Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 07:22 AM JST

PDB ID	:	7W39
EMDB ID	:	EMD-32274
Title	:	Structure of USP14-bound human 26S proteasome in state EA2.1_UBL
Authors	:	Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on	:	2021-11-25
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

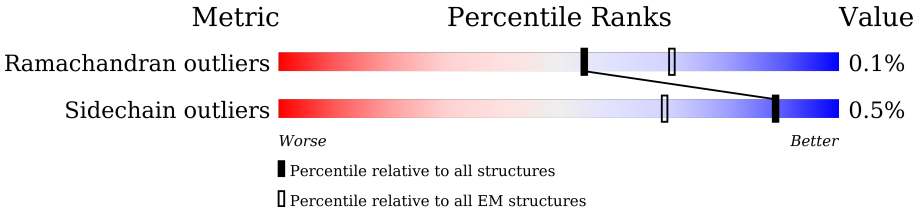
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	154571	4023
Sidechain outliers	154315	3826

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	87% · 13%
3	C	398	89% · 9%
4	D	418	91% 9%
5	E	403	6% 95% · ·
6	F	439	7% 94% 5%
7	G	246	99% ·
7	g	246	99% ·
8	H	234	99% ·

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Mol	Chain	Length	Quality of chain
8	h	234	99%
9	I	261	95%
9	i	261	96%
10	J	248	96%
10	j	248	96%
11	K	241	97%
11	k	241	97%
12	L	269	88% 12%
12	l	269	88% 12%
13	M	255	94% 6%
13	m	255	94% 6%
14	N	239	85% 15%
14	n	239	85% 15%
15	O	277	79% 21%
15	o	277	79% 21%
16	P	205	100%
16	p	205	100%
17	Q	201	99%
17	q	201	99%
18	R	263	76% 24%
18	r	263	76% 24%
19	S	241	88% 12%
19	s	241	88% 12%
20	T	264	82% 18%
20	t	264	81% 18%

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Mol	Chain	Length	Quality of chain
21	U	953	85% 15%
22	V	534	83% 17%
23	W	456	97%
24	X	422	90% 10%
25	Y	389	96%
26	Z	324	86% 12%
27	a	376	98%
28	b	377	50% 49%
29	c	310	92% 7%
30	d	350	73% 27%
31	e	70	71% 29%
32	f	908	15% 97%
33	u	76	100%
34	v	10	90% 10%
35	x	494	15% 15% 85%

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 106442 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	3018	1901	515	587	15	0	0

- Molecule 3 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	363	2864	1808	515	525	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 proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	389	3097	1947	552	581	17	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	415	3251	2038	561	634	18	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	244	1889	1198	316	362	13	0	0
7	g	244	1880	1193	318	356	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	1805	1152	305	342	6	0	0
8	h	232	1805	1154	307	338	6	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	1958	1236	336	376	10	1	0
9	i	250	1955	1234	336	375	10	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	1880	1179	333	363	5	0	0
10	j	239	1861	1168	332	356	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	1777	1117	295	354	11	0	0
11	k	234	1782	1119	295	357	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	238	1866	1169	336	350	11	0	0
12	l	238	1861	1165	335	350	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	1876	1191	321	353	11	0	0
13	m	240	1881	1193	321	356	11	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	202	1514	949	258	295	12	0	0
14	n	202	1510	947	258	293	12	0	0

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	220	1649	1038	279	320	12	0	0
15	o	220	1659	1044	283	320	12	0	0

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	204	1587	1010	264	294	19	0	0
16	p	204	1591	1013	265	294	19	0	0

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	199	1588	1017	270	292	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	q	199	1588	1017	270	292	9	0	0

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	201	1559	982	274	294	9	0	0
18	r	201	1559	982	274	294	9	0	0

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	213	1641	1041	281	309	10	0	0
19	s	213	1654	1047	284	313	10	0	0

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	216	1683	1062	291	318	12	0	0
20	t	216	1687	1064	291	320	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	812	6334	4023	1078	1189	44	0	0

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	444	3612	2301	645	653	13	0	0

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	446	3635	2302	622	687	24	0	0

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	380	3009	1918	509	570	12	0	0

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	373	2995	1911	510	559	15	0	0

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	257	2116	1371	346	390	9	0	0

- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	e	50	425	260	65	100	0	0

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	889	6866	4315	1174	1331	46	0	0

- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	u	76	601	378	105	117	1	0	0

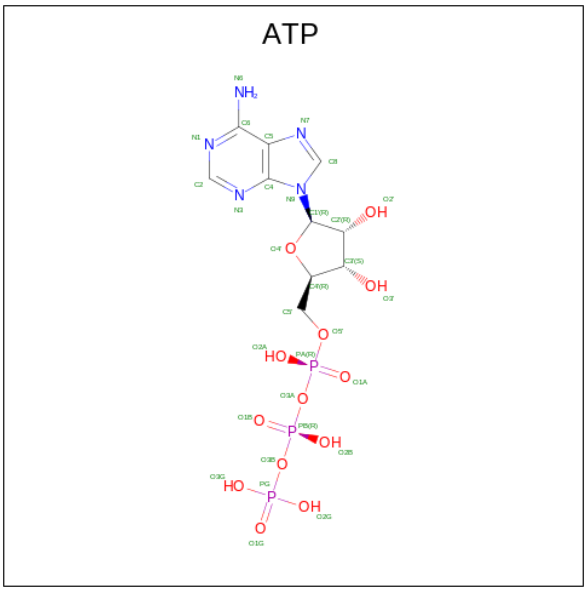
- Molecule 34 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	v	10	53	32	11	10	0	0

- Molecule 35 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	x	76	588	378	96	108	6	0	0

- Molecule 36 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).

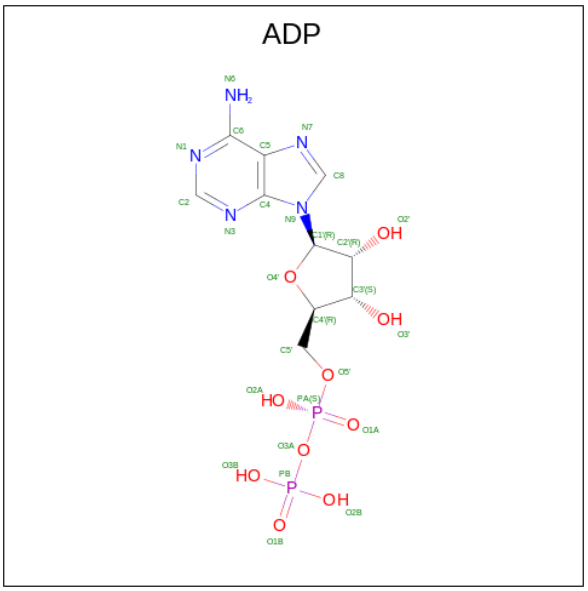


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 38 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
38	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
38	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	c	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

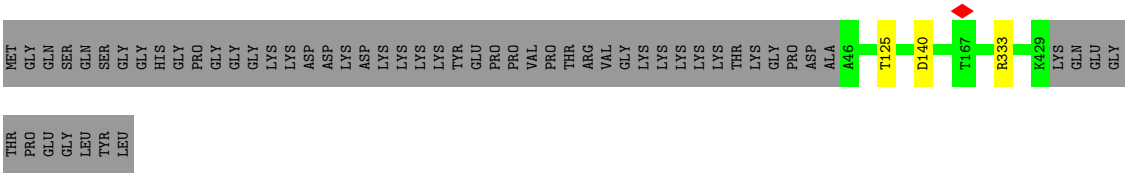
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

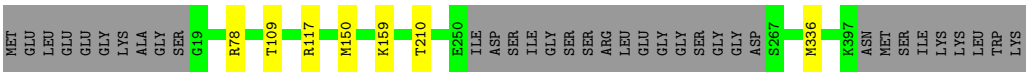
• Molecule 2: 26S protease regulatory subunit 4

Chain B:



• Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8

Chain C:

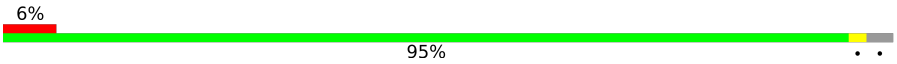


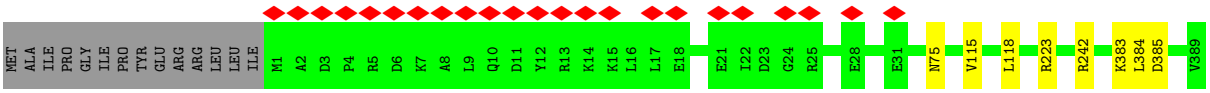
• Molecule 4: 26S protease regulatory subunit 6B

Chain D:

• Molecule 5: 26S proteasome regulatory subunit 10B

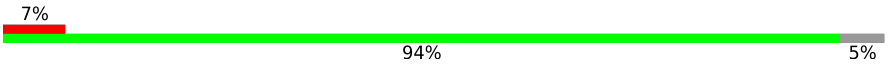
Chain E:

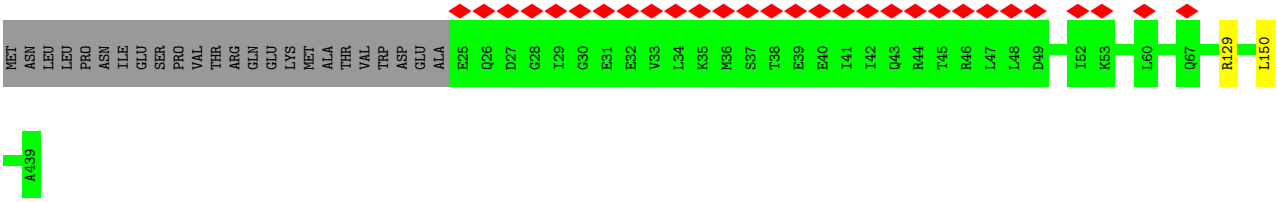




• Molecule 6: 26S protease regulatory subunit 6A

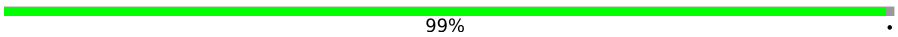
Chain F:





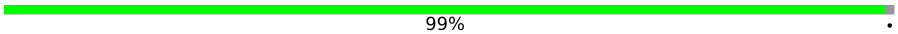
• Molecule 7: Proteasome subunit alpha type-6

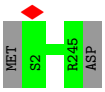
Chain G:



• Molecule 7: Proteasome subunit alpha type-6

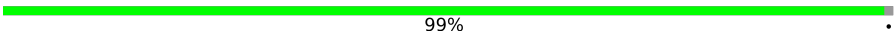
Chain g:

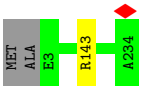




• Molecule 8: Proteasome subunit alpha type-2

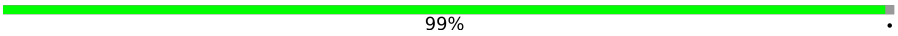
Chain H:

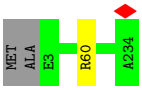




• Molecule 8: Proteasome subunit alpha type-2

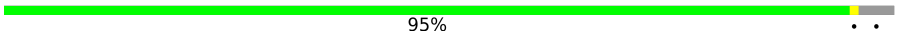
Chain h:

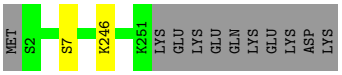




• Molecule 9: Proteasome subunit alpha type-4

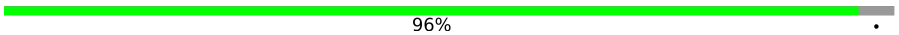
Chain I:





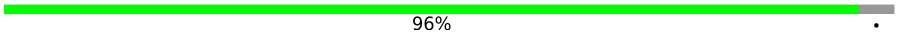
• Molecule 9: Proteasome subunit alpha type-4

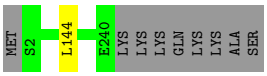
Chain i:



• Molecule 10: Proteasome subunit alpha type-7

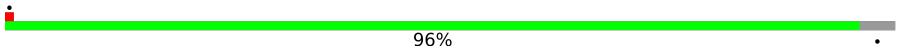
Chain J:

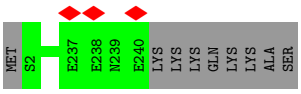




• Molecule 10: Proteasome subunit alpha type-7

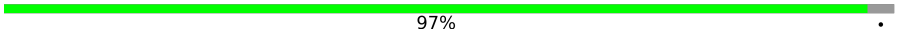
Chain j:





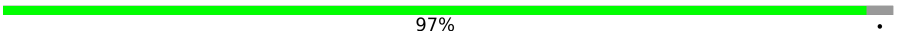
• Molecule 11: Proteasome subunit alpha type-5

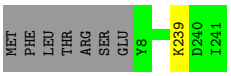
Chain K:



• Molecule 11: Proteasome subunit alpha type-5

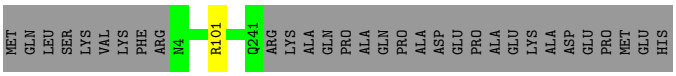
Chain k:





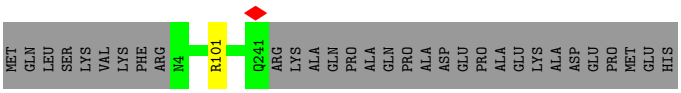
• Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L:



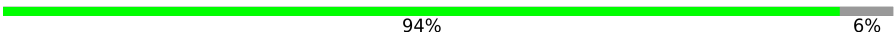
• Molecule 12: Isoform Long of Proteasome subunit alpha type-1

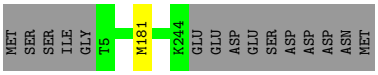
Chain l:



• Molecule 13: Proteasome subunit alpha type-3

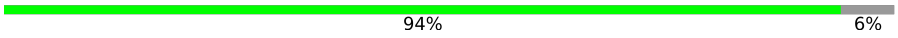
Chain M:

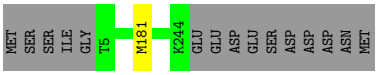




• Molecule 13: Proteasome subunit alpha type-3

Chain m:



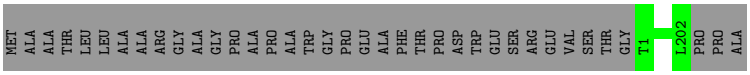


• Molecule 14: Proteasome subunit beta type-6

Chain N:

• Molecule 14: Proteasome subunit beta type-6

Chain n:



• Molecule 15: Proteasome subunit beta type-7

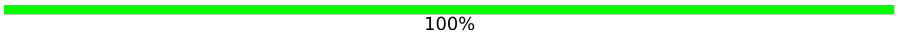
Chain O:

• Molecule 15: Proteasome subunit beta type-7

Chain o:

• Molecule 16: Proteasome subunit beta type-3

Chain P:



• Molecule 16: Proteasome subunit beta type-3

Chain p: 100%

• Molecule 17: Proteasome subunit beta type-2

Chain Q: 99%

• Molecule 17: Proteasome subunit beta type-2

Chain q: 99%

• Molecule 18: Proteasome subunit beta type-5

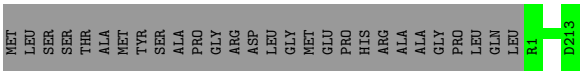
Chain R: 76% 24%

• Molecule 18: Proteasome subunit beta type-5

Chain r: 76% 24%

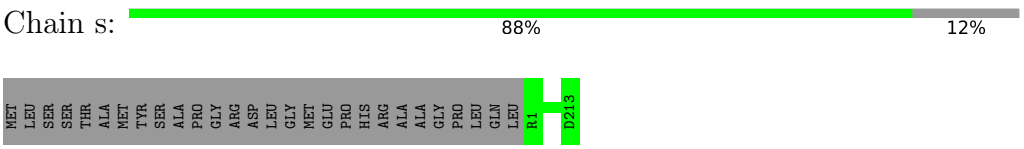
• Molecule 19: Proteasome subunit beta type-1

Chain S: 88% 12%



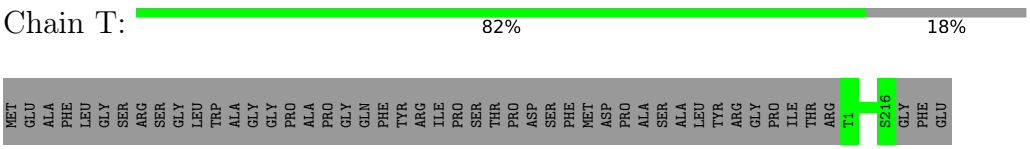
• Molecule 19: Proteasome subunit beta type-1

Chain s:



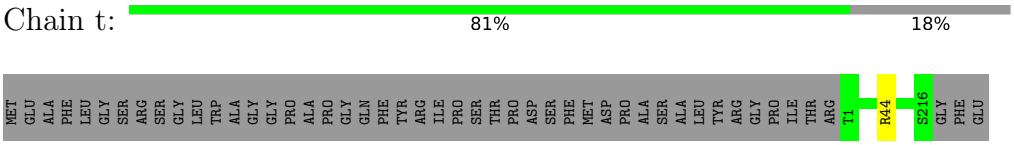
• Molecule 20: Proteasome subunit beta type-4

Chain T:



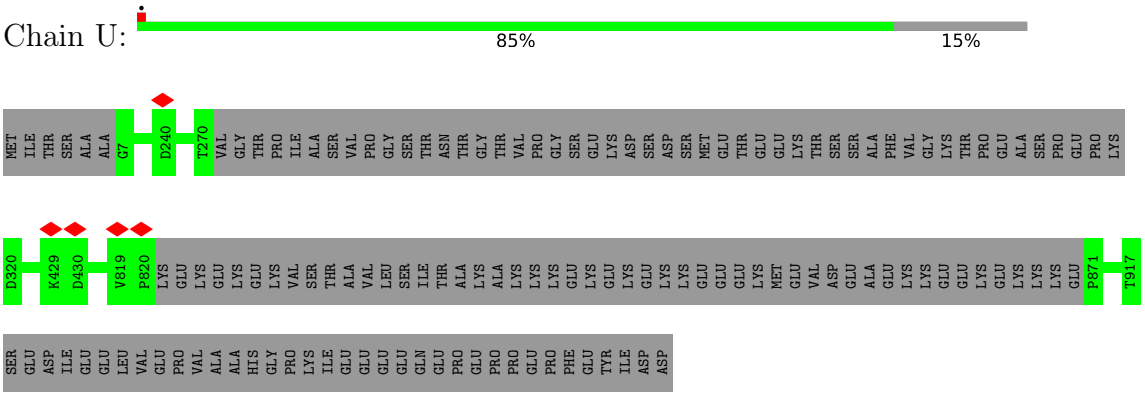
• Molecule 20: Proteasome subunit beta type-4

Chain t:



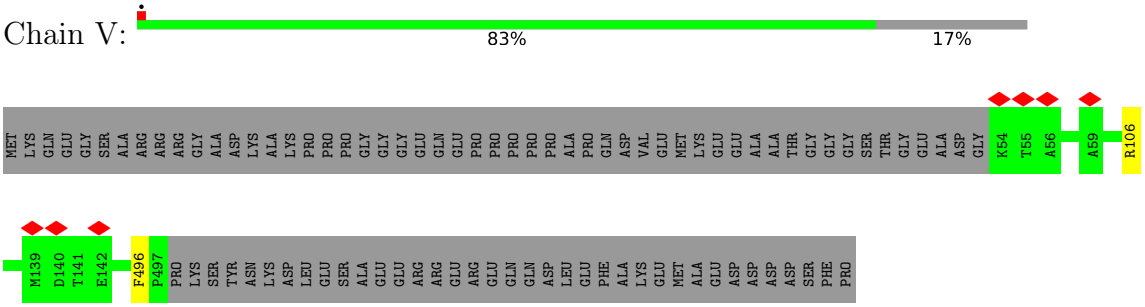
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U:



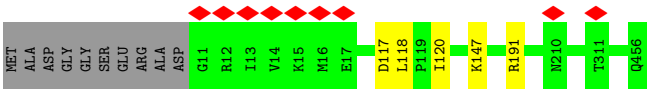
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



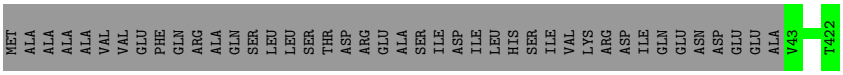
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



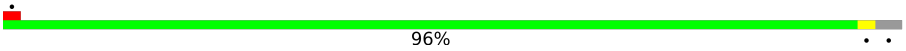
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

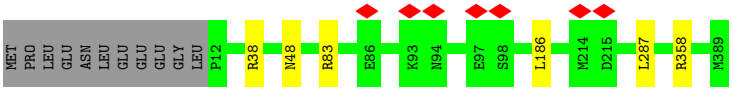
Chain X:



• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

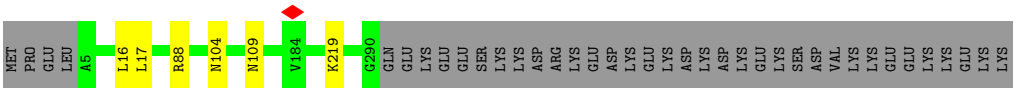
Chain Y:





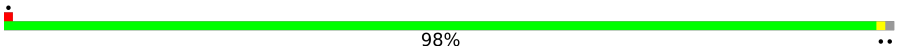
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

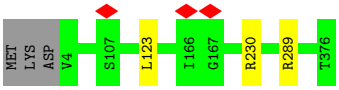
Chain Z:



• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

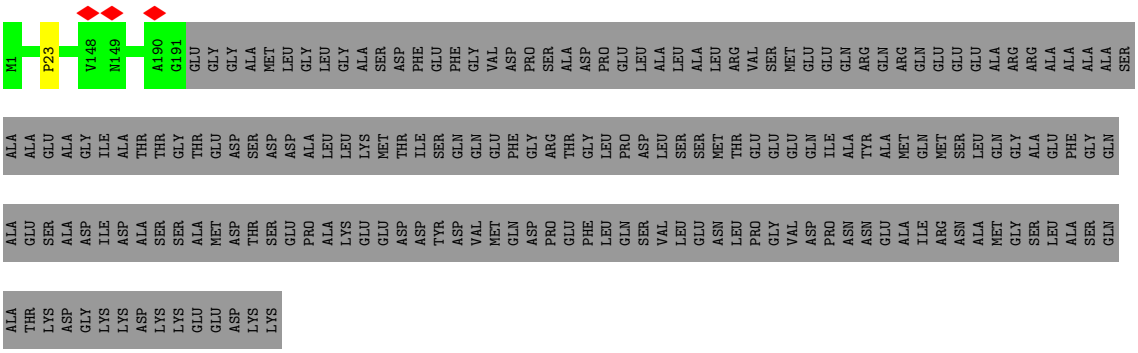
Chain a:





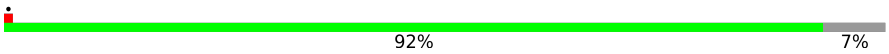
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

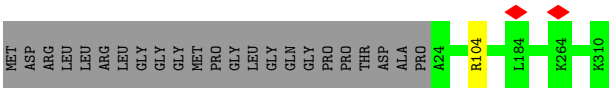
Chain b:



• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

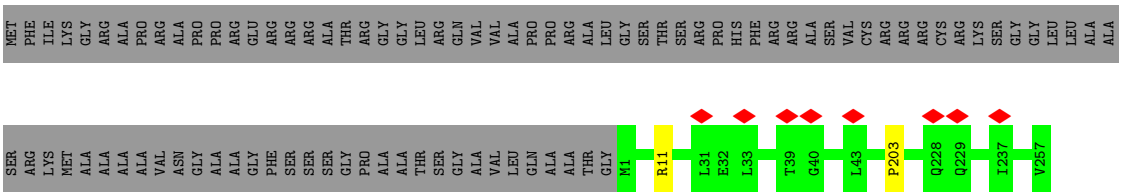
Chain c:





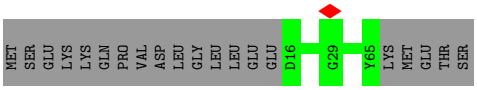
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



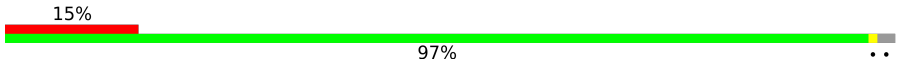
• Molecule 31: 26S proteasome complex subunit DSS1

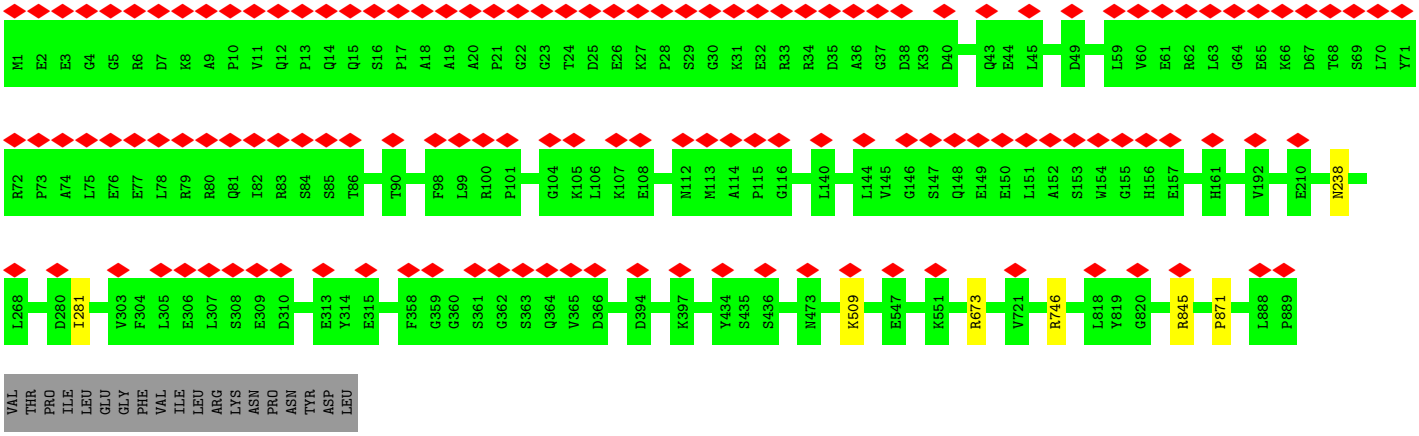
Chain e:



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

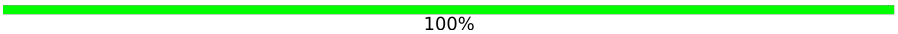
Chain f:





• Molecule 33: Ubiquitin

Chain u:



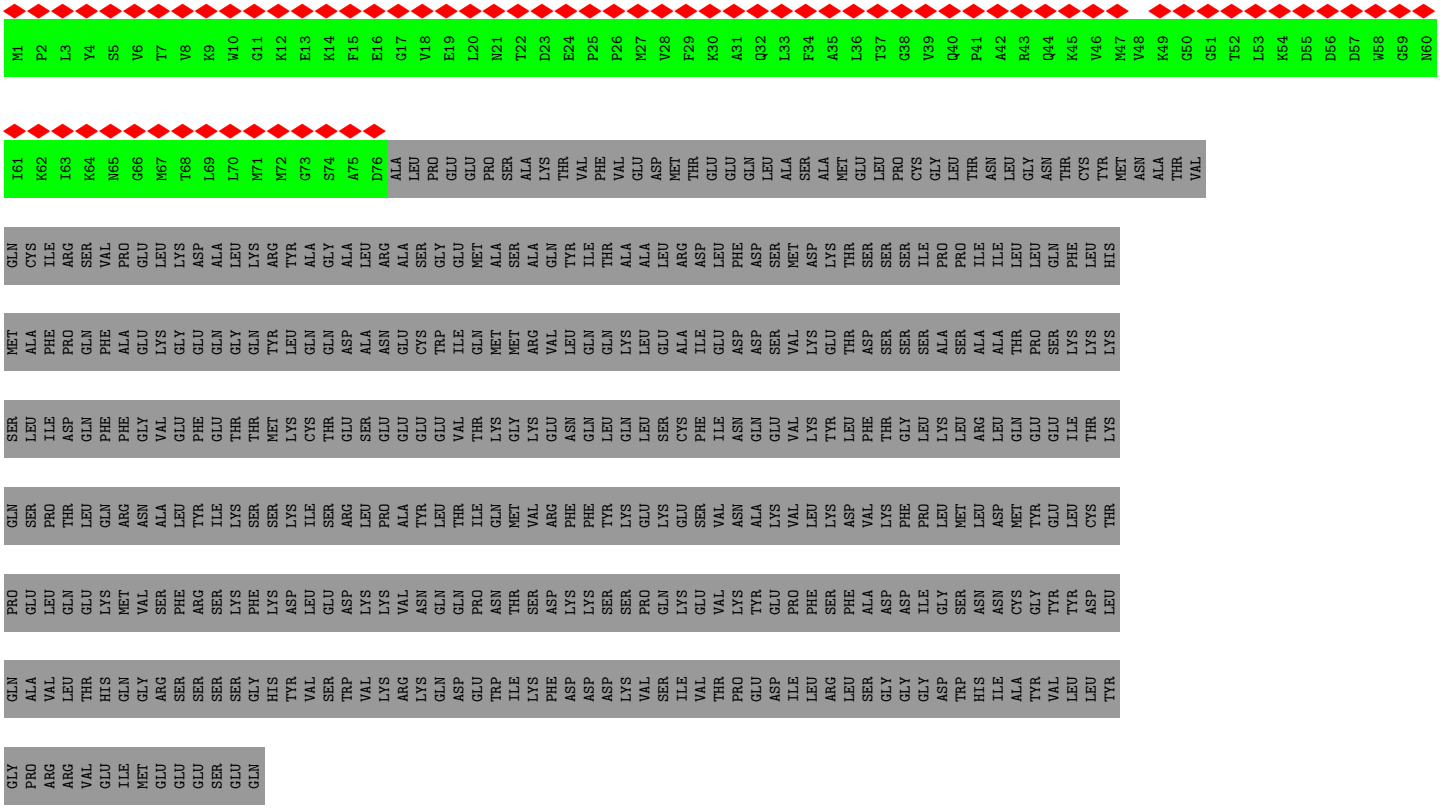
There are no outlier residues recorded for this chain.

• Molecule 34: Substrate

Chain v:

• Molecule 35: Ubiquitin carboxyl-terminal hydrolase 14

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294653	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.28	0/3148	0.59	1/4250 (0.0%)
2	B	0.27	0/3061	0.58	1/4129 (0.0%)
3	C	0.28	0/2902	0.60	0/3904
4	D	0.29	0/3089	0.59	0/4168
5	E	0.28	0/3145	0.57	0/4233
6	F	0.29	0/3292	0.56	1/4435 (0.0%)
7	G	0.29	0/1923	0.53	0/2601
7	g	0.29	0/1914	0.52	0/2590
8	H	0.30	0/1844	0.52	0/2499
8	h	0.29	0/1844	0.50	0/2497
9	I	0.29	0/1991	0.56	0/2685
9	i	0.28	0/1985	0.52	0/2677
10	J	0.29	0/1906	0.55	1/2573 (0.0%)
10	j	0.27	0/1887	0.55	0/2549
11	K	0.28	0/1804	0.50	0/2436
11	k	0.27	0/1809	0.50	0/2444
12	L	0.28	0/1901	0.52	0/2570
12	l	0.27	0/1896	0.53	0/2565
13	M	0.29	0/1911	0.51	0/2573
13	m	0.28	0/1916	0.50	0/2580
14	N	0.29	0/1540	0.51	0/2085
14	n	0.28	0/1536	0.50	0/2080
15	O	0.28	0/1676	0.54	0/2271
15	o	0.27	0/1686	0.52	0/2282
16	P	0.28	0/1616	0.55	0/2180
16	p	0.28	0/1620	0.54	0/2184
17	Q	0.28	0/1621	0.51	0/2194
17	q	0.29	0/1621	0.52	0/2194
18	R	0.29	0/1590	0.54	0/2147
18	r	0.29	0/1590	0.53	0/2147
19	S	0.29	0/1671	0.54	0/2252
19	s	0.29	0/1684	0.54	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	T	0.29	0/1716	0.53	0/2323
20	t	0.29	0/1720	0.53	0/2328
21	U	0.29	0/6449	0.57	0/8729
22	V	0.28	0/3681	0.53	0/4969
23	W	0.30	0/3683	0.62	0/4952
24	X	0.27	0/3053	0.55	0/4115
25	Y	0.31	0/3173	0.64	1/4273 (0.0%)
26	Z	0.32	0/2324	0.59	0/3150
27	a	0.29	0/3053	0.60	0/4133
28	b	0.27	0/1478	0.59	0/2001
29	c	0.31	0/2302	0.60	0/3110
30	d	0.28	0/2162	0.59	0/2919
31	e	0.27	0/437	0.51	0/595
32	f	0.27	0/6980	0.63	1/9433 (0.0%)
33	u	0.30	0/607	0.59	0/816
34	v	0.20	0/8	0.17	0/8
35	x	0.25	0/599	0.47	0/805
All	All	0.29	0/108044	0.56	6/145901 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	144	LEU	CA-CB-CG	5.55	128.06	115.30
2	B	140	ASP	CB-CG-OD1	5.54	123.29	118.30
32	f	281	ILE	CG1-CB-CG2	-5.47	99.37	111.40
1	A	51	ASP	CB-CG-OD1	5.25	123.02	118.30
25	Y	186	LEU	CA-CB-CG	5.18	127.21	115.30
6	F	150	LEU	CA-CB-CG	5.07	126.96	115.30

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%)	344 (88%)	48 (12%)	0	100	100
2	B	382/440 (87%)	359 (94%)	23 (6%)	0	100	100
3	C	359/398 (90%)	330 (92%)	29 (8%)	0	100	100
4	D	378/418 (90%)	343 (91%)	35 (9%)	0	100	100
5	E	387/403 (96%)	362 (94%)	24 (6%)	1 (0%)	41	74
6	F	413/439 (94%)	387 (94%)	26 (6%)	0	100	100
7	G	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
7	g	242/246 (98%)	226 (93%)	16 (7%)	0	100	100
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
9	I	249/261 (95%)	240 (96%)	9 (4%)	0	100	100
9	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
10	j	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
11	K	232/241 (96%)	220 (95%)	11 (5%)	1 (0%)	34	69
11	k	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
12	L	236/269 (88%)	231 (98%)	5 (2%)	0	100	100
12	l	236/269 (88%)	228 (97%)	8 (3%)	0	100	100
13	M	238/255 (93%)	237 (100%)	1 (0%)	0	100	100
13	m	238/255 (93%)	237 (100%)	1 (0%)	0	100	100
14	N	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	194 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
17	Q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
17	q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
18	R	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
18	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
20	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
20	t	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
21	U	806/953 (85%)	765 (95%)	41 (5%)	0	100	100
22	V	442/534 (83%)	434 (98%)	7 (2%)	1 (0%)	47	79
23	W	444/456 (97%)	421 (95%)	23 (5%)	0	100	100
24	X	378/422 (90%)	357 (94%)	21 (6%)	0	100	100
25	Y	376/389 (97%)	335 (89%)	41 (11%)	0	100	100
26	Z	284/324 (88%)	261 (92%)	23 (8%)	0	100	100
27	a	371/376 (99%)	343 (92%)	28 (8%)	0	100	100
28	b	189/377 (50%)	172 (91%)	16 (8%)	1 (0%)	29	67
29	c	285/310 (92%)	259 (91%)	26 (9%)	0	100	100
30	d	255/350 (73%)	225 (88%)	29 (11%)	1 (0%)	34	69
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
32	f	887/908 (98%)	760 (86%)	126 (14%)	1 (0%)	51	83
33	u	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
34	v	1/10 (10%)	0	0	1 (100%)	0	0
35	x	74/494 (15%)	71 (96%)	3 (4%)	0	100	100
All	All	13434/15468 (87%)	12634 (94%)	793 (6%)	7 (0%)	54	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	d	203	PRO
5	E	242	ARG
22	V	496	PHE
34	v	25	LYS
32	f	871	PRO

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Mol	Chain	Res	Type
28	b	23	PRO
11	K	130	PRO

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%)	334 (99%)	3 (1%)	78	91
2	B	339/385 (88%)	337 (99%)	2 (1%)	86	94
3	C	314/346 (91%)	307 (98%)	7 (2%)	52	79
4	D	333/366 (91%)	333 (100%)	0	100	100
5	E	341/353 (97%)	334 (98%)	7 (2%)	53	79
6	F	357/379 (94%)	356 (100%)	1 (0%)	92	96
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	202 (100%)	0	100	100
8	H	188/191 (98%)	187 (100%)	1 (0%)	88	95
8	h	188/191 (98%)	187 (100%)	1 (0%)	88	95
9	I	207/221 (94%)	204 (99%)	3 (1%)	67	86
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	201 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	194 (100%)	1 (0%)	88	95
12	L	202/230 (88%)	201 (100%)	1 (0%)	88	95
12	l	201/230 (87%)	200 (100%)	1 (0%)	88	95
13	M	196/212 (92%)	195 (100%)	1 (0%)	88	95
13	m	198/212 (93%)	197 (100%)	1 (0%)	88	95
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	178 (99%)	1 (1%)	86	94
21	U	692/816 (85%)	692 (100%)	0	100	100
22	V	390/460 (85%)	389 (100%)	1 (0%)	92	96
23	W	410/416 (99%)	405 (99%)	5 (1%)	71	88
24	X	327/362 (90%)	327 (100%)	0	100	100
25	Y	334/344 (97%)	329 (98%)	5 (2%)	65	85
26	Z	257/295 (87%)	251 (98%)	6 (2%)	50	78
27	a	333/336 (99%)	330 (99%)	3 (1%)	78	91
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	251 (100%)	1 (0%)	91	95
30	d	231/294 (79%)	230 (100%)	1 (0%)	91	95
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	745/763 (98%)	740 (99%)	5 (1%)	84	94
33	u	68/68 (100%)	68 (100%)	0	100	100
34	v	1/1 (100%)	1 (100%)	0	100	100
35	x	64/439 (15%)	64 (100%)	0	100	100
All	All	11490/13134 (88%)	11432 (100%)	58 (0%)	89	95

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG

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Mol	Chain	Res	Type
1	A	297	ARG
1	A	403	ILE
2	B	125	THR
2	B	333	ARG
3	C	78	ARG
3	C	109	THR
3	C	117	ARG
3	C	150	MET
3	C	159	LYS
3	C	210	THR
3	C	336	MET
5	E	75	ASN
5	E	115	VAL
5	E	118	LEU
5	E	223	ARG
5	E	383	LYS
5	E	384	LEU
5	E	385	ASP
6	F	129	ARG
8	H	143	ARG
9	I	7[A]	SER
9	I	7[B]	SER
9	I	246	LYS
12	L	101	ARG
13	M	181	MET
22	V	106	ARG
23	W	117	ASP
23	W	118	LEU
23	W	120	ILE
23	W	147	LYS
23	W	191	ARG
25	Y	38	ARG
25	Y	48	ASN
25	Y	83	ARG
25	Y	287	LEU
25	Y	358	ARG
26	Z	16	LEU
26	Z	17	LEU
26	Z	88	ARG
26	Z	104	ASN
26	Z	109	ASN
26	Z	219	LYS

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Mol	Chain	Res	Type
27	a	123	LEU
27	a	230	ARG
27	a	289	ARG
29	c	104	ARG
30	d	11	ARG
32	f	238	ASN
32	f	509	LYS
32	f	673	ARG
32	f	746	ARG
32	f	845	ARG
8	h	60	ARG
11	k	239	LYS
12	l	101	ARG
13	m	181	MET
20	t	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	117	GLN
9	I	146	GLN
17	Q	61	GLN
19	S	160	ASN
21	U	70	HIS
24	X	334	ASN
30	d	60	GLN
32	f	371	ASN
7	g	150	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
38	ADP	F	501	37	24,29,29	0.94	1 (4%)	29,45,45	1.58	4 (13%)
38	ADP	C	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.55	4 (13%)
36	ATP	A	501	37	26,33,33	0.64	0	31,52,52	0.78	1 (3%)
36	ATP	B	501	37	26,33,33	0.61	0	31,52,52	0.74	1 (3%)
36	ATP	D	501	37	26,33,33	0.93	1 (3%)	31,52,52	1.43	5 (16%)
36	ATP	E	501	37	26,33,33	0.64	0	31,52,52	0.73	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	ADP	F	501	37	-	5/12/32/32	0/3/3/3
38	ADP	C	501	-	-	2/12/32/32	0/3/3/3
36	ATP	A	501	37	-	4/18/38/38	0/3/3/3
36	ATP	B	501	37	-	5/18/38/38	0/3/3/3
36	ATP	D	501	37	-	3/18/38/38	0/3/3/3
36	ATP	E	501	37	-	5/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ATP	C5-C4	2.46	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	501	ADP	C5-C4	2.44	1.47	1.40
38	C	501	ADP	C5-C4	2.43	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	F	501	ADP	PA-O3A-PB	-3.94	119.29	132.83
38	C	501	ADP	C3'-C2'-C1'	3.90	106.85	100.98
38	F	501	ADP	C3'-C2'-C1'	3.75	106.63	100.98
38	C	501	ADP	PA-O3A-PB	-3.70	120.14	132.83
38	F	501	ADP	N3-C2-N1	-3.26	123.59	128.68
38	C	501	ADP	N3-C2-N1	-3.23	123.64	128.68
36	D	501	ATP	N3-C2-N1	-3.18	123.71	128.68
36	D	501	ATP	PA-O3A-PB	-2.95	122.71	132.83
36	D	501	ATP	C3'-C2'-C1'	2.90	105.35	100.98
36	D	501	ATP	PB-O3B-PG	-2.68	123.64	132.83
38	C	501	ADP	C4-C5-N7	-2.53	106.76	109.40
38	F	501	ADP	C4-C5-N7	-2.31	107.00	109.40
36	E	501	ATP	C5-C6-N6	2.30	123.85	120.35
36	B	501	ATP	C5-C6-N6	2.28	123.82	120.35
36	A	501	ATP	C5-C6-N6	2.28	123.81	120.35
36	D	501	ATP	C4-C5-N7	-2.08	107.23	109.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	501	ATP	C5'-O5'-PA-O3A
36	B	501	ATP	C5'-O5'-PA-O1A
36	D	501	ATP	C5'-O5'-PA-O1A
36	E	501	ATP	C5'-O5'-PA-O3A
38	C	501	ADP	C5'-O5'-PA-O2A
38	C	501	ADP	C5'-O5'-PA-O3A
38	F	501	ADP	PA-O3A-PB-O3B
38	F	501	ADP	C5'-O5'-PA-O2A
38	F	501	ADP	C5'-O5'-PA-O3A
38	F	501	ADP	O4'-C4'-C5'-O5'
38	F	501	ADP	C3'-C4'-C5'-O5'
36	B	501	ATP	O4'-C4'-C5'-O5'
36	B	501	ATP	C3'-C4'-C5'-O5'
36	A	501	ATP	PG-O3B-PB-O2B
36	A	501	ATP	C5'-O5'-PA-O2A

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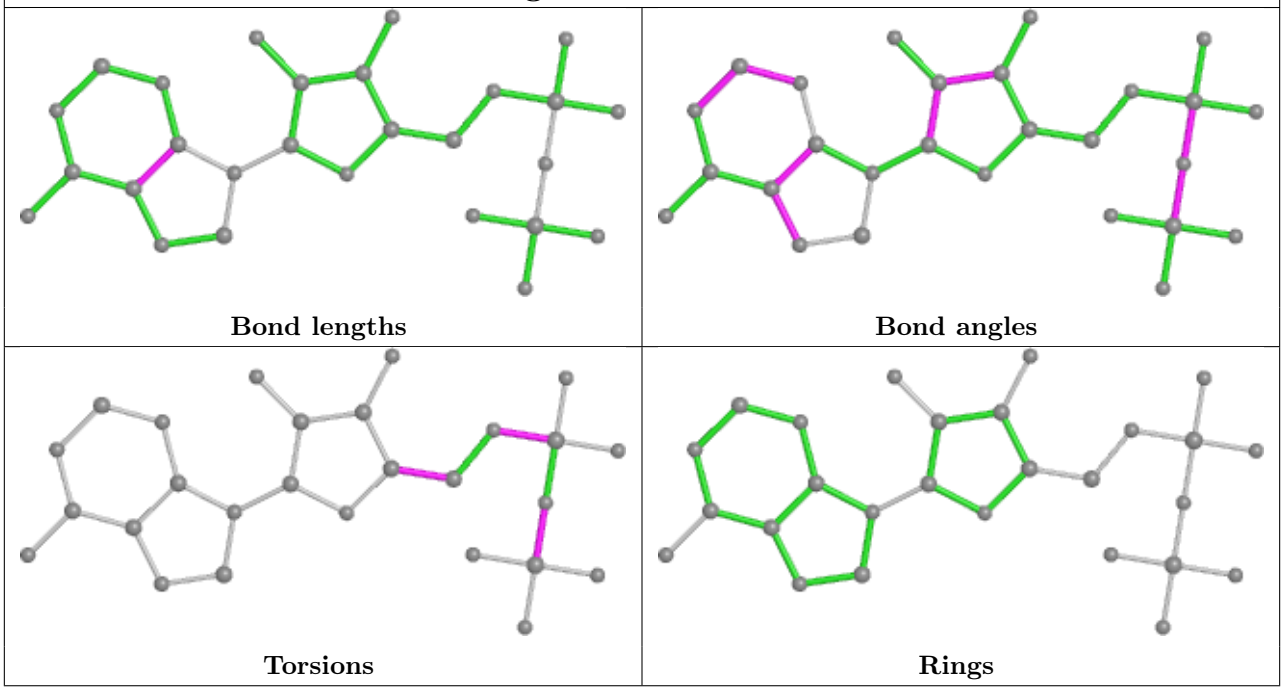
Mol	Chain	Res	Type	Atoms
36	B	501	ATP	C5'-O5'-PA-O2A
36	E	501	ATP	C5'-O5'-PA-O1A
36	D	501	ATP	PB-O3A-PA-O2A
36	B	501	ATP	C5'-O5'-PA-O3A
36	D	501	ATP	C5'-O5'-PA-O3A
36	A	501	ATP	PG-O3B-PB-O1B
36	E	501	ATP	PA-O3A-PB-O1B
36	E	501	ATP	PA-O3A-PB-O2B
36	E	501	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

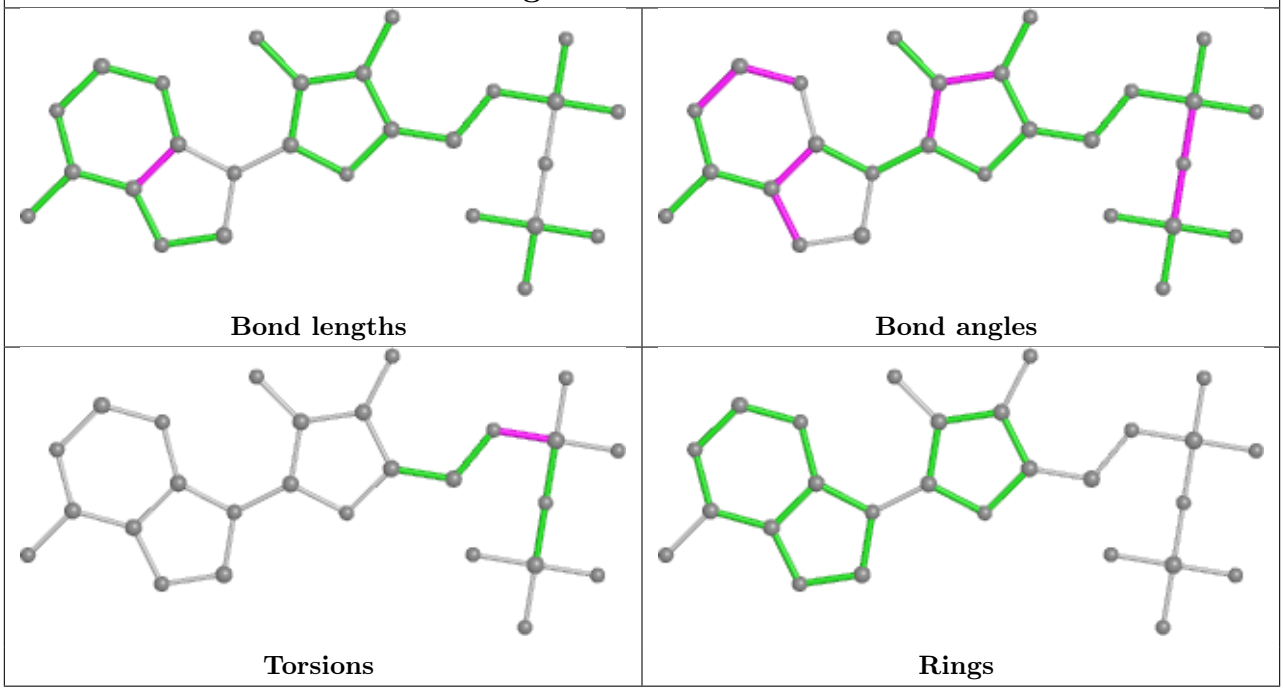
No monomer is involved in short contacts.

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.

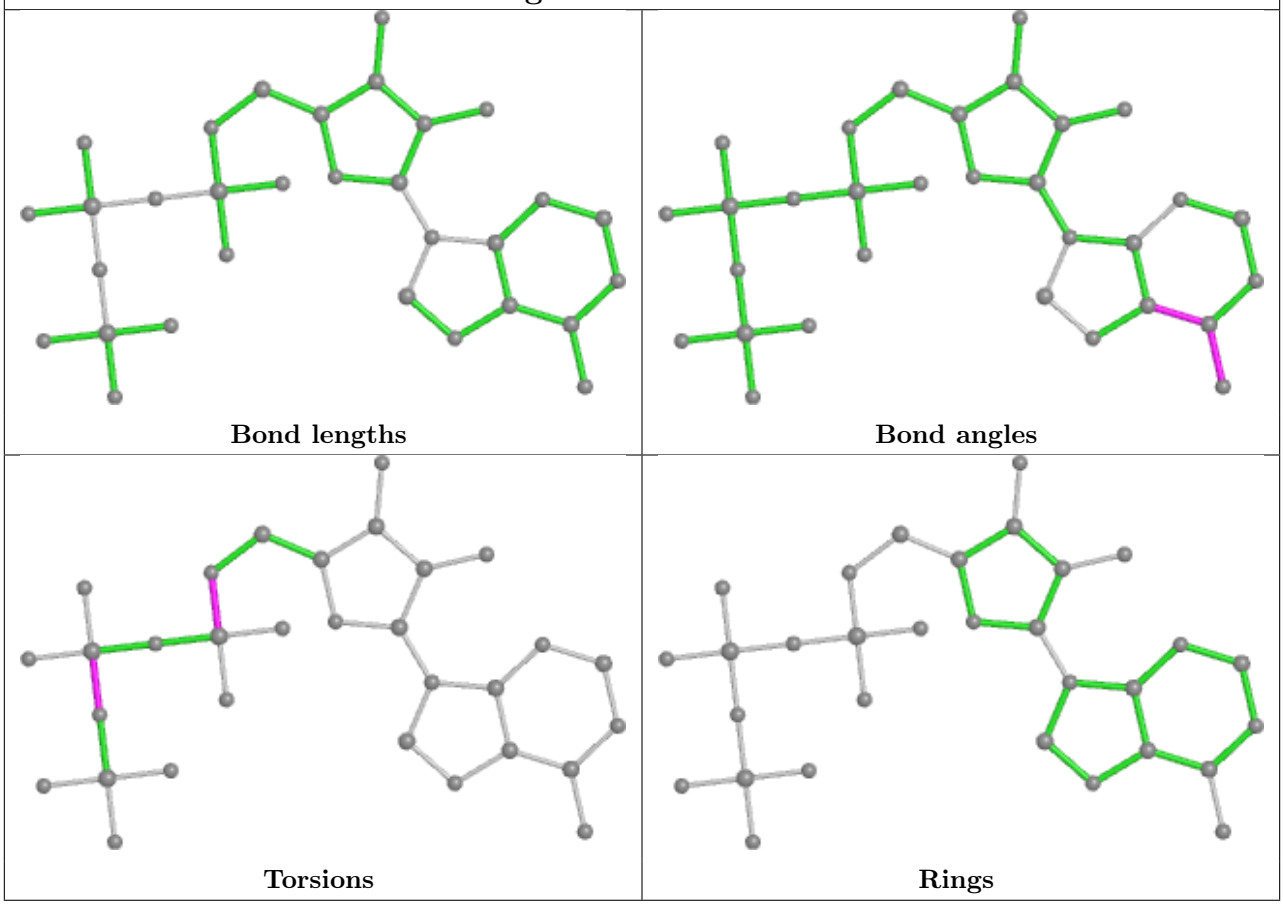
Ligand ADP F 501



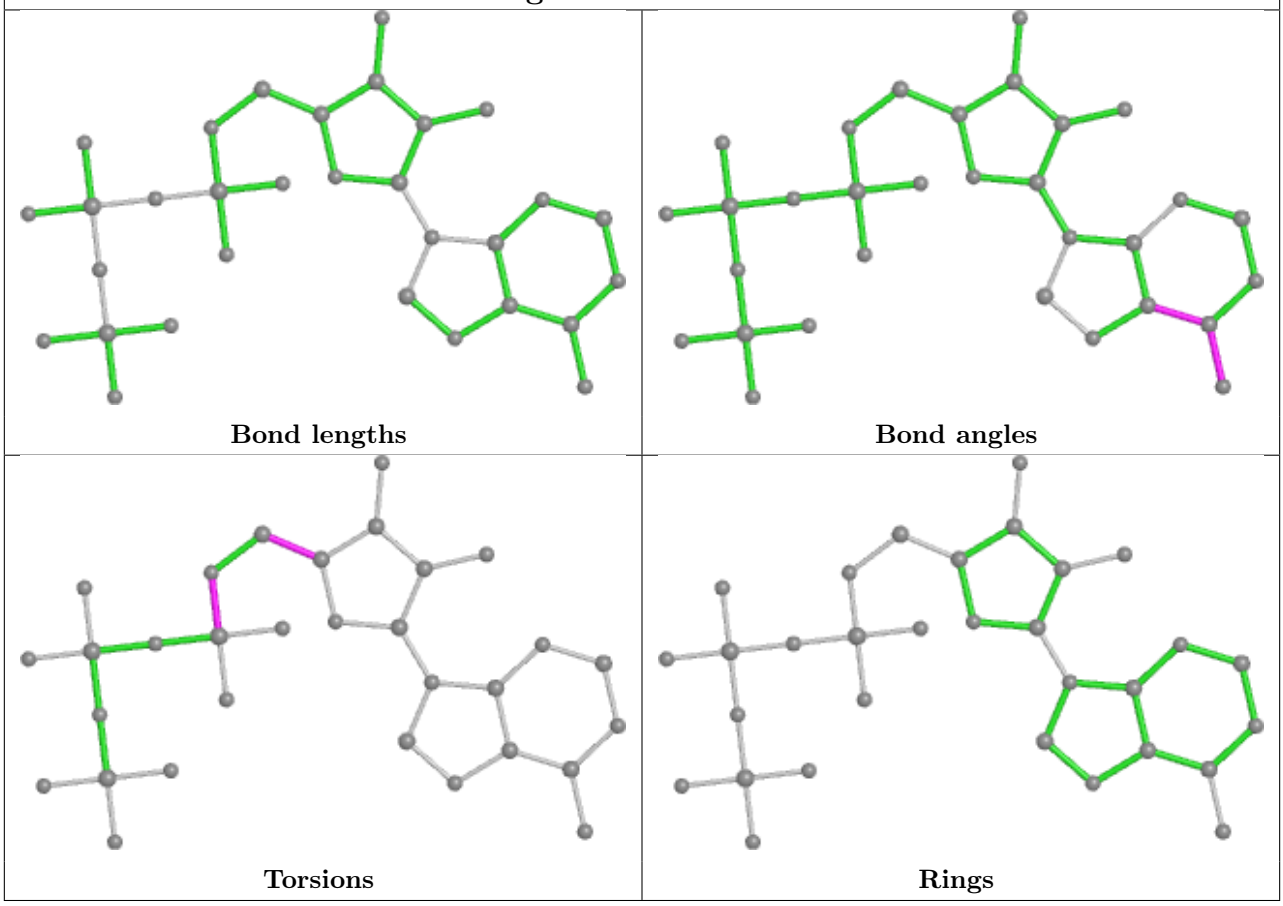
Ligand ADP C 501



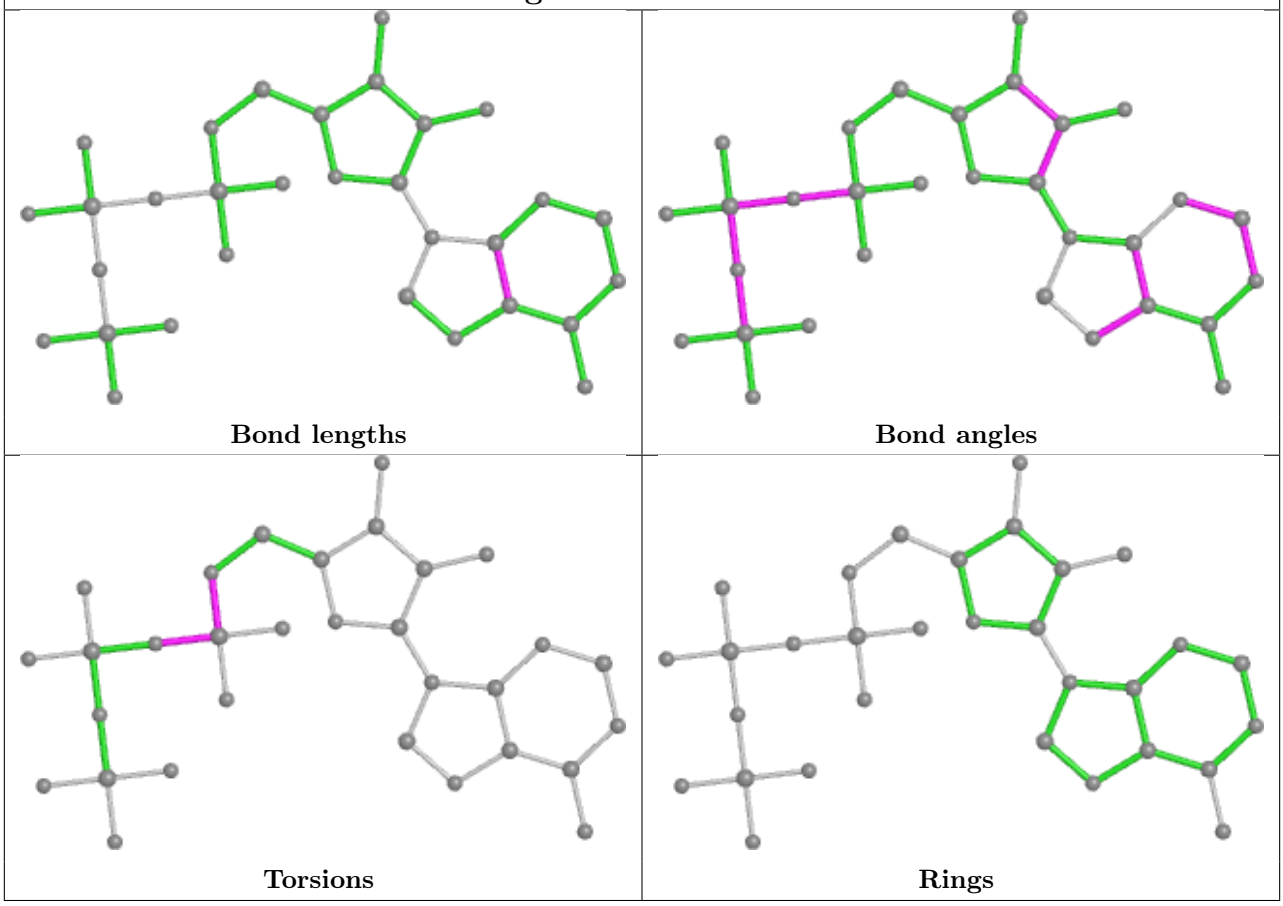
Ligand ATP A 501



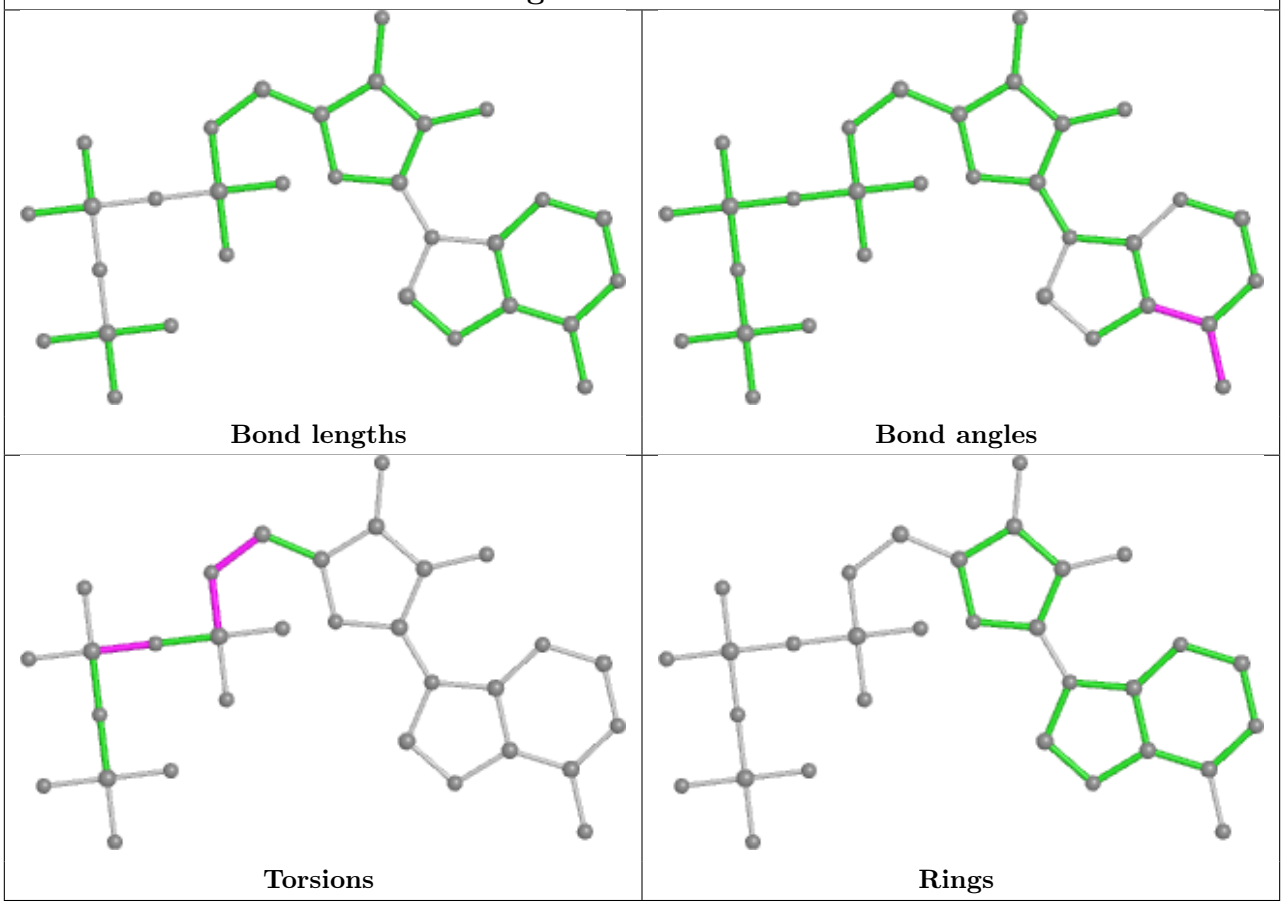
Ligand ATP B 501



Ligand ATP D 501



Ligand ATP E 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.

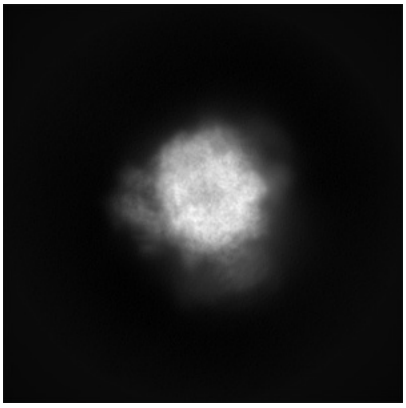
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32274. These allow visual inspection of the internal detail of the map and identification of artifacts.

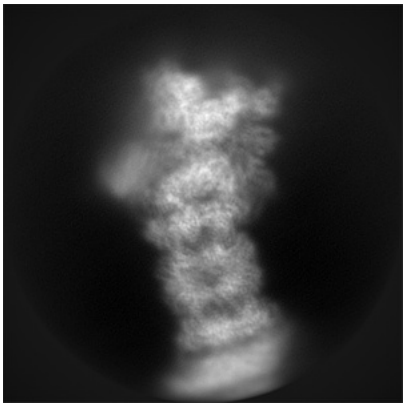
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

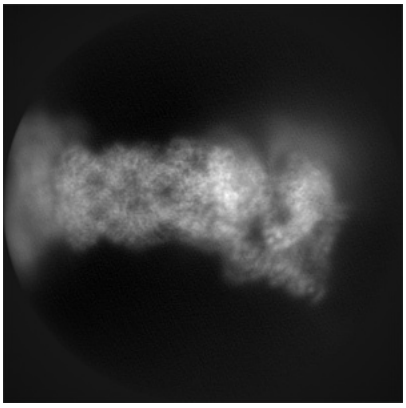
6.1.1 Primary map



X



Y

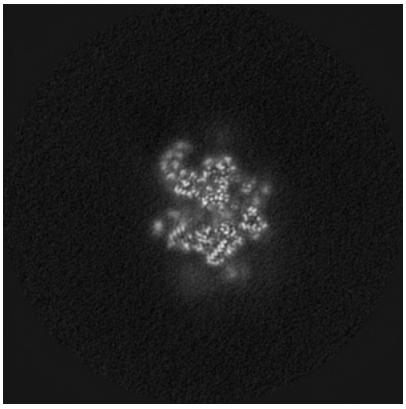


Z

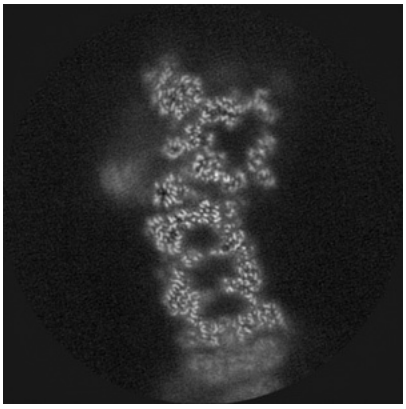
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

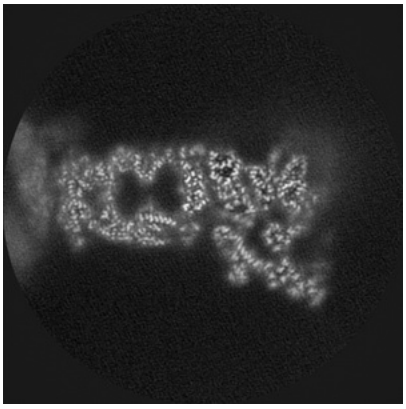
6.2.1 Primary map



X Index: 320



Y Index: 320

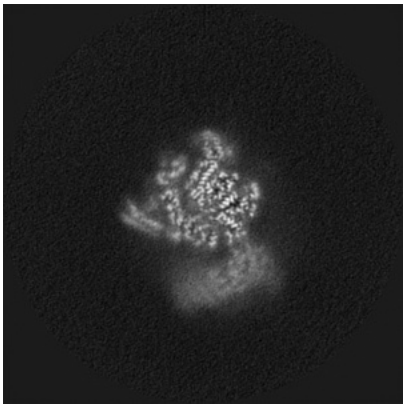


Z Index: 320

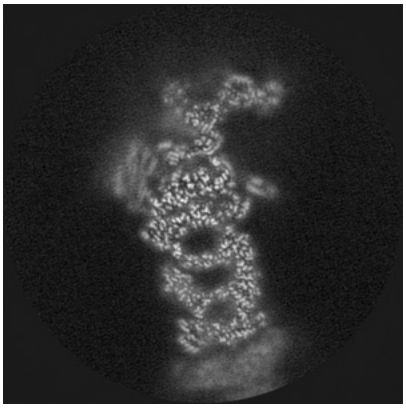
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

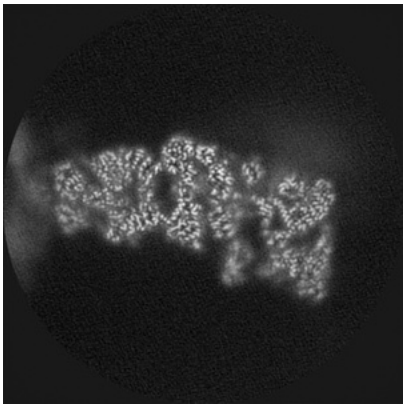
6.3.1 Primary map



X Index: 360



Y Index: 360



Z Index: 296

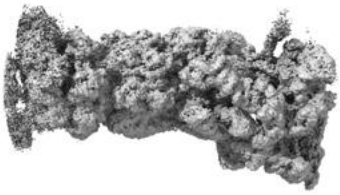
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

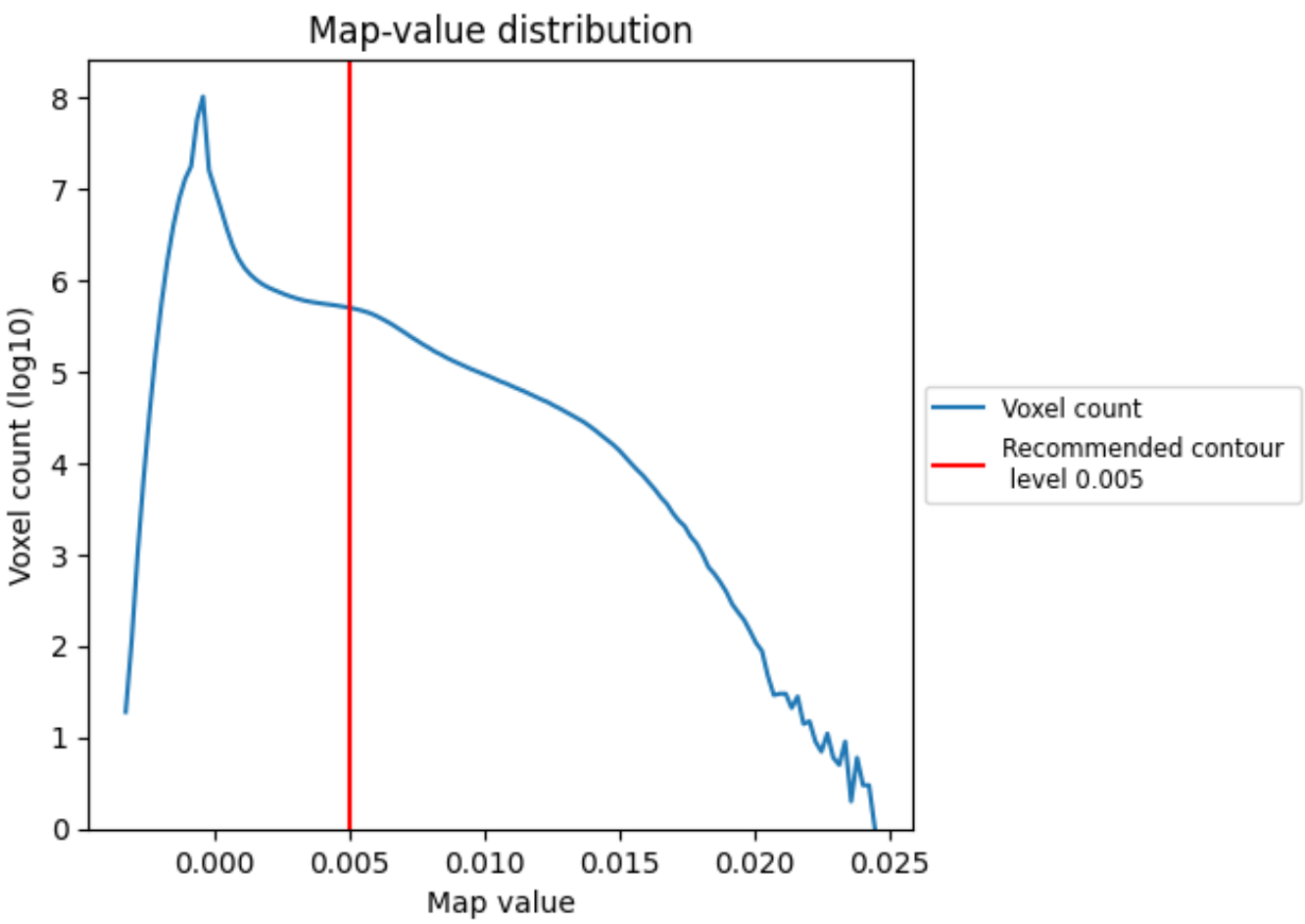
6.5 Mask visualisation (i)

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

7 Map analysis (i)

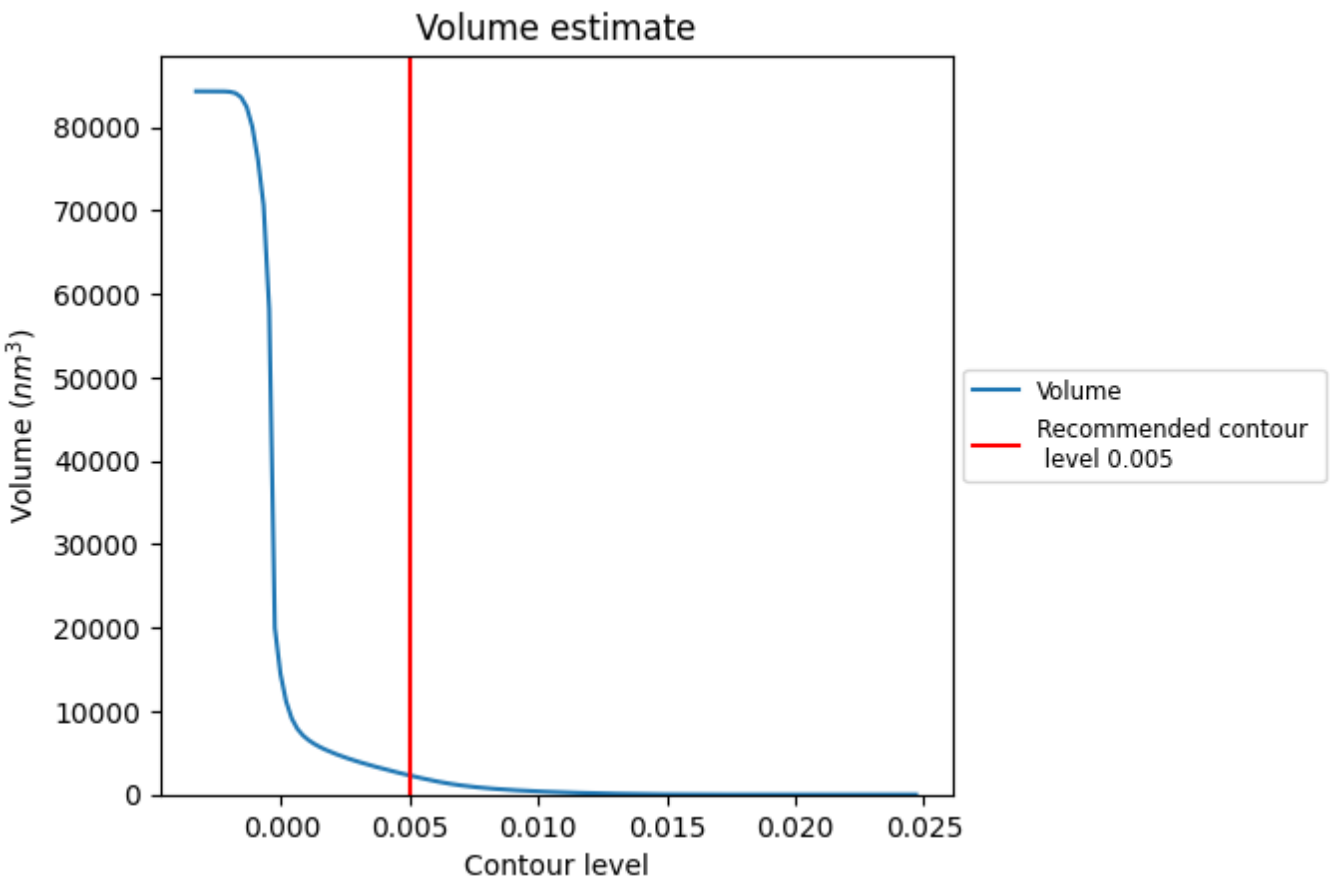
This section contains the results of statistical analysis of the map.

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.

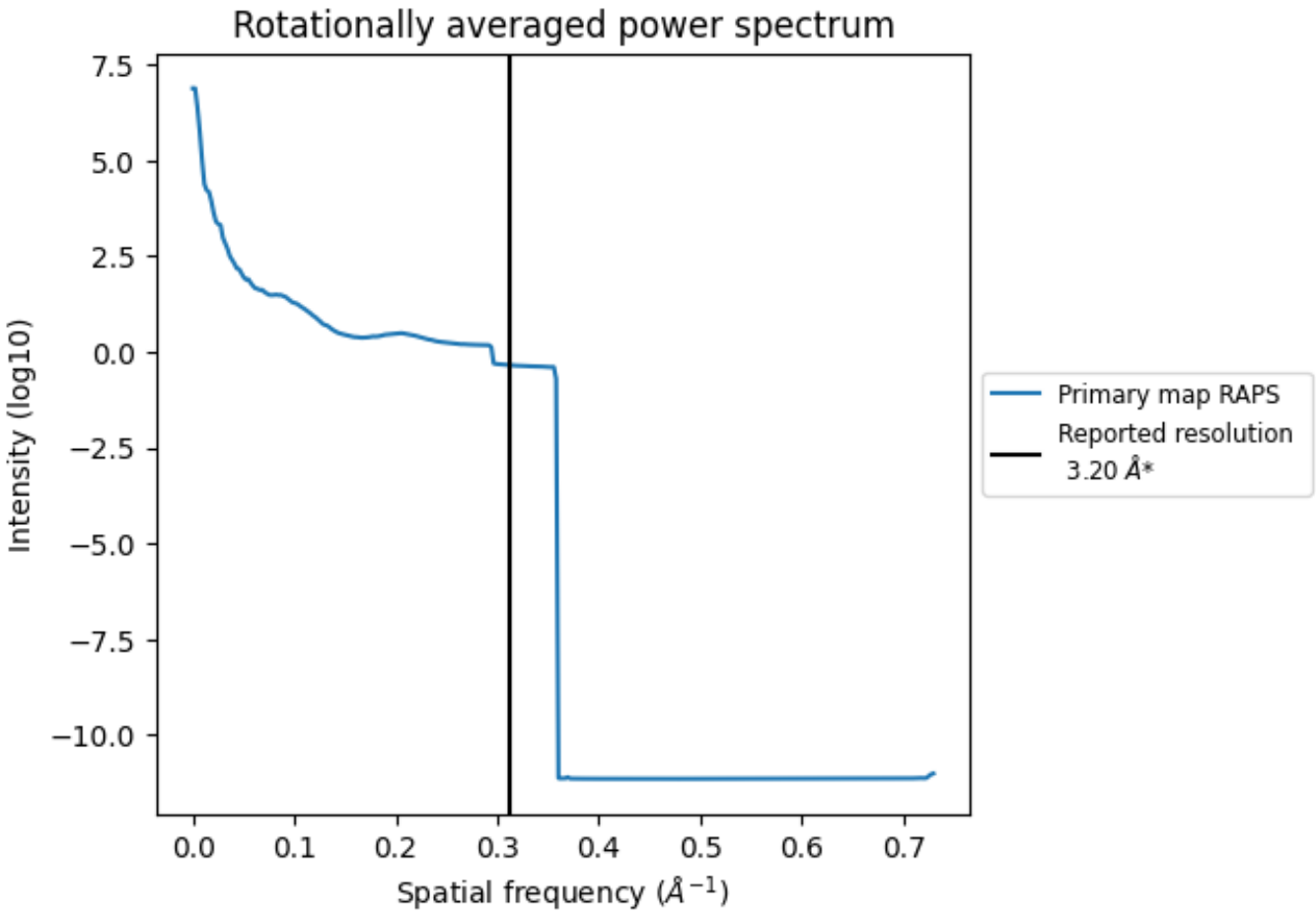
7.2 Volume estimate (i)



The volume at the recommended contour level is 2293 nm^3; this corresponds to an approximate mass of 2072 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 0.312 Å^{-1}

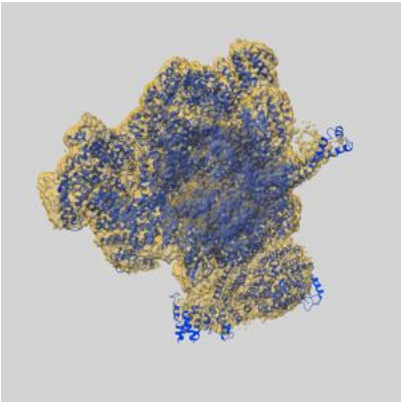
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

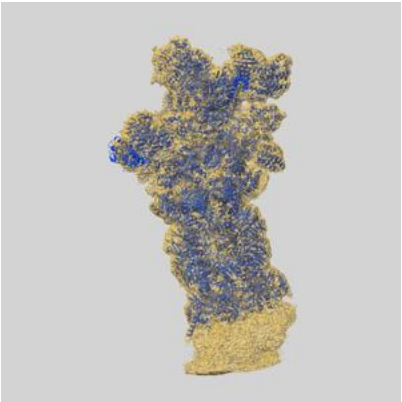
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32274 and PDB model 7W39. Per-residue inclusion information can be found in section 3 on page 13.

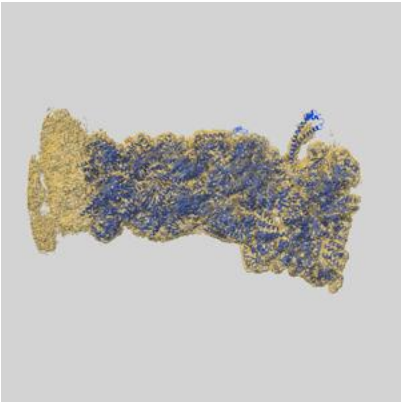
9.1 Map-model overlay (i)



X



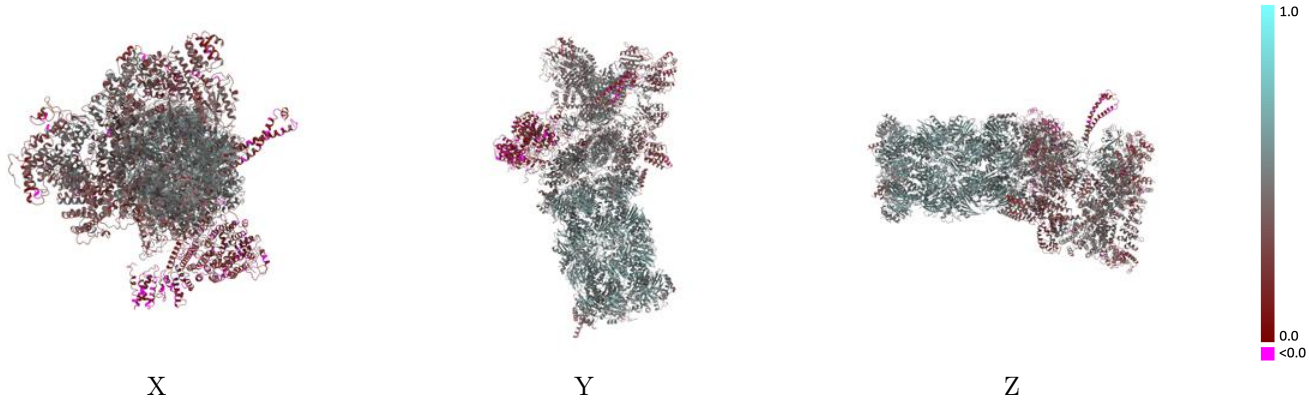
Y



Z

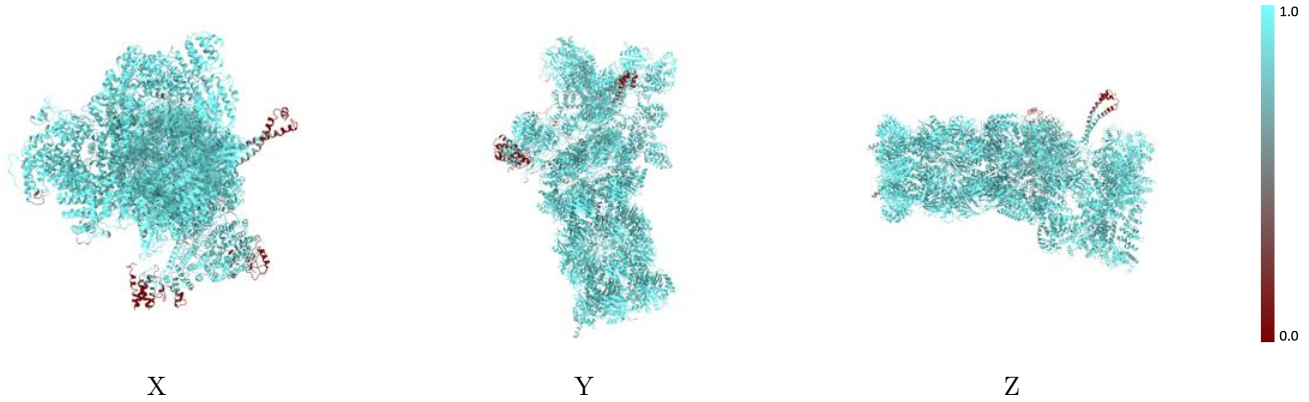
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



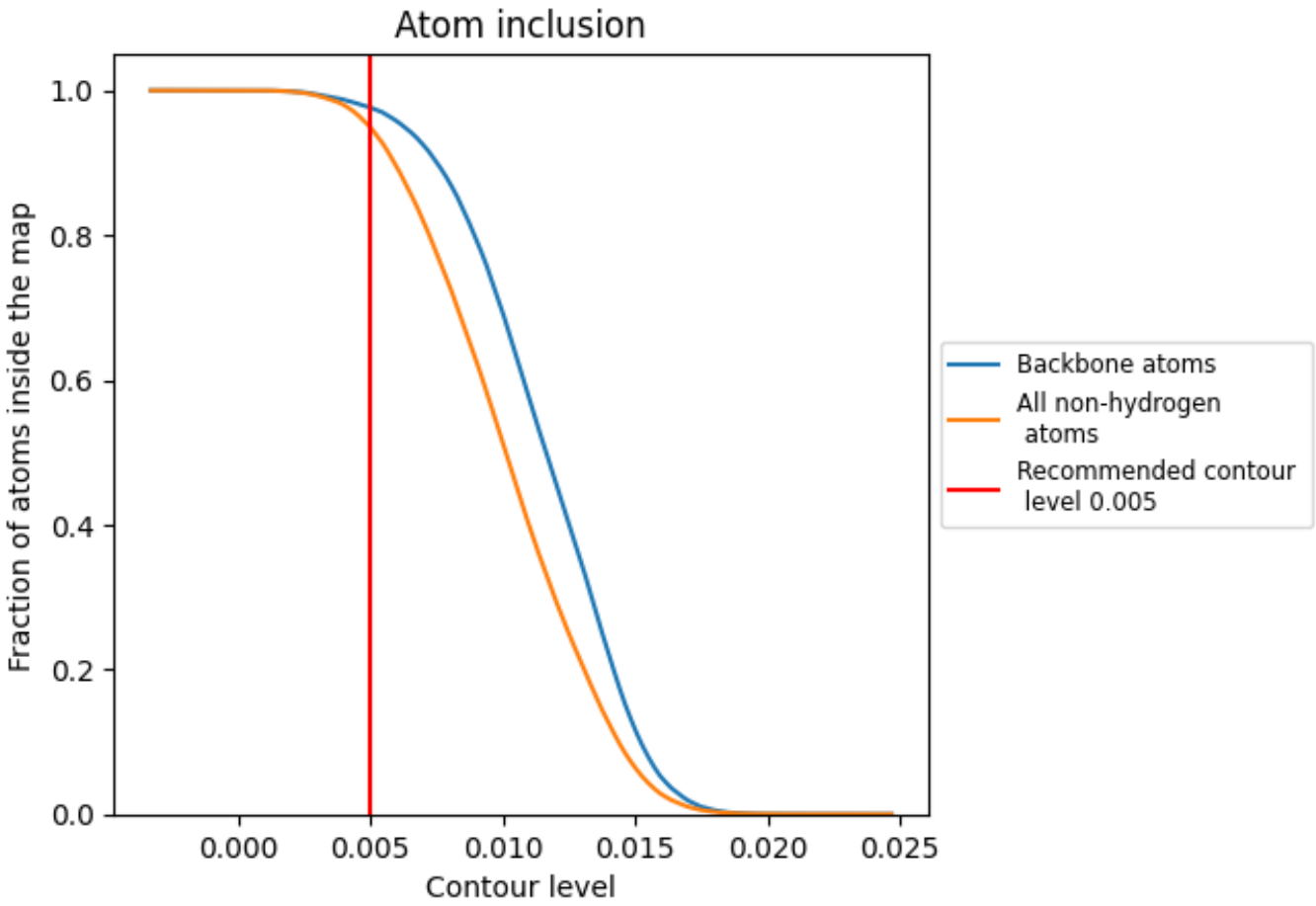
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9489	0.4300
A	0.9716	0.4240
B	0.9707	0.3860
C	0.9806	0.3870
D	0.9814	0.4160
E	0.9209	0.4150
F	0.8974	0.4180
G	0.9844	0.5180
H	0.9859	0.5230
I	0.9838	0.5070
J	0.9755	0.4870
K	0.9813	0.5210
L	0.9890	0.5360
M	0.9896	0.5200
N	0.9906	0.5510
O	0.9920	0.5430
P	0.9949	0.5460
Q	0.9903	0.5400
R	0.9934	0.5370
S	0.9913	0.5410
T	0.9896	0.5540
U	0.9590	0.3940
V	0.9503	0.3900
W	0.9122	0.3110
X	0.9472	0.3350
Y	0.9409	0.3110
Z	0.9649	0.4110
a	0.9278	0.3210
b	0.9362	0.3480
c	0.9682	0.4440
d	0.8945	0.2820
e	0.9427	0.3440
f	0.7912	0.1480
g	0.9772	0.5220
h	0.9853	0.5180

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Chain	Atom inclusion	Q-score
i	0.9619	0.4920
j	0.9565	0.4590
k	0.9757	0.5060
l	0.9857	0.5290
m	0.9804	0.5160
n	0.9953	0.5610
o	0.9914	0.5490
p	0.9968	0.5530
q	0.9948	0.5480
r	0.9940	0.5510
s	0.9864	0.5440
t	0.9866	0.5570
u	0.9780	0.4550
v	1.0000	0.2250
x	0.0240	0.1320