



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 12:27 PM JST

PDB ID : 8JTI
EMDB ID : EMD-36645
Title : Cryo-EM structure of human 26S RP (Eb state) bound to K11/K48-branched ubiquitin (Ub) chain composed of four Ub.
Authors : Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on : 2023-06-21
Resolution : 3.80 Å (reported)
Based on initial model : 6MSB

This is a wwPDB EM Validation Summary 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:

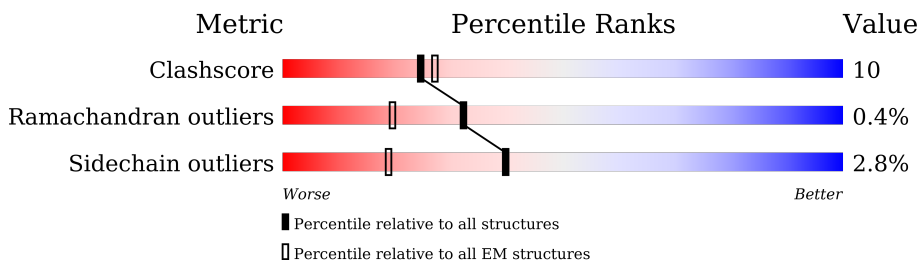
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.80 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.






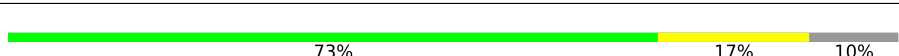
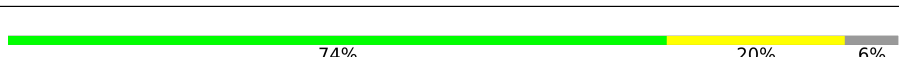
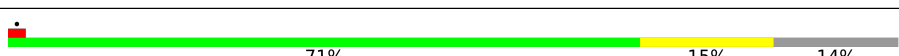
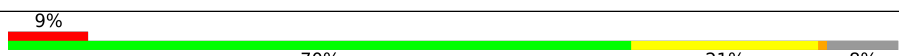
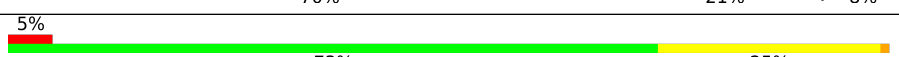

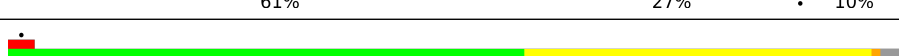
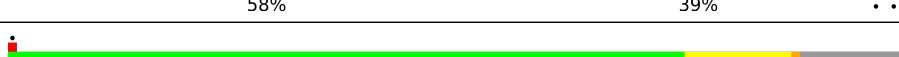

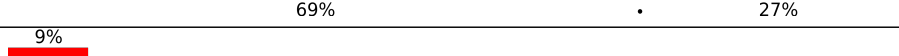

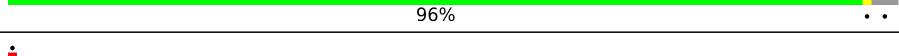
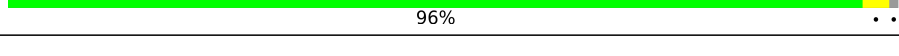

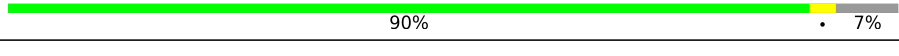
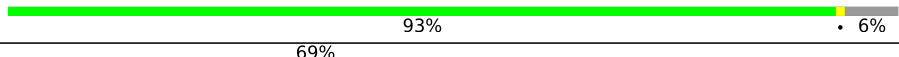
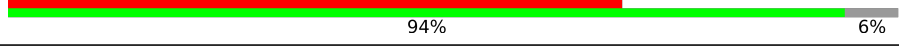
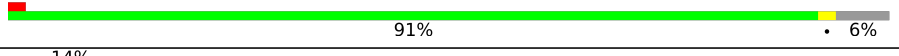
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	406	
4	D	418	
5	E	389	
6	F	439	
7	G	246	
8	H	234	

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Mol	Chain	Length	Quality of chain
9	I	261	
10	J	248	
11	K	241	
12	L	263	
13	M	255	
14	U	953	
15	V	534	
16	W	456	
17	X	422	
18	Y	389	
19	Z	324	
20	d	350	
21	e	70	
22	f	908	
23	a	376	
24	b	377	
25	c	310	
26	u	81	
26	v	81	
26	w	81	
26	x	81	

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 67839 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	3096	1951	543	584	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	3004	1895	515	580	14	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	365	2868	1811	515	526	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 26S protease regulatory subunit 10B.

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

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

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

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	U	815	6361	4040	1083	1194	44	0	0

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	V	493	3315	2075	622	611	7	0	0

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	W	456	3292	2064	584	630	14	0	0

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	380	2793	1763	487	534	9	0	0

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	d	257	2053	1332	336	376	9	0	0

- Molecule 21 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	49	Total	C	N	O	S	0	0
			280	171	52	56	1		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	f	880	Total	C	N	O	0	0
			4338	2578	880	880		

- 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
			2995	1911	510	559	15		

- 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		

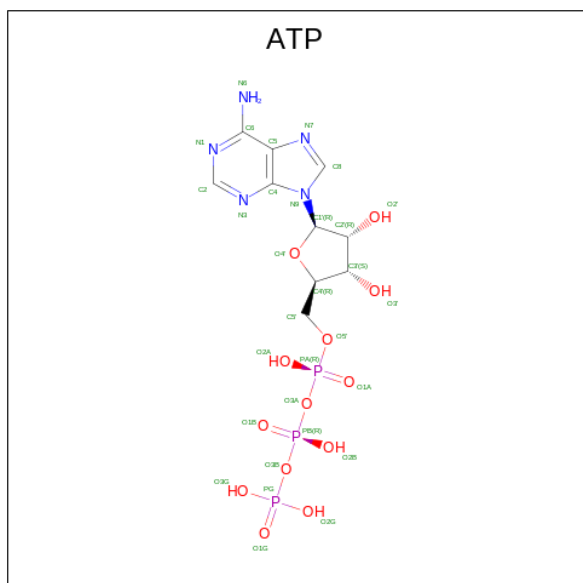
- Molecule 26 is a protein called Polyubiquitin-B.

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
			603	378	107	117	1		
26	x	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
26	w	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There are 24 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
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
x	-4	GLY	-	linker	UNP P0CG47
x	-3	SER	-	linker	UNP P0CG47
x	-2	GLY	-	linker	UNP P0CG47
x	-1	GLY	-	linker	UNP P0CG47
x	0	SER	-	linker	UNP P0CG47
x	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: $C_{10}H_{16}N_5O_{13}P_3$).

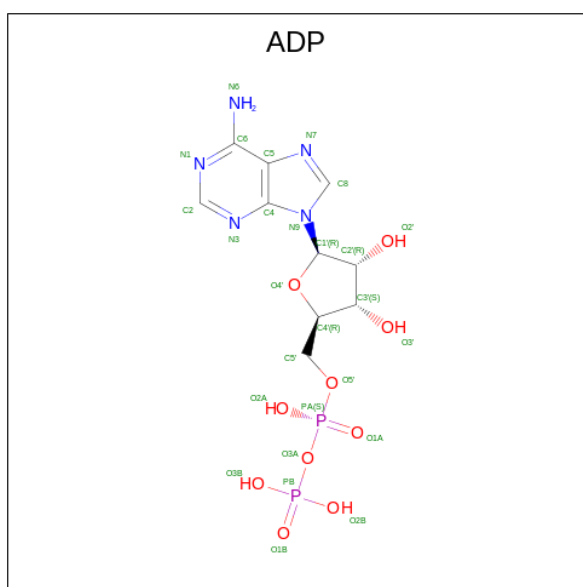


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
27	A	1	Total 31	C 10	N 5	O 13	P 3	0
27	B	1	Total 31	C 10	N 5	O 13	P 3	0
27	D	1	Total 31	C 10	N 5	O 13	P 3	0
27	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

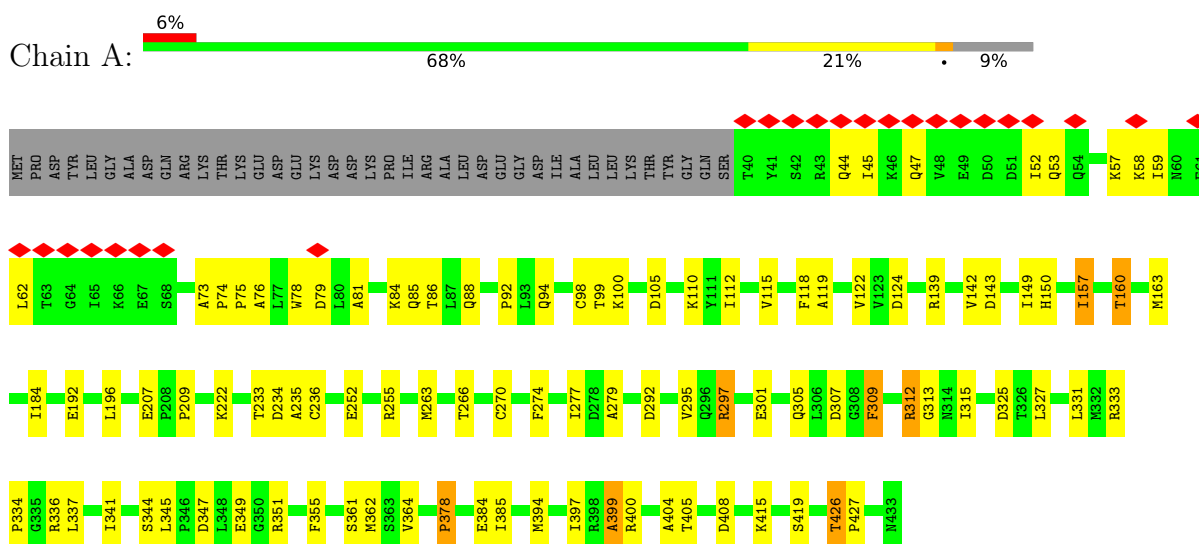


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	C	1	27	10	5	10	2	0
29	F	1	27	10	5	10	2	0

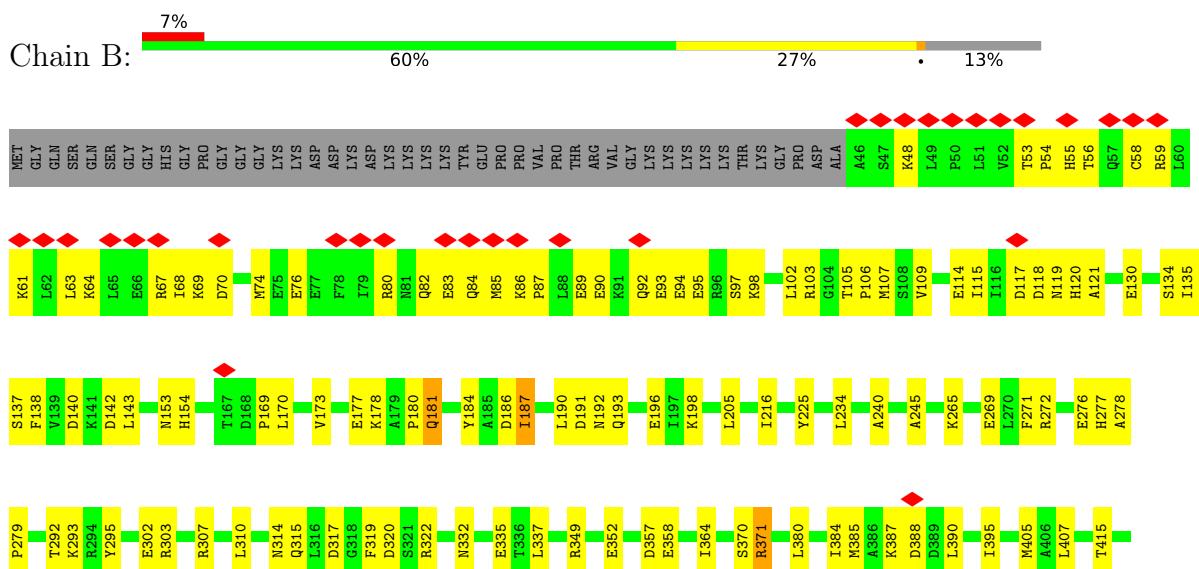
3 Residue-property plots [i](#)

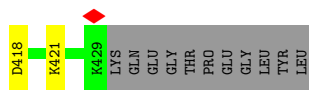
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

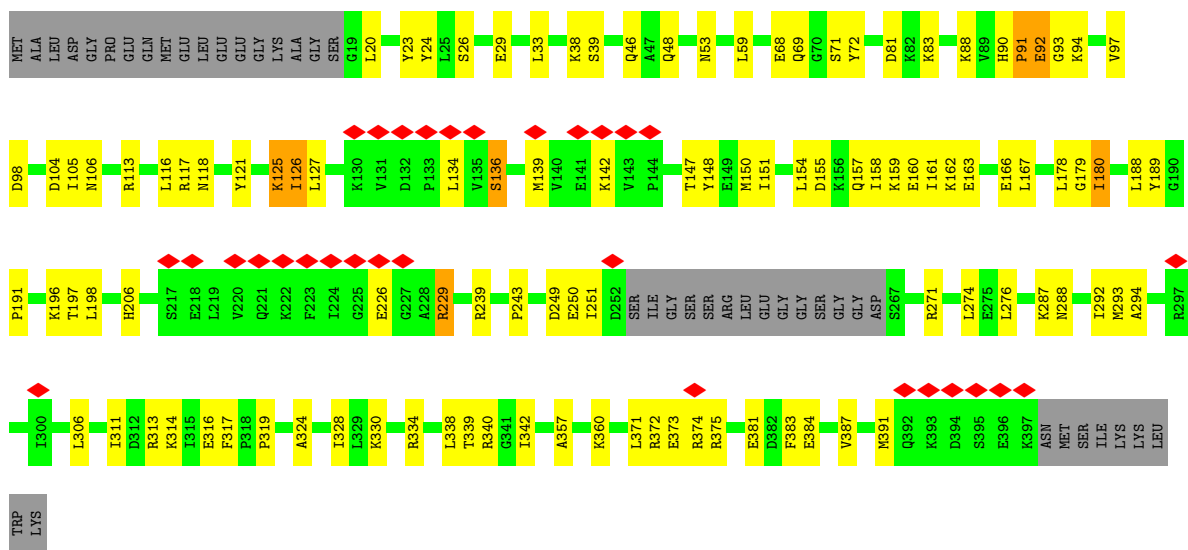


- Molecule 2: 26S protease regulatory subunit 4

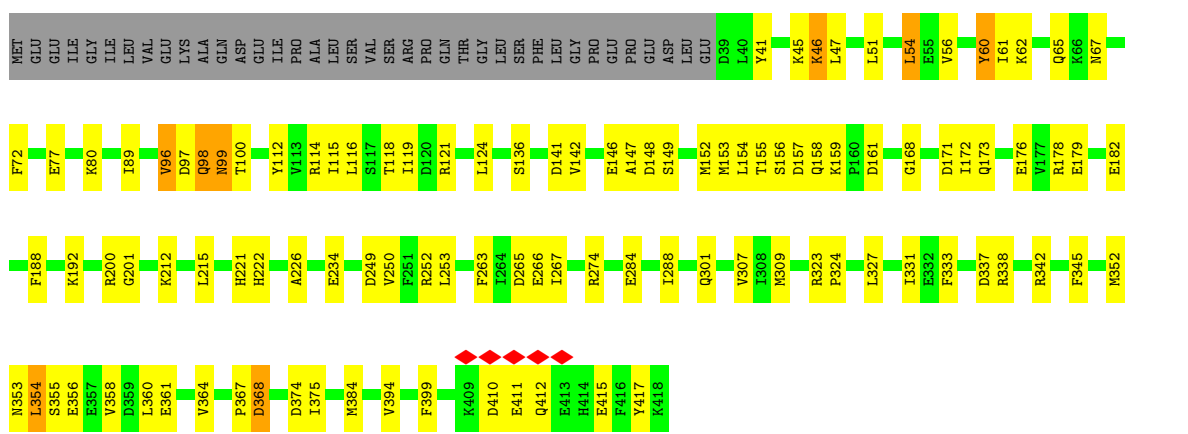




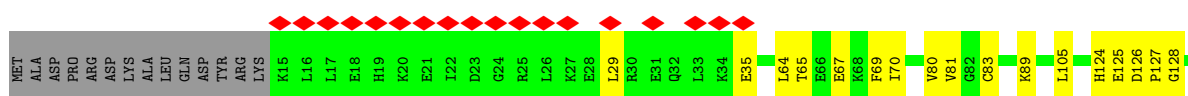
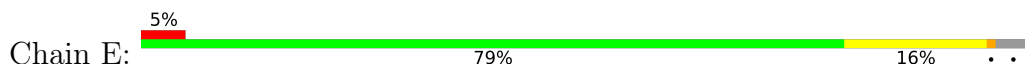
• Molecule 3: 26S protease regulatory subunit 8



• Molecule 4: 26S protease regulatory subunit 6B

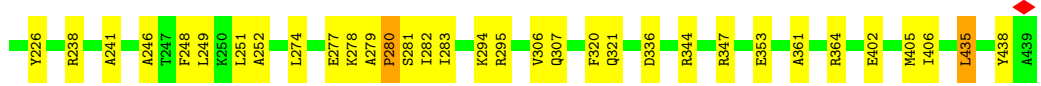
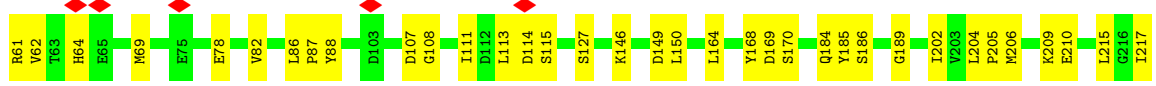
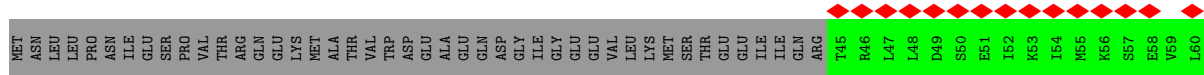
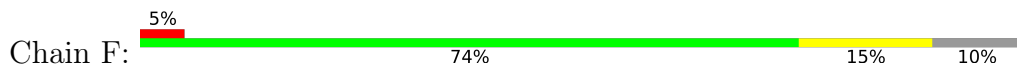


• Molecule 5: 26S protease regulatory subunit 10B

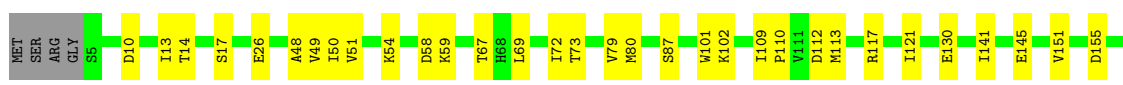
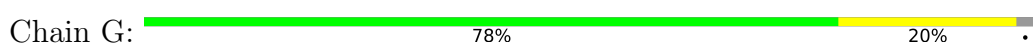




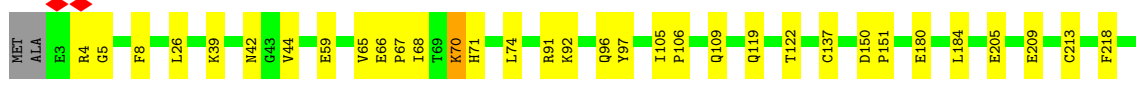
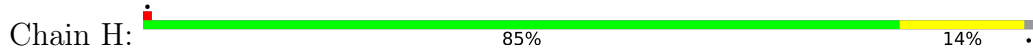
• Molecule 6: 26S protease regulatory subunit 6A



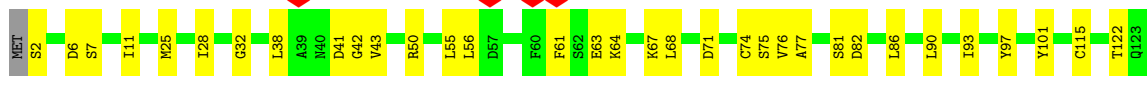
• Molecule 7: Proteasome subunit alpha type-6

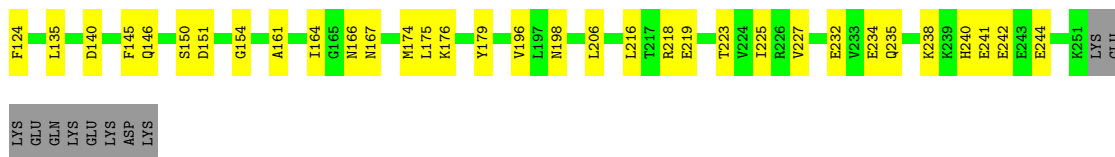


• Molecule 8: Proteasome subunit alpha type-2

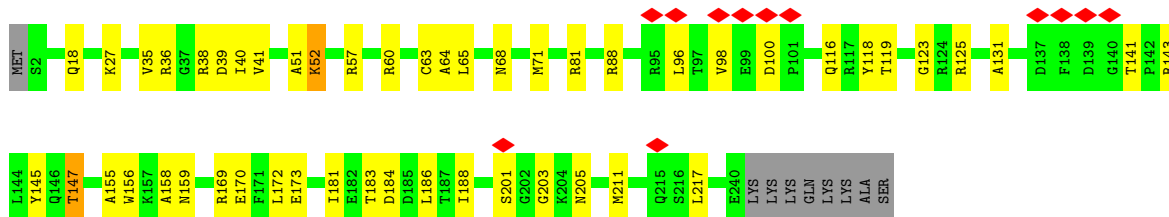
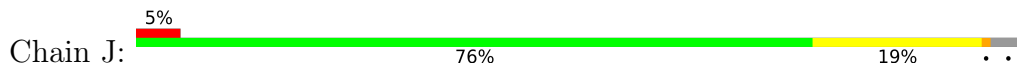


• Molecule 9: Proteasome subunit alpha type-4

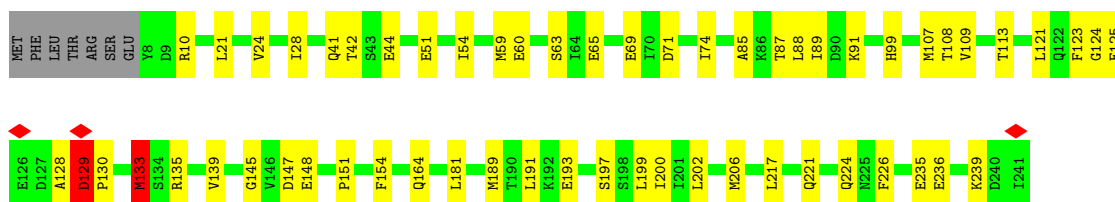




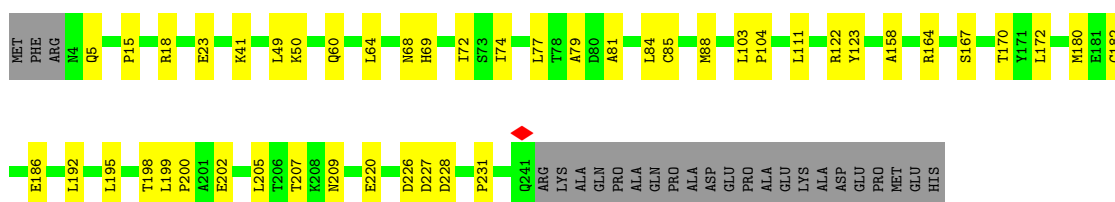
• Molecule 10: Proteasome subunit alpha type-7



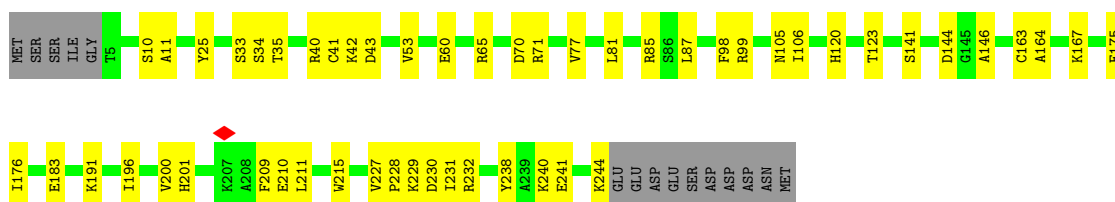
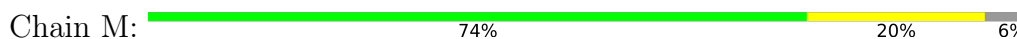
• Molecule 11: Proteasome subunit alpha type-5



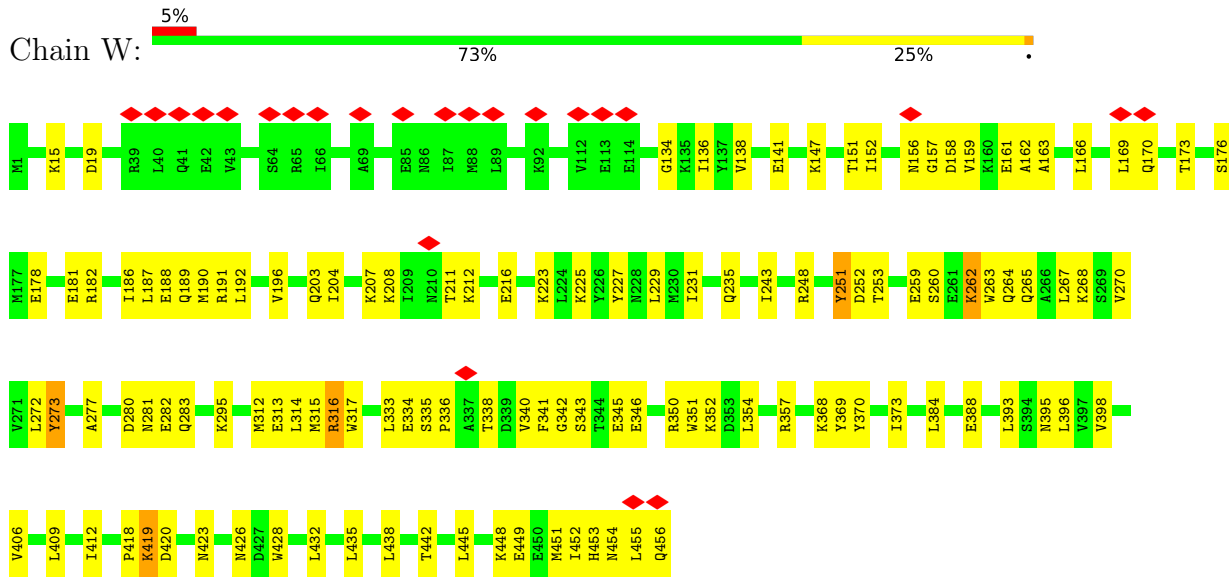
• Molecule 12: Proteasome subunit alpha type-1



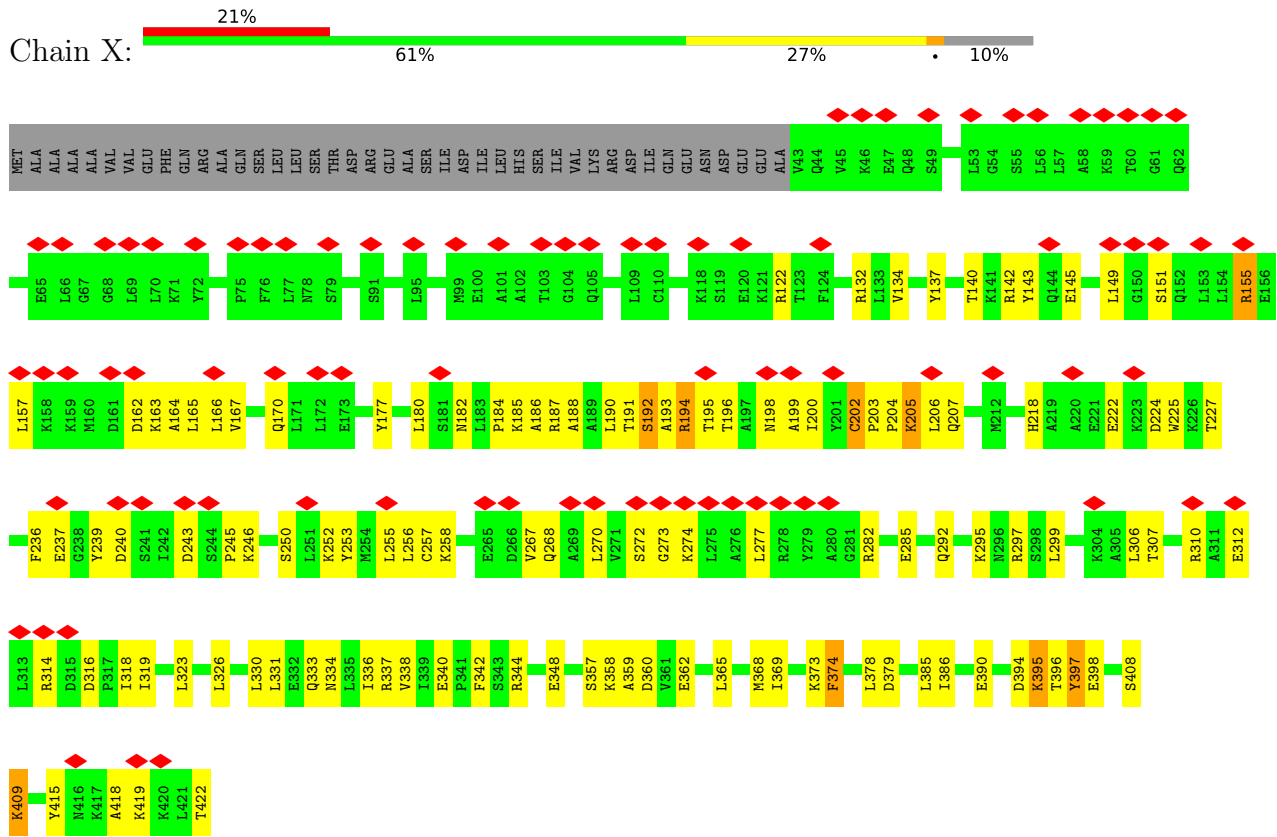
• Molecule 13: Proteasome subunit alpha type-3



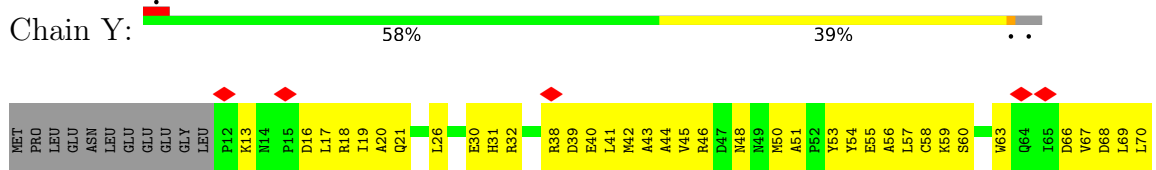
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 1

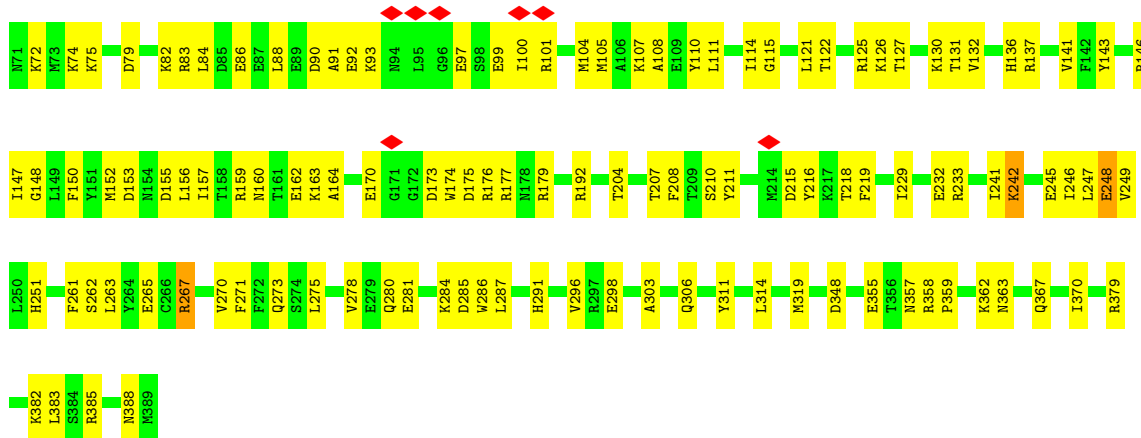


• Molecule 17: 26S proteasome non-ATPase regulatory subunit 11

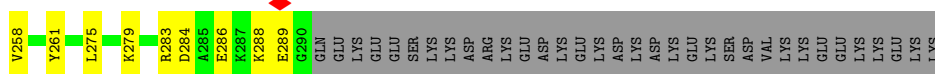
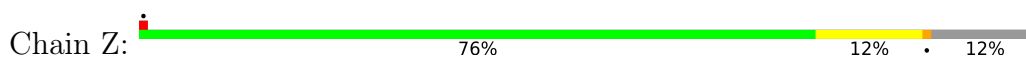


• Molecule 18: 26S proteasome non-ATPase regulatory subunit 6

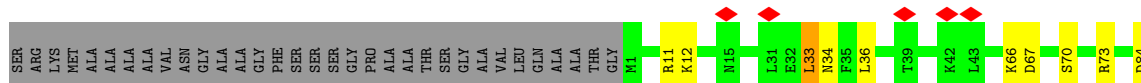
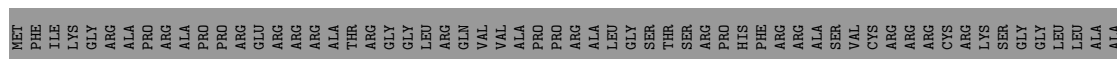




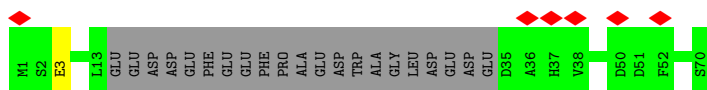
- Molecule 19: 26S proteasome non-ATPase regulatory subunit 7



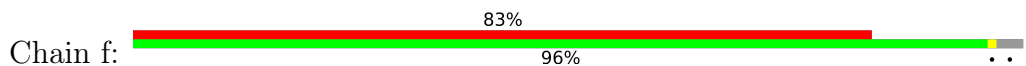
- Molecule 20: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 21: 26S proteasome complex subunit DSS1



- Molecule 22: 26S proteasome non-ATPase regulatory subunit 2



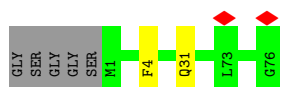
• Molecule 26: Polyubiquitin-B

Chain x:  14% 93% 6%



• Molecule 26: Polyubiquitin-B

Chain w:  91% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	50.794	Depositor
Minimum map value	-23.427	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	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: MG, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/3148	0.66	0/4250
2	B	0.49	0/3047	0.63	0/4111
3	C	0.42	0/2905	0.62	0/3910
4	D	0.52	0/3089	0.61	0/4168
5	E	0.57	0/3025	0.69	0/4073
6	F	0.56	0/3134	0.65	0/4225
7	G	0.46	0/1859	0.56	0/2523
8	H	0.43	0/1743	0.53	0/2372
9	I	0.38	0/1942	0.55	0/2628
10	J	0.42	0/1737	0.57	0/2369
11	K	0.41	0/1786	0.56	0/2419
12	L	0.46	0/1885	0.59	0/2552
13	M	0.47	0/1891	0.56	0/2552
14	U	0.51	0/6476	0.62	0/8764
15	V	0.42	0/3360	0.60	0/4587
16	W	0.40	0/3332	0.56	0/4514
17	X	0.35	0/2831	0.53	0/3835
18	Y	0.46	0/3173	0.59	0/4273
19	Z	0.63	0/2324	0.64	0/3150
20	d	0.39	0/2096	0.59	0/2835
21	e	0.29	0/279	0.59	0/379
22	f	0.24	0/4336	0.45	0/6030
23	a	0.39	0/3053	0.58	0/4133
24	b	0.48	0/1478	0.67	0/2001
25	c	0.61	0/2302	0.65	0/3110
26	u	0.51	0/609	0.62	0/819
26	v	0.28	0/609	0.53	0/819
26	w	0.38	0/609	0.64	0/819
26	x	0.29	0/609	0.56	0/819
All	All	0.47	0/68667	0.60	0/93039

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	3138	78	0
2	B	3004	0	3063	93	0
3	C	2868	0	2964	81	0
4	D	3039	0	3075	80	0
5	E	2979	0	3052	45	0
6	F	3093	0	3165	44	0
7	G	1826	0	1796	35	0
8	H	1708	0	1594	23	0
9	I	1912	0	1851	50	0
10	J	1713	0	1537	39	0
11	K	1759	0	1707	41	0
12	L	1850	0	1822	31	0
13	M	1856	0	1814	34	0
14	U	6361	0	6397	83	0
15	V	3315	0	2757	82	0
16	W	3292	0	2975	100	0
17	X	2793	0	2662	83	0
18	Y	3115	0	3120	129	0
19	Z	2281	0	2312	38	0
20	d	2053	0	2029	0	0
21	e	280	0	190	0	0
22	f	4338	0	2026	0	0
23	a	2995	0	3012	0	0
24	b	1458	0	1505	0	0
25	c	2260	0	2276	0	0
26	u	603	0	629	0	0
26	v	603	0	629	0	0
26	w	603	0	629	0	0
26	x	603	0	629	0	0
27	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	31	0	12	0	0
27	D	31	0	12	1	0
27	E	31	0	12	2	0
28	A	1	0	0	0	0
28	B	1	0	0	0	0
28	D	1	0	0	0	0
28	E	1	0	0	0	0
28	F	1	0	0	0	0
29	C	27	0	12	3	0
29	F	27	0	12	1	0
All	All	67839	0	64427	1097	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1097 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:TYR:HB2	14:U:603:LEU:HD21	1.51	0.93
9:I:42:GLY:HA2	9:I:216:LEU:O	1.70	0.92
7:G:50:ILE:HG21	7:G:79:VAL:HG21	1.50	0.91
15:V:270:LEU:HD12	15:V:271:VAL:HG13	1.54	0.88
6:F:111:ILE:HG22	6:F:113:LEU:H	1.37	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/433 (90%)	337 (86%)	51 (13%)	4 (1%)	13	44
2	B	382/440 (87%)	337 (88%)	42 (11%)	3 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	361/406 (89%)	328 (91%)	32 (9%)	1 (0%)	37	69
4	D	378/418 (90%)	335 (89%)	41 (11%)	2 (0%)	25	58
5	E	373/389 (96%)	342 (92%)	31 (8%)	0	100	100
6	F	393/439 (90%)	358 (91%)	32 (8%)	3 (1%)	16	49
7	G	238/246 (97%)	224 (94%)	14 (6%)	0	100	100
8	H	230/234 (98%)	216 (94%)	14 (6%)	0	100	100
9	I	248/261 (95%)	227 (92%)	21 (8%)	0	100	100
10	J	237/248 (96%)	217 (92%)	19 (8%)	1 (0%)	30	63
11	K	232/241 (96%)	210 (90%)	19 (8%)	3 (1%)	10	39
12	L	236/263 (90%)	214 (91%)	22 (9%)	0	100	100
13	M	238/255 (93%)	219 (92%)	19 (8%)	0	100	100
14	U	809/953 (85%)	750 (93%)	59 (7%)	0	100	100
15	V	489/534 (92%)	423 (86%)	65 (13%)	1 (0%)	44	74
16	W	454/456 (100%)	412 (91%)	40 (9%)	2 (0%)	30	63
17	X	378/422 (90%)	342 (90%)	33 (9%)	3 (1%)	16	49
18	Y	376/389 (97%)	337 (90%)	39 (10%)	0	100	100
19	Z	284/324 (88%)	260 (92%)	24 (8%)	0	100	100
20	d	255/350 (73%)	208 (82%)	46 (18%)	1 (0%)	30	63
21	e	45/70 (64%)	32 (71%)	13 (29%)	0	100	100
22	f	876/908 (96%)	727 (83%)	141 (16%)	8 (1%)	14	45
23	a	371/376 (99%)	343 (92%)	27 (7%)	1 (0%)	37	69
24	b	189/377 (50%)	164 (87%)	24 (13%)	1 (0%)	25	58
25	c	285/310 (92%)	256 (90%)	29 (10%)	0	100	100
26	u	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
26	v	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
26	w	74/81 (91%)	70 (95%)	4 (5%)	0	100	100
26	x	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
All	All	9045/10066 (90%)	8105 (90%)	906 (10%)	34 (0%)	32	63

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	128	ALA

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Mol	Chain	Res	Type
15	V	344	ASP
20	d	33	LEU
22	f	344	VAL
22	f	353	LEU

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	337/372 (91%)	330 (98%)	7 (2%)	48	66
2	B	334/385 (87%)	323 (97%)	11 (3%)	33	56
3	C	311/352 (88%)	296 (95%)	15 (5%)	21	46
4	D	333/366 (91%)	318 (96%)	15 (4%)	23	47
5	E	329/341 (96%)	321 (98%)	8 (2%)	44	62
6	F	339/379 (89%)	331 (98%)	8 (2%)	44	62
7	G	193/210 (92%)	193 (100%)	0	100	100
8	H	164/191 (86%)	162 (99%)	2 (1%)	67	77
9	I	193/221 (87%)	192 (100%)	1 (0%)	86	90
10	J	154/211 (73%)	148 (96%)	6 (4%)	27	51
11	K	189/203 (93%)	185 (98%)	4 (2%)	48	66
12	L	198/224 (88%)	195 (98%)	3 (2%)	60	74
13	M	192/212 (91%)	191 (100%)	1 (0%)	86	90
14	U	695/816 (85%)	677 (97%)	18 (3%)	41	61
15	V	236/460 (51%)	231 (98%)	5 (2%)	48	66
16	W	291/416 (70%)	280 (96%)	11 (4%)	28	52
17	X	262/362 (72%)	244 (93%)	18 (7%)	13	37
18	Y	334/344 (97%)	326 (98%)	8 (2%)	44	62
19	Z	257/295 (87%)	253 (98%)	4 (2%)	58	73
20	d	212/294 (72%)	198 (93%)	14 (7%)	14	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	e	12/63 (19%)	11 (92%)	1 (8%)	9	32
23	a	333/336 (99%)	323 (97%)	10 (3%)	36	58
24	b	167/312 (54%)	164 (98%)	3 (2%)	54	71
25	c	252/268 (94%)	244 (97%)	8 (3%)	34	56
26	u	68/70 (97%)	67 (98%)	1 (2%)	60	74
26	v	68/70 (97%)	68 (100%)	0	100	100
26	w	68/70 (97%)	66 (97%)	2 (3%)	37	58
26	x	68/70 (97%)	67 (98%)	1 (2%)	60	74
All	All	6589/7913 (83%)	6404 (97%)	185 (3%)	40	59

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	X	155	ARG
19	Z	257	MET
17	X	192	SER
17	X	398	GLU
20	d	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
15	V	266	GLN
15	V	299	GLN
26	w	41	GLN
20	d	252	GLN
24	b	12	ASN

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 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
27	ATP	D	501	28	26,33,33	0.80	0	31,52,52	0.92	2 (6%)
27	ATP	A	501	28	26,33,33	0.80	0	31,52,52	0.93	2 (6%)
29	ADP	C	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.63	4 (13%)
29	ADP	F	501	28	24,29,29	1.09	1 (4%)	29,45,45	1.63	5 (17%)
27	ATP	B	501	28	26,33,33	0.74	0	31,52,52	0.90	2 (6%)
27	ATP	E	401	28	26,33,33	0.82	1 (3%)	31,52,52	0.94	2 (6%)

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
27	ATP	D	501	28	-	3/18/38/38	0/3/3/3
27	ATP	A	501	28	-	5/18/38/38	0/3/3/3
29	ADP	C	501	-	-	2/12/32/32	0/3/3/3
29	ADP	F	501	28	-	4/12/32/32	0/3/3/3
27	ATP	B	501	28	-	3/18/38/38	0/3/3/3
27	ATP	E	401	28	-	7/18/38/38	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	C2'-C1'	-2.45	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	501	ADP	C5-C4	2.24	1.46	1.40
27	E	401	ATP	C8-N7	-2.04	1.31	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	501	ADP	PA-O3A-PB	-4.77	116.44	132.83
29	C	501	ADP	PA-O3A-PB	-4.57	117.16	132.83
29	C	501	ADP	C3'-C2'-C1'	3.97	106.95	100.98
29	F	501	ADP	N3-C2-N1	-3.20	123.67	128.68
29	C	501	ADP	C4-C5-N7	-3.04	106.23	109.40

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	501	ATP	C5'-O5'-PA-O1A
27	E	401	ATP	PB-O3B-PG-O2G
27	E	401	ATP	C5'-O5'-PA-O1A
27	E	401	ATP	C5'-O5'-PA-O2A
27	E	401	ATP	O4'-C4'-C5'-O5'

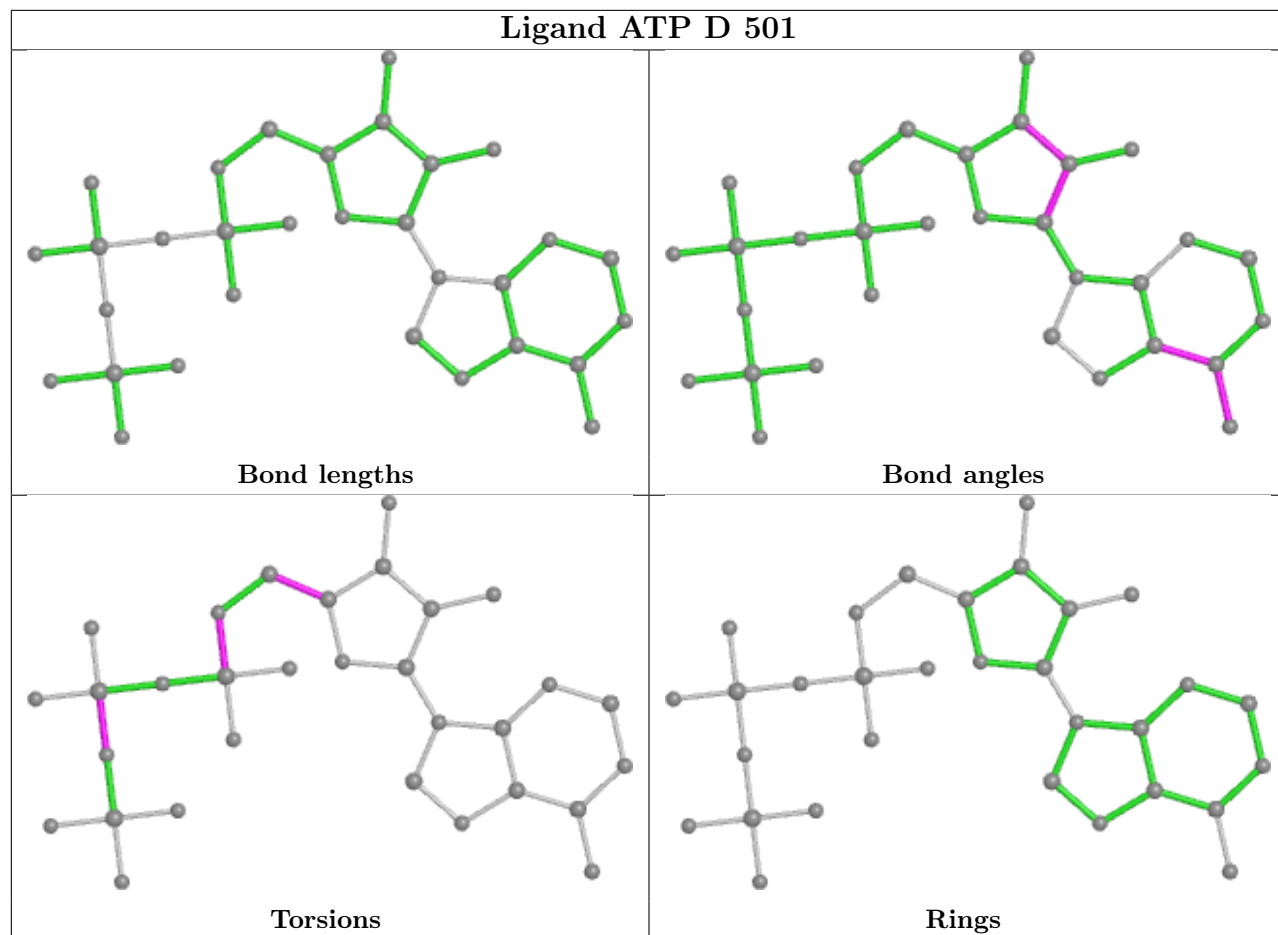
There are no ring outliers.

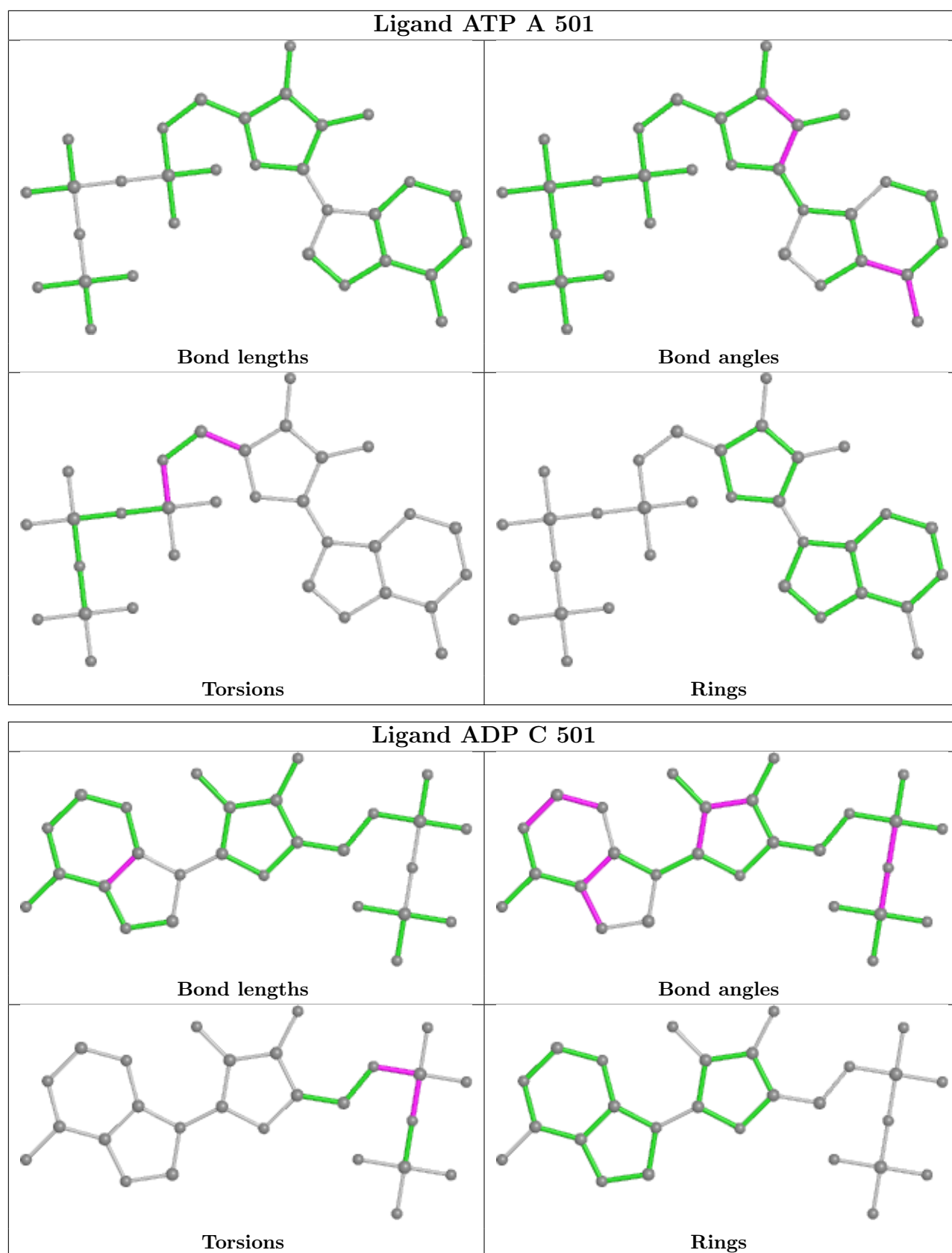
4 monomers are involved in 7 short contacts:

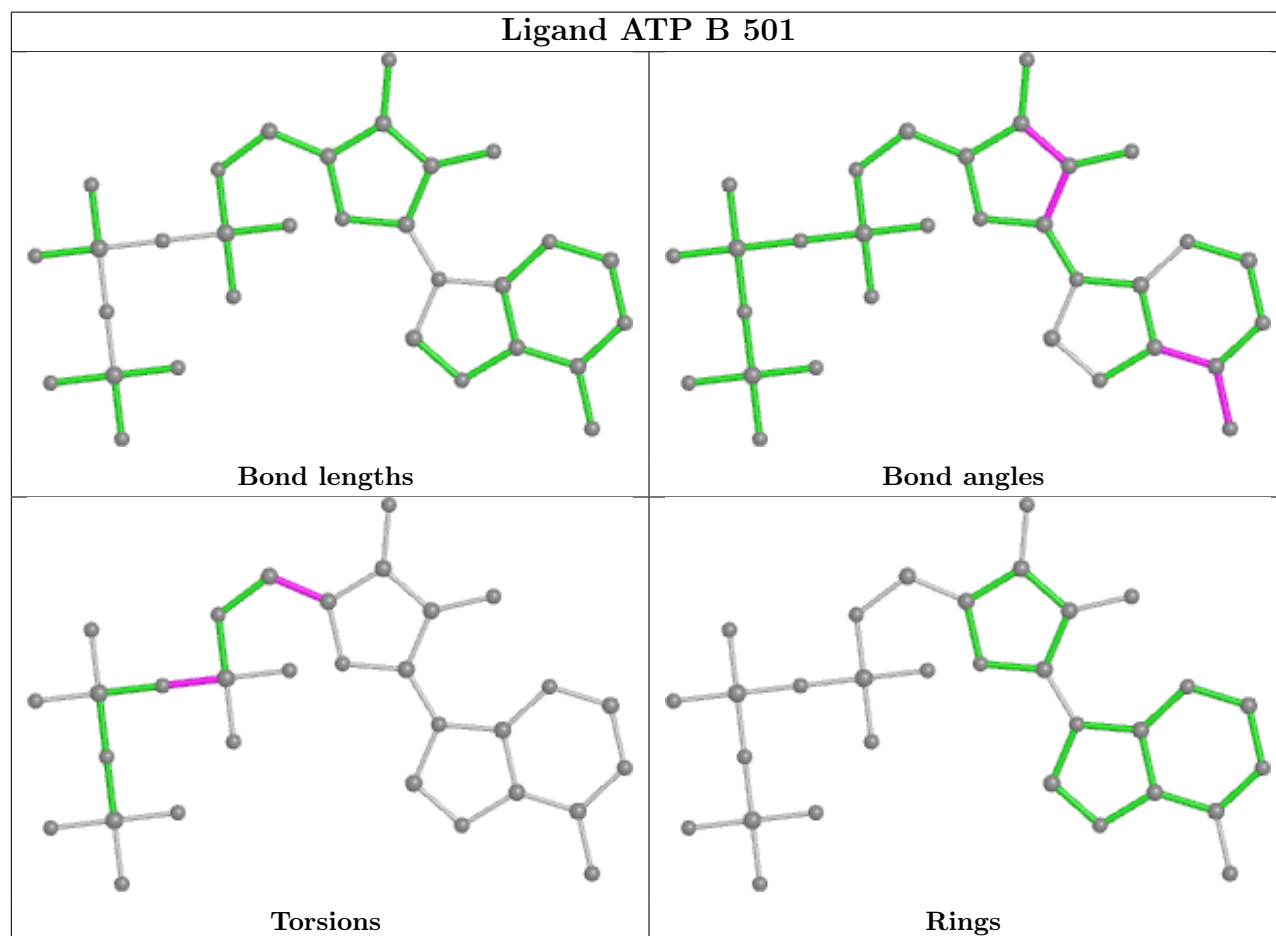
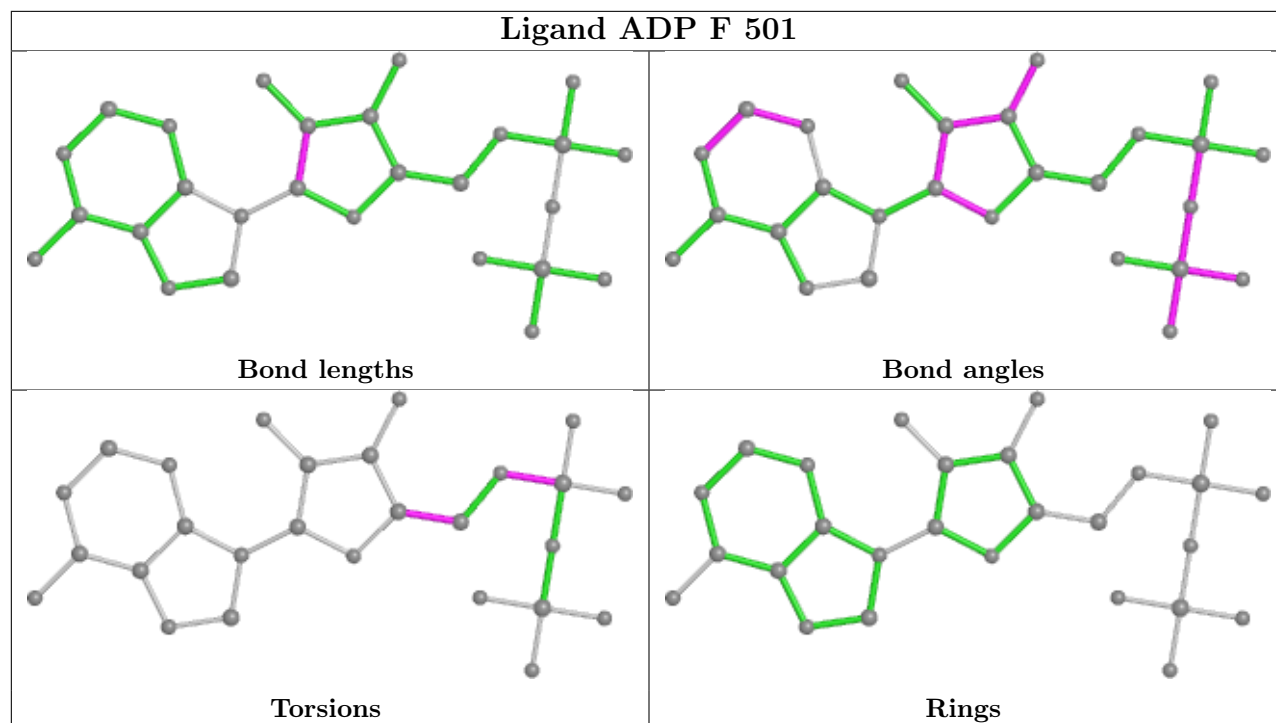
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	501	ATP	1	0
29	C	501	ADP	3	0
29	F	501	ADP	1	0
27	E	401	ATP	2	0

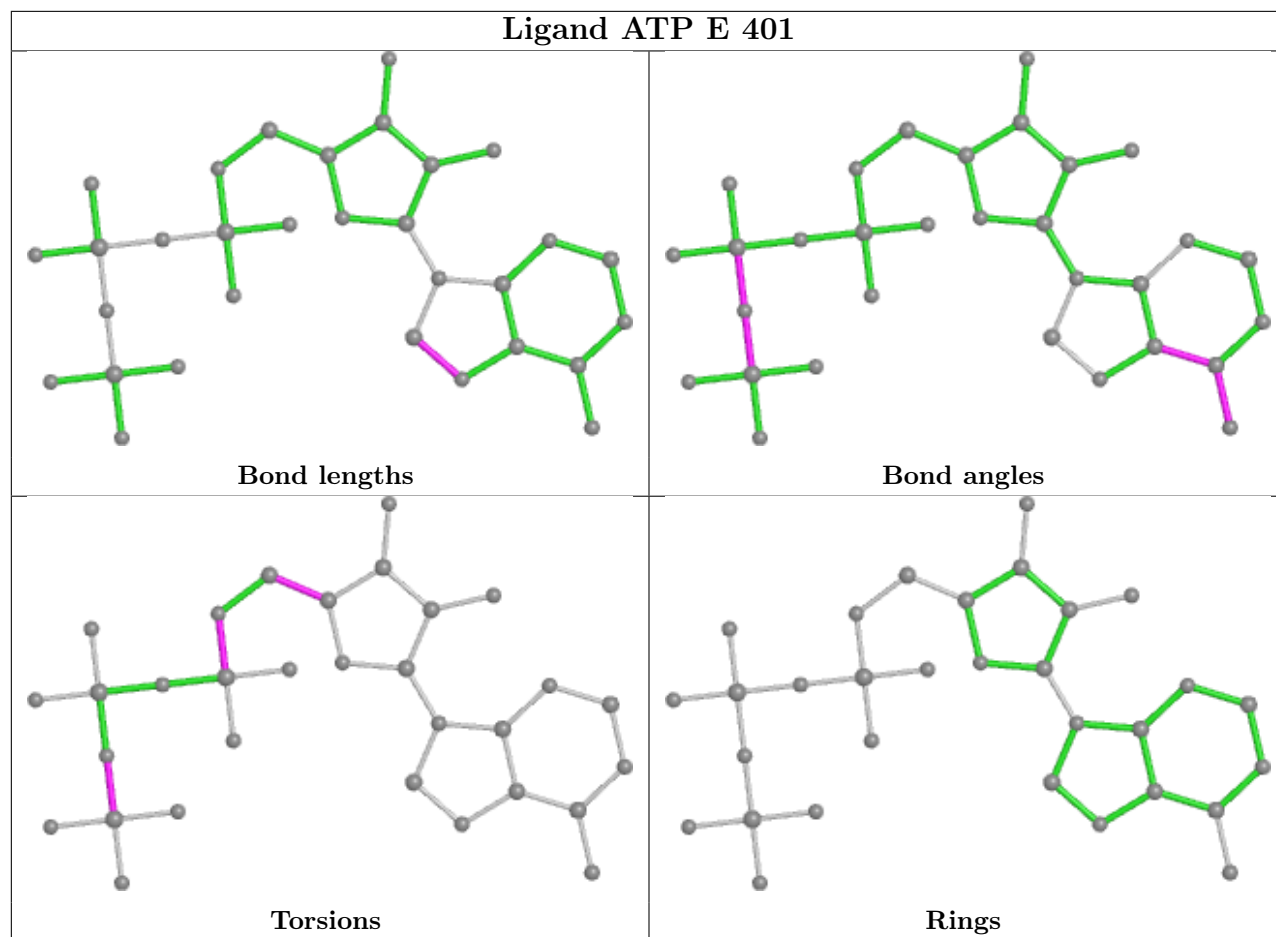
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

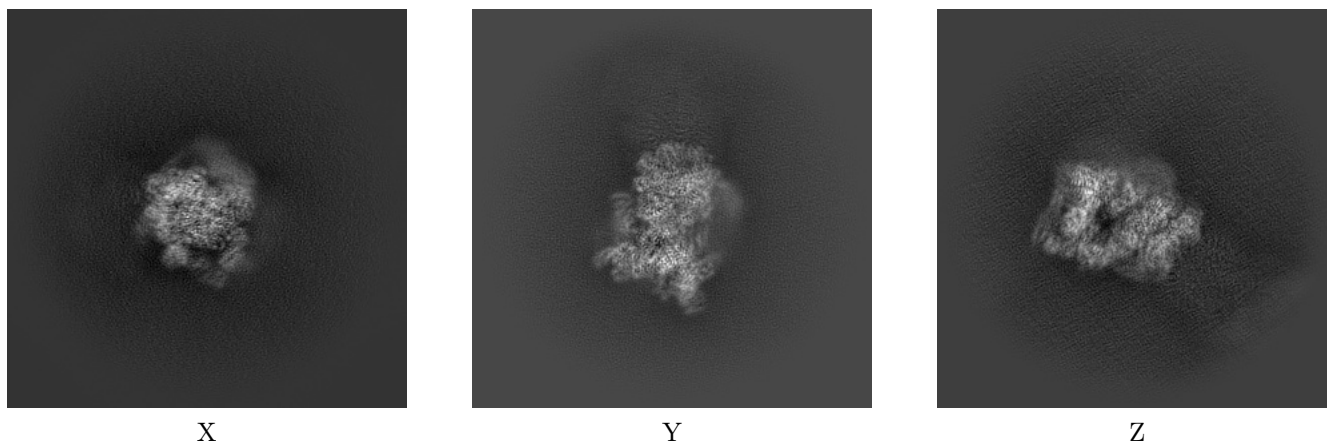
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36645. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

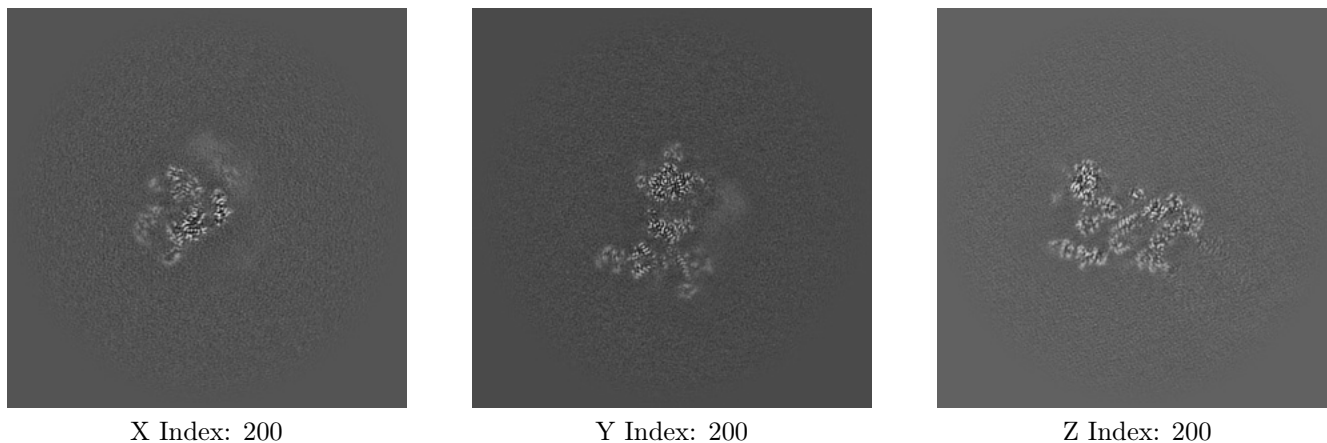
6.1.1 Primary map



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

6.2 Central slices [i](#)

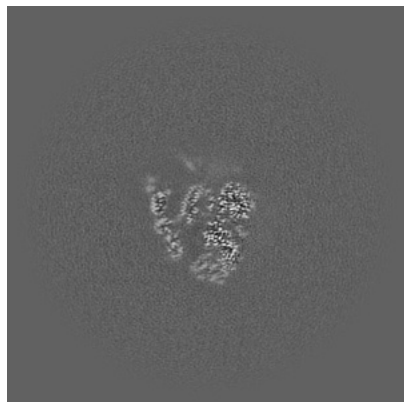
6.2.1 Primary map



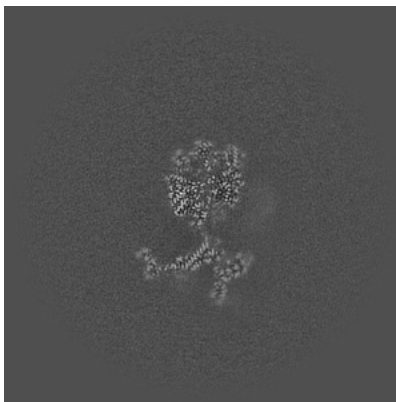
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

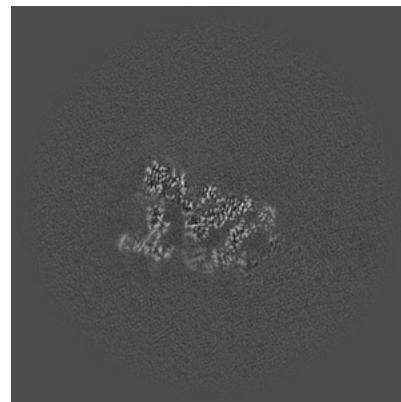
6.3.1 Primary map



X Index: 153



Y Index: 188

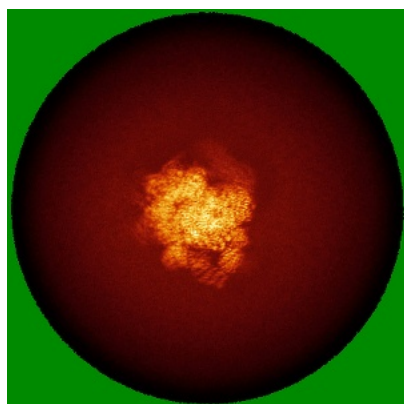


Z Index: 191

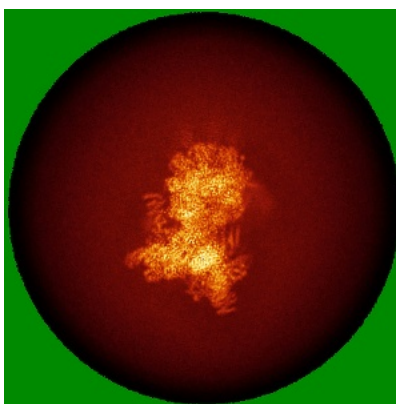
The images above show the largest variance slices of the map in three orthogonal directions.

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

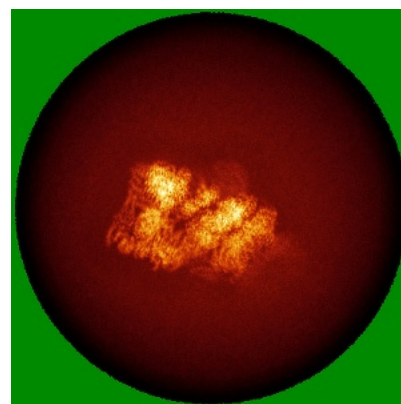
6.4.1 Primary map



X



Y

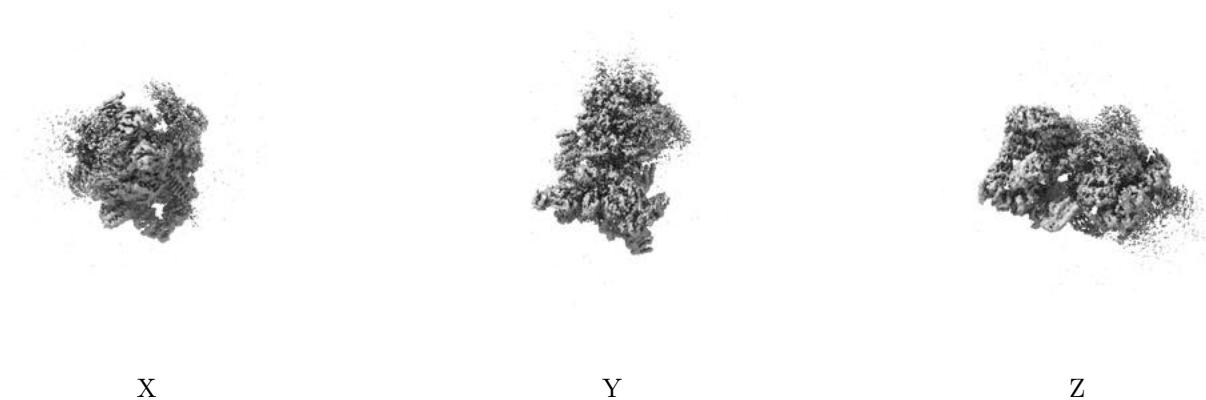


Z

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



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

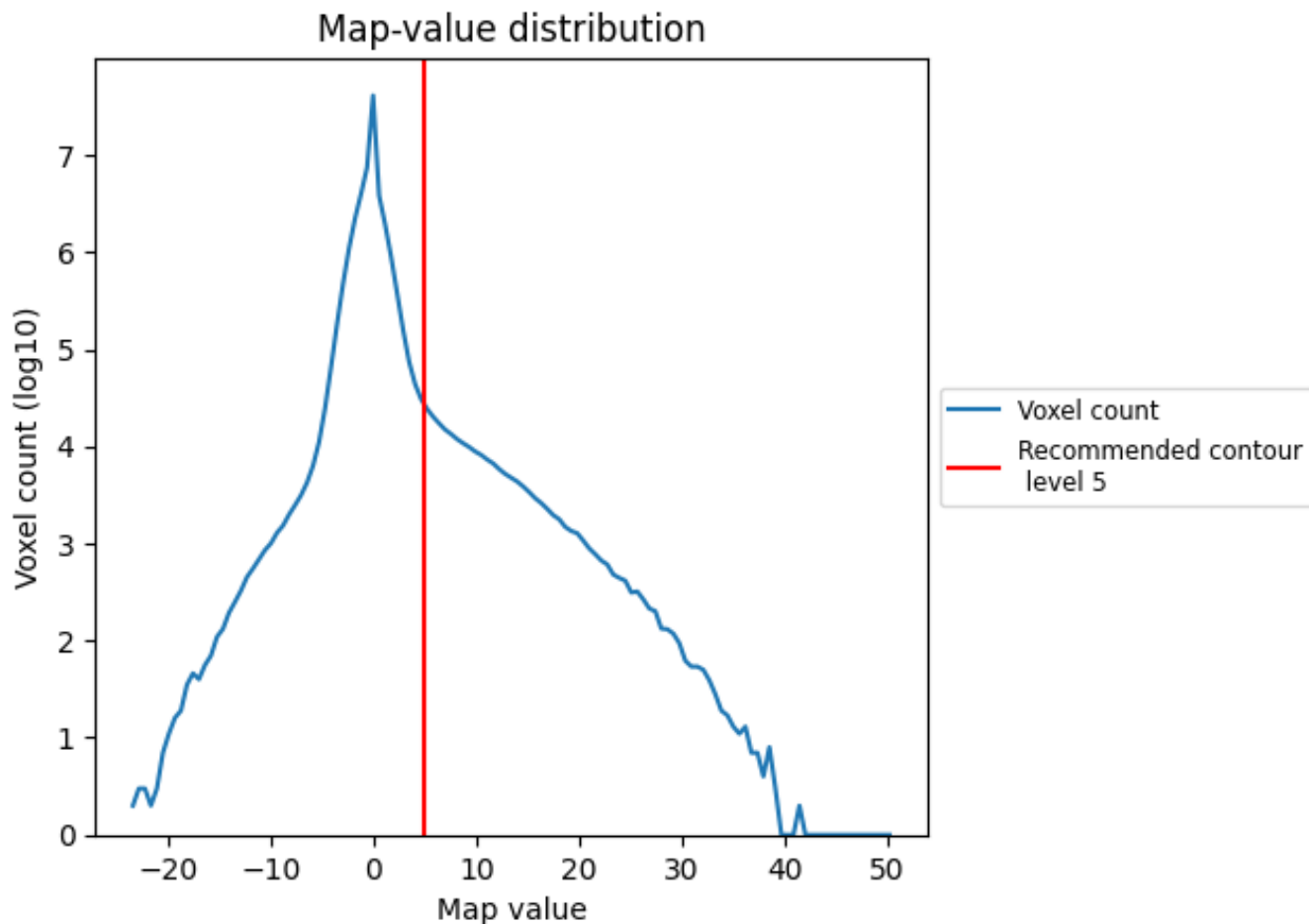
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

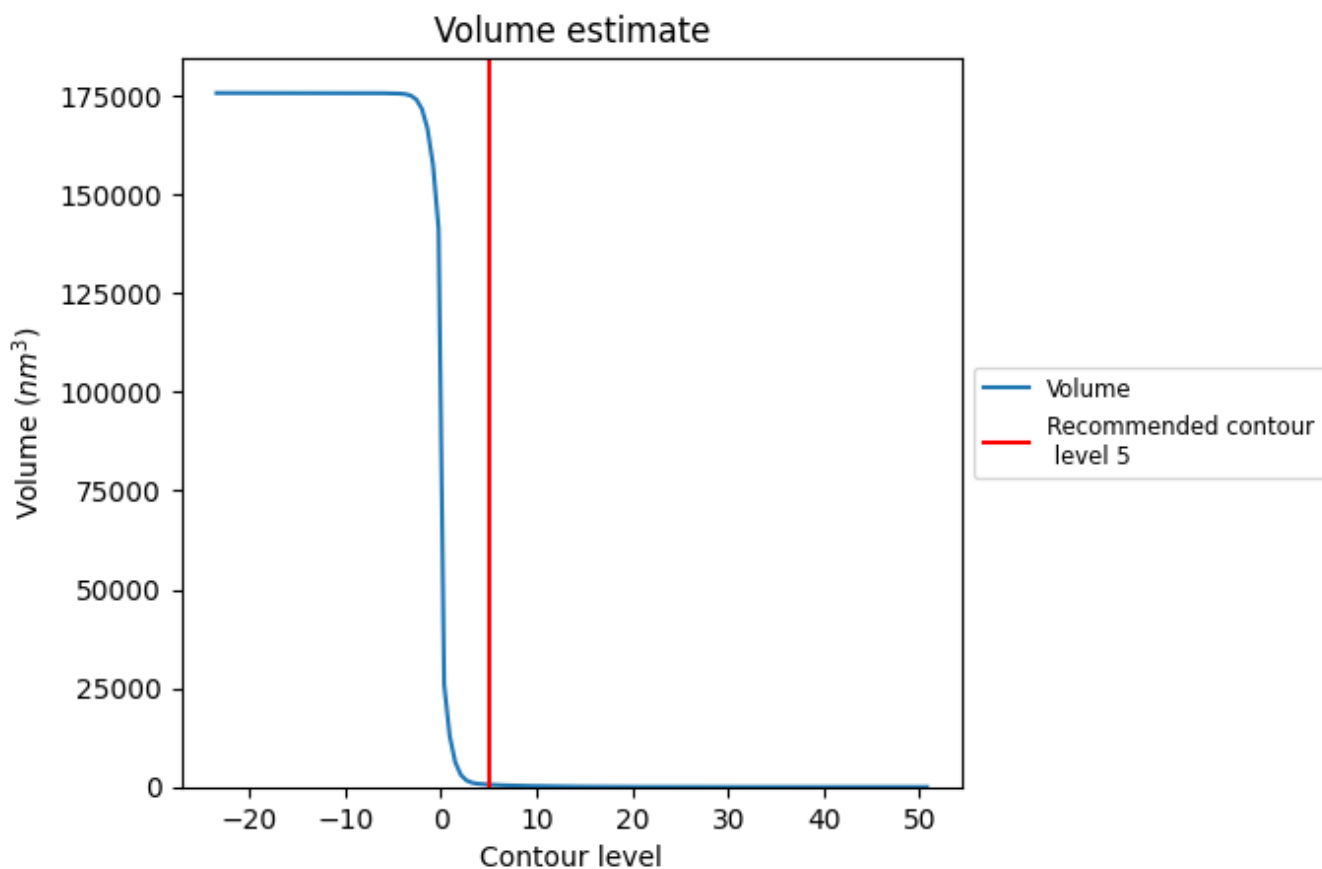
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

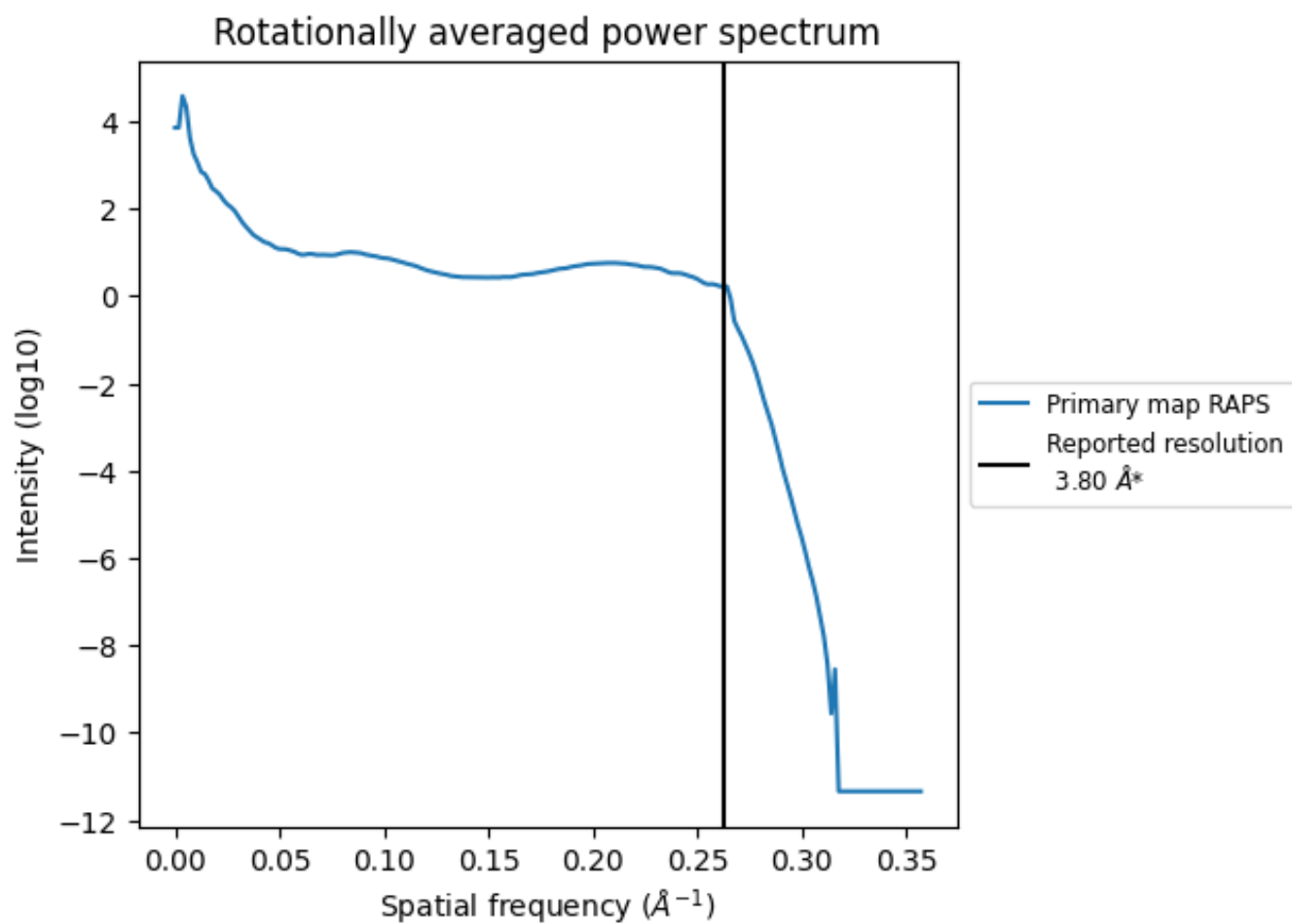
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 587 nm^3 ; this corresponds to an approximate mass of 530 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

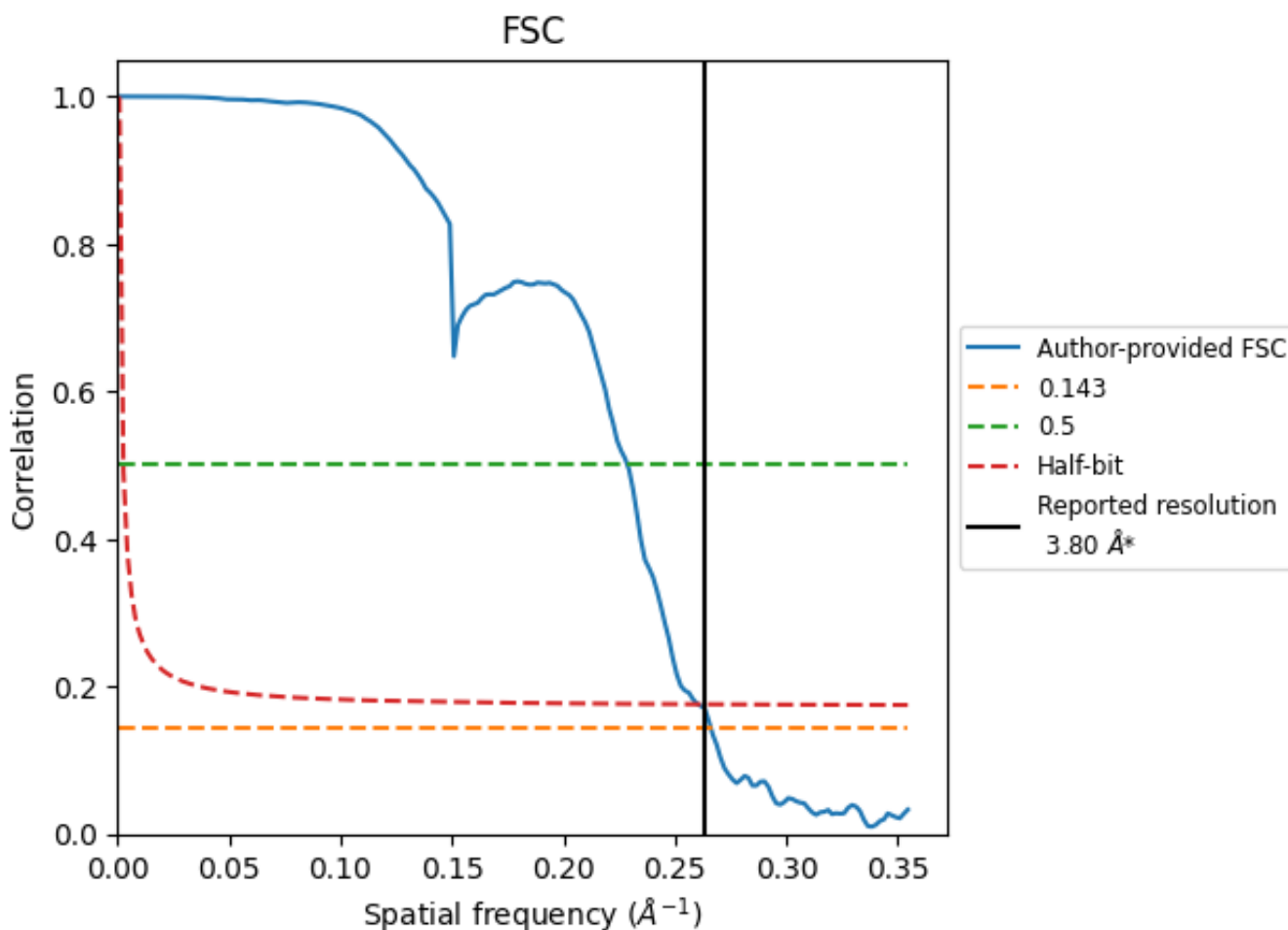


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

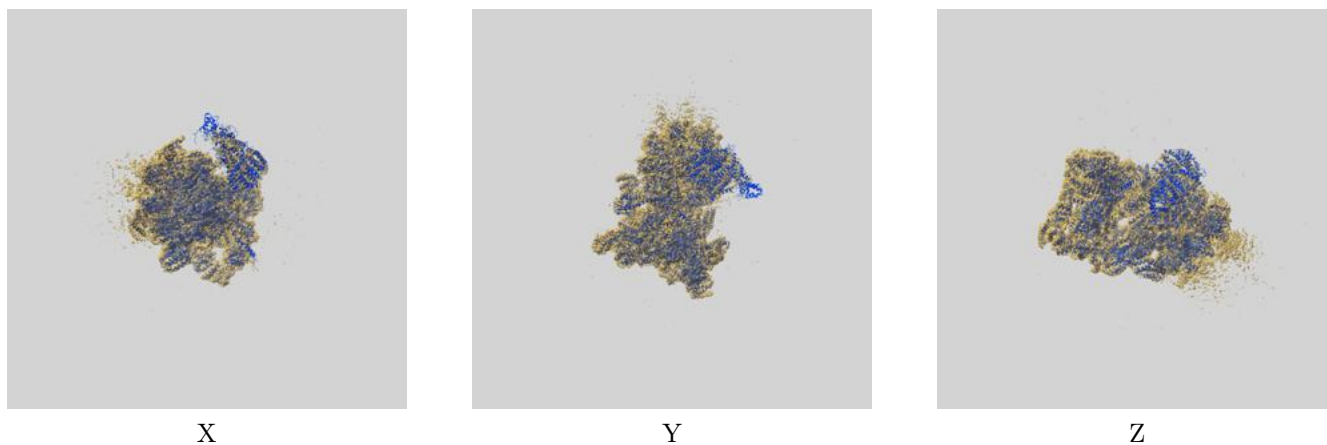
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.37	3.84
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

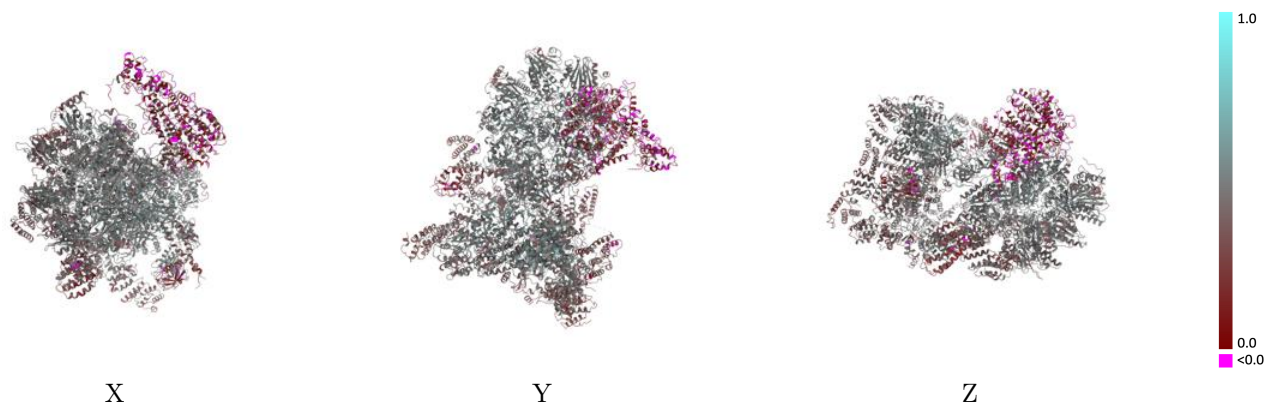
This section contains information regarding the fit between EMDB map EMD-36645 and PDB model 8JTI. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



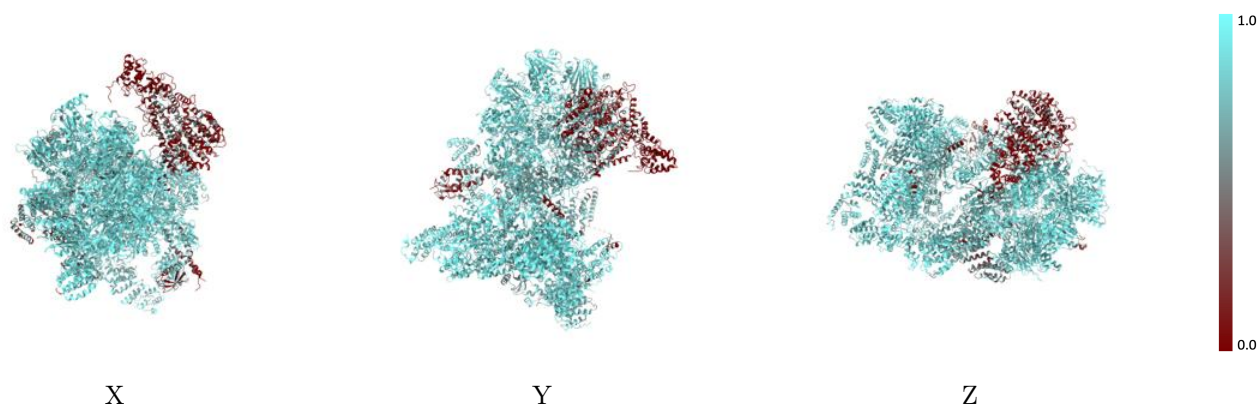
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



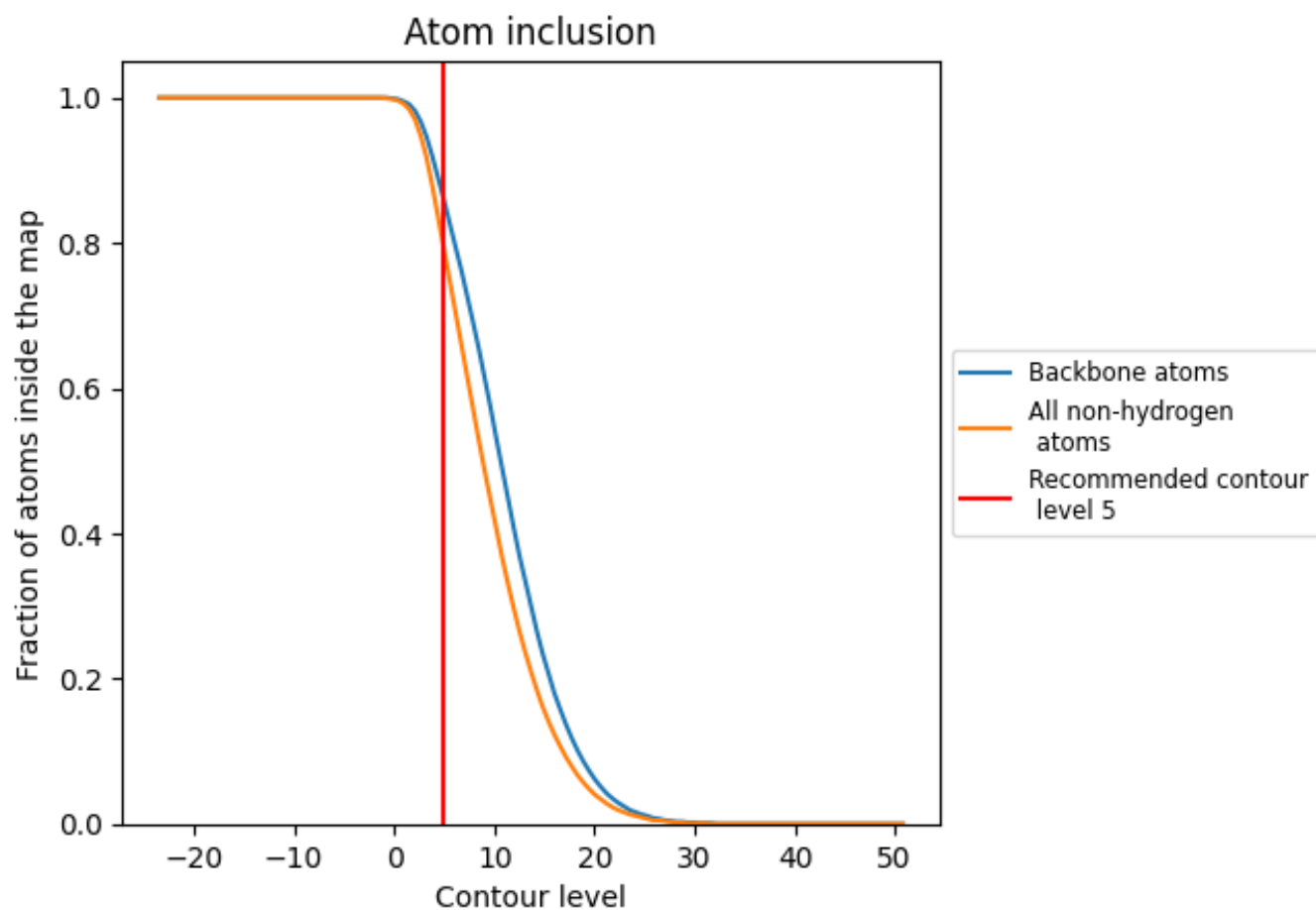
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.4230
A	 0.8510	 0.4690
B	 0.7980	 0.4490
C	 0.7880	 0.4450
D	 0.8520	 0.4740
E	 0.8650	 0.4910
F	 0.8530	 0.4870
G	 0.8750	 0.4800
H	 0.8750	 0.4650
I	 0.8260	 0.4350
J	 0.8450	 0.4500
K	 0.8570	 0.4740
L	 0.8850	 0.4830
M	 0.8750	 0.4640
U	 0.8730	 0.4550
V	 0.8310	 0.3900
W	 0.8360	 0.3810
X	 0.6250	 0.3710
Y	 0.8330	 0.3710
Z	 0.8730	 0.4800
a	 0.8450	 0.4070
b	 0.8980	 0.4580
c	 0.8920	 0.5020
d	 0.8040	 0.3550
e	 0.7860	 0.3390
f	 0.1810	 0.1890
u	 0.9340	 0.4690
v	 0.2430	 0.2040
w	 0.8290	 0.4200
x	 0.5880	 0.3900

