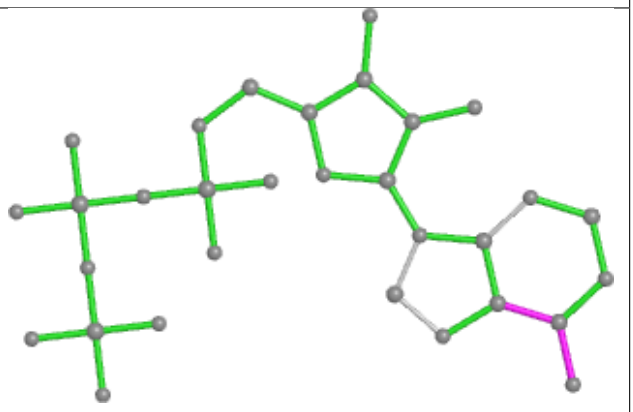


Rings

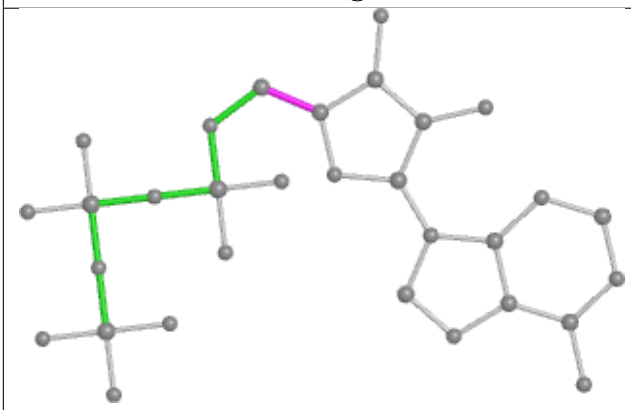
Ligand ATP A 501



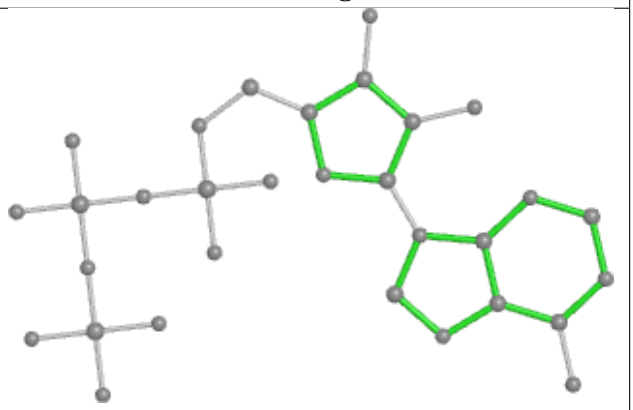
Bond lengths



Bond angles

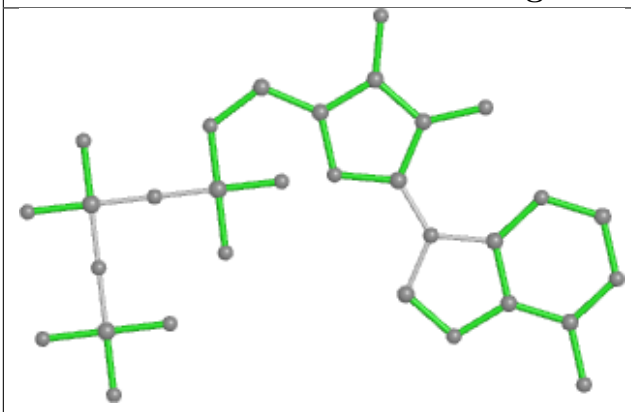


Torsions

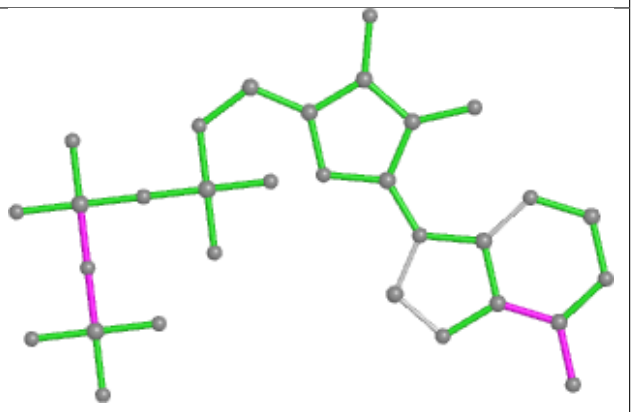


Rings

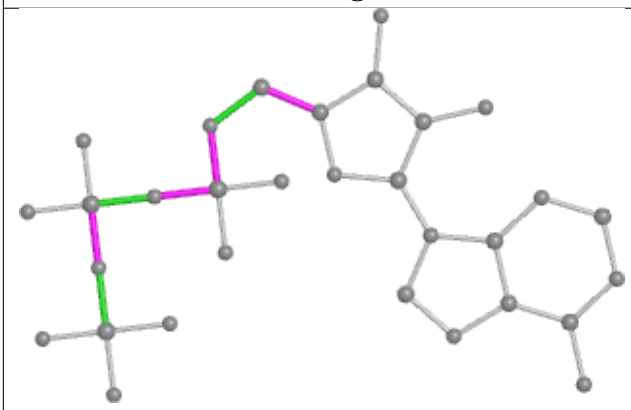
Ligand ATP E 401



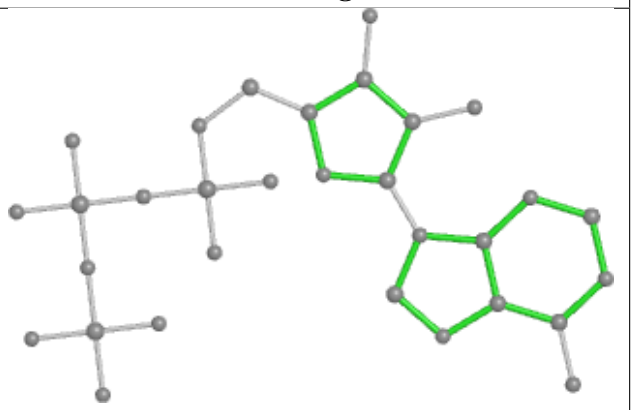
Bond lengths



Bond angles

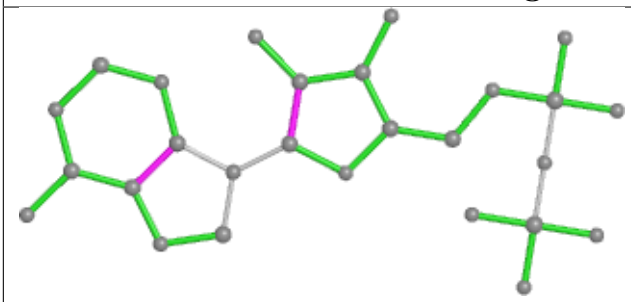


Torsions

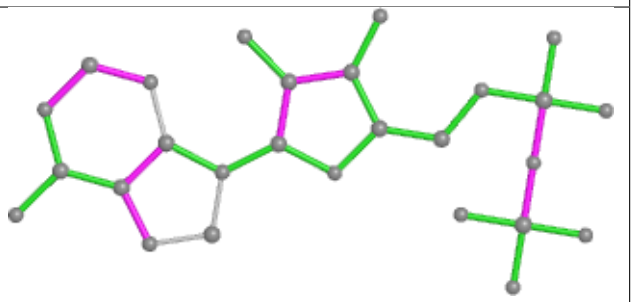


Rings

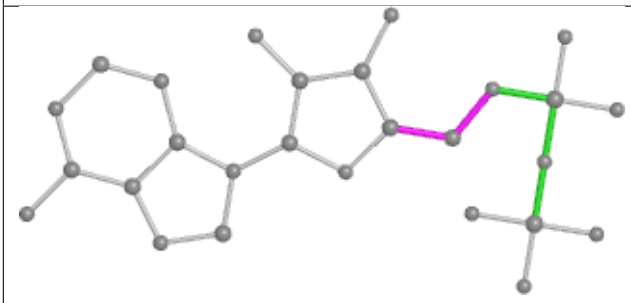
Ligand ADP F 501



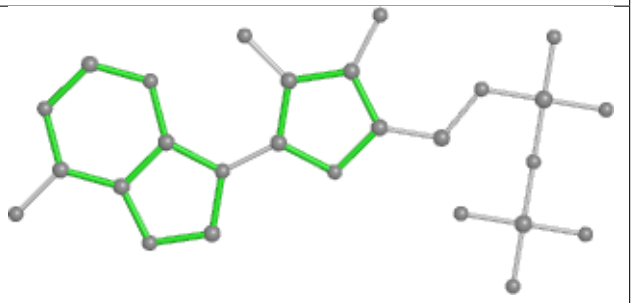
Bond lengths



Bond angles

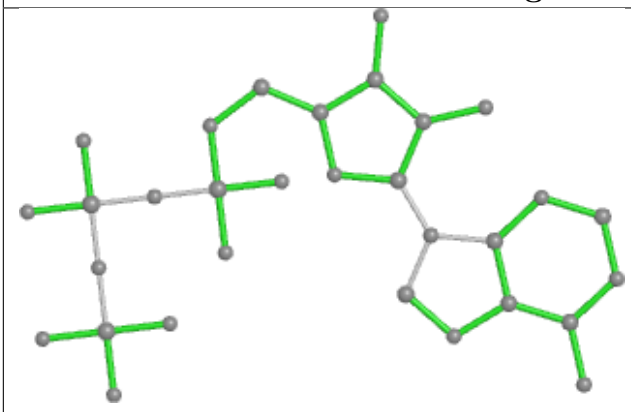


Torsions

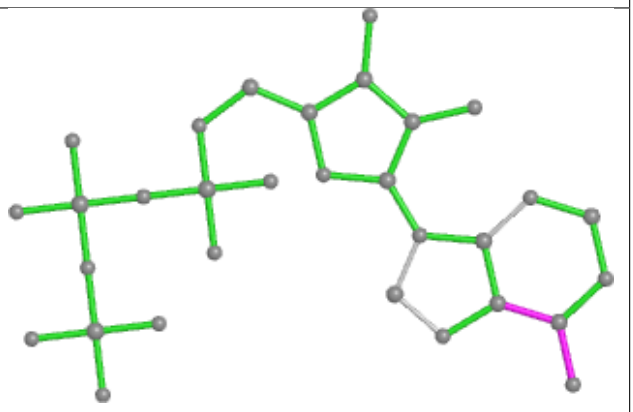


Rings

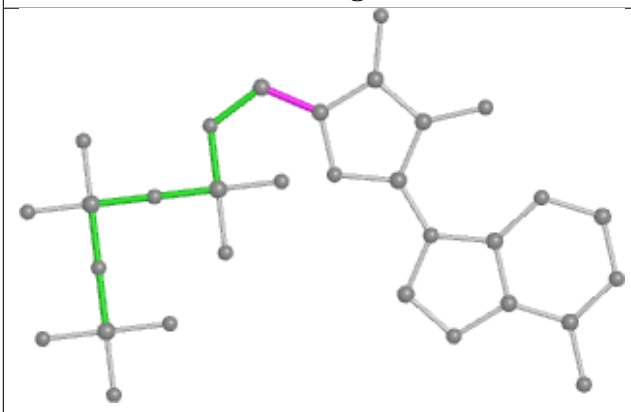
Ligand ATP B 501



Bond lengths



Bond angles



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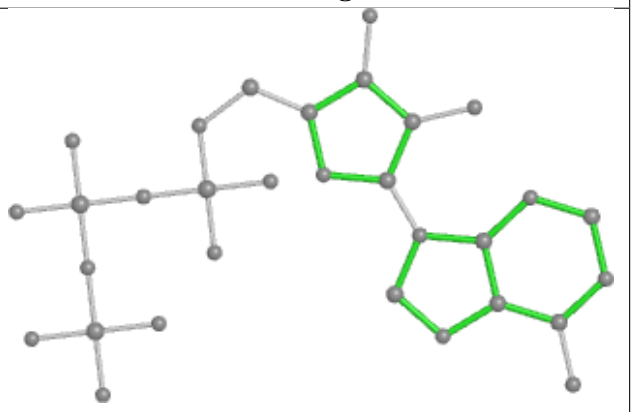
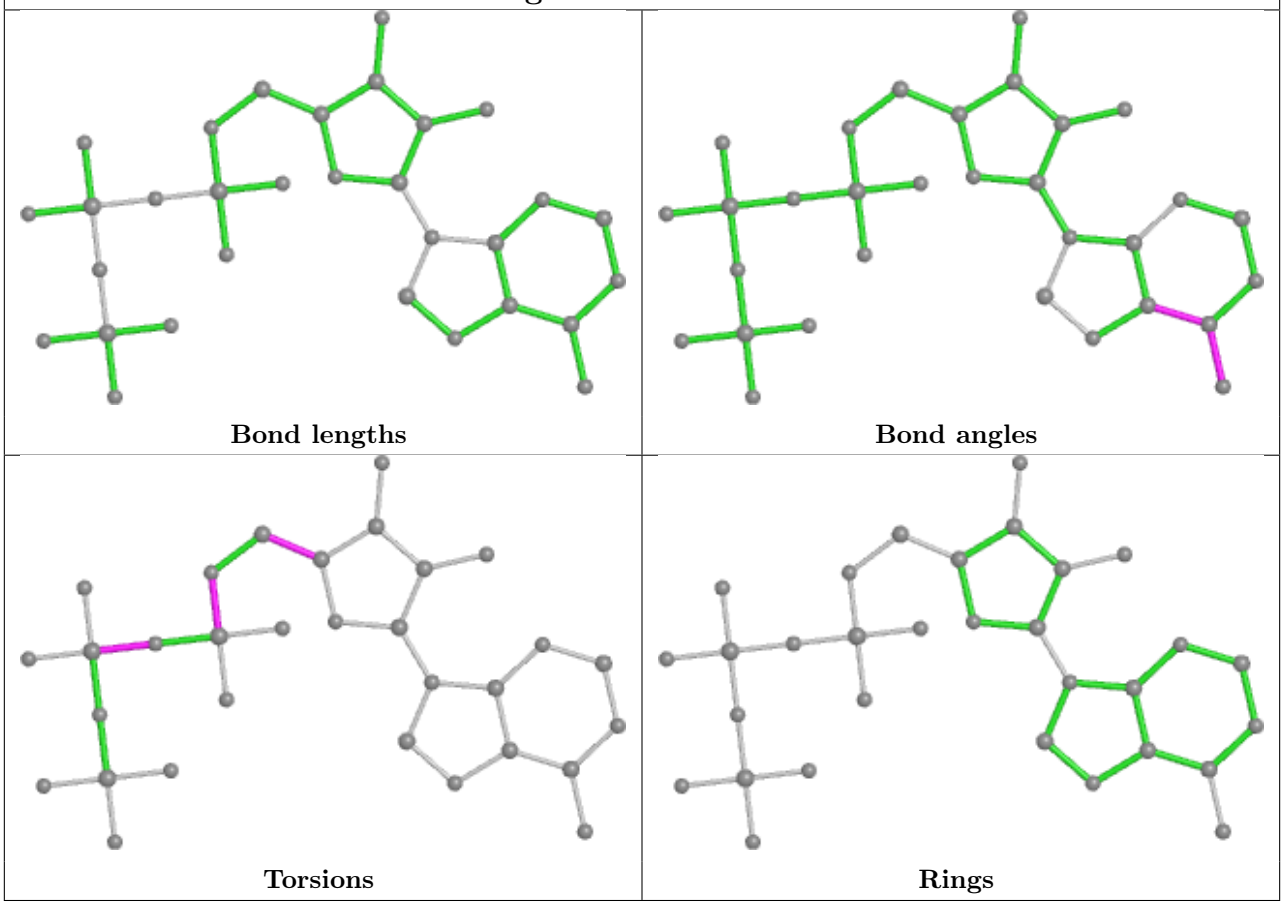


Rings

Ligand ATP D 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

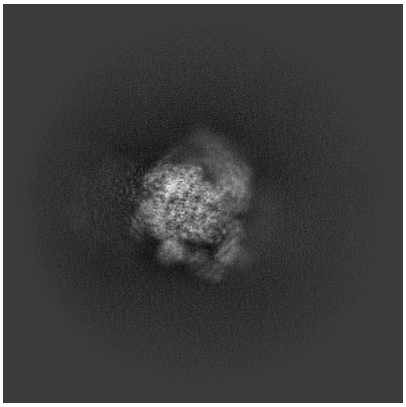
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36605. These allow visual inspection of the internal detail of the map and identification of artifacts.

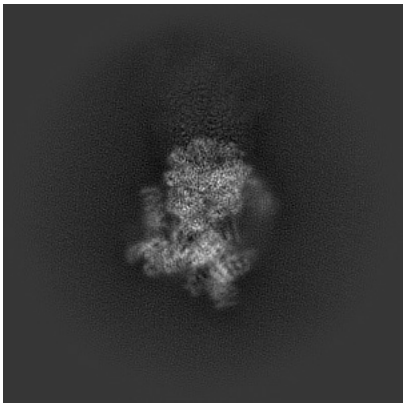
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

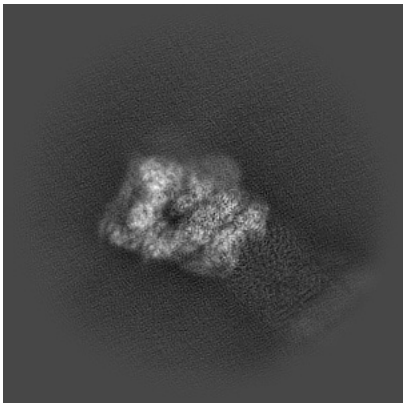
6.1.1 Primary map



X



Y

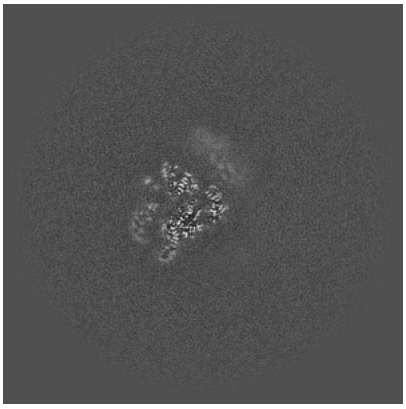


Z

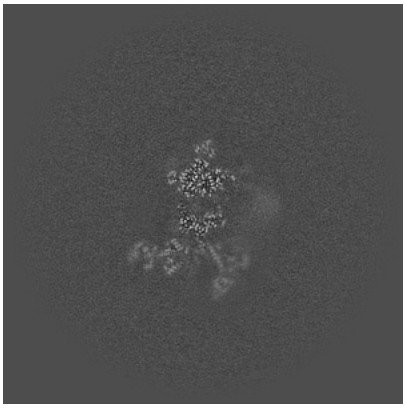
The images above show the map projected in three orthogonal directions.

6.2 Central slices

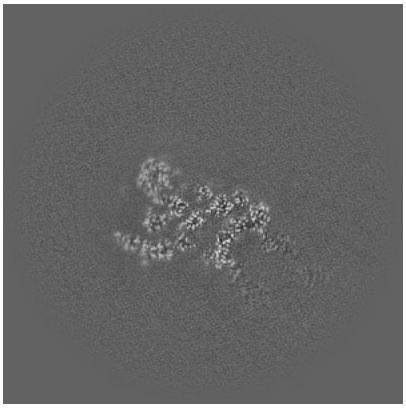
6.2.1 Primary map



X Index: 200



Y Index: 200

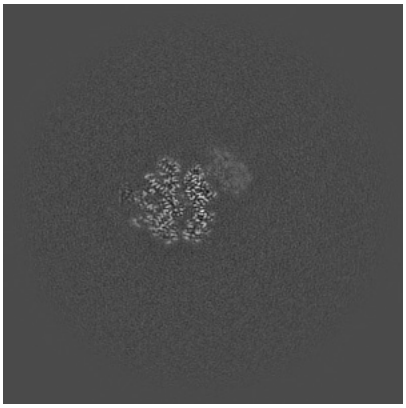


Z Index: 200

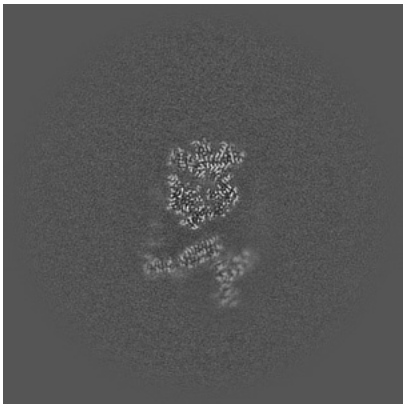
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

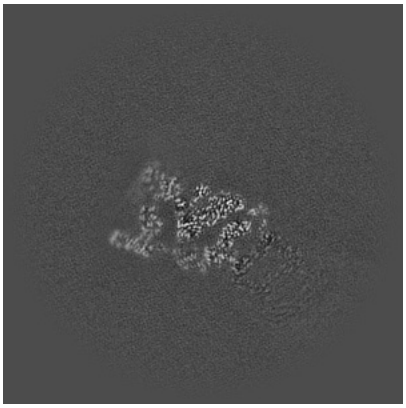
6.3.1 Primary map



X Index: 226



Y Index: 182

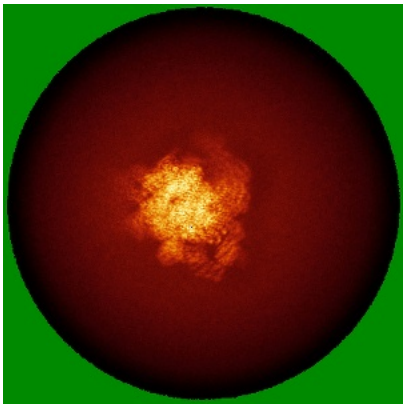


Z Index: 190

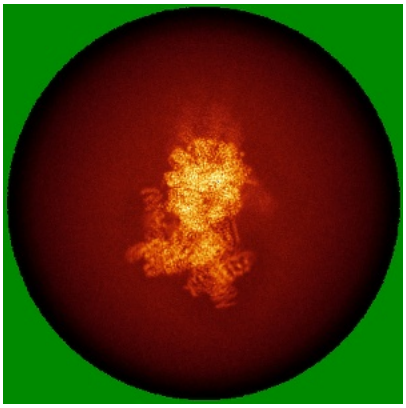
The images above show the largest variance slices of the map in three orthogonal directions.

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

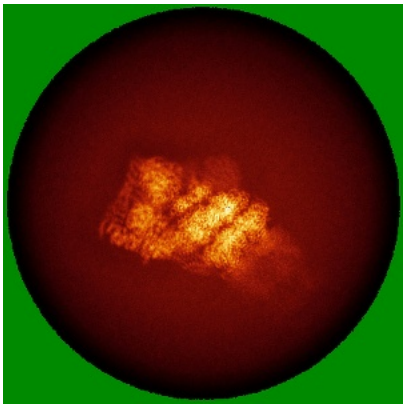
6.4.1 Primary map



X



Y



Z

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 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

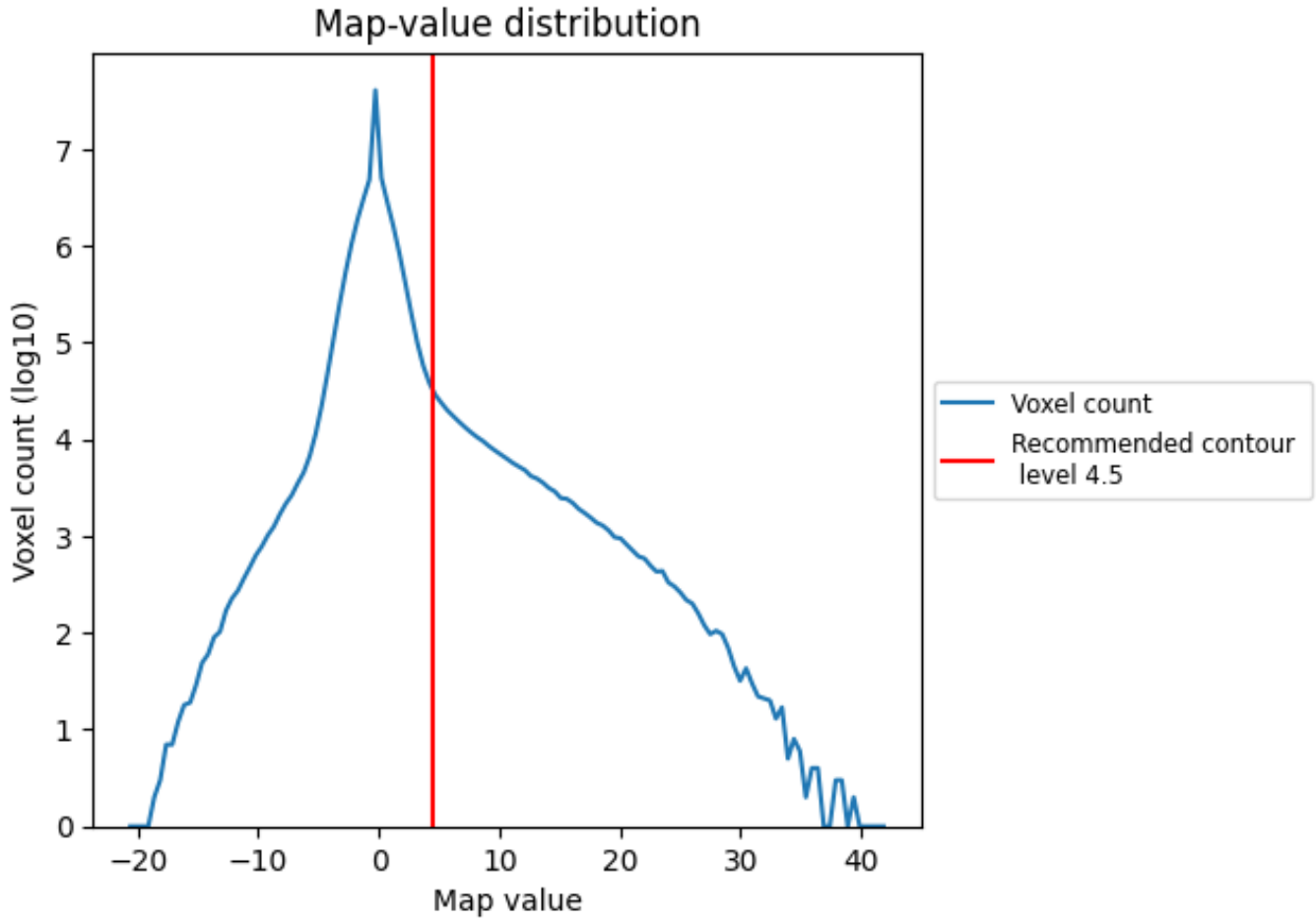
6.6 Mask visualisation (i)

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

7 Map analysis

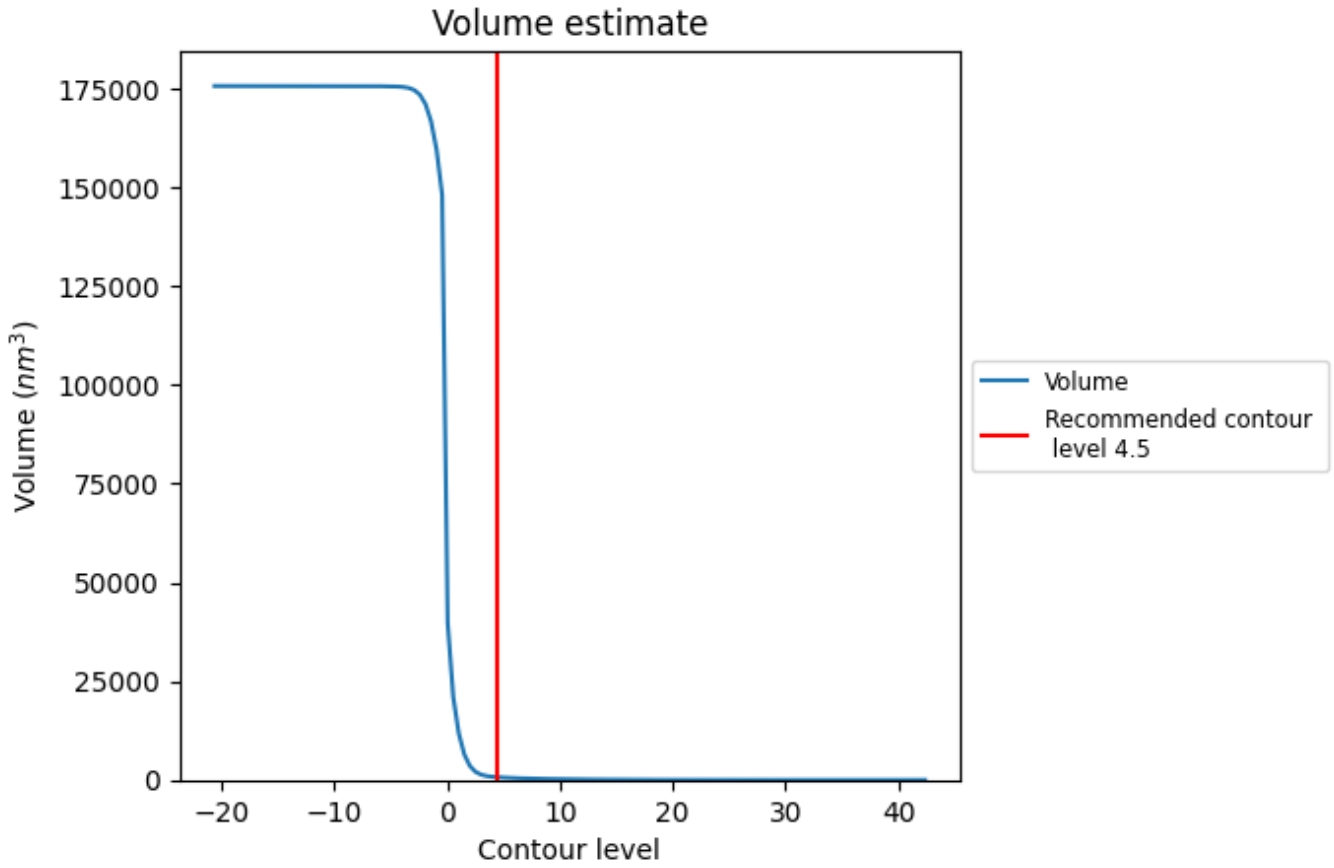
This section contains the results of statistical analysis of the map.

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.

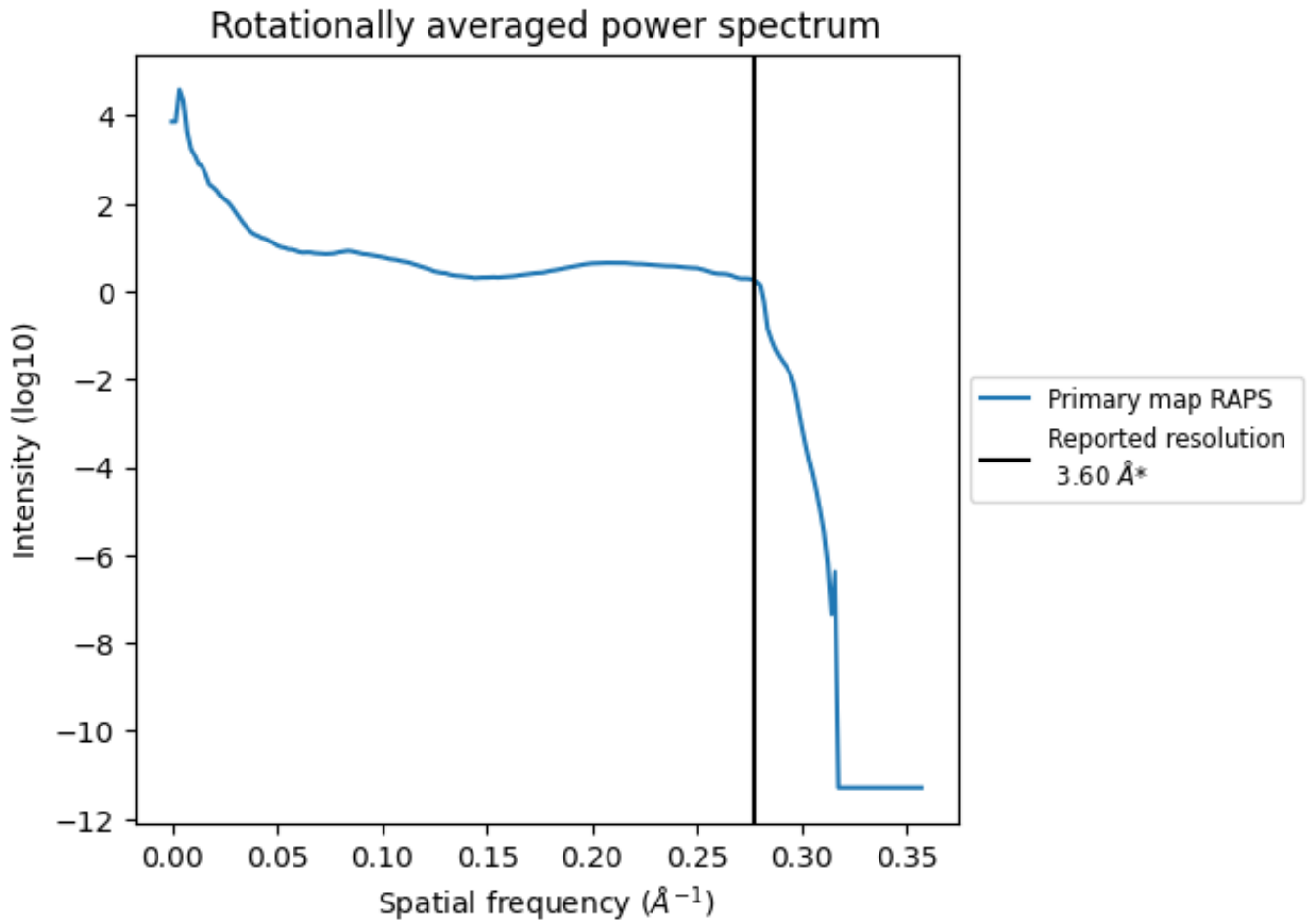
7.2 Volume estimate



The volume at the recommended contour level is 687 nm^3; this corresponds to an approximate mass of 621 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)

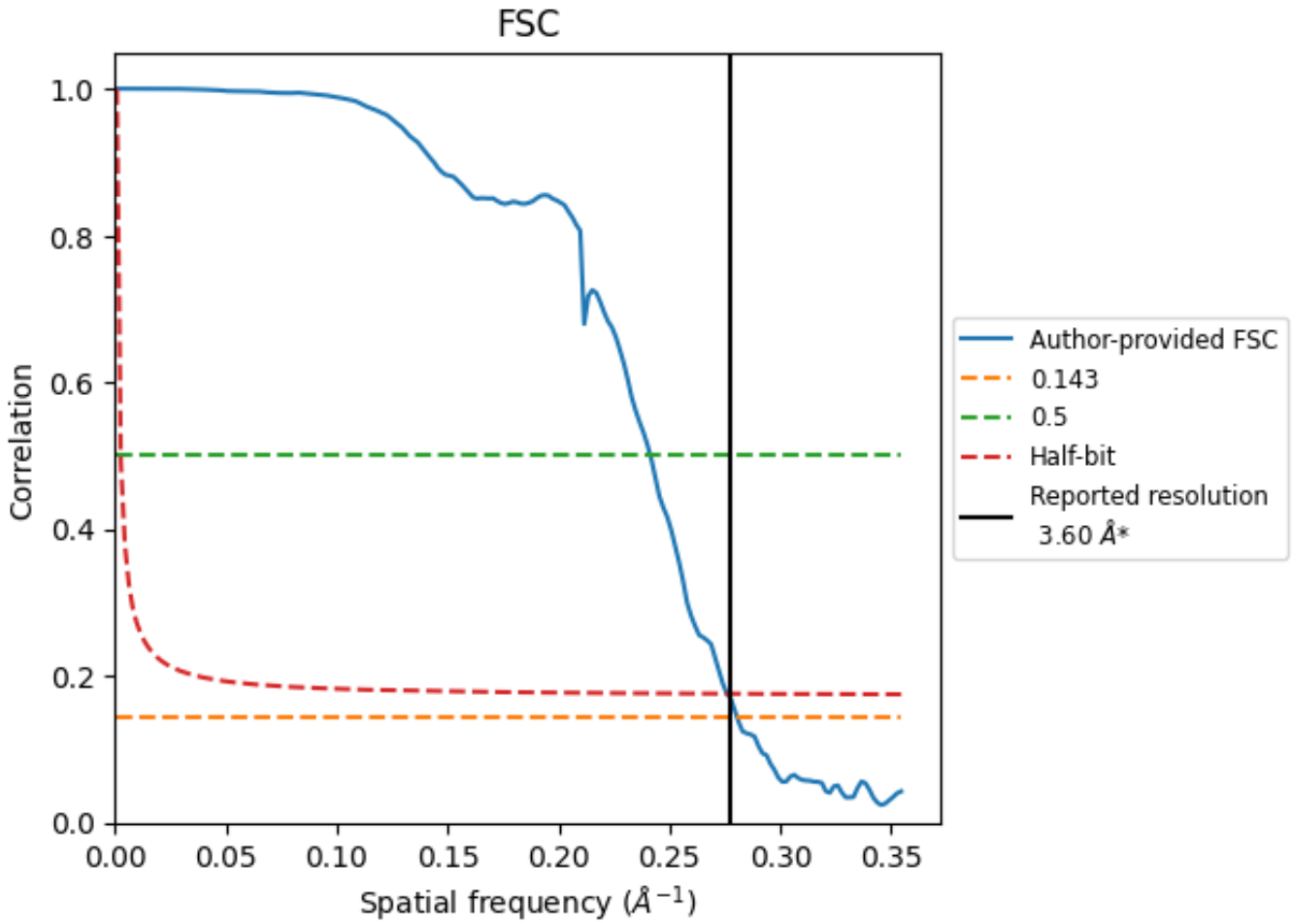


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

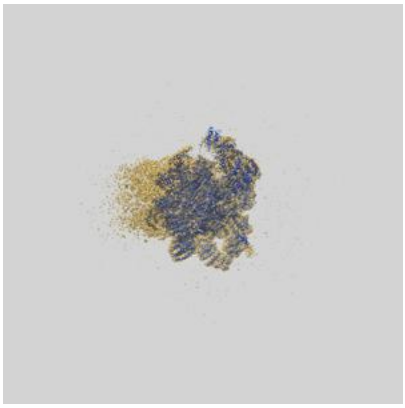
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.14	3.62
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

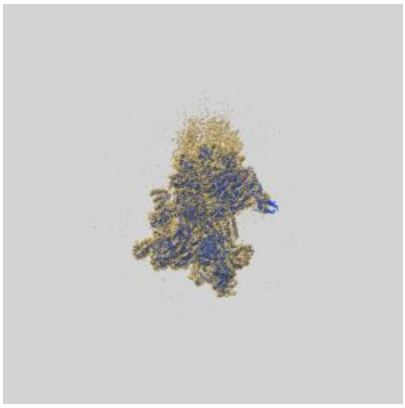
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36605 and PDB model 8JRT. Per-residue inclusion information can be found in section 3 on page 10.

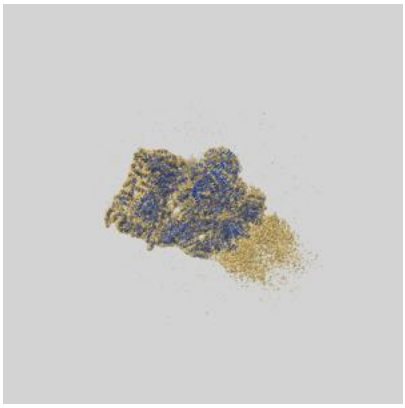
9.1 Map-model overlay



X



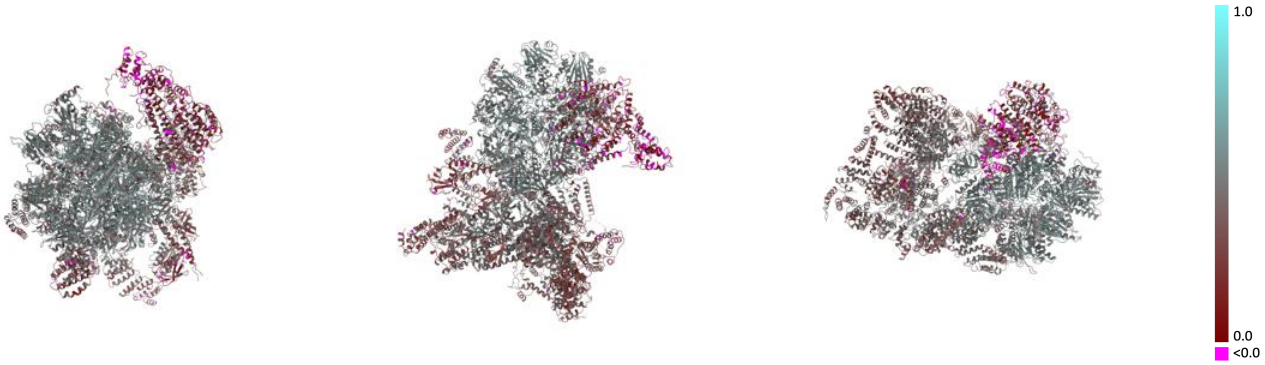
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

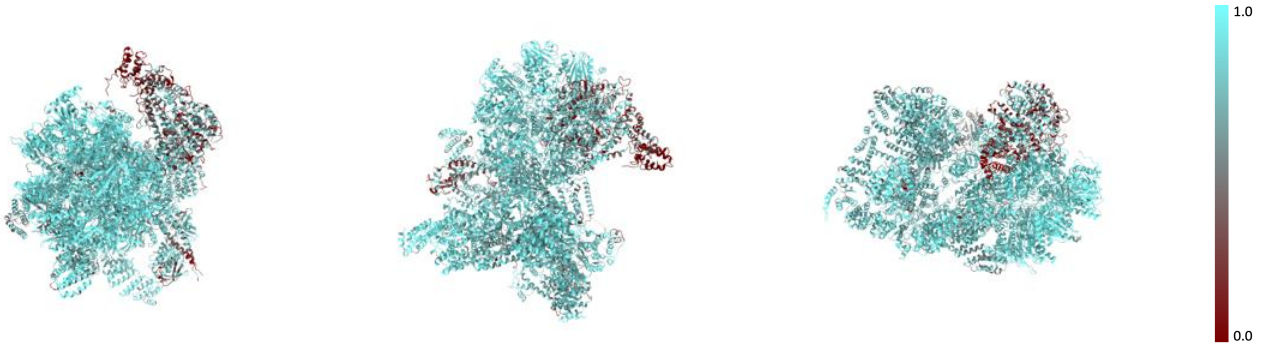
9.2 Q-score mapped to coordinate model (i)



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.

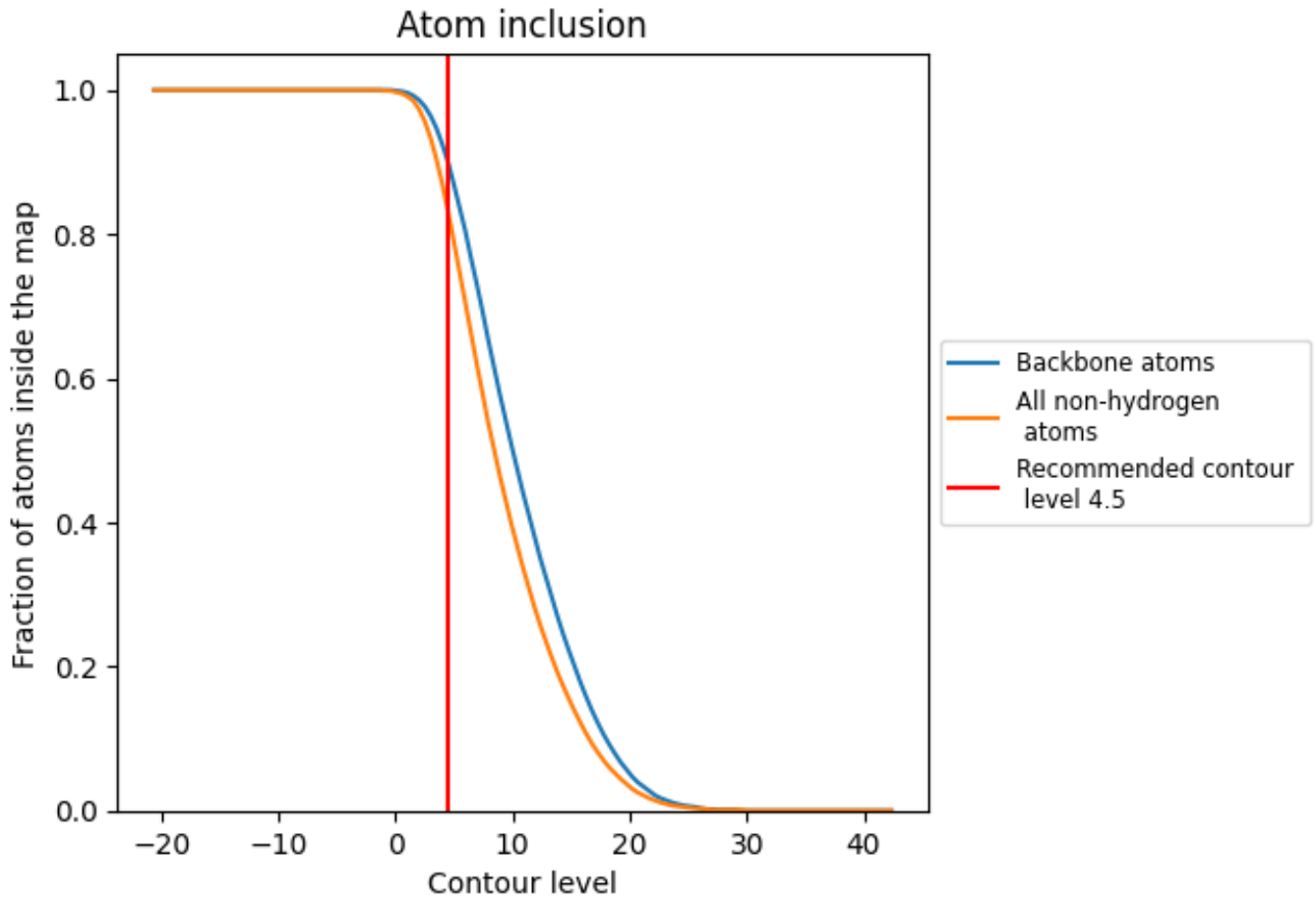
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.4230
A	0.9060	0.4920
B	0.8720	0.4740
C	0.8700	0.4840
D	0.8910	0.4930
E	0.8880	0.4990
F	0.8640	0.5000
G	0.9350	0.5030
H	0.9340	0.5090
I	0.9230	0.4880
J	0.9310	0.5010
K	0.9270	0.5120
L	0.9480	0.5180
M	0.9170	0.4950
U	0.8080	0.3650
V	0.8240	0.3650
W	0.8340	0.3780
X	0.7440	0.4070
Y	0.8720	0.4110
Z	0.8600	0.4480
a	0.9020	0.3880
b	0.8560	0.3500
c	0.8600	0.4520
d	0.8330	0.3730
e	0.7370	0.3820
f	0.4280	0.2020
u	0.7640	0.3050
v	0.4260	0.1980
w	0.4950	0.2660