Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 07:24 AM JST

PDB ID	:	7W3A
EMDB ID	:	EMD-32275
Title	:	Structure of USP14-bound human 26S proteasome in substrate-engaged state ED4_USP14
Authors	:	Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on	:	2021-11-25
Resolution	:	3.50 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:

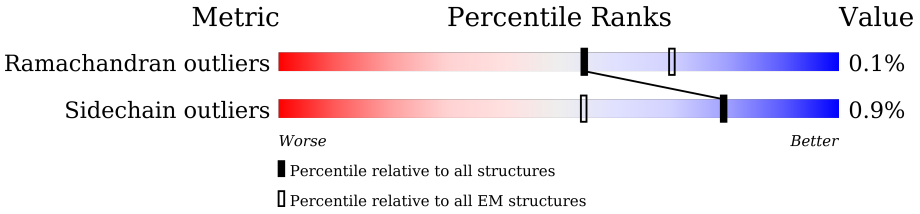
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.50 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	93% • 5%
2	B	440	92% • 7%
3	C	398	98% • •
4	D	418	89% • 9%
5	E	403	96% • •
6	F	439	90% • 9%
7	G	246	97% •
7	g	246	98% • •
8	H	234	99% •

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Mol	Chain	Length	Quality of chain
8	h	234	99%
9	I	261	94% 5%
9	i	261	96%
10	J	248	96%
10	j	248	96%
11	K	241	98%
11	k	241	97%
12	L	269	88% 11%
12	l	269	88% 12%
13	M	255	95% 5%
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	v	34	100%
22	x	494	10%, 99%
23	y	76	100%
24	U	953	91%, 8%
25	V	534	82%, 17%
26	W	456	96%
27	X	422	89%, 10%
28	Y	389	96%
29	Z	324	86%, 12%
30	a	376	97%
31	b	377	51%, 49%
32	c	310	92%, 7%
33	d	350	73%, 27%
34	f	908	9%, 97%
35	e	70	70%, 29%

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 110889 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	413	3229	2034	566	611	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	411	3207	2022	548	622	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	396	3105	1954	558	576	17	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	400	3133	1972	540	603	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	240	1867	1187	312	355	13	0	0
7	g	244	1879	1193	318	355	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	1801	1149	304	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	248	1933	1222	330	371	10	0	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	1861	1166	327	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	238	1813	1139	302	361	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	240	1876	1175	338	352	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	242	1890	1200	323	356	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	203	1521	954	259	296	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	1645	1035	278	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	1578	1012	267	290	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	1549	977	270	293	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	1650	1044	283	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 Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	v	34	170	102	34	34	0	0

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	x	494	3929	2485	647	769	28	0	0

- Molecule 23 is a protein called Ubiquitin.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	U	872	6828	4328	1157	1298	45	0	0

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Y	389	3202	2041	545	598	18	0	0

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

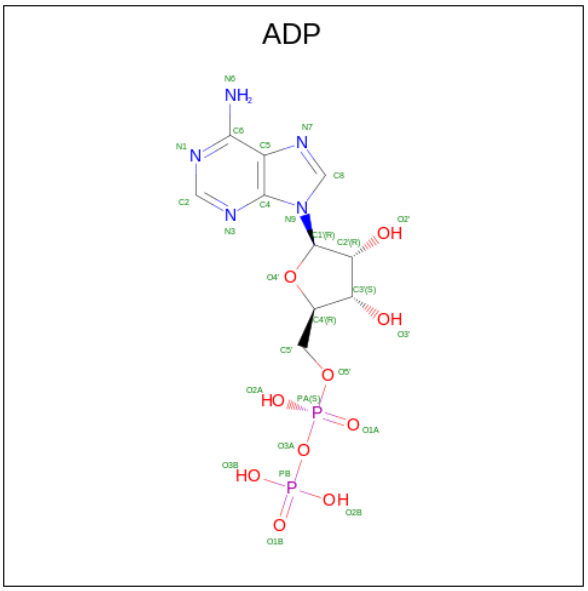
- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 35 is a protein called 26S proteasome complex subunit DSS1.

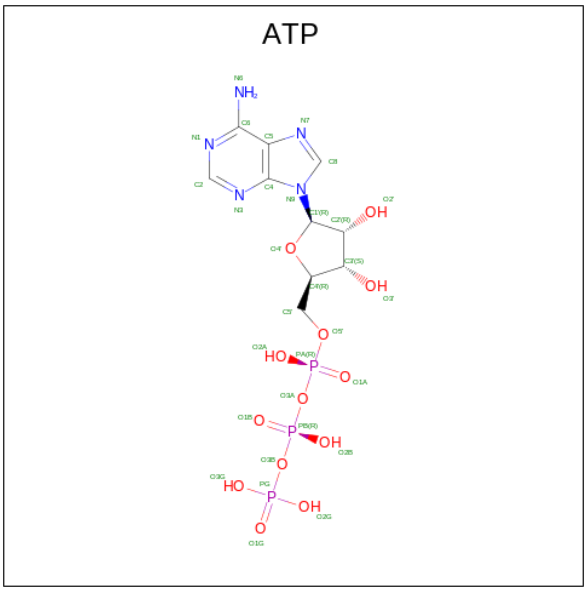
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	e	50	425	260	65	100	0	0

- Molecule 36 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
36	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 37 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
37	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

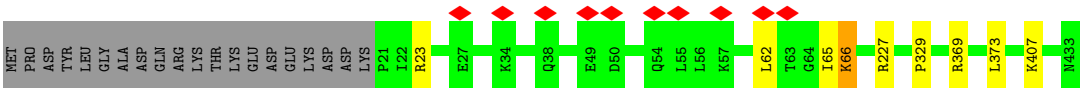
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
38	c	1	1	1	0

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.

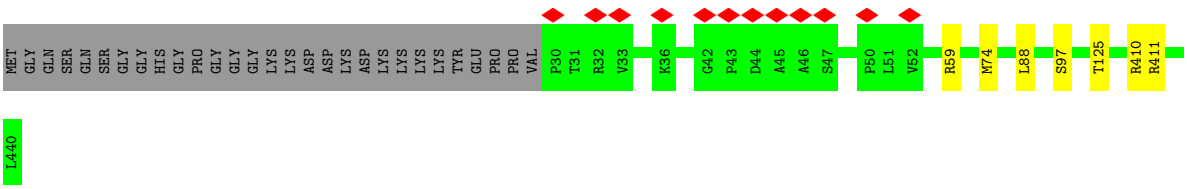
• Molecule 1: 26S protease regulatory subunit 7

Chain A: 93% 5%



• Molecule 2: 26S protease regulatory subunit 4

Chain B: 92% 7%

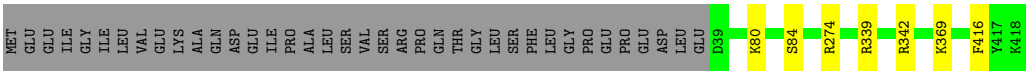


• Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8

Chain C: 98%

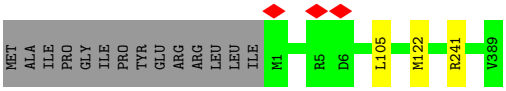
• Molecule 4: 26S protease regulatory subunit 6B

Chain D: 89% 9%



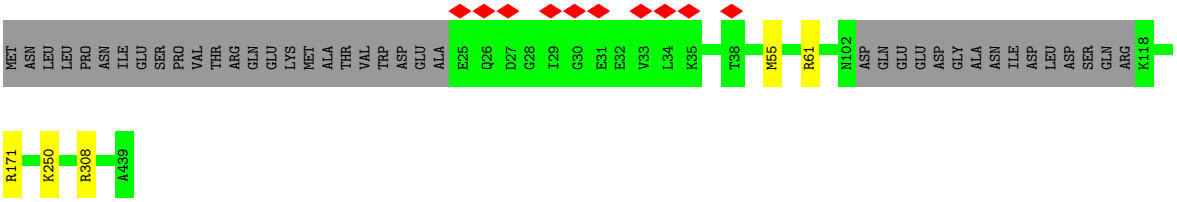
• Molecule 5: 26S proteasome regulatory subunit 10B

Chain E: 96%



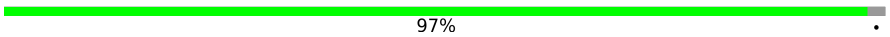
• Molecule 6: 26S protease regulatory subunit 6A

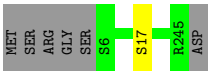
Chain F:



• Molecule 7: Proteasome subunit alpha type-6

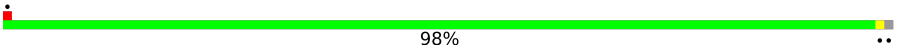
Chain G:

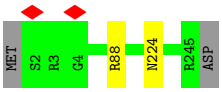




• Molecule 7: Proteasome subunit alpha type-6

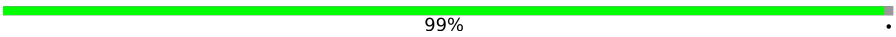
Chain g:

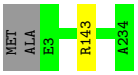




• Molecule 8: Proteasome subunit alpha type-2

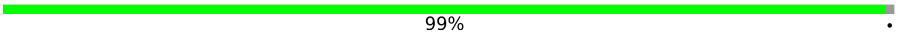
Chain H:





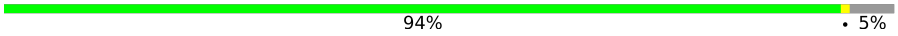
• Molecule 8: Proteasome subunit alpha type-2

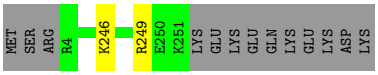
Chain h:



• Molecule 9: Proteasome subunit alpha type-4

Chain I:



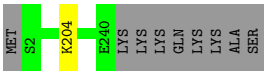


• Molecule 9: Proteasome subunit alpha type-4

Chain i: 96%

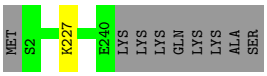
• Molecule 10: Proteasome subunit alpha type-7

Chain J: 96%



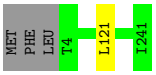
• Molecule 10: Proteasome subunit alpha type-7

Chain j: 96%



• Molecule 11: Proteasome subunit alpha type-5

Chain K: 98%

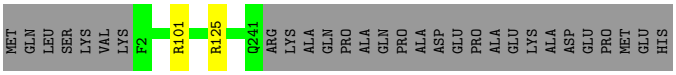


• Molecule 11: Proteasome subunit alpha type-5

Chain k: 97%

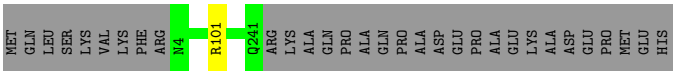
• Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L: 88% 11%



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

Chain l: 88% 12%

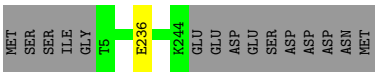


• Molecule 13: Proteasome subunit alpha type-3

Chain M: 95% 5%

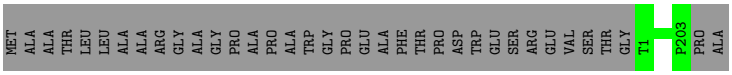
• Molecule 13: Proteasome subunit alpha type-3

Chain m: 94% 6%



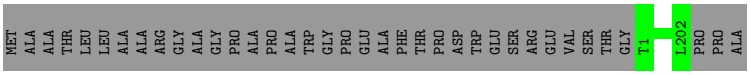
• Molecule 14: Proteasome subunit beta type-6

Chain N: 85% 15%



• Molecule 14: Proteasome subunit beta type-6

Chain n: 85% 15%

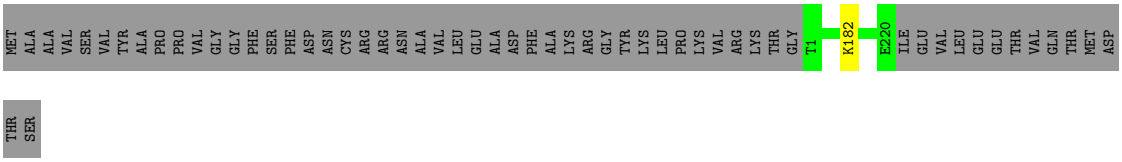


• Molecule 15: Proteasome subunit beta type-7

Chain O: 79% 21%

• Molecule 15: Proteasome subunit beta type-7

Chain o: 79% 21%



• Molecule 16: Proteasome subunit beta type-3

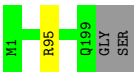
Chain P: 100%

• Molecule 16: Proteasome subunit beta type-3

Chain p: 100%

• Molecule 17: Proteasome subunit beta type-2

Chain Q: 99%

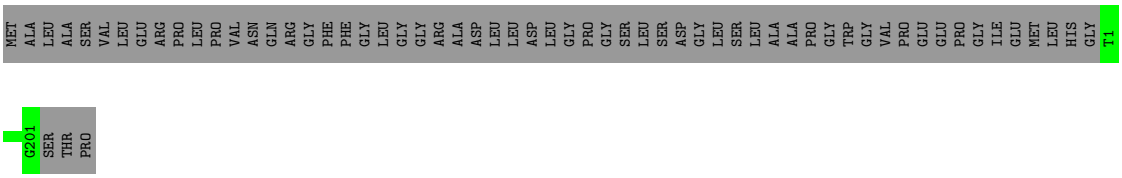


• Molecule 17: Proteasome subunit beta type-2

Chain q: 99%

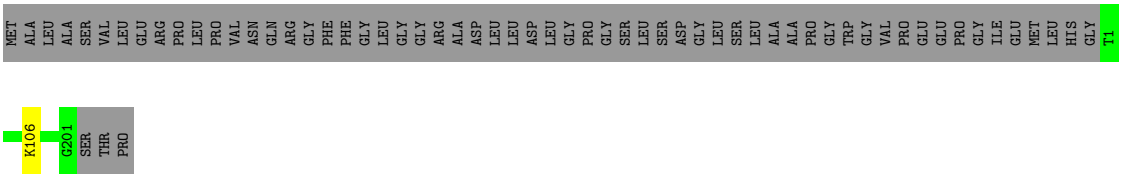
• Molecule 18: Proteasome subunit beta type-5

Chain R: 76% 24%



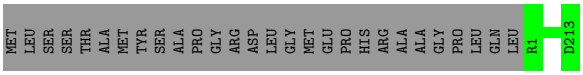
• Molecule 18: Proteasome subunit beta type-5

Chain r: 76% 24%



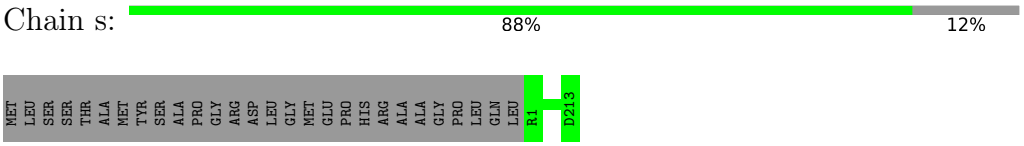
• Molecule 19: Proteasome subunit beta type-1

Chain S: 88% 12%



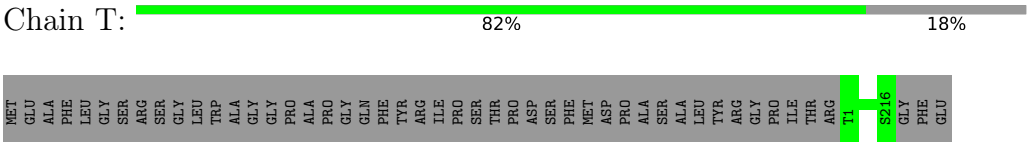
• Molecule 19: Proteasome subunit beta type-1

Chain s:



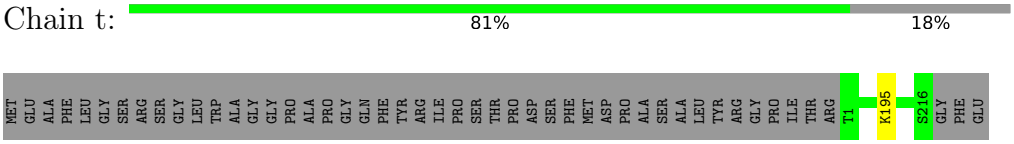
• Molecule 20: Proteasome subunit beta type-4

Chain T:



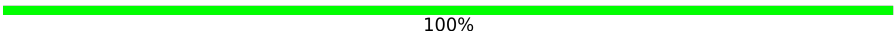
• Molecule 20: Proteasome subunit beta type-4

Chain t:



• Molecule 21: Substrate

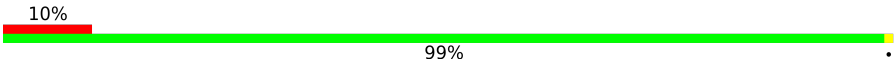
Chain v:

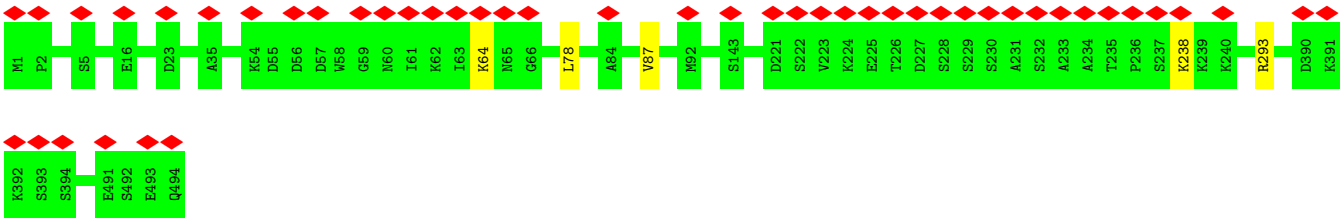


There are no outlier residues recorded for this chain.

• Molecule 22: Ubiquitin carboxyl-terminal hydrolase 14

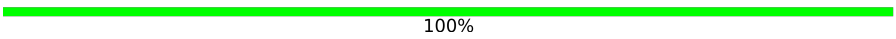
Chain x:





• Molecule 23: Ubiquitin

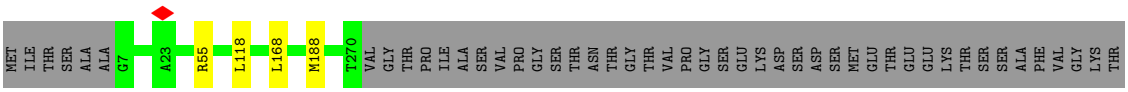
Chain y:

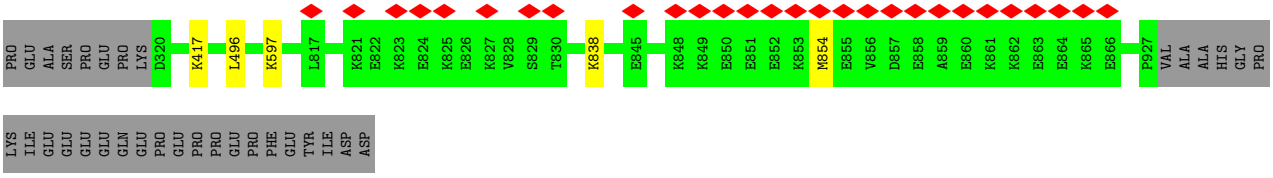


There are no outlier residues recorded for this chain.

• Molecule 24: 26S proteasome non-ATPase regulatory subunit 1

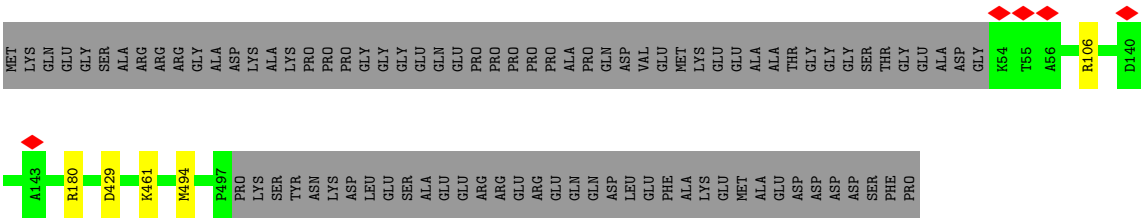
Chain U:





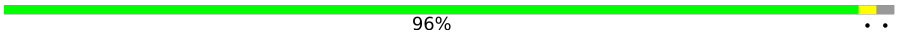
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



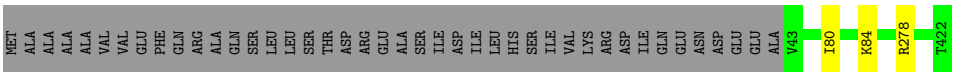
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



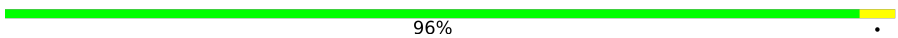
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



• Molecule 28: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:

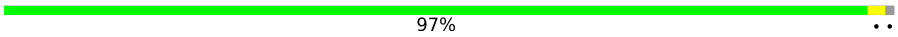


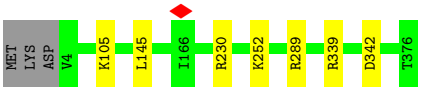
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:

• Molecule 30: 26S proteasome non-ATPase regulatory subunit 13

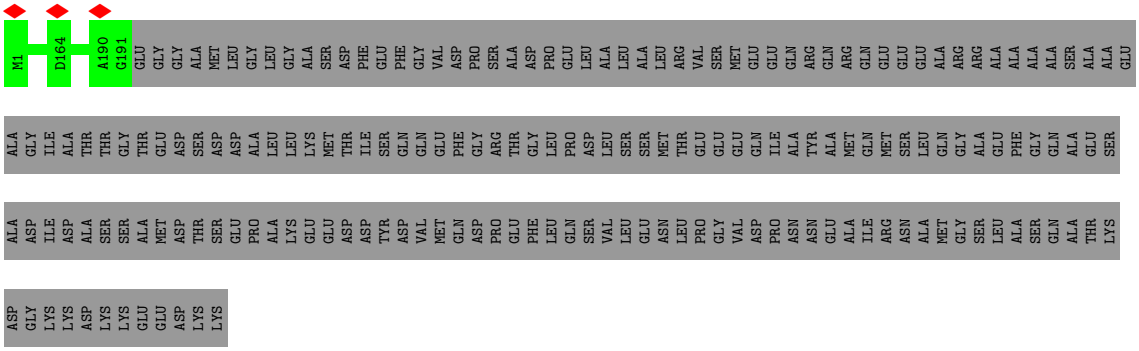
Chain a:





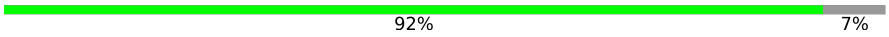
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 4

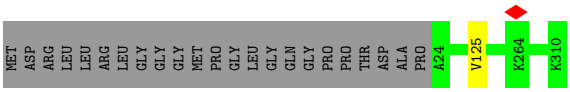
Chain b:



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 14

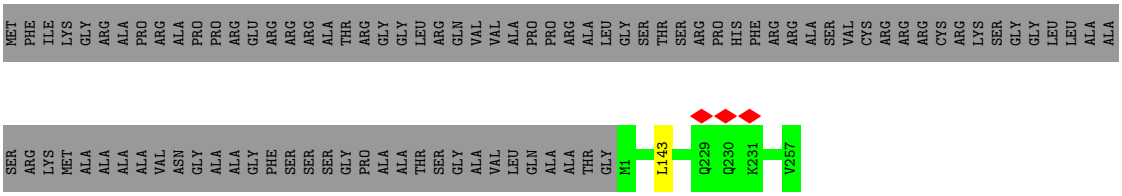
Chain c:





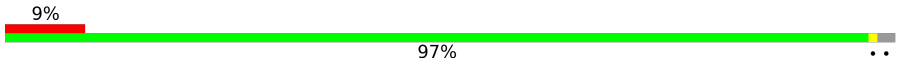
• Molecule 33: 26S proteasome non-ATPase regulatory subunit 8

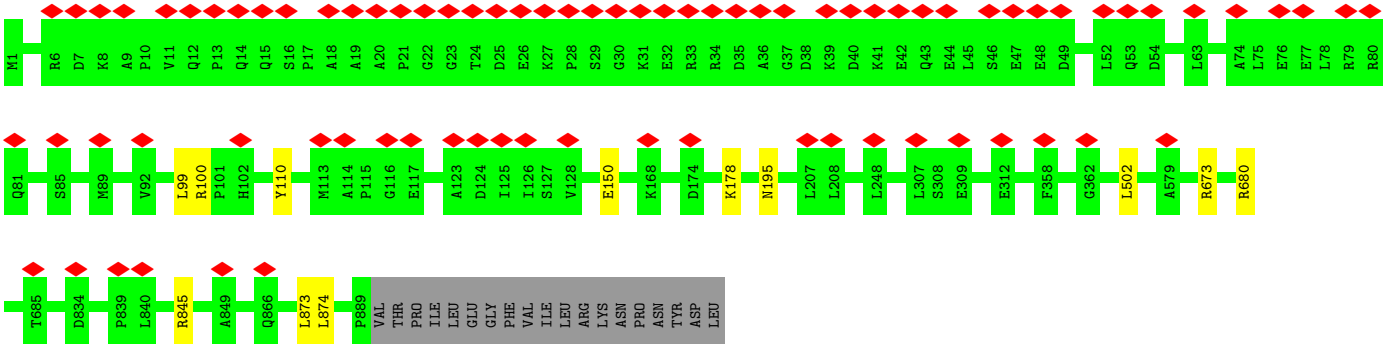
Chain d:



• Molecule 34: 26S proteasome non-ATPase regulatory subunit 2

Chain f:





• Molecule 35: 26S proteasome complex subunit DSS1

Chain e:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66910	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	0.024	Depositor
Minimum map value	-0.005	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: ADP, ZN, 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	0.26	0/3283	0.58	0/4433
2	B	0.27	0/3254	0.57	0/4388
3	C	0.28	0/3146	0.60	0/4226
4	D	0.29	0/3089	0.58	0/4168
5	E	0.27	0/3145	0.57	1/4233 (0.0%)
6	F	0.27	0/3173	0.55	1/4273 (0.0%)
7	G	0.30	0/1901	0.54	0/2572
7	g	0.28	0/1913	0.53	0/2589
8	H	0.29	0/1840	0.50	0/2495
8	h	0.28	0/1844	0.52	0/2497
9	I	0.27	0/1963	0.53	0/2650
9	i	0.28	0/1985	0.55	0/2677
10	J	0.27	0/1887	0.56	0/2553
10	j	0.28	0/1887	0.56	0/2549
11	K	0.27	0/1841	0.52	1/2486 (0.0%)
11	k	0.26	0/1809	0.50	0/2444
12	L	0.27	0/1911	0.53	0/2584
12	l	0.26	0/1896	0.52	0/2565
13	M	0.28	0/1925	0.52	0/2592
13	m	0.29	0/1916	0.55	0/2580
14	N	0.27	0/1548	0.51	0/2097
14	n	0.28	0/1536	0.51	0/2080
15	O	0.27	0/1672	0.54	0/2267
15	o	0.27	0/1686	0.54	0/2282
16	P	0.28	0/1616	0.54	0/2180
16	p	0.27	0/1620	0.54	0/2184
17	Q	0.28	0/1621	0.51	0/2194
17	q	0.28	0/1611	0.50	0/2182
18	R	0.28	0/1590	0.53	0/2147
18	r	0.30	0/1580	0.55	0/2135
19	S	0.28	0/1671	0.55	0/2252
19	s	0.28	0/1680	0.54	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	T	0.28	0/1716	0.53	0/2323
20	t	0.27	0/1720	0.54	0/2328
22	x	0.26	0/4002	0.51	0/5390
23	y	0.27	0/607	0.57	0/816
24	U	0.28	0/6945	0.60	3/9382 (0.0%)
25	V	0.28	0/3681	0.56	2/4969 (0.0%)
26	W	0.27	0/3683	0.60	1/4952 (0.0%)
27	X	0.27	0/3053	0.56	1/4115 (0.0%)
28	Y	0.29	0/3261	0.62	2/4393 (0.0%)
29	Z	0.28	0/2324	0.60	0/3150
30	a	0.26	0/3053	0.57	1/4133 (0.0%)
31	b	0.29	0/1478	0.61	0/2001
32	c	0.28	0/2302	0.60	0/3110
33	d	0.28	0/2162	0.61	1/2919 (0.0%)
34	f	0.27	0/6980	0.61	2/9433 (0.0%)
35	e	0.29	0/437	0.48	0/595
All	All	0.28	0/112443	0.56	16/151827 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	U	168	LEU	CA-CB-CG	5.97	129.02	115.30
6	F	55	MET	CA-CB-CG	5.88	123.30	113.30
28	Y	260	LEU	CB-CG-CD2	-5.84	101.07	111.00
30	a	145	LEU	CA-CB-CG	5.73	128.49	115.30
24	U	118	LEU	CA-CB-CG	5.73	128.47	115.30
34	f	99	LEU	C-N-CA	5.57	135.63	121.70
25	V	494	MET	CA-CB-CG	5.54	122.71	113.30
5	E	105	LEU	CA-CB-CG	5.51	127.98	115.30
11	K	121	LEU	CA-CB-CG	5.49	127.93	115.30
25	V	429	ASP	CB-CG-OD1	5.33	123.10	118.30
26	W	88	MET	CA-CB-CG	5.33	122.35	113.30
24	U	496	LEU	CA-CB-CG	5.27	127.43	115.30
33	d	143	LEU	CA-CB-CG	5.23	127.32	115.30
34	f	502	LEU	CA-CB-CG	5.20	127.26	115.30
28	Y	287	LEU	CA-CB-CG	5.16	127.17	115.30
27	X	80	ILE	CG1-CB-CG2	-5.11	100.17	111.40

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	411/433 (95%)	361 (88%)	48 (12%)	2 (0%)	29	68
2	B	409/440 (93%)	367 (90%)	42 (10%)	0	100	100
3	C	394/398 (99%)	351 (89%)	39 (10%)	4 (1%)	15	54
4	D	378/418 (90%)	337 (89%)	40 (11%)	1 (0%)	41	75
5	E	387/403 (96%)	357 (92%)	30 (8%)	0	100	100
6	F	396/439 (90%)	360 (91%)	36 (9%)	0	100	100
7	G	238/246 (97%)	225 (94%)	13 (6%)	0	100	100
7	g	242/246 (98%)	234 (97%)	8 (3%)	0	100	100
8	H	230/234 (98%)	216 (94%)	14 (6%)	0	100	100
8	h	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
9	I	246/261 (94%)	234 (95%)	12 (5%)	0	100	100
9	i	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
10	J	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
10	j	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
11	K	236/241 (98%)	229 (97%)	7 (3%)	0	100	100
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	238/269 (88%)	225 (94%)	13 (6%)	0	100	100
12	l	236/269 (88%)	224 (95%)	12 (5%)	0	100	100
13	M	240/255 (94%)	232 (97%)	8 (3%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
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%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
19	s	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
20	T	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
22	x	492/494 (100%)	469 (95%)	22 (4%)	1 (0%)	47	81
23	y	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
24	U	868/953 (91%)	785 (90%)	83 (10%)	0	100	100
25	V	442/534 (83%)	432 (98%)	10 (2%)	0	100	100
26	W	444/456 (97%)	415 (94%)	28 (6%)	1 (0%)	47	81
27	X	378/422 (90%)	357 (94%)	21 (6%)	0	100	100
28	Y	387/389 (100%)	349 (90%)	35 (9%)	3 (1%)	19	58
29	Z	284/324 (88%)	243 (86%)	41 (14%)	0	100	100
30	a	371/376 (99%)	345 (93%)	26 (7%)	0	100	100
31	b	189/377 (50%)	170 (90%)	19 (10%)	0	100	100
32	c	285/310 (92%)	244 (86%)	41 (14%)	0	100	100
33	d	255/350 (73%)	222 (87%)	33 (13%)	0	100	100
34	f	887/908 (98%)	778 (88%)	107 (12%)	2 (0%)	47	81
35	e	48/70 (69%)	41 (85%)	7 (15%)	0	100	100
All	All	13990/15458 (90%)	13036 (93%)	940 (7%)	14 (0%)	54	84

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO

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Mol	Chain	Res	Type
3	C	224	ILE
4	D	416	PHE
22	x	87	VAL
34	f	100	ARG
28	Y	8	GLU
1	A	66	LYS
3	C	90	HIS
3	C	91	PRO
26	W	140	ILE
28	Y	2	PRO
34	f	110	TYR
3	C	131	VAL
28	Y	211	TYR

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	349/372 (94%)	341 (98%)	8 (2%)	50	77
2	B	357/385 (93%)	350 (98%)	7 (2%)	55	79
3	C	340/346 (98%)	337 (99%)	3 (1%)	78	90
4	D	333/366 (91%)	327 (98%)	6 (2%)	59	81
5	E	341/353 (97%)	339 (99%)	2 (1%)	86	94
6	F	344/379 (91%)	340 (99%)	4 (1%)	71	87
7	G	202/210 (96%)	201 (100%)	1 (0%)	88	94
7	g	201/210 (96%)	199 (99%)	2 (1%)	76	88
8	H	187/191 (98%)	186 (100%)	1 (0%)	88	94
8	h	188/191 (98%)	188 (100%)	0	100	100
9	I	202/221 (91%)	200 (99%)	2 (1%)	76	88
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	196 (100%)	1 (0%)	88	94
10	j	196/211 (93%)	195 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/230 (88%)	200 (99%)	2 (1%)	76	88
12	l	201/230 (87%)	200 (100%)	1 (0%)	88	94
13	M	198/212 (93%)	198 (100%)	0	100	100
13	m	198/212 (93%)	197 (100%)	1 (0%)	88	94
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (100%)	0	100	100
15	o	181/228 (79%)	180 (99%)	1 (1%)	86	94
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%)	167 (99%)	1 (1%)	86	94
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	153 (99%)	1 (1%)	86	94
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	177 (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
22	x	439/439 (100%)	435 (99%)	4 (1%)	78	90
23	y	68/68 (100%)	68 (100%)	0	100	100
24	U	748/816 (92%)	742 (99%)	6 (1%)	81	91
25	V	390/460 (85%)	387 (99%)	3 (1%)	81	91
26	W	410/416 (99%)	405 (99%)	5 (1%)	71	87
27	X	327/362 (90%)	325 (99%)	2 (1%)	86	94
28	Y	344/344 (100%)	331 (96%)	13 (4%)	33	65
29	Z	257/295 (87%)	250 (97%)	7 (3%)	44	73
30	a	333/336 (99%)	327 (98%)	6 (2%)	59	81
31	b	167/312 (54%)	167 (100%)	0	100	100
32	c	252/268 (94%)	251 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	d	231/294 (79%)	231 (100%)	0	100	100
34	f	745/763 (98%)	737 (99%)	8 (1%)	73	88
35	e	44/63 (70%)	43 (98%)	1 (2%)	50	77
All	All	11960/13133 (91%)	11858 (99%)	102 (1%)	79	90

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	62	LEU
1	A	65	ILE
1	A	66	LYS
1	A	227	ARG
1	A	369	ARG
1	A	373	LEU
1	A	407	LYS
2	B	59	ARG
2	B	74	MET
2	B	88	LEU
2	B	97	SER
2	B	125	THR
2	B	410	ARG
2	B	411	ARG
3	C	101	LYS
3	C	109	THR
3	C	210	THR
4	D	80	LYS
4	D	84	SER
4	D	274	ARG
4	D	339	ARG
4	D	342	ARG
4	D	369	LYS
5	E	122	MET
5	E	241	ARG
6	F	61	ARG
6	F	171	ARG
6	F	250	LYS
6	F	308	ARG
7	G	17	SER
8	H	143	ARG
9	I	246	LYS

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Mol	Chain	Res	Type
9	I	249	ARG
10	J	204	LYS
12	L	101	ARG
12	L	125	ARG
17	Q	95	ARG
7	g	88	ARG
7	g	224	ASN
10	j	227	LYS
12	l	101	ARG
13	m	236	GLU
15	o	182	LYS
18	r	106	LYS
20	t	195	LYS
22	x	64	LYS
22	x	78	LEU
22	x	238	LYS
22	x	293	ARG
24	U	55	ARG
24	U	188	MET
24	U	417	LYS
24	U	597	LYS
24	U	838	LYS
24	U	854	MET
25	V	106	ARG
25	V	180	ARG
25	V	461	LYS
26	W	118	LEU
26	W	142	ARG
26	W	191	ARG
26	W	315	MET
26	W	329	ARG
27	X	84	LYS
27	X	278	ARG
28	Y	5	ASN
28	Y	6	LEU
28	Y	13	LYS
28	Y	23	ARG
28	Y	46	ARG
28	Y	113	ARG
28	Y	205	VAL
28	Y	208	PHE
28	Y	209	THR

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Mol	Chain	Res	Type
28	Y	210	SER
28	Y	211	TYR
28	Y	212	GLU
28	Y	214	MET
29	Z	33	LYS
29	Z	143	GLU
29	Z	145	HIS
29	Z	149	THR
29	Z	151	THR
29	Z	175	LEU
29	Z	176	LEU
30	a	105	LYS
30	a	230	ARG
30	a	252	LYS
30	a	289	ARG
30	a	339	ARG
30	a	342	ASP
32	c	125	VAL
34	f	150	GLU
34	f	178	LYS
34	f	195	ASN
34	f	673	ARG
34	f	680	ARG
34	f	845	ARG
34	f	873	LEU
34	f	874	LEU
35	e	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	53	ASN
22	x	473	HIS
24	U	135	ASN
24	U	373	ASN
26	W	395	ASN
34	f	148	GLN
34	f	815	HIS

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 7 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
37	ATP	C	501	-	26,33,33	0.62	0	31,52,52	0.84	1 (3%)
37	ATP	F	501	-	26,33,33	0.64	0	31,52,52	0.77	1 (3%)
37	ATP	E	501	-	26,33,33	0.62	0	31,52,52	0.73	2 (6%)
36	ADP	A	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
37	ATP	D	501	-	26,33,33	0.64	0	31,52,52	0.75	1 (3%)
36	ADP	B	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)

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
37	ATP	C	501	-	-	6/18/38/38	0/3/3/3
37	ATP	F	501	-	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ATP	E	501	-	-	3/18/38/38	0/3/3/3
36	ADP	A	501	-	-	2/12/32/32	0/3/3/3
37	ATP	D	501	-	-	8/18/38/38	0/3/3/3
36	ADP	B	501	-	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	501	ADP	C5-C4	2.48	1.47	1.40
36	A	501	ADP	C5-C4	2.41	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	A	501	ADP	PA-O3A-PB	-3.95	119.26	132.83
36	B	501	ADP	C3'-C2'-C1'	3.72	106.58	100.98
36	A	501	ADP	C3'-C2'-C1'	3.48	106.22	100.98
36	B	501	ADP	PA-O3A-PB	-3.43	121.06	132.83
36	B	501	ADP	N3-C2-N1	-3.13	123.78	128.68
36	A	501	ADP	N3-C2-N1	-3.10	123.84	128.68
36	A	501	ADP	C4-C5-N7	-2.75	106.53	109.40
36	B	501	ADP	C4-C5-N7	-2.51	106.78	109.40
37	C	501	ATP	C5-C6-N6	2.30	123.84	120.35
37	F	501	ATP	C5-C6-N6	2.30	123.84	120.35
37	D	501	ATP	C5-C6-N6	2.28	123.82	120.35
37	E	501	ATP	C5-C6-N6	2.27	123.80	120.35
37	E	501	ATP	PB-O3B-PG	2.01	139.71	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	501	ADP	C5'-O5'-PA-O3A
36	B	501	ADP	C5'-O5'-PA-O2A
36	B	501	ADP	C5'-O5'-PA-O3A
36	B	501	ADP	C3'-C4'-C5'-O5'
37	C	501	ATP	C5'-O5'-PA-O2A
37	D	501	ATP	PB-O3B-PG-O3G
37	D	501	ATP	C5'-O5'-PA-O2A
37	F	501	ATP	O4'-C4'-C5'-O5'

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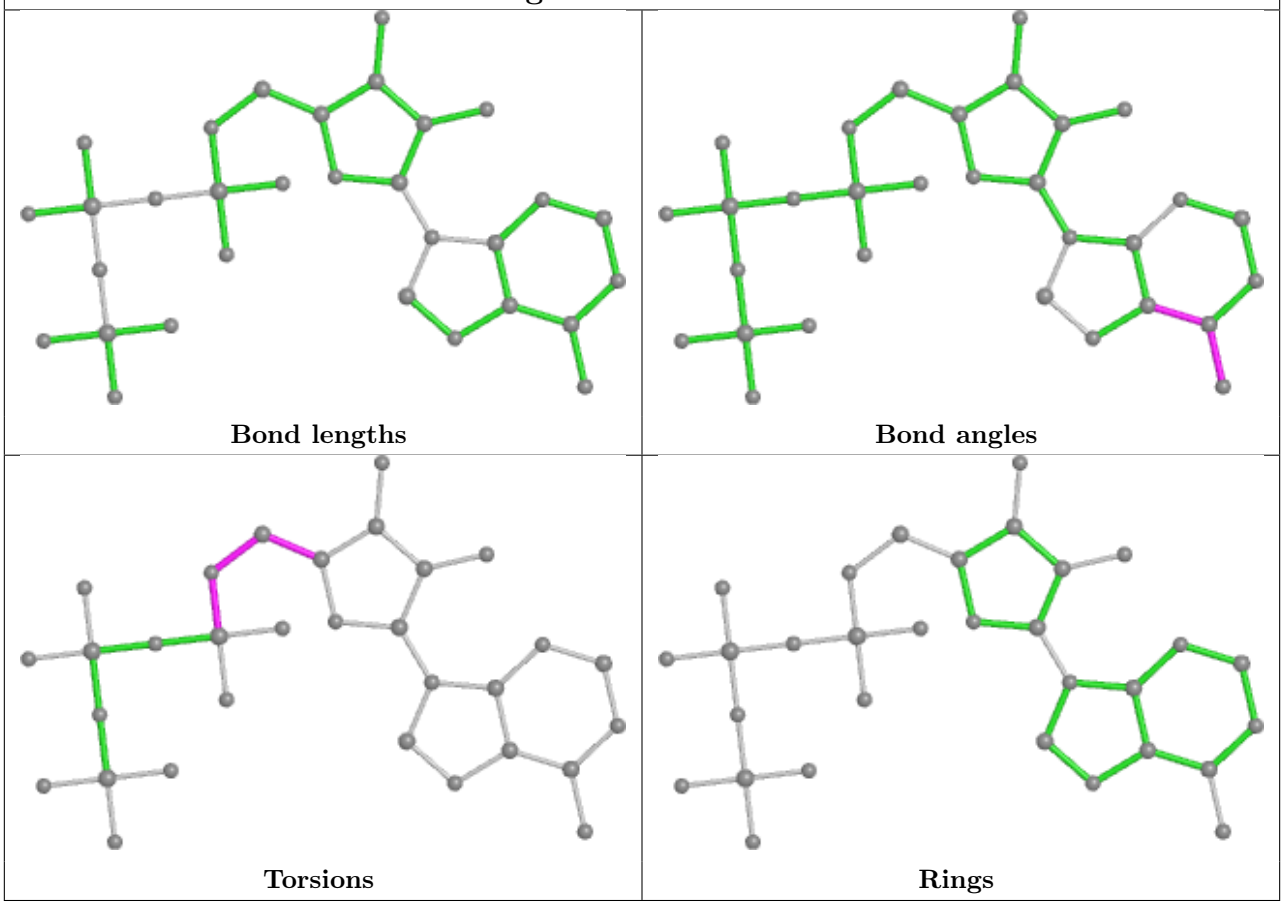
Mol	Chain	Res	Type	Atoms
36	B	501	ADP	O4'-C4'-C5'-O5'
37	C	501	ATP	C3'-C4'-C5'-O5'
37	F	501	ATP	C3'-C4'-C5'-O5'
37	C	501	ATP	O4'-C4'-C5'-O5'
37	D	501	ATP	O4'-C4'-C5'-O5'
37	C	501	ATP	C5'-O5'-PA-O3A
37	D	501	ATP	C5'-O5'-PA-O3A
37	E	501	ATP	C5'-O5'-PA-O3A
36	B	501	ADP	C4'-C5'-O5'-PA
37	C	501	ATP	C4'-C5'-O5'-PA
36	A	501	ADP	C5'-O5'-PA-O1A
37	C	501	ATP	C5'-O5'-PA-O1A
37	D	501	ATP	C5'-O5'-PA-O1A
37	E	501	ATP	PG-O3B-PB-O2B
37	F	501	ATP	C4'-C5'-O5'-PA
37	D	501	ATP	PB-O3B-PG-O1G
37	E	501	ATP	C4'-C5'-O5'-PA
37	D	501	ATP	PG-O3B-PB-O1B
37	D	501	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

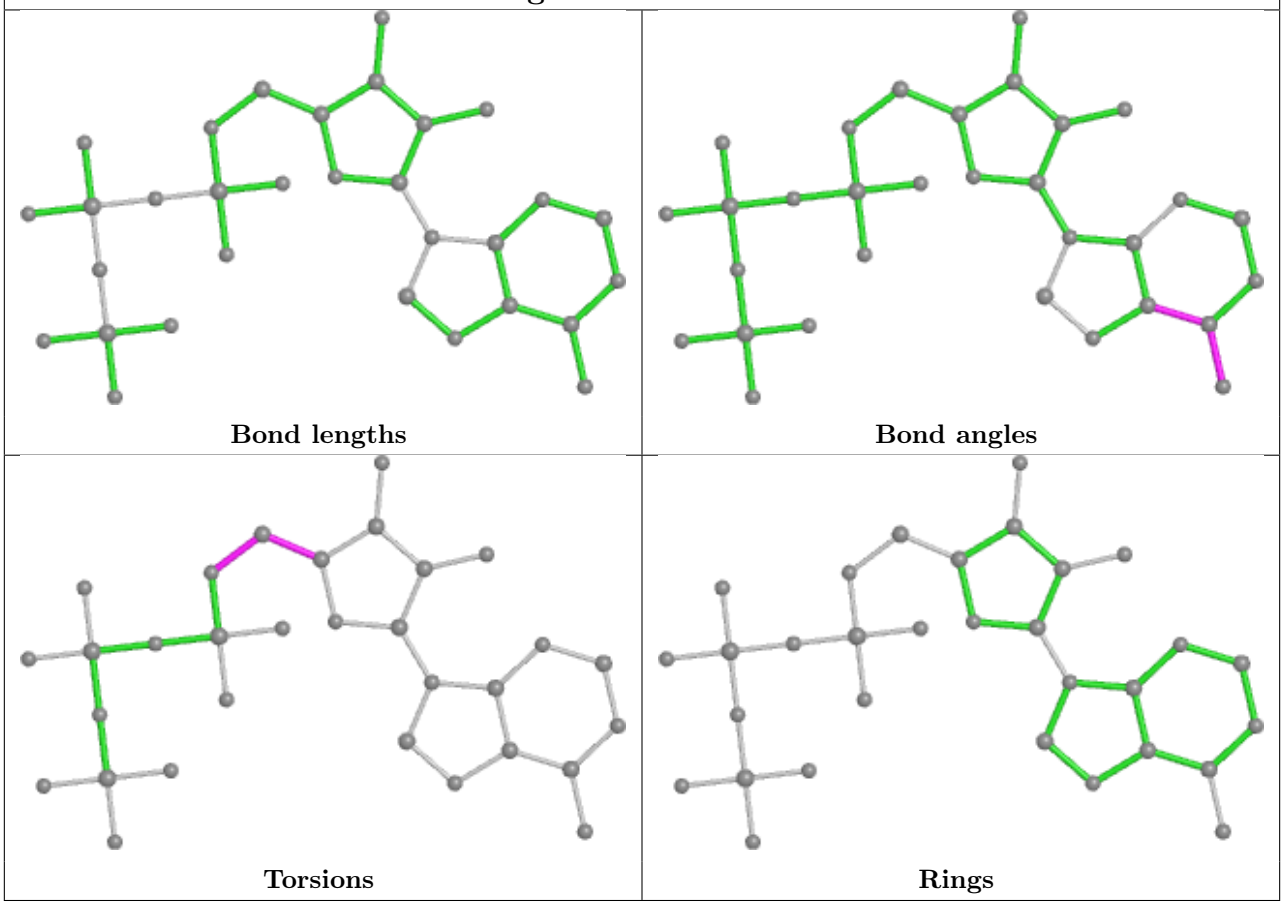
No monomer is involved in short contacts.

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.

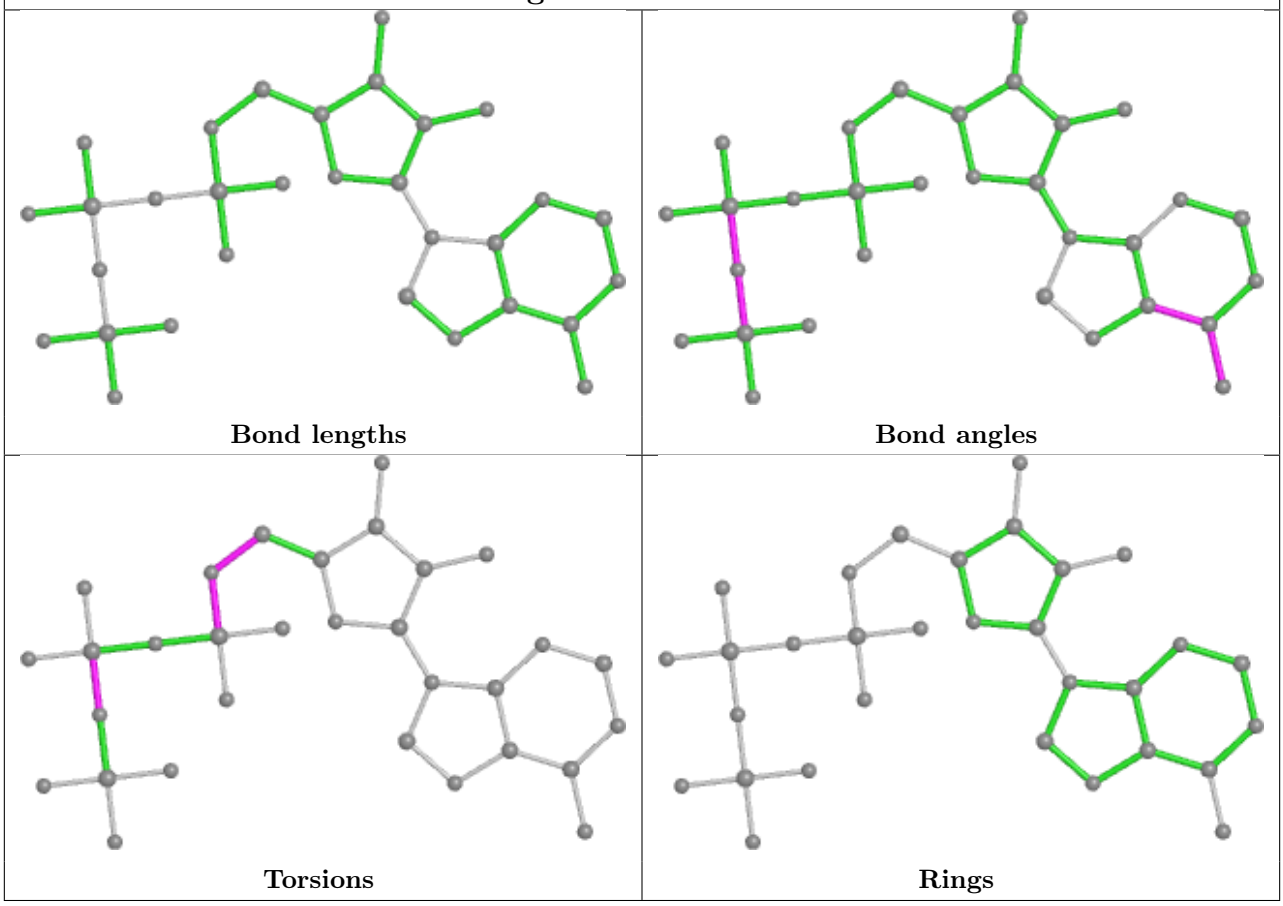
Ligand ATP C 501



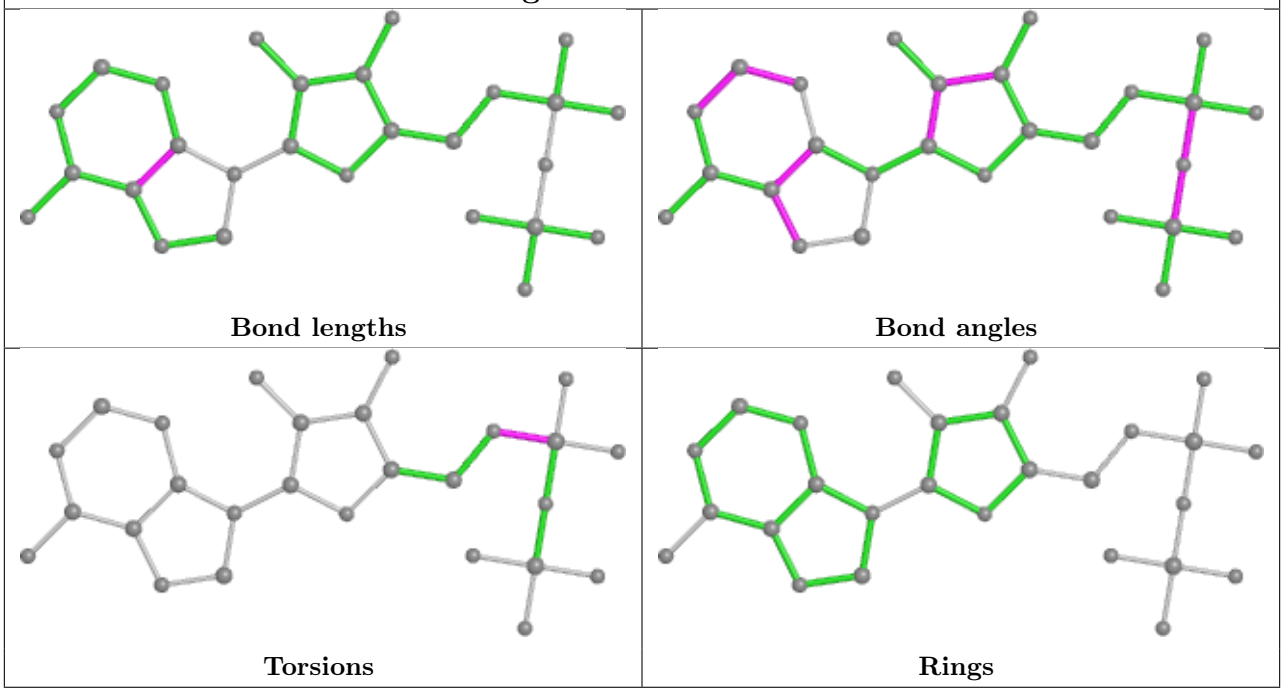
Ligand ATP F 501



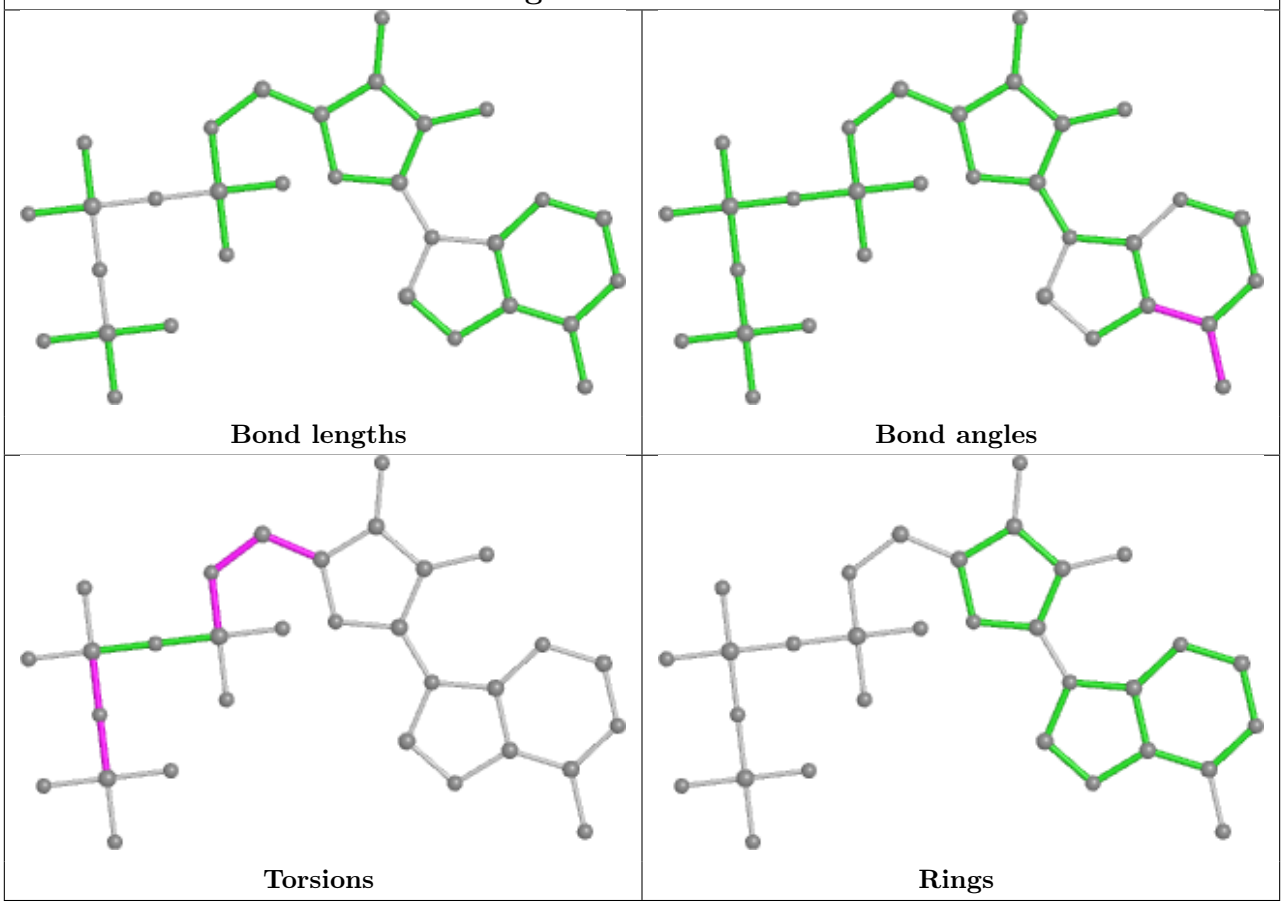
Ligand ATP E 501



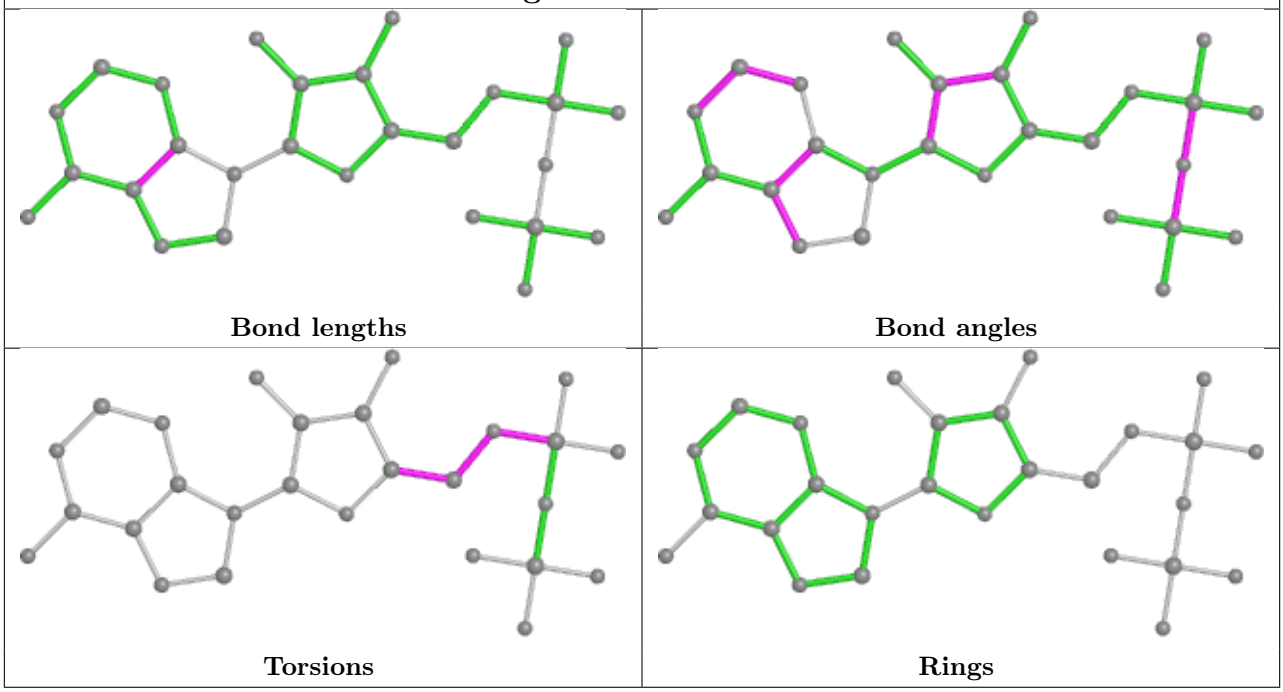
Ligand ADP A 501



Ligand ATP D 501



Ligand ADP B 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.

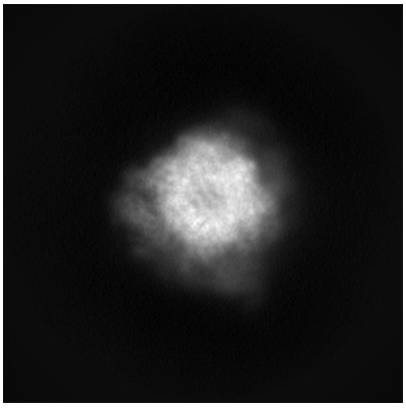
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32275. These allow visual inspection of the internal detail of the map and identification of artifacts.

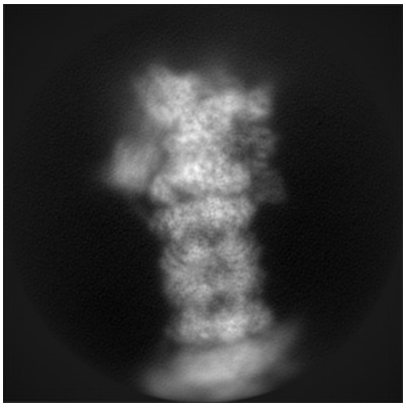
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

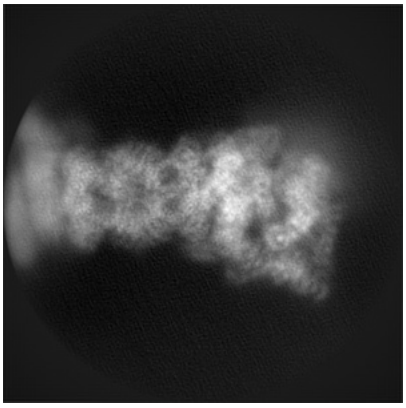
6.1.1 Primary map



X



Y

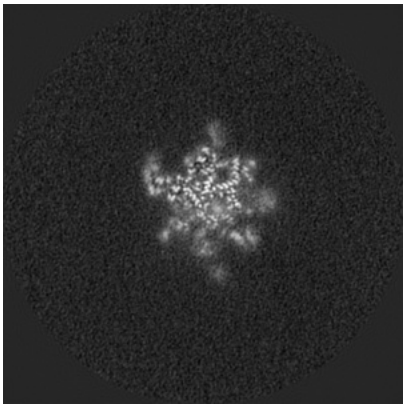


Z

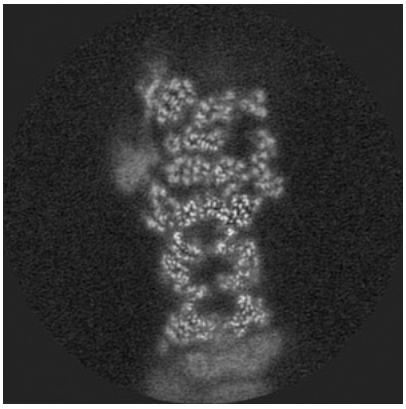
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

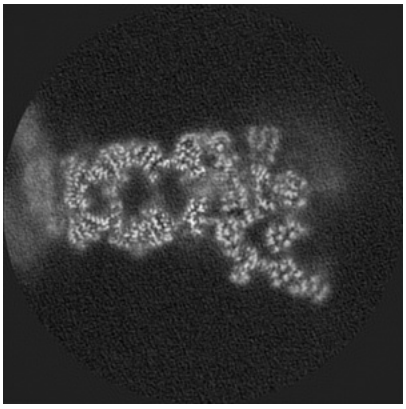
6.2.1 Primary map



X Index: 320



Y Index: 320

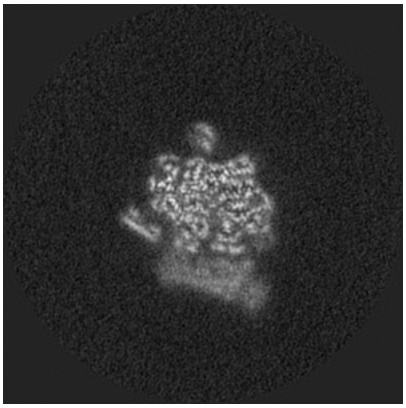


Z Index: 320

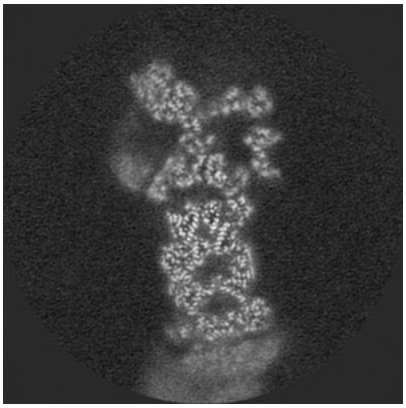
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

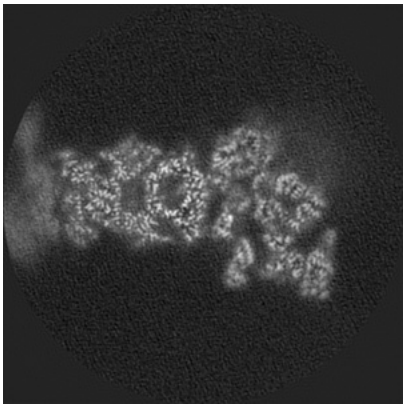
6.3.1 Primary map



X Index: 359



Y Index: 302



Z Index: 298

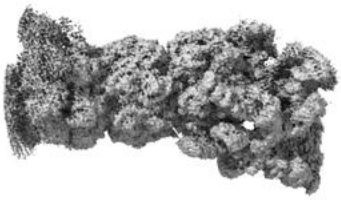
The images above show the largest variance slices of the map in three orthogonal directions.

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.

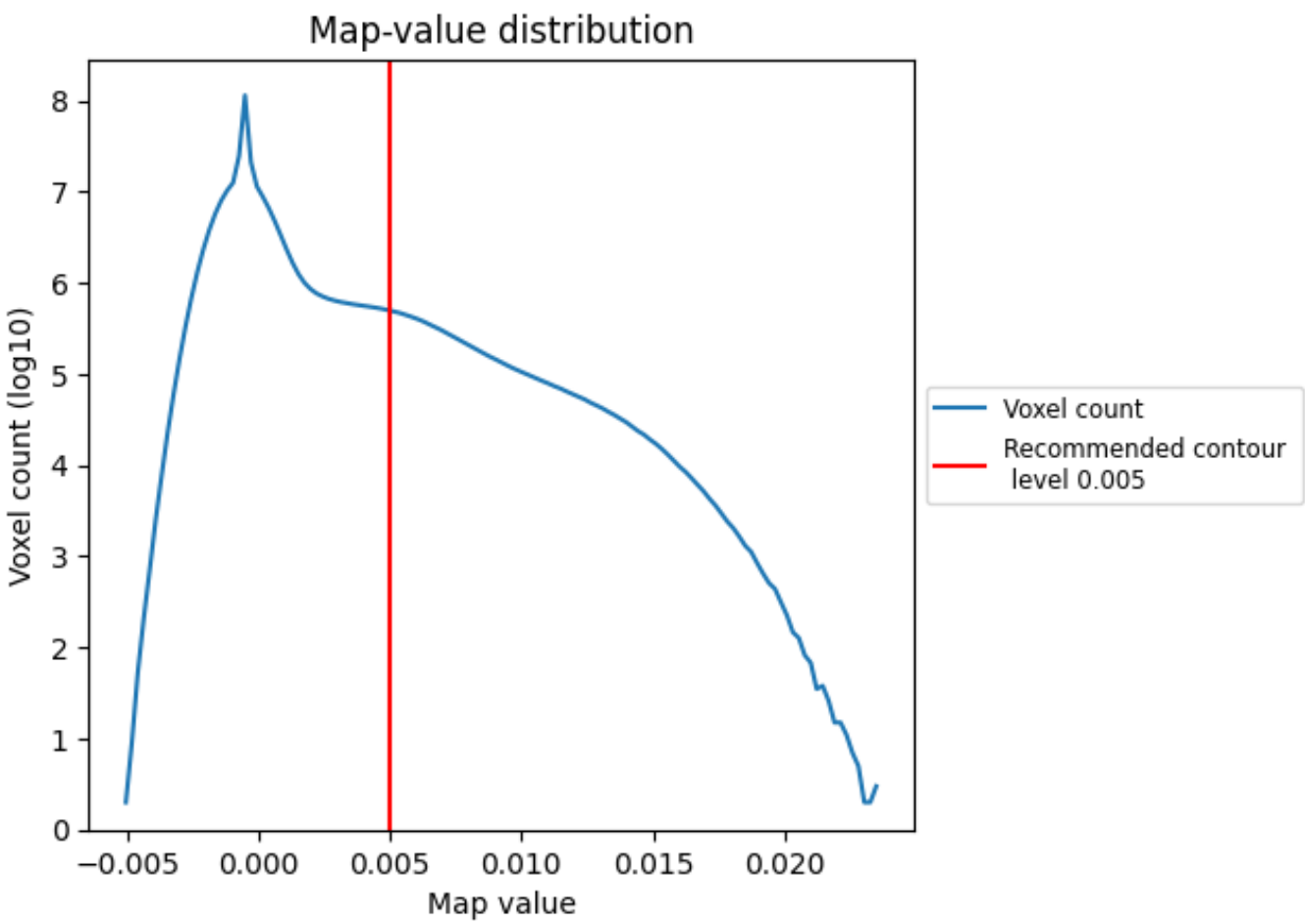
6.5 Mask visualisation (i)

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

7 Map analysis (i)

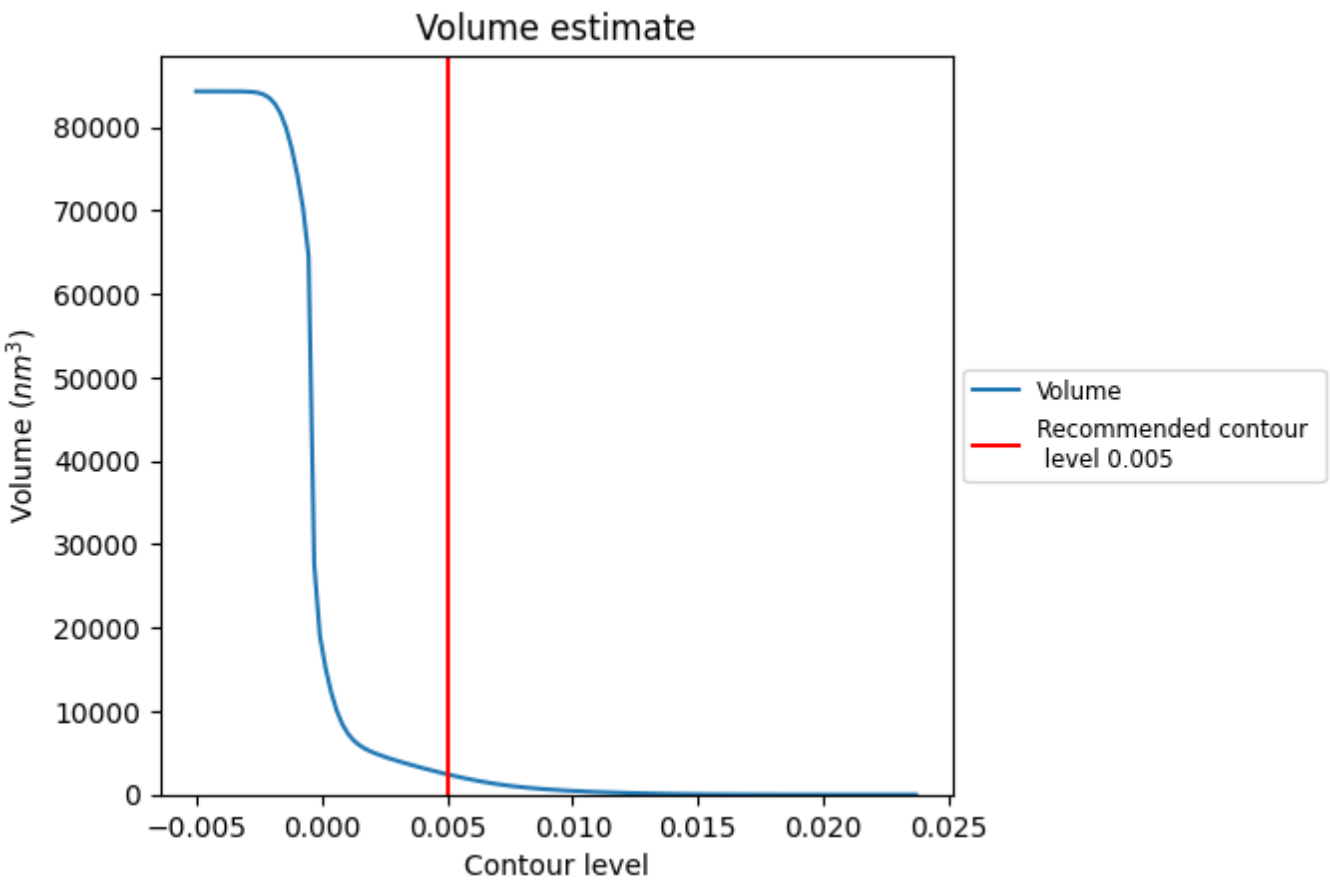
This section contains the results of statistical analysis of the map.

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.

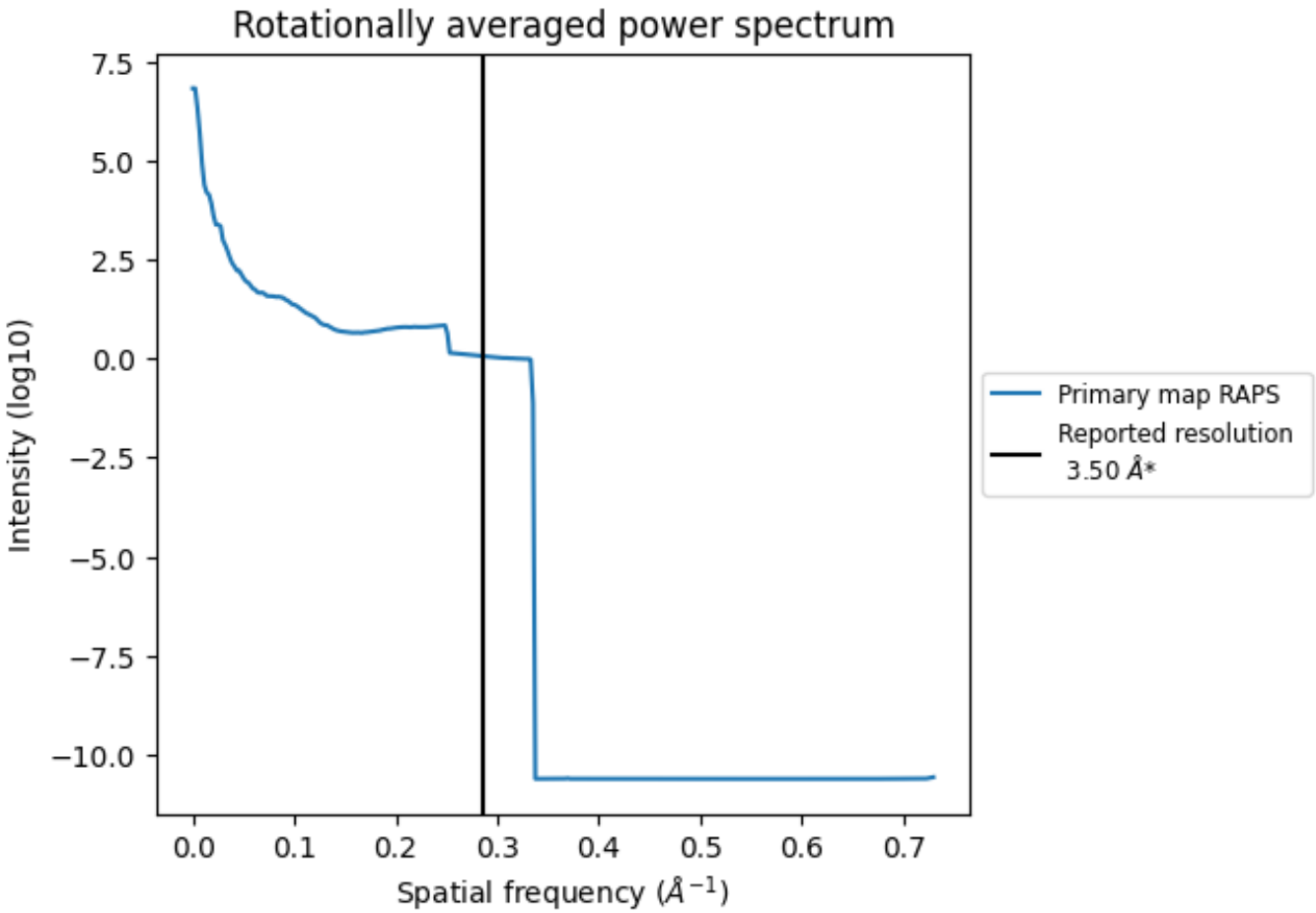
7.2 Volume estimate (i)



The volume at the recommended contour level is 2426 nm^3; this corresponds to an approximate mass of 2191 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 0.286 Å^{-1}

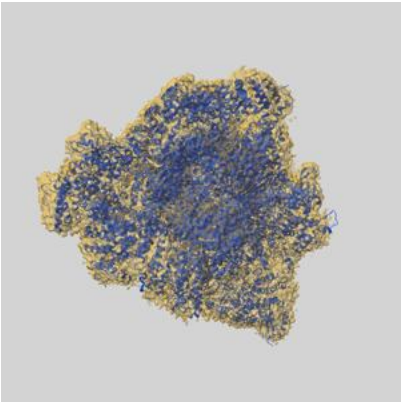
8 Fourier-Shell correlation (i)

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

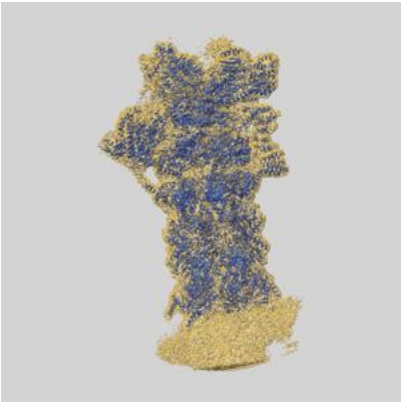
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32275 and PDB model 7W3A. Per-residue inclusion information can be found in section 3 on page 13.

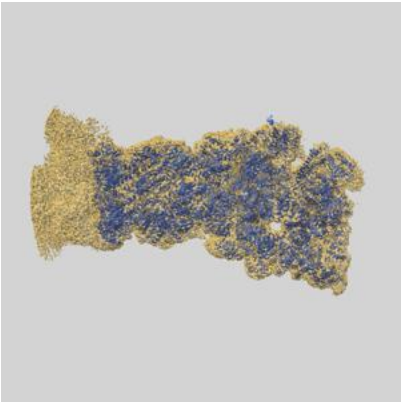
9.1 Map-model overlay (i)



X



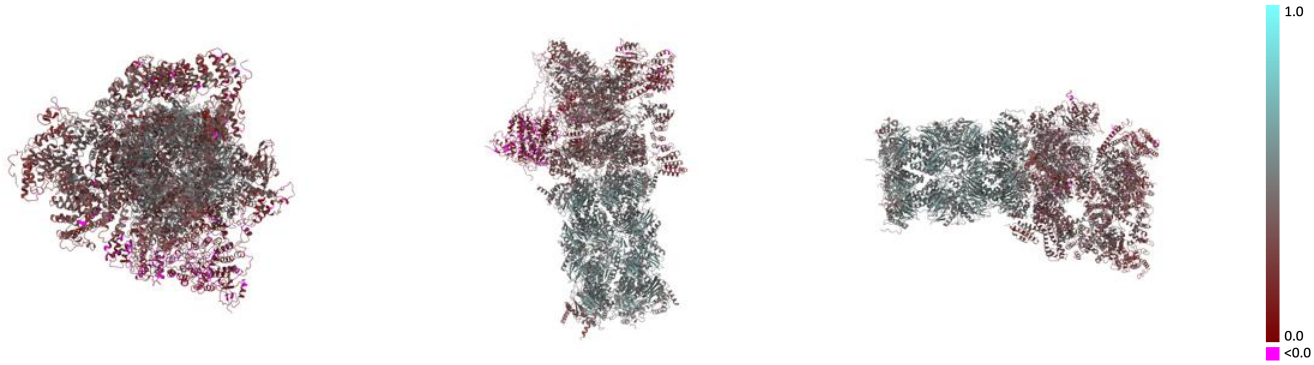
Y



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.

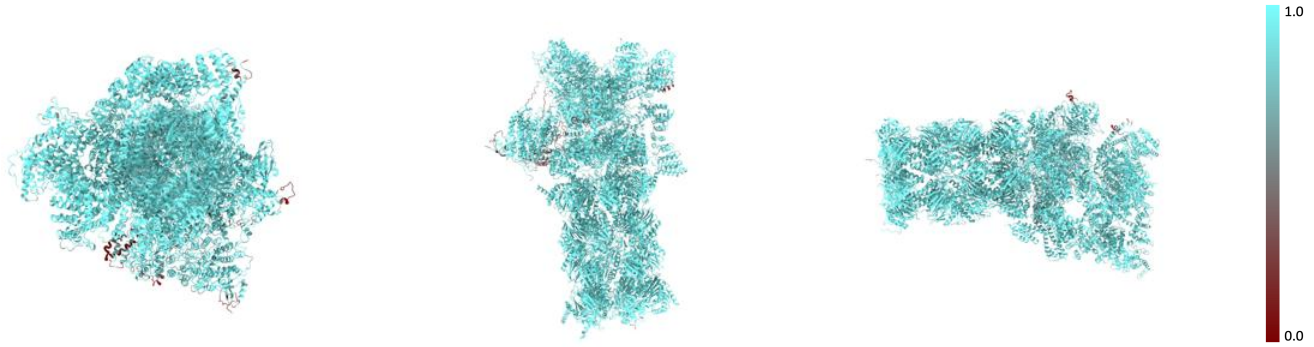
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

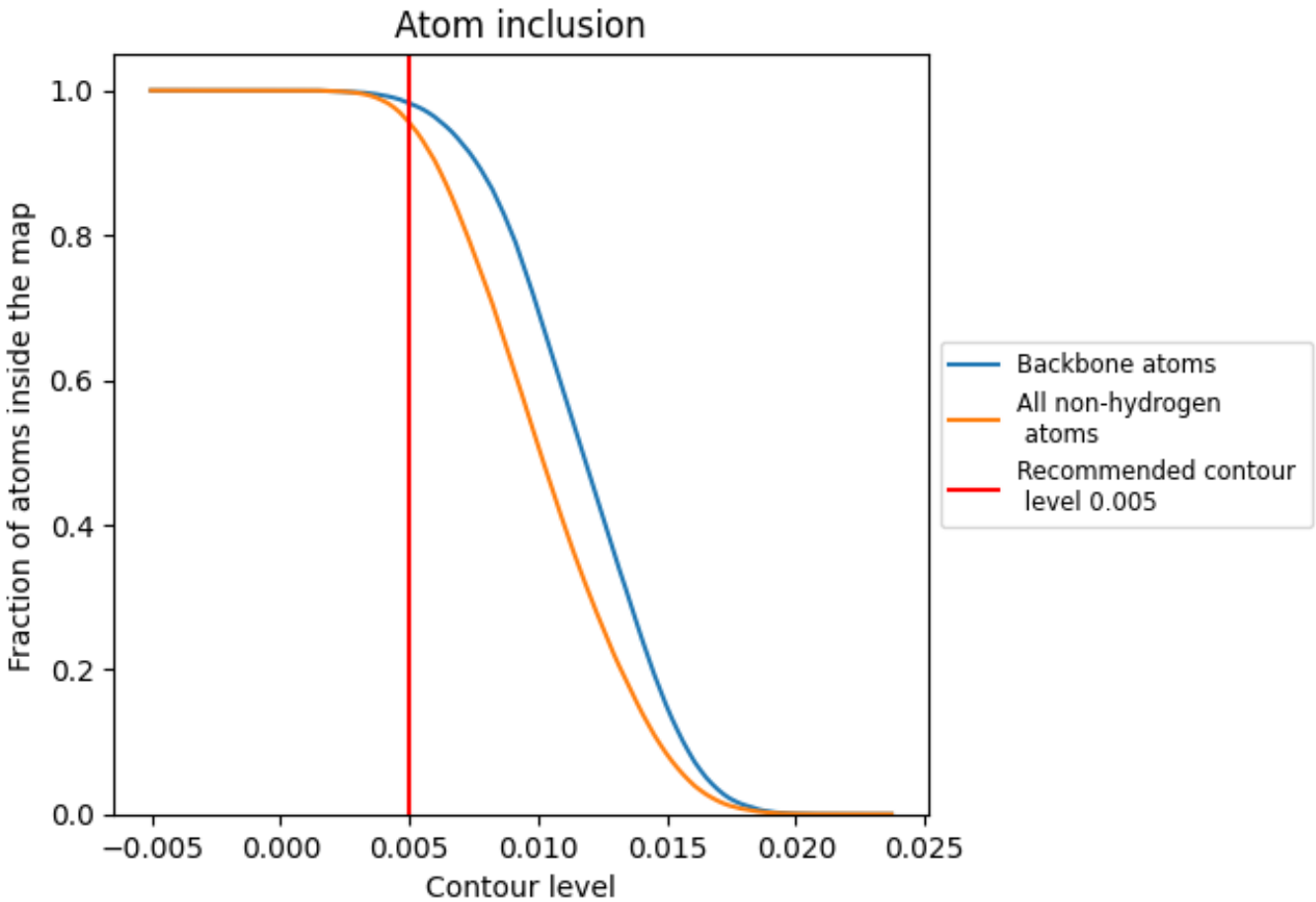
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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	0.9554	0.3900
A	0.9426	0.3320
B	0.9252	0.3000
C	0.9632	0.3300
D	0.9734	0.3670
E	0.9575	0.3680
F	0.9418	0.3660
G	0.9869	0.4970
H	0.9887	0.4940
I	0.9837	0.4810
J	0.9807	0.4780
K	0.9838	0.4900
L	0.9924	0.5040
M	0.9870	0.5010
N	0.9879	0.5190
O	0.9926	0.5120
P	0.9923	0.5220
Q	0.9903	0.5170
R	0.9947	0.5210
S	0.9932	0.5090
T	0.9859	0.5260
U	0.9226	0.3270
V	0.9503	0.3300
W	0.9310	0.2950
X	0.9614	0.3500
Y	0.9535	0.3300
Z	0.9733	0.3350
a	0.9461	0.2830
b	0.9473	0.2680
c	0.9659	0.3420
d	0.9253	0.2580
e	0.9451	0.3200
f	0.8629	0.1480
g	0.9783	0.4950
h	0.9830	0.4980

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Chain	Atom inclusion	Q-score
i	0.9739	0.4700
j	0.9686	0.4350
k	0.9768	0.4740
l	0.9890	0.5060
m	0.9777	0.4930
n	0.9946	0.5270
o	0.9902	0.5170
p	0.9936	0.5220
q	0.9948	0.5190
r	0.9960	0.5250
s	0.9901	0.5130
t	0.9884	0.5220
v	0.9882	0.3420
x	0.8519	0.2700
y	0.9409	0.3260