Full wwPDB EM Validation Report (i)

Nov 7, 2022 – 10:47 PM EST

PDB ID	:	6MSB
EMDB ID	:	EMD-9216
Title	:	Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors	:	Mao, Y.D.
Deposited on	:	2018-10-16
Resolution	:	3.00 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:

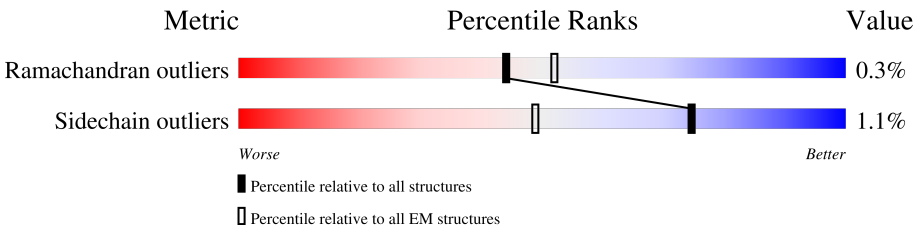
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.00 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	U	953	84% • 15%
2	V	534	11% 93% • 5%
3	W	456	7% 97% •
4	X	422	88% • 10%
5	Y	389	96% • •
6	Z	324	85% • 12%
7	a	376	98% • •
8	b	377	50% 49%
9	c	309	88% 5% 7%

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Mol	Chain	Length	Quality of chain
10	d	349	5% 72% 26%
11	e	70	9% 54% 43%
12	f	908	16% 94%
13	A	433	87% 9%
14	B	440	85% 13%
15	C	398	88% 9%
16	D	418	87% 9%
17	E	403	91% 7%
18	F	439	85% 14%
19	u	76	99% 100%
19	w	76	91% 100%
20	G	245	98%
20	g	245	98%
21	H	233	99%
21	h	233	99%
22	I	260	95%
22	i	260	95%
23	J	247	95%
23	j	247	95%
24	K	240	94% 5%
24	k	240	94% 5%
25	L	268	88% 11%
25	l	268	88% 11%
26	M	254	93% 6%
26	m	254	93% 6%

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Mol	Chain	Length	Quality of chain
27	N	238	80% 20%
27	n	238	80% 20%
28	O	276	80% 20%
28	o	276	80% 20%
29	P	204	100%
29	p	204	100%
30	Q	201	97%
30	q	201	97%
31	R	262	77% 23%
31	r	262	77% 23%
32	S	240	89% 11%
32	s	240	89% 11%
33	T	263	81% 18%
33	t	263	81% 18%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 104938 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 proteasome non-ATPase regulatory subunit 1.

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

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	508	3994	2530	712	738	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	456	3703	2339	635	704	25	0	0

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e	40	334	200	55	77	2	0	0

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A	394	3096	1951	543	584	18	0	0

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B	384	3018	1901	515	587	15	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C	363	2864	1808	515	525	16	0	0

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	E	375	2860	1796	512	536	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	376	2858	1802	496	545	15	0	0

- Molecule 19 is a protein called Ubiquitin.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47
w	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	J	239	1713	1062	311	335	5	0	0
23	j	239	1704	1056	308	335	5	0	0

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	K	228	1722	1080	284	348	10	0	0
24	k	228	1722	1080	284	348	10	0	0

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

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

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

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	N	191	1430	893	245	280	12	0	0
27	n	191	1430	893	245	280	12	0	0

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	O	220	1643	1033	280	318	12	0	0
28	o	220	1643	1033	280	318	12	0	0

- Molecule 29 is a protein called Proteasome subunit beta type-3.

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

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Q	199	1570	1006	265	290	9	0	0
30	q	199	1570	1006	265	290	9	0	0

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	R	201	1548	974	273	292	9	0	0
31	r	201	1548	974	273	292	9	0	0

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	S	213	1641	1036	282	313	10	0	0
32	s	213	1644	1039	282	313	10	0	0

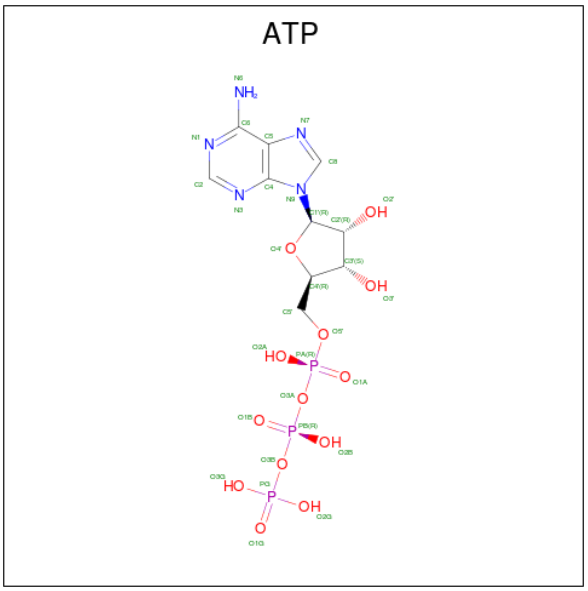
- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	T	215	1667	1052	285	318	12	0	0
33	t	215	1667	1052	285	318	12	0	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

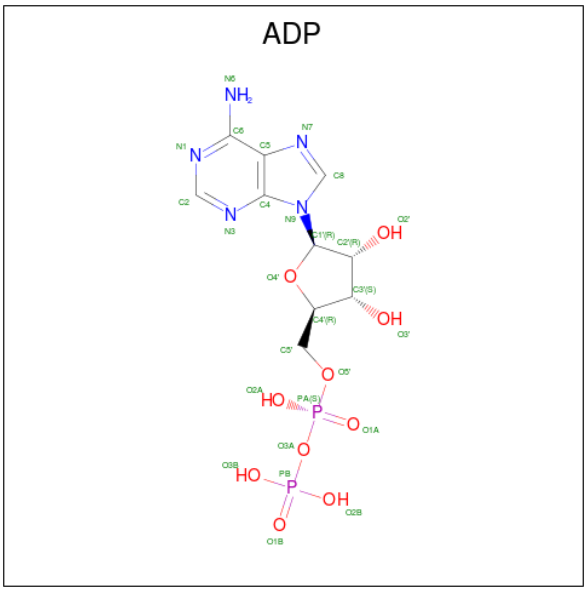


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



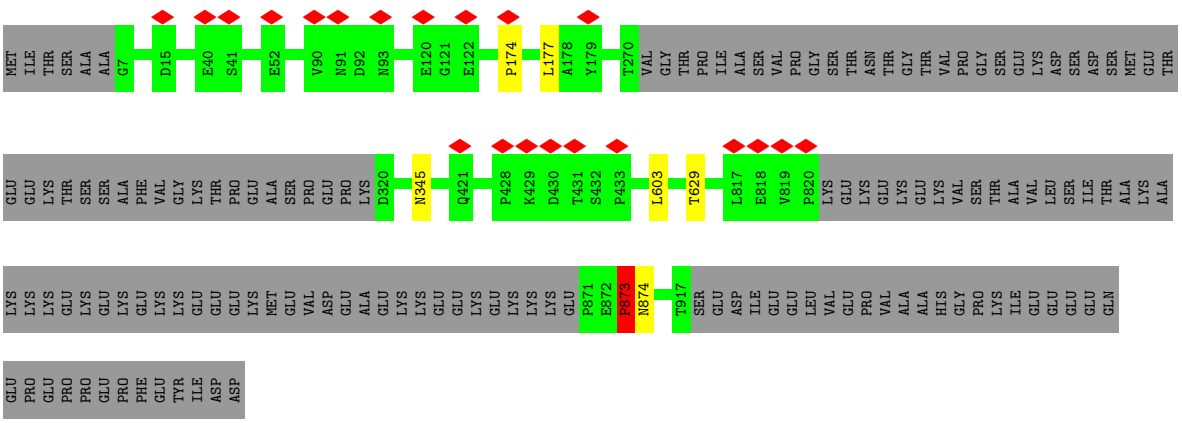
Mol	Chain	Residues	Atoms					AltConf
37	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
37	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

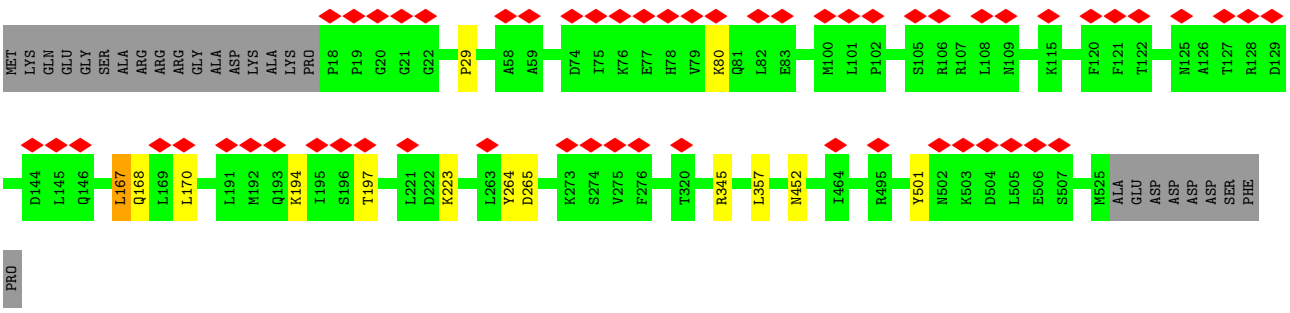
• Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 84% 15%



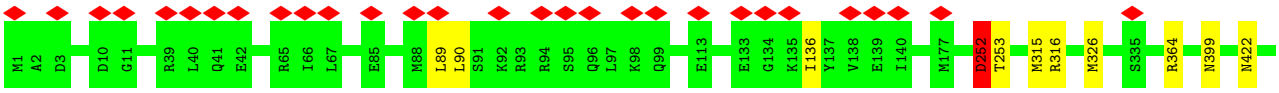
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

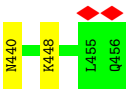
Chain V: 11% 93% 5%



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

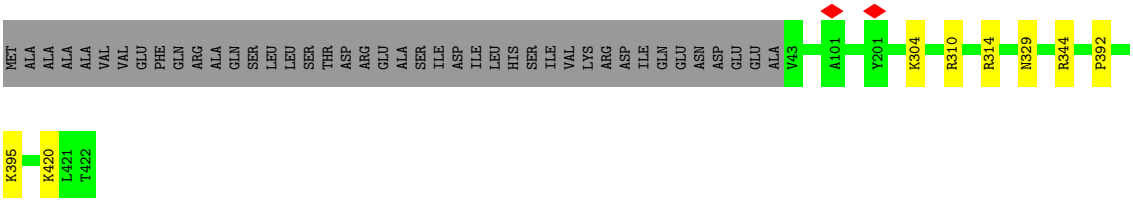
Chain W: 7% 97%





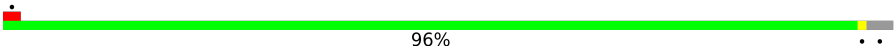
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

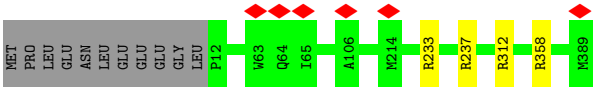
Chain X:



• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

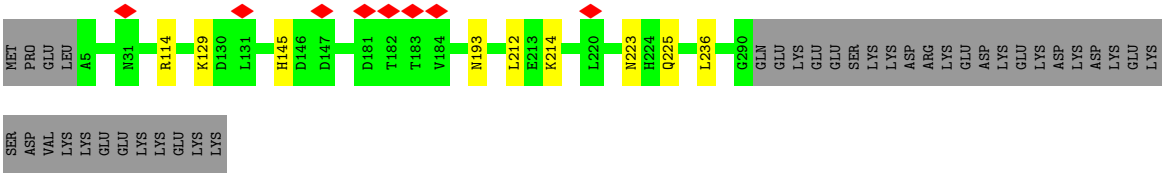
Chain Y:





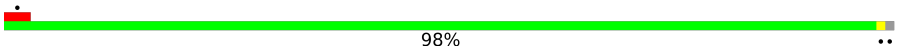
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

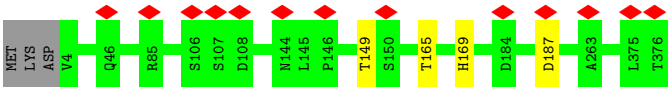
Chain Z:



• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

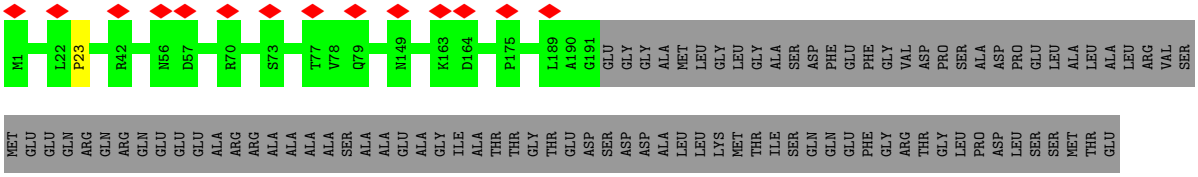
Chain a:

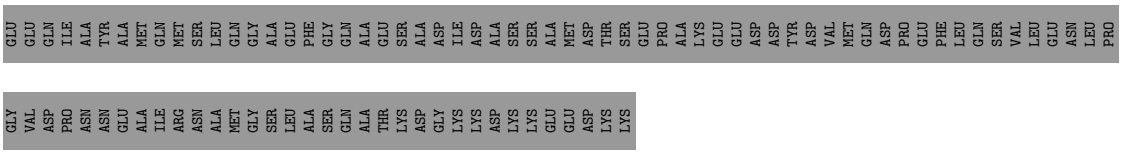




• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



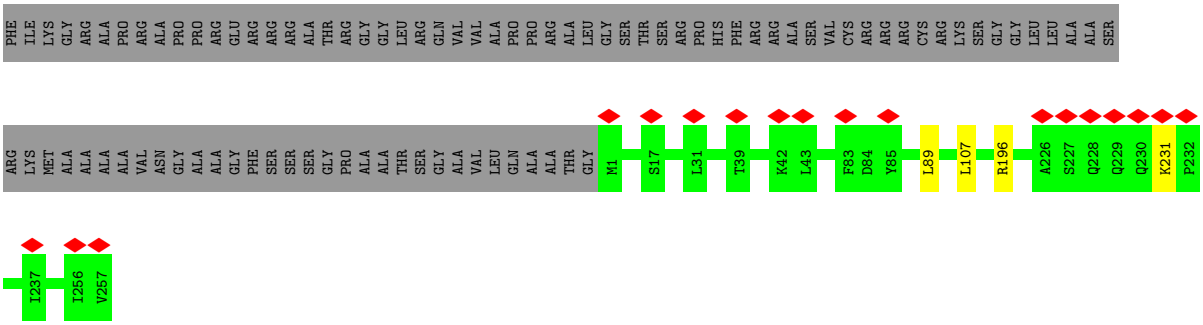


- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain c:

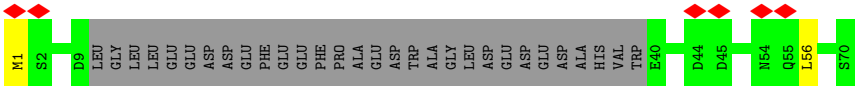
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



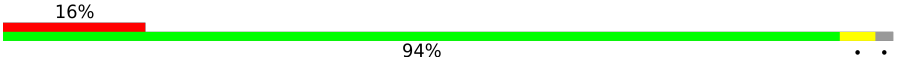
- Molecule 11: 26S proteasome complex subunit SEM1

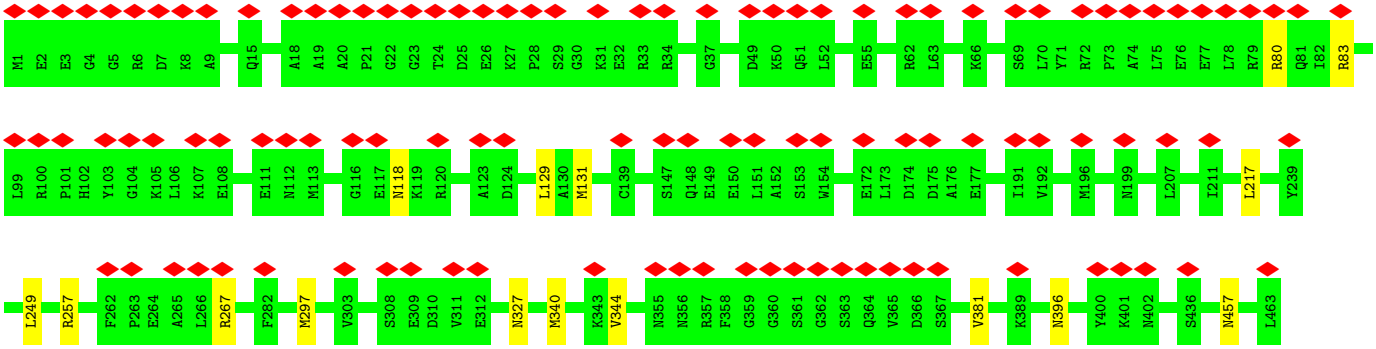
Chain e:

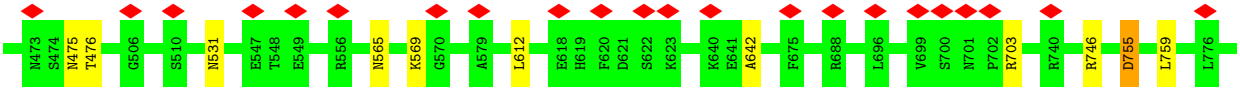


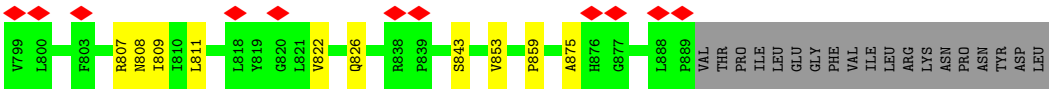
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain f:



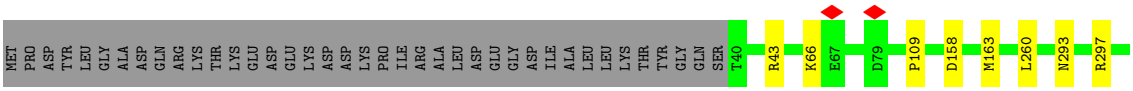






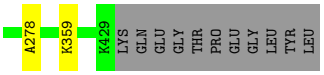
• Molecule 13: 26S proteasome regulatory subunit 7

Chain A:



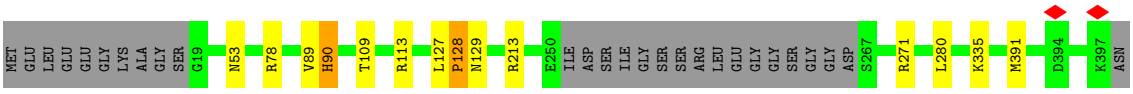
• Molecule 14: 26S proteasome regulatory subunit 4

Chain B:



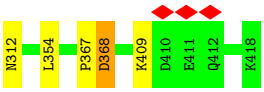
• Molecule 15: 26S proteasome regulatory subunit 8

Chain C:



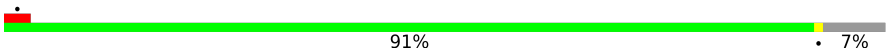
• Molecule 16: 26S proteasome regulatory subunit 6B

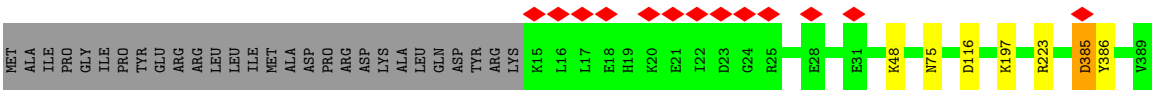
Chain D:



• Molecule 17: 26S proteasome regulatory subunit 10B

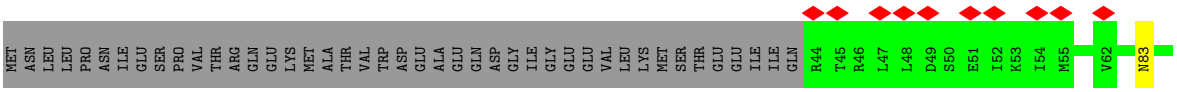
Chain E:





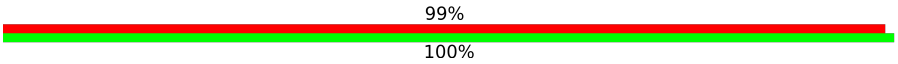
• Molecule 18: 26S proteasome regulatory subunit 6A

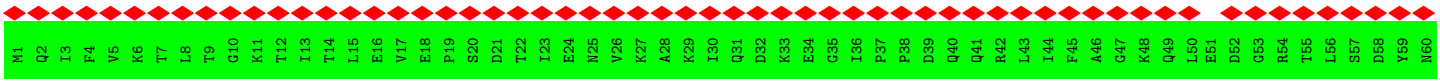
Chain F:

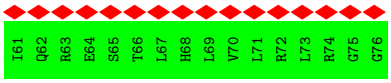


• Molecule 19: Ubiquitin

Chain u:

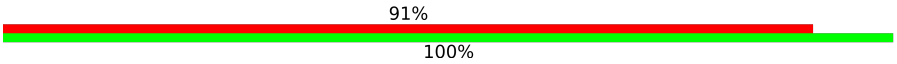


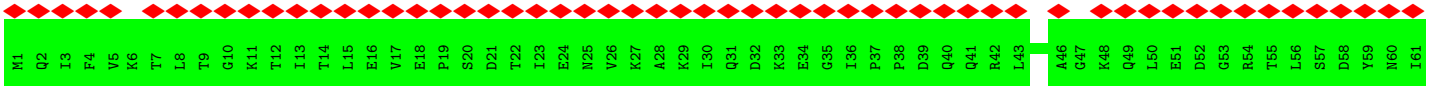


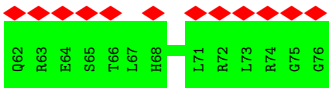


• Molecule 19: Ubiquitin

Chain w:

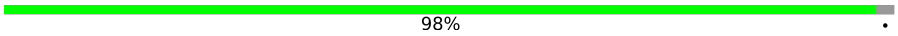


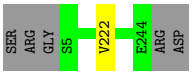




• Molecule 20: Proteasome subunit alpha type-6

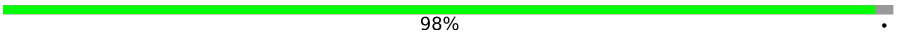
Chain G:

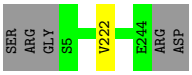




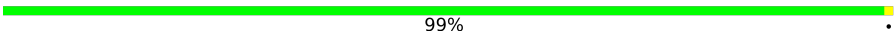
• Molecule 20: Proteasome subunit alpha type-6

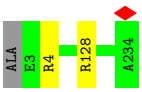
Chain g:



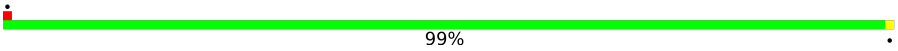


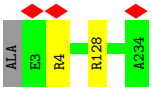
• Molecule 21: Proteasome subunit alpha type-2

Chain H: 

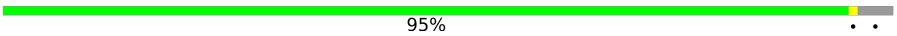


• Molecule 21: Proteasome subunit alpha type-2

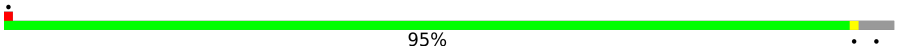
Chain h: 

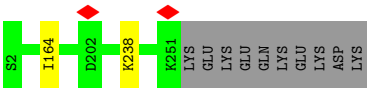


• Molecule 22: Proteasome subunit alpha type-4

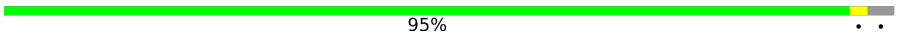
Chain I: 

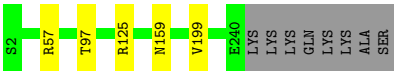
• Molecule 22: Proteasome subunit alpha type-4

Chain i: 

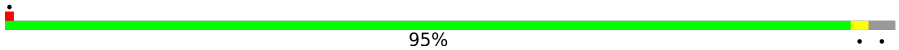


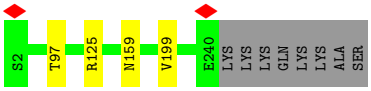
• Molecule 23: Proteasome subunit alpha type-7

Chain J: 



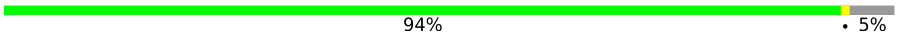
• Molecule 23: Proteasome subunit alpha type-7

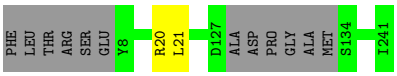
Chain j: 



• Molecule 24: Proteasome subunit alpha type-5

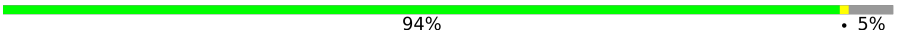
Chain K:

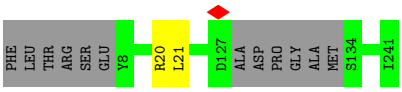




• Molecule 24: Proteasome subunit alpha type-5

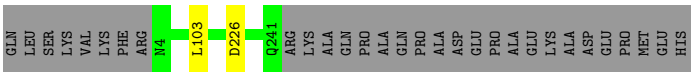
Chain k:





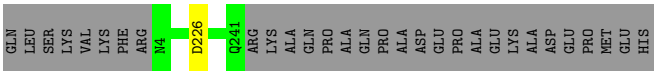
• Molecule 25: Proteasome subunit alpha type-1

Chain L:



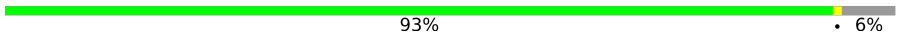
• Molecule 25: Proteasome subunit alpha type-1

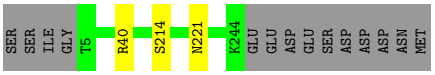
Chain l:



• Molecule 26: Proteasome subunit alpha type-3

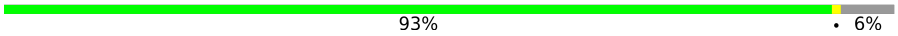
Chain M:

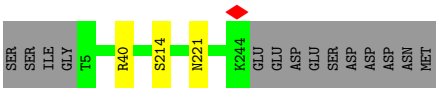




• Molecule 26: Proteasome subunit alpha type-3

Chain m:





• Molecule 27: Proteasome subunit beta type-6

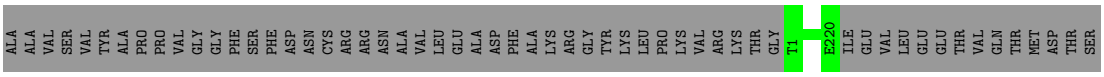
Chain N:

• Molecule 27: Proteasome subunit beta type-6

Chain n: 80% 20%

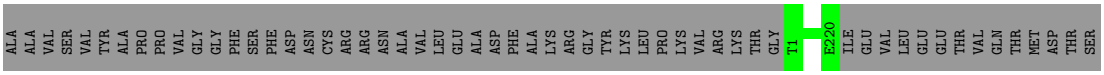
• Molecule 28: Proteasome subunit beta type-7

Chain O: 80% 20%



• Molecule 28: Proteasome subunit beta type-7

Chain o: 80% 20%



• Molecule 29: Proteasome subunit beta type-3

Chain P: 100%

There are no outlier residues recorded for this chain.

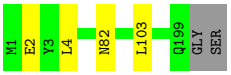
• Molecule 29: Proteasome subunit beta type-3

Chain p: 100%

There are no outlier residues recorded for this chain.

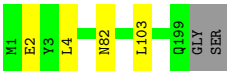
• Molecule 30: Proteasome subunit beta type-2

Chain Q: 97%



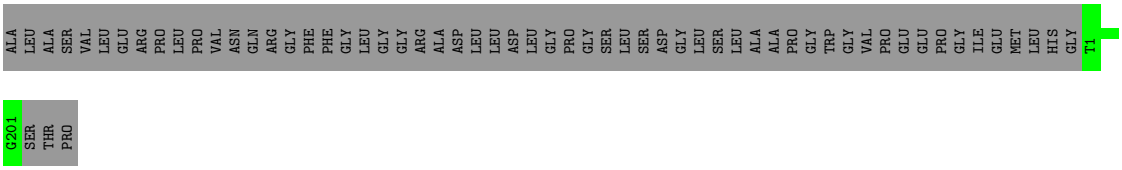
• Molecule 30: Proteasome subunit beta type-2

Chain q: 97%



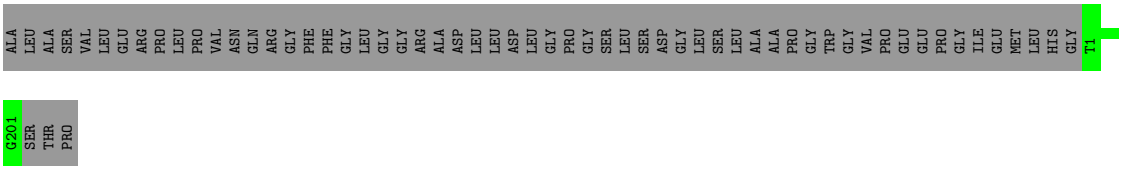
• Molecule 31: Proteasome subunit beta type-5

Chain R: 77% 23%



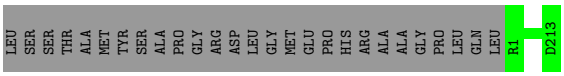
• Molecule 31: Proteasome subunit beta type-5

Chain r: 77% 23%



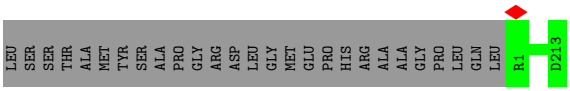
• Molecule 32: Proteasome subunit beta type-1

Chain S: 89% 11%



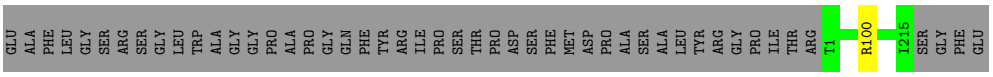
• Molecule 32: Proteasome subunit beta type-1

Chain s: 89% 11%



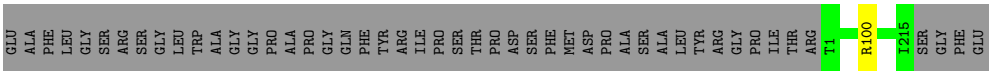
• Molecule 33: Proteasome subunit beta type-4

Chain T: 81% 18%



• Molecule 33: Proteasome subunit beta type-4

Chain t: 81% 18%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105157	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 ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	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: MG, ATP, ZN, 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	U	0.33	0/6449	0.58	4/8729 (0.0%)
2	V	0.34	0/4072	0.65	3/5510 (0.1%)
3	W	0.33	0/3751	0.63	2/5042 (0.0%)
4	X	0.32	0/3053	0.59	0/4115
5	Y	0.37	0/3173	0.62	0/4273
6	Z	0.32	0/2324	0.64	2/3150 (0.1%)
7	a	0.30	0/3053	0.60	1/4133 (0.0%)
8	b	0.29	0/1478	0.61	0/2001
9	c	0.37	0/2302	0.67	0/3110
10	d	0.33	0/2162	0.67	2/2919 (0.1%)
11	e	0.31	0/338	0.69	1/450 (0.2%)
12	f	0.32	0/6980	0.70	5/9433 (0.1%)
13	A	0.45	0/3148	0.65	2/4250 (0.0%)
14	B	0.42	0/3061	0.64	1/4129 (0.0%)
15	C	0.40	0/2902	0.63	1/3904 (0.0%)
16	D	0.44	0/3089	0.64	0/4168
17	E	0.40	0/2904	0.61	1/3924 (0.0%)
18	F	0.43	0/2896	0.59	0/3912
19	u	0.27	0/609	0.49	0/819
19	w	0.27	0/609	0.49	0/819
20	G	0.41	0/1859	0.56	0/2523
20	g	0.41	0/1859	0.56	0/2523
21	H	0.44	0/1743	0.53	0/2372
21	h	0.44	0/1743	0.53	0/2372
22	I	0.38	0/1942	0.58	1/2628 (0.0%)
22	i	0.37	0/1942	0.58	1/2628 (0.0%)
23	J	0.43	0/1737	0.59	0/2369
23	j	0.32	0/1728	0.55	0/2358
24	K	0.38	0/1747	0.57	1/2364 (0.0%)
24	k	0.37	0/1747	0.57	1/2364 (0.0%)
25	L	0.42	0/1885	0.61	2/2552 (0.1%)
25	l	0.42	0/1885	0.61	1/2552 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	M	0.41	0/1891	0.55	0/2552
26	m	0.41	0/1891	0.55	0/2552
27	N	0.36	0/1454	0.51	0/1967
27	n	0.36	0/1454	0.51	0/1967
28	O	0.38	0/1670	0.54	0/2265
28	o	0.38	0/1670	0.54	0/2265
29	P	0.38	0/1620	0.52	0/2184
29	p	0.38	0/1620	0.52	0/2184
30	Q	0.40	0/1603	0.57	1/2174 (0.0%)
30	q	0.40	0/1603	0.57	1/2174 (0.0%)
31	R	0.41	0/1579	0.51	0/2134
31	r	0.41	0/1579	0.51	0/2134
32	S	0.39	0/1671	0.51	0/2253
32	s	0.36	0/1674	0.51	0/2257
33	T	0.39	0/1700	0.54	0/2305
33	t	0.39	0/1700	0.54	0/2305
All	All	0.38	0/106549	0.60	34/144067 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1
2	V	0	2
3	W	0	2
5	Y	0	1
6	Z	0	2
7	a	0	1
9	c	0	2
12	f	0	9
13	A	0	2
14	B	0	1
15	C	0	5
16	D	0	4
17	E	0	2
18	F	0	1
20	G	0	1
20	g	0	1
23	J	0	1
23	j	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	M	0	1
26	m	0	1
30	Q	0	1
30	q	0	1
All	All	0	43

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	310	ASP	CB-CG-OD1	8.20	125.68	118.30
3	W	89	LEU	CA-CB-CG	7.57	132.70	115.30
11	e	56	LEU	CA-CB-CG	7.44	132.42	115.30
12	f	759	LEU	CA-CB-CG	6.86	131.09	115.30
1	U	603	LEU	CA-CB-CG	6.71	130.74	115.30
1	U	177	LEU	CA-CB-CG	6.59	130.46	115.30
12	f	129	LEU	CA-CB-CG	6.54	130.34	115.30
25	L	226	ASP	CB-CG-OD1	6.28	123.96	118.30
25	l	226	ASP	CB-CG-OD1	6.27	123.94	118.30
2	V	167	LEU	CA-CB-CG	6.09	129.31	115.30
14	B	140	ASP	CB-CG-OD1	6.07	123.76	118.30
2	V	170	LEU	CA-CB-CG	5.92	128.91	115.30
2	V	357	LEU	CA-CB-CG	5.75	128.52	115.30
17	E	116	ASP	CB-CG-OD1	5.75	123.47	118.30
10	d	89	LEU	CA-CB-CG	5.57	128.11	115.30
12	f	217	LEU	CA-CB-CG	5.52	128.01	115.30
12	f	811	LEU	CA-CB-CG	5.45	127.83	115.30
1	U	603	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	U	873	PRO	C-N-CA	5.43	135.26	121.70
3	W	252	ASP	C-N-CA	5.38	135.15	121.70
6	Z	236	LEU	CA-CB-CG	5.38	127.66	115.30
10	d	107	LEU	CA-CB-CG	5.33	127.55	115.30
24	K	21	LEU	CA-CB-CG	5.27	127.42	115.30
24	k	21	LEU	CA-CB-CG	5.27	127.41	115.30
12	f	612	LEU	CA-CB-CG	5.25	127.37	115.30
15	C	280	LEU	CA-CB-CG	5.24	127.35	115.30
7	a	187	ASP	CB-CG-OD1	5.20	122.98	118.30
30	q	103	LEU	CA-CB-CG	5.20	127.25	115.30
30	Q	103	LEU	CA-CB-CG	5.19	127.25	115.30
13	A	260	LEU	CB-CG-CD1	-5.19	102.18	111.00
22	I	164	ILE	CG1-CB-CG2	-5.15	100.07	111.40
22	i	164	ILE	CG1-CB-CG2	-5.14	100.08	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	212	LEU	CA-CB-CG	5.12	127.09	115.30
25	L	103	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	158	ASP	Peptide
13	A	400	ARG	Peptide
14	B	278	ALA	Peptide
15	C	127	LEU	Peptide
15	C	128	PRO	Peptide
15	C	129	ASN	Peptide
15	C	89	VAL	Peptide
15	C	90	HIS	Peptide
16	D	125	LYS	Peptide
16	D	354	LEU	Peptide
16	D	368	ASP	Peptide
16	D	83	GLN	Peptide
17	E	385	ASP	Peptide
17	E	75	ASN	Peptide
18	F	344	ARG	Peptide
20	G	222	VAL	Peptide
23	J	199	VAL	Peptide
26	M	214	SER	Peptide
30	Q	2	GLU	Peptide
1	U	873	PRO	Peptide
2	V	264	TYR	Peptide
2	V	501	TYR	Peptide
3	W	252	ASP	Peptide
3	W	315	MET	Peptide
5	Y	233	ARG	Peptide
6	Z	145	HIS	Peptide
6	Z	223	ASN	Peptide
7	a	169	HIS	Peptide
9	c	155	VAL	Peptide
9	c	84	VAL	Peptide
12	f	249	LEU	Peptide
12	f	257	ARG	Peptide
12	f	340	MET	Peptide
12	f	642	ALA	Peptide
12	f	755	ASP	Peptide

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Mol	Chain	Res	Type	Group
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	843	SER	Peptide
12	f	875	ALA	Peptide
20	g	222	VAL	Peptide
23	j	199	VAL	Peptide
26	m	214	SER	Peptide
30	q	2	GLU	Peptide

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	U	806/953 (85%)	738 (92%)	65 (8%)	3 (0%)	34	72
2	V	506/534 (95%)	453 (90%)	49 (10%)	4 (1%)	19	57
3	W	454/456 (100%)	407 (90%)	43 (10%)	4 (1%)	17	55
4	X	378/422 (90%)	353 (93%)	24 (6%)	1 (0%)	41	76
5	Y	376/389 (97%)	342 (91%)	34 (9%)	0	100	100
6	Z	284/324 (88%)	243 (86%)	41 (14%)	0	100	100
7	a	371/376 (99%)	337 (91%)	33 (9%)	1 (0%)	41	76
8	b	189/377 (50%)	175 (93%)	13 (7%)	1 (0%)	29	68
9	c	285/309 (92%)	244 (86%)	38 (13%)	3 (1%)	14	50
10	d	255/349 (73%)	216 (85%)	39 (15%)	0	100	100
11	e	36/70 (51%)	22 (61%)	14 (39%)	0	100	100
12	f	887/908 (98%)	715 (81%)	165 (19%)	7 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A	392/433 (90%)	342 (87%)	48 (12%)	2 (0%)	29	68
14	B	382/440 (87%)	348 (91%)	33 (9%)	1 (0%)	41	76
15	C	359/398 (90%)	333 (93%)	24 (7%)	2 (1%)	25	64
16	D	378/418 (90%)	334 (88%)	38 (10%)	6 (2%)	9	40
17	E	373/403 (93%)	335 (90%)	36 (10%)	2 (0%)	29	68
18	F	372/439 (85%)	338 (91%)	33 (9%)	1 (0%)	41	76
19	u	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
19	w	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
20	G	238/245 (97%)	223 (94%)	15 (6%)	0	100	100
20	g	238/245 (97%)	223 (94%)	15 (6%)	0	100	100
21	H	230/233 (99%)	224 (97%)	6 (3%)	0	100	100
21	h	230/233 (99%)	224 (97%)	6 (3%)	0	100	100
22	I	248/260 (95%)	229 (92%)	19 (8%)	0	100	100
22	i	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
23	J	237/247 (96%)	218 (92%)	18 (8%)	1 (0%)	34	72
23	j	237/247 (96%)	220 (93%)	16 (7%)	1 (0%)	34	72
24	K	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
24	k	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
25	L	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
25	l	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
26	M	238/254 (94%)	222 (93%)	16 (7%)	0	100	100
26	m	238/254 (94%)	222 (93%)	16 (7%)	0	100	100
27	N	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
27	n	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
28	O	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
28	o	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
29	P	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
29	p	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
30	Q	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
30	q	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
31	R	199/262 (76%)	188 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	r	199/262 (76%)	188 (94%)	11 (6%)	0	100	100
32	S	211/240 (88%)	204 (97%)	7 (3%)	0	100	100
32	s	211/240 (88%)	200 (95%)	11 (5%)	0	100	100
33	T	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
33	t	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
All	All	13391/15012 (89%)	12242 (91%)	1109 (8%)	40 (0%)	44	76

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	167	LEU
15	C	90	HIS
1	U	874	ASN
2	V	168	GLN
16	D	84	SER
17	E	386	TYR
2	V	265	ASP
3	W	252	ASP
4	X	392	PRO
7	a	149	THR
12	f	118	ASN
12	f	476	THR
12	f	808	ASN
15	C	128	PRO
16	D	126	PRO
1	U	873	PRO
12	f	853	VAL
12	f	859	PRO
13	A	425	ALA
14	B	87	PRO
16	D	154	LEU
16	D	368	ASP
17	E	385	ASP
23	J	97	THR
3	W	136	ILE
9	c	158	ASP
12	f	475	ASN
13	A	109	PRO
23	j	97	THR
3	W	316	ARG

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Mol	Chain	Res	Type
16	D	85	ILE
18	F	165	PRO
1	U	174	PRO
9	c	157	ILE
12	f	755	ASP
16	D	367	PRO
3	W	253	THR
8	b	23	PRO
2	V	29	PRO
9	c	156	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	692/816 (85%)	690 (100%)	2 (0%)	92	97
2	V	415/460 (90%)	409 (99%)	6 (1%)	67	88
3	W	416/416 (100%)	409 (98%)	7 (2%)	60	85
4	X	327/362 (90%)	320 (98%)	7 (2%)	53	82
5	Y	334/344 (97%)	331 (99%)	3 (1%)	78	92
6	Z	257/295 (87%)	252 (98%)	5 (2%)	57	84
7	a	333/336 (99%)	332 (100%)	1 (0%)	92	97
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	242 (96%)	10 (4%)	31	68
10	d	231/293 (79%)	229 (99%)	2 (1%)	78	92
11	e	38/63 (60%)	37 (97%)	1 (3%)	46	78
12	f	745/763 (98%)	728 (98%)	17 (2%)	50	80
13	A	337/372 (91%)	327 (97%)	10 (3%)	41	75
14	B	339/385 (88%)	333 (98%)	6 (2%)	59	85
15	C	314/346 (91%)	306 (98%)	8 (2%)	47	79
16	D	333/366 (91%)	324 (97%)	9 (3%)	44	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	E	298/353 (84%)	295 (99%)	3 (1%)	76	91
18	F	296/379 (78%)	293 (99%)	3 (1%)	76	91
19	u	68/68 (100%)	68 (100%)	0	100	100
19	w	68/68 (100%)	68 (100%)	0	100	100
20	G	193/209 (92%)	193 (100%)	0	100	100
20	g	193/209 (92%)	193 (100%)	0	100	100
21	H	164/190 (86%)	162 (99%)	2 (1%)	71	90
21	h	164/190 (86%)	162 (99%)	2 (1%)	71	90
22	I	193/220 (88%)	192 (100%)	1 (0%)	88	96
22	i	193/220 (88%)	192 (100%)	1 (0%)	88	96
23	J	154/210 (73%)	151 (98%)	3 (2%)	57	84
23	j	152/210 (72%)	150 (99%)	2 (1%)	69	89
24	K	186/202 (92%)	185 (100%)	1 (0%)	88	96
24	k	186/202 (92%)	185 (100%)	1 (0%)	88	96
25	L	198/229 (86%)	198 (100%)	0	100	100
25	l	198/229 (86%)	198 (100%)	0	100	100
26	M	192/211 (91%)	190 (99%)	2 (1%)	76	91
26	m	192/211 (91%)	190 (99%)	2 (1%)	76	91
27	N	148/180 (82%)	147 (99%)	1 (1%)	84	94
27	n	148/180 (82%)	147 (99%)	1 (1%)	84	94
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	177 (100%)	0	100	100
29	P	173/173 (100%)	173 (100%)	0	100	100
29	p	173/173 (100%)	173 (100%)	0	100	100
30	Q	164/171 (96%)	162 (99%)	2 (1%)	71	90
30	q	164/171 (96%)	162 (99%)	2 (1%)	71	90
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	175/198 (88%)	175 (100%)	0	100	100
33	T	175/214 (82%)	174 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	t	175/214 (82%)	174 (99%)	1 (1%)	86 95
All	All	11147/12734 (88%)	11022 (99%)	125 (1%)	74 90

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	345	ASN
1	U	629	THR
2	V	80	LYS
2	V	194	LYS
2	V	197	THR
2	V	223	LYS
2	V	345	ARG
2	V	452	ASN
3	W	90	LEU
3	W	326	MET
3	W	364	ARG
3	W	399	ASN
3	W	422	ASN
3	W	440	ASN
3	W	448	LYS
4	X	304	LYS
4	X	310	ARG
4	X	314	ARG
4	X	329	ASN
4	X	344	ARG
4	X	395	LYS
4	X	420	LYS
5	Y	237	ARG
5	Y	312	ARG
5	Y	358	ARG
6	Z	114	ARG
6	Z	129	LYS
6	Z	193	ASN
6	Z	214	LYS
6	Z	225	GLN
7	a	165	THR
9	c	49	VAL
9	c	104	ARG
9	c	164	ASN
9	c	166	ASN
9	c	180	ASN

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Mol	Chain	Res	Type
9	c	197	ASN
9	c	232	GLN
9	c	251	LEU
9	c	254	ASN
9	c	277	LYS
10	d	196	ARG
10	d	231	LYS
11	e	1	MET
12	f	80	ARG
12	f	83	ARG
12	f	131	MET
12	f	267	ARG
12	f	297	MET
12	f	327	ASN
12	f	344	VAL
12	f	381	VAL
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	569	LYS
12	f	703	ARG
12	f	746	ARG
12	f	822	VAL
12	f	826	GLN
13	A	43	ARG
13	A	66	LYS
13	A	163	MET
13	A	293	ASN
13	A	297	ARG
13	A	304	ASN
13	A	312	ARG
13	A	360	ARG
13	A	403	ILE
13	A	428	ARG
14	B	48	LYS
14	B	125	THR
14	B	143	LEU
14	B	170	LEU
14	B	241	ASN
14	B	359	LYS
15	C	53	ASN

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Mol	Chain	Res	Type
15	C	78	ARG
15	C	109	THR
15	C	113	ARG
15	C	213	ARG
15	C	271	ARG
15	C	335	LYS
15	C	391	MET
16	D	66	LYS
16	D	67	ASN
16	D	81	ARG
16	D	152	MET
16	D	153	MET
16	D	231	VAL
16	D	257	ASN
16	D	312	ASN
16	D	409	LYS
17	E	48	LYS
17	E	197	LYS
17	E	223	ARG
18	F	83	ASN
18	F	184	GLN
18	F	430	LYS
21	H	4	ARG
21	H	128	ARG
22	I	238	LYS
23	J	57	ARG
23	J	125	ARG
23	J	159	ASN
24	K	20	ARG
26	M	40	ARG
26	M	221	ASN
27	N	28	ASN
30	Q	4	LEU
30	Q	82	ASN
33	T	100	ARG
21	h	4	ARG
21	h	128	ARG
22	i	238	LYS
23	j	125	ARG
23	j	159	ASN
24	k	20	ARG
26	m	40	ARG

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Mol	Chain	Res	Type
26	m	221	ASN
27	n	28	ASN
30	q	4	LEU
30	q	82	ASN
33	t	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	207	ASN
1	U	345	ASN
1	U	377	HIS
1	U	415	HIS
1	U	595	ASN
1	U	647	HIS
2	V	247	GLN
2	V	257	ASN
2	V	260	HIS
2	V	283	ASN
2	V	401	ASN
2	V	427	GLN
2	V	452	ASN
3	W	41	GLN
3	W	203	GLN
3	W	399	ASN
4	X	213	GLN
4	X	333	GLN
5	Y	48	ASN
5	Y	136	HIS
5	Y	363	ASN
6	Z	109	ASN
6	Z	231	GLN
6	Z	256	GLN
6	Z	277	ASN
6	Z	278	ASN
7	a	12	GLN
7	a	23	HIS
7	a	193	GLN
7	a	212	ASN
7	a	231	GLN
7	a	264	ASN
7	a	267	GLN

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Mol	Chain	Res	Type
7	a	345	GLN
7	a	370	GLN
8	b	142	ASN
9	c	101	GLN
9	c	130	GLN
9	c	164	ASN
9	c	166	ASN
9	c	180	ASN
9	c	197	ASN
9	c	232	GLN
9	c	241	ASN
9	c	298	GLN
10	d	15	ASN
10	d	116	HIS
11	e	63	HIS
12	f	118	ASN
12	f	171	GLN
12	f	213	GLN
12	f	291	GLN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	614	HIS
12	f	715	HIS
12	f	737	ASN
12	f	752	HIS
12	f	786	GLN
12	f	848	GLN
13	A	60	ASN
13	A	85	GLN
13	A	293	ASN
13	A	304	ASN
14	B	195	GLN
15	C	36	ASN
15	C	48	GLN
15	C	53	ASN
15	C	171	HIS
16	D	91	GLN
16	D	133	HIS

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Mol	Chain	Res	Type
16	D	173	GLN
16	D	221	HIS
16	D	222	HIS
16	D	257	ASN
16	D	312	ASN
16	D	353	ASN
18	F	83	ASN
19	u	25	ASN
19	u	41	GLN
19	w	25	ASN
19	w	41	GLN
22	I	109	GLN
23	J	85	ASN
23	J	159	ASN
24	K	99	HIS
24	K	214	ASN
25	L	4	ASN
25	L	21	GLN
26	M	97	ASN
26	M	221	ASN
27	N	28	ASN
27	N	110	GLN
28	O	66	HIS
28	O	165	ASN
29	P	93	ASN
30	Q	71	ASN
31	R	29	GLN
31	R	38	ASN
33	T	81	HIS
23	j	159	ASN
24	k	99	HIS
24	k	214	ASN
25	l	4	ASN
26	m	97	ASN
26	m	221	ASN
27	n	28	ASN
27	n	110	GLN
28	o	66	HIS
28	o	165	ASN
29	p	93	ASN
31	r	29	GLN
31	r	38	ASN

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Mol	Chain	Res	Type
33	t	81	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 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	$\#\|Z\| > 2$
37	ADP	C	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.64	4 (13%)
35	ATP	D	501	36	26,33,33	0.90	1 (3%)	31,52,52	1.64	5 (16%)
35	ATP	E	401	36	26,33,33	0.91	1 (3%)	31,52,52	1.68	6 (19%)
35	ATP	B	501	36	26,33,33	0.94	1 (3%)	31,52,52	1.76	4 (12%)
35	ATP	A	501	36	26,33,33	0.96	1 (3%)	31,52,52	1.74	5 (16%)
37	ADP	F	501	36	24,29,29	0.93	1 (4%)	29,45,45	1.48	5 (17%)

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	ADP	C	501	-	-	4/12/32/32	0/3/3/3
35	ATP	D	501	36	-	3/18/38/38	0/3/3/3
35	ATP	E	401	36	-	0/18/38/38	0/3/3/3
35	ATP	B	501	36	-	3/18/38/38	0/3/3/3
35	ATP	A	501	36	-	1/18/38/38	0/3/3/3
37	ADP	F	501	36	-	5/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	501	ADP	C5-C4	2.20	1.46	1.40
35	D	501	ATP	C5-C4	2.15	1.46	1.40
35	E	401	ATP	C5-C4	2.11	1.46	1.40
35	B	501	ATP	C5-C4	2.08	1.46	1.40
35	A	501	ATP	C5-C4	2.07	1.46	1.40
37	F	501	ADP	C5-C4	2.05	1.46	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	501	ATP	PA-O3A-PB	-4.86	116.16	132.83
35	B	501	ATP	PA-O3A-PB	-4.81	116.33	132.83
35	D	501	ATP	PA-O3A-PB	-4.67	116.80	132.83
35	E	401	ATP	PA-O3A-PB	-4.62	116.97	132.83
37	C	501	ADP	PA-O3A-PB	-4.31	118.03	132.83
35	A	501	ATP	PB-O3B-PG	-4.22	118.34	132.83
37	C	501	ADP	C3'-C2'-C1'	4.12	107.19	100.98
37	F	501	ADP	PA-O3A-PB	-4.12	118.69	132.83
35	D	501	ATP	PB-O3B-PG	-4.06	118.88	132.83
35	B	501	ATP	C3'-C2'-C1'	3.97	106.96	100.98
35	E	401	ATP	PB-O3B-PG	-3.90	119.46	132.83
35	B	501	ATP	PB-O3B-PG	-3.69	120.16	132.83
35	B	501	ATP	N3-C2-N1	-3.45	123.28	128.68
35	E	401	ATP	C3'-C2'-C1'	3.29	105.93	100.98
37	F	501	ADP	C3'-C2'-C1'	3.16	105.73	100.98
35	D	501	ATP	N3-C2-N1	-3.13	123.78	128.68
35	A	501	ATP	C3'-C2'-C1'	3.13	105.69	100.98
35	E	401	ATP	N3-C2-N1	-3.12	123.80	128.68
37	C	501	ADP	N3-C2-N1	-3.08	123.87	128.68
35	A	501	ATP	N3-C2-N1	-2.99	124.00	128.68
37	F	501	ADP	N3-C2-N1	-2.92	124.11	128.68
35	D	501	ATP	C3'-C2'-C1'	2.77	105.15	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	501	ADP	C4-C5-N7	-2.46	106.83	109.40
35	D	501	ATP	C4-C5-N7	-2.29	107.02	109.40
35	A	501	ATP	C4-C5-N7	-2.28	107.03	109.40
35	E	401	ATP	O3G-PG-O2G	2.23	116.15	107.64
35	E	401	ATP	C4-C5-N7	-2.11	107.20	109.40
37	F	501	ADP	C4-C5-N7	-2.09	107.22	109.40
37	F	501	ADP	O3B-PB-O2B	2.02	115.34	107.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
37	C	501	ADP	PA-O3A-PB-O3B
37	C	501	ADP	C5'-O5'-PA-O3A
37	F	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C3'-C4'-C5'-O5'
37	F	501	ADP	PA-O3A-PB-O1B
37	F	501	ADP	PA-O3A-PB-O2B
35	B	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C5'-O5'-PA-O3A
37	C	501	ADP	C5'-O5'-PA-O2A
35	D	501	ATP	O4'-C4'-C5'-O5'
35	A	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O1A
37	C	501	ADP	PA-O3A-PB-O1B

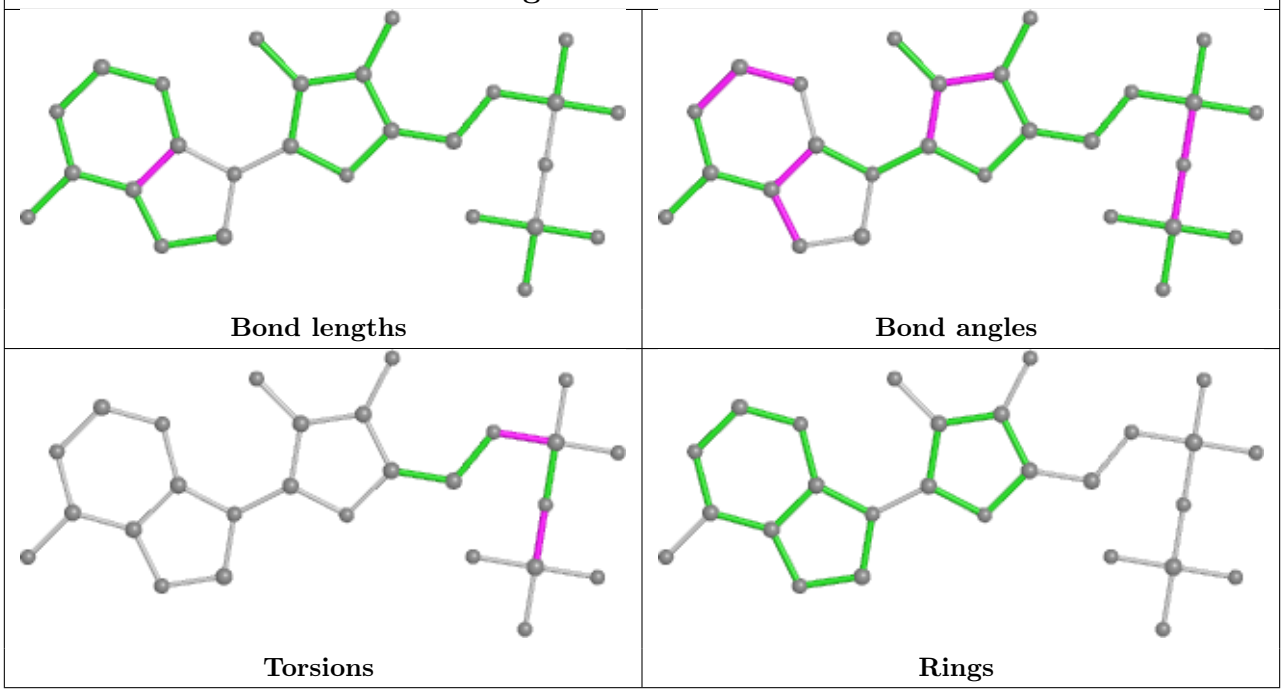
There are no ring outliers.

No monomer is involved in short contacts.

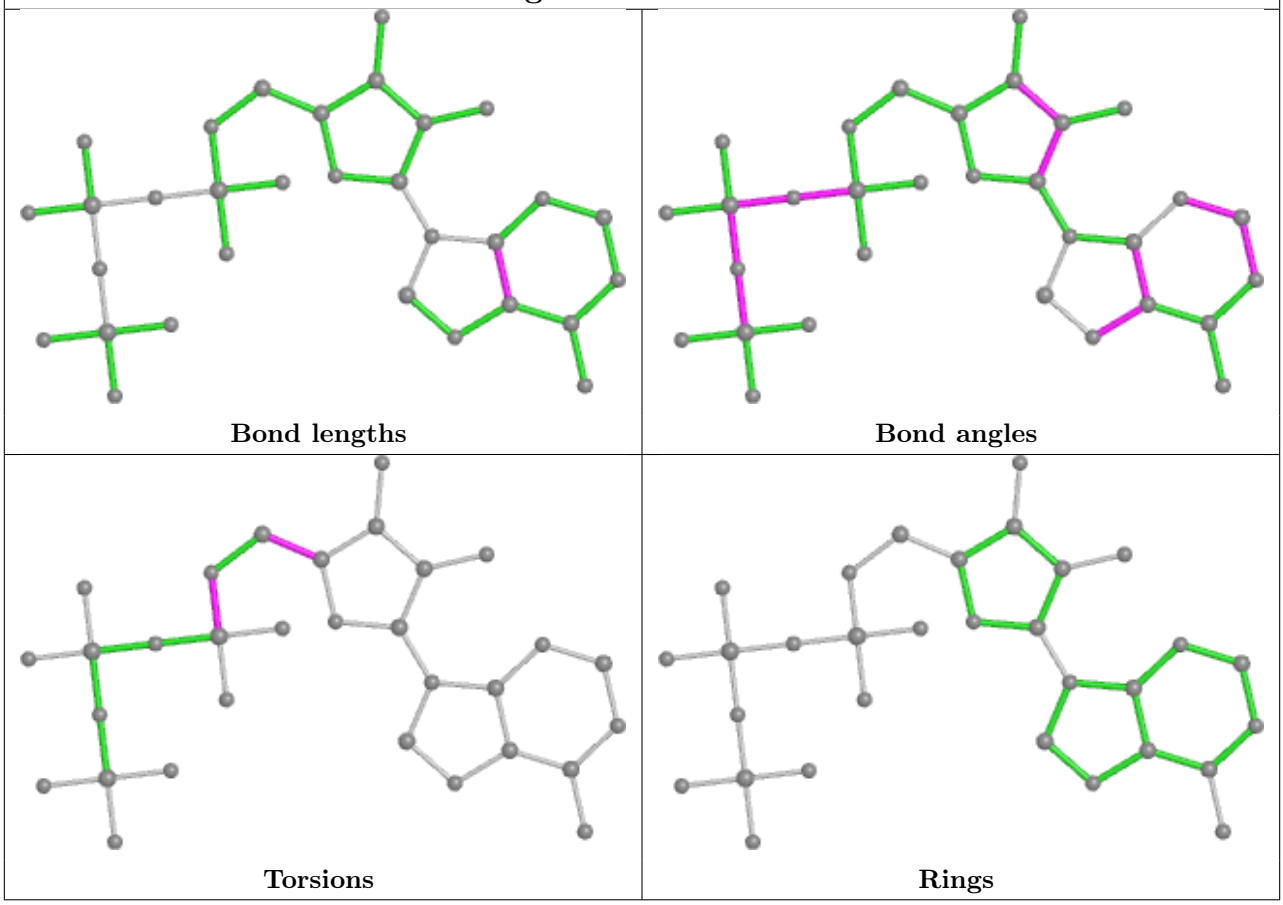
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

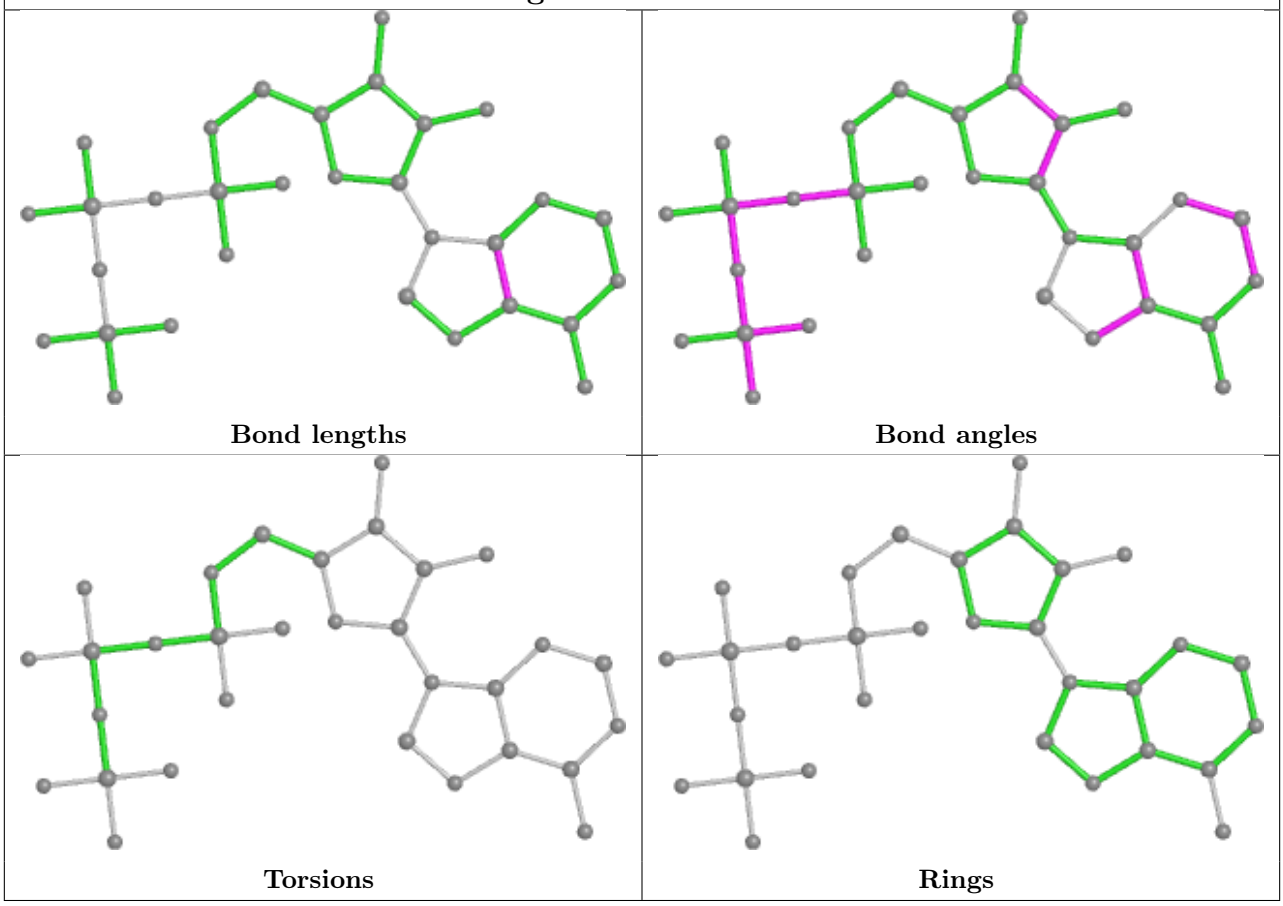
Ligand ADP C 501



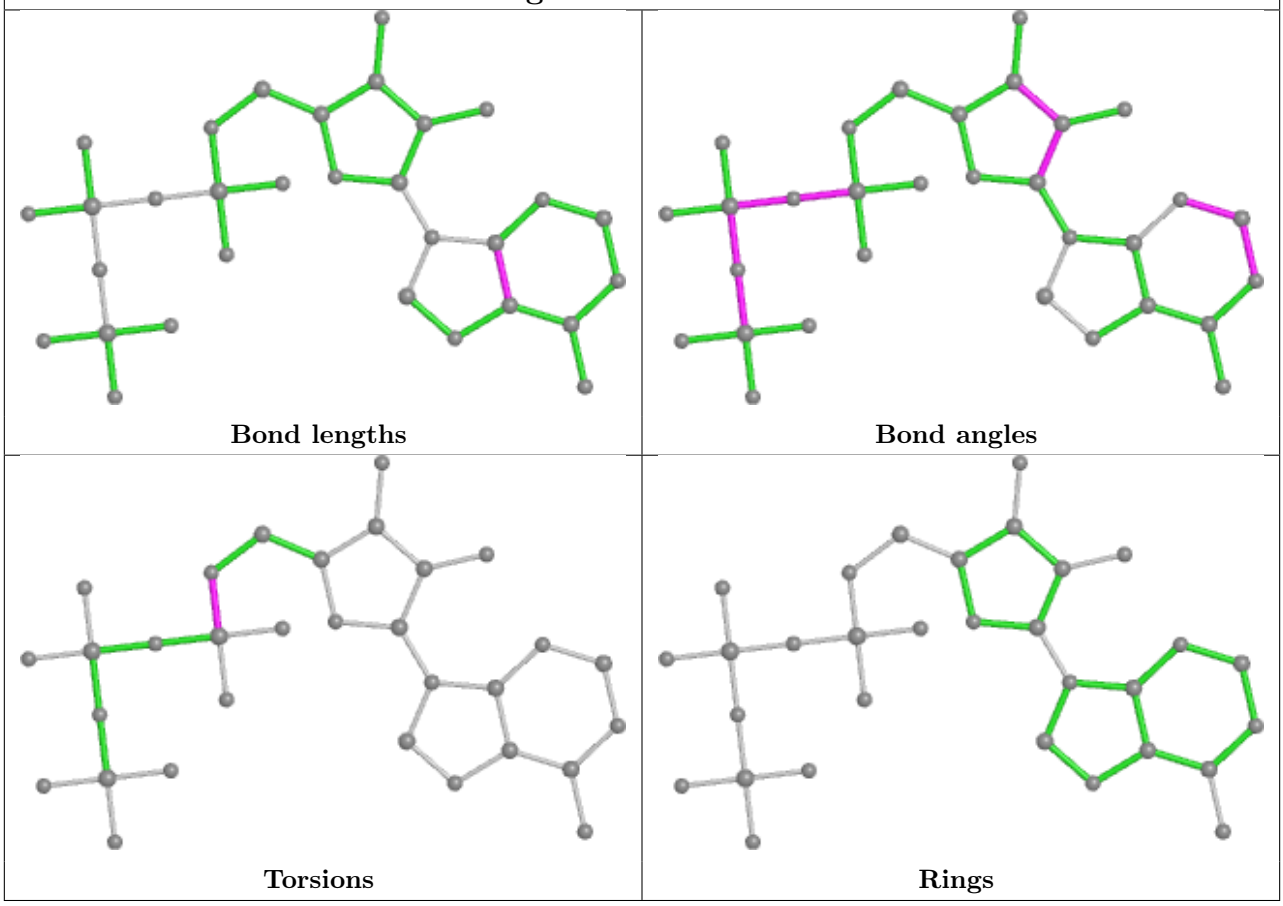
Ligand ATP D 501



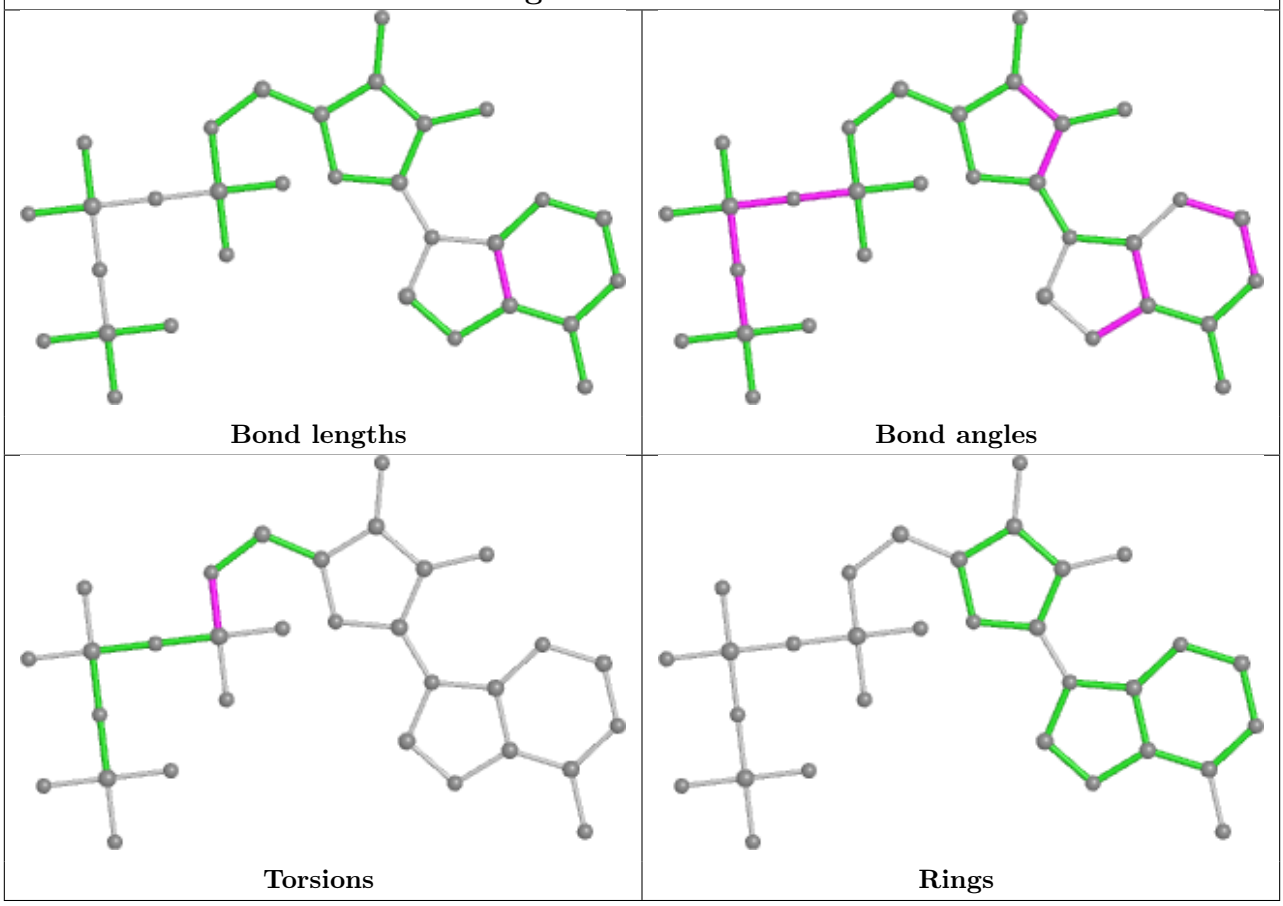
Ligand ATP E 401



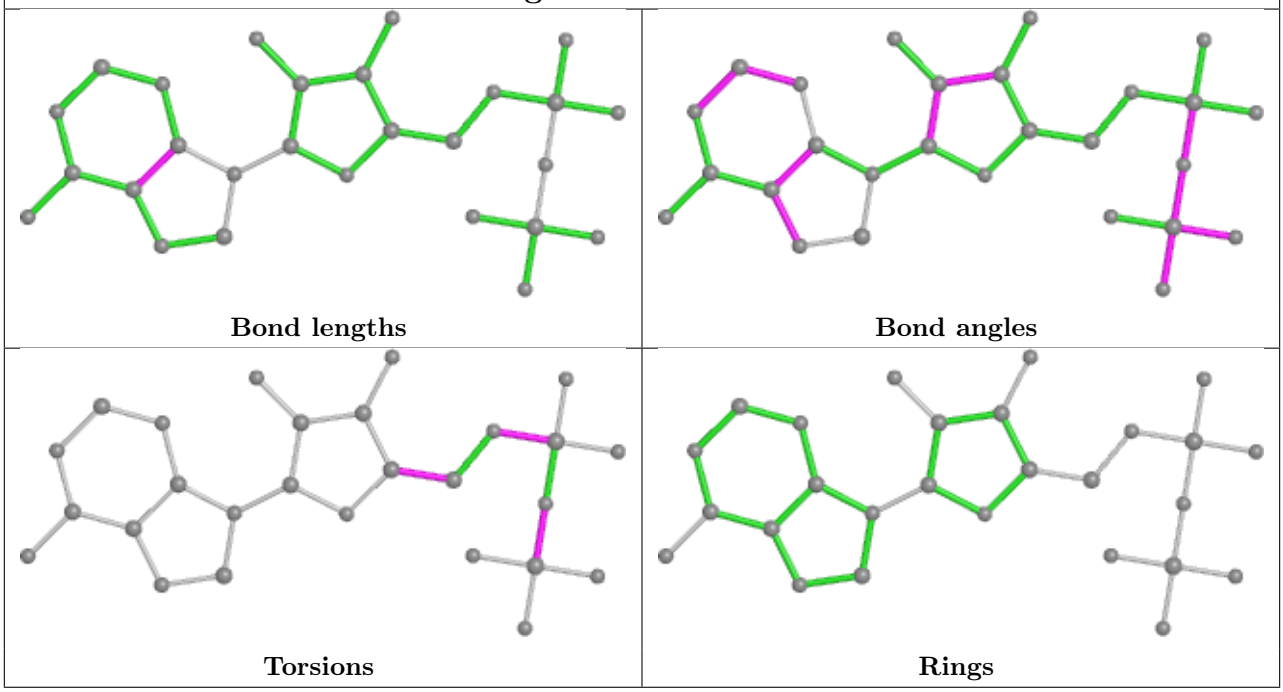
Ligand ATP B 501



Ligand ATP A 501



Ligand ADP F 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.

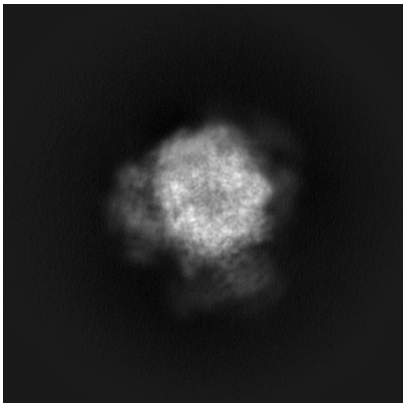
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9216. These allow visual inspection of the internal detail of the map and identification of artifacts.

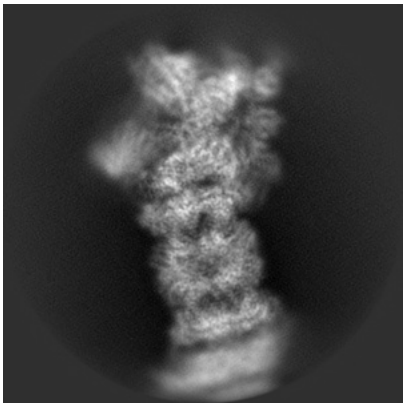
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

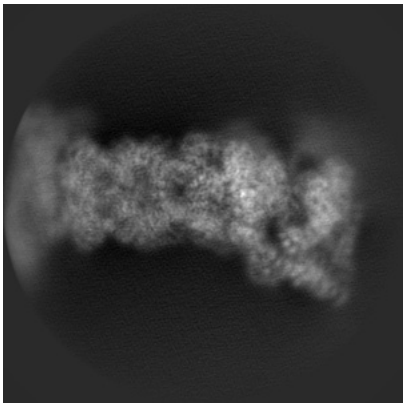
6.1.1 Primary map



X



Y

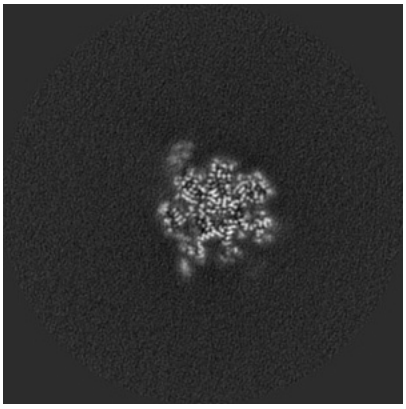


Z

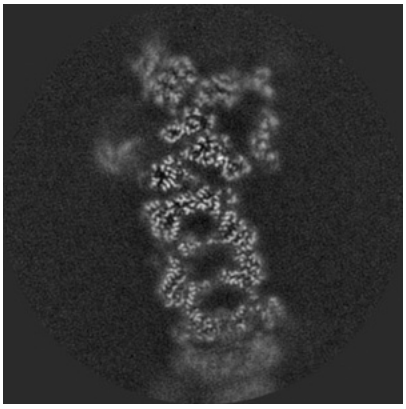
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

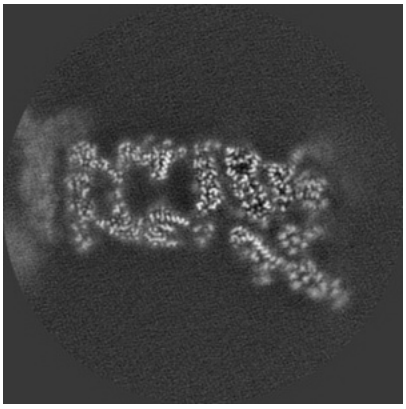
6.2.1 Primary map



X Index: 300



Y Index: 300

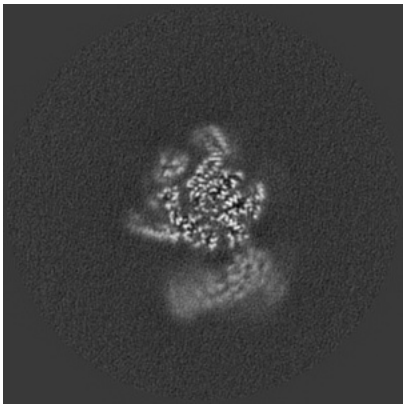


Z Index: 300

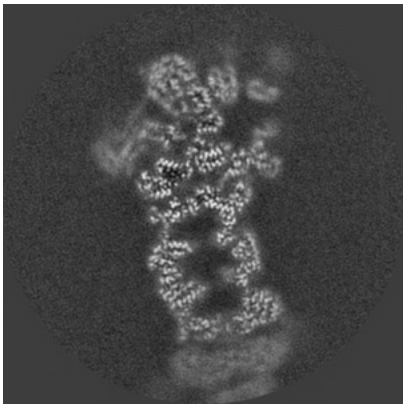
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

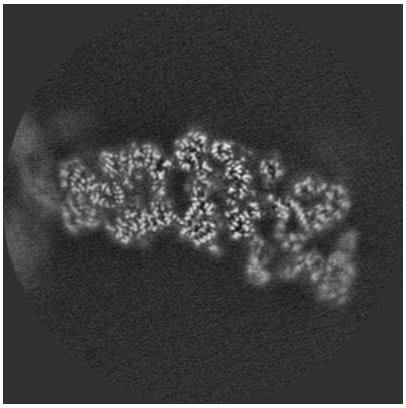
6.3.1 Primary map



X Index: 364



Y Index: 315



Z Index: 275

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 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

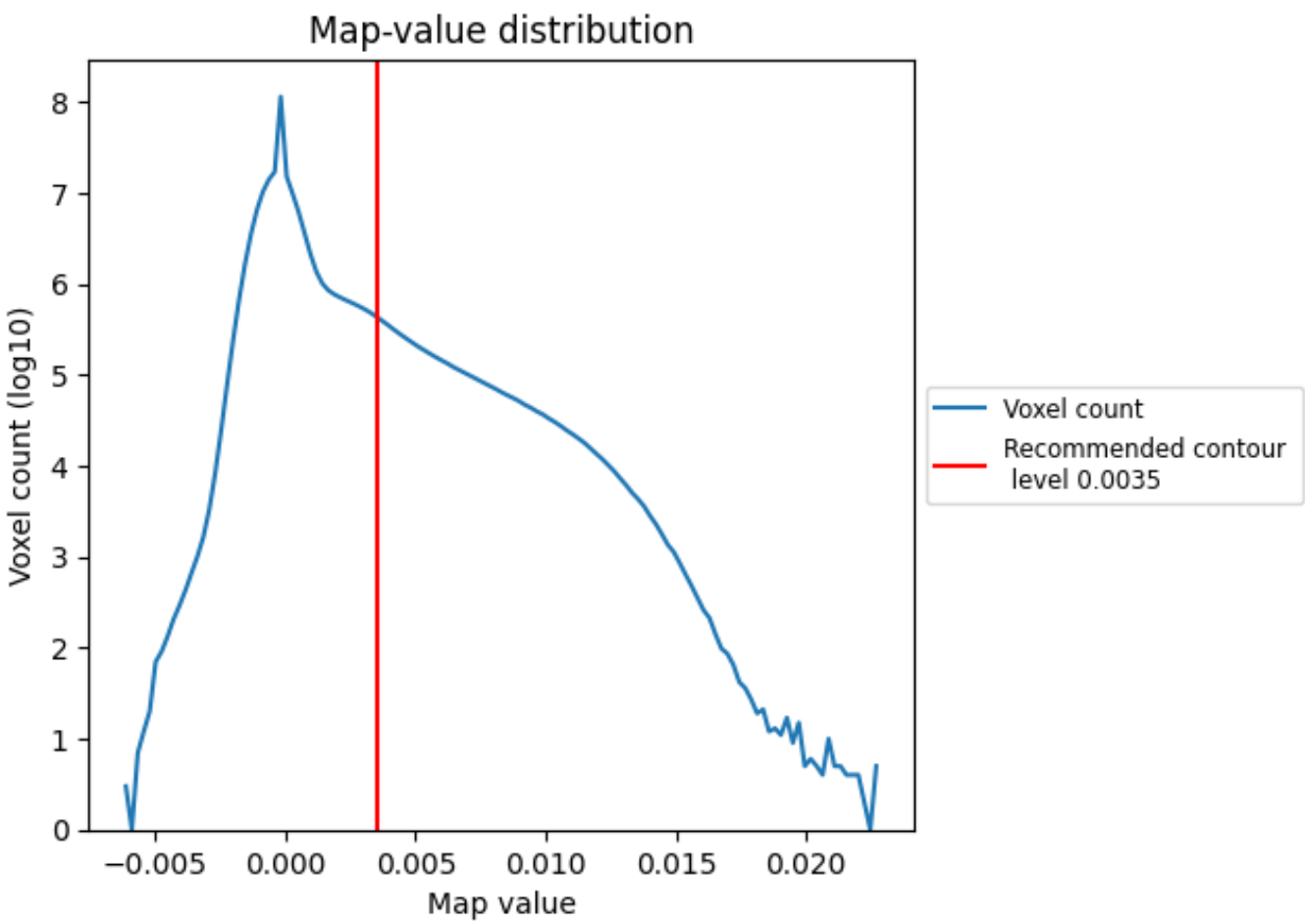
6.5 Mask visualisation (i)

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

7 Map analysis (i)

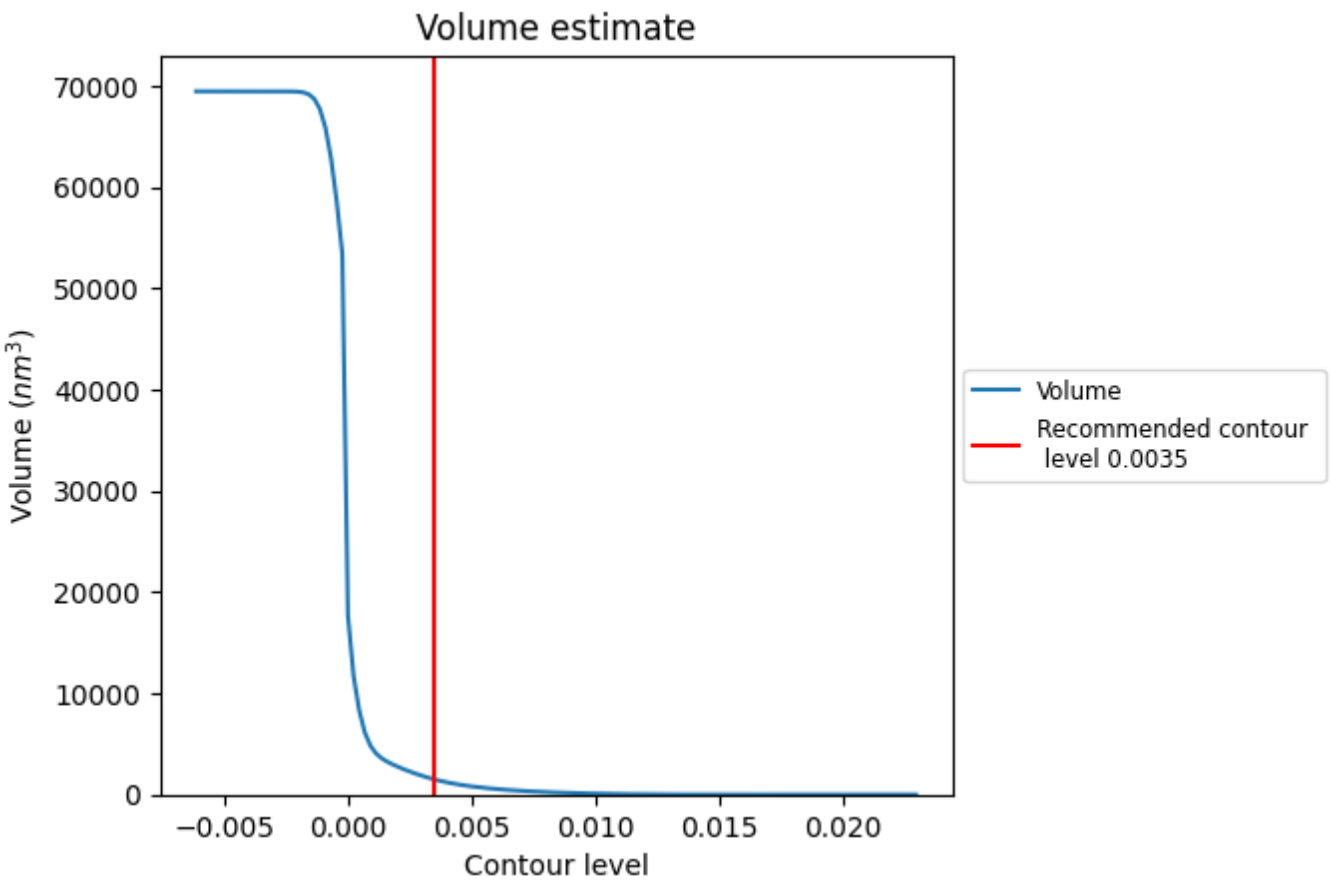
This section contains the results of statistical analysis of the map.

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.

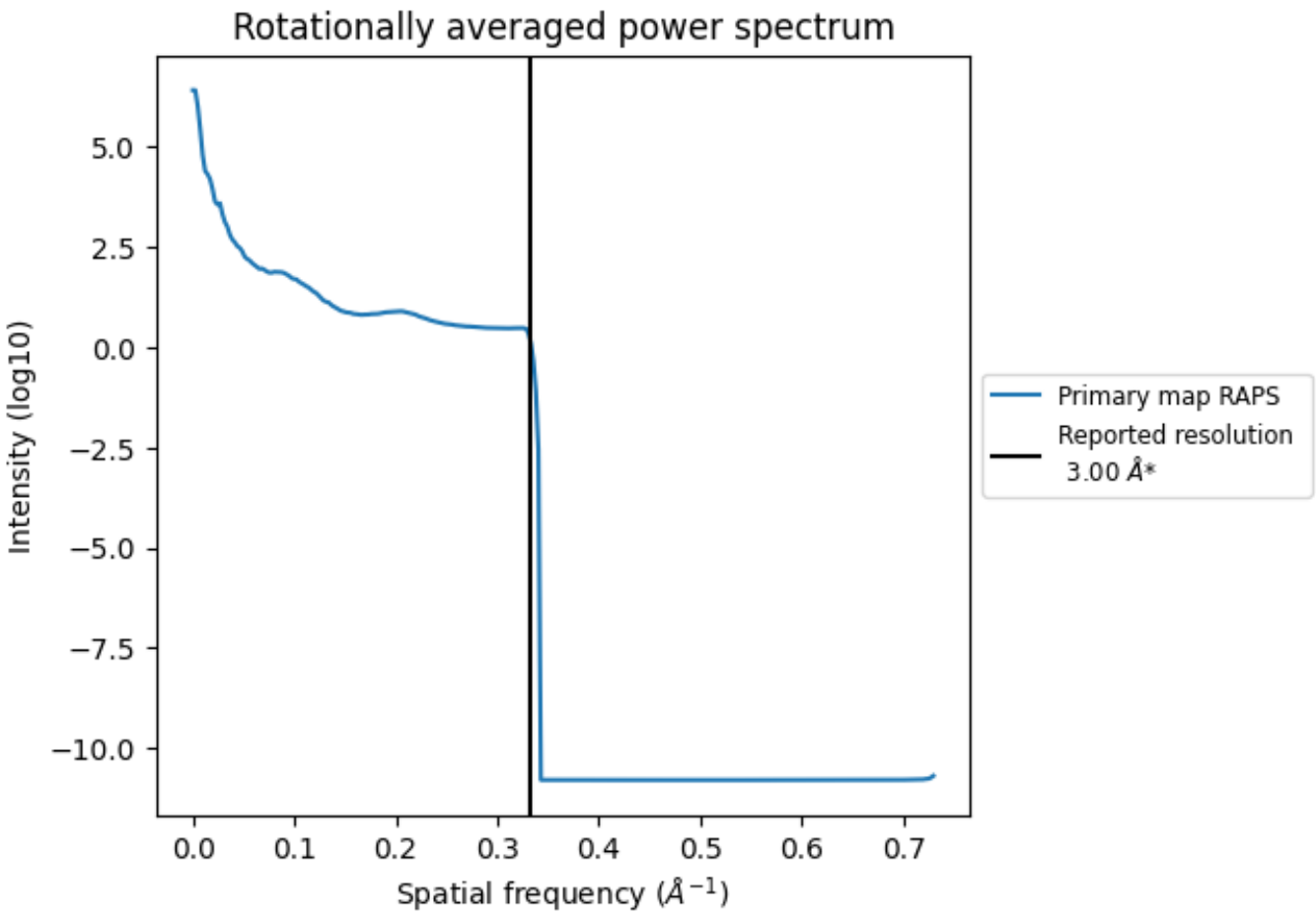
7.2 Volume estimate (i)



The volume at the recommended contour level is 1494 nm^3; this corresponds to an approximate mass of 1350 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 0.333 Å^{-1}

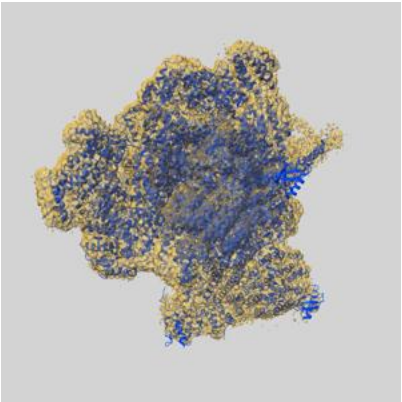
8 Fourier-Shell correlation (i)

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

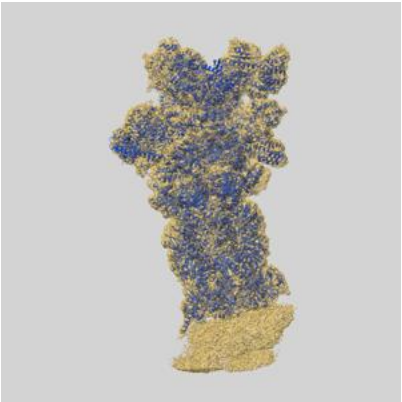
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9216 and PDB model 6MSB. Per-residue inclusion information can be found in section 3 on page 13.

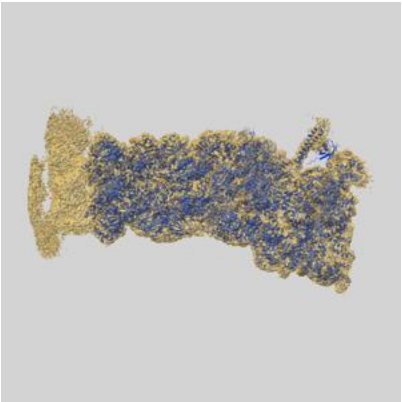
9.1 Map-model overlay (i)



X



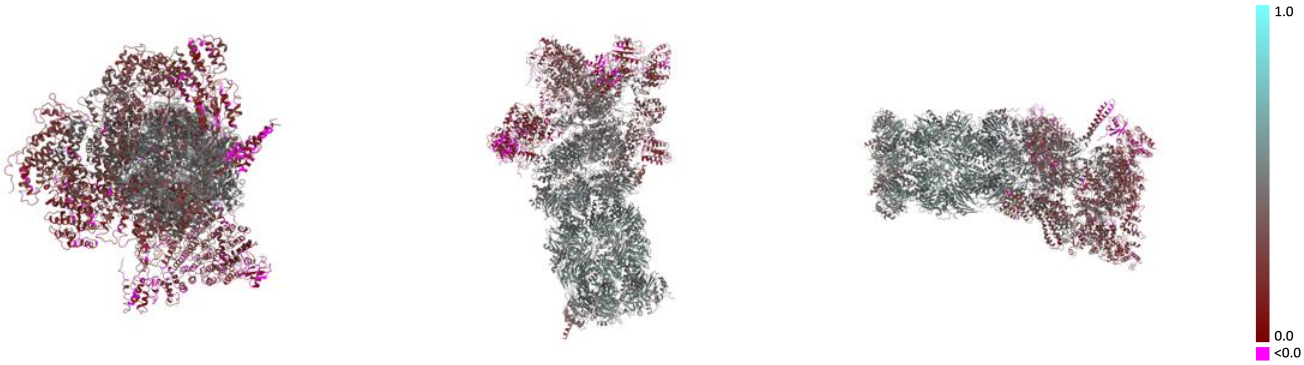
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0035 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.

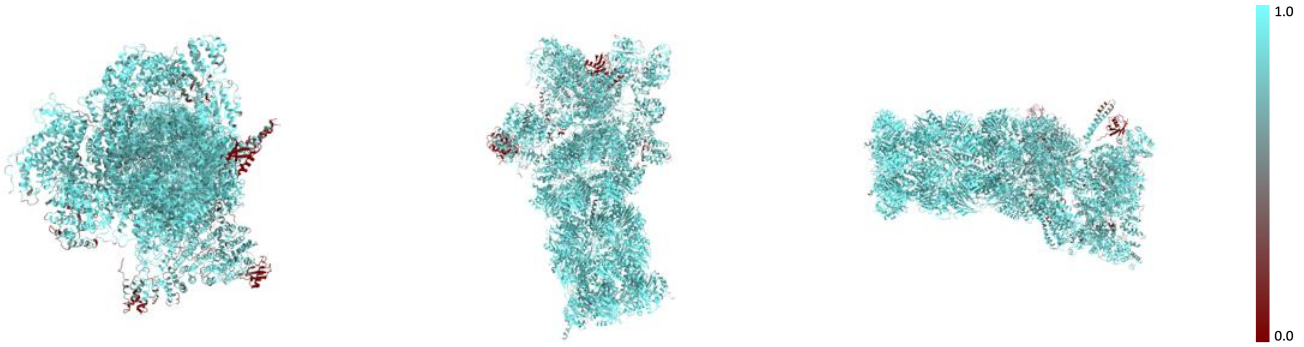
9.2 Q-score mapped to coordinate model (i)



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.

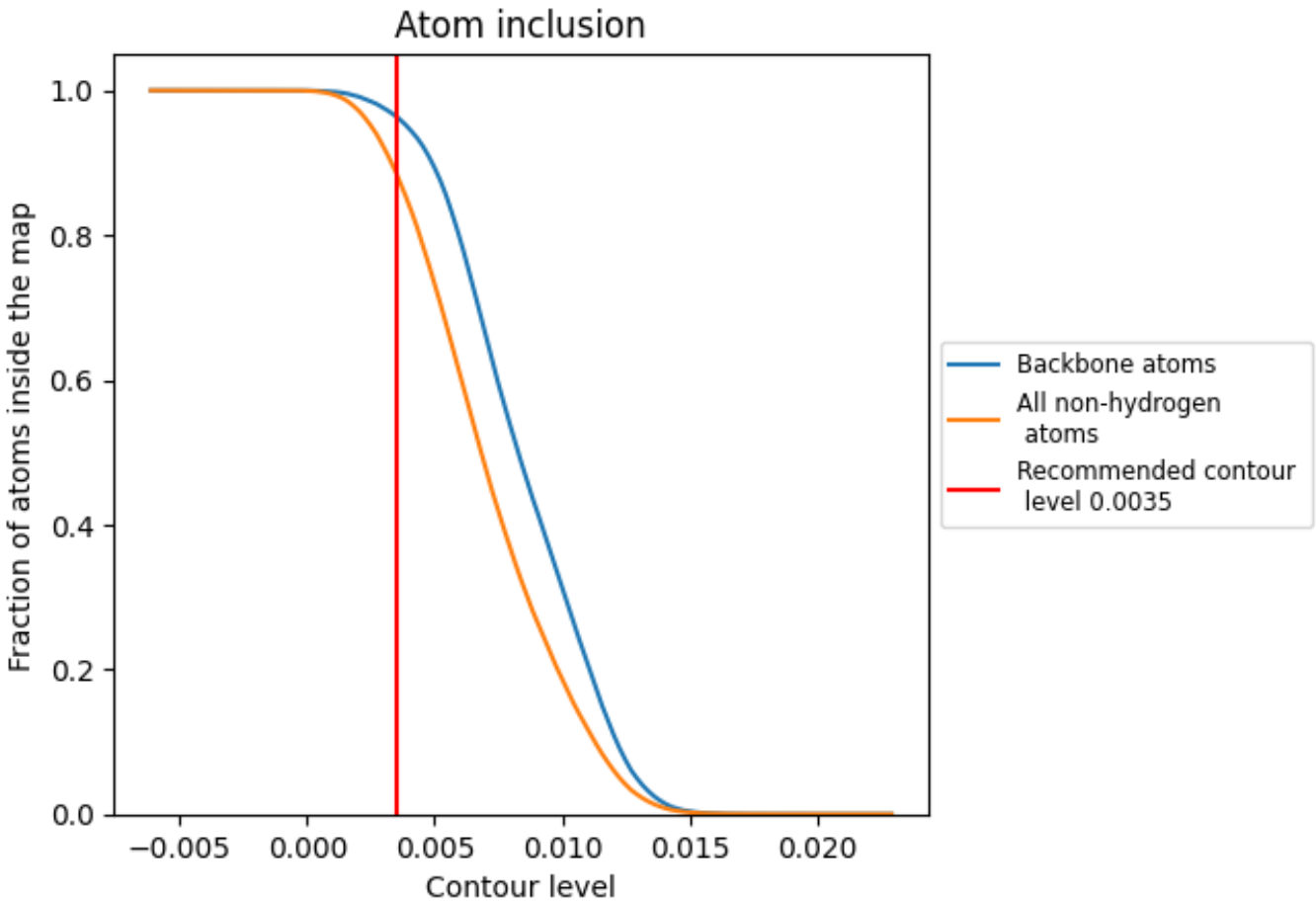
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0035).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8857	0.3890
A	0.9040	0.4330
B	0.9083	0.4270
C	0.9135	0.4390
D	0.9017	0.4280
E	0.9029	0.4250
F	0.8979	0.4340
G	0.9460	0.4920
H	0.9547	0.4990
I	0.9461	0.4700
J	0.9558	0.4710
K	0.9472	0.4850
L	0.9530	0.4930
M	0.9411	0.4780
N	0.9642	0.5170
O	0.9783	0.5130
P	0.9667	0.5180
Q	0.9668	0.5080
R	0.9713	0.5140
S	0.9595	0.5110
T	0.9624	0.5220
U	0.8623	0.2700
V	0.7858	0.2310
W	0.7956	0.2470
X	0.8474	0.3230
Y	0.8944	0.3210
Z	0.8506	0.3090
a	0.8505	0.2480
b	0.8015	0.1550
c	0.8687	0.3650
d	0.8126	0.2180
e	0.7545	0.1620
f	0.7194	0.1610
g	0.9521	0.4910
h	0.9458	0.4970

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Chain	Atom inclusion	Q-score
i	0.9082	0.4430
j	0.9310	0.4280
k	0.9420	0.4730
l	0.9563	0.4860
m	0.9345	0.4740
n	0.9700	0.5250
o	0.9727	0.5190
p	0.9706	0.5230
q	0.9720	0.5160
r	0.9806	0.5290
s	0.9677	0.5150
t	0.9692	0.5250
u	0.0203	-0.0160
w	0.1081	0.0120